Supporting Information

VIBE-QC: an open-source, general-purpose electronic-structure code for molecules and solids developed with generative AI

Michael F. Peintinger
Mulliken Center for Theoretical Chemistry, University of Bonn, Bonn, Germany
mpei@vibe-qc.com; mpei@uni-bonn.de

This document collects the computational details, the full validation tables, the periodic convergence data, an example of the per-job provenance and citation artifacts, the job-queue architecture, the complete validation database, and representative listings of the input scripts for the calculations reported in the main text (the complete set is distributed with the source archive). All calculations use the VIBE-QC 0.15 release series. Script identifiers (M01–M20, P01–P10) match the test set distributed with the manuscript.

Contents

S1 Computational details **2**

S2 Test set **4**
S2.1 Large-molecule coverage 4
S2.2 Additional release-matrix coverage 5
S2.3 Automated regression-suite structure 5

S3 Per-method benchmarks **7**
S3.1 Molecular method benchmarks 8
S3.2 Two-code consensus reference energies 10
S3.3 Additional methods against ORCA 6 11
S3.4 Literature-benchmark artifacts 13
S3.5 Semiempirical methods 13
S3.6 RIJCOSX SCF and gradient against ORCA, per method 14

S4 Periodic benchmarks and convergence data **14**
S4.1 Periodic methods against the matched reference 14
S4.2 Periodic capabilities not validated at this release 14
S4.3 GDF fitting-cutoff convergence 16
S4.4 Brillouin-zone mesh convergence 16
S4.5 First multi-route band-gap comparison 16
S4.6 Internal check: Ewald lattice-sum primitive 17
S4.7 Comparison against published reference values 17

S5 Per-job artifacts **18**
S5.1 Provenance manifest (`.system`) 18
S5.2 Automatic citation manifest (`.references` / `.bibtex`) 19
S5.3 The QVF visualization archive 19

S5.4 Additional VIBE-VIEW panels 19

S6 The VIBE-QUEUE job scheduler **19**
S6.1 Motivation and design invariants 20
S6.2 Resource enforcement 21
S6.3 Remote and fleet execution 22
S6.4 The external batch-scheduler backend 22

S7 Input listings **23**
S7.1 Molecular: RHF single point (M01) 23
S7.2 Molecular: MP2 family (M04) 24
S7.3 Molecular: non-mean-field solvers (M10) 25
S7.4 Periodic: multi-$\boldsymbol{k}$ GDF on LiH (P02) 25
S7.5 Periodic: bipolar-expansion route on MgO (P03) 26
S7.6 Periodic: band structure and DOS of silicon (P04) 27

S8 Complete validation database **28**

S1 Computational details

Software. Unless a row states otherwise, calculations were produced with the VIBE-QC 0.15 release series, built from source by the bootstrap script against the vendored native dependencies in Table S1. Because the series is under active development, a version string alone does not identify a build: every archived artifact records its exact build, vendored-library versions, and host in a `.system` manifest (Section S5), and that manifest is the object a reported value is pinned to. Values reported in this work are taken only from artifacts whose manifest records a release-line build; development-branch artifacts are excluded. The settings below are the global defaults, with per-calculation settings given in the input listings (Section S7).

Table S1: Native and build-time dependencies used by the release build. Header-only build dependencies are not reported as calculation runtime values.

Library	Version	License
LIBINT	2.13.1	LGPL-3.0
LIBXC	7.0.0	MPL-2.0
SPGLIB	2.7.0	BSD-3-Clause
LIBECPINT	1.0.7	MIT
FFTW3	3.3.9	GPL-2.0-or-later
EIGEN	5.0.1-compatible	MPL-2.0 (header-only)
`pybind11`	≥2.12	BSD-3-Clause (build-time, header-only)

Reference programs. Cross-code comparisons used ORCA 6.1.1 for molecular methods, OPENMOLCAS for CAS and multireference methods, PYSCF for periodic Gaussian density fitting, CRYSTAL 23 for the bipolar-expansion route and the periodic-XC comparisons, and GPAW for the Gaussian-and-plane-waves route. Every reference program was run out of process as an independent oracle; VIBE-QC links against numerical libraries only and never against another quantum-chemistry program's runtime. Basis, auxiliary

basis, integration grid, convergence thresholds, frozen-core treatment, and k-mesh were matched to the VIBE-QC run in each comparison, and both inputs and both full outputs are archived with the calculation.

Hardware. The reported calculations were run through `vq` on five workstation-class hosts and two university clusters. The workstations were an Intel Core i9-10885H (8 physical / 16 logical cores, 62 GB), an AMD Ryzen 9 9950X (16 / 32 cores, 64 GB), an AMD Ryzen 9 5950X (16 / 32 cores, 126 GB), and an Intel Core i5-8400 (6 cores, 32 GB), all under Manjaro Linux 7.0.10/7.0.13, together with an Apple M5 Max (18 cores, 128 GB) under macOS 26.5.1. The remainder ran on a PBS/Torque cluster whose nodes span Intel Xeon X5670 (12 cores, 94 GB), Xeon E5-2620 (12 cores, 252 GB), Xeon Silver 4114 (20 cores, 93 GB), and AMD Opteron 6376 (32 / 64 cores, 252 GB) partitions under openSUSE Tumbleweed 6.5.x, and on a Slurm cluster with Intel Xeon Platinum 8468 nodes (96 cores, 1008 GB) under AlmaLinux 9.6. Node-level hostnames are pseudonymized in the archived manifests. The manifests record 1–128 OpenMP threads for the reported calculations. The BLAS/LAPACK backend was OpenBLAS with LAPACKE on Linux and Accelerate on macOS.

Default convergence and grid settings. Unless overridden in the input, the molecular SCF used the SAD initial guess, Pulay DIIS with an eight-vector subspace, an energy convergence threshold of $1 \times 10^{-7}\ E_\mathrm{h}$ (tightened to $1 \times 10^{-10}\ E_\mathrm{h}$ for the post-SCF correlation references), and the default Treutler–Ahlrichs/Lebedev integration grid. Periodic calculations used the GDF route by default with the production-default fitting cutoff, the SAD guess, and an energy threshold of $1 \times 10^{-7}\ E_\mathrm{h}$; tighter cutoffs used in the parity studies are stated explicitly in Section S4.

Cross-platform reproducibility. Two rows were repeated on two independent clusters from the same build to separate host effects from method effects. The M01 RHF/def2-TZVP and M02 UHF/def2-TZVP decks were each run on a Slurm host and on a PBS/Torque host. The two VIBE-QC total energies agree to $1.4 \times 10^{-13}\ E_\mathrm{h}$ for M01 and are bit-identical for M02, and each run separately matches its own ORCA 6.1.1 reference on its own host, by $1.231 \times 10^{-9}\ E_\mathrm{h}$ and $2.831 \times 10^{-10}\ E_\mathrm{h}$. This is a reproducibility observation for those two rows; it is not a scaling result and it does not extend the accuracy claims those rows carry.

Timing measurements. Timings follow a separate protocol from the accuracy comparisons and are never harvested from the accuracy runs, because those were produced under heterogeneous allocations. For a timing pair, the VIBE-QC run and its reference run are executed on the same host and node with one allocated CPU per process and identical requested memory and wall-time limits; the inputs and numerical settings remain those of the accepted accuracy comparison. A timing row is reported only when both processes yield elapsed wall time, active CPU time, peak resident-set size, allocated CPU count, and the primary solver iteration count, taken from program output or from scheduler accounting. Reference runs shorter than 10 s are excluded as startup-dominated, and archived outputs that carry internal component timings but no process-level resource measurement are not substituted: the reference is rerun in the same resource envelope instead.

S2 Test set

The test set comprises molecular (Table S2) and periodic (Table S5) validation scripts, driven entirely through the high-level `run_job` and `run_periodic_job` API. Each script writes the standard artifact bundle (Section S5); the full listings are in Section S7.

Table S2: Molecular test set. Each row is one input script.

ID	Script	System / basis	Method(s)
M01	`m01_rhf_h2o.py`	H_2O / def2-TZVP	RHF
M02	`m02_uhf_oh.py`	$OH(^2\Pi)$ / def2-TZVP	UHF
M03	`m03_dft_functional_ladder.py`	H_2O / def2-TZVP	PBE, PBE0, B3LYP, r^{2}SCAN, ωB97X
M04	`m04_mp2_family.py`	H_2O / cc-pVTZ	MP2, SCS-MP2, SOS-MP2 (RI)
M05	`m05_double_hybrid_b2plyp.py`	H_2O / cc-pVTZ	B2PLYP
M06	`m06_composite_3c.py`	$(H_2O)_2$	hf-3c, r^{2}SCAN-3c
M07	`m07_dispersion_geomopt.py`	$(H_2O)_2$ / def2-TZVP	PBE0-D3(BJ) + opt
M08	`m08_solvation_cpcm_cosmo.py`	CH_3COOH / def2-TZVP	B3LYP + CPCM, COSMO
M09	`m09_ecp_heavy.py`	I_2 / dhf-TZVP	RHF + ECP
M10	`m10_wavefunction_solvers.py`	H_2/6-31G; N_2/cc-pVDZ	FCI; selected-CI, DMRG
M11	`m11_cas_multireference.py`	N_2 / cc-pVDZ	CASCI, CASSCF, NEVPT2, CASPT2*
M12	`m12_coupled_cluster.py`	H_2O / cc-pVDZ	CCSD, CCSD(T)
M13	`m13_semiempirical.py`	C_2H_5OH	PM6, SCC-DFTB, GFN2-xTB*
M14	`m14_hessian_ir.py`	H_2O / def2-TZVP	RHF analytic Hessian + IR
M15	`m15_rohf_roks.py`	NH_2 / def2-TZVP	ROHF, ROKS
M16	`m16_dlpno.py`	n-butane / cc-pVDZ	DLPNO-MP2/CCSD/CCSD(T)
M17	`m17_excited_states.py`	CH_2O / def2-SVP	TDDFT (Casida), TDA/CIS
M18	`m18_ovgf_ip.py`	H_2O / def2-TZVP	GF2 / OVGF (IP; smoke)
M19	`m19_new_functionals.py`	H_2O	r^{2}SCAN01, ωB97X-V, ωB97M-V, revDSD-PBEP86-D4
M20	`m20_benzene_application.py`	C_6H_6 / def2-TZVP	PBE0-D3(BJ) opt; DLPNO-CCSD(T) audit held

* experimental/provisional in the 0.15 series; gated behind an environment flag.

S2.1 Large-molecule coverage

The release-paper calculation set also includes a large-molecule smoke batch with attached ORCA single-point references. These runs exercise the same provenance, QVF, Molden, population, and cube-output paths on larger molecular AO spaces. Table S3 reports the fetched VIBE-QC coverage artifacts. The ORCA references were rerun serially after its parallel startup failed on that cluster, so only the RHF rows are used as clean parity checks.

The four alkane-formula rows (LM01–LM04) are *synthetic straight-chain structures*, not relaxed molecular geometries. They were produced by an internal chain generator that places the hydrogens of each internal methylene from a carbon–carbon-derived offset; the resulting coordinates carry over-long internal C–H bonds (up to 1.18 Å, against a physical 1.09 Å) and short H $\cdots$ H contacts (down to 1.14 Å). We therefore treat these rows strictly as VIBE-QC-VS-ORCA agreement tests on a fixed, identical set of atomic coordinates in a large AO space, and make no physical claim about *n*-octane or *n*-dodecane. LM05, a benzene dimer, is a genuine physical geometry and is unaffected.

The LM01, LM03, and LM04 rows were subsequently repeated on a later release build of the 0.15 series, with matched ORCA 6.1.1 references. All three reproduce the VIBE-QC total energies tabulated above

Table S3: Fetched large-molecule coverage. Energies are total VIBE-QC energies from the archived `.out` files. LM01–LM04 are synthetic straight-chain structures with a known geometry defect (see text) and are used only as fixed-coordinate VIBE-QC-vs-ORCA agreement tests, not as physical alkane benchmarks.

ID	System	Method / basis	Status	E_{tot} / E_{h}
LM01	synthetic C_8H_{18} chain	RHF / STO-3G	converged, QVF	−306.6793935231
LM02	synthetic C_8H_{18} chain	RKS-PBE / def2-SVP	converged, QVF	−313.1624959631
LM03	synthetic $C_{12}H_{26}$ chain	RHF / STO-3G	converged, QVF	−459.1244786257
LM04	synthetic $C_{12}H_{26}$ chain	RKS-PBE / STO-3G	converged, QVF	−462.5765005417
LM05	benzene dimer	RKS-PBE0-D3(BJ) / def2-SVP	converged, QVF	−463.6017562931

The `.system` manifests record the exact VIBE-QC build and branch. ORCA 6.1.1 serial fallback references give RHF total-energy differences of 2.50×10^{-8} and 3.71×10^{-8} E_{h} for LM01 and LM03. The DFT rows remain coverage/convention checks with differences 6.44×10^{-4}, 5.48×10^{-3}, and 2.64×10^{-2} E_{h} for LM02, LM04, and LM05.

at the precision displayed, and reproduce the tabulated reference differences 2.50×10^{-8}, 3.71×10^{-8}, and 5.48×10^{-3} E_{h}; the LM03 and LM04 differences agree with their original values to 8.8×10^{-12} and 2.1×10^{-7} E_{h}. The LM04 comparison is grid-convention-limited rather than SCF-limited, because its ORCA deck carries no `DEFGRID` keyword and the row therefore compares the two programs' default integration grids. LM02 and LM05 are not promoted from that repeat, and their entries above remain artifacts of the original build.

Reproducibility caveat: initial-guess dependence of LM01. That repeat also established that the LM01 system supports at least three distinct closed-shell RHF/STO-3G stationary points. Varying only the initial guess on a single release binary gives −306.679 393 523 1 E_{h} (`SAP`, and `AUTO`, which selects it), −306.638 682 864 5 E_{h} (`PATOM`, `SAD`, `HCORE`, `MINAO`), and −306.494 698 185 0 E_{h} (`HUECKEL`). All three converge cleanly to positive-gap solutions, so these are genuinely different solutions of the same SCF equations rather than convergence artifacts. The value tabulated above is the lowest of the three, the `SAP/AUTO` solution, which is also the one the matched ORCA reference reproduces. We record this as a reproducibility caveat rather than a defect. We attribute the near-degeneracy to the strained synthetic geometry rather than to any physical property of an alkane: the over-long internal C–H bonds and 1.14 Å H $\cdots$ H contacts noted above give a compressed, near-degenerate manifold of low-lying closed-shell solutions, so reproducing the tabulated LM01 number requires the `SAP` guess specifically. We make no claim that any one guess is preferable in general, nor that the list above is exhaustive.

S2.2 Additional release-matrix coverage

Beyond the canonical validation rows, the release matrix includes small method-by-system smoke batches used to exercise the same output and provenance path on additional combinations. Table S4 lists the first landed batch. These rows are not independent-oracle benchmarks. They are archived coverage runs from an earlier build in the series and are reported as coverage rather than as paper values.

S2.3 Automated regression-suite structure

The automated test infrastructure has two distinct layers. The first is the repo-wide `pytest` suite, which is broad engineering and scientific regression coverage. It verifies numerical kernels, API behavior, physics conventions, data provenance, failure gates, and output artifacts. The second is the standalone

Table S4: Additional release-matrix coverage. All values are total energies taken from the archived `.out` files.

Case	System	Method	Basis	E / E_h
`A_rhf_h2o`	H_2O	RHF	STO-3G	−74.9644538631
`A_pbe_h2o`	H_2O	RKS-PBE	STO-3G	−75.2342885566
`A_b3lyp_h2o`	H_2O	RKS-B3LYP	STO-3G	−75.2826476567
`A_pbe0_h2o`	H_2O	RKS-PBE0	STO-3G	−75.2519152837
`A_r2scan_h2o`	H_2O	RKS-r^{2}SCAN	STO-3G	−75.2937248441
`A_wb97x_h2o`	H_2O	RKS-ωB97X	STO-3G	−75.3129220111
`A_rhf_nh3`	NH_3	RHF	STO-3G	−55.4550218289
`A_pbe_nh3`	NH_3	RKS-PBE	STO-3G	−55.7105508231

Table S5: Periodic test set. Each row is one input script.

ID	Script	System / basis	Route	k-mesh
P01	`p01_mgo_gamma_gdf.py`	MgO / def2-SVP	GDF, RKS-PBE	Γ
P02	`p02_lih_multik_gdf.py`	LiH / STO-3G	GDF, KRHF	(2, 2, 2)
P03	`p03_mgo_multik_bipole.py`	MgO / STO-3G	BIPOLE, KRHF	(2, 2, 2)
P04	`p04_si_bands_dos.py`	Si / def2-SVP	GDF, RKS-PBE	(4, 4, 4)
P05	`p05_nacl_symmetry.py`	NaCl / def2-SVP	GDF + SYM6	(4, 4, 4)
P06	`p06_periodic_dispersion.py`	fcc Ne / def2-SVP	GDF + D3(BJ)	(4, 4, 4)
P07	`p07_gpw_si.py`	Si / def2-SVP	GPW, RKS-PBE	(4, 4, 4)
P08	`p08_gapw_lif.py`	LiF / def2-SVP	GAPW (experimental*)	(4, 4, 4)
P09	`p09_periodic_ecp.py`	Ag, Au, W / pob-TZVP-REV2	GDF + periodic ECP	(4, 4, 4)
P10	`p10_coop_cohp.py`	NaCl / def2-SVP	GDF + COOP/COHP, Mayer	(4, 4, 4)

* GAPW is experimental in the 0.15 series and is excluded from the validated benchmarks; GPW (P07) is the production periodic-DFT route.

`examples/regression` scientific parity runner, a curated set of end-to-end calculations with retained inputs and outputs. Only a subset of the `pytest` suite is direct cross-code parity, so the counts in Table S6 should not be read as thousands of independent oracle calculations.

Table S6: Regression-suite and parity-runner counts at the `v0.15.132` snapshot (collection only; no tests executed).

Item	Count
`pytest` test files present	733
`pytest` files with collected tests	726
Collected `pytest` test items	15576
Active `examples/regression` cases	44
Active molecular parity cases	40
Active periodic parity cases	4
Full default parity-run program rows, when ORCA and PySCF are available	128

Table S7 gives an approximate first-match classification of the `v0.15.132` collection by test-module name, generated by the classifier script distributed with the paper (`scripts/classify_tests_v015132.py`). It is intended to show the breadth of the regression surface, not to replace the method-by-method validation tables in Section S3.

The full suite includes tests or runners that mention external implementations at the file level, including PySCF (117 files), ORCA (40), CP2K (12), CRYSTAL (77), GPAW (6), Psi4 (5), MOPAC (2), xTB (27), DFTD3 (7), DFTD4 (9), and ASE (391). These mentions include true parity checks, parser tests, optional-interface tests, fixtures, and documentation/provenance tests.

Table S7: Approximate first-match classification of collected `pytest` items by test-module name at the `v0.15.132` snapshot.

Area	Tests
Periodic solids: $\boldsymbol{k}$ meshes, Ewald, GDF/GPW/BIPOLE, slabs, bands	4450
Molecular SCF, DFT, XC, grids, convergence controls	1822
Citations, provenance, documentation, release hygiene	2746
Post-HF, coupled cluster, multireference, CAS/MRPT/FCI	1770
Basis sets, ECPs, integrals, DF/RI, numerical kernels	648
Semiempirical, MSINDO, DFTB, xTB	841
Output files, QVF, cubes, visualization, I/O formats	972
Molecular gradients, Hessians, optimization, properties	439
CCM/AICCM periodic cluster models	639
ASE, NEB, MD, MLIP, workflow integration	253
Dispersion and corrections	383
Symmetry and structural utilities	188
Other focused regression tests	425

The 44 active standalone parity cases cover atomic and diatomic smoke systems (H_2, Ne, HF), small closed-shell molecules (CH_4, NH_3, H_2O, H_2CO), RHF and RKS-LDA/PBE/BLYP/B3LYP, MP2, density-fitted RHF and RKS-PBE examples, benzene, open-shell O_2 and O_3 stress cases, and a noncovalent S22 subset. The active periodic cases are Ne fcc, LiH, NaCl, and MgO rocksalts. At this snapshot the active periodic parity cases all use STO-3G/RKS-LDA/$1 \times 1 \times 1$ settings and are best viewed as useful bug-finding cases; recent paper reruns still show open periodic numerical failures, so they are not presented as an all-green periodic validation suite.

S3 Per-method benchmarks

This section gives one benchmark per implemented method, each against a single reference program matched to the formalism: Orca 6 for molecular methods wherever Orca implements the feature; OpenMolcas for the complete-active-space and multireference methods; PySCF for the periodic Gaussian-density-fitting route; and Crystal 23 for the periodic bipolar-expansion route. Table S8 records the reference-program versions and settings. All vibe-qc numbers come from the archived test set; reference programs are run out-of-process. The agreement column is tiered by the limiting quantity rather than by a single threshold. Mean-field rows are SCF-limited and agree at the nanohartree scale: RHF/UHF/ROHF to $1.2 \times 10^{-9}\ E_\mathrm{h}$ and ECP energies to $1.4 \times 10^{-8}\ E_\mathrm{h}$ against Orca. The complete-active-space energies match a matched OpenMolcas reference but are held pending a tagged-release rerun, and the full-configuration-interaction solver is checked for cross-release reproducibility, spanning a development build and the tagged release, rather than against an external oracle. Correlated and density-functional rows are limited by density fitting and integration grids rather than by SCF convergence, and agree at the tens-of-microhartree to sub-millihartree scale when those approximations define the comparison: MP2 reaches $2.5 \times 10^{-5}\ E_\mathrm{h}$, SOS-MP2 $6.5 \times 10^{-5}\ E_\mathrm{h}$, the single H_2O DF-CCSD(T) benchmark is $1.4 \times 10^{-4}\ E_\mathrm{h}$, and the KS-DFT ladder is $1.5 \times 10^{-4}\ E_\mathrm{h}$. The 0.15-series route matrix separates this from conventional all-electron CCSD(T), which agrees with Orca to $3.3 \times 10^{-7}\ E_\mathrm{h}$ or better over H_2O and CO basis-set checks. Periodic solid rows are kept as separate open blockers: the point-charge Madelung foundation is exact to about 1×10^{-11}, but matched SCF cross-code comparisons remain gauge-held under constant

electrostatic-convention offsets rather than parity, with the tightest matched LiH multi-$\boldsymbol{k}$ GDF/PySCF point at $1.6 \times 10^{-3}\ E_\mathrm{h}$ and the MgO BIPOLE/Crystal 23 comparison at a $0.64\ E_\mathrm{h}$ gauge offset.

Table S8: Reference programs used as cross-code oracles, with the version and the key settings matched to the vibe-qc run.

Program	Version	Matched settings
Orca 6	6.1.1	same basis/aux, `TightSCF`, grid
OpenMolcas	26.02 (`pymolcas` py2.30)	same basis, active space, `RASSCF`/`CASPT2` settings
PySCF	2.13.1	same basis/aux, k-mesh, `exxdiv`
Crystal 23	23	same basis, TOLINTEG, shrinking factor
GPAW	26.7.0	same basis, k-mesh, functional

S3.1 Molecular method benchmarks

Table S9: Molecular methods validated against matched reference programs; the CASCI, CASSCF, NEVPT2, and CASPT2 rows are validated against OpenMolcas. $|\Delta E|$ is the absolute difference in total energy, or correlation energy where the row notes "corr", in hartree.

Method	System / basis	Quantity	Agreement
RHF	H_2O / def2-TZVP	total	1.2×10^{-9}
UHF	OH / def2-TZVP	total	2.8×10^{-10}
ROHF	NH_2 / def2-TZVP	total	3.4×10^{-10}
ROKS-PBE	NH_2 / def2-TZVP	total	9.1×10^{-5}
RKS-PBE	H_2O / def2-TZVP	total	1.4×10^{-4}
RKS-PBE0	H_2O / def2-TZVP	total	1.3×10^{-4}
RKS-r^{2}SCAN	H_2O / def2-TZVP	total	1.5×10^{-4}
RKS-r^{2}SCAN01	H_2O / def2-SVP	total	3.9×10^{-6}
RKS-ωB97X-V	H_2O / cc-pVDZ	total	7.8×10^{-5}
RKS-ωB97M-V	H_2O / cc-pVDZ	total	8.1×10^{-5}
MP2 (all-e corr)	H_2O / cc-pVTZ	corr	2.5×10^{-5}
SCS-MP2 (all-e corr)	H_2O / cc-pVTZ	corr	5.2×10^{-5}
SOS-MP2 (all-e corr)	H_2O / cc-pVTZ	corr	6.5×10^{-5}
CCSD(T) (all-e conv.)	H_2O, CO / cc-pVXZ, def2-XVP	total	$\leq 3.3 \times 10^{-7}$
DF-CCSD (all-e corr)	H_2O / cc-pVDZ	corr	1.37×10^{-4}
DF-CCSD(T) (all-e corr)	H_2O / cc-pVDZ	corr	held: explicit-pair comparison pending
FNO-CCSD(T) (all-e, no trunc.)	H_2O / cc-pVDZ	corr	held: explicit-pair comparison pending
DF-UCCSD(T) (all-e corr)	OH / cc-pVDZ	corr	held: explicit-pair comparison pending
CASCI	N_2 / cc-pVDZ (6e,6o)	total	8.2×10^{-9}
CASSCF	N_2 / cc-pVDZ (6e,6o)	total	$\leq 3.0 \times 10^{-10}$

Method	System / basis	Quantity	Agreement
CASSCF grad.	N_2 / cc-pVDZ	$\|\nabla\|$	held: VIBE-QC leg pending
NEVPT2	N_2 / cc-pVDZ	total	2.0×10^{-6}
CASPT2	N_2 / cc-pVDZ	total	held: 8.9×10^{-5} residual in the second-order correction
FCI	H_2 / 6-31G	total	1.4×10^{-11}
selected-CI (corr)	N_2 / cc-pVDZ	corr	held: solver-side estimator defect
DMRG (corr)	N_2 / cc-pVDZ	corr	held (ref. pending)
TDDFT (1^1B_2)	CH_2O / def2-SVP	ω / eV	4.4×10^{-3}
CIS (1^1B_2)	CH_2O / def2-SVP	ω / eV	7.6×10^{-4}
GF2 / OVGF (IP)	H_2O / def2-TZVP	IP / eV	held: no oracle in ORCA
RHF analytic Hessian	H_2O / def2-TZVP	freq / cm^{-1}	0.11 cm^{-1}
ECP (dhf-ECP)	I_2 / dhf-TZVP	total	1.32×10^{-8}

The I_2/dhf-TZVP ECP row above is a matched small-core comparison. It must not be conflated with a separate H_2S/LANL2DZ comparison, whose case label requested an ECP but whose Python input supplied only the orbital-basis name. That VIBE-QC job retained all 18 electrons, while ORCA applied the sulfur ECP and correlated the 8-valence-electron problem; the resulting −78.628 E_h difference is an input construction failure and is excluded from numerical validation.

For the M18 propagator row the archived VIBE-QC smoke value is 11.2155 eV. ORCA 6.1.1 does not implement the OVGF or GF2 propagator methods, so no direct cross-code comparison exists for this row; the underlying Hartree–Fock orbital energies are compared against ORCA in the main text, and an IP-EOM-CCSD accuracy oracle on the same geometry is pending.

Every correlated row above states its frozen-core convention in the method column: "all-e" rows correlate all electrons on both sides. The VIBE-QC default for canonical and density-fitted CCSD/CCSD(T) freezes one noble-gas chemical core per atom, so the all-electron rows pin the convention explicitly; DLPNO and MP2 routes correlate all electrons by default.

For the M12 closed-shell and corresponding open-shell coupled-cluster comparisons, the original archived comparison mixed ORCA `NoFrozenCore` references with VIBE-QC's default frozen-core convention. The reported DF row in Table S9 therefore uses the later explicit all-electron density-fitted VIBE-QC rerun, with a residual difference against conventional ORCA of 1.37×10^{-4} E_h for H_2O DF-CCSD. The corresponding density-fitted triples comparisons (H_2O DF-CCSD(T), OH DF-UCCSD(T), and the no-truncation FNO-CCSD(T) check) predate the corrected density-fitting path of the current release line. Re-execution of fourteen correlated cases on the corrected route reproduces every earlier default-route total energy to within 1.1×10^{-9} E_h, so the correction moved no default-route number; the triples cells remain held pending an explicit density-fitted versus conventional pair comparison, which the corrected route makes

possible for the first time. A guarded route matrix adds an all-electron conventional CCSD(T) comparison: exact-SCF conventional VIBE-QC CCSD(T) agrees with exact-SCF conventional ORCA to $3.3 \times 10^{-7}\ E_h$ or better over H_2O and CO with cc-pVDZ, cc-pVTZ, def2-SVP, and def2-TZVP bases.

The M17 PBE0-TDA excitation energies are 4.0354 eV, 8.5374 eV, 9.2501 eV, 9.9332 eV and 10.3588 eV, with a maximum printed-root difference of 4.4×10^{-3} eV against ORCA 6.1.1.

S3.2 Two-code consensus reference energies

Alongside the per-method benchmarks, a two-code consensus reference suite (ASCENT) is maintained with the input library and will be described separately. A consensus value is created only when VIBE-QC and ORCA, executed independently at identical geometry, basis set, and protocol, agree within a per-atom tolerance; when the spread exceeds the tolerance, no value is stored. Table S10 lists the complete citable set at the 2026-08-14 snapshot: 44 canonical RHF total energies (38 distinct system–basis pairs, with protocol-variant contracts collapsed onto their shared value) and one exact FCI energy. The largest cross-code spread in the set is $3.1 \times 10^{-9}\ E_h$. Four contract checks are open at this snapshot and produce no consensus value: the LiH/cc-pVDZ cross-code contract ($1.1 \times 10^{-4}\ E_h$, attributed to a cc-pVDZ basis-revision difference between the reference program's built-in library and the BSE-sourced set; the same comparison passes at $5.1 \times 10^{-11}\ E_h$ with the revision matched explicitly), an MgO-cluster cross-code contract ($1.1 \times 10^{-1}\ E_h$), a RIJCOSX-versus-canonical approximation contract (H_2O/STO-3G, $7.8 \times 10^{-4}\ E_h$ against a $6 \times 10^{-4}\ E_h$ window), and a GFN2-xTB cross-code contract measured on an earlier build and awaiting re-measurement. System identifiers are the input-library identifiers; `n-alkane:2` is ethane. These values carry no external archive identifier yet. As an independent check, the release-line VIBE-QC runs recorded in the validation database reproduce all 44 consensus cells within their windows, with a largest deviation of $1.6 \times 10^{-9}\ E_h$ from the stored values; those comparisons appear as rows of Table S21.

Table S10: Two-code consensus reference energies: canonical RHF total energies on which VIBE-QC and ORCA agree at identical geometry, basis, and protocol, plus one exact FCI energy. The spread column is the absolute difference between the two codes' energies.

System	Basis	E / E_h	Spread / E_h
`atom-mg`	3-21G	−198.468103018	2.1×10^{-10}
`atom-mg`	6-31G**	−199.595219247	4.6×10^{-10}
`atom-mg`	cc-pVDZ	−199.608297028	3.5×10^{-10}
`atom-mg`	def2-SVP	−199.534810664	2.8×10^{-10}
`atom-mg`	STO-3G	−197.007353900	1.5×10^{-10}
`c2h4`	STO-3G	−77.072178778	9.1×10^{-10}
`ch2o`	STO-3G	−112.353831892	7.0×10^{-12}
`ch4`	3-21G	−39.976830650	1.7×10^{-10}
`ch4`	STO-3G	−39.726809171	1.6×10^{-10}
`co`	3-21G	−112.093296738	4.2×10^{-11}
`co`	STO-3G	−111.224558696	3.9×10^{-10}
`co2`	STO-3G	−185.064695683	1.3×10^{-9}
`h2`	3-21G	−1.122928328	9.0×10^{-12}
`h2`	6-31G**	−1.131277627	2.5×10^{-11}
`h2`	aug-cc-pVDZ	−1.128793349	7.6×10^{-11}

System	Basis	E / E_h	Spread / E_h
h2	cc-pVDZ	−1.128714959	6.5×10^{-11}
h2	def2-SVP	−1.128906379	1.8×10^{-11}
h2 (7 protocol variants)	def2-TZVP	−1.132530993	8.0×10^{-12}
h2	STO-3G	−1.116684387	2.2×10^{-10}
h2o	3-21G	−75.585408880	1.1×10^{-10}
h2o	STO-3G	−74.963023139	5.3×10^{-10}
h2o-dimer	STO-3G	−149.934156936	6.4×10^{-10}
h2o2	STO-3G	−148.673974044	2.5×10^{-9}
hf	3-21G	−99.459751767	1.2×10^{-10}
hf	STO-3G	−98.570779986	3.9×10^{-10}
lih	3-21G	−7.929586512	7.1×10^{-11}
lih	STO-3G	−7.862023860	2.3×10^{-10}
n-alkane:2	STO-3G	−78.305264172	3.9×10^{-10}
n2	3-21G	−108.300238170	7.1×10^{-10}
n2	STO-3G	−107.495975031	1.3×10^{-9}
nacl-cluster:1	STO-3G	−614.480650190	2.6×10^{-9}
nh3	3-21G	−55.870191524	1.5×10^{-10}
nh3	STO-3G	−55.454507814	3.7×10^{-10}
s22-ammonia-dimer	STO-3G	−110.786163275	3.1×10^{-9}
s22-methane-dimer	STO-3G	−79.441572974	4.9×10^{-10}
s22-water-dimer	STO-3G	−149.935375927	5.3×10^{-10}
water-cluster:1	STO-3G	−74.962928247	5.8×10^{-10}
water-cluster:2	STO-3G	−149.813556355	1.7×10^{-9}
h2 (FCI)	STO-3G	−1.137270175	exact

S3.3 Additional methods against ORCA 6

These are the ORCA-specific method families beyond the core molecular rows in Table S9. Table S11 reports the glycine/def2-TZVP RIJCOSX set (SCF energy and analytic gradient), the DLPNO pilot hierarchy, the composite "-3c" methods, and continuum solvation component audits.

Exact-algorithm agreement. Where VIBE-QC and ORCA run the same algorithm with the same settings, the total energies agree at the numerical floor. Across the matched RHF, UHF, and ROHF comparisons the largest absolute difference is 1.54×10^{-9} E_h; a five-basis H_2O_2 RHF series from STO-3G through cc-pVTZ agrees within 2.55×10^{-9} E_h. Matched ROKS-PBE comparisons are grid-limited rather than SCF-limited and span 2.5×10^{-5}–1.3×10^{-4} E_h. The MP2 family spans a wider range, 7.17×10^{-9}–1.016×10^{-4} E_h, whose upper end is a density-fitting effect: the rows that avoid an auxiliary basis mismatch, O_2 across five bases and LiH/def2-TZVP, stay within 1.40×10^{-7} E_h. The ECP path was validated after a provenance failure, when a reconstructed input silently omitted the ECP declaration; with the ECP applied explicitly the I_2 energy is −589.344 400 824 577 E_h against −589.344 400 837 791 E_h from ORCA 6.1.1, a difference of 1.32×10^{-8} E_h.

Coupled cluster. The canonical, non-density-fitted route is the parity claim; the matched density-fitted CCSD comparison carries a residual of 0.137 mE_h. The density-fitted triples comparisons are held pend-

Table S11: Methods benchmarked or audited against ORCA 6.1.1.

Method	System / basis	Quantity	Agreement
RIJCOSX (RHF/UHF/B3LYP/PBE0)	glycine / def2-TZVP	E_{SCF}	$\leq 2.7 \times 10^{-4}\ E_h$
RIJCOSX analytic gradient	glycine / def2-TZVP	$\lvert\nabla\rvert$	held: $4.3 \times 10^{-3}\ E_h\ a_0^{-1}$ RMS
DLPNO-MP2 (corr)	n-butane / cc-pVDZ	corr	pilot: $3.762 \times 10^{-3}\ E_h$
DLPNO-CCSD (corr)	n-butane / cc-pVDZ	corr	pilot: $-3.813 \times 10^{-3}\ E_h$
DLPNO-CCSD(T) (corr)	n-butane / cc-pVDZ	corr	pilot: $-5.909 \times 10^{-3}\ E_h$
DLPNO-UMP2 (corr)	C_3H_5• / cc-pVTZ	corr	smoke: current QVF; parity pending
HF-3c	$(H_2O)_2$ / MINIX	total	$1.7 \times 10^{-9}\ E_h$
HF-3c gCP + SRB	$(H_2O)_2$ / MINIX	corr. terms	$4.0 \times 10^{-9}\ E_h$
r^{2}SCAN-3c	$(H_2O)_2$ / def2-mTZVPP	total	held: $1.3 \times 10^{-3}\ E_h$
r^{2}SCAN-3c, SCF half	$(H_2O)_2$ / def2-mTZVPP	E_{SCF}	held: $1.2 \times 10^{-3}\ E_h$ RI conv.
r^{2}SCAN-3c, D4 term	$(H_2O)_2$ / def2-mTZVPP	E_{disp}	defect: $6.0 \times 10^{-5}\ E_h$
r^{2}SCAN-3c, gCP	$(H_2O)_2$ / def2-mTZVPP	gCP	$2.0 \times 10^{-9}\ E_h$
B2PLYP	H_2O / cc-pVTZ	total	$1.4 \times 10^{-6}\ E_h$
B2PLYP, KS half	H_2O / cc-pVTZ	E_{SCF}	$1.3 \times 10^{-6}\ E_h$
B2PLYP, scaled MP2	H_2O / cc-pVTZ	E_{corr}	$7.7 \times 10^{-8}\ E_h$
revDSD-PBEP86-D4	H_2O / cc-pVTZ	total	held: $2.185 \times 10^{-3}\ E_h$ conv.
D4 dispersion (PBE0)	$(H_2O)_2$ / def2-TZVP	E_{disp}	$2.0 \times 10^{-9}\ E_h$
PBE0-D3(BJ) optimization	$(H_2O)_2$ / def2-TZVP	E, r_{OO}	$3.1 \times 10^{-4}\ E_h$, 3.5×10^{-3} Å
CPCM (water)	CH_3COOH / def2-TZVP	ΔG_{solv}	held: component cmp.
COSMO (water)	CH_3COOH / def2-TZVP	ΔG_{solv}	held: no oracle

ing reruns on the corrected density-fitting path of the current release line. Two comparisons were rejected as settings mismatches rather than implementation differences, at 2.808 mE_h and 35.373 mE_h, because VIBE-QC froze one orbital where ORCA froze none; the corrected all-electron reruns are the values reported in Table S9.

Local correlation. The DLPNO hierarchy is reported as convention-held rather than as parity. Against ORCA TightPNO the released VIBE-QC defaults differ by $-3.813 \times 10^{-3}\ E_h$ for DLPNO-CCSD and $-5.909 \times 10^{-3}\ E_h$ for DLPNO-CCSD(T) on the M16 system, and by 0.43–1.18 mE_h on the smaller library cases. The truncation defaults differ on both sides, so these differences measure the default settings, not the correctness of the local-correlation implementation, and we do not present them as a parity result.

Conventions that must be matched before a comparison is valid. Three classes of row are held for definitional rather than numerical reasons. First, basis-set revision: for LiH the ORCA basis *label* selects a different primitive contraction than VIBE-QC resolves, giving apparent differences of 1.14×10^{-4}, 1.45×10^{-5}, and $-1.54 \times 10^{-7}\ E_h$ across cc-pVDZ, cc-pVTZ, and cc-pVQZ; regenerating the ORCA basis explicitly from the same primitives brings the same comparisons to within $5.1 \times 10^{-11}\ E_h$, and those explicit controls are the values we report. Second, integration grid: a thirteen-row LiH series comparing ORCA DefGrid3 against the VIBE-QC default grid differs by 4.10×10^{-6}–$4.02 \times 10^{-4}\ E_h$, which is a grid specification difference and is excluded from parity claims. Third, solvation and double hybrids: the M08 CPCM in-solvent total differs from ORCA by $-9.28 \times 10^{-4}\ E_h$ and the M19 revDSD-PBEP86-

D4 total by $2.185 \times 10^{-3}\ E_\mathrm{h}$. Solvated total energies embed a model-dependent reference state and must be compared through matched solvent-response components, so the solvation row remains held. The revDSD difference is localized by term-by-term decomposition to the local-correlation composition flavor of the Kohn–Sham half (PZ81 against the VWN5 of the defining paper's reference implementation); the remainder is attributable to a documented 2019-versus-2021 dispersion-parameter revision and the reference integration floor, and the row remains held pending a rerun with the matched composition.

Timing. A colocated control illustrates the timing protocol of Section S1. For LiH CCSD(T)/cc-pVQZ, run sequentially in one allocation with one CPU and 8 GiB each, VIBE-QC used 21.71 s wall, 21.03 s active CPU, and 932.47 MiB peak RSS, against 35.30 s, 17.03 s, and 369.16 MiB for ORCA 6.1.1: symmetric ratios of 1.63, 1.24, and 2.53, all within the factor-of-ten gate. Two efficiency defects are open and disclosed. The DLPNO routes run 6–11 times slower than ORCA at one core on the same inputs, and the RIJCOSX SCF is similarly slow while remaining accurate, the two newly measured UKS rows differing from ORCA by $2.079 \times 10^{-4}\ E_\mathrm{h}$ (B3LYP) and $2.431 \times 10^{-4}\ E_\mathrm{h}$ (PBE0). The static memory pre-flight is conservative by a wide margin, with a median requested-to-peak ratio of 26.3 across the successful runs, which costs queue throughput but never under-allocates.

S3.4 Literature-benchmark artifacts

Table S12 reports the water-dimer interaction energy from the S22 set [1] computed with and without the D3(BJ) correction, as a check that the dispersion correction enters the interaction energy with the expected magnitude and sign.

Table S12: Water-dimer PBE/def2-TZVP interaction energies from the S22 calculation set.

Route	E_dimer / E_h	E_monomer / E_h	ΔE_int / kcal mol^{-1}
PBE, no dispersion	−152.7627101655	−76.3765380594	−6.0455
PBE-D3(BJ)	−152.7653804355	−76.3772423994	−6.8371

S3.5 Semiempirical methods

The semiempirical methods sit outside the five DFT/WFT reference programs used for the main parity tables. Their appropriate external oracles are method-specific: `xtb` for GFN2-xTB, MOPAC for PM6, DFTB+ for SCC-DFTB, the Bonn MSINDO implementation for MSINDO, and the `mace-torch` model engine for MACE. Table S13 therefore reports the release-paper archive status rather than claiming parity for rows whose matched out-of-process reference outputs have not yet been promoted into the paper bundle.

The scale of what remains open here should be stated plainly, because the semiempirical family is the largest single block of attempted work in the database and the smallest block of completed work. Of its 791 comparisons, spanning SCC-DFTB, DFTB0, PM6, GFN2-xTB, MSINDO, OM2, and OM3 against DFTB+, `xtb`, MOPAC, and the Bonn MSINDO implementation, 742 are blocked, 31 are `artifact-incomplete`, and 18 lack a completed reference. None has yet closed. The semiempirical route carries substantial method development that is the subject of a separate article, and no quantitative semiempirical claim is made in the present paper.

Table S13: Semiempirical and MLIP methods against their reference implementations.

Method	System	Reference impl.	Status
GFN2-xTB	ethanol	`xtb` (Grimme)	experimental; excluded from this paper
PM6	ethanol	MOPAC	production path; MOPAC parity pending
SCC-DFTB	ethanol	DFTB+	implementation smoke; DFTB+ parity pending
MSINDO	ethanol	Bonn MSINDO	validated in code suite; paper row pending
MACE-MP	ethanol	`mace-torch`	optional engine not installed here

S3.6 RIJCOSX SCF and gradient against Orca, per method

Table S14 resolves the RIJCOSX comparison by method. The SCF energies agree to a few times $1 \times 10^{-4}\ E_\mathrm{h}$ throughout, which is the expected size of a COSX grid difference, while the analytic gradient does not yet reach parity and is reported as such.

Table S14: Per-method RIJCOSX parity against Orca 6.1.1, glycine/def2-TZVP. Maximum absolute SCF-energy difference across the current 0.15-series refresh is $2.649 \times 10^{-4}\ E_\mathrm{h}$. The RHF analytic gradient is measured against an Orca `EnGrad` reference on the same geometry and does not reach parity; the remaining gradient rows are unfilled.

Method	$\lvert\Delta E_\mathrm{SCF}\rvert$ / E_h	max $\lvert\Delta(\partial E/\partial R)\rvert$ / ($E_\mathrm{h}\,a_0^{-1}$)
RHF	2.648×10^{-4}	1.04×10^{-2}
UHF	2.649×10^{-4}	held
RKS-B3LYP	2.079×10^{-4}	held
RKS-PBE0	2.431×10^{-4}	held
UKS-B3LYP	2.079×10^{-4}	held
UKS-PBE0	2.431×10^{-4}	held
Maximum	2.649×10^{-4}	held

S4 Periodic benchmarks and convergence data

S4.1 Periodic methods against the matched reference

Table S15 gives the periodic quantities that reach a reported number, each against the reference matched to its formalism: PySCF.pbc for the Gaussian-density-fitting (GDF) route and Crystal 23 for the bipolar-expansion route. Every row is gauge-held rather than a parity claim, apart from the Madelung foundation. The periodic capabilities that ship but are not validated at this release are enumerated in Section S4.2, with the blocker that stops each one.

S4.2 Periodic capabilities not validated at this release

The following capabilities are implemented and run, but none produces a reportable number in the 0.15 series. They are recorded here so that the benchmark table above contains only rows that carry a value.

- **GPW RKS-PBE**, Si / def2-SVP $(4, 4, 4)$: non-converged.
- **GDF multi-*k* KRKS-PBE**, MgO / def2-SVP $(4, 4, 4)$: non-converged runaway SCF.
- **GDF multi-*k* KUKS**, NiO / pob-TZVP-REV2: no complete artifact.

Table S15: Periodic-method benchmarks, one reference per route.

Route / quantity	System / basis	k-mesh	Reference	Agreement
GDF **Γ** RHF	MgO / STO-3G	Γ	PySCF	held: $-4.596 \times 10^{-1}\ E_\mathrm{h}$ gauge
GDF multi-$\boldsymbol{k}$ KRHF	LiH / STO-3G	(2, 2, 2)	PySCF	held: $1.585 \times 10^{-3}\ E_\mathrm{h}$
Periodic XC energy	MgO / STO-3G, LDA	(2, 2, 2)	Crystal 23 SHRINK 2	held: $-1.033\ E_\mathrm{h}$ gauge
Periodic XC energy	MgO / STO-3G, PBE	(2, 2, 2)	Crystal 23 SHRINK 2	held: $-1.034\ E_\mathrm{h}$ gauge
Periodic XC energy	MgO / STO-3G, r^{2}SCAN	(2, 2, 2)	Crystal 23 SHRINK 2	held: $-1.034\ E_\mathrm{h}$ gauge
BIPOLE multi-$\boldsymbol{k}$ KRHF	MgO / STO-3G	(2, 2, 2)	Crystal 23	held: $6.434 \times 10^{-1}\ E_\mathrm{h}$ gauge; sidecars valid

Capabilities not validated at this release, including GPW, all-electron GAPW, periodic ECPs, DFT+U, COOP/COHP, mixed density fitting, and the BIPOLE analytic gradient, are listed in Section S4.2.

- **Mixed density fitting**, MgO / def2-SVP: the overlap matrix loses positive definiteness.
- **BIPOLE analytic gradient**, MgO / STO-3G: no complete artifact.
- **Periodic ECPs**, Ag and Au fcc: a closed-shell RKS input is used for an odd electron count. W bcc: offline ECP resolution fails.
- **COOP / COHP**, NaCl / def2-SVP: a 297 GiB complex-array allocation.
- **DFT+U**, NiO / pob-TZVP-REV2: `std::bad_alloc`.
- **Bulk equation-of-state observables**, Si, MgO, LiF: non-converged or runaway scan points.
- **Brillouin-zone mesh convergence**, Si: a 38.9 GiB Ewald-cache allocation at $k = 2$ and $k = 4$, non-converged at $k = 6$.
- **Bands and densities of states**: the Si target is non-converged, and the graphene and hexagonal boron nitride examples return a nonphysical negative indirect gap under the default integer-occupation profile.
- **Space-group symmetry**, NaCl: a 1225 GB GDF memory guard.
- **All-electron GAPW**: experimental, with a known exchange-derivative issue.

These are current outcomes, not pending values. Each blocker is recorded, with the failing run, in the calculation archive distributed with the paper, and, where the run emitted one, in the machine-readable failure record.

The 0.15-series P03 BIPOLE KRHF MgO calculation completed and wrote `.out`, `.system`, population sidecars, density, DOS, bond-order, and QVF artifacts. The total energy is $-271.212\,957\,677\,3\ E_\mathrm{h}$, giving $E_\mathrm{vibe-qc} - E_\mathrm{CRYSTAL23} = 6.434\,388 \times 10^{-1}\ \mathrm{E_h}$ against the sealed SHRINK-2 HF reference, so the absolute-energy row remains held. The property sidecars are usable: Mulliken charges are $\pm 0.843566\,e$,

Löwdin charges are ±0.703709 e, the Mg–O Mayer order is 1.645 991, and the ordinary three-dimensional bulk dipole is cleanly marked unsupported. The corresponding LiH BIPOLE calculation gives $E = -7.919\,877\,978\,2\ \mathrm{E_h}$ on the 0.15 series; the DFT+U/GPW target remains failed.

The 0.15-series MgO GDF/XC calculations completed LDA, PBE, and r^{2}SCAN with total energies −271.531 535 514 7 E_h, −272.799 650 390 4 E_h and −272.963 026 737 0 E_h. They are not promoted as CRYSTAL 23 parity: the absolute offsets against the sealed SHRINK-2 references remain about −1.033 E_h, −1.034 E_h and −1.034 E_h. Cross-build repeats reproduce the P01, P02, and MgO GDF/XC totals at table precision, confirming that those values are stable across builds.

The $\mathbf{\Gamma}$ GDF baseline for P01 is complete at $E = -271.509\,106\,034\,5\ \mathrm{E_h}$, which leaves the held PySCF-gauge difference of $-4.596 \times 10^{-1}\ E_\mathrm{h}$.

A group of periodic rows is not reportable at all in this release, and we list them explicitly rather than quoting the numbers their failed runs produced. The multi-$\boldsymbol{k}$ MgO/def2-SVP case, the Si band-structure and DOS row (P04), and the Si k-convergence series do not reach SCF convergence; the k-convergence series additionally hits an unguarded Ewald-cache allocation of 38.9 GiB at the smaller meshes. The equation-of-state scans for Si, MgO, and LiF return non-converged or runaway points at most volumes, so no bulk observable (a_0, B, band gap) is derived from them. The periodic-ECP row (P09), the COOP/COHP row (P10), and the DFT+U case likewise have no complete artifact. These are recorded as open blockers in Section S4.2; the MgO GDF/XC case runs cleanly but remains convention-held on the absolute-energy comparison.

S4.3 GDF fitting-cutoff convergence

Table S16 reports the multi-$\boldsymbol{k}$ KRHF energy of primitive LiH at a $(2, 2, 2)$ mesh as a function of the GDF fitting cutoff, against the PySCF `KRHF.density_fit` reference. The tight cutoff is stable but remains $1.585\,179 \times 10^{-3}\ E_\mathrm{h}$ above the archived PySCF reference, so the row is retained as a hardening audit rather than as a promoted parity claim.

Table S16: Primitive LiH $(2, 2, 2)$ KRHF energy versus GDF fitting cutoff, against PySCF.

Cutoff	E / E_h	ΔE vs PySCF/ E_h
production default	−7.9203949568	$1.608\,278 \times 10^{-3}\ E_\mathrm{h}$
tight	−7.9204180555	$1.585\,179 \times 10^{-3}\ E_\mathrm{h}$

S4.4 Brillouin-zone mesh convergence

No Monkhorst–Pack mesh-convergence table is reported for this release. The Si/def2-SVP series fails at $k = 2$ and $k = 4$ on a 38.9 GiB Ewald-cache allocation and does not converge at $k = 6$. The irreducible-$\boldsymbol{k}$ versus full-mesh check, which would confirm that the SPGLIB symmetry reduction is exact, therefore awaits a fresh successful rerun (Section S4.2).

S4.5 First multi-route band-gap comparison

The first held band-gap comparisons across two Fock-build routes are recorded at the 2026-08-14 database state. Table S17 reports sampled-$\boldsymbol{k}$-set gaps for LiF (pob-TZVP-REV2, PBE, $(2, 2, 2)$ mesh) from the

GDF and GPW routes against a matched-mesh GPAW reference, together with the diamond GDF value. The GPW values are at the 300 E_h production cutoff and are not cutoff-converged. The diamond GPW leg does not produce a number: the route's Bloch-metric positivity gate refuses the calculation (minimum raw eigenvalue 6.9×10^{-5} against a 10^{-4} floor) rather than proceeding with dropped directions. The NaCl GAPW leg fails by tens of eV and is recorded under the experimental GAPW gating. All rows are held pending a band-gap tolerance class.

Table S17: Sampled-$\boldsymbol{k}$-set band gaps (eV) from two Fock-build routes against a matched-mesh GPAW reference, PBE, (2, 2, 2) mesh, pob-TZVP-REV2. Held pending a band-gap tolerance class; the GPW values are not converged with respect to the plane-wave cutoff.

System	Route	Gap	Ref. (GPAW)	Δ
LiF	GDF	8.5427	8.8629	−0.320
LiF	GPW	8.6830	8.8629	−0.180
C (diamond)	GDF	4.5324	4.5594	−0.027

S4.6 Internal check: Ewald lattice-sum primitive

The following is an internal unit check of the reciprocal-space lattice-sum primitive, not a cross-code validation. The Madelung constant of a lattice is an exact geometric sum, so reproducing it confirms only that the Ewald machinery converges to the right mathematical limit; it says nothing about the self-consistent electrostatic convention that the single-point comparisons in Table S15 probe. It is recorded here for completeness because a failure of this check would invalidate everything built on top of it.

Table S18: Internal convergence check of the Ewald lattice-sum primitive against the exact geometric Madelung constants.

Lattice	VIBE-QC	Accepted	Deviation
NaCl (rocksalt)	1.7475645946	1.7475645946	6.34×10^{-12}
CsCl	1.7626747729	1.7626747758	2.86×10^{-9}
ZnS (zincblende)	1.6380550534	1.6380550533	3.41×10^{-11}
2D square lattice	1.6155426267	1.6155426267	1.24×10^{-11}

The zincblende ZnS entry uses the sphalerite Madelung constant normalized by the nearest-neighbor separation, 1.63805505338879. Comparison against the rounded value 1.6380 would give an artificial 5.51×10^{-5} residual.

S4.7 Comparison against published reference values

Beyond the matched out-of-process reference runs, the periodic test systems are also compared against values published in the literature. The pob-TZVP basis-set paper [2] tabulates periodic total energies per unit cell for a set of cubic ionic solids computed with CRYSTAL, at both the Hartree–Fock and the PW1PW level, for the CRYSTAL standard basis sets and for pob-TZVP. Two of those compounds, LiH and NaCl, are also part of the periodic test set of this paper, which makes them a direct external check that is independent of the reference programs executed here.

Table S19 reproduces the published values and pairs them with the corresponding VIBE-QC results. Reproducing these numbers requires the pob-TZVP basis and the matching lattice constants and truncation

settings of the original work, so the VIBE-QC column is filled from dedicated pob-TZVP runs (bipolar-expansion route, $(2, 2, 2)$ mesh, real-space cutoffs of 20–25 a_0, energy convergence $1 \times 10^{-9}\,E_\mathrm{h}$) rather than from the STO-3G rows of Table S15. The VIBE-QC values agree with the published CRYSTAL values to between 1.0 mE_h and 19.6 mE_h. These are external consistency checks rather than parity claims: the two codes differ in their lattice-sum truncation schemes, and the quoted values are not converged with respect to the real-space cutoff, whose confirmation runs did not complete. The agreement is nevertheless three orders of magnitude tighter than the held STO-3G dense-core rows of Table S15, because the pob-TZVP systems avoid the dense-core fitting deficit discussed there. The corresponding MgO calculations did not complete within their allocated wall time and are not reported.

Table S19: Periodic total energies per unit cell (E_h) compared against the published values of Ref. [2], which were obtained with CRYSTAL. HF denotes Hartree–Fock; the PW1PW columns use the same hybrid functional as the original work. VIBE-QC values use the pob-TZVP basis and the published structures.

	HF		PW1PW	
Compound	Ref. (pob-TZVP)	VIBE-QC	Ref. (pob-TZVP)	VIBE-QC
LiH	−8.060732	−8.059734	−8.149050	−8.129497
NaCl	−621.504227	−621.519103	−622.617190	−622.624367

S5 Per-job artifacts

Every job writes a self-describing artifact bundle. This section shows the provenance and citation artifacts for a representative molecular job; the structure is identical for periodic jobs.

S5.1 Provenance manifest (`.system`)

The `.system` file is a TOML manifest pinning the build, host, and runtime so a reported result is traceable to an exact code state. A representative manifest is shown below (illustrative format; the live values are filled at run time).

Listing S1: Representative `.system` manifest.

```
[build]
version = "<filled at run time>"
commit = "<filled at run time>"
libint = "2.13.1"
libxc = "7.0.0"
spglib = "2.7.0"
libecpint = "1.0.7"

[host]
cpu = "<filled at run time>"
cores = "<filled at run time>"
memory_gb = "<filled at run time>"
os = "<filled at run time>"

[run]
omp_threads = "<filled at run time>"
```

```
fingerprint = "<filled at run time>"
```

S5.2 Automatic citation manifest (`.references` / `.bibtex`)

Each job assembles, from a single citation database, the list of papers for every method, functional, basis set, ECP, and linked library it used, and writes them as a human-readable `.references` file and a ready-to-use `.bibtex` file. For the closed-shell PBE0-D3(BJ)/def2-TZVP job (M07) the manifest contains, among others, the def2 basis [3], the PBE0 functional [4, 5], the D3(BJ) correction [6, 7], LIBINT [8], and LIBXC [9]. The user therefore receives the exact citation list their own Methods section should carry, without manual bookkeeping.

S5.3 The QVF visualization archive

When a job is run with `output_qvf=True` it writes a QVF archive (integer major version, 1 for molecular and 2 once a periodic section is present) bundling, as available, the structure, molecular orbitals, density, band structure and density of states, spectra, and optimization trajectory. The VIBE-VIEW viewer reads the archive directly and renders each component interactively in the browser. The archive is a versioned container so that older files remain readable as the schema evolves; conventional formats (`.molden`, extended XYZ, POSCAR, XSF, BXSF, CIF, Gaussian cube) are written alongside for interoperability.

S5.4 Additional VIBE-VIEW panels

The main article shows two representative viewer panels. The remaining panels used during this work are collected here. All are unmodified screenshots taken from the same archives the validation tables report, with the producing host redacted before capture.

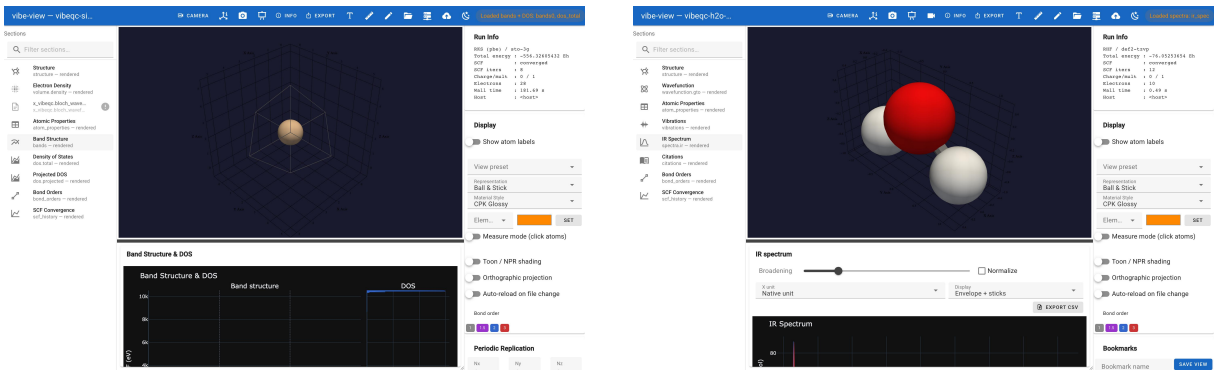

Figure S1: The two-dimensional panels, interactive Plotly charts rendered below the 3-D viewport. Left: the band-structure and density-of-states panel for a silicon test calculation (RKS PBE/STO-3G, GPW route). The minimal basis puts the silicon core states tens of keV below the valence manifold, and the automatic energy range follows the data, so this figure shows the panel rather than a converged band structure. Right: the computed IR spectrum of M14 water (RHF/def2-TZVP) with Lorentzian broadening.

S6 The VIBE-QUEUE job scheduler

The calculations in this work were dispatched, supervised, and collected with VIBE-QUEUE (CLI name `vq`), the job scheduler bundled with VIBE-QC. This section records the parts that bear on reproducibility of the

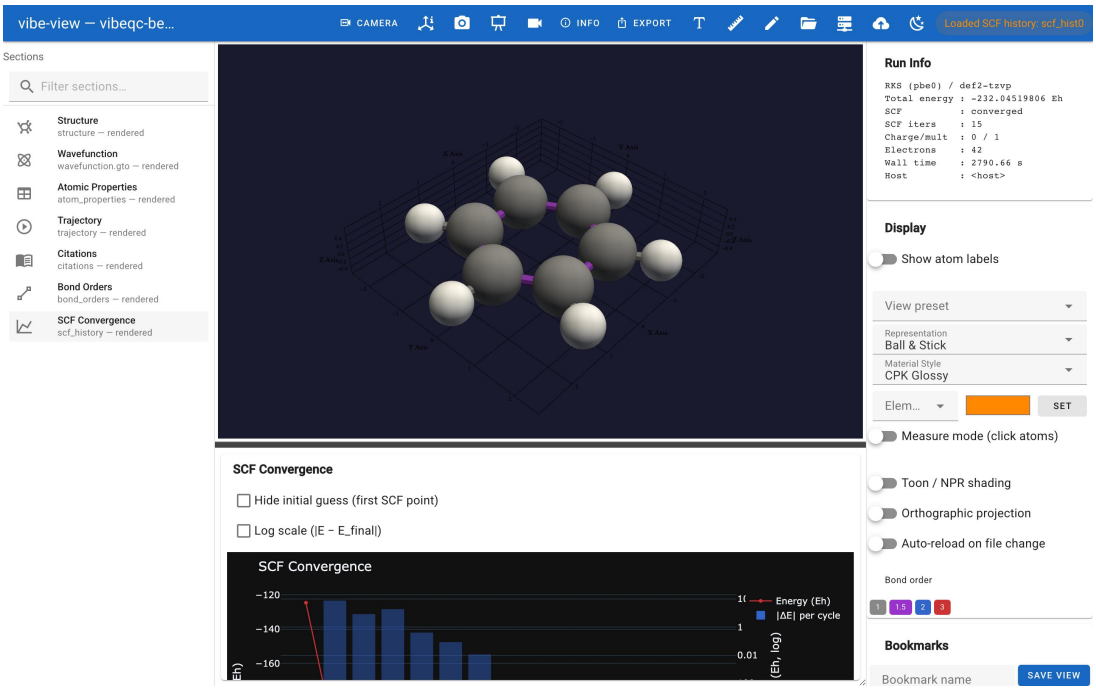

Figure S2: A full VIBE-VIEW session: the structure viewport, the sidebar with section picker and file selector, and the embedded citation panel with BibTeX export. The provenance bar identifies the loaded QVF archive and its producing code.

reported results: the design invariants, the resource enforcement that makes a reported wall time and peak memory meaningful, the remote execution model, and the external batch-scheduler backend. The full component model, on-disk state contract, and deployment guide are part of the software documentation rather than of this paper. Capabilities that are gated or on the roadmap are identified as such.

S6.1 Motivation and design invariants

Electronic-structure jobs are long-running and memory-intensive, and interactive execution is fragile: a single under-provisioned SCF can trigger the host's out-of-memory (OOM) killer and terminate unrelated processes, and a job started in an interactive shell does not survive a daemon, shell, or machine restart. VIBE-QUEUE makes this workload robust on shared workstations. Its design target is, deliberately, a personal batch scheduler rather than a cluster resource manager: it schedules one host well and delegates to a site batch scheduler when the workload exceeds a single machine. It is explicitly *not* a workflow-DAG engine, a distributed compute-graph runtime, a container orchestrator, or a multi-tenant service; those concerns are left to the tools built for them.

Six invariants hold across every release and shape everything below. **(i) Backend-agnostic specification:** the on-disk job description is declarative and dispatcher-independent, so the same specification is consumed unchanged by the local-process backend and by the external-scheduler backend. **(ii) Explicit restart semantics:** a daemon restart never silently re-runs a job; recovery is opt-in and reuses the original workspace. **(iii) No data loss on crash:** a job's workspace and specification are persisted to disk, atomically, before any process is started. **(iv) Single-language core:** the command-line interface, daemon, watchdog, adapters, and web service are all Python, with no compiled service to deploy. **(v) User-space first:** the whole system runs without root, as `vq daemon run` in a terminal multiplexer; a system service

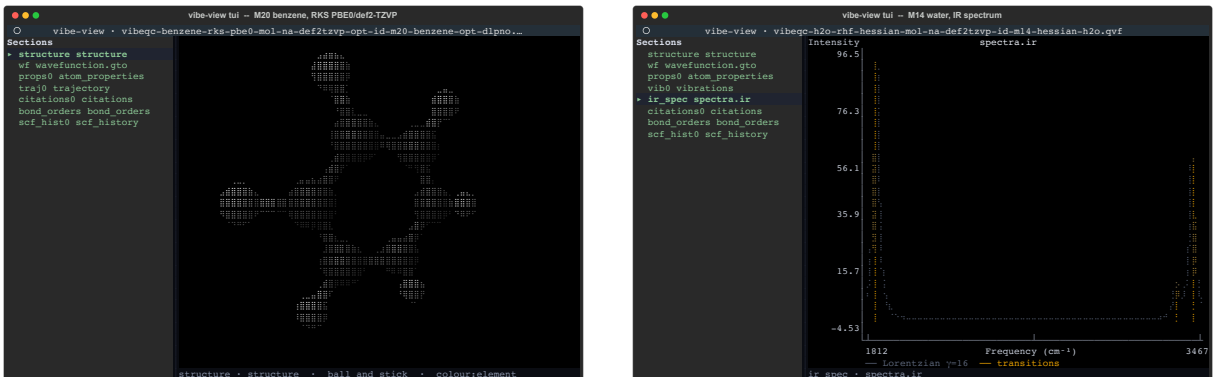

Figure S3: The terminal renderer, which prints a structure or a spectrum directly in a text console for use over a remote session without a browser.

is a supported production upgrade, not a requirement. **(vi) Versioned state:** the job-specification schema is versioned and migrated on read, never silently mutated, so specifications written by an earlier release remain readable.

S6.2 Resource enforcement

Resource safety is layered: an estimate before the job starts, a hard kernel limit while it runs, and a sampling sentinel that catches what the kernel limit does not.

Pre-flight and placement. VIBE-QC itself carries a static memory pre-flight that sizes the integral, orbital, grid, and periodic tensors before any allocation and refuses to start a job that will not fit (described in the main text). VIBE-QUEUE uses the same estimate, or an explicit request, to place a job: the auto-placement mode reads live free memory from each candidate host's `/proc/meminfo` and chooses the host on which the job actually fits, by memory headroom first and CPU headroom second, rather than the nominally largest box.

cgroup-enforced limits. On Linux, each job is launched into its own cgroup v2 scope via `systemd-run`, with the memory ceiling and CPU quota set as scope properties, so the kernel enforces the memory limit and OOM-kills the job *inside its own scope* without touching its neighbors. On a host without cgroup delegation the watchdog still enforces the limits by `/proc` sampling, less precisely but without a separate code path.

The watchdog. The watchdog samples each running job a few times a minute, recording resident memory and CPU usage to the per-job `samples.jsonl` and stamping a liveness heartbeat. It escalates a limit breach from `SIGTERM` to `SIGKILL` after a grace period and records the matching terminal reason, such as `OOM_KILLED`, `STARVED`, or `TIME_EXCEEDED`. A separate host-pressure guard protects the whole machine: when total memory pressure crosses an upper threshold the watchdog `SIGSTOP`s the running jobs to freeze their footprint and avert a cascade OOM, and `SIGCONT`s exactly those jobs once pressure falls back below a lower threshold, leaving user-suspended jobs alone.

S6.3 Remote and fleet execution

VIBE-QUEUE dispatches to a remote workstation or server over SSH without requiring a persistent daemon on every target: the client stages the payload, invokes `vq` on the remote host, and reads results back through the same artifact bundle. A submitted job receives a clean per-job scratch directory, exported to the job as the environment variable `$VQ_WORKDIR`, into which all intermediate and large data are written; the workspace and that scratch directory are retrieved afterwards. The readback verbs are uniform across local and remote hosts: `vq status` for the specification and a tail of standard error, `vq logs` for the full output streams, `vq fetch` for the workspace, and a bulk variant that pulls every terminal job at once. Across a fleet, queue and health queries fan out to all configured hosts in parallel with per-host failures isolated, and a host can be marked administratively down so that submissions and fan-out queries route around it. Listing S2 shows the typical submit-and-collect cycle.

Listing S2: A representative submit-and-collect cycle.

```
# submit a vibe-qc job to a workstation, 8 cores, 32 GB, 6 h wall time
vq submit workstation m07_pbe0_def2tzvp.py \
 --adapter vibeqc --cpus 8 --mem-mb 32000 --wall-time 6h

# or let vq place it on whichever host it fits
vq submit auto m07_pbe0_def2tzvp.py --adapter vibeqc

vq status abcd1234 # state + stderr tail
vq logs abcd1234 # full stdout/stderr
vq fetch workstation abcd1234 -o ~/results/
```

S6.4 The external batch-scheduler backend

On a shared HPC system the site's batch scheduler manages the nodes, so the local-process backend does not apply. VIBE-QUEUE therefore abstracts dispatch behind a *dispatcher* seam with two implementations behind one interface (`start`, `poll`, `signal`, `reattach`). The local dispatcher wraps process-group `Popen` as described above. The scheduler dispatcher instead drives an external batch scheduler over SSH, translating the same declarative job specification into a submission through a pluggable *dialect*: the CPU, memory, and wall-time requests map to the scheduler's resource flags, and the scheduler's own job states map back onto the internal job states. Shipped dialects include PBS/Torque and Slurm. Beyond the original Torque 2.5.12 validation, the PBS backend has been exercised across the queue targets of a university PBS/Torque cluster. PBS Pro and SGE share the dispatcher interface.

The deployment model keeps VIBE-QUEUE off the cluster and stateless on it: the cluster's head node runs no VIBE-QUEUE daemon, and a separate always-on driver daemon owns the cluster's jobs, submitting them with the configured scheduler dialect over SSH, reconciling their scheduler state, and staging the results back into the local state tree. When a job runs under the external scheduler the watchdog degrades to telemetry-only, because the scheduler owns enforcement; the job still records the same event log and exit marker, so the readback verbs and the provenance trail are unchanged. As of the release line reported here the full path is wired end to end: a submission to a scheduler-configured host forwards to the driver daemon and reaches the configured external-scheduler backend, and is *config-gated*: only a host declared

with a scheduler dialect and a driver triggers it, so every ordinary host is unaffected.

Both shipped dialects have been exercised end to end on university systems. On the Slurm route, production-shaped VIBE-QC and ORCA submissions were dispatched, ran to completion, and were retrieved through the ordinary readback verbs. On the PBS/Torque route the VIBE-QC environment was installed and validated across five queue targets; all jobs exited successfully and every fetched workspace contains a valid QVF archive together with the `.system` manifest, output files, scheduler script, and scheduler logs. A representative probe, an RHF/STO-3G calculation on a twenty-water cluster, converged in 19 SCF iterations to $E = -1499.343\,640\,976\,0\,\mathrm{E_h}$ with an identical energy at 64 and at 128 OpenMP threads, and process-CPU to wall-time ratios of 30.95× and 59.89× respectively.

These runs validate OpenMP execution and the queue-to-scheduler integration. They are not a scaling study: the two thread counts sit on different queue targets and are therefore not a controlled series, and they are not an MPI result at all, since the release-line MPI surface is limited to an optional `mpi4py` substrate and an experimental GPW z-slab overlay, with production distributed-memory execution deferred to the roadmap.

S7 Input listings

Complete listings of representative input scripts follow, reproduced verbatim from the test set distributed with this manuscript. The complete test set (twenty molecular and ten periodic inputs) is in the `test-set/` directory of the source archive and follows the same pattern.

S7.1 Molecular: RHF single point (M01)

```
"""M01 - Closed-shell RHF, H2O / def2-TZVP.

Baseline mean-field reference. Parity target: PySCF RHF to ~1e-9 Ha,
ORCA 6.1.1 to ~1e-6 Ha (same libint integral family vs independent
implementation).
"""
from pathlib import Path
import vibeqc as vq

OUT = Path(__file__).resolve().parents[1] / "outputs"
OUT.mkdir(exist_ok=True)

mol = vq.Molecule([
    vq.Atom(8, [0.0,  0.00,  0.00]),
    vq.Atom(1, [0.0,  1.43, -0.98]),
    vq.Atom(1, [0.0, -1.43, -0.98]),
])

vq.run_job(
    mol,
    basis="def2-tzvp",
    method="rhf",
```

```
    output=OUT / "m01_rhf_h2o",
    output_qvf=True,      # write the .qvf archive for vibe-view
    citations=True,       # write .bibtex / .references manifest
)
```

S7.2 Molecular: MP2 family (M04)

```
"""M04 - MP2 family on top of RHF, H2O / cc-pVTZ.

Canonical MP2, spin-component-scaled SCS-MP2, scaled-opposite-spin
SOS-MP2, all via the RI (density-fitting) path on a shared RHF
reference. The wrapper auto-resolves cc-pvtz -> cc-pvtz-ri for the
auxiliary basis. Preferred paper oracle: ORCA MP2-family correlation
energies where ORCA implements the feature.
"""
from pathlib import Path
import vibeqc as vq

OUT = Path(__file__).resolve().parents[1] / "outputs"
OUT.mkdir(exist_ok=True)
STEM = OUT / "m04_mp2_family_h2o"

mol = vq.Molecule([
    vq.Atom(8, [0.0,  0.00,  0.00]),
    vq.Atom(1, [0.0,  1.43, -0.98]),
    vq.Atom(1, [0.0, -1.43, -0.98]),
])

# RHF reference + standard artefact bundle.
vq.run_job(mol, basis="cc-pvtz", method="rhf", output=STEM,
           output_qvf=True, citations=True)

basis = vq.BasisSet(mol, "cc-pvtz")
opts = vq.RHFOptions()
opts.conv_tol_energy = 1e-10
hf = vq.run_rhf(mol, basis, opts)

mp2 = vq.run_mp2(mol, basis, hf)         # c_os = c_ss = 1
scs = vq.run_scs_mp2(mol, basis, hf)     # c_os = 6/5, c_ss = 1/3
sos = vq.run_sos_mp2(mol, basis, hf)     # c_os = 1.3, c_ss = 0

with open(STEM.with_suffix(".out"), "a") as fh:
    fh.write("\n=== post-SCF correlation (RI on RHF / cc-pVTZ) ===\n")
    fh.write(f"  E(RHF)          = {hf.energy:16.10f} Ha\n")
    fh.write(f"  E_corr(MP2)     = {mp2.e_correlation:16.10f} Ha\n")
    fh.write(f"  E_corr(SCS-MP2) = {scs.e_correlation:16.10f} Ha\n")
    fh.write(f"  E_corr(SOS-MP2) = {sos.e_correlation:16.10f} Ha\n")
```

S7.3 Molecular: non-mean-field solvers (M10)

```
"""M10 - Non-mean-field solvers (vibeqc.solvers).

Three entries to the wavefunction-method suite, all on small active
spaces so the set runs on a laptop:

  - Full CI          : method="fci" (exact in the orbital basis; H2/6-31G)
  - Selected CI      : method="selected_ci" (CIPSI-style heat-bath)
  - DMRG             : method="dmrg" (two-site MPS)

FCI on H2/6-31G is verified against PySCF FCI to machine precision.
The approximate solvers are run in a (6e, 6o) active space on N2;
widen active_space=(n_elec, n_orb) for production accuracy.
"""
from pathlib import Path
import vibeqc as vq

OUT = Path(__file__).resolve().parents[1] / "outputs"
OUT.mkdir(exist_ok=True)

# --- Full CI on H2 / 6-31G (exact reference) --------------------------
h2 = vq.Molecule([vq.Atom(1, [0.0, 0.0, 0.0]), vq.Atom(1, [0.0, 0.0, 1.4])])
vq.run_job(h2, basis="6-31g", method="fci",
           output=OUT / "m10_fci_h2", citations=True)

# --- Approximate solvers on N2 / cc-pVDZ, (6e, 6o) --------------------
n2 = vq.Molecule([vq.Atom(7, [0.0, 0.0, 0.0]), vq.Atom(7, [0.0, 0.0, 2.074])])
for method in ["selected_ci", "dmrg"]:
    vq.run_job(
        n2,
        basis="cc-pvdz",
        method=method,
        active_space=(6, 6),
        output=OUT / f"m10_{method}_n2",
        citations=True,
    )
```

S7.4 Periodic: multi-*k* GDF on LiH (P02)

```
"""P02 - Multi-k periodic HF via GDF, LiH primitive FCC, (2,2,2).

The headline periodic-parity calculation: multi-k KRHF on the
primitive rocksalt LiH cell with a 2x2x2 Monkhorst-Pack mesh through
the native Gaussian-density-fitting path. This is the case that closed
the four-cycle GDF deferral at v0.11.0, reaching ~ -1.0 uHa parity vs
PySCF KRHF.density_fit() at the tight (30-bohr) cutoff. The default
production cutoff is looser and trades accuracy for cost.
"""
```

```
from pathlib import Path
import numpy as np
import vibeqc as vq
from vibeqc.periodic_runner import run_periodic_job

OUT = Path(__file__).resolve().parents[1] / "outputs"
OUT.mkdir(exist_ok=True)

ANG2BOHR = 1.0 / 0.529177210903
a = 4.084 * ANG2BOHR                        # LiH rocksalt lattice constant
lattice = (a / 2.0) * np.array([[0.0, 1.0, 1.0],
                                [1.0, 0.0, 1.0],
                                [1.0, 1.0, 0.0]])
atoms = [vq.Atom(3, [0.0, 0.0, 0.0]),
         vq.Atom(1, [a / 2.0, a / 2.0, a / 2.0])]
sysp = vq.PeriodicSystem(3, lattice, atoms)
basis = vq.BasisSet(sysp.unit_cell_molecule(), "sto-3g")

run_periodic_job(
    sysp, basis,
    method="RHF",
    jk_method="gdf",
    kpoints=(2, 2, 2),
    output=OUT / "p02_lih_multik_gdf",
    output_qvf=True,
    citations=True,
    max_iter=80, conv_tol_energy=1e-8, initial_guess="SAD",
)
```

S7.5 Periodic: bipolar-expansion route on MgO (P03)

```
"""P03 - Multi-k periodic HF via the BIPOLE driver, MgO primitive, (2,2,2).

The CRYSTAL-gauge multipole (BIPOLE) Fock-build route. This is the
path used in the end-to-end CRYSTAL-parity workstream. The CRYSTAL-
alpha / Ewald-omega gauge unification (v0.10.0 "cluster-A1 fix")
aligns the BIPOLE and Ewald gauges so the SCF energy is meaningful
across routes. Compare directly against P02 on the same physics.
"""
from pathlib import Path
import numpy as np
import vibeqc as vq
from vibeqc.periodic_runner import run_periodic_job

OUT = Path(__file__).resolve().parents[1] / "outputs"
OUT.mkdir(exist_ok=True)

ANG2BOHR = 1.0 / 0.529177210903
```

```
a = 4.21 * ANG2BOHR
lattice = (a / 2.0) * np.array([[0.0, 1.0, 1.0],
                                [1.0, 0.0, 1.0],
                                [1.0, 1.0, 0.0]])
atoms = [vq.Atom(12, [0.0, 0.0, 0.0]),
         vq.Atom(8, [a / 2.0, a / 2.0, a / 2.0])]
sysp = vq.PeriodicSystem(3, lattice, atoms)
basis = vq.BasisSet(sysp.unit_cell_molecule(), "sto-3g")

run_periodic_job(
    sysp, basis,
    method="RHF",
    jk_method="bipole",
    kpoints=(2, 2, 2),
    multipole_l_max=2,
    output=OUT / "p03_mgo_multik_bipole",
    output_qvf=True,
    citations=True,
    max_iter=60, conv_tol_energy=1e-7, initial_guess="SAD",
    ewald_precision=1e-8,
)
```

S7.6 Periodic: band structure and DOS of silicon (P04)

```
"""P04 - Band structure + density of states, Si diamond / def2-SVP.

Multi-k RKS-PBE SCF on the 2-atom primitive diamond cell, then a band
structure along the standard HPKOT k-path and a density of states.
Both are embedded in the .qvf archive so vibe-view renders interactive
band-structure and DOS plots. Demonstrates the periodic property
surface and the visualization pipeline.

The band-structure helper API may differ slightly between releases;
if vq.band_structure is unavailable in your build, drop the
band_structure= argument and the SCF + QVF still run.
"""
from pathlib import Path
import numpy as np
import vibeqc as vq
from vibeqc.periodic_runner import run_periodic_job

OUT = Path(__file__).resolve().parents[1] / "outputs"
OUT.mkdir(exist_ok=True)

ANG2BOHR = 1.0 / 0.529177210903
a = 5.431 * ANG2BOHR
lattice = (a / 2.0) * np.array([[0.0, 1.0, 1.0],
                                [1.0, 0.0, 1.0],
```

```
                                [1.0, 1.0, 0.0]])
atoms = [vq.Atom(14, [0.0, 0.0, 0.0]),
         vq.Atom(14, [a / 4.0, a / 4.0, a / 4.0])]
sysp = vq.PeriodicSystem(3, lattice, atoms)
basis = vq.BasisSet(sysp.unit_cell_molecule(), "def2-svp")

# Optional: precompute a band structure to embed in the QVF archive.
bands = None
if hasattr(vq, "band_structure"):
    try:
        bands = vq.band_structure(sysp, basis, kpoints=(4, 4, 4))
    except Exception:
        bands = None

run_periodic_job(
    sysp, basis,
    method="RKS", functional="pbe",
    jk_method="gdf",
    kpoints=(4, 4, 4),
    band_structure=bands,
    output=OUT / "p04_si_bands_dos",
    output_qvf=True,
    citations=True,
    smearing_temperature="small-gap",
    max_iter=100, conv_tol_energy=1e-7, initial_guess="SAD",
)
```

S8 Complete validation database

The preceding sections report the per-method benchmarks in curated form: one canonical system per capability, chosen to be readable. This section reports the underlying database in full. Every comparison that has been attempted for this release appears below, including those that produced no number, so that the selected rows above can be placed against the whole attempt surface rather than against a summary of it.

The tables are generated directly from the calculation database and are not maintained by hand. Table S20 gives the disposition of the complete set; Table S21 and Table S22 give the individual comparisons, grouped by method family and preceded in each block by that family's counts and, where completed comparisons exist, the median and maximum absolute deviation over them.

Reading the verdict column. A comparison reaches a number only when both codes ran to completion and produced the artifacts required to establish that they were solving the same problem. Where that did not happen, the deviation column carries the reason instead:

- `pass` and `fail`: both sides completed and the deviation is reported. `fail` means the row missed its stated tolerance, which is not the same as a defect in the method. A large share of the present

failures are comparisons in which an integration grid or a frozen-core convention was not matched between the two programs, and these are being reduced by matched reruns rather than by relaxing the tolerance.

- `held`: both codes completed, but the comparison is retained under a stated convention or gauge offset rather than promoted as a parity claim.
- `incomplete`: the comparison record could not be evaluated to a pass/fail verdict.
- `reference-missing`: VIBE-QC completed but the reference program did not, so no comparison exists.
- `artifact-incomplete`: the calculation ran but its bundle lacks a file the comparison requires.
- `blocked`: the case did not reach a usable state, most often on a resource guard or a route that fails closed. `blocked-reference-leg` marks the same condition on the reference side.
- `pass-pending-tolerance`: both sides completed and the deviation is recorded, but the tolerance class for the quantity has not yet been fixed, so no pass/fail verdict is assigned.
- `recorded-no-tolerance-class`: the value is recorded without a tolerance class and carries no verdict.
- `reference-property-measured`: a reference-side property was measured; the paired VIBE-QC value is not yet available.
- `queued`: staged but not yet executed at the cut.

We report the unfiltered set deliberately. A validation campaign of this size has a long tail, and the accurate summary of it is that the molecular stack is now densely covered, across mean-field, density-functional, perturbative, coupled-cluster, excited-state, and propagator routes, while the periodic routes have broad attempt coverage with no closed cross-code comparison yet, as the main article states in its limitations. At the 2026-08-14 database snapshot used for this paper, 58 percent of the comparisons complete on both sides and report a deviation, and 43 percent pass their stated tolerance. Suppressing the rest would make the covered fraction look larger than it is, and would also hide the two most useful diagnostics in the table: which routes fail systematically, and which fail only where a convention has not been matched.

Table S20: Disposition of every comparison in the validation database.

Verdict	Molecular	Periodic
pass	3239	0
pass-pending-tolerance	14	26
held	1106	65
fail	1063	67
recorded-no-tolerance-class	9	4
reference-property-measured	0	19
incomplete	7	2
artifact-incomplete	407	14
reference-missing	137	9
blocked-reference-leg	1	0
blocked	1194	65
queued	23	13
Total	7200	284

Table S21: Complete molecular validation database, grouped by method family. Every comparison in the archive is listed, including those that did not produce a number. $|\Delta|$ is given for completed comparisons (in hartree unless the quantity names another unit); otherwise the column carries the verdict.

Method	System / basis	Ref.	Quantity	$\lvert\Delta\rvert$
Hartree–Fock				
150 pass, 32 fail, 28 blocked. Median $\lvert\Delta E\rvert$ 4.3×10^{-10}, max 8.3×10^{-7} E_h.				
RHF	atom-mg / 3-21g	orca	energy total ha	1.05×10^{-10}
RHF	atom-mg / 6-31gss	orca	energy total ha	2.29×10^{-10}
RHF	atom-mg / cc-pvdz	orca	energy total ha	1.74×10^{-10}
RHF	atom-mg / def2-svp	orca	energy total ha	1.42×10^{-10}
RHF	atom-mg / sto-3g	orca	energy total ha	7.75×10^{-11}
RHF	c2h4 / sto-3g	orca	energy total ha	4.55×10^{-10}
RHF	ch2o / sto-3g	orca	energy total ha	3.50×10^{-12}
RHF	ch4 / 3-21g	orca	energy total ha	8.35×10^{-11}
RHF	ch4 / sto-3g	orca	energy total ha	8.15×10^{-11}
RHF	co2 / sto-3g	orca	energy total ha	6.61×10^{-10}
RHF	co / 3-21g	orca	energy total ha	2.10×10^{-11}
RHF	co / sto-3g	orca	energy total ha	1.93×10^{-10}
RHF	h2 / 3-21g	orca	energy total ha	4.50×10^{-12}
RHF	h2 / 6-31gss	orca	energy total ha	1.25×10^{-11}
RHF	h2 / aug-cc-pvdz	orca	energy total ha	3.80×10^{-11}
RHF	h2 / cc-pvdz	orca	energy total ha	3.25×10^{-11}
RHF	h2 / def2-svp	orca	energy total ha	9.00×10^{-12}
RHF	h2 / def2-tzvp	orca	energy total ha	4.00×10^{-12}
RHF	h2 / def2-tzvp	orca	energy total ha	3.50×10^{-12}
RHF	h2 / def2-tzvp	orca	energy total ha	4.00×10^{-12}
RHF	h2 / def2-tzvp	orca	energy total ha	4.00×10^{-12}
RHF	h2 / def2-tzvp	orca	energy total ha	4.00×10^{-12}
RHF	h2 / def2-tzvp	orca	energy total ha	4.00×10^{-12}
RHF	h2 / def2-tzvp	orca	energy total ha	4.00×10^{-12}
RHF	h2 / sto-3g	orca	energy total ha	1.08×10^{-10}
RHF	h2o-dimer / sto-3g	orca	energy total ha	3.22×10^{-10}
RHF	h2o2 / sto-3g	orca	energy total ha	1.28×10^{-9}
RHF	h2o / 3-21g	orca	energy total ha	5.30×10^{-11}
RHF	h2o / sto-3g	orca	energy total ha	2.64×10^{-10}
RHF	hf / 3-21g	orca	energy total ha	6.05×10^{-11}
RHF	hf / sto-3g	orca	energy total ha	1.93×10^{-10}
RHF	lih / 3-21g	orca	energy total ha	3.55×10^{-11}
RHF	lih / sto-3g	orca	energy total ha	1.15×10^{-10}
RHF	n-alkane:2 / sto-3g	orca	energy total ha	1.95×10^{-10}
RHF	n2 / 3-21g	orca	energy total ha	3.55×10^{-10}
RHF	n2 / sto-3g	orca	energy total ha	6.49×10^{-10}
RHF	nacl-cluster:1 / sto-3g	orca	energy total ha	1.28×10^{-9}
RHF	nh3 / 3-21g	orca	energy total ha	7.65×10^{-11}
RHF	nh3 / sto-3g	orca	energy total ha	1.84×10^{-10}
RHF	s22-ammonia-dimer / sto-3g	orca	energy total ha	1.56×10^{-9}
RHF	s22-methane-dimer / sto-3g	orca	energy total ha	2.45×10^{-10}
RHF	s22-water-dimer / sto-3g	orca	energy total ha	2.65×10^{-10}
RHF	water-cluster:1 / sto-3g	orca	energy total ha	2.88×10^{-10}
RHF	water-cluster:2 / sto-3g	orca	energy total ha	8.44×10^{-10}
UHF	h2o / cc-pvdz	orca	scf total energy ha	4.58×10^{-10}
ROHF	h2o / cc-pvdz	orca	scf total energy ha	4.17×10^{-10}
UHF	h2o / aug-cc-pvdz	orca	scf total energy ha	4.55×10^{-10}
RHF	h2o / cc-pvdz	orca	scf total energy ha	2.06×10^{-9}
UHF	h2o / cc-pvdz	orca	scf total energy ha	2.21×10^{-9}
ROHF	h2o / cc-pvdz	orca	scf total energy ha	1.99×10^{-9}
UHF	co / cc-pvdz	orca	scf total energy ha	1.06×10^{-9}
ROHF	co / cc-pvdz	orca	scf total energy ha	1.59×10^{-9}

Table S21, continued.

Method	System / basis	Ref.	Quantity	$\lvert\Delta\rvert$
UHF	co / aug-cc-pvdz	orca	scf total energy ha	9.04×10^{-10}
UHF	benzene / cc-pvdz	orca	scf total energy ha	1.40×10^{-9}
UHF	n2 / cc-pvdz	orca	scf total energy ha	2.76×10^{-10}
ROHF	n2 / cc-pvdz	orca	scf total energy ha	4.23×10^{-10}
UHF	n2 / cc-pvdz	orca	scf total energy ha	2.50×10^{-9}
RHF	o2-triplet / cc-pvdz	orca	scf total energy ha	1.18×10^{-9}
RHF	h2o / cc-pvtz	orca	scf total energy ha	4.96×10^{-10}
RHF	h2o / cc-pvqz	orca	scf total energy ha	3.87×10^{-10}
RHF	h2o / cc-pv5z	orca	scf total energy ha	5.32×10^{-10}
RHF	h2o / aug-cc-pvqz	orca	scf total energy ha	6.46×10^{-10}
RHF	h2o / def2-qzvpp	orca	scf total energy ha	5.33×10^{-10}
RHF	ch4 / cc-pvqz	orca	scf total energy ha	1.67×10^{-10}
RHF	ch4 / cc-pv5z	orca	scf total energy ha	7.26×10^{-10}
RHF	ch4 / def2-qzvpp	orca	scf total energy ha	4.32×10^{-10}
RHF	co / cc-pvqz	orca	scf total energy ha	9.22×10^{-10}
RHF	co / cc-pv5z	orca	scf total energy ha	7.38×10^{-10}
RHF	benzene / cc-pvtz	orca	scf total energy ha	1.04×10^{-7}
RHF	benzene / cc-pvqz	orca	scf total energy ha	6.10×10^{-8}
RHF	benzene / def2-qzvpp	orca	scf total energy ha	3.39×10^{-8}
RHF	ch4 / cc-pvqz	orca	scf total energy ha	1.67×10^{-10}
RHF	ch4 / cc-pv5z	orca	scf total energy ha	7.26×10^{-10}
RHF	h2 / aug-cc-pv5z	orca	scf total energy ha	8.25×10^{-9}
RHF	h2 / aug-cc-pv5z	orca	scf total energy ha	6.22×10^{-9}
RHF	h2 / aug-cc-pv5z	orca	scf total energy ha	3.51×10^{-9}
RHF	h2o / aug-cc-pvqz	orca	scf total energy ha	6.46×10^{-10}
RHF	h2o / aug-cc-pv5z	orca	scf total energy ha	6.37×10^{-10}
RHF	benzene / aug-cc-pvtz	orca	scf total energy ha	1.22×10^{-7}
RHF	benzene / def2-qzvppd	orca	scf total energy ha	6.38×10^{-9}
RHF	h2 / aug-cc-pv5z	orca	scf total energy ha	8.25×10^{-9}
RHF	h2 / aug-cc-pv5z	orca	scf total energy ha	8.25×10^{-9}
RHF	naphthalene / sto-3g	orca	scf total energy ha	4.11×10^{-9}
RHF	naphthalene / def2-svp	orca	scf total energy ha	4.79×10^{-9}
RHF	h2 / cc-pvdz	orca	scf total energy ha	1.00×10^{-12}
RHF	h2 / cc-pvdz	orca	scf total energy ha	9.12×10^{-10}
RHF	h2 / cc-pvdz	orca	scf total energy ha	1.34×10^{-9}
RHF	h2 / cc-pvdz	orca	scf total energy ha	1.32×10^{-9}
RHF	h2 / cc-pvdz	orca	scf total energy ha	9.64×10^{-10}
RHF	h2 / cc-pvdz	orca	scf total energy ha	3.57×10^{-10}
RHF	n2 / cc-pvdz	orca	scf total energy ha	8.34×10^{-10}
UHF	n2 / cc-pvdz	orca	scf total energy ha	8.34×10^{-10}
RHF	n2 / cc-pvdz	orca	scf total energy ha	5.94×10^{-9}
UHF	n2 / cc-pvdz	orca	scf total energy ha	5.91×10^{-9}
RHF	n2 / cc-pvdz	orca	scf total energy ha	6.00×10^{-9}
UHF	n2 / cc-pvdz	orca	scf total energy ha	6.02×10^{-9}
RHF	n2 / cc-pvdz	orca	scf total energy ha	5.02×10^{-9}
UHF	n2 / cc-pvdz	orca	scf total energy ha	5.17×10^{-9}
RHF	c2h4-twisted / cc-pvdz	orca	scf total energy ha	5.38×10^{-10}
UHF	c2h4-twisted / cc-pvdz	orca	scf total energy ha	6.44×10^{-10}
UHF	c2h4-twisted / cc-pvdz	orca	scf total energy ha	2.24×10^{-9}
UHF	c2h4-twisted / cc-pvdz	orca	scf total energy ha	1.51×10^{-9}
UHF	o2-triplet / cc-pvdz	orca	scf total energy ha	1.20×10^{-9}
ROHF	o2-triplet / cc-pvdz	orca	scf total energy ha	1.25×10^{-9}
UHF	oh-radical / cc-pvdz	orca	scf total energy ha	2.89×10^{-10}
UHF	o2-triplet / cc-pvtz	orca	scf total energy ha	1.26×10^{-9}
ROHF	o2-triplet / cc-pvtz	orca	scf total energy ha	1.34×10^{-9}
UHF	oh-radical / cc-pvtz	orca	scf total energy ha	3.19×10^{-10}
UHF	fecl3 / def2-svp	orca	scf total energy ha	1.34×10^{-9}
RHF	ferrocene / def2-svp	orca	scf total energy ha	8.34×10^{-7}

Table S21, continued.

Method	System / basis	Ref.	Quantity	$\lvert\Delta\rvert$
RHF	cr-co6 / def2-svp	orca	scf total energy ha	1.07×10^{-8}
RHF	ni-co4 / def2-svp	orca	scf total energy ha	2.57×10^{-8}
RHF	ni-co4 / lanl2dz	orca	scf total energy ha	1.19×10^{-7}
RHF	ni-co4 / lanl2dz	orca	scf total energy ha	1.19×10^{-7}
RHF	n2 / cc-pvdz	openmolcas	total energy ha	0
RHF	n2 / cc-pvdz	openmolcas	total energy ha	0
RHF	n2 / cc-pvtz	openmolcas	total energy ha	0
RHF	n2 / cc-pvdz	openmolcas	total energy ha	0
RHF	n2 / cc-pvdz	openmolcas	total energy ha	0
RHF	hf-molecule / cc-pvdz	openmolcas	total energy ha	0
RHF	hf-molecule / cc-pvdz	openmolcas	total energy ha	0
RHF	h2o / cc-pvdz	openmolcas	total energy ha	0
RHF	c2 / cc-pvdz	openmolcas	total energy ha	0
RHF	Ba-atom / dhf-qzvp	orca	total energy ha	1.20×10^{-8}
RHF	Ba-atom / dhf-svp	orca	total energy ha	1.21×10^{-8}
RHF	Ba-atom / dhf-tzvp	orca	total energy ha	1.20×10^{-8}
RHF	Ba-atom / lanl08	orca	total energy ha	1.80×10^{-11}
RHF	Ba-atom / lanl2dz	orca	total energy ha	9.00×10^{-12}
RHF	Cd-atom / dhf-qzvp	orca	total energy ha	6.20×10^{-11}
RHF	Cd-atom / dhf-svp	orca	total energy ha	7.50×10^{-11}
RHF	Cd-atom / dhf-tzvp	orca	total energy ha	3.40×10^{-11}
RHF	Cd-atom / lanl08	orca	total energy ha	2.90×10^{-11}
RHF	Cd-atom / lanl2dz	orca	total energy ha	5.30×10^{-11}
RHF	cr-co6 / lanl2dz	orca	total energy ha	2.25×10^{-7}
UHF	fecl3 / lanl08	orca	total energy ha	1.57×10^{-7}
UHF	fecl3 / lanl2dz	orca	total energy ha	1.94×10^{-7}
RHF	ferrocene / lanl2dz	orca	total energy ha	8.26×10^{-8}
RHF	Hg-atom / dhf-qzvp	orca	total energy ha	1.17×10^{-10}
RHF	Hg-atom / dhf-svp	orca	total energy ha	1.74×10^{-10}
RHF	Hg-atom / dhf-tzvp	orca	total energy ha	4.20×10^{-11}
RHF	Hg-atom / lanl08	orca	total energy ha	6.00×10^{-11}
RHF	Hg-atom / lanl2dz	orca	total energy ha	9.30×10^{-11}
RHF	ni-co4 / lanl2dz	orca	total energy ha	1.19×10^{-7}
RHF	Xe-atom / dhf-qzvp	orca	total energy ha	9.40×10^{-11}
RHF	Xe-atom / dhf-svp	orca	total energy ha	9.50×10^{-11}
RHF	Xe-atom / dhf-tzvp	orca	total energy ha	9.50×10^{-11}
RHF	Xe-atom / lanl08	orca	total energy ha	3.50×10^{-11}
RHF	Xe-atom / lanl2dz	orca	total energy ha	3.40×10^{-11}
RHF	Zn-atom / lanl08	orca	total energy ha	4.30×10^{-11}
RHF	Zn-atom / lanl2dz	orca	total energy ha	4.90×10^{-11}
UHF	benzene / cc-pvdz	orca	scf total energy ha	2.66×10^{-3}
ROHF	benzene / cc-pvdz	orca	scf total energy ha	6.72×10^{-4}
ROHF	n2 / cc-pvdz	orca	scf total energy ha	1.29×10^{-1}
UHF	lih / aug-cc-pvdz	orca	scf total energy ha	1.87×10^{-5}
UHF	o2-triplet / cc-pvdz	orca	scf total energy ha	7.60×10^{-2}
ROHF	o2-triplet / cc-pvdz	orca	scf total energy ha	n/a
RHF	lih / aug-cc-pvqz	orca	scf total energy ha	2.63×10^{-6}
RHF	naphthalene / def2-tzvp	orca	scf total energy ha	1.58×10^{-6}
RHF	porphine / sto-3g	orca	scf total energy ha	5.24×10^{-2}
RHF	porphine / def2-svp	orca	scf total energy ha	2.41×10^{-3}
RHF	crambin / sto-3g	orca	scf total energy ha	5.83×10^{-4}
RHF	crambin / def2-svp	orca	scf total energy ha	3.98×10^{-2}
RHF	c10h22 / def2-svp	orca	scf total energy ha	1.36×10^{-6}
RHF	c16h34 / def2-svp	orca	scf total energy ha	2.83×10^{-6}
RHF	c20h42 / def2-svp	orca	scf total energy ha	4.01×10^{-6}
RHF	c30h62 / def2-svp	orca	scf total energy ha	7.51×10^{-6}
RHF	c20h42 / def2-tzvp	orca	scf total energy ha	1.02×10^{-4}
RHF	c2h4-twisted / cc-pvdz	orca	scf total energy ha	3.08×10^{-2}

Table S21, continued.

Method	System / basis	Ref.	Quantity	$\lvert\Delta\rvert$
UHF	c2h4-twisted / cc-pvdz	orca	scf total energy ha	3.08×10^{-2}
ROHF	oh-radical / cc-pvdz	orca	scf total energy ha	6.08×10^{-4}
ROHF	oh-radical / cc-pvtz	orca	scf total energy ha	1.36×10^{-3}
ROHF	fecl3 / def2-svp	orca	scf total energy ha	n/a
UHF	fecl3 / def2-svp	orca	scf total energy ha	n/a
ROHF	fecl3 / def2-svp	orca	scf total energy ha	n/a
ROHF	fecl3 / def2-tzvp	orca	scf total energy ha	5.20×10^{-1}
UHF	fecl3 / def2-tzvp	orca	scf total energy ha	6.08×10^{-2}
ROHF	fecl3 / def2-tzvp	orca	scf total energy ha	2.63×10^{-2}
UHF	ferrocene / def2-svp	orca	scf total energy ha	1.93×10^{-1}
ROHF	ferrocene / def2-svp	orca	scf total energy ha	3.23×10^{-2}
ROHF	cr-co6 / def2-svp	orca	scf total energy ha	n/a
UHF	ni-co4 / def2-svp	orca	scf total energy ha	n/a
ROHF	ni-co4 / def2-svp	orca	scf total energy ha	n/a
RHF	h2 / ma-def2-tzvp	orca	energy total ha	blocked
RHF	acetamide / def2-svp	orca	total energy ha	blocked
RHF	cr-co6 / sto-3g	orca	total energy ha	blocked
RHF	porphine / def2-tzvp	orca	total energy ha	blocked
ROHF	fecl3 / def2-svp	orca	total energy ha	blocked
RHF	s22-ethene-ethyne / def2-svp	orca	total energy ha	blocked
RHF	hf / def2-svp	orca	total energy ha	blocked
RHF	hf / cc-pvdz	orca	total energy ha	blocked
RHF	hf / cc-pvqz	orca	total energy ha	blocked
RHF	imidazole / sto-3g	orca	total energy ha	blocked
RHF	imidazole / def2-svp	orca	total energy ha	blocked
RHF	imidazole / def2-tzvp	orca	total energy ha	blocked
RHF	imidazole / cc-pvdz	orca	total energy ha	blocked
RHF	imidazole / cc-pvtz	orca	total energy ha	blocked
RHF	n2 / sto-3g	orca	total energy ha	blocked
RHF	n2 / def2-tzvp	orca	total energy ha	blocked
RHF	naphthalene / cc-pvtz	orca	total energy ha	blocked
RHF	nh3 / def2-svp	orca	total energy ha	blocked
RHF	ni-co4 / cc-pvdz	orca	total energy ha	blocked
UHF	o2-triplet / sto-3g	orca	total energy ha	blocked
RHF	propanamide / def2-svp	orca	total energy ha	blocked
RHF	pyrimidine / def2-svp	orca	total energy ha	blocked
RHF	pyrrole / cc-pvdz	orca	total energy ha	blocked
RHF	tetrazine / sto-3g	orca	total energy ha	blocked
RHF	thymine / def2-svp	orca	total energy ha	blocked
RHF	triazine / def2-svp	orca	total energy ha	blocked
RHF	triazine / cc-pvtz	orca	total energy ha	blocked
RHF	uracil / cc-pvdz	orca	total energy ha	blocked
Self-consistent field				
387 pass, 379 fail, 4 incomplete, 22 artifact-incomplete, 43 blocked. Median $\lvert\Delta E\rvert$ 8.1×10^{-6}, max 5.5×10^{-3} E_h.				
RHF	glycine / def2-tzvp	orca	total energy ha	4.56×10^{-4}
UHF	glycine / def2-tzvp	orca	total energy ha	4.56×10^{-4}
UHF	glycine / def2-tzvp	orca	total energy ha	4.56×10^{-4}
RHF	h2 / sto-3g	orca	total energy ha	3.12×10^{-9}
RHF	h2o / sto-3g	orca	total energy ha	1.03×10^{-8}
RHF	n-octane / sto-3g	orca	total energy ha	2.50×10^{-8}
RHF	n-dodecane / sto-3g	orca	total energy ha	3.71×10^{-8}
RKS/pbe	n-dodecane / sto-3g	orca	total energy ha	5.48×10^{-3}
RHF	h2o / def2-tzvp	orca	total energy ha	1.42×10^{-13}
RHF	h2o / def2-tzvp	orca	total energy ha	1.23×10^{-9}
RHF	h2o / def2-tzvp	orca	total energy ha	1.23×10^{-9}
UHF	oh / def2-tzvp	orca	total energy ha	0
UHF	oh / def2-tzvp	orca	total energy ha	2.83×10^{-10}

Table S21, continued.

Method	System / basis	Ref.	Quantity	$\lvert\Delta\rvert$
UHF	oh / def2-tzvp	orca	total energy ha	2.83×10^{-10}
RKS/b3lyp	h2o / def2-tzvp	orca	total energy ha	1.15×10^{-4}
RKS/pbe0	h2o / def2-tzvp	orca	total energy ha	1.32×10^{-4}
RKS/pbe	h2o / def2-tzvp	orca	total energy ha	1.44×10^{-4}
RKS/r2scan	h2o / def2-tzvp	orca	total energy ha	1.50×10^{-4}
RKS/wb97x	h2o / def2-tzvp	orca	total energy ha	1.37×10^{-4}
ROHF	nh2 / def2-tzvp	orca	total energy ha	3.41×10^{-10}
RHF	h2o / def2-svp	orca	total energy ha	1.66×10^{-8}
RHF	h2o / def2-svp	orca	total energy ha	1.66×10^{-8}
RHF	h2o / def2-svp	orca	total energy ha	1.66×10^{-8}
UHF	oh-radical / def2-svp	orca	total energy ha	2.22×10^{-9}
UHF	oh-radical / def2-svp	orca	total energy ha	2.22×10^{-9}
UHF	oh-radical / def2-svp	orca	total energy ha	2.19×10^{-9}
ROHF	nh2-radical / def2-svp	orca	total energy ha	2.19×10^{-9}
ROHF	nh2-radical / def2-svp	orca	total energy ha	2.19×10^{-9}
ROHF	nh2-radical / def2-svp	orca	total energy ha	2.16×10^{-9}
RHF	h2o / sto-3g	orca	total energy ha	5.35×10^{-9}
UHF	oh-radical / sto-3g	orca	total energy ha	7.73×10^{-9}
ROHF	nh2-radical / sto-3g	orca	total energy ha	9.79×10^{-9}
RHF	h2o / def2-svp	orca	total energy ha	1.66×10^{-8}
RHF	h2o / sto-3g	orca	total energy ha	5.35×10^{-9}
RHF	h2o / def2-tzvp	orca	total energy ha	1.69×10^{-8}
UHF	oh-radical / def2-svp	orca	total energy ha	2.22×10^{-9}
UHF	oh-radical / sto-3g	orca	total energy ha	7.73×10^{-9}
UHF	oh-radical / def2-tzvp	orca	total energy ha	2.58×10^{-9}
ROHF	nh2-radical / def2-svp	orca	total energy ha	2.19×10^{-9}
ROHF	nh2-radical / sto-3g	orca	total energy ha	9.79×10^{-9}
ROHF	nh2-radical / def2-tzvp	orca	total energy ha	3.47×10^{-9}
RHF	acetic-acid / sto-3g	orca	total energy ha	4.48×10^{-9}
RHF	c2h4 / sto-3g	orca	total energy ha	9.11×10^{-10}
RHF	acetic-acid / def2-svp	orca	total energy ha	2.96×10^{-9}
RHF	c2h4 / def2-svp	orca	total energy ha	1.23×10^{-10}
RHF	acetic-acid / def2-tzvp	orca	total energy ha	2.28×10^{-9}
RHF	c2h4 / def2-tzvp	orca	total energy ha	4.49×10^{-10}
RHF	acetic-acid / cc-pvdz	orca	total energy ha	3.51×10^{-9}
RHF	c2h4 / cc-pvdz	orca	total energy ha	5.39×10^{-10}
RHF	c2h4 / cc-pvtz	orca	total energy ha	6.43×10^{-10}
RKS/pbe	c2h4 / def2-svp	orca	total energy ha	2.53×10^{-5}
RKS/pbe	c2h4 / def2-tzvp	orca	total energy ha	4.25×10^{-5}
RKS/pbe	c2h4 / cc-pvdz	orca	total energy ha	1.90×10^{-5}
RKS/pbe	c2h4 / cc-pvtz	orca	total energy ha	3.75×10^{-5}
RKS/pbe0	c2h4 / sto-3g	orca	total energy ha	4.07×10^{-5}
RKS/pbe0	acetic-acid / def2-svp	orca	total energy ha	4.88×10^{-5}
RKS/pbe0	c2h4 / def2-svp	orca	total energy ha	1.89×10^{-5}
RKS/pbe0	c2h4 / def2-tzvp	orca	total energy ha	3.35×10^{-5}
RKS/pbe0	acetic-acid / cc-pvdz	orca	total energy ha	4.80×10^{-5}
RKS/pbe0	c2h4 / cc-pvdz	orca	total energy ha	1.43×10^{-5}
RKS/pbe0	c2h4 / cc-pvtz	orca	total energy ha	2.90×10^{-5}
RKS/b3lyp	acetic-acid / sto-3g	orca	total energy ha	3.13×10^{-5}
RKS/b3lyp	c2h4 / sto-3g	orca	total energy ha	2.78×10^{-5}
RKS/b3lyp	acetic-acid / def2-svp	orca	total energy ha	1.13×10^{-5}
RKS/b3lyp	c2h4 / def2-svp	orca	total energy ha	9.62×10^{-6}
RKS/b3lyp	acetic-acid / def2-tzvp	orca	total energy ha	3.29×10^{-5}
RKS/b3lyp	c2h4 / def2-tzvp	orca	total energy ha	1.96×10^{-5}
RKS/b3lyp	acetic-acid / cc-pvdz	orca	total energy ha	1.01×10^{-5}
RKS/b3lyp	c2h4 / cc-pvdz	orca	total energy ha	4.83×10^{-6}
RKS/b3lyp	c2h4 / cc-pvtz	orca	total energy ha	1.70×10^{-5}
MP2	c2h4 / sto-3g	orca	total energy ha	1.04×10^{-8}

Table S21, continued.

Method	System / basis	Ref.	Quantity	$\lvert\Delta\rvert$
RKS/wb97x	acetic-acid / def2-svp	orca	total energy ha	2.76×10^{-5}
RKS/wb97x	acetic-acid / def2-tzvp	orca	total energy ha	4.61×10^{-5}
RKS/wb97x	acetic-acid / cc-pvdz	orca	total energy ha	1.62×10^{-5}
RKS/wb97x-v	acetic-acid / sto-3g	orca	total energy ha	1.33×10^{-5}
RKS/wb97m-v	acetic-acid / sto-3g	orca	total energy ha	1.29×10^{-5}
RKS/tpss	acetic-acid / sto-3g	orca	total energy ha	4.61×10^{-5}
RKS/tpss	acetic-acid / def2-svp	orca	total energy ha	1.92×10^{-5}
RKS/tpss	acetic-acid / def2-tzvp	orca	total energy ha	4.18×10^{-5}
RKS/tpss	acetic-acid / cc-pvdz	orca	total energy ha	1.60×10^{-5}
RHF	co2 / sto-3g	orca	total energy ha	1.32×10^{-9}
RHF	co2 / def2-svp	orca	total energy ha	1.77×10^{-9}
RHF	co2 / def2-tzvp	orca	total energy ha	1.85×10^{-9}
RHF	co2 / cc-pvdz	orca	total energy ha	1.27×10^{-9}
RHF	co2 / cc-pvtz	orca	total energy ha	1.24×10^{-9}
RHF	co2 / cc-pvqz	orca	total energy ha	1.32×10^{-9}
RKS/pbe	co2 / sto-3g	orca	total energy ha	3.23×10^{-5}
RKS/pbe	co2 / def2-svp	orca	total energy ha	2.62×10^{-5}
RKS/pbe	co2 / def2-tzvp	orca	total energy ha	3.32×10^{-5}
RKS/pbe	co2 / cc-pvdz	orca	total energy ha	2.83×10^{-5}
RKS/pbe	co2 / cc-pvtz	orca	total energy ha	4.32×10^{-5}
RKS/pbe0	co2 / sto-3g	orca	total energy ha	2.40×10^{-5}
RKS/pbe0	co2 / def2-svp	orca	total energy ha	1.88×10^{-5}
RKS/pbe0	co2 / def2-tzvp	orca	total energy ha	2.43×10^{-5}
RKS/pbe0	co2 / cc-pvdz	orca	total energy ha	2.03×10^{-5}
RKS/pbe0	co2 / cc-pvtz	orca	total energy ha	3.18×10^{-5}
RKS/pbe0	co2 / cc-pvqz	orca	total energy ha	2.40×10^{-5}
RKS/b3lyp	co2 / sto-3g	orca	total energy ha	4.11×10^{-6}
RKS/b3lyp	co2 / def2-svp	orca	total energy ha	8.19×10^{-6}
RKS/b3lyp	co2 / def2-tzvp	orca	total energy ha	2.39×10^{-6}
RKS/b3lyp	co2 / cc-pvdz	orca	total energy ha	5.96×10^{-6}
RKS/b3lyp	co2 / cc-pvtz	orca	total energy ha	8.13×10^{-6}
RKS/b3lyp	co2 / cc-pvqz	orca	total energy ha	2.78×10^{-6}
MP2	co2 / sto-3g	orca	total energy ha	1.30×10^{-7}
MP2	co2 / def2-svp	orca	total energy ha	3.85×10^{-7}
MP2	co2 / def2-tzvp	orca	total energy ha	8.68×10^{-8}
MP2	co2 / cc-pvdz	orca	total energy ha	1.75×10^{-7}
MP2	co2 / cc-pvtz	orca	total energy ha	2.83×10^{-9}
MP2	co2 / cc-pvqz	orca	total energy ha	6.88×10^{-9}
RHF	h2o2 / sto-3g	orca	total energy ha	2.55×10^{-9}
RHF	h2o2 / def2-svp	orca	total energy ha	1.15×10^{-9}
RHF	h2o2 / def2-tzvp	orca	total energy ha	6.68×10^{-10}
RHF	h2o2 / cc-pvdz	orca	total energy ha	1.04×10^{-9}
RHF	h2o2 / cc-pvtz	orca	total energy ha	7.42×10^{-10}
RHF	h2o2 / cc-pvqz	orca	total energy ha	1.82×10^{-10}
RKS/pbe	h2o2 / sto-3g	orca	total energy ha	3.06×10^{-5}
RKS/pbe	h2o2 / def2-svp	orca	total energy ha	2.94×10^{-5}
RKS/pbe	h2o2 / def2-tzvp	orca	total energy ha	3.25×10^{-5}
RKS/pbe	h2o2 / cc-pvdz	orca	total energy ha	2.52×10^{-5}
RKS/pbe	h2o2 / cc-pvtz	orca	total energy ha	3.27×10^{-5}
RKS/pbe	h2o2 / cc-pvqz	orca	total energy ha	3.28×10^{-5}
RKS/pbe0	h2o2 / sto-3g	orca	total energy ha	2.26×10^{-5}
RKS/pbe0	h2o2 / def2-svp	orca	total energy ha	2.17×10^{-5}
RKS/pbe0	h2o2 / def2-tzvp	orca	total energy ha	2.34×10^{-5}
RKS/pbe0	h2o2 / cc-pvdz	orca	total energy ha	1.86×10^{-5}
RKS/pbe0	h2o2 / cc-pvtz	orca	total energy ha	2.40×10^{-5}
RKS/pbe0	h2o2 / cc-pvqz	orca	total energy ha	2.37×10^{-5}
RKS/b3lyp	h2o2 / sto-3g	orca	total energy ha	6.13×10^{-6}
RKS/b3lyp	h2o2 / def2-svp	orca	total energy ha	4.03×10^{-7}

Table S21, continued.

Method	System / basis	Ref.	Quantity	$\lvert\Delta\rvert$
RKS/b3lyp	h2o2 / def2-tzvp	orca	total energy ha	3.23×10^{-6}
RKS/b3lyp	h2o2 / cc-pvdz	orca	total energy ha	3.62×10^{-6}
RKS/b3lyp	h2o2 / cc-pvtz	orca	total energy ha	2.86×10^{-6}
RKS/b3lyp	h2o2 / cc-pvqz	orca	total energy ha	3.81×10^{-6}
MP2	h2o2 / sto-3g	orca	total energy ha	3.58×10^{-8}
MP2	h2o2 / def2-svp	orca	total energy ha	3.12×10^{-8}
MP2	h2o2 / def2-tzvp	orca	total energy ha	9.68×10^{-8}
MP2	h2o2 / cc-pvdz	orca	total energy ha	1.91×10^{-8}
MP2	h2o2 / cc-pvtz	orca	total energy ha	2.91×10^{-8}
MP2	h2o2 / cc-pvqz	orca	total energy ha	3.29×10^{-8}
RHF	lih / sto-3g	orca	total energy ha	2.30×10^{-10}
RHF	lih / def2-svp	orca	total energy ha	1.40×10^{-11}
RHF	lih / def2-tzvp	orca	total energy ha	2.90×10^{-11}
RHF	lih / cc-pvdz	orca	total energy ha	5.10×10^{-11}
RHF	lih / cc-pvtz	orca	total energy ha	3.00×10^{-11}
RHF	lih / cc-pvqz	orca	total energy ha	3.90×10^{-11}
RKS/pbe	lih / sto-3g	orca	total energy ha	1.53×10^{-5}
RKS/pbe	lih / def2-svp	orca	total energy ha	2.77×10^{-5}
RKS/pbe	lih / def2-tzvp	orca	total energy ha	1.13×10^{-5}
RKS/pbe	lih / cc-pvtz	orca	total energy ha	8.66×10^{-6}
RKS/pbe	lih / cc-pvqz	orca	total energy ha	8.00×10^{-6}
RKS/pbe0	lih / sto-3g	orca	total energy ha	1.04×10^{-5}
RKS/pbe0	lih / def2-svp	orca	total energy ha	1.74×10^{-5}
RKS/pbe0	lih / def2-tzvp	orca	total energy ha	6.87×10^{-6}
RKS/pbe0	lih / cc-pvtz	orca	total energy ha	4.63×10^{-6}
RKS/pbe0	lih / cc-pvqz	orca	total energy ha	4.37×10^{-6}
RKS/b3lyp	lih / sto-3g	orca	total energy ha	7.32×10^{-6}
RKS/b3lyp	lih / def2-svp	orca	total energy ha	1.87×10^{-5}
RKS/b3lyp	lih / def2-tzvp	orca	total energy ha	2.79×10^{-6}
RKS/b3lyp	lih / cc-pvtz	orca	total energy ha	1.49×10^{-6}
RKS/b3lyp	lih / cc-pvqz	orca	total energy ha	1.04×10^{-7}
MP2	lih / def2-tzvp	orca	total energy ha	7.17×10^{-9}
MP2	lih / cc-pvdz	orca	total energy ha	5.21×10^{-5}
MP2	lih / cc-pvtz	orca	total energy ha	1.02×10^{-4}
MP2	lih / cc-pvqz	orca	total energy ha	3.57×10^{-5}
UHF	o2-triplet / sto-3g	orca	total energy ha	1.40×10^{-11}
UHF	o2-triplet / def2-svp	orca	total energy ha	1.39×10^{-9}
UHF	o2-triplet / def2-tzvp	orca	total energy ha	1.27×10^{-9}
UHF	o2-triplet / cc-pvdz	orca	total energy ha	1.20×10^{-9}
UHF	o2-triplet / cc-pvtz	orca	total energy ha	1.26×10^{-9}
UHF	o2-triplet / cc-pvqz	orca	total energy ha	1.25×10^{-9}
ROHF	o2-triplet / sto-3g	orca	total energy ha	1.90×10^{-11}
ROHF	o2-triplet / def2-svp	orca	total energy ha	1.54×10^{-9}
ROHF	o2-triplet / def2-tzvp	orca	total energy ha	1.44×10^{-9}
ROHF	o2-triplet / cc-pvdz	orca	total energy ha	1.25×10^{-9}
ROHF	o2-triplet / cc-pvtz	orca	total energy ha	1.34×10^{-9}
ROHF	o2-triplet / cc-pvqz	orca	total energy ha	1.23×10^{-9}
ROKS/pbe	o2-triplet / sto-3g	orca	total energy ha	2.52×10^{-5}
ROKS/pbe	o2-triplet / def2-svp	orca	total energy ha	1.29×10^{-4}
ROKS/pbe	o2-triplet / def2-tzvp	orca	total energy ha	8.25×10^{-5}
ROKS/pbe	o2-triplet / cc-pvdz	orca	total energy ha	1.08×10^{-4}
ROKS/pbe	o2-triplet / cc-pvtz	orca	total energy ha	7.23×10^{-5}
ROKS/pbe	o2-triplet / cc-pvqz	orca	total energy ha	7.73×10^{-5}
MP2	o2-triplet / def2-svp	orca	total energy ha	5.45×10^{-8}
MP2	o2-triplet / def2-tzvp	orca	total energy ha	6.20×10^{-8}
MP2	o2-triplet / cc-pvdz	orca	total energy ha	1.40×10^{-7}
MP2	o2-triplet / cc-pvtz	orca	total energy ha	3.28×10^{-8}
MP2	o2-triplet / cc-pvqz	orca	total energy ha	2.92×10^{-8}

Table S21, continued.

Method	System / basis	Ref.	Quantity	$\lvert\Delta\rvert$
RKS/pbe	cyclopropene / cc-pvtz	orca	total energy ha	4.90×10^{-5}
RKS/pbe0	cyclopropene / cc-pvtz	orca	total energy ha	4.12×10^{-5}
MP2	cyclopropene / sto-3g	orca	total energy ha	3.87×10^{-5}
MP2	cyclopropene / def2-svp	orca	total energy ha	4.42×10^{-8}
MP2	cyclopropene / def2-tzvp	orca	total energy ha	6.85×10^{-8}
MP2	cyclopropene / cc-pvdz	orca	total energy ha	4.84×10^{-8}
MP2	cyclopropene / cc-pvtz	orca	total energy ha	3.85×10^{-8}
RKS/r2scan	cyclopropene / def2-svp	orca	total energy ha	1.39×10^{-5}
RKS/r2scan	cyclopropene / def2-tzvp	orca	total energy ha	3.91×10^{-7}
RKS/r2scan	cyclopropene / cc-pvdz	orca	total energy ha	1.93×10^{-5}
RKS/r2scan	cyclopropene / cc-pvtz	orca	total energy ha	4.29×10^{-5}
RHF	s22-ammonia-dimer / sto-3g	orca	total energy ha	3.13×10^{-9}
RHF	s22-ammonia-dimer / def2-svp	orca	total energy ha	1.36×10^{-9}
RHF	s22-ammonia-dimer / def2-tzvp	orca	total energy ha	1.21×10^{-9}
RHF	s22-ammonia-dimer / cc-pvdz	orca	total energy ha	1.49×10^{-9}
RHF	s22-ammonia-dimer / cc-pvtz	orca	total energy ha	1.07×10^{-9}
RKS/pbe	s22-ammonia-dimer / sto-3g	orca	total energy ha	4.84×10^{-5}
RKS/pbe	s22-ammonia-dimer / def2-svp	orca	total energy ha	4.74×10^{-5}
RKS/pbe	s22-ammonia-dimer / def2-tzvp	orca	total energy ha	4.42×10^{-5}
RKS/pbe0	s22-ammonia-dimer / sto-3g	orca	total energy ha	3.81×10^{-5}
RKS/pbe0	s22-ammonia-dimer / def2-svp	orca	total energy ha	3.60×10^{-5}
RKS/pbe0	s22-ammonia-dimer / def2-tzvp	orca	total energy ha	3.45×10^{-5}
RKS/pbe0	s22-ammonia-dimer / cc-pvdz	orca	total energy ha	3.87×10^{-5}
RKS/b3lyp	s22-ammonia-dimer / sto-3g	orca	total energy ha	1.34×10^{-5}
RKS/b3lyp	s22-ammonia-dimer / def2-svp	orca	total energy ha	1.56×10^{-5}
RKS/b3lyp	s22-ammonia-dimer / def2-tzvp	orca	total energy ha	1.25×10^{-5}
RKS/b3lyp	s22-ammonia-dimer / cc-pvdz	orca	total energy ha	1.94×10^{-5}
UHF	fecl3 / sto-3g	orca	total energy ha	1.93×10^{-9}
UHF	fecl3 / def2-svp	orca	total energy ha	1.34×10^{-9}
MP2	fecl3 / sto-3g	orca	total energy ha	7.90×10^{-8}
MP2	fecl3 / def2-svp	orca	total energy ha	1.54×10^{-7}
RHF	s22-water-dimer / sto-3g	orca	total energy ha	5.29×10^{-10}
RHF	s22-water-dimer / def2-svp	orca	total energy ha	5.31×10^{-10}
RHF	s22-water-dimer / def2-tzvp	orca	total energy ha	9.22×10^{-10}
RHF	s22-water-dimer / cc-pvdz	orca	total energy ha	4.05×10^{-10}
RHF	s22-water-dimer / cc-pvtz	orca	total energy ha	1.07×10^{-9}
RKS/pbe	s22-water-dimer / sto-3g	orca	total energy ha	2.31×10^{-5}
RKS/pbe	s22-water-dimer / def2-svp	orca	total energy ha	2.50×10^{-5}
RKS/pbe	s22-water-dimer / def2-tzvp	orca	total energy ha	2.92×10^{-5}
RKS/pbe	s22-water-dimer / cc-pvdz	orca	total energy ha	2.49×10^{-5}
RKS/pbe	s22-water-dimer / cc-pvtz	orca	total energy ha	3.66×10^{-5}
RKS/pbe0	s22-water-dimer / sto-3g	orca	total energy ha	1.66×10^{-5}
RKS/pbe0	s22-water-dimer / def2-svp	orca	total energy ha	1.81×10^{-5}
RKS/pbe0	s22-water-dimer / def2-tzvp	orca	total energy ha	2.11×10^{-5}
RKS/pbe0	s22-water-dimer / cc-pvdz	orca	total energy ha	1.80×10^{-5}
RKS/pbe0	s22-water-dimer / cc-pvtz	orca	total energy ha	2.67×10^{-5}
RKS/b3lyp	s22-water-dimer / sto-3g	orca	total energy ha	3.12×10^{-6}
RKS/b3lyp	s22-water-dimer / def2-svp	orca	total energy ha	3.96×10^{-6}
RKS/b3lyp	s22-water-dimer / def2-tzvp	orca	total energy ha	2.19×10^{-7}
RKS/b3lyp	s22-water-dimer / cc-pvdz	orca	total energy ha	3.98×10^{-6}
RKS/b3lyp	s22-water-dimer / cc-pvtz	orca	total energy ha	5.60×10^{-6}
MP2	s22-water-dimer / sto-3g	orca	total energy ha	7.10×10^{-9}
RKS/pbe	nitromethane / cc-pvtz	orca	total energy ha	2.98×10^{-5}
RKS/pbe0	nitromethane / def2-tzvp	orca	total energy ha	4.15×10^{-5}
RKS/pbe0	nitromethane / cc-pvtz	orca	total energy ha	2.08×10^{-5}
RKS/b3lyp	nitromethane / def2-svp	orca	total energy ha	2.61×10^{-5}
RKS/b3lyp	nitromethane / def2-tzvp	orca	total energy ha	5.99×10^{-6}
RKS/b3lyp	nitromethane / cc-pvdz	orca	total energy ha	2.67×10^{-5}

Table S21, continued.

Method	System / basis	Ref.	Quantity	$\lvert\Delta\rvert$
RKS/b3lyp	nitromethane / cc-pvtz	orca	total energy ha	5.91×10^{-6}
MP2	nitromethane / sto-3g	orca	total energy ha	1.39×10^{-7}
MP2	nitromethane / def2-svp	orca	total energy ha	7.44×10^{-8}
MP2	nitromethane / def2-tzvp	orca	total energy ha	3.16×10^{-7}
MP2	nitromethane / cc-pvdz	orca	total energy ha	1.46×10^{-7}
MP2	nitromethane / cc-pvtz	orca	total energy ha	4.44×10^{-7}
RKS/wb97x	nitromethane / sto-3g	orca	total energy ha	3.09×10^{-6}
RKS/wb97x	nitromethane / def2-svp	orca	total energy ha	1.27×10^{-5}
RKS/wb97x	nitromethane / def2-tzvp	orca	total energy ha	2.94×10^{-6}
RKS/wb97x	nitromethane / cc-pvdz	orca	total energy ha	5.82×10^{-6}
RKS/wb97x	nitromethane / cc-pvtz	orca	total energy ha	5.44×10^{-7}
RKS/wb97x-v	nitromethane / def2-svp	orca	total energy ha	7.69×10^{-6}
RKS/wb97x-v	nitromethane / cc-pvtz	orca	total energy ha	1.88×10^{-5}
RKS/wb97m-v	nitromethane / def2-tzvp	orca	total energy ha	8.38×10^{-6}
RKS/tpss	nitromethane / def2-svp	orca	total energy ha	1.50×10^{-5}
RKS/tpss	nitromethane / def2-tzvp	orca	total energy ha	1.10×10^{-5}
RKS/tpss	nitromethane / cc-pvdz	orca	total energy ha	1.85×10^{-5}
RKS/tpss	nitromethane / cc-pvtz	orca	total energy ha	1.78×10^{-5}
RHF	tetrazine / def2-svp	orca	total energy ha	5.45×10^{-9}
RKS/pbe0	tetrazine / sto-3g	orca	total energy ha	4.01×10^{-5}
RKS/pbe0	tetrazine / def2-svp	orca	total energy ha	7.35×10^{-6}
RKS/pbe0	tetrazine / cc-pvdz	orca	total energy ha	6.44×10^{-6}
RKS/b3lyp	tetrazine / sto-3g	orca	total energy ha	6.02×10^{-6}
RKS/wb97x-v	tetrazine / sto-3g	orca	total energy ha	2.62×10^{-5}
RHF	urea / sto-3g	orca	total energy ha	1.11×10^{-10}
RHF	urea / def2-svp	orca	total energy ha	3.04×10^{-9}
RHF	urea / def2-tzvp	orca	total energy ha	2.24×10^{-9}
RHF	urea / cc-pvdz	orca	total energy ha	2.17×10^{-9}
RKS/pbe	urea / def2-tzvp	orca	total energy ha	3.72×10^{-5}
RKS/pbe0	urea / sto-3g	orca	total energy ha	3.97×10^{-5}
RKS/pbe0	urea / def2-tzvp	orca	total energy ha	2.82×10^{-5}
RKS/b3lyp	urea / sto-3g	orca	total energy ha	1.03×10^{-5}
RKS/b3lyp	urea / def2-svp	orca	total energy ha	2.99×10^{-5}
RKS/b3lyp	urea / cc-pvdz	orca	total energy ha	2.29×10^{-5}
RKS/wb97x	urea / sto-3g	orca	total energy ha	1.98×10^{-5}
RKS/wb97x	urea / def2-svp	orca	total energy ha	8.44×10^{-6}
RKS/wb97x	urea / def2-tzvp	orca	total energy ha	3.30×10^{-6}
RKS/wb97x	urea / cc-pvdz	orca	total energy ha	5.60×10^{-7}
RKS/wb97x-v	urea / sto-3g	orca	total energy ha	3.82×10^{-6}
RKS/wb97m-v	urea / sto-3g	orca	total energy ha	8.58×10^{-6}
RKS/tpss	urea / sto-3g	orca	total energy ha	4.16×10^{-6}
RKS/tpss	urea / def2-svp	orca	total energy ha	4.71×10^{-5}
RKS/tpss	urea / cc-pvdz	orca	total energy ha	4.08×10^{-5}
RHF	formaldehyde / def2-tzvp	orca	total energy ha	1.19×10^{-9}
RHF	formaldehyde / def2-tzvp	orca	total energy ha	1.47×10^{-8}
RHF	acetic-acid / def2-svp	orca	dielectric scaling ratio	n/a
RHF	acetic-acid / def2-svp	orca	dielectric scaling ratio	n/a
RHF	acetic-acid / def2-svp	orca	dielectric scaling ratio	n/a
RHF	acetic-acid / def2-svp	orca	dielectric scaling ratio	n/a
RHF	acetic-acid / def2-svp	orca	total energy ha	2.96×10^{-9}
RHF	acetic-acid / def2-svp	orca	dielectric interaction energy ha	8.07×10^{-4}
RHF	acetic-acid / def2-svp	orca	solvation shift ha	7.63×10^{-4}
RHF	acetic-acid / def2-svp	orca	dielectric scaling ratio	n/a
RHF	acetic-acid / def2-svp	orca	solvation shift ha	9.82×10^{-4}
RHF	acetic-acid / def2-svp	orca	dielectric scaling ratio	n/a
RHF	acetic-acid / def2-svp	orca	dielectric scaling ratio	n/a
RHF	acetic-acid / def2-svp	orca	dielectric scaling ratio	n/a

Table S21, continued.

Method	System / basis	Ref.	Quantity	$\lvert\Delta\rvert$
RHF	ch2o / def2-svp	orca	dielectric scaling ratio	n/a
RHF	ch2o / def2-svp	orca	dielectric scaling ratio	n/a
RHF	ch2o / def2-svp	orca	solvation shift ha	9.77×10^{-4}
RHF	ch2o / def2-svp	orca	dielectric scaling ratio	n/a
RHF	ch2o / def2-svp	orca	dielectric scaling ratio	n/a
RHF	ch2o / def2-svp	orca	total energy ha	9.35×10^{-10}
RHF	ch2o / def2-tzvp	orca	total energy ha	1.02×10^{-9}
RHF	ch2o / sto-3g	orca	total energy ha	6.99×10^{-12}
RHF	ch2o / def2-svp	orca	dielectric interaction energy ha	5.07×10^{-4}
RHF	ch2o / def2-svp	orca	solvation shift ha	4.61×10^{-4}
RHF	ch2o / def2-svp	orca	dielectric scaling ratio	n/a
RHF	ch2o / def2-tzvp	orca	dielectric interaction energy ha	5.29×10^{-4}
RHF	ch2o / def2-tzvp	orca	solvation shift ha	4.80×10^{-4}
RHF	ch2o / def2-tzvp	orca	dielectric scaling ratio	n/a
RHF	ch2o / sto-3g	orca	dielectric interaction energy ha	1.82×10^{-4}
RHF	ch2o / sto-3g	orca	solvation shift ha	1.73×10^{-4}
RHF	ch2o / sto-3g	orca	dielectric scaling ratio	n/a
RHF	ch2o / def2-svp	orca	dielectric interaction energy ha	6.76×10^{-4}
RHF	ch2o / def2-svp	orca	solvation shift ha	6.00×10^{-4}
RHF	ch2o / def2-svp	orca	dielectric scaling ratio	n/a
RHF	ch2o / def2-tzvp	orca	dielectric interaction energy ha	7.08×10^{-4}
RHF	ch2o / def2-tzvp	orca	solvation shift ha	6.24×10^{-4}
RHF	ch2o / def2-tzvp	orca	dielectric scaling ratio	n/a
RHF	ch2o / sto-3g	orca	dielectric interaction energy ha	2.37×10^{-4}
RHF	ch2o / sto-3g	orca	solvation shift ha	2.22×10^{-4}
RHF	ch2o / sto-3g	orca	dielectric scaling ratio	n/a
RHF	ch2o / def2-svp	orca	dielectric scaling ratio	n/a
RHF	ch2o / def2-svp	orca	dielectric scaling ratio	n/a
RHF	ch2o / sto-3g	orca	dielectric interaction energy ha	5.84×10^{-4}
RHF	ch2o / sto-3g	orca	solvation shift ha	5.04×10^{-4}
RHF	ch2o / sto-3g	orca	dielectric interaction energy ha	5.89×10^{-4}
RHF	ch2o / sto-3g	orca	solvation shift ha	5.08×10^{-4}
RHF	ethanol / def2-svp	orca	dielectric scaling ratio	n/a
RHF	ethanol / def2-svp	orca	dielectric scaling ratio	n/a
RHF	ethanol / def2-svp	orca	dielectric scaling ratio	n/a
RHF	ethanol / def2-svp	orca	dielectric scaling ratio	n/a
RHF	ethanol / def2-svp	orca	total energy ha	1.09×10^{-9}
RHF	ethanol / def2-svp	orca	dielectric interaction energy ha	6.49×10^{-4}
RHF	ethanol / def2-svp	orca	solvation shift ha	6.22×10^{-4}
RHF	ethanol / def2-svp	orca	dielectric scaling ratio	n/a
RHF	ethanol / def2-svp	orca	dielectric interaction energy ha	8.42×10^{-4}
RHF	ethanol / def2-svp	orca	solvation shift ha	7.97×10^{-4}
RHF	ethanol / def2-svp	orca	dielectric scaling ratio	n/a
RHF	ethanol / def2-svp	orca	dielectric scaling ratio	n/a
RHF	ethanol / def2-svp	orca	dielectric scaling ratio	n/a
RHF	h2o / def2-svp	orca	dielectric scaling ratio	n/a
RHF	h2o / def2-svp	orca	dielectric scaling ratio	n/a
RHF	h2o / def2-svp	orca	dielectric scaling ratio	n/a

Table S21, continued.

Method	System / basis	Ref.	Quantity	$\lvert\Delta\rvert$
RHF	h2o / def2-svp	orca	dielectric scaling ratio	n/a
RHF	h2o / def2-svp	orca	total energy ha	3.95×10^{-10}
RHF	h2o / def2-tzvp	orca	total energy ha	4.59×10^{-10}
RHF	h2o / sto-3g	orca	total energy ha	5.28×10^{-10}
RHF	h2o / def2-svp	orca	dielectric interaction energy ha	6.37×10^{-4}
RHF	h2o / def2-svp	orca	solvation shift ha	6.04×10^{-4}
RHF	h2o / def2-svp	orca	dielectric scaling ratio	n/a
RHF	h2o / def2-tzvp	orca	dielectric interaction energy ha	7.09×10^{-4}
RHF	h2o / def2-tzvp	orca	solvation shift ha	6.71×10^{-4}
RHF	h2o / def2-tzvp	orca	dielectric scaling ratio	n/a
RHF	h2o / sto-3g	orca	dielectric interaction energy ha	4.19×10^{-4}
RHF	h2o / sto-3g	orca	solvation shift ha	4.07×10^{-4}
RHF	h2o / sto-3g	orca	dielectric scaling ratio	n/a
RHF	h2o / def2-svp	orca	dielectric interaction energy ha	8.30×10^{-4}
RHF	h2o / def2-svp	orca	solvation shift ha	7.76×10^{-4}
RHF	h2o / def2-svp	orca	dielectric scaling ratio	n/a
RHF	h2o / def2-tzvp	orca	dielectric interaction energy ha	9.25×10^{-4}
RHF	h2o / def2-tzvp	orca	solvation shift ha	8.62×10^{-4}
RHF	h2o / def2-tzvp	orca	dielectric scaling ratio	n/a
RHF	h2o / sto-3g	orca	dielectric interaction energy ha	5.39×10^{-4}
RHF	h2o / sto-3g	orca	solvation shift ha	5.19×10^{-4}
RHF	h2o / sto-3g	orca	dielectric scaling ratio	n/a
RHF	h2o / def2-svp	orca	dielectric scaling ratio	n/a
RHF	h2o / def2-svp	orca	dielectric scaling ratio	n/a
RHF	nh3 / def2-svp	orca	dielectric scaling ratio	n/a
RHF	nh3 / def2-svp	orca	dielectric scaling ratio	n/a
RHF	nh3 / def2-svp	orca	dielectric scaling ratio	n/a
RHF	nh3 / def2-svp	orca	dielectric scaling ratio	n/a
RHF	nh3 / def2-svp	orca	total energy ha	3.71×10^{-10}
RHF	nh3 / def2-svp	orca	dielectric interaction energy ha	5.25×10^{-4}
RHF	nh3 / def2-svp	orca	solvation shift ha	4.99×10^{-4}
RHF	nh3 / def2-svp	orca	dielectric scaling ratio	n/a
RHF	nh3 / def2-svp	orca	dielectric interaction energy ha	6.84×10^{-4}
RHF	nh3 / def2-svp	orca	solvation shift ha	6.41×10^{-4}
RHF	nh3 / def2-svp	orca	dielectric scaling ratio	n/a
RHF	nh3 / def2-svp	orca	dielectric scaling ratio	n/a
RHF	nh3 / def2-svp	orca	dielectric scaling ratio	n/a
RKS/pbe	acetic-acid / sto-3g	orca	total energy ha	2.15×10^{-3}
RKS/pbe	acetic-acid / sto-3g	orca	total energy ha	8.15×10^{-5}
RKS/pbe	c2h4 / sto-3g	orca	total energy ha	9.12×10^{-4}
RKS/pbe	c2h4 / sto-3g	orca	total energy ha	5.41×10^{-5}
RKS/pbe	acetic-acid / def2-svp	orca	total energy ha	3.03×10^{-4}
RKS/pbe	acetic-acid / def2-svp	orca	total energy ha	6.64×10^{-5}
RKS/pbe	c2h4 / def2-svp	orca	total energy ha	1.27×10^{-4}
RKS/pbe	acetic-acid / def2-tzvp	orca	total energy ha	3.08×10^{-4}
RKS/pbe	acetic-acid / def2-tzvp	orca	total energy ha	9.02×10^{-5}
RKS/pbe	c2h4 / def2-tzvp	orca	total energy ha	1.28×10^{-4}
RKS/pbe	acetic-acid / cc-pvdz	orca	total energy ha	2.79×10^{-4}
RKS/pbe	acetic-acid / cc-pvdz	orca	total energy ha	6.46×10^{-5}
RKS/pbe	c2h4 / cc-pvdz	orca	total energy ha	1.09×10^{-4}

Table S21, continued.

Method	System / basis	Ref.	Quantity	$\lvert\Delta\rvert$
RKS/pbe	c2h4 / cc-pvtz	orca	total energy ha	1.51×10^{-4}
RKS/pbe0	acetic-acid / sto-3g	orca	total energy ha	2.15×10^{-3}
RKS/pbe0	acetic-acid / sto-3g	orca	total energy ha	6.15×10^{-5}
RKS/pbe0	c2h4 / sto-3g	orca	total energy ha	9.07×10^{-4}
RKS/pbe0	acetic-acid / def2-svp	orca	total energy ha	2.62×10^{-4}
RKS/pbe0	c2h4 / def2-svp	orca	total energy ha	1.25×10^{-4}
RKS/pbe0	acetic-acid / def2-tzvp	orca	total energy ha	3.02×10^{-4}
RKS/pbe0	acetic-acid / def2-tzvp	orca	total energy ha	6.77×10^{-5}
RKS/pbe0	c2h4 / def2-tzvp	orca	total energy ha	1.15×10^{-4}
RKS/pbe0	acetic-acid / cc-pvdz	orca	total energy ha	2.35×10^{-4}
RKS/pbe0	c2h4 / cc-pvdz	orca	total energy ha	1.06×10^{-4}
RKS/pbe0	acetic-acid / cc-pvtz	orca	total energy ha	3.42×10^{-4}
RKS/pbe0	acetic-acid / cc-pvtz	orca	total energy ha	7.60×10^{-5}
RKS/pbe0	c2h4 / cc-pvtz	orca	total energy ha	1.39×10^{-4}
RKS/b3lyp	acetic-acid / sto-3g	orca	total energy ha	2.12×10^{-3}
RKS/b3lyp	c2h4 / sto-3g	orca	total energy ha	8.95×10^{-4}
RKS/b3lyp	acetic-acid / def2-svp	orca	total energy ha	2.67×10^{-4}
RKS/b3lyp	c2h4 / def2-svp	orca	total energy ha	1.17×10^{-4}
RKS/b3lyp	acetic-acid / def2-tzvp	orca	total energy ha	2.76×10^{-4}
RKS/b3lyp	c2h4 / def2-tzvp	orca	total energy ha	1.22×10^{-4}
RKS/b3lyp	acetic-acid / cc-pvdz	orca	total energy ha	1.99×10^{-4}
RKS/b3lyp	c2h4 / cc-pvdz	orca	total energy ha	9.59×10^{-5}
RKS/b3lyp	c2h4 / cc-pvtz	orca	total energy ha	1.51×10^{-4}
RKS/wb97x	acetic-acid / sto-3g	orca	total energy ha	2.11×10^{-3}
RKS/wb97x	acetic-acid / def2-svp	orca	total energy ha	2.50×10^{-4}
RKS/wb97x	acetic-acid / def2-tzvp	orca	total energy ha	2.56×10^{-4}
RKS/wb97x	acetic-acid / cc-pvdz	orca	total energy ha	2.18×10^{-4}
RKS/wb97x	acetic-acid / cc-pvtz	orca	total energy ha	3.09×10^{-4}
RKS/wb97x	acetic-acid / cc-pvtz	orca	total energy ha	5.33×10^{-5}
RKS/wb97x-v	acetic-acid / sto-3g	orca	total energy ha	2.11×10^{-3}
RKS/wb97m-v	acetic-acid / sto-3g	orca	total energy ha	2.12×10^{-3}
RKS/r2scan	acetic-acid / sto-3g	orca	total energy ha	1.80×10^{-3}
RKS/r2scan	acetic-acid / sto-3g	orca	total energy ha	2.94×10^{-4}
RKS/r2scan	acetic-acid / def2-svp	orca	total energy ha	4.12×10^{-4}
RKS/r2scan	acetic-acid / def2-svp	orca	total energy ha	1.53×10^{-4}
RKS/r2scan	acetic-acid / def2-tzvp	orca	total energy ha	3.80×10^{-4}
RKS/r2scan	acetic-acid / def2-tzvp	orca	total energy ha	1.39×10^{-4}
RKS/r2scan	acetic-acid / cc-pvdz	orca	total energy ha	3.73×10^{-4}
RKS/r2scan	acetic-acid / cc-pvdz	orca	total energy ha	1.35×10^{-4}
RKS/tpss	acetic-acid / sto-3g	orca	total energy ha	2.11×10^{-3}
RKS/tpss	acetic-acid / def2-svp	orca	total energy ha	2.55×10^{-4}
RKS/tpss	acetic-acid / def2-tzvp	orca	total energy ha	2.54×10^{-4}
RKS/tpss	acetic-acid / cc-pvdz	orca	total energy ha	2.34×10^{-4}
RKS/pbe	co2 / sto-3g	orca	total energy ha	1.63×10^{-3}
RKS/pbe	co2 / def2-svp	orca	total energy ha	8.99×10^{-5}
RKS/pbe	co2 / def2-tzvp	orca	total energy ha	5.44×10^{-5}
RKS/pbe	co2 / cc-pvdz	orca	total energy ha	7.40×10^{-5}
RKS/pbe	co2 / cc-pvtz	orca	total energy ha	5.47×10^{-5}
RKS/pbe	co2 / cc-pvqz	orca	total energy ha	5.44×10^{-5}
RKS/pbe0	co2 / sto-3g	orca	total energy ha	1.62×10^{-3}
RKS/pbe0	co2 / def2-svp	orca	total energy ha	7.05×10^{-5}
RKS/pbe0	co2 / def2-tzvp	orca	total energy ha	5.13×10^{-5}
RKS/pbe0	co2 / cc-pvdz	orca	total energy ha	5.58×10^{-5}
RKS/pbe0	co2 / cc-pvtz	orca	total energy ha	6.50×10^{-5}
RKS/pbe0	co2 / cc-pvqz	orca	total energy ha	4.82×10^{-5}
RKS/b3lyp	co2 / sto-3g	orca	total energy ha	1.60×10^{-3}
RKS/b3lyp	co2 / def2-svp	orca	total energy ha	5.64×10^{-5}
RKS/b3lyp	co2 / def2-tzvp	orca	total energy ha	9.41×10^{-6}

Table S21, continued.

Method	System / basis	Ref.	Quantity	$\lvert\Delta\rvert$
RKS/b3lyp	co2 / cc-pvdz	orca	total energy ha	3.06×10^{-5}
RKS/b3lyp	co2 / cc-pvtz	orca	total energy ha	1.06×10^{-5}
RKS/b3lyp	co2 / cc-pvqz	orca	total energy ha	2.19×10^{-5}
RKS/pbe	h2o2 / sto-3g	orca	total energy ha	1.55×10^{-3}
RKS/pbe	h2o2 / def2-svp	orca	total energy ha	2.54×10^{-4}
RKS/pbe	h2o2 / def2-tzvp	orca	total energy ha	3.03×10^{-4}
RKS/pbe	h2o2 / cc-pvdz	orca	total energy ha	2.29×10^{-4}
RKS/pbe	h2o2 / cc-pvtz	orca	total energy ha	3.49×10^{-4}
RKS/pbe	h2o2 / cc-pvqz	orca	total energy ha	3.75×10^{-4}
RKS/pbe0	h2o2 / sto-3g	orca	total energy ha	1.54×10^{-3}
RKS/pbe0	h2o2 / def2-svp	orca	total energy ha	2.52×10^{-4}
RKS/pbe0	h2o2 / def2-tzvp	orca	total energy ha	3.12×10^{-4}
RKS/pbe0	h2o2 / cc-pvdz	orca	total energy ha	2.28×10^{-4}
RKS/pbe0	h2o2 / cc-pvtz	orca	total energy ha	3.45×10^{-4}
RKS/pbe0	h2o2 / cc-pvqz	orca	total energy ha	3.67×10^{-4}
RKS/b3lyp	h2o2 / sto-3g	orca	total energy ha	1.52×10^{-3}
RKS/b3lyp	h2o2 / def2-svp	orca	total energy ha	2.26×10^{-4}
RKS/b3lyp	h2o2 / def2-tzvp	orca	total energy ha	2.83×10^{-4}
RKS/b3lyp	h2o2 / cc-pvdz	orca	total energy ha	2.02×10^{-4}
RKS/b3lyp	h2o2 / cc-pvtz	orca	total energy ha	3.35×10^{-4}
RKS/b3lyp	h2o2 / cc-pvqz	orca	total energy ha	3.58×10^{-4}
RHF	lih / cc-pvdz	orca	total energy ha	1.14×10^{-4}
RHF	lih / cc-pvtz	orca	total energy ha	1.45×10^{-5}
RHF	lih / cc-pvqz	orca	total energy ha	1.54×10^{-7}
RKS/pbe	lih / sto-3g	orca	total energy ha	4.02×10^{-4}
RKS/pbe	lih / def2-svp	orca	total energy ha	7.75×10^{-6}
RKS/pbe	lih / def2-tzvp	orca	total energy ha	2.60×10^{-5}
RKS/pbe	lih / cc-pvdz	orca	total energy ha	1.05×10^{-4}
RKS/pbe	lih / cc-pvdz	orca	total energy ha	1.04×10^{-4}
RKS/pbe	lih / cc-pvtz	orca	total energy ha	1.71×10^{-5}
RKS/pbe	lih / cc-pvqz	orca	total energy ha	1.49×10^{-5}
RKS/pbe0	lih / sto-3g	orca	total energy ha	4.01×10^{-4}
RKS/pbe0	lih / def2-svp	orca	total energy ha	6.66×10^{-6}
RKS/pbe0	lih / def2-tzvp	orca	total energy ha	1.41×10^{-5}
RKS/pbe0	lih / cc-pvdz	orca	total energy ha	1.11×10^{-4}
RKS/pbe0	lih / cc-pvdz	orca	total energy ha	1.06×10^{-4}
RKS/pbe0	lih / cc-pvtz	orca	total energy ha	1.30×10^{-5}
RKS/pbe0	lih / cc-pvqz	orca	total energy ha	1.09×10^{-5}
RKS/b3lyp	lih / sto-3g	orca	total energy ha	3.97×10^{-4}
RKS/b3lyp	lih / def2-svp	orca	total energy ha	4.10×10^{-6}
RKS/b3lyp	lih / def2-tzvp	orca	total energy ha	1.88×10^{-5}
RKS/b3lyp	lih / cc-pvdz	orca	total energy ha	1.13×10^{-4}
RKS/b3lyp	lih / cc-pvdz	orca	total energy ha	1.03×10^{-4}
RKS/b3lyp	lih / cc-pvtz	orca	total energy ha	9.61×10^{-6}
RKS/b3lyp	lih / cc-pvqz	orca	total energy ha	8.48×10^{-6}
MP2	lih / sto-3g	orca	total energy ha	1.29×10^{-2}
MP2	lih / def2-svp	orca	total energy ha	2.21×10^{-2}
ROKS/pbe	o2-triplet / sto-3g	orca	total energy ha	1.27×10^{-3}
MP2	o2-triplet / sto-3g	orca	total energy ha	9.65×10^{-2}
RKS/pbe	cyclopropene / def2-svp	orca	total energy ha	2.04×10^{-4}
RKS/pbe	cyclopropene / def2-svp	orca	total energy ha	8.52×10^{-5}
RKS/pbe	cyclopropene / def2-tzvp	orca	total energy ha	2.35×10^{-4}
RKS/pbe	cyclopropene / def2-tzvp	orca	total energy ha	7.32×10^{-5}
RKS/pbe	cyclopropene / cc-pvdz	orca	total energy ha	2.19×10^{-4}
RKS/pbe	cyclopropene / cc-pvdz	orca	total energy ha	7.86×10^{-5}
RKS/pbe	cyclopropene / cc-pvtz	orca	total energy ha	2.42×10^{-4}
RKS/pbe0	cyclopropene / def2-svp	orca	total energy ha	2.02×10^{-4}
RKS/pbe0	cyclopropene / def2-svp	orca	total energy ha	6.83×10^{-5}

Table S21, continued.

Method	System / basis	Ref.	Quantity	$\lvert\Delta\rvert$
RKS/pbe0	cyclopropene / def2-tzvp	orca	total energy ha	2.12×10^{-4}
RKS/pbe0	cyclopropene / def2-tzvp	orca	total energy ha	5.93×10^{-5}
RKS/pbe0	cyclopropene / cc-pvdz	orca	total energy ha	2.19×10^{-4}
RKS/pbe0	cyclopropene / cc-pvdz	orca	total energy ha	6.33×10^{-5}
RKS/pbe0	cyclopropene / cc-pvtz	orca	total energy ha	2.32×10^{-4}
RKS/b3lyp	cyclopropene / def2-svp	orca	total energy ha	1.82×10^{-4}
RKS/b3lyp	cyclopropene / def2-svp	orca	total energy ha	8.53×10^{-5}
RKS/b3lyp	cyclopropene / def2-tzvp	orca	total energy ha	2.20×10^{-4}
RKS/b3lyp	cyclopropene / def2-tzvp	orca	total energy ha	9.19×10^{-5}
RKS/b3lyp	cyclopropene / cc-pvdz	orca	total energy ha	1.97×10^{-4}
RKS/b3lyp	cyclopropene / cc-pvdz	orca	total energy ha	7.96×10^{-5}
RKS/b3lyp	cyclopropene / cc-pvtz	orca	total energy ha	2.31×10^{-4}
RKS/b3lyp	cyclopropene / cc-pvtz	orca	total energy ha	6.09×10^{-5}
RKS/wb97x	cyclopropene / def2-svp	orca	total energy ha	1.58×10^{-4}
RKS/wb97x	cyclopropene / def2-svp	orca	total energy ha	1.32×10^{-4}
RKS/wb97x	cyclopropene / def2-tzvp	orca	total energy ha	1.80×10^{-4}
RKS/wb97x	cyclopropene / def2-tzvp	orca	total energy ha	9.90×10^{-5}
RKS/wb97x	cyclopropene / cc-pvdz	orca	total energy ha	1.62×10^{-4}
RKS/wb97x	cyclopropene / cc-pvdz	orca	total energy ha	1.39×10^{-4}
RKS/wb97x	cyclopropene / cc-pvtz	orca	total energy ha	1.95×10^{-4}
RKS/wb97x	cyclopropene / cc-pvtz	orca	total energy ha	9.55×10^{-5}
RKS/wb97x-v	cyclopropene / def2-tzvp	orca	total energy ha	1.88×10^{-4}
RKS/wb97x-v	cyclopropene / def2-tzvp	orca	total energy ha	8.46×10^{-5}
RKS/wb97m-v	cyclopropene / def2-tzvp	orca	total energy ha	2.12×10^{-4}
RKS/wb97m-v	cyclopropene / def2-tzvp	orca	total energy ha	6.33×10^{-5}
RKS/r2scan	cyclopropene / def2-svp	orca	total energy ha	3.14×10^{-4}
RKS/r2scan	cyclopropene / def2-tzvp	orca	total energy ha	3.03×10^{-4}
RKS/r2scan	cyclopropene / cc-pvdz	orca	total energy ha	3.37×10^{-4}
RKS/r2scan	cyclopropene / cc-pvtz	orca	total energy ha	3.44×10^{-4}
RKS/tpss	cyclopropene / def2-svp	orca	total energy ha	1.75×10^{-4}
RKS/tpss	cyclopropene / def2-svp	orca	total energy ha	1.16×10^{-4}
RKS/tpss	cyclopropene / def2-tzvp	orca	total energy ha	1.99×10^{-4}
RKS/tpss	cyclopropene / def2-tzvp	orca	total energy ha	1.04×10^{-4}
RKS/tpss	cyclopropene / cc-pvdz	orca	total energy ha	1.89×10^{-4}
RKS/tpss	cyclopropene / cc-pvdz	orca	total energy ha	1.10×10^{-4}
RKS/tpss	cyclopropene / cc-pvtz	orca	total energy ha	2.07×10^{-4}
RKS/tpss	cyclopropene / cc-pvtz	orca	total energy ha	8.66×10^{-5}
RKS/pbe	s22-ammonia-dimer / sto-3g	orca	total energy ha	1.20×10^{-3}
RKS/pbe	s22-ammonia-dimer / def2-svp	orca	total energy ha	2.97×10^{-4}
RKS/pbe	s22-ammonia-dimer / def2-tzvp	orca	total energy ha	2.47×10^{-4}
RKS/pbe	s22-ammonia-dimer / cc-pvdz	orca	total energy ha	2.32×10^{-4}
RKS/pbe	s22-ammonia-dimer / cc-pvdz	orca	total energy ha	5.11×10^{-5}
RKS/pbe0	s22-ammonia-dimer / sto-3g	orca	total energy ha	1.19×10^{-3}
RKS/pbe0	s22-ammonia-dimer / def2-svp	orca	total energy ha	2.92×10^{-4}
RKS/pbe0	s22-ammonia-dimer / def2-tzvp	orca	total energy ha	2.29×10^{-4}
RKS/pbe0	s22-ammonia-dimer / cc-pvdz	orca	total energy ha	2.27×10^{-4}
RKS/b3lyp	s22-ammonia-dimer / sto-3g	orca	total energy ha	1.17×10^{-3}
RKS/b3lyp	s22-ammonia-dimer / def2-svp	orca	total energy ha	2.79×10^{-4}
RKS/b3lyp	s22-ammonia-dimer / def2-tzvp	orca	total energy ha	2.35×10^{-4}
RKS/b3lyp	s22-ammonia-dimer / cc-pvdz	orca	total energy ha	2.14×10^{-4}
UHF	fecl3 / cc-pvdz	orca	total energy ha	1.06×10^{-1}
UKS/pbe	fecl3 / sto-3g	orca	total energy ha	2.15×10^{-2}
UKS/pbe	fecl3 / sto-3g	orca	total energy ha	2.69×10^{-4}
UKS/pbe	fecl3 / def2-svp	orca	total energy ha	4.25×10^{-4}
UKS/pbe	fecl3 / def2-svp	orca	total energy ha	1.40×10^{-4}
UKS/pbe	fecl3 / def2-tzvp	orca	total energy ha	2.19×10^{-4}
UKS/pbe	fecl3 / def2-tzvp	orca	total energy ha	2.36×10^{-4}
UKS/pbe	fecl3 / cc-pvtz	orca	total energy ha	2.26×10^{-4}

Table S21, continued.

Method	System / basis	Ref.	Quantity	$\lvert\Delta\rvert$
MP2	fecl3 / cc-pvdz	orca	total energy ha	6.85×10^{-2}
MP2	fecl3 / cc-pvtz	orca	total energy ha	6.71×10^{-2}
RKS/pbe	s22-water-dimer / sto-3g	orca	total energy ha	1.50×10^{-3}
RKS/pbe	s22-water-dimer / def2-svp	orca	total energy ha	2.05×10^{-4}
RKS/pbe	s22-water-dimer / def2-tzvp	orca	total energy ha	2.53×10^{-4}
RKS/pbe	s22-water-dimer / cc-pvdz	orca	total energy ha	1.77×10^{-4}
RKS/pbe	s22-water-dimer / cc-pvtz	orca	total energy ha	3.15×10^{-4}
RKS/pbe0	s22-water-dimer / sto-3g	orca	total energy ha	1.50×10^{-3}
RKS/pbe0	s22-water-dimer / def2-svp	orca	total energy ha	1.98×10^{-4}
RKS/pbe0	s22-water-dimer / def2-tzvp	orca	total energy ha	2.27×10^{-4}
RKS/pbe0	s22-water-dimer / cc-pvdz	orca	total energy ha	1.69×10^{-4}
RKS/pbe0	s22-water-dimer / cc-pvtz	orca	total energy ha	2.99×10^{-4}
RKS/b3lyp	s22-water-dimer / sto-3g	orca	total energy ha	1.48×10^{-3}
RKS/b3lyp	s22-water-dimer / def2-svp	orca	total energy ha	1.74×10^{-4}
RKS/b3lyp	s22-water-dimer / def2-tzvp	orca	total energy ha	2.32×10^{-4}
RKS/b3lyp	s22-water-dimer / cc-pvdz	orca	total energy ha	1.46×10^{-4}
RKS/b3lyp	s22-water-dimer / cc-pvtz	orca	total energy ha	2.90×10^{-4}
RKS/pbe	nitromethane / def2-svp	orca	total energy ha	2.85×10^{-4}
RKS/pbe	nitromethane / def2-svp	orca	total energy ha	7.85×10^{-5}
RKS/pbe	nitromethane / def2-tzvp	orca	total energy ha	2.28×10^{-4}
RKS/pbe	nitromethane / def2-tzvp	orca	total energy ha	5.67×10^{-5}
RKS/pbe	nitromethane / cc-pvdz	orca	total energy ha	2.60×10^{-4}
RKS/pbe	nitromethane / cc-pvdz	orca	total energy ha	8.10×10^{-5}
RKS/pbe	nitromethane / cc-pvtz	orca	total energy ha	2.39×10^{-4}
RKS/pbe0	nitromethane / def2-svp	orca	total energy ha	2.76×10^{-4}
RKS/pbe0	nitromethane / def2-svp	orca	total energy ha	5.76×10^{-5}
RKS/pbe0	nitromethane / def2-tzvp	orca	total energy ha	2.09×10^{-4}
RKS/pbe0	nitromethane / cc-pvtz	orca	total energy ha	2.13×10^{-4}
RKS/b3lyp	nitromethane / def2-svp	orca	total energy ha	2.43×10^{-4}
RKS/b3lyp	nitromethane / def2-tzvp	orca	total energy ha	1.88×10^{-4}
RKS/b3lyp	nitromethane / cc-pvdz	orca	total energy ha	2.19×10^{-4}
RKS/b3lyp	nitromethane / cc-pvtz	orca	total energy ha	2.06×10^{-4}
RKS/wb97x	nitromethane / sto-3g	orca	total energy ha	2.27×10^{-3}
RKS/wb97x	nitromethane / def2-svp	orca	total energy ha	2.28×10^{-4}
RKS/wb97x	nitromethane / def2-tzvp	orca	total energy ha	1.73×10^{-4}
RKS/wb97x	nitromethane / cc-pvdz	orca	total energy ha	1.96×10^{-4}
RKS/wb97x	nitromethane / cc-pvtz	orca	total energy ha	1.88×10^{-4}
RKS/wb97x-v	nitromethane / def2-svp	orca	total energy ha	2.24×10^{-4}
RKS/wb97x-v	nitromethane / cc-pvtz	orca	total energy ha	1.76×10^{-4}
RKS/wb97m-v	nitromethane / def2-tzvp	orca	total energy ha	1.87×10^{-4}
RKS/r2scan	nitromethane / def2-svp	orca	total energy ha	4.05×10^{-4}
RKS/r2scan	nitromethane / def2-svp	orca	total energy ha	1.99×10^{-4}
RKS/r2scan	nitromethane / def2-tzvp	orca	total energy ha	2.98×10^{-4}
RKS/r2scan	nitromethane / def2-tzvp	orca	total energy ha	1.08×10^{-4}
RKS/r2scan	nitromethane / cc-pvdz	orca	total energy ha	3.79×10^{-4}
RKS/r2scan	nitromethane / cc-pvdz	orca	total energy ha	1.96×10^{-4}
RKS/r2scan	nitromethane / cc-pvtz	orca	total energy ha	3.37×10^{-4}
RKS/r2scan	nitromethane / cc-pvtz	orca	total energy ha	1.29×10^{-4}
RKS/tpss	nitromethane / def2-svp	orca	total energy ha	2.37×10^{-4}
RKS/tpss	nitromethane / def2-tzvp	orca	total energy ha	1.71×10^{-4}
RKS/tpss	nitromethane / cc-pvdz	orca	total energy ha	2.13×10^{-4}
RKS/tpss	nitromethane / cc-pvtz	orca	total energy ha	1.79×10^{-4}
RHF	tetrazine / cc-pvdz	orca	total energy ha	4.92×10^{-2}
RHF	tetrazine / cc-pvtz	orca	total energy ha	5.05×10^{-2}
RKS/pbe0	tetrazine / sto-3g	orca	total energy ha	2.85×10^{-3}
RKS/pbe0	tetrazine / def2-svp	orca	total energy ha	4.52×10^{-4}
RKS/pbe0	tetrazine / cc-pvdz	orca	total energy ha	4.04×10^{-4}
RKS/b3lyp	tetrazine / sto-3g	orca	total energy ha	2.80×10^{-3}

Table S21, continued.

Method	System / basis	Ref.	Quantity	$\lvert\Delta\rvert$
RKS/wb97x	tetrazine / sto-3g	orca	total energy ha	2.82×10^{-3}
RKS/wb97x	tetrazine / sto-3g	orca	total energy ha	7.35×10^{-5}
RKS/wb97x	tetrazine / def2-svp	orca	total energy ha	4.20×10^{-4}
RKS/wb97x	tetrazine / def2-svp	orca	total energy ha	1.36×10^{-4}
RKS/wb97x	tetrazine / def2-tzvp	orca	total energy ha	2.96×10^{-4}
RKS/wb97x	tetrazine / def2-tzvp	orca	total energy ha	6.24×10^{-5}
RKS/wb97x	tetrazine / cc-pvdz	orca	total energy ha	3.80×10^{-4}
RKS/wb97x	tetrazine / cc-pvdz	orca	total energy ha	1.23×10^{-4}
RKS/wb97x-v	tetrazine / sto-3g	orca	total energy ha	2.80×10^{-3}
RKS/wb97m-v	tetrazine / sto-3g	orca	total energy ha	2.82×10^{-3}
RKS/wb97m-v	tetrazine / sto-3g	orca	total energy ha	5.46×10^{-5}
RKS/pbe	urea / sto-3g	orca	total energy ha	2.14×10^{-3}
RKS/pbe	urea / sto-3g	orca	total energy ha	5.26×10^{-5}
RKS/pbe	urea / def2-svp	orca	total energy ha	3.97×10^{-4}
RKS/pbe	urea / def2-svp	orca	total energy ha	9.71×10^{-5}
RKS/pbe	urea / def2-tzvp	orca	total energy ha	3.15×10^{-4}
RKS/pbe	urea / cc-pvdz	orca	total energy ha	3.47×10^{-4}
RKS/pbe	urea / cc-pvdz	orca	total energy ha	8.90×10^{-5}
RKS/pbe0	urea / sto-3g	orca	total energy ha	2.13×10^{-3}
RKS/pbe0	urea / def2-svp	orca	total energy ha	3.92×10^{-4}
RKS/pbe0	urea / def2-svp	orca	total energy ha	7.20×10^{-5}
RKS/pbe0	urea / def2-tzvp	orca	total energy ha	3.18×10^{-4}
RKS/pbe0	urea / cc-pvdz	orca	total energy ha	3.38×10^{-4}
RKS/pbe0	urea / cc-pvdz	orca	total energy ha	6.56×10^{-5}
RKS/b3lyp	urea / sto-3g	orca	total energy ha	2.11×10^{-3}
RKS/b3lyp	urea / def2-svp	orca	total energy ha	3.57×10^{-4}
RKS/b3lyp	urea / cc-pvdz	orca	total energy ha	3.10×10^{-4}
RKS/wb97x	urea / sto-3g	orca	total energy ha	2.10×10^{-3}
RKS/wb97x	urea / def2-svp	orca	total energy ha	3.46×10^{-4}
RKS/wb97x	urea / def2-tzvp	orca	total energy ha	2.63×10^{-4}
RKS/wb97x	urea / cc-pvdz	orca	total energy ha	2.92×10^{-4}
RKS/wb97x-v	urea / sto-3g	orca	total energy ha	2.10×10^{-3}
RKS/wb97m-v	urea / sto-3g	orca	total energy ha	2.11×10^{-3}
RKS/r2scan	urea / sto-3g	orca	total energy ha	1.93×10^{-3}
RKS/r2scan	urea / sto-3g	orca	total energy ha	1.44×10^{-4}
RKS/r2scan	urea / def2-svp	orca	total energy ha	5.20×10^{-4}
RKS/r2scan	urea / def2-svp	orca	total energy ha	1.92×10^{-4}
RKS/r2scan	urea / cc-pvdz	orca	total energy ha	4.78×10^{-4}
RKS/r2scan	urea / cc-pvdz	orca	total energy ha	1.88×10^{-4}
RKS/tpss	urea / sto-3g	orca	total energy ha	2.09×10^{-3}
RKS/tpss	urea / def2-svp	orca	total energy ha	3.44×10^{-4}
RKS/tpss	urea / cc-pvdz	orca	total energy ha	2.97×10^{-4}
RHF	acetic-acid / def2-svp	orca	dielectric interaction energy ha	2.59×10^{-3}
RHF	acetic-acid / def2-svp	orca	solvation shift ha	2.19×10^{-3}
RHF	acetic-acid / def2-svp	orca	dielectric interaction energy ha	2.64×10^{-3}
RHF	acetic-acid / def2-svp	orca	solvation shift ha	2.23×10^{-3}
RHF	acetic-acid / def2-svp	orca	dielectric interaction energy ha	1.75×10^{-3}
RHF	acetic-acid / def2-svp	orca	solvation shift ha	1.56×10^{-3}
RHF	acetic-acid / def2-svp	orca	dielectric interaction energy ha	1.99×10^{-3}
RHF	acetic-acid / def2-svp	orca	solvation shift ha	1.74×10^{-3}
RHF	acetic-acid / def2-svp	orca	dielectric interaction energy ha	1.06×10^{-3}
RHF	acetic-acid / def2-svp	orca	dielectric interaction energy ha	2.07×10^{-3}

Table S21, continued.

Method	System / basis	Ref.	Quantity	$\lvert\Delta\rvert$
RHF	acetic-acid / def2-svp	orca	solvation shift ha	1.80×10^{-3}
RHF	acetic-acid / def2-svp	orca	dielectric interaction energy ha	2.25×10^{-3}
RHF	acetic-acid / def2-svp	orca	solvation shift ha	1.94×10^{-3}
RHF	acetic-acid / def2-svp	orca	dielectric interaction energy ha	2.67×10^{-3}
RHF	acetic-acid / def2-svp	orca	solvation shift ha	2.25×10^{-3}
RHF	acetic-acid / def2-svp	orca	dielectric interaction energy ha	2.70×10^{-3}
RHF	acetic-acid / def2-svp	orca	solvation shift ha	2.27×10^{-3}
RHF	ch2o / def2-svp	orca	dielectric interaction energy ha	1.84×10^{-3}
RHF	ch2o / def2-svp	orca	solvation shift ha	1.42×10^{-3}
RHF	ch2o / def2-svp	orca	dielectric interaction energy ha	1.89×10^{-3}
RHF	ch2o / def2-svp	orca	solvation shift ha	1.44×10^{-3}
RHF	ch2o / def2-svp	orca	dielectric interaction energy ha	1.18×10^{-3}
RHF	ch2o / def2-svp	orca	dielectric interaction energy ha	1.37×10^{-3}
RHF	ch2o / def2-svp	orca	solvation shift ha	1.11×10^{-3}
RHF	ch2o / def2-svp	orca	dielectric interaction energy ha	1.43×10^{-3}
RHF	ch2o / def2-svp	orca	solvation shift ha	1.15×10^{-3}
RHF	ch2o / def2-svp	orca	dielectric interaction energy ha	1.57×10^{-3}
RHF	ch2o / def2-svp	orca	solvation shift ha	1.24×10^{-3}
RHF	ch2o / def2-svp	orca	dielectric interaction energy ha	1.91×10^{-3}
RHF	ch2o / def2-svp	orca	solvation shift ha	1.46×10^{-3}
RHF	ch2o / def2-tzvp	orca	dielectric interaction energy ha	2.05×10^{-3}
RHF	ch2o / def2-tzvp	orca	solvation shift ha	1.54×10^{-3}
RHF	ch2o / def2-svp	orca	dielectric interaction energy ha	1.93×10^{-3}
RHF	ch2o / def2-svp	orca	solvation shift ha	1.47×10^{-3}
RHF	ch2o / def2-tzvp	orca	dielectric interaction energy ha	2.07×10^{-3}
RHF	ch2o / def2-tzvp	orca	solvation shift ha	1.55×10^{-3}
RHF	ethanol / def2-svp	orca	dielectric interaction energy ha	1.97×10^{-3}
RHF	ethanol / def2-svp	orca	solvation shift ha	1.74×10^{-3}
RHF	ethanol / def2-svp	orca	dielectric interaction energy ha	2.01×10^{-3}
RHF	ethanol / def2-svp	orca	solvation shift ha	1.77×10^{-3}
RHF	ethanol / def2-svp	orca	dielectric interaction energy ha	1.36×10^{-3}
RHF	ethanol / def2-svp	orca	solvation shift ha	1.25×10^{-3}
RHF	ethanol / def2-svp	orca	dielectric interaction energy ha	1.54×10^{-3}
RHF	ethanol / def2-svp	orca	solvation shift ha	1.40×10^{-3}
RHF	ethanol / def2-svp	orca	dielectric interaction energy ha	1.60×10^{-3}
RHF	ethanol / def2-svp	orca	solvation shift ha	1.44×10^{-3}
RHF	ethanol / def2-svp	orca	dielectric interaction energy ha	1.73×10^{-3}
RHF	ethanol / def2-svp	orca	solvation shift ha	1.55×10^{-3}

Table S21, continued.

Method	System / basis	Ref.	Quantity	$\lvert\Delta\rvert$
RHF	ethanol / def2-svp	orca	dielectric interaction energy ha	2.03×10^{-3}
RHF	ethanol / def2-svp	orca	solvation shift ha	1.78×10^{-3}
RHF	ethanol / def2-svp	orca	dielectric interaction energy ha	2.05×10^{-3}
RHF	ethanol / def2-svp	orca	solvation shift ha	1.80×10^{-3}
RHF	h2o / def2-svp	orca	dielectric interaction energy ha	1.97×10^{-3}
RHF	h2o / def2-svp	orca	solvation shift ha	1.71×10^{-3}
RHF	h2o / def2-svp	orca	dielectric interaction energy ha	2.01×10^{-3}
RHF	h2o / def2-svp	orca	solvation shift ha	1.74×10^{-3}
RHF	h2o / def2-svp	orca	dielectric interaction energy ha	1.36×10^{-3}
RHF	h2o / def2-svp	orca	solvation shift ha	1.22×10^{-3}
RHF	h2o / def2-svp	orca	dielectric interaction energy ha	1.54×10^{-3}
RHF	h2o / def2-svp	orca	solvation shift ha	1.37×10^{-3}
RHF	h2o / def2-svp	orca	dielectric interaction energy ha	1.59×10^{-3}
RHF	h2o / def2-svp	orca	solvation shift ha	1.42×10^{-3}
RHF	h2o / def2-svp	orca	dielectric interaction energy ha	1.73×10^{-3}
RHF	h2o / def2-svp	orca	solvation shift ha	1.52×10^{-3}
RHF	h2o / def2-svp	orca	dielectric interaction energy ha	2.03×10^{-3}
RHF	h2o / def2-svp	orca	solvation shift ha	1.76×10^{-3}
RHF	h2o / def2-tzvp	orca	dielectric interaction energy ha	2.29×10^{-3}
RHF	h2o / def2-tzvp	orca	solvation shift ha	1.96×10^{-3}
RHF	h2o / sto-3g	orca	dielectric interaction energy ha	1.23×10^{-3}
RHF	h2o / sto-3g	orca	solvation shift ha	1.14×10^{-3}
RHF	h2o / def2-svp	orca	dielectric interaction energy ha	2.05×10^{-3}
RHF	h2o / def2-svp	orca	solvation shift ha	1.77×10^{-3}
RHF	h2o / def2-tzvp	orca	dielectric interaction energy ha	2.31×10^{-3}
RHF	h2o / def2-tzvp	orca	solvation shift ha	1.98×10^{-3}
RHF	h2o / sto-3g	orca	dielectric interaction energy ha	1.24×10^{-3}
RHF	h2o / sto-3g	orca	solvation shift ha	1.14×10^{-3}
RHF	nh3 / def2-svp	orca	dielectric interaction energy ha	1.63×10^{-3}
RHF	nh3 / def2-svp	orca	solvation shift ha	1.41×10^{-3}
RHF	nh3 / def2-svp	orca	dielectric interaction energy ha	1.66×10^{-3}
RHF	nh3 / def2-svp	orca	solvation shift ha	1.44×10^{-3}
RHF	nh3 / def2-svp	orca	dielectric interaction energy ha	1.12×10^{-3}
RHF	nh3 / def2-svp	orca	solvation shift ha	1.01×10^{-3}
RHF	nh3 / def2-svp	orca	dielectric interaction energy ha	1.27×10^{-3}
RHF	nh3 / def2-svp	orca	solvation shift ha	1.13×10^{-3}
RHF	nh3 / def2-svp	orca	dielectric interaction energy ha	1.31×10^{-3}
RHF	nh3 / def2-svp	orca	solvation shift ha	1.17×10^{-3}

Table S21, continued.

Method	System / basis	Ref.	Quantity	$\lvert\Delta\rvert$
RHF	nh3 / def2-svp	orca	dielectric interaction energy ha	1.43×10^{-3}
RHF	nh3 / def2-svp	orca	solvation shift ha	1.26×10^{-3}
RHF	nh3 / def2-svp	orca	dielectric interaction energy ha	1.68×10^{-3}
RHF	nh3 / def2-svp	orca	solvation shift ha	1.45×10^{-3}
RHF	nh3 / def2-svp	orca	dielectric interaction energy ha	1.69×10^{-3}
RHF	nh3 / def2-svp	orca	solvation shift ha	1.46×10^{-3}
RKS/wb97x	acetic-acid / sto-3g	orca	total energy ha	incomplete
RKS/pbe	co2 / cc-pvqz	orca	total energy ha	incomplete
RKS/pbe	h2o2 / sto-3g	orca	total energy ha	incomplete
UKS/pbe	fecl3 / cc-pvtz	orca	total energy ha	incomplete
RHF	h2 / sto-3g	orca	total energy ha	artifact-incomplete
RHF	h2 / def2-tzvp	orca	total energy ha	artifact-incomplete
RHF	h2o / sto-3g	orca	total energy ha	artifact-incomplete
RHF	h2o / def2-svp	orca	total energy ha	artifact-incomplete
RHF	ch4 / def2-svp	orca	total energy ha	artifact-incomplete
RHF	nh3 / def2-svp	orca	total energy ha	artifact-incomplete
RHF	co / def2-svp	orca	total energy ha	artifact-incomplete
RHF	n2 / def2-svp	orca	total energy ha	artifact-incomplete
UHF	oh-radical / sto-3g	orca	total energy ha	artifact-incomplete
UHF	o2-triplet / def2-svp	orca	total energy ha	artifact-incomplete
RHF	ammonia-water-dimer / sto-3g	orca	total energy ha	artifact-incomplete
RHF	ne2 / sto-3g	orca	total energy ha	artifact-incomplete
RHF	ar2 / sto-3g	orca	total energy ha	artifact-incomplete
RHF	h2o / def2-svp	orca	total energy ha	artifact-incomplete
UHF	oh-radical / def2-svp	orca	total energy ha	artifact-incomplete
ROHF	nh2-radical / def2-svp	orca	total energy ha	artifact-incomplete
RHF	h2o / sto-3g	orca	total energy ha	artifact-incomplete
RHF	h2o / sto-3g	orca	total energy ha	artifact-incomplete
UHF	oh-radical / sto-3g	orca	total energy ha	artifact-incomplete
UHF	oh-radical / sto-3g	orca	total energy ha	artifact-incomplete
ROHF	nh2-radical / sto-3g	orca	total energy ha	artifact-incomplete
ROHF	nh2-radical / sto-3g	orca	total energy ha	artifact-incomplete
RKS/b2plyp	acetic-acid / sto-3g	orca	total energy ha	blocked
RKS/b2plyp	acetic-acid / def2-svp	orca	total energy ha	blocked
RKS/b2plyp	acetic-acid / def2-tzvp	orca	total energy ha	blocked
RKS/b2plyp	acetic-acid / cc-pvdz	orca	total energy ha	blocked
RKS/dsd-pbep86	acetic-acid / sto-3g	orca	total energy ha	blocked
RKS/dsd-pbep86	acetic-acid / def2-svp	orca	total energy ha	blocked
RKS/dsd-pbep86	acetic-acid / def2-tzvp	orca	total energy ha	blocked
RKS/dsd-pbep86	acetic-acid / cc-pvdz	orca	total energy ha	blocked
RHF	lih / cc-pvdz	orca	total energy ha	blocked
UKS/pbe	o2-triplet / sto-3g	orca	total energy ha	blocked
UKS/pbe	o2-triplet / def2-svp	orca	total energy ha	blocked
UKS/pbe	o2-triplet / def2-tzvp	orca	total energy ha	blocked
UKS/pbe	o2-triplet / cc-pvdz	orca	total energy ha	blocked
UKS/pbe	o2-triplet / cc-pvtz	orca	total energy ha	blocked
UKS/pbe	o2-triplet / cc-pvqz	orca	total energy ha	blocked
RKS/b2plyp	cyclopropene / def2-svp	orca	total energy ha	blocked
RKS/b2plyp	cyclopropene / cc-pvdz	orca	total energy ha	blocked
RKS/b2plyp	cyclopropene / cc-pvtz	orca	total energy ha	blocked
RKS/dsd-pbep86	cyclopropene / def2-svp	orca	total energy ha	blocked
RKS/dsd-pbep86	cyclopropene / cc-pvdz	orca	total energy ha	blocked
RKS/dsd-pbep86	cyclopropene / cc-pvtz	orca	total energy ha	blocked
RKS/b2plyp	nitromethane / def2-svp	orca	total energy ha	blocked
RKS/b2plyp	nitromethane / cc-pvdz	orca	total energy ha	blocked

Table S21, continued.

Method	System / basis	Ref.	Quantity	$\lvert\Delta\rvert$
RKS/b2plyp	nitromethane / cc-pvtz	orca	total energy ha	blocked
RKS/dsd-pbep86	nitromethane / def2-svp	orca	total energy ha	blocked
RKS/dsd-pbep86	nitromethane / cc-pvdz	orca	total energy ha	blocked
RKS/dsd-pbep86	nitromethane / cc-pvtz	orca	total energy ha	blocked
RKS/b2plyp	tetrazine / sto-3g	orca	total energy ha	blocked
RKS/b2plyp	tetrazine / def2-svp	orca	total energy ha	blocked
RKS/b2plyp	tetrazine / cc-pvdz	orca	total energy ha	blocked
RKS/dsd-pbep86	tetrazine / sto-3g	orca	total energy ha	blocked
RKS/dsd-pbep86	tetrazine / def2-svp	orca	total energy ha	blocked
RKS/dsd-pbep86	tetrazine / cc-pvdz	orca	total energy ha	blocked
RKS/b2plyp	urea / sto-3g	orca	total energy ha	blocked
RKS/b2plyp	urea / def2-svp	orca	total energy ha	blocked
RKS/b2plyp	urea / def2-tzvp	orca	total energy ha	blocked
RKS/b2plyp	urea / cc-pvdz	orca	total energy ha	blocked
RKS/dsd-pbep86	urea / sto-3g	orca	total energy ha	blocked
RKS/dsd-pbep86	urea / def2-svp	orca	total energy ha	blocked
RKS/dsd-pbep86	urea / def2-tzvp	orca	total energy ha	blocked
RKS/dsd-pbep86	urea / cc-pvdz	orca	total energy ha	blocked
RHF	formaldehyde / def2-tzvp	orca	total energy ha	blocked
RHF	formaldehyde / def2-tzvp	orca	total energy ha	blocked

Kohn–Sham DFT

888 pass, 38 held, 166 fail, 1 incomplete, 35 artifact-incomplete, 182 blocked, 1 queued. Median $\lvert\Delta E\rvert$ 2.2×10^{-4}, max $3.5 \times 10^{-2}\ E_\mathrm{h}$.

RKS/b3lyp	glycine / def2-tzvp	orca	total energy ha	2.16×10^{-4}
RKS/pbe0	glycine / def2-tzvp	orca	total energy ha	2.56×10^{-4}
UKS/b3lyp	glycine / def2-tzvp	orca	total energy ha	2.16×10^{-4}
UKS/b3lyp	glycine / def2-tzvp	orca	total energy ha	2.16×10^{-4}
UKS/pbe0	glycine / def2-tzvp	orca	total energy ha	2.56×10^{-4}
UKS/pbe0	glycine / def2-tzvp	orca	total energy ha	2.56×10^{-4}
UKS/pbe	bh9-01-15p / def2-qzvpp	literature	total energy ha	0
UKS/pbe	bh9-01-15r / def2-qzvpp	literature	total energy ha	0
UKS/pbe	bh9-01-15ts / def2-qzvpp	literature	total energy ha	0
UKS/pbe	bh9-01-17p / def2-qzvpp	literature	total energy ha	0
UKS/pbe	bh9-01-17r / def2-qzvpp	literature	total energy ha	0
UKS/pbe	bh9-01-17ts / def2-qzvpp	literature	total energy ha	0
UKS/pbe	bh9-01-18p / def2-qzvpp	literature	total energy ha	1.00×10^{-10}
UKS/pbe	bh9-01-18r / def2-qzvpp	literature	total energy ha	0
UKS/pbe	bh9-01-18ts / def2-qzvpp	literature	total energy ha	0
UKS/pbe	bh9-01-19p / def2-qzvpp	literature	total energy ha	0
UKS/pbe	bh9-01-19r / def2-qzvpp	literature	total energy ha	0
UKS/pbe	bh9-01-19ts / def2-qzvpp	literature	total energy ha	1.00×10^{-10}
UKS/pbe	bh9-01-20p / def2-qzvpp	literature	total energy ha	0
UKS/pbe	bh9-01-20r / def2-qzvpp	literature	total energy ha	0
UKS/pbe	bh9-01-20ts / def2-qzvpp	literature	total energy ha	0
UKS/pbe	bh9-01-21p / def2-qzvpp	literature	total energy ha	0
UKS/pbe	bh9-01-21r / def2-qzvpp	literature	total energy ha	1.00×10^{-10}
UKS/pbe	bh9-01-21ts / def2-qzvpp	literature	total energy ha	0
UKS/pbe	bh9-01-22p / def2-qzvpp	literature	total energy ha	1.00×10^{-10}
UKS/pbe	bh9-01-22r / def2-qzvpp	literature	total energy ha	0
UKS/pbe	bh9-01-22ts / def2-qzvpp	literature	total energy ha	0
UKS/pbe	bh9-01-23p / def2-qzvpp	literature	total energy ha	0
UKS/pbe	bh9-01-23r / def2-qzvpp	literature	total energy ha	0
UKS/pbe	bh9-01-23ts / def2-qzvpp	literature	total energy ha	0
UKS/pbe	bh9-01-24p / def2-qzvpp	literature	total energy ha	0
UKS/pbe	bh9-01-24r / def2-qzvpp	literature	total energy ha	0
UKS/pbe	bh9-01-24ts / def2-qzvpp	literature	total energy ha	0
UKS/pbe	bh9-01-25p / def2-qzvpp	literature	total energy ha	1.00×10^{-10}

Table S21, continued.

Method	System / basis	Ref.	Quantity	$\lvert\Delta\rvert$
UKS/pbe	bh9-01-25r / def2-qzvpp	literature	total energy ha	0
UKS/pbe	bh9-01-25ts / def2-qzvpp	literature	total energy ha	0
UKS/pbe	bh9-01-26p / def2-qzvpp	literature	total energy ha	0
UKS/pbe	bh9-01-26r / def2-qzvpp	literature	total energy ha	0
UKS/pbe	bh9-01-26ts / def2-qzvpp	literature	total energy ha	0
UKS/pbe	bh9-01-27p / def2-qzvpp	literature	total energy ha	0
UKS/pbe	bh9-01-27r / def2-qzvpp	literature	total energy ha	0
UKS/pbe	bh9-01-27ts / def2-qzvpp	literature	total energy ha	0
UKS/pbe	bh9-01-28p / def2-qzvpp	literature	total energy ha	1.00×10^{-10}
UKS/pbe	bh9-01-28r / def2-qzvpp	literature	total energy ha	0
UKS/pbe	bh9-01-28ts / def2-qzvpp	literature	total energy ha	0
UKS/pbe	bh9-01-29p / def2-qzvpp	literature	total energy ha	0
UKS/pbe	bh9-01-29r / def2-qzvpp	literature	total energy ha	0
UKS/pbe	bh9-01-29ts / def2-qzvpp	literature	total energy ha	0
UKS/pbe	bh9-01-30p / def2-qzvpp	literature	total energy ha	0
UKS/pbe	bh9-01-30r / def2-qzvpp	literature	total energy ha	0
UKS/pbe	bh9-01-30ts / def2-qzvpp	literature	total energy ha	0
UKS/pbe	bh9-01-31p / def2-qzvpp	literature	total energy ha	0
UKS/pbe	bh9-01-31r / def2-qzvpp	literature	total energy ha	0
UKS/pbe	bh9-01-31ts / def2-qzvpp	literature	total energy ha	0
UKS/pbe	bh9-01-32p / def2-qzvpp	literature	total energy ha	0
UKS/pbe	bh9-01-32r / def2-qzvpp	literature	total energy ha	0
UKS/pbe	bh9-01-32ts / def2-qzvpp	literature	total energy ha	0
UKS/pbe	bh9-01-10 / def2-qzvpp	literature	barrier height forward kcal mol	9.50×10^{-3}
UKS/pbe	bh9-01-10 / def2-qzvpp	literature	barrier height reverse kcal mol	1.19×10^{-2}
UKS/pbe	bh9-01-10 / def2-qzvpp	literature	reaction energy kcal mol	2.44×10^{-3}
UKS/pbe	bh9-01-11 / def2-qzvpp	literature	barrier height forward kcal mol	7.76×10^{-3}
UKS/pbe	bh9-01-11 / def2-qzvpp	literature	barrier height reverse kcal mol	1.67×10^{-3}
UKS/pbe	bh9-01-11 / def2-qzvpp	literature	reaction energy kcal mol	6.08×10^{-3}
UKS/pbe	bh9-01-12 / def2-qzvpp	literature	barrier height forward kcal mol	4.12×10^{-3}
UKS/pbe	bh9-01-12 / def2-qzvpp	literature	barrier height reverse kcal mol	7.48×10^{-3}
UKS/pbe	bh9-01-12 / def2-qzvpp	literature	reaction energy kcal mol	3.36×10^{-3}
UKS/pbe	bh9-01-13 / def2-qzvpp	literature	barrier height forward kcal mol	6.00×10^{-3}
UKS/pbe	bh9-01-13 / def2-qzvpp	literature	barrier height reverse kcal mol	1.13×10^{-2}
UKS/pbe	bh9-01-13 / def2-qzvpp	literature	reaction energy kcal mol	5.32×10^{-3}
UKS/pbe	bh9-01-14 / def2-qzvpp	literature	barrier height forward kcal mol	3.77×10^{-3}
UKS/pbe	bh9-01-14 / def2-qzvpp	literature	barrier height reverse kcal mol	8.58×10^{-3}
UKS/pbe	bh9-01-14 / def2-qzvpp	literature	reaction energy kcal mol	4.81×10^{-3}
UKS/pbe	bh9-01-15 / def2-qzvpp	literature	barrier height forward kcal mol	9.44×10^{-3}
UKS/pbe	bh9-01-15 / def2-qzvpp	literature	barrier height reverse kcal mol	2.65×10^{-3}
UKS/pbe	bh9-01-15 / def2-qzvpp	literature	reaction energy kcal mol	6.79×10^{-3}
UKS/pbe	bh9-01-16 / def2-qzvpp	literature	barrier height forward kcal mol	7.09×10^{-3}
UKS/pbe	bh9-01-16 / def2-qzvpp	literature	barrier height reverse kcal mol	4.16×10^{-3}
UKS/pbe	bh9-01-16 / def2-qzvpp	literature	reaction energy kcal mol	2.95×10^{-3}

Table S21, continued.

Method	System / basis	Ref.	Quantity	$\lvert\Delta\rvert$
UKS/pbe	bh9-01-17 / def2-qzvpp	literature	barrier height forward kcal mol	7.66×10^{-3}
UKS/pbe	bh9-01-17 / def2-qzvpp	literature	barrier height reverse kcal mol	5.40×10^{-3}
UKS/pbe	bh9-01-17 / def2-qzvpp	literature	reaction energy kcal mol	2.26×10^{-3}
UKS/pbe	bh9-01-18 / def2-qzvpp	literature	barrier height forward kcal mol	4.62×10^{-3}
UKS/pbe	bh9-01-18 / def2-qzvpp	literature	barrier height reverse kcal mol	1.01×10^{-2}
UKS/pbe	bh9-01-18 / def2-qzvpp	literature	reaction energy kcal mol	5.48×10^{-3}
UKS/pbe	bh9-01-19 / def2-qzvpp	literature	barrier height forward kcal mol	5.56×10^{-3}
UKS/pbe	bh9-01-19 / def2-qzvpp	literature	barrier height reverse kcal mol	7.89×10^{-3}
UKS/pbe	bh9-01-19 / def2-qzvpp	literature	reaction energy kcal mol	2.35×10^{-3}
UKS/pbe	bh9-01-1 / def2-qzvpp	literature	barrier height forward kcal mol	7.79×10^{-3}
UKS/pbe	bh9-01-1 / def2-qzvpp	literature	barrier height reverse kcal mol	2.49×10^{-3}
UKS/pbe	bh9-01-1 / def2-qzvpp	literature	reaction energy kcal mol	5.31×10^{-3}
UKS/pbe	bh9-01-20 / def2-qzvpp	literature	barrier height forward kcal mol	5.08×10^{-3}
UKS/pbe	bh9-01-20 / def2-qzvpp	literature	barrier height reverse kcal mol	6.56×10^{-3}
UKS/pbe	bh9-01-20 / def2-qzvpp	literature	reaction energy kcal mol	1.49×10^{-3}
UKS/pbe	bh9-01-21 / def2-qzvpp	literature	barrier height forward kcal mol	5.86×10^{-3}
UKS/pbe	bh9-01-21 / def2-qzvpp	literature	barrier height reverse kcal mol	1.16×10^{-2}
UKS/pbe	bh9-01-21 / def2-qzvpp	literature	reaction energy kcal mol	5.79×10^{-3}
UKS/pbe	bh9-01-22 / def2-qzvpp	literature	barrier height forward kcal mol	4.60×10^{-3}
UKS/pbe	bh9-01-22 / def2-qzvpp	literature	barrier height reverse kcal mol	8.13×10^{-3}
UKS/pbe	bh9-01-22 / def2-qzvpp	literature	reaction energy kcal mol	3.51×10^{-3}
UKS/pbe	bh9-01-23 / def2-qzvpp	literature	barrier height forward kcal mol	6.67×10^{-3}
UKS/pbe	bh9-01-23 / def2-qzvpp	literature	barrier height reverse kcal mol	3.29×10^{-3}
UKS/pbe	bh9-01-23 / def2-qzvpp	literature	reaction energy kcal mol	3.38×10^{-3}
UKS/pbe	bh9-01-24 / def2-qzvpp	literature	barrier height forward kcal mol	5.65×10^{-3}
UKS/pbe	bh9-01-24 / def2-qzvpp	literature	barrier height reverse kcal mol	6.45×10^{-3}
UKS/pbe	bh9-01-24 / def2-qzvpp	literature	reaction energy kcal mol	7.81×10^{-4}
UKS/pbe	bh9-01-25 / def2-qzvpp	literature	barrier height forward kcal mol	1.82×10^{-3}
UKS/pbe	bh9-01-25 / def2-qzvpp	literature	barrier height reverse kcal mol	1.06×10^{-2}
UKS/pbe	bh9-01-25 / def2-qzvpp	literature	reaction energy kcal mol	8.83×10^{-3}
UKS/pbe	bh9-01-26 / def2-qzvpp	literature	barrier height forward kcal mol	9.48×10^{-3}
UKS/pbe	bh9-01-26 / def2-qzvpp	literature	barrier height reverse kcal mol	5.09×10^{-3}
UKS/pbe	bh9-01-26 / def2-qzvpp	literature	reaction energy kcal mol	4.38×10^{-3}
UKS/pbe	bh9-01-27 / def2-qzvpp	literature	barrier height forward kcal mol	2.78×10^{-3}

Table S21, continued.

Method	System / basis	Ref.	Quantity	$\lvert\Delta\rvert$
UKS/pbe	bh9-01-27 / def2-qzvpp	literature	barrier height reverse kcal mol	1.09×10^{-2}
UKS/pbe	bh9-01-27 / def2-qzvpp	literature	reaction energy kcal mol	8.16×10^{-3}
UKS/pbe	bh9-01-28 / def2-qzvpp	literature	barrier height forward kcal mol	6.77×10^{-3}
UKS/pbe	bh9-01-28 / def2-qzvpp	literature	barrier height reverse kcal mol	8.68×10^{-3}
UKS/pbe	bh9-01-28 / def2-qzvpp	literature	reaction energy kcal mol	1.91×10^{-3}
UKS/pbe	bh9-01-29 / def2-qzvpp	literature	barrier height forward kcal mol	4.19×10^{-3}
UKS/pbe	bh9-01-29 / def2-qzvpp	literature	barrier height reverse kcal mol	8.73×10^{-3}
UKS/pbe	bh9-01-29 / def2-qzvpp	literature	reaction energy kcal mol	4.54×10^{-3}
UKS/pbe	bh9-01-2 / def2-qzvpp	literature	barrier height forward kcal mol	6.54×10^{-3}
UKS/pbe	bh9-01-2 / def2-qzvpp	literature	barrier height reverse kcal mol	1.60×10^{-3}
UKS/pbe	bh9-01-2 / def2-qzvpp	literature	reaction energy kcal mol	4.93×10^{-3}
UKS/pbe	bh9-01-30 / def2-qzvpp	literature	barrier height forward kcal mol	6.34×10^{-3}
UKS/pbe	bh9-01-30 / def2-qzvpp	literature	barrier height reverse kcal mol	3.95×10^{-3}
UKS/pbe	bh9-01-30 / def2-qzvpp	literature	reaction energy kcal mol	2.39×10^{-3}
UKS/pbe	bh9-01-31 / def2-qzvpp	literature	barrier height forward kcal mol	4.74×10^{-3}
UKS/pbe	bh9-01-31 / def2-qzvpp	literature	barrier height reverse kcal mol	8.57×10^{-3}
UKS/pbe	bh9-01-31 / def2-qzvpp	literature	reaction energy kcal mol	3.83×10^{-3}
UKS/pbe	bh9-01-32 / def2-qzvpp	literature	barrier height forward kcal mol	7.57×10^{-3}
UKS/pbe	bh9-01-32 / def2-qzvpp	literature	barrier height reverse kcal mol	3.28×10^{-3}
UKS/pbe	bh9-01-32 / def2-qzvpp	literature	reaction energy kcal mol	4.29×10^{-3}
UKS/pbe	bh9-01-3 / def2-qzvpp	literature	barrier height forward kcal mol	6.89×10^{-3}
UKS/pbe	bh9-01-3 / def2-qzvpp	literature	barrier height reverse kcal mol	4.87×10^{-3}
UKS/pbe	bh9-01-3 / def2-qzvpp	literature	reaction energy kcal mol	2.03×10^{-3}
UKS/pbe	bh9-01-4 / def2-qzvpp	literature	barrier height forward kcal mol	8.22×10^{-3}
UKS/pbe	bh9-01-4 / def2-qzvpp	literature	barrier height reverse kcal mol	2.02×10^{-3}
UKS/pbe	bh9-01-4 / def2-qzvpp	literature	reaction energy kcal mol	6.20×10^{-3}
UKS/pbe	bh9-01-5 / def2-qzvpp	literature	barrier height forward kcal mol	7.78×10^{-3}
UKS/pbe	bh9-01-5 / def2-qzvpp	literature	barrier height reverse kcal mol	6.50×10^{-3}
UKS/pbe	bh9-01-5 / def2-qzvpp	literature	reaction energy kcal mol	1.28×10^{-3}
UKS/pbe	bh9-01-6 / def2-qzvpp	literature	barrier height forward kcal mol	6.39×10^{-3}
UKS/pbe	bh9-01-6 / def2-qzvpp	literature	barrier height reverse kcal mol	1.18×10^{-2}
UKS/pbe	bh9-01-6 / def2-qzvpp	literature	reaction energy kcal mol	5.41×10^{-3}
UKS/pbe	bh9-01-7 / def2-qzvpp	literature	barrier height forward kcal mol	5.91×10^{-3}
UKS/pbe	bh9-01-7 / def2-qzvpp	literature	barrier height reverse kcal mol	6.95×10^{-3}
UKS/pbe	bh9-01-7 / def2-qzvpp	literature	reaction energy kcal mol	1.04×10^{-3}

Table S21, continued.

Method	System / basis	Ref.	Quantity	$\lvert\Delta\rvert$
UKS/pbe	bh9-01-8 / def2-qzvpp	literature	barrier height forward kcal mol	8.87×10^{-3}
UKS/pbe	bh9-01-8 / def2-qzvpp	literature	barrier height reverse kcal mol	7.52×10^{-3}
UKS/pbe	bh9-01-8 / def2-qzvpp	literature	reaction energy kcal mol	1.37×10^{-3}
RKS/UKS/pbe	bh9-01-9 / def2-qzvpp	literature	barrier height forward kcal mol	8.29×10^{-3}
UKS/pbe	bh9-01-9 / def2-qzvpp	literature	barrier height reverse kcal mol	3.46×10^{-3}
RKS/UKS/pbe	bh9-01-9 / def2-qzvpp	literature	reaction energy kcal mol	4.83×10^{-3}
RKS/pbe	bh9-02-104p / def2-qzvpp	literature	total energy ha	1.00×10^{-10}
RKS/pbe	bh9-02-104r / def2-qzvpp	literature	total energy ha	1.00×10^{-10}
RKS/pbe	bh9-02-104ts / def2-qzvpp	literature	total energy ha	0
RKS/pbe	bh9-02-105p / def2-qzvpp	literature	total energy ha	1.00×10^{-10}
RKS/pbe	bh9-02-105r / def2-qzvpp	literature	total energy ha	0
RKS/pbe	bh9-02-105ts / def2-qzvpp	literature	total energy ha	0
RKS/pbe	bh9-02-109p / def2-qzvpp	literature	total energy ha	0
RKS/pbe	bh9-02-109r / def2-qzvpp	literature	total energy ha	0
RKS/pbe	bh9-02-109ts / def2-qzvpp	literature	total energy ha	0
RKS/pbe	bh9-02-110p / def2-qzvpp	literature	total energy ha	0
RKS/pbe	bh9-02-110ts / def2-qzvpp	literature	total energy ha	0
RKS/pbe	bh9-02-111p / def2-qzvpp	literature	total energy ha	0
RKS/pbe	bh9-02-111r / def2-qzvpp	literature	total energy ha	1.00×10^{-10}
RKS/pbe	bh9-02-111ts / def2-qzvpp	literature	total energy ha	0
RKS/pbe	bh9-02-128p / def2-qzvpp	literature	total energy ha	0
RKS/pbe	bh9-02-128r / def2-qzvpp	literature	total energy ha	0
RKS/pbe	bh9-02-128ts / def2-qzvpp	literature	total energy ha	0
RKS/pbe	bh9-02-135p / def2-qzvpp	literature	total energy ha	0
RKS/pbe	bh9-02-135r / def2-qzvpp	literature	total energy ha	0
RKS/pbe	bh9-02-135ts / def2-qzvpp	literature	total energy ha	0
RKS/pbe	bh9-02-140p / def2-qzvpp	literature	total energy ha	1.00×10^{-10}
RKS/pbe	bh9-02-140r / def2-qzvpp	literature	total energy ha	0
RKS/pbe	bh9-02-140ts / def2-qzvpp	literature	total energy ha	0
RKS/pbe	bh9-02-21p / def2-qzvpp	literature	total energy ha	0
RKS/pbe	bh9-02-21r / def2-qzvpp	literature	total energy ha	0
RKS/pbe	bh9-02-21ts / def2-qzvpp	literature	total energy ha	1.00×10^{-10}
RKS/pbe	bh9-02-24p / def2-qzvpp	literature	total energy ha	0
RKS/pbe	bh9-02-24r / def2-qzvpp	literature	total energy ha	0
RKS/pbe	bh9-02-24ts / def2-qzvpp	literature	total energy ha	0
RKS/pbe	bh9-02-25p / def2-qzvpp	literature	total energy ha	0
RKS/pbe	bh9-02-25r / def2-qzvpp	literature	total energy ha	0
RKS/pbe	bh9-02-25ts / def2-qzvpp	literature	total energy ha	0
RKS/pbe	bh9-02-32p / def2-qzvpp	literature	total energy ha	0
RKS/pbe	bh9-02-32ts / def2-qzvpp	literature	total energy ha	1.00×10^{-10}
RKS/pbe	bh9-02-42p / def2-qzvpp	literature	total energy ha	0
RKS/pbe	bh9-02-42ts / def2-qzvpp	literature	total energy ha	0
RKS/pbe	bh9-02-43p / def2-qzvpp	literature	total energy ha	0
RKS/pbe	bh9-02-43ts / def2-qzvpp	literature	total energy ha	0
RKS/pbe	bh9-02-44p / def2-qzvpp	literature	total energy ha	0
RKS/pbe	bh9-02-44ts / def2-qzvpp	literature	total energy ha	0
RKS/pbe	bh9-02-47p / def2-qzvpp	literature	total energy ha	0
RKS/pbe	bh9-02-47ts / def2-qzvpp	literature	total energy ha	0
RKS/pbe	bh9-02-56p / def2-qzvpp	literature	total energy ha	0
RKS/pbe	bh9-02-56ts / def2-qzvpp	literature	total energy ha	0
RKS/pbe	bh9-02-5p / def2-qzvpp	literature	total energy ha	0
RKS/pbe	bh9-02-5r / def2-qzvpp	literature	total energy ha	0
RKS/pbe	bh9-02-5ts / def2-qzvpp	literature	total energy ha	0
RKS/pbe	bh9-02-6p / def2-qzvpp	literature	total energy ha	0

Table S21, continued.

Method	System / basis	Ref.	Quantity	$\lvert\Delta\rvert$
RKS/pbe	bh9-02-6r / def2-qzvpp	literature	total energy ha	0
RKS/pbe	bh9-02-6ts / def2-qzvpp	literature	total energy ha	0
RKS/pbe	bh9-02-96p / def2-qzvpp	literature	total energy ha	0
RKS/pbe	bh9-02-96r / def2-qzvpp	literature	total energy ha	0
RKS/pbe	bh9-02-96ts / def2-qzvpp	literature	total energy ha	1.00×10^{-10}
RKS/pbe	bh9-02-104 / def2-qzvpp	literature	barrier height forward kcal mol	5.15×10^{-3}
RKS/pbe	bh9-02-104 / def2-qzvpp	literature	barrier height reverse kcal mol	8.63×10^{-3}
RKS/pbe	bh9-02-104 / def2-qzvpp	literature	reaction energy kcal mol	3.48×10^{-3}
RKS/pbe	bh9-02-105 / def2-qzvpp	literature	barrier height forward kcal mol	5.10×10^{-3}
RKS/pbe	bh9-02-105 / def2-qzvpp	literature	barrier height reverse kcal mol	6.29×10^{-3}
RKS/pbe	bh9-02-105 / def2-qzvpp	literature	reaction energy kcal mol	1.19×10^{-3}
RKS/pbe	bh9-02-109 / def2-qzvpp	literature	barrier height forward kcal mol	9.38×10^{-3}
RKS/pbe	bh9-02-109 / def2-qzvpp	literature	barrier height reverse kcal mol	2.56×10^{-3}
RKS/pbe	bh9-02-109 / def2-qzvpp	literature	reaction energy kcal mol	6.82×10^{-3}
RKS/pbe	bh9-02-110 / def2-qzvpp	literature	barrier height forward kcal mol	9.38×10^{-3}
RKS/pbe	bh9-02-110 / def2-qzvpp	literature	barrier height reverse kcal mol	1.48×10^{-2}
RKS/pbe	bh9-02-110 / def2-qzvpp	literature	reaction energy kcal mol	5.44×10^{-3}
RKS/pbe	bh9-02-111 / def2-qzvpp	literature	barrier height forward kcal mol	6.79×10^{-3}
RKS/pbe	bh9-02-111 / def2-qzvpp	literature	barrier height reverse kcal mol	1.16×10^{-2}
RKS/pbe	bh9-02-111 / def2-qzvpp	literature	reaction energy kcal mol	4.87×10^{-3}
RKS/pbe	bh9-02-128 / def2-qzvpp	literature	barrier height forward kcal mol	1.91×10^{-2}
RKS/pbe	bh9-02-128 / def2-qzvpp	literature	barrier height reverse kcal mol	4.60×10^{-3}
RKS/pbe	bh9-02-128 / def2-qzvpp	literature	reaction energy kcal mol	1.45×10^{-2}
RKS/pbe	bh9-02-134 / def2-qzvpp	literature	barrier height forward kcal mol	1.30×10^{-2}
RKS/pbe	bh9-02-134 / def2-qzvpp	literature	barrier height reverse kcal mol	1.38×10^{-2}
RKS/pbe	bh9-02-134 / def2-qzvpp	literature	reaction energy kcal mol	8.15×10^{-4}
RKS/pbe	bh9-02-135 / def2-qzvpp	literature	barrier height forward kcal mol	1.21×10^{-2}
RKS/pbe	bh9-02-135 / def2-qzvpp	literature	barrier height reverse kcal mol	1.71×10^{-2}
RKS/pbe	bh9-02-135 / def2-qzvpp	literature	reaction energy kcal mol	5.01×10^{-3}
RKS/pbe	bh9-02-136 / def2-qzvpp	literature	barrier height forward kcal mol	1.50×10^{-2}
RKS/pbe	bh9-02-136 / def2-qzvpp	literature	barrier height reverse kcal mol	1.67×10^{-2}
RKS/pbe	bh9-02-136 / def2-qzvpp	literature	reaction energy kcal mol	1.78×10^{-3}
RKS/pbe	bh9-02-139 / def2-qzvpp	literature	barrier height forward kcal mol	1.09×10^{-2}
RKS/pbe	bh9-02-139 / def2-qzvpp	literature	barrier height reverse kcal mol	1.21×10^{-2}
RKS/pbe	bh9-02-139 / def2-qzvpp	literature	reaction energy kcal mol	1.18×10^{-3}
RKS/pbe	bh9-02-140 / def2-qzvpp	literature	barrier height forward kcal mol	2.29×10^{-2}

Table S21, continued.

Method	System / basis	Ref.	Quantity	$\lvert\Delta\rvert$
RKS/pbe	bh9-02-140 / def2-qzvpp	literature	barrier height reverse kcal mol	5.89×10^{-3}
RKS/pbe	bh9-02-140 / def2-qzvpp	literature	reaction energy kcal mol	1.70×10^{-2}
RKS/pbe	bh9-02-21 / def2-qzvpp	literature	barrier height forward kcal mol	9.98×10^{-3}
RKS/pbe	bh9-02-21 / def2-qzvpp	literature	barrier height reverse kcal mol	1.94×10^{-2}
RKS/pbe	bh9-02-21 / def2-qzvpp	literature	reaction energy kcal mol	9.40×10^{-3}
RKS/pbe	bh9-02-24 / def2-qzvpp	literature	barrier height forward kcal mol	8.78×10^{-3}
RKS/pbe	bh9-02-24 / def2-qzvpp	literature	barrier height reverse kcal mol	1.69×10^{-2}
RKS/pbe	bh9-02-24 / def2-qzvpp	literature	reaction energy kcal mol	8.08×10^{-3}
RKS/pbe	bh9-02-25 / def2-qzvpp	literature	barrier height forward kcal mol	7.56×10^{-3}
RKS/pbe	bh9-02-25 / def2-qzvpp	literature	barrier height reverse kcal mol	1.79×10^{-2}
RKS/pbe	bh9-02-25 / def2-qzvpp	literature	reaction energy kcal mol	1.04×10^{-2}
RKS/pbe	bh9-02-32 / def2-qzvpp	literature	barrier height forward kcal mol	1.02×10^{-3}
RKS/pbe	bh9-02-32 / def2-qzvpp	literature	barrier height reverse kcal mol	1.59×10^{-2}
RKS/pbe	bh9-02-32 / def2-qzvpp	literature	reaction energy kcal mol	1.69×10^{-2}
RKS/pbe	bh9-02-42 / def2-qzvpp	literature	barrier height forward kcal mol	1.03×10^{-3}
RKS/pbe	bh9-02-42 / def2-qzvpp	literature	barrier height reverse kcal mol	1.37×10^{-2}
RKS/pbe	bh9-02-42 / def2-qzvpp	literature	reaction energy kcal mol	1.47×10^{-2}
RKS/pbe	bh9-02-43 / def2-qzvpp	literature	barrier height forward kcal mol	4.57×10^{-4}
RKS/pbe	bh9-02-43 / def2-qzvpp	literature	barrier height reverse kcal mol	1.55×10^{-2}
RKS/pbe	bh9-02-43 / def2-qzvpp	literature	reaction energy kcal mol	1.51×10^{-2}
RKS/pbe	bh9-02-44 / def2-qzvpp	literature	barrier height forward kcal mol	3.97×10^{-3}
RKS/pbe	bh9-02-44 / def2-qzvpp	literature	barrier height reverse kcal mol	1.92×10^{-2}
RKS/pbe	bh9-02-44 / def2-qzvpp	literature	reaction energy kcal mol	1.52×10^{-2}
RKS/pbe	bh9-02-45 / def2-qzvpp	literature	barrier height forward kcal mol	5.90×10^{-3}
RKS/pbe	bh9-02-45 / def2-qzvpp	literature	barrier height reverse kcal mol	1.18×10^{-2}
RKS/pbe	bh9-02-45 / def2-qzvpp	literature	reaction energy kcal mol	5.89×10^{-3}
RKS/pbe	bh9-02-47 / def2-qzvpp	literature	barrier height forward kcal mol	2.22×10^{-4}
RKS/pbe	bh9-02-47 / def2-qzvpp	literature	barrier height reverse kcal mol	7.30×10^{-3}
RKS/pbe	bh9-02-47 / def2-qzvpp	literature	reaction energy kcal mol	7.52×10^{-3}
RKS/pbe	bh9-02-56 / def2-qzvpp	literature	barrier height forward kcal mol	4.83×10^{-3}
RKS/pbe	bh9-02-56 / def2-qzvpp	literature	barrier height reverse kcal mol	1.42×10^{-2}
RKS/pbe	bh9-02-56 / def2-qzvpp	literature	reaction energy kcal mol	9.38×10^{-3}
RKS/pbe	bh9-02-58 / def2-qzvpp	literature	barrier height forward kcal mol	4.50×10^{-3}
RKS/pbe	bh9-02-58 / def2-qzvpp	literature	barrier height reverse kcal mol	1.78×10^{-2}
RKS/pbe	bh9-02-58 / def2-qzvpp	literature	reaction energy kcal mol	1.33×10^{-2}

Table S21, continued.

Method	System / basis	Ref.	Quantity	$\lvert\Delta\rvert$
RKS/pbe	bh9-02-59 / def2-qzvpp	literature	barrier height forward kcal mol	4.38×10^{-3}
RKS/pbe	bh9-02-59 / def2-qzvpp	literature	barrier height reverse kcal mol	1.84×10^{-2}
RKS/pbe	bh9-02-59 / def2-qzvpp	literature	reaction energy kcal mol	1.40×10^{-2}
RKS/pbe	bh9-02-5 / def2-qzvpp	literature	barrier height forward kcal mol	1.58×10^{-2}
RKS/pbe	bh9-02-5 / def2-qzvpp	literature	barrier height reverse kcal mol	7.61×10^{-3}
RKS/pbe	bh9-02-5 / def2-qzvpp	literature	reaction energy kcal mol	8.22×10^{-3}
RKS/pbe	bh9-02-6 / def2-qzvpp	literature	barrier height forward kcal mol	1.56×10^{-2}
RKS/pbe	bh9-02-6 / def2-qzvpp	literature	barrier height reverse kcal mol	8.84×10^{-3}
RKS/pbe	bh9-02-6 / def2-qzvpp	literature	reaction energy kcal mol	6.76×10^{-3}
RKS/pbe	bh9-02-96 / def2-qzvpp	literature	barrier height forward kcal mol	7.74×10^{-3}
RKS/pbe	bh9-02-96 / def2-qzvpp	literature	barrier height reverse kcal mol	1.19×10^{-3}
RKS/pbe	bh9-02-96 / def2-qzvpp	literature	reaction energy kcal mol	6.55×10^{-3}
RKS/pbe	bh9-02-98 / def2-qzvpp	literature	barrier height forward kcal mol	9.37×10^{-3}
RKS/pbe	bh9-02-98 / def2-qzvpp	literature	barrier height reverse kcal mol	5.24×10^{-3}
RKS/pbe	bh9-02-98 / def2-qzvpp	literature	reaction energy kcal mol	4.13×10^{-3}
RKS/pbe	bh9-02-99 / def2-qzvpp	literature	barrier height forward kcal mol	7.04×10^{-3}
RKS/pbe	bh9-02-99 / def2-qzvpp	literature	barrier height reverse kcal mol	3.33×10^{-3}
RKS/pbe	bh9-02-99 / def2-qzvpp	literature	reaction energy kcal mol	3.71×10^{-3}
UKS/pbe	bh9-03-10ts / def2-qzvpp	literature	total energy ha	9.98×10^{-11}
UKS/pbe	bh9-03-11ts / def2-qzvpp	literature	total energy ha	0
UKS/pbe	bh9-03-12p1 / def2-qzvpp	literature	total energy ha	0
RKS/pbe	bh9-03-12r1 / def2-qzvpp	literature	total energy ha	0
UKS/pbe	bh9-03-12ts / def2-qzvpp	literature	total energy ha	0
UKS/pbe	bh9-03-13ts / def2-qzvpp	literature	total energy ha	1.00×10^{-10}
UKS/pbe	bh9-03-15p1 / def2-qzvpp	literature	total energy ha	0
RKS/pbe	bh9-03-15r1 / def2-qzvpp	literature	total energy ha	0
UKS/pbe	bh9-03-15ts / def2-qzvpp	literature	total energy ha	1.00×10^{-10}
UKS/pbe	bh9-03-3ts / def2-qzvpp	literature	total energy ha	0
UKS/pbe	bh9-03-4ts / def2-qzvpp	literature	total energy ha	1.00×10^{-10}
UKS/pbe	bh9-03-5ts / def2-qzvpp	literature	total energy ha	0
UKS/pbe	bh9-03-6ts / def2-qzvpp	literature	total energy ha	0
UKS/pbe	bh9-03-7p1 / def2-qzvpp	literature	total energy ha	0
RKS/pbe	bh9-03-7r1 / def2-qzvpp	literature	total energy ha	0
UKS/pbe	bh9-03-7ts / def2-qzvpp	literature	total energy ha	0
UKS/pbe	bh9-03-8p1 / def2-qzvpp	literature	total energy ha	0
RKS/pbe	bh9-03-8r1 / def2-qzvpp	literature	total energy ha	0
UKS/pbe	bh9-03-8ts / def2-qzvpp	literature	total energy ha	1.00×10^{-10}
UKS/pbe	bh9-03-9ts / def2-qzvpp	literature	total energy ha	0
RKS/UKS/pbe	bh9-03-10 / def2-qzvpp	literature	barrier height forward kcal mol	2.87×10^{-2}
RKS/UKS/pbe	bh9-03-10 / def2-qzvpp	literature	barrier height reverse kcal mol	1.62×10^{-2}
RKS/UKS/pbe	bh9-03-10 / def2-qzvpp	literature	reaction energy kcal mol	1.26×10^{-2}
RKS/UKS/pbe	bh9-03-11 / def2-qzvpp	literature	barrier height forward kcal mol	8.99×10^{-3}

Table S21, continued.

Method	System / basis	Ref.	Quantity	$\lvert\Delta\rvert$
RKS/UKS/pbe	bh9-03-11 / def2-qzvpp	literature	barrier height reverse kcal mol	4.25×10^{-4}
RKS/UKS/pbe	bh9-03-11 / def2-qzvpp	literature	reaction energy kcal mol	9.44×10^{-3}
RKS/UKS/pbe	bh9-03-12 / def2-qzvpp	literature	barrier height forward kcal mol	3.50×10^{-2}
RKS/UKS/pbe	bh9-03-12 / def2-qzvpp	literature	barrier height reverse kcal mol	1.57×10^{-2}
RKS/UKS/pbe	bh9-03-12 / def2-qzvpp	literature	reaction energy kcal mol	1.93×10^{-2}
RKS/UKS/pbe	bh9-03-13 / def2-qzvpp	literature	barrier height forward kcal mol	1.16×10^{-3}
RKS/UKS/pbe	bh9-03-13 / def2-qzvpp	literature	barrier height reverse kcal mol	1.57×10^{-2}
RKS/UKS/pbe	bh9-03-13 / def2-qzvpp	literature	reaction energy kcal mol	1.45×10^{-2}
RKS/UKS/pbe	bh9-03-15 / def2-qzvpp	literature	barrier height forward kcal mol	3.35×10^{-2}
RKS/UKS/pbe	bh9-03-15 / def2-qzvpp	literature	barrier height reverse kcal mol	1.67×10^{-2}
RKS/UKS/pbe	bh9-03-15 / def2-qzvpp	literature	reaction energy kcal mol	1.69×10^{-2}
RKS/UKS/pbe	bh9-03-1 / def2-qzvpp	literature	barrier height forward kcal mol	3.13×10^{-2}
RKS/UKS/pbe	bh9-03-1 / def2-qzvpp	literature	barrier height reverse kcal mol	1.70×10^{-2}
RKS/UKS/pbe	bh9-03-1 / def2-qzvpp	literature	reaction energy kcal mol	1.43×10^{-2}
RKS/UKS/pbe	bh9-03-2 / def2-qzvpp	literature	barrier height forward kcal mol	2.73×10^{-2}
RKS/UKS/pbe	bh9-03-2 / def2-qzvpp	literature	barrier height reverse kcal mol	1.96×10^{-2}
RKS/UKS/pbe	bh9-03-2 / def2-qzvpp	literature	reaction energy kcal mol	7.63×10^{-3}
RKS/UKS/pbe	bh9-03-3 / def2-qzvpp	literature	barrier height forward kcal mol	1.72×10^{-2}
RKS/UKS/pbe	bh9-03-3 / def2-qzvpp	literature	barrier height reverse kcal mol	1.53×10^{-3}
RKS/UKS/pbe	bh9-03-3 / def2-qzvpp	literature	reaction energy kcal mol	1.56×10^{-2}
RKS/UKS/pbe	bh9-03-4 / def2-qzvpp	literature	barrier height forward kcal mol	1.79×10^{-2}
RKS/UKS/pbe	bh9-03-4 / def2-qzvpp	literature	barrier height reverse kcal mol	6.78×10^{-3}
RKS/UKS/pbe	bh9-03-4 / def2-qzvpp	literature	reaction energy kcal mol	1.12×10^{-2}
RKS/UKS/pbe	bh9-03-5 / def2-qzvpp	literature	barrier height forward kcal mol	1.23×10^{-2}
RKS/UKS/pbe	bh9-03-5 / def2-qzvpp	literature	barrier height reverse kcal mol	1.65×10^{-2}
RKS/UKS/pbe	bh9-03-5 / def2-qzvpp	literature	reaction energy kcal mol	4.26×10^{-3}
RKS/UKS/pbe	bh9-03-6 / def2-qzvpp	literature	barrier height forward kcal mol	1.27×10^{-2}
RKS/UKS/pbe	bh9-03-6 / def2-qzvpp	literature	barrier height reverse kcal mol	1.26×10^{-3}
RKS/UKS/pbe	bh9-03-6 / def2-qzvpp	literature	reaction energy kcal mol	1.14×10^{-2}
RKS/UKS/pbe	bh9-03-7 / def2-qzvpp	literature	barrier height forward kcal mol	3.34×10^{-2}
RKS/UKS/pbe	bh9-03-7 / def2-qzvpp	literature	barrier height reverse kcal mol	1.65×10^{-2}
RKS/UKS/pbe	bh9-03-7 / def2-qzvpp	literature	reaction energy kcal mol	1.69×10^{-2}
RKS/UKS/pbe	bh9-03-8 / def2-qzvpp	literature	barrier height forward kcal mol	3.30×10^{-2}
RKS/UKS/pbe	bh9-03-8 / def2-qzvpp	literature	barrier height reverse kcal mol	1.67×10^{-2}
RKS/UKS/pbe	bh9-03-8 / def2-qzvpp	literature	reaction energy kcal mol	1.63×10^{-2}

Table S21, continued.

Method	System / basis	Ref.	Quantity	$\lvert\Delta\rvert$
RKS/UKS/pbe	bh9-03-9 / def2-qzvpp	literature	reaction energy kcal mol	1.18×10^{-2}
UKS/pbe	bh9-04-10ts / def2-qzvpp	literature	total energy ha	0
UKS/pbe	bh9-04-11ts / def2-qzvpp	literature	total energy ha	0
UKS/pbe	bh9-04-12ts / def2-qzvpp	literature	total energy ha	0
UKS/pbe	bh9-04-13ts / def2-qzvpp	literature	total energy ha	0
UKS/pbe	bh9-04-14ts / def2-qzvpp	literature	total energy ha	0
UKS/pbe	bh9-04-15ts / def2-qzvpp	literature	total energy ha	0
UKS/pbe	bh9-04-16ts / def2-qzvpp	literature	total energy ha	9.99×10^{-11}
UKS/pbe	bh9-04-17ts / def2-qzvpp	literature	total energy ha	0
UKS/pbe	bh9-04-18p / def2-qzvpp	literature	total energy ha	0
UKS/pbe	bh9-04-18r / def2-qzvpp	literature	total energy ha	9.99×10^{-11}
UKS/pbe	bh9-04-18ts / def2-qzvpp	literature	total energy ha	0
UKS/pbe	bh9-04-19p / def2-qzvpp	literature	total energy ha	1.00×10^{-10}
UKS/pbe	bh9-04-19r / def2-qzvpp	literature	total energy ha	0
UKS/pbe	bh9-04-19ts / def2-qzvpp	literature	total energy ha	1.00×10^{-10}
UKS/pbe	bh9-04-20p / def2-qzvpp	literature	total energy ha	0
UKS/pbe	bh9-04-20r / def2-qzvpp	literature	total energy ha	0
UKS/pbe	bh9-04-20ts / def2-qzvpp	literature	total energy ha	0
UKS/pbe	bh9-04-21p / def2-qzvpp	literature	total energy ha	0
UKS/pbe	bh9-04-21r / def2-qzvpp	literature	total energy ha	0
UKS/pbe	bh9-04-21ts / def2-qzvpp	literature	total energy ha	0
UKS/pbe	bh9-04-22ts / def2-qzvpp	literature	total energy ha	0
UKS/pbe	bh9-04-23ts / def2-qzvpp	literature	total energy ha	0
UKS/pbe	bh9-04-24ts / def2-qzvpp	literature	total energy ha	0
UKS/pbe	bh9-04-25ts / def2-qzvpp	literature	total energy ha	1.00×10^{-10}
UKS/pbe	bh9-04-26ts / def2-qzvpp	literature	total energy ha	0
UKS/pbe	bh9-04-27ts / def2-qzvpp	literature	total energy ha	1.00×10^{-10}
UKS/pbe	bh9-04-28p / def2-qzvpp	literature	total energy ha	0
UKS/pbe	bh9-04-28r / def2-qzvpp	literature	total energy ha	1.00×10^{-10}
UKS/pbe	bh9-04-28ts / def2-qzvpp	literature	total energy ha	1.00×10^{-10}
UKS/pbe	bh9-04-29ts / def2-qzvpp	literature	total energy ha	0
UKS/pbe	bh9-04-30ts / def2-qzvpp	literature	total energy ha	0
UKS/pbe	bh9-04-31p / def2-qzvpp	literature	total energy ha	0
UKS/pbe	bh9-04-31r / def2-qzvpp	literature	total energy ha	0
UKS/pbe	bh9-04-31ts / def2-qzvpp	literature	total energy ha	0
UKS/pbe	bh9-04-32ts / def2-qzvpp	literature	total energy ha	0
UKS/pbe	bh9-04-33ts / def2-qzvpp	literature	total energy ha	0
UKS/pbe	bh9-04-34ts / def2-qzvpp	literature	total energy ha	0
UKS/pbe	bh9-04-35ts / def2-qzvpp	literature	total energy ha	0
UKS/pbe	bh9-04-36p / def2-qzvpp	literature	total energy ha	0
UKS/pbe	bh9-04-36r / def2-qzvpp	literature	total energy ha	0
UKS/pbe	bh9-04-36ts / def2-qzvpp	literature	total energy ha	0
UKS/pbe	bh9-04-37p / def2-qzvpp	literature	total energy ha	0
UKS/pbe	bh9-04-37r / def2-qzvpp	literature	total energy ha	0
UKS/pbe	bh9-04-37ts / def2-qzvpp	literature	total energy ha	0
UKS/pbe	bh9-04-38ts / def2-qzvpp	literature	total energy ha	0
UKS/pbe	bh9-04-39ts / def2-qzvpp	literature	total energy ha	0
UKS/pbe	bh9-04-9ts / def2-qzvpp	literature	total energy ha	0
RKS/UKS/pbe	bh9-04-10 / def2-qzvpp	literature	barrier height forward kcal mol	2.38×10^{-2}
RKS/UKS/pbe	bh9-04-10 / def2-qzvpp	literature	barrier height reverse kcal mol	1.02×10^{-2}
RKS/UKS/pbe	bh9-04-10 / def2-qzvpp	literature	reaction energy kcal mol	1.36×10^{-2}
RKS/UKS/pbe	bh9-04-11 / def2-qzvpp	literature	barrier height reverse kcal mol	1.94×10^{-2}
RKS/UKS/pbe	bh9-04-11 / def2-qzvpp	literature	reaction energy kcal mol	1.45×10^{-2}
RKS/UKS/pbe	bh9-04-12 / def2-qzvpp	literature	barrier height forward kcal mol	2.06×10^{-2}

Table S21, continued.

Method	System / basis	Ref.	Quantity	$\lvert\Delta\rvert$
RKS/UKS/pbe	bh9-04-12 / def2-qzvpp	literature	barrier height reverse kcal mol	1.44×10^{-2}
RKS/UKS/pbe	bh9-04-12 / def2-qzvpp	literature	reaction energy kcal mol	6.19×10^{-3}
RKS/UKS/pbe	bh9-04-13 / def2-qzvpp	literature	barrier height forward kcal mol	1.91×10^{-2}
RKS/UKS/pbe	bh9-04-13 / def2-qzvpp	literature	barrier height reverse kcal mol	1.82×10^{-2}
RKS/UKS/pbe	bh9-04-13 / def2-qzvpp	literature	reaction energy kcal mol	8.78×10^{-4}
RKS/UKS/pbe	bh9-04-14 / def2-qzvpp	literature	barrier height forward kcal mol	2.03×10^{-2}
RKS/UKS/pbe	bh9-04-14 / def2-qzvpp	literature	barrier height reverse kcal mol	1.98×10^{-2}
RKS/UKS/pbe	bh9-04-14 / def2-qzvpp	literature	reaction energy kcal mol	4.90×10^{-4}
RKS/UKS/pbe	bh9-04-15 / def2-qzvpp	literature	barrier height forward kcal mol	1.88×10^{-2}
RKS/UKS/pbe	bh9-04-15 / def2-qzvpp	literature	barrier height reverse kcal mol	2.56×10^{-2}
RKS/UKS/pbe	bh9-04-15 / def2-qzvpp	literature	reaction energy kcal mol	6.77×10^{-3}
RKS/UKS/pbe	bh9-04-16 / def2-qzvpp	literature	barrier height forward kcal mol	1.91×10^{-2}
RKS/UKS/pbe	bh9-04-16 / def2-qzvpp	literature	barrier height reverse kcal mol	1.36×10^{-2}
RKS/UKS/pbe	bh9-04-16 / def2-qzvpp	literature	reaction energy kcal mol	5.43×10^{-3}
RKS/UKS/pbe	bh9-04-17 / def2-qzvpp	literature	barrier height forward kcal mol	2.00×10^{-2}
RKS/UKS/pbe	bh9-04-17 / def2-qzvpp	literature	barrier height reverse kcal mol	2.18×10^{-2}
RKS/UKS/pbe	bh9-04-17 / def2-qzvpp	literature	reaction energy kcal mol	1.83×10^{-3}
UKS/pbe	bh9-04-18 / def2-qzvpp	literature	barrier height forward kcal mol	1.53×10^{-2}
UKS/pbe	bh9-04-18 / def2-qzvpp	literature	barrier height reverse kcal mol	6.88×10^{-3}
UKS/pbe	bh9-04-18 / def2-qzvpp	literature	reaction energy kcal mol	8.37×10^{-3}
UKS/pbe	bh9-04-19 / def2-qzvpp	literature	barrier height forward kcal mol	9.26×10^{-3}
UKS/pbe	bh9-04-19 / def2-qzvpp	literature	barrier height reverse kcal mol	9.09×10^{-3}
UKS/pbe	bh9-04-19 / def2-qzvpp	literature	reaction energy kcal mol	1.71×10^{-4}
UKS/pbe	bh9-04-1 / def2-qzvpp	literature	barrier height forward kcal mol	1.62×10^{-2}
UKS/pbe	bh9-04-1 / def2-qzvpp	literature	barrier height reverse kcal mol	1.13×10^{-2}
UKS/pbe	bh9-04-1 / def2-qzvpp	literature	reaction energy kcal mol	4.84×10^{-3}
UKS/pbe	bh9-04-20 / def2-qzvpp	literature	barrier height forward kcal mol	8.79×10^{-3}
UKS/pbe	bh9-04-20 / def2-qzvpp	literature	barrier height reverse kcal mol	1.54×10^{-2}
UKS/pbe	bh9-04-20 / def2-qzvpp	literature	reaction energy kcal mol	6.60×10^{-3}
UKS/pbe	bh9-04-21 / def2-qzvpp	literature	barrier height forward kcal mol	9.99×10^{-3}
UKS/pbe	bh9-04-21 / def2-qzvpp	literature	barrier height reverse kcal mol	1.45×10^{-2}
UKS/pbe	bh9-04-21 / def2-qzvpp	literature	reaction energy kcal mol	4.45×10^{-3}
RKS/UKS/pbe	bh9-04-22 / def2-qzvpp	literature	barrier height forward kcal mol	1.29×10^{-2}
RKS/UKS/pbe	bh9-04-22 / def2-qzvpp	literature	barrier height reverse kcal mol	2.25×10^{-3}
RKS/UKS/pbe	bh9-04-22 / def2-qzvpp	literature	reaction energy kcal mol	1.06×10^{-2}

Table S21, continued.

Method	System / basis	Ref.	Quantity	$\lvert\Delta\rvert$
RKS/UKS/pbe	bh9-04-23 / def2-qzvpp	literature	barrier height forward kcal mol	1.24×10^{-2}
RKS/UKS/pbe	bh9-04-23 / def2-qzvpp	literature	barrier height reverse kcal mol	2.50×10^{-3}
RKS/UKS/pbe	bh9-04-23 / def2-qzvpp	literature	reaction energy kcal mol	9.94×10^{-3}
RKS/UKS/pbe	bh9-04-24 / def2-qzvpp	literature	barrier height forward kcal mol	1.72×10^{-2}
RKS/UKS/pbe	bh9-04-24 / def2-qzvpp	literature	barrier height reverse kcal mol	1.32×10^{-2}
RKS/UKS/pbe	bh9-04-24 / def2-qzvpp	literature	reaction energy kcal mol	4.04×10^{-3}
RKS/UKS/pbe	bh9-04-25 / def2-qzvpp	literature	barrier height forward kcal mol	1.69×10^{-2}
RKS/UKS/pbe	bh9-04-25 / def2-qzvpp	literature	barrier height reverse kcal mol	2.01×10^{-2}
RKS/UKS/pbe	bh9-04-25 / def2-qzvpp	literature	reaction energy kcal mol	3.24×10^{-3}
RKS/UKS/pbe	bh9-04-26 / def2-qzvpp	literature	barrier height forward kcal mol	1.67×10^{-2}
RKS/UKS/pbe	bh9-04-26 / def2-qzvpp	literature	barrier height reverse kcal mol	1.99×10^{-2}
RKS/UKS/pbe	bh9-04-26 / def2-qzvpp	literature	reaction energy kcal mol	3.20×10^{-3}
RKS/UKS/pbe	bh9-04-27 / def2-qzvpp	literature	barrier height forward kcal mol	1.76×10^{-2}
RKS/UKS/pbe	bh9-04-27 / def2-qzvpp	literature	barrier height reverse kcal mol	2.08×10^{-2}
RKS/UKS/pbe	bh9-04-27 / def2-qzvpp	literature	reaction energy kcal mol	3.22×10^{-3}
UKS/pbe	bh9-04-28 / def2-qzvpp	literature	barrier height forward kcal mol	1.31×10^{-2}
UKS/pbe	bh9-04-28 / def2-qzvpp	literature	barrier height reverse kcal mol	8.72×10^{-3}
UKS/pbe	bh9-04-28 / def2-qzvpp	literature	reaction energy kcal mol	4.37×10^{-3}
RKS/UKS/pbe	bh9-04-29 / def2-qzvpp	literature	barrier height forward kcal mol	1.23×10^{-2}
RKS/UKS/pbe	bh9-04-29 / def2-qzvpp	literature	barrier height reverse kcal mol	2.55×10^{-3}
RKS/UKS/pbe	bh9-04-29 / def2-qzvpp	literature	reaction energy kcal mol	9.78×10^{-3}
RKS/UKS/pbe	bh9-04-2 / def2-qzvpp	literature	barrier height forward kcal mol	2.37×10^{-2}
RKS/UKS/pbe	bh9-04-2 / def2-qzvpp	literature	barrier height reverse kcal mol	1.82×10^{-2}
RKS/UKS/pbe	bh9-04-2 / def2-qzvpp	literature	reaction energy kcal mol	5.47×10^{-3}
RKS/UKS/pbe	bh9-04-30 / def2-qzvpp	literature	barrier height forward kcal mol	1.42×10^{-2}
RKS/UKS/pbe	bh9-04-30 / def2-qzvpp	literature	barrier height reverse kcal mol	1.30×10^{-2}
RKS/UKS/pbe	bh9-04-30 / def2-qzvpp	literature	reaction energy kcal mol	1.23×10^{-3}
UKS/pbe	bh9-04-31 / def2-qzvpp	literature	barrier height forward kcal mol	9.97×10^{-3}
UKS/pbe	bh9-04-31 / def2-qzvpp	literature	barrier height reverse kcal mol	5.72×10^{-3}
UKS/pbe	bh9-04-31 / def2-qzvpp	literature	reaction energy kcal mol	4.25×10^{-3}
RKS/UKS/pbe	bh9-04-32 / def2-qzvpp	literature	reaction energy kcal mol	4.27×10^{-3}
RKS/UKS/pbe	bh9-04-33 / def2-qzvpp	literature	reaction energy kcal mol	2.76×10^{-3}
RKS/UKS/pbe	bh9-04-34 / def2-qzvpp	literature	reaction energy kcal mol	3.97×10^{-3}
RKS/UKS/pbe	bh9-04-35 / def2-qzvpp	literature	barrier height forward kcal mol	1.53×10^{-2}
RKS/UKS/pbe	bh9-04-35 / def2-qzvpp	literature	barrier height reverse kcal mol	1.02×10^{-2}
RKS/UKS/pbe	bh9-04-35 / def2-qzvpp	literature	reaction energy kcal mol	5.13×10^{-3}

Table S21, continued.

Method	System / basis	Ref.	Quantity	$\lvert\Delta\rvert$
UKS/pbe	bh9-04-36 / def2-qzvpp	literature	barrier height forward kcal mol	1.35×10^{-2}
UKS/pbe	bh9-04-36 / def2-qzvpp	literature	barrier height reverse kcal mol	1.82×10^{-2}
UKS/pbe	bh9-04-36 / def2-qzvpp	literature	reaction energy kcal mol	4.64×10^{-3}
UKS/pbe	bh9-04-37 / def2-qzvpp	literature	barrier height forward kcal mol	1.09×10^{-2}
UKS/pbe	bh9-04-37 / def2-qzvpp	literature	barrier height reverse kcal mol	1.85×10^{-2}
UKS/pbe	bh9-04-37 / def2-qzvpp	literature	reaction energy kcal mol	7.53×10^{-3}
RKS/UKS/pbe	bh9-04-38 / def2-qzvpp	literature	barrier height forward kcal mol	1.32×10^{-2}
RKS/UKS/pbe	bh9-04-38 / def2-qzvpp	literature	barrier height reverse kcal mol	1.17×10^{-2}
RKS/UKS/pbe	bh9-04-38 / def2-qzvpp	literature	reaction energy kcal mol	1.41×10^{-3}
RKS/UKS/pbe	bh9-04-39 / def2-qzvpp	literature	barrier height forward kcal mol	1.13×10^{-2}
RKS/UKS/pbe	bh9-04-39 / def2-qzvpp	literature	barrier height reverse kcal mol	3.77×10^{-3}
RKS/UKS/pbe	bh9-04-39 / def2-qzvpp	literature	reaction energy kcal mol	7.49×10^{-3}
RKS/UKS/pbe	bh9-04-3 / def2-qzvpp	literature	barrier height forward kcal mol	1.06×10^{-2}
RKS/UKS/pbe	bh9-04-3 / def2-qzvpp	literature	barrier height reverse kcal mol	1.00×10^{-2}
RKS/UKS/pbe	bh9-04-3 / def2-qzvpp	literature	reaction energy kcal mol	5.49×10^{-4}
UKS/pbe	bh9-04-4 / def2-qzvpp	literature	barrier height forward kcal mol	1.55×10^{-2}
UKS/pbe	bh9-04-4 / def2-qzvpp	literature	barrier height reverse kcal mol	1.09×10^{-2}
UKS/pbe	bh9-04-4 / def2-qzvpp	literature	reaction energy kcal mol	4.53×10^{-3}
RKS/UKS/pbe	bh9-04-5 / def2-qzvpp	literature	barrier height forward kcal mol	1.50×10^{-2}
RKS/UKS/pbe	bh9-04-5 / def2-qzvpp	literature	barrier height reverse kcal mol	1.55×10^{-2}
RKS/UKS/pbe	bh9-04-5 / def2-qzvpp	literature	reaction energy kcal mol	4.52×10^{-4}
RKS/UKS/pbe	bh9-04-6 / def2-qzvpp	literature	barrier height forward kcal mol	1.11×10^{-2}
RKS/UKS/pbe	bh9-04-6 / def2-qzvpp	literature	barrier height reverse kcal mol	8.82×10^{-3}
RKS/UKS/pbe	bh9-04-6 / def2-qzvpp	literature	reaction energy kcal mol	2.29×10^{-3}
RKS/UKS/pbe	bh9-04-7 / def2-qzvpp	literature	barrier height forward kcal mol	1.39×10^{-2}
RKS/UKS/pbe	bh9-04-7 / def2-qzvpp	literature	barrier height reverse kcal mol	1.00×10^{-2}
RKS/UKS/pbe	bh9-04-7 / def2-qzvpp	literature	reaction energy kcal mol	3.93×10^{-3}
UKS/pbe	bh9-04-8 / def2-qzvpp	literature	barrier height forward kcal mol	9.73×10^{-3}
UKS/pbe	bh9-04-8 / def2-qzvpp	literature	barrier height reverse kcal mol	1.40×10^{-2}
UKS/pbe	bh9-04-8 / def2-qzvpp	literature	reaction energy kcal mol	4.22×10^{-3}
RKS/UKS/pbe	bh9-04-9 / def2-qzvpp	literature	barrier height forward kcal mol	2.34×10^{-2}
RKS/UKS/pbe	bh9-04-9 / def2-qzvpp	literature	barrier height reverse kcal mol	9.50×10^{-3}
RKS/UKS/pbe	bh9-04-9 / def2-qzvpp	literature	reaction energy kcal mol	1.39×10^{-2}
RKS/pbe	bh9-05-5ts / def2-qzvpp	literature	total energy ha	0
RKS/pbe	bh9-05-6p / def2-qzvpp	literature	total energy ha	0
RKS/pbe	bh9-05-6r / def2-qzvpp	literature	total energy ha	0

Table S21, continued.

Method	System / basis	Ref.	Quantity	$\lvert\Delta\rvert$
RKS/pbe	bh9-05-6ts / def2-qzvpp	literature	total energy ha	0
RKS/pbe	bh9-05-7ts / def2-qzvpp	literature	total energy ha	0
RKS/pbe	bh9-05-1 / def2-qzvpp	literature	barrier height forward kcal mol	1.15×10^{-2}
RKS/pbe	bh9-05-1 / def2-qzvpp	literature	barrier height reverse kcal mol	1.06×10^{-2}
RKS/pbe	bh9-05-1 / def2-qzvpp	literature	reaction energy kcal mol	9.19×10^{-4}
RKS/pbe	bh9-05-2 / def2-qzvpp	literature	barrier height forward kcal mol	1.13×10^{-2}
RKS/pbe	bh9-05-2 / def2-qzvpp	literature	barrier height reverse kcal mol	9.79×10^{-3}
RKS/pbe	bh9-05-2 / def2-qzvpp	literature	reaction energy kcal mol	1.58×10^{-3}
RKS/pbe	bh9-05-3 / def2-qzvpp	literature	barrier height forward kcal mol	8.94×10^{-3}
RKS/pbe	bh9-05-3 / def2-qzvpp	literature	barrier height reverse kcal mol	7.79×10^{-3}
RKS/pbe	bh9-05-3 / def2-qzvpp	literature	reaction energy kcal mol	1.15×10^{-3}
RKS/pbe	bh9-05-4 / def2-qzvpp	literature	barrier height forward kcal mol	4.24×10^{-3}
RKS/pbe	bh9-05-4 / def2-qzvpp	literature	barrier height reverse kcal mol	1.29×10^{-2}
RKS/pbe	bh9-05-4 / def2-qzvpp	literature	reaction energy kcal mol	8.71×10^{-3}
RKS/pbe	bh9-05-5 / def2-qzvpp	literature	barrier height forward kcal mol	2.57×10^{-2}
RKS/pbe	bh9-05-5 / def2-qzvpp	literature	barrier height reverse kcal mol	2.80×10^{-2}
RKS/pbe	bh9-05-5 / def2-qzvpp	literature	reaction energy kcal mol	2.30×10^{-3}
RKS/pbe	bh9-05-6 / def2-qzvpp	literature	barrier height forward kcal mol	9.74×10^{-3}
RKS/pbe	bh9-05-6 / def2-qzvpp	literature	barrier height reverse kcal mol	9.45×10^{-3}
RKS/pbe	bh9-05-6 / def2-qzvpp	literature	reaction energy kcal mol	2.92×10^{-4}
RKS/pbe	bh9-05-7 / def2-qzvpp	literature	barrier height forward kcal mol	2.54×10^{-2}
RKS/pbe	bh9-05-7 / def2-qzvpp	literature	barrier height reverse kcal mol	2.50×10^{-2}
RKS/pbe	bh9-05-7 / def2-qzvpp	literature	reaction energy kcal mol	4.23×10^{-4}
UKS/pbe	bh9-06-3p / def2-qzvpp	literature	total energy ha	0
UKS/pbe	bh9-06-3ts / def2-qzvpp	literature	total energy ha	0
UKS/pbe	bh9-06-4p / def2-qzvpp	literature	total energy ha	0
UKS/pbe	bh9-06-4ts / def2-qzvpp	literature	total energy ha	1.00×10^{-10}
RKS/pbe	bh9-06-5p / def2-qzvpp	literature	total energy ha	0
RKS/pbe	bh9-06-5ts / def2-qzvpp	literature	total energy ha	0
UKS/pbe	bh9-06-6p / def2-qzvpp	literature	total energy ha	0
UKS/pbe	bh9-06-6ts / def2-qzvpp	literature	total energy ha	0
UKS/pbe	bh9-06-7ts / def2-qzvpp	literature	total energy ha	0
RKS/UKS/pbe	bh9-06-1 / def2-qzvpp	literature	barrier height forward kcal mol	1.56×10^{-2}
RKS/UKS/pbe	bh9-06-1 / def2-qzvpp	literature	barrier height reverse kcal mol	1.59×10^{-2}
RKS/UKS/pbe	bh9-06-1 / def2-qzvpp	literature	reaction energy kcal mol	3.19×10^{-4}
RKS/UKS/pbe	bh9-06-2 / def2-qzvpp	literature	barrier height forward kcal mol	3.85×10^{-3}
UKS/pbe	bh9-06-2 / def2-qzvpp	literature	barrier height reverse kcal mol	8.80×10^{-3}
RKS/UKS/pbe	bh9-06-2 / def2-qzvpp	literature	reaction energy kcal mol	4.97×10^{-3}
RKS/UKS/pbe	bh9-06-3 / def2-qzvpp	literature	barrier height forward kcal mol	3.45×10^{-3}

Table S21, continued.

Method	System / basis	Ref.	Quantity	$\lvert\Delta\rvert$
UKS/pbe	bh9-06-3 / def2-qzvpp	literature	barrier height reverse kcal mol	1.05×10^{-2}
RKS/UKS/pbe	bh9-06-3 / def2-qzvpp	literature	reaction energy kcal mol	7.05×10^{-3}
RKS/UKS/pbe	bh9-06-4 / def2-qzvpp	literature	barrier height forward kcal mol	2.36×10^{-3}
UKS/pbe	bh9-06-4 / def2-qzvpp	literature	barrier height reverse kcal mol	1.16×10^{-2}
RKS/UKS/pbe	bh9-06-4 / def2-qzvpp	literature	reaction energy kcal mol	9.22×10^{-3}
RKS/pbe	bh9-06-5 / def2-qzvpp	literature	barrier height forward kcal mol	3.90×10^{-3}
RKS/pbe	bh9-06-5 / def2-qzvpp	literature	barrier height reverse kcal mol	4.14×10^{-3}
RKS/pbe	bh9-06-5 / def2-qzvpp	literature	reaction energy kcal mol	2.28×10^{-4}
RKS/UKS/pbe	bh9-06-6 / def2-qzvpp	literature	barrier height forward kcal mol	1.63×10^{-3}
UKS/pbe	bh9-06-6 / def2-qzvpp	literature	barrier height reverse kcal mol	1.03×10^{-2}
RKS/UKS/pbe	bh9-06-6 / def2-qzvpp	literature	reaction energy kcal mol	8.62×10^{-3}
RKS/UKS/pbe	bh9-06-7 / def2-qzvpp	literature	barrier height forward kcal mol	9.34×10^{-3}
RKS/UKS/pbe	bh9-06-7 / def2-qzvpp	literature	barrier height reverse kcal mol	9.37×10^{-3}
RKS/UKS/pbe	bh9-06-7 / def2-qzvpp	literature	reaction energy kcal mol	4.71×10^{-5}
RKS/pbe	bh9-07-10p1 / def2-qzvpp	literature	total energy ha	0
RKS/pbe	bh9-07-10r1 / def2-qzvpp	literature	total energy ha	0
RKS/pbe	bh9-07-10ts / def2-qzvpp	literature	total energy ha	1.00×10^{-10}
RKS/pbe	bh9-07-4ts / def2-qzvpp	literature	total energy ha	0
RKS/pbe	bh9-07-5p / def2-qzvpp	literature	total energy ha	0
RKS/pbe	bh9-07-5r / def2-qzvpp	literature	total energy ha	0
RKS/pbe	bh9-07-5ts / def2-qzvpp	literature	total energy ha	0
RKS/pbe	bh9-07-10 / def2-qzvpp	literature	barrier height forward kcal mol	1.05×10^{-2}
RKS/pbe	bh9-07-10 / def2-qzvpp	literature	barrier height reverse kcal mol	1.18×10^{-2}
RKS/pbe	bh9-07-10 / def2-qzvpp	literature	reaction energy kcal mol	1.34×10^{-3}
RKS/pbe	bh9-07-1 / def2-qzvpp	literature	barrier height forward kcal mol	8.50×10^{-3}
RKS/pbe	bh9-07-1 / def2-qzvpp	literature	barrier height reverse kcal mol	1.21×10^{-2}
RKS/pbe	bh9-07-1 / def2-qzvpp	literature	reaction energy kcal mol	3.63×10^{-3}
RKS/pbe	bh9-07-2 / def2-qzvpp	literature	barrier height forward kcal mol	2.60×10^{-3}
RKS/pbe	bh9-07-2 / def2-qzvpp	literature	barrier height reverse kcal mol	5.53×10^{-4}
RKS/pbe	bh9-07-2 / def2-qzvpp	literature	reaction energy kcal mol	2.05×10^{-3}
RKS/pbe	bh9-07-3 / def2-qzvpp	literature	barrier height forward kcal mol	9.22×10^{-3}
RKS/pbe	bh9-07-3 / def2-qzvpp	literature	barrier height reverse kcal mol	1.09×10^{-2}
RKS/pbe	bh9-07-3 / def2-qzvpp	literature	reaction energy kcal mol	1.68×10^{-3}
RKS/pbe	bh9-07-4 / def2-qzvpp	literature	barrier height forward kcal mol	1.74×10^{-2}
RKS/pbe	bh9-07-4 / def2-qzvpp	literature	barrier height reverse kcal mol	9.08×10^{-3}
RKS/pbe	bh9-07-4 / def2-qzvpp	literature	reaction energy kcal mol	8.29×10^{-3}
RKS/pbe	bh9-07-5 / def2-qzvpp	literature	barrier height forward kcal mol	8.12×10^{-3}

Table S21, continued.

Method	System / basis	Ref.	Quantity	$\lvert\Delta\rvert$
RKS/pbe	bh9-07-5 / def2-qzvpp	literature	barrier height reverse kcal mol	1.43×10^{-2}
RKS/pbe	bh9-07-5 / def2-qzvpp	literature	reaction energy kcal mol	6.13×10^{-3}
RKS/pbe	bh9-07-9 / def2-qzvpp	literature	barrier height forward kcal mol	9.64×10^{-3}
RKS/pbe	bh9-07-9 / def2-qzvpp	literature	barrier height reverse kcal mol	1.33×10^{-2}
RKS/pbe	bh9-07-9 / def2-qzvpp	literature	reaction energy kcal mol	3.63×10^{-3}
RKS/pbe	bh9-08-3r1 / def2-qzvpp	literature	total energy ha	0
RKS/pbe	bh9-08-3ts / def2-qzvpp	literature	total energy ha	0
RKS/pbe	bh9-08-4p / def2-qzvpp	literature	total energy ha	0
RKS/pbe	bh9-08-4ts / def2-qzvpp	literature	total energy ha	0
RKS/pbe	bh9-08-5p1 / def2-qzvpp	literature	total energy ha	0
RKS/pbe	bh9-08-5ts / def2-qzvpp	literature	total energy ha	0
RKS/pbe	bh9-08-1 / def2-qzvpp	literature	barrier height forward kcal mol	1.73×10^{-2}
RKS/pbe	bh9-08-1 / def2-qzvpp	literature	barrier height reverse kcal mol	6.71×10^{-3}
RKS/pbe	bh9-08-1 / def2-qzvpp	literature	reaction energy kcal mol	1.06×10^{-2}
RKS/pbe	bh9-08-2 / def2-qzvpp	literature	barrier height forward kcal mol	1.47×10^{-2}
RKS/pbe	bh9-08-2 / def2-qzvpp	literature	barrier height reverse kcal mol	6.50×10^{-3}
RKS/pbe	bh9-08-2 / def2-qzvpp	literature	reaction energy kcal mol	8.20×10^{-3}
RKS/pbe	bh9-08-3 / def2-qzvpp	literature	barrier height reverse kcal mol	6.99×10^{-3}
RKS/pbe	bh9-08-3 / def2-qzvpp	literature	reaction energy kcal mol	1.90×10^{-2}
RKS/pbe	bh9-08-4 / def2-qzvpp	literature	barrier height forward kcal mol	9.88×10^{-3}
RKS/pbe	bh9-08-4 / def2-qzvpp	literature	barrier height reverse kcal mol	1.36×10^{-2}
RKS/pbe	bh9-08-4 / def2-qzvpp	literature	reaction energy kcal mol	3.76×10^{-3}
RKS/pbe	bh9-08-5 / def2-qzvpp	literature	barrier height forward kcal mol	7.08×10^{-3}
RKS/pbe	bh9-08-5 / def2-qzvpp	literature	barrier height reverse kcal mol	1.61×10^{-2}
RKS/pbe	bh9-08-5 / def2-qzvpp	literature	reaction energy kcal mol	9.01×10^{-3}
RKS/pbe	bh9-09-10p / def2-qzvpp	literature	total energy ha	0
RKS/pbe	bh9-09-10r / def2-qzvpp	literature	total energy ha	0
RKS/pbe	bh9-09-10ts / def2-qzvpp	literature	total energy ha	0
RKS/pbe	bh9-09-11p / def2-qzvpp	literature	total energy ha	0
RKS/pbe	bh9-09-11ts / def2-qzvpp	literature	total energy ha	9.99×10^{-11}
RKS/pbe	bh9-09-12p / def2-qzvpp	literature	total energy ha	0
RKS/pbe	bh9-09-12ts / def2-qzvpp	literature	total energy ha	0
RKS/pbe	bh9-09-7p / def2-qzvpp	literature	total energy ha	0
RKS/pbe	bh9-09-7ts / def2-qzvpp	literature	total energy ha	0
RKS/pbe	bh9-09-8p / def2-qzvpp	literature	total energy ha	0
RKS/pbe	bh9-09-8ts / def2-qzvpp	literature	total energy ha	0
RKS/pbe	bh9-09-9p / def2-qzvpp	literature	total energy ha	0
RKS/pbe	bh9-09-9ts / def2-qzvpp	literature	total energy ha	0
RKS/pbe	bh9-09-10 / def2-qzvpp	literature	barrier height forward kcal mol	1.28×10^{-3}
RKS/pbe	bh9-09-10 / def2-qzvpp	literature	barrier height reverse kcal mol	1.13×10^{-2}
RKS/pbe	bh9-09-10 / def2-qzvpp	literature	reaction energy kcal mol	1.26×10^{-2}
RKS/pbe	bh9-09-11 / def2-qzvpp	literature	barrier height forward kcal mol	1.67×10^{-2}

Table S21, continued.

Method	System / basis	Ref.	Quantity	$\lvert\Delta\rvert$
RKS/pbe	bh9-09-11 / def2-qzvpp	literature	barrier height reverse kcal mol	1.12×10^{-2}
RKS/pbe	bh9-09-11 / def2-qzvpp	literature	reaction energy kcal mol	5.47×10^{-3}
RKS/pbe	bh9-09-12 / def2-qzvpp	literature	barrier height forward kcal mol	1.91×10^{-3}
RKS/pbe	bh9-09-12 / def2-qzvpp	literature	barrier height reverse kcal mol	1.89×10^{-3}
RKS/pbe	bh9-09-12 / def2-qzvpp	literature	reaction energy kcal mol	1.94×10^{-5}
RKS/pbe	bh9-09-1 / def2-qzvpp	literature	barrier height forward kcal mol	8.06×10^{-3}
RKS/pbe	bh9-09-1 / def2-qzvpp	literature	barrier height reverse kcal mol	1.91×10^{-3}
RKS/pbe	bh9-09-1 / def2-qzvpp	literature	reaction energy kcal mol	6.14×10^{-3}
RKS/pbe	bh9-09-2 / def2-qzvpp	literature	barrier height forward kcal mol	9.82×10^{-3}
RKS/pbe	bh9-09-2 / def2-qzvpp	literature	barrier height reverse kcal mol	1.98×10^{-3}
RKS/pbe	bh9-09-2 / def2-qzvpp	literature	reaction energy kcal mol	7.82×10^{-3}
RKS/pbe	bh9-09-3 / def2-qzvpp	literature	barrier height forward kcal mol	1.35×10^{-2}
RKS/pbe	bh9-09-3 / def2-qzvpp	literature	barrier height reverse kcal mol	1.28×10^{-2}
RKS/pbe	bh9-09-3 / def2-qzvpp	literature	reaction energy kcal mol	7.03×10^{-4}
RKS/pbe	bh9-09-4 / def2-qzvpp	literature	barrier height forward kcal mol	9.54×10^{-3}
RKS/pbe	bh9-09-4 / def2-qzvpp	literature	barrier height reverse kcal mol	1.11×10^{-2}
RKS/pbe	bh9-09-4 / def2-qzvpp	literature	reaction energy kcal mol	1.57×10^{-3}
RKS/pbe	bh9-09-5 / def2-qzvpp	literature	barrier height forward kcal mol	1.13×10^{-2}
RKS/pbe	bh9-09-5 / def2-qzvpp	literature	barrier height reverse kcal mol	1.98×10^{-2}
RKS/pbe	bh9-09-5 / def2-qzvpp	literature	reaction energy kcal mol	8.43×10^{-3}
RKS/pbe	bh9-09-6 / def2-qzvpp	literature	barrier height forward kcal mol	7.92×10^{-3}
RKS/pbe	bh9-09-6 / def2-qzvpp	literature	barrier height reverse kcal mol	1.10×10^{-2}
RKS/pbe	bh9-09-6 / def2-qzvpp	literature	reaction energy kcal mol	3.02×10^{-3}
RKS/pbe	bh9-09-7 / def2-qzvpp	literature	barrier height forward kcal mol	1.17×10^{-2}
RKS/pbe	bh9-09-7 / def2-qzvpp	literature	barrier height reverse kcal mol	7.57×10^{-3}
RKS/pbe	bh9-09-7 / def2-qzvpp	literature	reaction energy kcal mol	4.18×10^{-3}
RKS/pbe	bh9-09-8 / def2-qzvpp	literature	barrier height forward kcal mol	9.31×10^{-3}
RKS/pbe	bh9-09-8 / def2-qzvpp	literature	barrier height reverse kcal mol	1.29×10^{-2}
RKS/pbe	bh9-09-8 / def2-qzvpp	literature	reaction energy kcal mol	3.63×10^{-3}
RKS/pbe	bh9-09-9 / def2-qzvpp	literature	barrier height forward kcal mol	7.40×10^{-3}
RKS/pbe	bh9-09-9 / def2-qzvpp	literature	barrier height reverse kcal mol	1.22×10^{-2}
RKS/pbe	bh9-09-9 / def2-qzvpp	literature	reaction energy kcal mol	4.84×10^{-3}
RKS/b3lyp	benzene / sto-3g	orca	total energy ha	4.32×10^{-5}
RKS/lda	benzene / sto-3g	orca	total energy ha	1.64×10^{-5}
RKS/tpss	benzene / def2-tzvp	orca	total energy ha	4.86×10^{-5}
RKS/tpss	benzene / sto-3g	orca	total energy ha	1.47×10^{-5}
RKS/wb97m-v	benzene / def2-svp	orca	total energy ha	4.92×10^{-5}

Table S21, continued.

Method	System / basis	Ref.	Quantity	$\lvert\Delta\rvert$
RKS/wb97m-v	benzene / def2-tzvp	orca	total energy ha	9.04×10^{-6}
RKS/wb97m-v	benzene / sto-3g	orca	total energy ha	6.04×10^{-6}
RKS/wb97x	benzene / sto-3g	orca	total energy ha	3.54×10^{-5}
RKS/wb97x-v	benzene / def2-svp	orca	total energy ha	7.64×10^{-6}
RKS/wb97x-v	benzene / def2-tzvp	orca	total energy ha	1.97×10^{-5}
RKS/wb97x-v	benzene / sto-3g	orca	total energy ha	1.23×10^{-5}
RKS/b3lyp	c2h4 / def2-svp	orca	total energy ha	9.62×10^{-6}
RKS/b3lyp	c2h4 / def2-tzvp	orca	total energy ha	1.96×10^{-5}
RKS/b3lyp	c2h4 / sto-3g	orca	total energy ha	2.78×10^{-5}
RKS/blyp	c2h4 / def2-svp	orca	total energy ha	1.10×10^{-5}
RKS/blyp	c2h4 / def2-tzvp	orca	total energy ha	2.04×10^{-5}
RKS/blyp	c2h4 / sto-3g	orca	total energy ha	3.27×10^{-5}
RKS/lda	c2h4 / def2-svp	orca	total energy ha	1.54×10^{-5}
RKS/lda	c2h4 / def2-tzvp	orca	total energy ha	3.03×10^{-5}
RKS/lda	c2h4 / sto-3g	orca	total energy ha	3.88×10^{-5}
RKS/pbe0	c2h4 / def2-svp	orca	total energy ha	1.89×10^{-5}
RKS/pbe0	c2h4 / def2-tzvp	orca	total energy ha	3.35×10^{-5}
RKS/pbe0	c2h4 / sto-3g	orca	total energy ha	4.07×10^{-5}
RKS/pbe	c2h4 / def2-svp	orca	total energy ha	2.53×10^{-5}
RKS/pbe	c2h4 / def2-tzvp	orca	total energy ha	4.25×10^{-5}
RKS/tpss	c2h4 / def2-svp	orca	total energy ha	2.16×10^{-6}
RKS/tpss	c2h4 / def2-tzvp	orca	total energy ha	1.95×10^{-5}
RKS/tpss	c2h4 / sto-3g	orca	total energy ha	4.72×10^{-5}
RKS/wb97m-v	c2h4 / def2-svp	orca	total energy ha	3.91×10^{-6}
RKS/wb97m-v	c2h4 / def2-tzvp	orca	total energy ha	2.77×10^{-6}
RKS/wb97m-v	c2h4 / sto-3g	orca	total energy ha	4.19×10^{-7}
RKS/wb97x	c2h4 / def2-svp	orca	total energy ha	1.43×10^{-5}
RKS/wb97x	c2h4 / def2-tzvp	orca	total energy ha	2.51×10^{-5}
RKS/wb97x	c2h4 / sto-3g	orca	total energy ha	1.59×10^{-5}
RKS/wb97x-v	c2h4 / def2-svp	orca	total energy ha	1.76×10^{-6}
RKS/wb97x-v	c2h4 / def2-tzvp	orca	total energy ha	7.47×10^{-6}
RKS/wb97x-v	c2h4 / sto-3g	orca	total energy ha	1.35×10^{-5}
RKS/b3lyp	ch4 / def2-svp	orca	total energy ha	3.76×10^{-5}
RKS/blyp	ch4 / def2-svp	orca	total energy ha	4.44×10^{-5}
RKS/pbe0	ch4 / def2-svp	orca	total energy ha	2.19×10^{-5}
RKS/pbe0	ch4 / def2-tzvp	orca	total energy ha	3.71×10^{-5}
RKS/pbe0	ch4 / sto-3g	orca	total energy ha	4.80×10^{-5}
RKS/pbe	ch4 / def2-svp	orca	total energy ha	2.77×10^{-5}
RKS/r2scan	ch4 / def2-svp	orca	total energy ha	3.28×10^{-6}
RKS/r2scan	ch4 / def2-tzvp	orca	total energy ha	1.56×10^{-6}
RKS/tpss	ch4 / def2-svp	orca	total energy ha	2.76×10^{-5}
RKS/wb97m-v	ch4 / def2-svp	orca	total energy ha	3.16×10^{-5}
RKS/wb97m-v	ch4 / def2-tzvp	orca	total energy ha	3.47×10^{-5}
RKS/wb97m-v	ch4 / sto-3g	orca	total energy ha	2.79×10^{-5}
RKS/wb97x	ch4 / def2-tzvp	orca	total energy ha	4.66×10^{-5}
RKS/wb97x	ch4 / sto-3g	orca	total energy ha	3.99×10^{-5}
RKS/wb97x-v	ch4 / def2-svp	orca	total energy ha	1.87×10^{-5}
RKS/wb97x-v	ch4 / def2-tzvp	orca	total energy ha	2.11×10^{-5}
RKS/wb97x-v	ch4 / sto-3g	orca	total energy ha	3.04×10^{-5}
RKS/b3lyp	co2 / def2-svp	orca	total energy ha	8.19×10^{-6}
RKS/b3lyp	co2 / def2-tzvp	orca	total energy ha	2.39×10^{-6}
RKS/b3lyp	co2 / sto-3g	orca	total energy ha	4.11×10^{-6}
RKS/blyp	co2 / def2-svp	orca	total energy ha	9.80×10^{-6}
RKS/blyp	co2 / def2-tzvp	orca	total energy ha	3.01×10^{-6}
RKS/blyp	co2 / sto-3g	orca	total energy ha	4.96×10^{-6}
RKS/lda	co2 / def2-svp	orca	total energy ha	9.80×10^{-6}
RKS/lda	co2 / def2-tzvp	orca	total energy ha	1.39×10^{-6}
RKS/lda	co2 / sto-3g	orca	total energy ha	3.60×10^{-6}

Table S21, continued.

Method	System / basis	Ref.	Quantity	$\lvert\Delta\rvert$
RKS/pbe0	co2 / def2-svp	orca	total energy ha	1.88×10^{-5}
RKS/pbe0	co2 / def2-tzvp	orca	total energy ha	2.43×10^{-5}
RKS/pbe0	co2 / sto-3g	orca	total energy ha	2.40×10^{-5}
RKS/pbe	co2 / def2-svp	orca	total energy ha	2.62×10^{-5}
RKS/pbe	co2 / def2-tzvp	orca	total energy ha	3.32×10^{-5}
RKS/pbe	co2 / sto-3g	orca	total energy ha	3.23×10^{-5}
RKS/tpss	co2 / def2-svp	orca	total energy ha	1.62×10^{-5}
RKS/tpss	co2 / def2-tzvp	orca	total energy ha	4.44×10^{-6}
RKS/tpss	co2 / sto-3g	orca	total energy ha	1.32×10^{-5}
RKS/wb97m-v	co2 / def2-svp	orca	total energy ha	6.80×10^{-6}
RKS/wb97m-v	co2 / def2-tzvp	orca	total energy ha	4.53×10^{-6}
RKS/wb97m-v	co2 / sto-3g	orca	total energy ha	2.00×10^{-6}
RKS/wb97x	co2 / def2-svp	orca	total energy ha	6.67×10^{-6}
RKS/wb97x	co2 / def2-tzvp	orca	total energy ha	8.61×10^{-6}
RKS/wb97x	co2 / sto-3g	orca	total energy ha	2.53×10^{-6}
RKS/wb97x-v	co2 / def2-svp	orca	total energy ha	1.68×10^{-5}
RKS/wb97x-v	co2 / def2-tzvp	orca	total energy ha	1.22×10^{-5}
RKS/wb97x-v	co2 / sto-3g	orca	total energy ha	7.59×10^{-6}
RKS/b3lyp	ethanol / def2-svp	orca	total energy ha	4.40×10^{-5}
RKS/b3lyp	ethanol / def2-tzvp	orca	total energy ha	4.18×10^{-5}
RKS/b3lyp	ethanol / sto-3g	orca	total energy ha	4.64×10^{-5}
RKS/tpss	ethanol / def2-tzvp	orca	total energy ha	4.84×10^{-5}
RKS/tpss	ethanol / sto-3g	orca	total energy ha	4.47×10^{-5}
RKS/wb97m-v	ethanol / def2-svp	orca	total energy ha	2.17×10^{-5}
RKS/wb97m-v	ethanol / def2-tzvp	orca	total energy ha	1.69×10^{-5}
RKS/wb97m-v	ethanol / sto-3g	orca	total energy ha	3.31×10^{-5}
RKS/wb97x-v	ethanol / def2-svp	orca	total energy ha	8.25×10^{-6}
RKS/wb97x-v	ethanol / def2-tzvp	orca	total energy ha	7.17×10^{-6}
RKS/wb97x-v	ethanol / sto-3g	orca	total energy ha	2.18×10^{-5}
RKS/b3lyp	glycine / def2-svp	orca	total energy ha	1.65×10^{-5}
RKS/b3lyp	glycine / sto-3g	orca	total energy ha	4.09×10^{-6}
RKS/blyp	glycine / def2-svp	orca	total energy ha	2.23×10^{-5}
RKS/blyp	glycine / sto-3g	orca	total energy ha	5.36×10^{-6}
RKS/lda	glycine / def2-svp	orca	total energy ha	1.43×10^{-5}
RKS/lda	glycine / sto-3g	orca	total energy ha	1.40×10^{-5}
RKS/pbe0	glycine / def2-svp	orca	total energy ha	2.48×10^{-5}
RKS/pbe	glycine / def2-svp	orca	total energy ha	3.38×10^{-5}
RKS/tpss	glycine / def2-svp	orca	total energy ha	3.01×10^{-5}
RKS/tpss	glycine / sto-3g	orca	total energy ha	1.96×10^{-5}
RKS/wb97m-v	glycine / def2-svp	orca	total energy ha	3.48×10^{-5}
RKS/wb97m-v	glycine / def2-tzvp	orca	total energy ha	2.30×10^{-5}
RKS/wb97m-v	glycine / sto-3g	orca	total energy ha	5.76×10^{-6}
RKS/wb97x	glycine / def2-tzvp	orca	total energy ha	2.34×10^{-5}
RKS/wb97x	glycine / sto-3g	orca	total energy ha	1.31×10^{-5}
RKS/wb97x-v	glycine / def2-svp	orca	total energy ha	2.37×10^{-5}
RKS/wb97x-v	glycine / def2-tzvp	orca	total energy ha	3.14×10^{-5}
RKS/wb97x-v	glycine / sto-3g	orca	total energy ha	6.91×10^{-6}
RKS/b3lyp	h2o / def2-svp	orca	total energy ha	7.60×10^{-6}
RKS/b3lyp	h2o / def2-tzvp	orca	total energy ha	3.75×10^{-7}
RKS/b3lyp	h2o / sto-3g	orca	total energy ha	2.04×10^{-6}
RKS/blyp	h2o / def2-svp	orca	total energy ha	9.57×10^{-6}
RKS/blyp	h2o / def2-tzvp	orca	total energy ha	7.99×10^{-7}
RKS/blyp	h2o / sto-3g	orca	total energy ha	2.93×10^{-6}
RKS/lda	h2o / def2-svp	orca	total energy ha	8.47×10^{-6}
RKS/lda	h2o / def2-tzvp	orca	total energy ha	4.23×10^{-7}
RKS/lda	h2o / sto-3g	orca	total energy ha	1.36×10^{-6}
RKS/pbe0	h2o / def2-svp	orca	total energy ha	1.64×10^{-5}
RKS/pbe0	h2o / def2-tzvp	orca	total energy ha	1.02×10^{-5}

Table S21, continued.

Method	System / basis	Ref.	Quantity	$\lvert\Delta\rvert$
RKS/pbe0	h2o / sto-3g	orca	total energy ha	9.05×10^{-6}
RKS/pbe	h2o / def2-svp	orca	total energy ha	2.24×10^{-5}
RKS/pbe	h2o / def2-tzvp	orca	total energy ha	1.45×10^{-5}
RKS/pbe	h2o / sto-3g	orca	total energy ha	1.33×10^{-5}
RKS/r2scan	h2o / def2-svp	orca	total energy ha	3.98×10^{-5}
RKS/r2scan	h2o / def2-tzvp	orca	total energy ha	1.18×10^{-5}
RKS/tpss	h2o / def2-svp	orca	total energy ha	1.77×10^{-5}
RKS/tpss	h2o / def2-tzvp	orca	total energy ha	2.06×10^{-6}
RKS/tpss	h2o / sto-3g	orca	total energy ha	1.12×10^{-5}
RKS/wb97m-v	h2o / def2-svp	orca	total energy ha	6.31×10^{-6}
RKS/wb97m-v	h2o / def2-tzvp	orca	total energy ha	6.69×10^{-7}
RKS/wb97m-v	h2o / sto-3g	orca	total energy ha	8.49×10^{-6}
RKS/wb97x	h2o / def2-svp	orca	total energy ha	4.52×10^{-6}
RKS/wb97x	h2o / def2-tzvp	orca	total energy ha	2.24×10^{-6}
RKS/wb97x	h2o / sto-3g	orca	total energy ha	8.92×10^{-6}
RKS/wb97x-v	h2o / def2-svp	orca	total energy ha	9.09×10^{-7}
RKS/wb97x-v	h2o / def2-tzvp	orca	total energy ha	4.82×10^{-6}
RKS/wb97x-v	h2o / sto-3g	orca	total energy ha	3.80×10^{-6}
RKS/b3lyp	hf / def2-svp	orca	total energy ha	1.08×10^{-6}
RKS/b3lyp	hf / def2-tzvp	orca	total energy ha	3.16×10^{-6}
RKS/b3lyp	hf / sto-3g	orca	total energy ha	3.19×10^{-6}
RKS/blyp	hf / def2-svp	orca	total energy ha	1.18×10^{-6}
RKS/blyp	hf / def2-tzvp	orca	total energy ha	3.71×10^{-6}
RKS/blyp	hf / sto-3g	orca	total energy ha	3.50×10^{-6}
RKS/lda	hf / def2-svp	orca	total energy ha	2.09×10^{-6}
RKS/lda	hf / def2-tzvp	orca	total energy ha	4.14×10^{-6}
RKS/lda	hf / sto-3g	orca	total energy ha	6.52×10^{-6}
RKS/pbe0	hf / def2-svp	orca	total energy ha	1.11×10^{-5}
RKS/pbe0	hf / def2-tzvp	orca	total energy ha	9.90×10^{-6}
RKS/pbe0	hf / sto-3g	orca	total energy ha	8.44×10^{-6}
RKS/pbe	hf / def2-svp	orca	total energy ha	1.53×10^{-5}
RKS/pbe	hf / def2-tzvp	orca	total energy ha	1.37×10^{-5}
RKS/pbe	hf / sto-3g	orca	total energy ha	1.21×10^{-5}
RKS/r2scan	hf / def2-svp	orca	total energy ha	2.13×10^{-6}
RKS/r2scan	hf / def2-tzvp	orca	total energy ha	1.32×10^{-5}
RKS/tpss	hf / def2-svp	orca	total energy ha	3.37×10^{-6}
RKS/tpss	hf / def2-tzvp	orca	total energy ha	2.36×10^{-6}
RKS/tpss	hf / sto-3g	orca	total energy ha	1.19×10^{-5}
RKS/wb97m-v	hf / def2-svp	orca	total energy ha	2.95×10^{-6}
RKS/wb97m-v	hf / def2-tzvp	orca	total energy ha	2.78×10^{-6}
RKS/wb97m-v	hf / sto-3g	orca	total energy ha	4.34×10^{-7}
RKS/wb97x	hf / def2-svp	orca	total energy ha	3.79×10^{-6}
RKS/wb97x	hf / def2-tzvp	orca	total energy ha	5.05×10^{-6}
RKS/wb97x	hf / sto-3g	orca	total energy ha	2.24×10^{-6}
RKS/wb97x-v	hf / def2-svp	orca	total energy ha	4.86×10^{-6}
RKS/wb97x-v	hf / def2-tzvp	orca	total energy ha	6.04×10^{-6}
RKS/wb97x-v	hf / sto-3g	orca	total energy ha	6.87×10^{-6}
RKS/b3lyp	methyl-chloride / def2-svp	orca	total energy ha	1.41×10^{-5}
RKS/b3lyp	methyl-chloride / def2-tzvp	orca	total energy ha	2.21×10^{-5}
RKS/b3lyp	methyl-chloride / sto-3g	orca	total energy ha	4.36×10^{-6}
RKS/blyp	methyl-chloride / def2-svp	orca	total energy ha	1.95×10^{-5}
RKS/blyp	methyl-chloride / def2-tzvp	orca	total energy ha	2.85×10^{-5}
RKS/blyp	methyl-chloride / sto-3g	orca	total energy ha	3.96×10^{-6}
RKS/lda	methyl-chloride / def2-svp	orca	total energy ha	5.47×10^{-6}
RKS/lda	methyl-chloride / def2-tzvp	orca	total energy ha	2.19×10^{-5}
RKS/lda	methyl-chloride / sto-3g	orca	total energy ha	7.68×10^{-6}
RKS/pbe0	methyl-chloride / def2-svp	orca	total energy ha	4.95×10^{-5}
RKS/pbe0	methyl-chloride / sto-3g	orca	total energy ha	2.81×10^{-5}

Table S21, continued.

Method	System / basis	Ref.	Quantity	$\lvert\Delta\rvert$
RKS/pbe	methyl-chloride / sto-3g	orca	total energy ha	3.92×10^{-5}
RKS/r2scan	methyl-chloride / def2-svp	orca	total energy ha	1.31×10^{-5}
RKS/r2scan	methyl-chloride / def2-tzvp	orca	total energy ha	2.89×10^{-5}
RKS/tpss	methyl-chloride / def2-svp	orca	total energy ha	4.39×10^{-5}
RKS/tpss	methyl-chloride / def2-tzvp	orca	total energy ha	3.70×10^{-5}
RKS/tpss	methyl-chloride / sto-3g	orca	total energy ha	7.91×10^{-6}
RKS/wb97m-v	methyl-chloride / def2-svp	orca	total energy ha	5.26×10^{-6}
RKS/wb97m-v	methyl-chloride / def2-tzvp	orca	total energy ha	9.46×10^{-6}
RKS/wb97m-v	methyl-chloride / sto-3g	orca	total energy ha	1.35×10^{-5}
RKS/wb97x	methyl-chloride / def2-svp	orca	total energy ha	2.32×10^{-5}
RKS/wb97x	methyl-chloride / def2-tzvp	orca	total energy ha	8.73×10^{-6}
RKS/wb97x	methyl-chloride / sto-3g	orca	total energy ha	3.99×10^{-5}
RKS/wb97x-v	methyl-chloride / def2-svp	orca	total energy ha	2.38×10^{-5}
RKS/wb97x-v	methyl-chloride / def2-tzvp	orca	total energy ha	1.87×10^{-5}
RKS/wb97x-v	methyl-chloride / sto-3g	orca	total energy ha	1.87×10^{-5}
RKS/b3lyp	nh3 / def2-svp	orca	total energy ha	9.47×10^{-8}
RKS/b3lyp	nh3 / def2-tzvp	orca	total energy ha	3.92×10^{-6}
RKS/b3lyp	nh3 / sto-3g	orca	total energy ha	3.07×10^{-7}
RKS/blyp	nh3 / def2-svp	orca	total energy ha	1.81×10^{-7}
RKS/blyp	nh3 / def2-tzvp	orca	total energy ha	5.04×10^{-6}
RKS/blyp	nh3 / sto-3g	orca	total energy ha	1.64×10^{-7}
RKS/lda	nh3 / def2-svp	orca	total energy ha	3.42×10^{-7}
RKS/lda	nh3 / def2-tzvp	orca	total energy ha	4.26×10^{-6}
RKS/lda	nh3 / sto-3g	orca	total energy ha	6.81×10^{-7}
RKS/pbe0	nh3 / def2-svp	orca	total energy ha	8.92×10^{-6}
RKS/pbe0	nh3 / def2-tzvp	orca	total energy ha	1.27×10^{-5}
RKS/pbe0	nh3 / sto-3g	orca	total energy ha	8.51×10^{-6}
RKS/pbe	nh3 / def2-svp	orca	total energy ha	1.18×10^{-5}
RKS/pbe	nh3 / def2-tzvp	orca	total energy ha	1.73×10^{-5}
RKS/pbe	nh3 / sto-3g	orca	total energy ha	1.13×10^{-5}
RKS/r2scan	nh3 / def2-svp	orca	total energy ha	4.49×10^{-5}
RKS/r2scan	nh3 / def2-tzvp	orca	total energy ha	3.98×10^{-5}
RKS/r2scan	nh3 / sto-3g	orca	total energy ha	4.96×10^{-6}
RKS/tpss	nh3 / def2-svp	orca	total energy ha	5.02×10^{-6}
RKS/tpss	nh3 / def2-tzvp	orca	total energy ha	6.23×10^{-7}
RKS/tpss	nh3 / sto-3g	orca	total energy ha	3.07×10^{-6}
RKS/wb97m-v	nh3 / def2-svp	orca	total energy ha	1.44×10^{-6}
RKS/wb97m-v	nh3 / def2-tzvp	orca	total energy ha	2.54×10^{-6}
RKS/wb97m-v	nh3 / sto-3g	orca	total energy ha	6.71×10^{-7}
RKS/wb97x	nh3 / def2-svp	orca	total energy ha	1.06×10^{-5}
RKS/wb97x	nh3 / def2-tzvp	orca	total energy ha	8.85×10^{-6}
RKS/wb97x	nh3 / sto-3g	orca	total energy ha	1.28×10^{-5}
RKS/wb97x-v	nh3 / def2-svp	orca	total energy ha	4.62×10^{-6}
RKS/wb97x-v	nh3 / def2-tzvp	orca	total energy ha	4.04×10^{-6}
RKS/wb97x-v	nh3 / sto-3g	orca	total energy ha	3.26×10^{-6}
RKS/lda	h2o / def2-svp	orca	total energy ha	3.42×10^{-8}
RKS/wb97x	h2o / def2-svp	orca	total energy ha	2.23×10^{-6}
RKS/wb97x-v	h2o / def2-svp	orca	total energy ha	3.76×10^{-6}
RKS/wb97m-v	h2o / def2-svp	orca	total energy ha	2.47×10^{-7}
UKS/b3lyp	oh-radical / def2-svp	orca	total energy ha	held
UKS/b3lyp	oh-radical / def2-tzvp	orca	total energy ha	held
UKS/blyp	oh-radical / def2-tzvp	orca	total energy ha	held
UKS/lda	oh-radical / def2-svp	orca	total energy ha	held
UKS/lda	oh-radical / def2-tzvp	orca	total energy ha	held
UKS/lda	oh-radical / sto-3g	orca	total energy ha	held
UKS/pbe0	oh-radical / def2-svp	orca	total energy ha	held
UKS/pbe	oh-radical / def2-svp	orca	total energy ha	held
UKS/pbe	oh-radical / def2-tzvp	orca	total energy ha	held

Table S21, continued.

Method	System / basis	Ref.	Quantity	$\lvert\Delta\rvert$
UKS/r2scan	oh-radical / def2-svp	orca	total energy ha	held
UKS/r2scan	oh-radical / def2-tzvp	orca	total energy ha	held
UKS/r2scan	oh-radical / sto-3g	orca	total energy ha	held
UKS/tpss	oh-radical / sto-3g	orca	total energy ha	held
UKS/wb97m-v	oh-radical / def2-tzvp	orca	total energy ha	held
UKS/wb97x	oh-radical / def2-svp	orca	total energy ha	held
UKS/wb97x-v	oh-radical / def2-svp	orca	total energy ha	held
UKS/wb97x-v	oh-radical / def2-tzvp	orca	total energy ha	held
UKS/wb97x-v	oh-radical / sto-3g	orca	total energy ha	held
UKS/b3lyp	sh-radical / def2-svp	orca	total energy ha	held
UKS/b3lyp	sh-radical / def2-tzvp	orca	total energy ha	held
UKS/blyp	sh-radical / def2-svp	orca	total energy ha	held
UKS/blyp	sh-radical / def2-tzvp	orca	total energy ha	held
UKS/blyp	sh-radical / sto-3g	orca	total energy ha	held
UKS/pbe	sh-radical / def2-svp	orca	total energy ha	held
UKS/pbe	sh-radical / def2-tzvp	orca	total energy ha	held
UKS/pbe	sh-radical / sto-3g	orca	total energy ha	held
UKS/r2scan	sh-radical / def2-svp	orca	total energy ha	held
UKS/r2scan	sh-radical / def2-tzvp	orca	total energy ha	held
UKS/r2scan	sh-radical / sto-3g	orca	total energy ha	held
UKS/tpss	sh-radical / def2-svp	orca	total energy ha	held
UKS/tpss	sh-radical / def2-tzvp	orca	total energy ha	held
UKS/wb97x	sh-radical / def2-svp	orca	total energy ha	held
UKS/wb97x	sh-radical / def2-tzvp	orca	total energy ha	held
UKS/pbe	oh-radical / def2-svp	orca	total energy ha	held
ROKS/pbe	nh2-radical / def2-svp	orca	total energy ha	held
RKS/pbe	h2o / def2-svp	orca	total energy ha	held
RKS/r2scan	h2o / def2-svp	orca	total energy ha	held
RKS/pbe0	h2o / def2-svp	orca	total energy ha	held
RKS/UKS/pbe	bh9-03-9 / def2-qzvpp	literature	barrier height forward kcal mol	9.43×10^{-2}
RKS/UKS/pbe	bh9-03-9 / def2-qzvpp	literature	barrier height reverse kcal mol	8.25×10^{-2}
RKS/UKS/pbe	bh9-04-11 / def2-qzvpp	literature	barrier height forward kcal mol	3.39×10^{-2}
RKS/UKS/pbe	bh9-04-32 / def2-qzvpp	literature	barrier height forward kcal mol	4.24×10^{-2}
RKS/UKS/pbe	bh9-04-32 / def2-qzvpp	literature	barrier height reverse kcal mol	3.81×10^{-2}
RKS/UKS/pbe	bh9-04-33 / def2-qzvpp	literature	barrier height forward kcal mol	4.41×10^{-2}
RKS/UKS/pbe	bh9-04-33 / def2-qzvpp	literature	barrier height reverse kcal mol	4.14×10^{-2}
RKS/UKS/pbe	bh9-04-34 / def2-qzvpp	literature	barrier height forward kcal mol	4.33×10^{-2}
RKS/UKS/pbe	bh9-04-34 / def2-qzvpp	literature	barrier height reverse kcal mol	3.94×10^{-2}
RKS/pbe	bh9-08-3 / def2-qzvpp	literature	barrier height forward kcal mol	2.60×10^{-2}
RKS/b3lyp	benzene / def2-svp	orca	total energy ha	1.40×10^{-4}
RKS/b3lyp	benzene / def2-tzvp	orca	total energy ha	9.53×10^{-5}
RKS/blyp	benzene / def2-svp	orca	total energy ha	1.72×10^{-4}
RKS/blyp	benzene / def2-tzvp	orca	total energy ha	1.16×10^{-4}
RKS/blyp	benzene / sto-3g	orca	total energy ha	5.85×10^{-5}
RKS/lda	benzene / def2-svp	orca	total energy ha	1.28×10^{-4}
RKS/lda	benzene / def2-tzvp	orca	total energy ha	9.38×10^{-5}
RKS/pbe0	benzene / def2-svp	orca	total energy ha	1.44×10^{-4}
RKS/pbe0	benzene / def2-tzvp	orca	total energy ha	1.06×10^{-4}

Table S21, continued.

Method	System / basis	Ref.	Quantity	$\lvert\Delta\rvert$
RKS/pbe0	benzene / sto-3g	orca	total energy ha	5.11×10^{-5}
RKS/pbe	benzene / def2-svp	orca	total energy ha	1.97×10^{-4}
RKS/pbe	benzene / def2-tzvp	orca	total energy ha	1.52×10^{-4}
RKS/pbe	benzene / sto-3g	orca	total energy ha	8.03×10^{-5}
RKS/r2scan	benzene / def2-svp	orca	total energy ha	4.34×10^{-4}
RKS/r2scan	benzene / def2-tzvp	orca	total energy ha	3.48×10^{-4}
RKS/r2scan	benzene / sto-3g	orca	total energy ha	2.42×10^{-4}
RKS/tpss	benzene / def2-svp	orca	total energy ha	9.86×10^{-5}
RKS/wb97x	benzene / def2-svp	orca	total energy ha	7.77×10^{-5}
RKS/wb97x	benzene / def2-tzvp	orca	total energy ha	8.97×10^{-5}
RKS/pbe	c2h4 / sto-3g	orca	total energy ha	5.41×10^{-5}
RKS/r2scan	c2h4 / def2-svp	orca	total energy ha	1.35×10^{-4}
RKS/r2scan	c2h4 / def2-tzvp	orca	total energy ha	1.24×10^{-4}
RKS/r2scan	c2h4 / sto-3g	orca	total energy ha	5.71×10^{-5}
RKS/b3lyp	ch4 / def2-tzvp	orca	total energy ha	5.18×10^{-5}
RKS/b3lyp	ch4 / sto-3g	orca	total energy ha	5.94×10^{-5}
RKS/blyp	ch4 / def2-tzvp	orca	total energy ha	6.54×10^{-5}
RKS/blyp	ch4 / sto-3g	orca	total energy ha	7.22×10^{-5}
RKS/lda	ch4 / def2-svp	orca	total energy ha	5.23×10^{-5}
RKS/lda	ch4 / def2-tzvp	orca	total energy ha	6.58×10^{-5}
RKS/lda	ch4 / sto-3g	orca	total energy ha	7.29×10^{-5}
RKS/pbe	ch4 / def2-tzvp	orca	total energy ha	5.09×10^{-5}
RKS/pbe	ch4 / sto-3g	orca	total energy ha	6.29×10^{-5}
RKS/r2scan	ch4 / sto-3g	orca	total energy ha	1.23×10^{-4}
RKS/tpss	ch4 / def2-tzvp	orca	total energy ha	5.71×10^{-5}
RKS/tpss	ch4 / sto-3g	orca	total energy ha	6.94×10^{-5}
RKS/wb97x	ch4 / def2-svp	orca	total energy ha	5.04×10^{-5}
RKS/r2scan	co2 / def2-svp	orca	total energy ha	1.08×10^{-4}
RKS/r2scan	co2 / def2-tzvp	orca	total energy ha	8.40×10^{-5}
RKS/r2scan	co2 / sto-3g	orca	total energy ha	2.87×10^{-4}
RKS/blyp	ethanol / def2-svp	orca	total energy ha	5.33×10^{-5}
RKS/blyp	ethanol / def2-tzvp	orca	total energy ha	5.09×10^{-5}
RKS/blyp	ethanol / sto-3g	orca	total energy ha	5.74×10^{-5}
RKS/lda	ethanol / def2-svp	orca	total energy ha	5.36×10^{-5}
RKS/lda	ethanol / def2-tzvp	orca	total energy ha	5.04×10^{-5}
RKS/lda	ethanol / sto-3g	orca	total energy ha	5.17×10^{-5}
RKS/pbe0	ethanol / def2-svp	orca	total energy ha	6.68×10^{-5}
RKS/pbe0	ethanol / def2-tzvp	orca	total energy ha	6.26×10^{-5}
RKS/pbe0	ethanol / sto-3g	orca	total energy ha	6.33×10^{-5}
RKS/pbe	ethanol / def2-svp	orca	total energy ha	8.87×10^{-5}
RKS/pbe	ethanol / def2-tzvp	orca	total energy ha	8.36×10^{-5}
RKS/pbe	ethanol / sto-3g	orca	total energy ha	8.43×10^{-5}
RKS/r2scan	ethanol / def2-svp	orca	total energy ha	2.07×10^{-4}
RKS/r2scan	ethanol / def2-tzvp	orca	total energy ha	1.75×10^{-4}
RKS/r2scan	ethanol / sto-3g	orca	total energy ha	8.79×10^{-5}
RKS/tpss	ethanol / def2-svp	orca	total energy ha	6.04×10^{-5}
RKS/wb97x	ethanol / def2-svp	orca	total energy ha	7.28×10^{-5}
RKS/wb97x	ethanol / def2-tzvp	orca	total energy ha	7.76×10^{-5}
RKS/wb97x	ethanol / sto-3g	orca	total energy ha	6.16×10^{-5}
RKS/b3lyp	glycine / def2-tzvp	orca	total energy ha	n/a
RKS/blyp	glycine / def2-tzvp	orca	total energy ha	n/a
RKS/lda	glycine / def2-tzvp	orca	total energy ha	n/a
RKS/pbe0	glycine / def2-tzvp	orca	total energy ha	n/a
RKS/pbe0	glycine / sto-3g	orca	total energy ha	5.26×10^{-5}
RKS/pbe	glycine / def2-tzvp	orca	total energy ha	n/a
RKS/pbe	glycine / sto-3g	orca	total energy ha	7.15×10^{-5}
RKS/r2scan	glycine / def2-svp	orca	total energy ha	2.13×10^{-4}
RKS/r2scan	glycine / def2-tzvp	orca	total energy ha	n/a

Table S21, continued.

Method	System / basis	Ref.	Quantity	$\lvert\Delta\rvert$
RKS/r2scan	glycine / sto-3g	orca	total energy ha	2.80×10^{-4}
RKS/tpss	glycine / def2-tzvp	orca	total energy ha	n/a
RKS/r2scan	h2o / sto-3g	orca	total energy ha	9.46×10^{-5}
RKS/r2scan	hf / sto-3g	orca	total energy ha	1.50×10^{-4}
RKS/pbe0	methyl-chloride / def2-tzvp	orca	total energy ha	5.18×10^{-5}
RKS/pbe	methyl-chloride / def2-svp	orca	total energy ha	6.82×10^{-5}
RKS/pbe	methyl-chloride / def2-tzvp	orca	total energy ha	7.03×10^{-5}
RKS/r2scan	methyl-chloride / sto-3g	orca	total energy ha	8.15×10^{-5}
UKS/b3lyp	oh-radical / sto-3g	orca	total energy ha	n/a
UKS/blyp	oh-radical / def2-svp	orca	total energy ha	n/a
UKS/blyp	oh-radical / sto-3g	orca	total energy ha	n/a
UKS/pbe0	oh-radical / def2-tzvp	orca	total energy ha	n/a
UKS/pbe0	oh-radical / sto-3g	orca	total energy ha	n/a
UKS/pbe	oh-radical / sto-3g	orca	total energy ha	n/a
UKS/tpss	oh-radical / def2-svp	orca	total energy ha	n/a
UKS/tpss	oh-radical / def2-tzvp	orca	total energy ha	n/a
UKS/wb97m-v	oh-radical / def2-svp	orca	total energy ha	n/a
UKS/wb97m-v	oh-radical / sto-3g	orca	total energy ha	n/a
UKS/wb97x	oh-radical / def2-tzvp	orca	total energy ha	n/a
UKS/wb97x	oh-radical / sto-3g	orca	total energy ha	n/a
UKS/b3lyp	sh-radical / sto-3g	orca	total energy ha	n/a
UKS/lda	sh-radical / def2-svp	orca	total energy ha	n/a
UKS/lda	sh-radical / def2-tzvp	orca	total energy ha	n/a
UKS/lda	sh-radical / sto-3g	orca	total energy ha	n/a
UKS/pbe0	sh-radical / def2-svp	orca	total energy ha	n/a
UKS/pbe0	sh-radical / def2-tzvp	orca	total energy ha	n/a
UKS/pbe0	sh-radical / sto-3g	orca	total energy ha	n/a
UKS/tpss	sh-radical / sto-3g	orca	total energy ha	n/a
UKS/wb97m-v	sh-radical / def2-svp	orca	total energy ha	n/a
UKS/wb97m-v	sh-radical / def2-tzvp	orca	total energy ha	n/a
UKS/wb97m-v	sh-radical / sto-3g	orca	total energy ha	n/a
UKS/wb97x	sh-radical / sto-3g	orca	total energy ha	n/a
UKS/wb97x-v	sh-radical / def2-svp	orca	total energy ha	n/a
UKS/wb97x-v	sh-radical / def2-tzvp	orca	total energy ha	n/a
UKS/wb97x-v	sh-radical / sto-3g	orca	total energy ha	n/a
RKS/lda	h2o / def2-svp	orca	total energy ha	8.14×10^{-5}
RKS/lda	h2o / def2-svp	orca	total energy ha	8.14×10^{-5}
UKS/pbe	oh-radical / def2-svp	orca	total energy ha	7.87×10^{-5}
UKS/pbe	oh-radical / def2-svp	orca	total energy ha	7.87×10^{-5}
ROKS/pbe	nh2-radical / def2-svp	orca	total energy ha	1.19×10^{-4}
ROKS/pbe	nh2-radical / def2-svp	orca	total energy ha	1.19×10^{-4}
RKS/pbe	h2o / def2-svp	orca	total energy ha	9.96×10^{-5}
RKS/pbe	h2o / def2-svp	orca	total energy ha	9.96×10^{-5}
RKS/r2scan	h2o / def2-svp	orca	total energy ha	7.36×10^{-5}
RKS/r2scan	h2o / def2-svp	orca	total energy ha	7.36×10^{-5}
RKS/pbe0	h2o / def2-svp	orca	total energy ha	1.03×10^{-4}
RKS/pbe0	h2o / def2-svp	orca	total energy ha	1.03×10^{-4}
RKS/wb97x	h2o / def2-svp	orca	total energy ha	9.22×10^{-5}
RKS/wb97x	h2o / def2-svp	orca	total energy ha	9.22×10^{-5}
RKS/wb97x-v	h2o / def2-svp	orca	total energy ha	8.92×10^{-5}
RKS/wb97x-v	h2o / def2-svp	orca	total energy ha	8.92×10^{-5}
RKS/wb97m-v	h2o / def2-svp	orca	total energy ha	9.37×10^{-5}
RKS/wb97m-v	h2o / def2-svp	orca	total energy ha	9.37×10^{-5}
RKS/lda	h2o / sto-3g	orca	total energy ha	7.76×10^{-4}
UKS/pbe	oh-radical / sto-3g	orca	total energy ha	7.42×10^{-4}
ROKS/pbe	nh2-radical / sto-3g	orca	total energy ha	5.57×10^{-4}
RKS/pbe	h2o / sto-3g	orca	total energy ha	7.92×10^{-4}
RKS/r2scan	h2o / sto-3g	orca	total energy ha	1.00×10^{-3}

Table S21, continued.

Method	System / basis	Ref.	Quantity	$\lvert\Delta\rvert$
RKS/pbe0	h2o / sto-3g	orca	total energy ha	7.94×10^{-4}
RKS/wb97x	h2o / sto-3g	orca	total energy ha	7.68×10^{-4}
RKS/wb97x-v	h2o / sto-3g	orca	total energy ha	7.84×10^{-4}
RKS/wb97m-v	h2o / sto-3g	orca	total energy ha	7.81×10^{-4}
RKS/lda	h2o / def2-svp	orca	total energy ha	8.14×10^{-5}
RKS/lda	h2o / sto-3g	orca	total energy ha	7.76×10^{-4}
RKS/lda	h2o / def2-tzvp	orca	total energy ha	1.25×10^{-4}
UKS/pbe	oh-radical / def2-svp	orca	total energy ha	7.87×10^{-5}
UKS/pbe	oh-radical / sto-3g	orca	total energy ha	7.42×10^{-4}
UKS/pbe	oh-radical / def2-tzvp	orca	total energy ha	9.17×10^{-5}
ROKS/pbe	nh2-radical / def2-svp	orca	total energy ha	1.19×10^{-4}
ROKS/pbe	nh2-radical / sto-3g	orca	total energy ha	5.57×10^{-4}
ROKS/pbe	nh2-radical / def2-tzvp	orca	total energy ha	9.09×10^{-5}
RKS/pbe	h2o / def2-svp	orca	total energy ha	9.96×10^{-5}
RKS/pbe	h2o / sto-3g	orca	total energy ha	7.92×10^{-4}
RKS/pbe	h2o / def2-tzvp	orca	total energy ha	1.44×10^{-4}
RKS/r2scan	h2o / def2-svp	orca	total energy ha	7.36×10^{-5}
RKS/r2scan	h2o / sto-3g	orca	total energy ha	1.00×10^{-3}
RKS/r2scan	h2o / def2-tzvp	orca	total energy ha	1.58×10^{-4}
RKS/pbe0	h2o / def2-svp	orca	total energy ha	1.03×10^{-4}
RKS/pbe0	h2o / sto-3g	orca	total energy ha	7.94×10^{-4}
RKS/pbe0	h2o / def2-tzvp	orca	total energy ha	1.34×10^{-4}
RKS/wb97x	h2o / def2-svp	orca	total energy ha	9.22×10^{-5}
RKS/wb97x	h2o / sto-3g	orca	total energy ha	7.68×10^{-4}
RKS/wb97x	h2o / def2-tzvp	orca	total energy ha	1.38×10^{-4}
RKS/wb97x-v	h2o / def2-svp	orca	total energy ha	8.92×10^{-5}
RKS/wb97x-v	h2o / sto-3g	orca	total energy ha	7.84×10^{-4}
RKS/wb97x-v	h2o / def2-tzvp	orca	total energy ha	1.38×10^{-4}
RKS/wb97m-v	h2o / def2-svp	orca	total energy ha	9.37×10^{-5}
RKS/wb97m-v	h2o / sto-3g	orca	total energy ha	7.81×10^{-4}
RKS/wb97m-v	h2o / def2-tzvp	orca	total energy ha	1.42×10^{-4}
RKS/pbe	n-octane / def2-svp	orca	total energy ha	incomplete
RKS/b3lyp	h2o / def2-tzvp	orca	total energy ha	artifact-incomplete
RKS/pbe	h2o / def2-tzvp	orca	total energy ha	artifact-incomplete
RKS/b3lyp	ch4 / def2-tzvp	orca	total energy ha	artifact-incomplete
RKS/b3lyp	nh3 / def2-tzvp	orca	total energy ha	artifact-incomplete
UKS/b3lyp	oh-radical / def2-tzvp	orca	total energy ha	artifact-incomplete
UKS/pbe	o2-triplet / def2-tzvp	orca	total energy ha	artifact-incomplete
RKS/b3lyp	h2o-dimer / def2-tzvp	orca	total energy ha	artifact-incomplete
RKS/b3lyp	methane-dimer / def2-tzvp	orca	total energy ha	artifact-incomplete
RKS/lda	h2o / def2-svp	orca	total energy ha	artifact-incomplete
UKS/pbe	oh-radical / def2-svp	orca	total energy ha	artifact-incomplete
ROKS/pbe	nh2-radical / def2-svp	orca	total energy ha	artifact-incomplete
RKS/pbe	h2o / def2-svp	orca	total energy ha	artifact-incomplete
RKS/r2scan	h2o / def2-svp	orca	total energy ha	artifact-incomplete
RKS/pbe0	h2o / def2-svp	orca	total energy ha	artifact-incomplete
RKS/wb97x	h2o / def2-svp	orca	total energy ha	artifact-incomplete
RKS/wb97x-v	h2o / def2-svp	orca	total energy ha	artifact-incomplete
RKS/wb97m-v	h2o / def2-svp	orca	total energy ha	artifact-incomplete
RKS/lda	h2o / sto-3g	orca	total energy ha	artifact-incomplete
RKS/lda	h2o / sto-3g	orca	total energy ha	artifact-incomplete
UKS/pbe	oh-radical / sto-3g	orca	total energy ha	artifact-incomplete
UKS/pbe	oh-radical / sto-3g	orca	total energy ha	artifact-incomplete
ROKS/pbe	nh2-radical / sto-3g	orca	total energy ha	artifact-incomplete
ROKS/pbe	nh2-radical / sto-3g	orca	total energy ha	artifact-incomplete
RKS/pbe	h2o / sto-3g	orca	total energy ha	artifact-incomplete
RKS/pbe	h2o / sto-3g	orca	total energy ha	artifact-incomplete
RKS/r2scan	h2o / sto-3g	orca	total energy ha	artifact-incomplete

Table S21, continued.

Method	System / basis	Ref.	Quantity	|Δ|
RKS/r2scan	h2o / sto-3g	orca	total energy ha	artifact-incomplete
RKS/pbe0	h2o / sto-3g	orca	total energy ha	artifact-incomplete
RKS/pbe0	h2o / sto-3g	orca	total energy ha	artifact-incomplete
RKS/wb97x	h2o / sto-3g	orca	total energy ha	artifact-incomplete
RKS/wb97x	h2o / sto-3g	orca	total energy ha	artifact-incomplete
RKS/wb97x-v	h2o / sto-3g	orca	total energy ha	artifact-incomplete
RKS/wb97x-v	h2o / sto-3g	orca	total energy ha	artifact-incomplete
RKS/wb97m-v	h2o / sto-3g	orca	total energy ha	artifact-incomplete
RKS/wb97m-v	h2o / sto-3g	orca	total energy ha	artifact-incomplete
RKS/UKS/pbe	bh9-03-12 / def2-qzvpp	literature	barrier height forward kcal mol	blocked
RKS/UKS/pbe	bh9-03-12 / def2-qzvpp	literature	reaction energy kcal mol	blocked
RKS/UKS/pbe	bh9-03-15 / def2-qzvpp	literature	barrier height forward kcal mol	blocked
RKS/UKS/pbe	bh9-03-15 / def2-qzvpp	literature	reaction energy kcal mol	blocked
RKS/UKS/pbe	bh9-03-1 / def2-qzvpp	literature	barrier height forward kcal mol	blocked
RKS/UKS/pbe	bh9-03-1 / def2-qzvpp	literature	reaction energy kcal mol	blocked
RKS/UKS/pbe	bh9-03-7 / def2-qzvpp	literature	barrier height forward kcal mol	blocked
RKS/UKS/pbe	bh9-03-7 / def2-qzvpp	literature	reaction energy kcal mol	blocked
RKS/UKS/pbe	bh9-03-8 / def2-qzvpp	literature	barrier height forward kcal mol	blocked
RKS/UKS/pbe	bh9-03-8 / def2-qzvpp	literature	reaction energy kcal mol	blocked
RKS/lda	h2o / def2-svp	orca	total energy ha	blocked
UKS/pbe	oh-radical / def2-svp	orca	total energy ha	blocked
ROKS/pbe	nh2-radical / def2-svp	orca	total energy ha	blocked
RKS/pbe	h2o / def2-svp	orca	total energy ha	blocked
RKS/r2scan	h2o / def2-svp	orca	total energy ha	blocked
RKS/pbe0	h2o / def2-svp	orca	total energy ha	blocked
RKS/wb97x	h2o / def2-svp	orca	total energy ha	blocked
RKS/wb97x-v	h2o / def2-svp	orca	total energy ha	blocked
RKS/wb97m-v	h2o / def2-svp	orca	total energy ha	blocked
RKS/pbe	acetamide / sto-3g	orca	total energy ha	blocked
RKS/pbe	acetamide / cc-pvdz	orca	total energy ha	blocked
RKS/b3lyp	crambin / cc-pvtz	orca	total energy ha	blocked
RKS/pbe	cr-co6 / def2-tzvp	orca	total energy ha	blocked
RKS/pbe	cyclopentadiene / sto-3g	orca	total energy ha	blocked
RKS/b3lyp	cyclopentadiene / sto-3g	orca	total energy ha	blocked
RKS/pbe0	cytosine / sto-3g	orca	total energy ha	blocked
UKS/pbe	fecl3 / cc-pvdz	orca	total energy ha	blocked
RKS/pbe	ferrocene / def2-svp	orca	total energy ha	blocked
RKS/pbe0	ferrocene / def2-tzvp	orca	total energy ha	blocked
RKS/pbe	furan / sto-3g	orca	total energy ha	blocked
RKS/pbe	glycine / def2-tzvp	orca	total energy ha	blocked
RKS/pbe0	glycine / cc-pvdz	orca	total energy ha	blocked
RKS/b3lyp	glycine / def2-svp	orca	total energy ha	blocked
RKS/pbe0	h2 / def2-tzvp	orca	total energy ha	blocked
RKS/pbe	hexatriene / def2-svp	orca	total energy ha	blocked
RKS/pbe	hexatriene / cc-pvtz	orca	total energy ha	blocked
RKS/pbe	hexatriene / cc-pvtz	orca	total energy ha	blocked
RKS/pbe0	hexatriene / sto-3g	orca	total energy ha	blocked
RKS/pbe0	hexatriene / sto-3g	orca	total energy ha	blocked
RKS/pbe0	hexatriene / cc-pvdz	orca	total energy ha	blocked
RKS/pbe0	hexatriene / cc-pvtz	orca	total energy ha	blocked
RKS/pbe	hf / def2-svp	orca	total energy ha	blocked
RKS/pbe	hf / cc-pvtz	orca	total energy ha	blocked
RKS/pbe0	hf / def2-svp	orca	total energy ha	blocked

Table S21, continued.

Method	System / basis	Ref.	Quantity	|Δ|
RKS/pbe0	hf / cc-pvdz	orca	total energy ha	blocked
RKS/pbe0	hf / cc-pvtz	orca	total energy ha	blocked
RKS/b3lyp	hf / def2-svp	orca	total energy ha	blocked
RKS/b3lyp	hf / def2-tzvp	orca	total energy ha	blocked
RKS/b3lyp	hf / cc-pvtz	orca	total energy ha	blocked
RKS/b3lyp	hf / cc-pvtz	orca	total energy ha	blocked
RKS/wb97x	hf / sto-3g	orca	total energy ha	blocked
RKS/wb97x	hf / def2-svp	orca	total energy ha	blocked
RKS/wb97x	hf / def2-tzvp	orca	total energy ha	blocked
RKS/wb97x	hf / cc-pvdz	orca	total energy ha	blocked
RKS/wb97x	hf / cc-pvtz	orca	total energy ha	blocked
RKS/wb97x-v	hf / sto-3g	orca	total energy ha	blocked
RKS/wb97x-v	hf / def2-svp	orca	total energy ha	blocked
RKS/wb97x-v	hf / def2-tzvp	orca	total energy ha	blocked
RKS/wb97x-v	hf / cc-pvdz	orca	total energy ha	blocked
RKS/wb97x-v	hf / cc-pvtz	orca	total energy ha	blocked
RKS/wb97m-v	hf / sto-3g	orca	total energy ha	blocked
RKS/wb97m-v	hf / def2-svp	orca	total energy ha	blocked
RKS/wb97m-v	hf / def2-tzvp	orca	total energy ha	blocked
RKS/wb97m-v	hf / cc-pvdz	orca	total energy ha	blocked
RKS/wb97m-v	hf / cc-pvtz	orca	total energy ha	blocked
RKS/r2scan	hf / sto-3g	orca	total energy ha	blocked
RKS/r2scan	hf / def2-svp	orca	total energy ha	blocked
RKS/r2scan	hf / def2-tzvp	orca	total energy ha	blocked
RKS/r2scan	hf / cc-pvdz	orca	total energy ha	blocked
RKS/r2scan	hf / cc-pvtz	orca	total energy ha	blocked
RKS/tpss	hf / sto-3g	orca	total energy ha	blocked
RKS/tpss	hf / def2-svp	orca	total energy ha	blocked
RKS/tpss	hf / def2-svp	orca	total energy ha	blocked
RKS/tpss	hf / def2-tzvp	orca	total energy ha	blocked
RKS/tpss	hf / cc-pvdz	orca	total energy ha	blocked
RKS/tpss	hf / cc-pvtz	orca	total energy ha	blocked
RKS/tpss	hf / cc-pvtz	orca	total energy ha	blocked
RKS/pbe	imidazole / sto-3g	orca	total energy ha	blocked
RKS/pbe	imidazole / def2-svp	orca	total energy ha	blocked
RKS/pbe	imidazole / def2-tzvp	orca	total energy ha	blocked
RKS/pbe	imidazole / cc-pvdz	orca	total energy ha	blocked
RKS/pbe	imidazole / cc-pvdz	orca	total energy ha	blocked
RKS/pbe	imidazole / cc-pvtz	orca	total energy ha	blocked
RKS/pbe	imidazole / cc-pvtz	orca	total energy ha	blocked
RKS/pbe0	imidazole / sto-3g	orca	total energy ha	blocked
RKS/pbe0	imidazole / def2-svp	orca	total energy ha	blocked
RKS/pbe0	imidazole / def2-tzvp	orca	total energy ha	blocked
RKS/pbe0	imidazole / cc-pvdz	orca	total energy ha	blocked
RKS/pbe0	imidazole / cc-pvdz	orca	total energy ha	blocked
RKS/pbe0	imidazole / cc-pvtz	orca	total energy ha	blocked
RKS/b3lyp	imidazole / sto-3g	orca	total energy ha	blocked
RKS/b3lyp	imidazole / def2-svp	orca	total energy ha	blocked
RKS/b3lyp	imidazole / def2-tzvp	orca	total energy ha	blocked
RKS/b3lyp	imidazole / cc-pvdz	orca	total energy ha	blocked
RKS/b3lyp	imidazole / cc-pvtz	orca	total energy ha	blocked
RKS/pbe	lih / sto-3g	orca	total energy ha	blocked
RKS/pbe	lih / sto-3g	orca	total energy ha	blocked
RKS/pbe	lih / cc-pvdz	orca	total energy ha	blocked
RKS/pbe0	lih / sto-3g	orca	total energy ha	blocked
RKS/pbe0	lih / def2-tzvp	orca	total energy ha	blocked
RKS/pbe0	lih / cc-pvqz	orca	total energy ha	blocked
RKS/pbe0	lih / cc-pvqz	orca	total energy ha	blocked

Table S21, continued.

Method	System / basis	Ref.	Quantity	|Δ|
RKS/b3lyp	lih / def2-svp	orca	total energy ha	blocked
RKS/b3lyp	lih / def2-tzvp	orca	total energy ha	blocked
RKS/b3lyp	lih / def2-tzvp	orca	total energy ha	blocked
RKS/b3lyp	lih / cc-pvdz	orca	total energy ha	blocked
RKS/b3lyp	lih / cc-pvtz	orca	total energy ha	blocked
RKS/wb97x	lih / sto-3g	orca	total energy ha	blocked
RKS/wb97x	lih / def2-svp	orca	total energy ha	blocked
RKS/wb97x	lih / def2-tzvp	orca	total energy ha	blocked
RKS/wb97x	lih / cc-pvdz	orca	total energy ha	blocked
RKS/wb97x	lih / cc-pvtz	orca	total energy ha	blocked
RKS/wb97x-v	lih / sto-3g	orca	total energy ha	blocked
RKS/wb97x-v	lih / def2-svp	orca	total energy ha	blocked
RKS/wb97x-v	lih / def2-svp	orca	total energy ha	blocked
RKS/wb97x-v	lih / def2-tzvp	orca	total energy ha	blocked
RKS/wb97x-v	lih / cc-pvdz	orca	total energy ha	blocked
RKS/wb97x-v	lih / cc-pvtz	orca	total energy ha	blocked
RKS/wb97m-v	lih / sto-3g	orca	total energy ha	blocked
RKS/wb97m-v	lih / def2-svp	orca	total energy ha	blocked
RKS/wb97m-v	lih / def2-tzvp	orca	total energy ha	blocked
RKS/wb97m-v	lih / cc-pvdz	orca	total energy ha	blocked
RKS/wb97m-v	lih / cc-pvtz	orca	total energy ha	blocked
RKS/r2scan	lih / sto-3g	orca	total energy ha	blocked
RKS/r2scan	lih / def2-svp	orca	total energy ha	blocked
RKS/r2scan	lih / def2-tzvp	orca	total energy ha	blocked
RKS/r2scan	lih / cc-pvdz	orca	total energy ha	blocked
RKS/r2scan	lih / cc-pvtz	orca	total energy ha	blocked
RKS/tpss	lih / sto-3g	orca	total energy ha	blocked
RKS/tpss	lih / def2-svp	orca	total energy ha	blocked
RKS/tpss	lih / def2-tzvp	orca	total energy ha	blocked
RKS/tpss	lih / cc-pvdz	orca	total energy ha	blocked
RKS/tpss	lih / cc-pvtz	orca	total energy ha	blocked
RKS/pbe	n2 / sto-3g	orca	total energy ha	blocked
RKS/wb97x-v	n2 / def2-tzvp	orca	total energy ha	blocked
RKS/wb97x-v	n2 / cc-pvdz	orca	total energy ha	blocked
RKS/r2scan	n2 / def2-tzvp	orca	total energy ha	blocked
RKS/b3lyp	naphthalene / sto-3g	orca	total energy ha	blocked
RKS/b3lyp	naphthalene / def2-tzvp	orca	total energy ha	blocked
RKS/wb97m-v	nh3 / sto-3g	orca	total energy ha	blocked
RKS/r2scan	nh3 / cc-pvdz	orca	total energy ha	blocked
RKS/pbe	ni-co4 / def2-svp	orca	total energy ha	blocked
RKS/pbe0	nitromethane / cc-pvdz	orca	total energy ha	blocked
RKS/wb97m-v	nitromethane / def2-svp	orca	total energy ha	blocked
RKS/wb97m-v	nitromethane / cc-pvtz	orca	total energy ha	blocked
RKS/pbe	norbornadiene / sto-3g	orca	total energy ha	blocked
RKS/pbe0	norbornadiene / def2-tzvp	orca	total energy ha	blocked
RKS/b3lyp	norbornadiene / cc-pvtz	orca	total energy ha	blocked
RKS/pbe0	p-benzoquinone / cc-pvtz	orca	total energy ha	blocked
RKS/b3lyp	p-benzoquinone / cc-pvdz	orca	total energy ha	blocked
RKS/pbe0	phenol / sto-3g	orca	total energy ha	blocked
RKS/b3lyp	phenol / def2-tzvp	orca	total energy ha	blocked
RKS/b3lyp	propanamide / def2-tzvp	orca	total energy ha	blocked
RKS/b3lyp	propanamide / cc-pvdz	orca	total energy ha	blocked
RKS/b3lyp	pyridazine / def2-tzvp	orca	total energy ha	blocked
RKS/b3lyp	pyridazine / cc-pvdz	orca	total energy ha	blocked
RKS/pbe0	pyridine / cc-pvtz	orca	total energy ha	blocked
RKS/b3lyp	pyridine / cc-pvtz	orca	total energy ha	blocked
RKS/pbe0	pyrimidine / def2-svp	orca	total energy ha	blocked
RKS/pbe0	pyrimidine / def2-tzvp	orca	total energy ha	blocked

Table S21, continued.

Method	System / basis	Ref.	Quantity	$\lvert\Delta\rvert$
RKS/pbe	pyrrole / def2-tzvp	orca	total energy ha	blocked
RKS/pbe	pyrrole / cc-pvdz	orca	total energy ha	blocked
RKS/pbe	pyrrole / cc-pvtz	orca	total energy ha	blocked
RKS/b3lyp	pyrrole / cc-pvtz	orca	total energy ha	blocked
RKS/wb97x	s22-ammonia-dimer / sto-3g	orca	total energy ha	blocked
RKS/wb97x	s22-ammonia-dimer / def2-tzvp	orca	total energy ha	blocked
RKS/wb97x	s22-ammonia-dimer / cc-pvdz	orca	total energy ha	blocked
RKS/pbe0	s22-benzene-methane / cc-pvdz	orca	total energy ha	blocked
RKS/b3lyp	s22-benzene-methane / sto-3g	orca	total energy ha	blocked
RKS/tpss	s22-water-dimer / def2-tzvp	orca	total energy ha	blocked
RKS/b3lyp	tetrazine / def2-svp	orca	total energy ha	blocked
RKS/b3lyp	tetrazine / cc-pvdz	orca	total energy ha	blocked
RKS/wb97x	tetrazine / cc-pvtz	orca	total energy ha	blocked
RKS/wb97x-v	tetrazine / def2-svp	orca	total energy ha	blocked
RKS/pbe0	thymine / cc-pvdz	orca	total energy ha	blocked
RKS/b3lyp	thymine / cc-pvdz	orca	total energy ha	blocked
RKS/b3lyp	triazine / def2-svp	orca	total energy ha	blocked
RKS/pbe	uracil / def2-tzvp	orca	total energy ha	blocked
RKS/pbe0	uracil / cc-pvdz	orca	total energy ha	blocked
RKS/pbe0	urea / cc-pvtz	orca	total energy ha	blocked
RKS/b3lyp	urea / def2-tzvp	orca	total energy ha	blocked
RKS/wb97m-v	urea / cc-pvdz	orca	total energy ha	blocked
RKS/wb97x	glycine / def2-svp	orca	total energy ha	queued
Noncovalent DFT				
85 pass, 528 held, 3 fail, 2 incomplete, 44 artifact-incomplete, 22 queued. Median $\lvert\Delta E\rvert$ 2.5×10^{-4}, max 9.4×10^{-4} E_h.				
RKS/pbe	s22-01-ammonia-dimer / def2-svp	orca	interaction energy kcal mol	6.45×10^{-6}
RKS/pbe	s22-01-ammonia-dimer / def2-svp	orca	total energy ha	3.55×10^{-4}
RKS/pbe	s22-01-ammonia-dimer / def2-svp	orca	total energy ha	1.81×10^{-4}
RKS/pbe	s22-01-ammonia-dimer / def2-svp	orca	total energy ha	1.81×10^{-4}
RKS/pbe	s22-02-water-dimer / def2-svp	orca	interaction energy kcal mol	7.64×10^{-6}
RKS/pbe	s22-02-water-dimer / def2-svp	orca	total energy ha	2.04×10^{-4}
RKS/pbe	s22-02-water-dimer / def2-svp	orca	total energy ha	1.06×10^{-4}
RKS/pbe	s22-02-water-dimer / def2-svp	orca	total energy ha	1.06×10^{-4}
RKS/pbe	s22-03-formic-acid-dimer / def2-svp	orca	interaction energy kcal mol	2.20×10^{-5}
RKS/pbe	s22-03-formic-acid-dimer / def2-svp	orca	total energy ha	3.74×10^{-4}
RKS/pbe	s22-03-formic-acid-dimer / def2-svp	orca	total energy ha	1.98×10^{-4}
RKS/pbe	s22-03-formic-acid-dimer / def2-svp	orca	total energy ha	1.98×10^{-4}
RKS/pbe	s22-04-formamide-dimer / def2-svp	orca	interaction energy kcal mol	6.82×10^{-5}
RKS/pbe	s22-04-formamide-dimer / def2-svp	orca	total energy ha	4.30×10^{-4}
RKS/pbe	s22-04-formamide-dimer / def2-svp	orca	total energy ha	2.49×10^{-4}
RKS/pbe	s22-04-formamide-dimer / def2-svp	orca	total energy ha	2.49×10^{-4}
RKS/pbe	s22-05-uracil-dimer-hb / def2-svp	orca	interaction energy kcal mol	6.79×10^{-5}
RKS/pbe	s22-05-uracil-dimer-hb / def2-svp	orca	total energy ha	9.38×10^{-4}
RKS/pbe	s22-05-uracil-dimer-hb / def2-svp	orca	total energy ha	5.03×10^{-4}
RKS/pbe	s22-05-uracil-dimer-hb / def2-svp	orca	total energy ha	5.03×10^{-4}
RKS/pbe	s22-06-2-pyridone-2-aminopyridine / def2-svp	orca	interaction energy kcal mol	5.78×10^{-5}
RKS/pbe	s22-06-2-pyridone-2-aminopyridine / def2-svp	orca	total energy ha	7.32×10^{-4}
RKS/pbe	s22-06-2-pyridone-2-aminopyridine / def2-svp	orca	total energy ha	3.80×10^{-4}
RKS/pbe	s22-06-2-pyridone-2-aminopyridine / def2-svp	orca	total energy ha	4.10×10^{-4}
RKS/pbe	s22-07-adenine-thymine-wc / def2-svp	orca	interaction energy kcal mol	7.47×10^{-5}
RKS/pbe	s22-07-adenine-thymine-wc / def2-svp	orca	total energy ha	5.94×10^{-4}

Table S21, continued.

Method	System / basis	Ref.	Quantity	$\lvert\Delta\rvert$
RKS/pbe	s22-07-adenine-thymine-wc / def2-svp	orca	total energy ha	5.77×10^{-4}
RKS/pbe	s22-08-methane-dimer / def2-svp	orca	interaction energy kcal mol	7.46×10^{-6}
RKS/pbe	s22-08-methane-dimer / def2-svp	orca	total energy ha	2.22×10^{-4}
RKS/pbe	s22-08-methane-dimer / def2-svp	orca	total energy ha	1.07×10^{-4}
RKS/pbe	s22-08-methane-dimer / def2-svp	orca	total energy ha	1.07×10^{-4}
RKS/pbe	s22-09-ethene-dimer / def2-svp	orca	interaction energy kcal mol	2.72×10^{-5}
RKS/pbe	s22-09-ethene-dimer / def2-svp	orca	total energy ha	2.84×10^{-4}
RKS/pbe	s22-09-ethene-dimer / def2-svp	orca	total energy ha	1.28×10^{-4}
RKS/pbe	s22-09-ethene-dimer / def2-svp	orca	total energy ha	1.28×10^{-4}
RKS/pbe	s22-10-benzene-ch4 / def2-svp	orca	interaction energy kcal mol	1.66×10^{-5}
RKS/pbe	s22-10-benzene-ch4 / def2-svp	orca	total energy ha	3.86×10^{-4}
RKS/pbe	s22-10-benzene-ch4 / def2-svp	orca	total energy ha	2.94×10^{-4}
RKS/pbe	s22-10-benzene-ch4 / def2-svp	orca	total energy ha	1.08×10^{-4}
RKS/pbe	s22-11-benzene-dimer-stack / def2-svp	orca	interaction energy kcal mol	1.27×10^{-5}
RKS/pbe	s22-11-benzene-dimer-stack / def2-svp	orca	total energy ha	5.67×10^{-4}
RKS/pbe	s22-11-benzene-dimer-stack / def2-svp	orca	total energy ha	2.90×10^{-4}
RKS/pbe	s22-11-benzene-dimer-stack / def2-svp	orca	total energy ha	2.90×10^{-4}
RKS/pbe	s22-12-pyrazine-dimer / def2-svp	orca	interaction energy kcal mol	1.74×10^{-6}
RKS/pbe	s22-12-pyrazine-dimer / def2-svp	orca	total energy ha	6.52×10^{-4}
RKS/pbe	s22-12-pyrazine-dimer / def2-svp	orca	total energy ha	3.30×10^{-4}
RKS/pbe	s22-12-pyrazine-dimer / def2-svp	orca	total energy ha	3.23×10^{-4}
RKS/pbe	s22-13-uracil-dimer-stack / def2-svp	orca	interaction energy kcal mol	1.54×10^{-5}
RKS/pbe	s22-13-uracil-dimer-stack / def2-svp	orca	total energy ha	5.00×10^{-4}
RKS/pbe	s22-13-uracil-dimer-stack / def2-svp	orca	total energy ha	5.00×10^{-4}
RKS/pbe	s22-14-indole-benzene-stack / def2-svp	orca	interaction energy kcal mol	1.45×10^{-5}
RKS/pbe	s22-14-indole-benzene-stack / def2-svp	orca	total energy ha	7.36×10^{-4}
RKS/pbe	s22-14-indole-benzene-stack / def2-svp	orca	total energy ha	3.01×10^{-4}
RKS/pbe	s22-14-indole-benzene-stack / def2-svp	orca	total energy ha	4.20×10^{-4}
RKS/pbe	s22-15-adenine-thymine-stack / def2-svp	orca	interaction energy kcal mol	3.48×10^{-5}
RKS/pbe	s22-15-adenine-thymine-stack / def2-svp	orca	total energy ha	5.89×10^{-4}
RKS/pbe	s22-15-adenine-thymine-stack / def2-svp	orca	total energy ha	5.76×10^{-4}
RKS/pbe	s22-16-ethene-ethyne / def2-svp	orca	interaction energy kcal mol	7.15×10^{-7}
RKS/pbe	s22-16-ethene-ethyne / def2-svp	orca	total energy ha	1.92×10^{-4}
RKS/pbe	s22-16-ethene-ethyne / def2-svp	orca	total energy ha	1.28×10^{-4}
RKS/pbe	s22-16-ethene-ethyne / def2-svp	orca	total energy ha	6.28×10^{-5}
RKS/pbe	s22-17-benzene-h2o / def2-svp	orca	interaction energy kcal mol	1.72×10^{-5}
RKS/pbe	s22-17-benzene-h2o / def2-svp	orca	total energy ha	3.71×10^{-4}
RKS/pbe	s22-17-benzene-h2o / def2-svp	orca	total energy ha	2.83×10^{-4}
RKS/pbe	s22-17-benzene-h2o / def2-svp	orca	total energy ha	1.05×10^{-4}
RKS/pbe	s22-18-benzene-nh3 / def2-svp	orca	interaction energy kcal mol	1.81×10^{-5}
RKS/pbe	s22-18-benzene-nh3 / def2-svp	orca	total energy ha	4.43×10^{-4}
RKS/pbe	s22-18-benzene-nh3 / def2-svp	orca	total energy ha	2.83×10^{-4}
RKS/pbe	s22-18-benzene-nh3 / def2-svp	orca	total energy ha	1.78×10^{-4}
RKS/pbe	s22-19-benzene-hcn / def2-svp	orca	interaction energy kcal mol	4.33×10^{-6}
RKS/pbe	s22-19-benzene-hcn / def2-svp	orca	total energy ha	3.55×10^{-4}
RKS/pbe	s22-19-benzene-hcn / def2-svp	orca	total energy ha	2.92×10^{-4}

Table S21, continued.

Method	System / basis	Ref.	Quantity	$\lvert\Delta\rvert$
RKS/pbe	s22-19-benzene-hcn / def2-svp	orca	total energy ha	6.73×10^{-5}
RKS/pbe	s22-20-benzene-dimer-t / def2-svp	orca	interaction energy kcal mol	1.25×10^{-5}
RKS/pbe	s22-20-benzene-dimer-t / def2-svp	orca	total energy ha	5.77×10^{-4}
RKS/pbe	s22-20-benzene-dimer-t / def2-svp	orca	total energy ha	3.04×10^{-4}
RKS/pbe	s22-20-benzene-dimer-t / def2-svp	orca	total energy ha	2.85×10^{-4}
RKS/pbe	s22-21-indole-benzene-t / def2-svp	orca	interaction energy kcal mol	4.27×10^{-5}
RKS/pbe	s22-21-indole-benzene-t / def2-svp	orca	total energy ha	6.68×10^{-4}
RKS/pbe	s22-21-indole-benzene-t / def2-svp	orca	total energy ha	2.89×10^{-4}
RKS/pbe	s22-21-indole-benzene-t / def2-svp	orca	total energy ha	4.22×10^{-4}
RKS/pbe	s22-22-phenol-dimer / def2-svp	orca	interaction energy kcal mol	2.43×10^{-5}
RKS/pbe	s22-22-phenol-dimer / def2-svp	orca	total energy ha	6.84×10^{-4}
RKS/pbe	s22-22-phenol-dimer / def2-svp	orca	total energy ha	3.64×10^{-4}
RKS/pbe	s22-22-phenol-dimer / def2-svp	orca	total energy ha	3.45×10^{-4}
RKS/pbe	s66x8-01-water-water-0.90re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-01-water-water-0.95re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-01-water-water-1.00re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-01-water-water-1.05re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-01-water-water-1.10re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-01-water-water-1.25re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-01-water-water-1.50re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-01-water-water-2.00re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-02-water-meoh-0.90re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-02-water-meoh-0.95re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-02-water-meoh-1.00re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-02-water-meoh-1.05re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-02-water-meoh-1.10re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-02-water-meoh-1.25re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-02-water-meoh-1.50re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-02-water-meoh-2.00re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-03-water-menh2-0.90re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-03-water-menh2-0.95re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-03-water-menh2-1.00re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-03-water-menh2-1.05re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-03-water-menh2-1.10re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-03-water-menh2-1.25re / def2-svp	literature	interaction energy kcal mol	held

Table S21, continued.

Method	System / basis	Ref.	Quantity	|Δ|
RKS/pbe	s66x8-03-water-menh2-1.50re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-03-water-menh2-2.00re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-04-water-peptide-0.90re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-04-water-peptide-0.95re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-04-water-peptide-1.00re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-04-water-peptide-1.05re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-04-water-peptide-1.10re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-04-water-peptide-1.25re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-04-water-peptide-1.50re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-04-water-peptide-2.00re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-05-meoh-meoh-0.90re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-05-meoh-meoh-0.95re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-05-meoh-meoh-1.00re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-05-meoh-meoh-1.05re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-05-meoh-meoh-1.10re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-05-meoh-meoh-1.25re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-05-meoh-meoh-1.50re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-05-meoh-meoh-2.00re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-06-meoh-menh2-0.90re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-06-meoh-menh2-0.95re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-06-meoh-menh2-1.00re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-06-meoh-menh2-1.05re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-06-meoh-menh2-1.10re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-06-meoh-menh2-1.25re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-06-meoh-menh2-1.50re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-06-meoh-menh2-2.00re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-07-meoh-peptide-0.90re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-07-meoh-peptide-0.95re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-07-meoh-peptide-1.00re / def2-svp	literature	interaction energy kcal mol	held

Table S21, continued.

Method	System / basis	Ref.	Quantity	|Δ|
RKS/pbe	s66x8-07-meoh-peptide-1.05re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-07-meoh-peptide-1.10re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-07-meoh-peptide-1.25re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-07-meoh-peptide-1.50re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-07-meoh-peptide-2.00re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-08-meoh-water-0.90re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-08-meoh-water-0.95re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-08-meoh-water-1.00re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-08-meoh-water-1.05re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-08-meoh-water-1.10re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-08-meoh-water-1.25re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-08-meoh-water-1.50re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-08-meoh-water-2.00re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-09-menh2-meoh-0.90re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-09-menh2-meoh-0.95re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-09-menh2-meoh-1.00re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-09-menh2-meoh-1.05re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-09-menh2-meoh-1.10re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-09-menh2-meoh-1.25re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-09-menh2-meoh-1.50re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-09-menh2-meoh-2.00re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-10-menh2-menh2-0.90re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-10-menh2-menh2-0.95re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-10-menh2-menh2-1.00re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-10-menh2-menh2-1.05re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-10-menh2-menh2-1.10re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-10-menh2-menh2-1.25re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-10-menh2-menh2-1.50re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-10-menh2-menh2-2.00re / def2-svp	literature	interaction energy kcal mol	held

Table S21, continued.

Method	System / basis	Ref.	Quantity	|Δ|
RKS/pbe	s66x8-11-menh2-peptide-0.90re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-11-menh2-peptide-0.95re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-11-menh2-peptide-1.00re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-11-menh2-peptide-1.05re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-11-menh2-peptide-1.10re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-11-menh2-peptide-1.25re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-11-menh2-peptide-1.50re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-11-menh2-peptide-2.00re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-12-menh2-water-0.90re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-12-menh2-water-0.95re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-12-menh2-water-1.00re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-12-menh2-water-1.05re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-12-menh2-water-1.10re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-12-menh2-water-1.25re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-12-menh2-water-1.50re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-12-menh2-water-2.00re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-13-peptide-meoh-0.90re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-13-peptide-meoh-0.95re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-13-peptide-meoh-1.00re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-13-peptide-meoh-1.05re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-13-peptide-meoh-1.10re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-13-peptide-meoh-1.25re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-13-peptide-meoh-1.50re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-13-peptide-meoh-2.00re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-14-peptide-menh2-0.90re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-14-peptide-menh2-0.95re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-14-peptide-menh2-1.00re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-14-peptide-menh2-1.05re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-14-peptide-menh2-1.10re / def2-svp	literature	interaction energy kcal mol	held

Table S21, continued.

Method	System / basis	Ref.	Quantity	|Δ|
RKS/pbe	s66x8-14-peptide-menh2-1.25re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-14-peptide-menh2-1.50re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-14-peptide-menh2-2.00re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-15-peptide-peptide-0.90re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-15-peptide-peptide-0.95re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-15-peptide-peptide-1.00re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-15-peptide-peptide-1.05re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-15-peptide-peptide-1.10re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-15-peptide-peptide-1.25re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-15-peptide-peptide-1.50re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-15-peptide-peptide-2.00re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-16-peptide-water-0.90re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-16-peptide-water-0.95re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-16-peptide-water-1.00re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-16-peptide-water-1.05re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-16-peptide-water-1.10re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-16-peptide-water-1.25re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-16-peptide-water-1.50re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-16-peptide-water-2.00re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-17-uracil-uracil-bp-0.90re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-17-uracil-uracil-bp-0.95re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-17-uracil-uracil-bp-1.00re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-17-uracil-uracil-bp-1.05re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-17-uracil-uracil-bp-1.10re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-17-uracil-uracil-bp-1.25re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-17-uracil-uracil-bp-1.50re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-17-uracil-uracil-bp-2.00re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-18-water-pyridine-0.90re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-18-water-pyridine-0.95re / def2-svp	literature	interaction energy kcal mol	held

Table S21, continued.

Method	System / basis	Ref.	Quantity	|Δ|
RKS/pbe	s66x8-18-water-pyridine-1.00re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-18-water-pyridine-1.05re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-18-water-pyridine-1.10re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-18-water-pyridine-1.25re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-18-water-pyridine-1.50re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-18-water-pyridine-2.00re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-19-meoh-pyridine-0.90re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-19-meoh-pyridine-0.95re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-19-meoh-pyridine-1.00re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-19-meoh-pyridine-1.05re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-19-meoh-pyridine-1.10re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-19-meoh-pyridine-1.25re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-19-meoh-pyridine-1.50re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-19-meoh-pyridine-2.00re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-20-acoh-acoh-0.90re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-20-acoh-acoh-0.95re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-20-acoh-acoh-1.00re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-20-acoh-acoh-1.05re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-20-acoh-acoh-1.10re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-20-acoh-acoh-1.25re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-20-acoh-acoh-1.50re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-20-acoh-acoh-2.00re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-21-acnh2-acnh2-0.90re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-21-acnh2-acnh2-0.95re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-21-acnh2-acnh2-1.00re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-21-acnh2-acnh2-1.05re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-21-acnh2-acnh2-1.10re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-21-acnh2-acnh2-1.25re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-21-acnh2-acnh2-1.50re / def2-svp	literature	interaction energy kcal mol	held

Table S21, continued.

Method	System / basis	Ref.	Quantity	|Δ|
RKS/pbe	s66x8-21-acnh2-acnh2-2.00re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-22-acoh-uracil-0.90re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-22-acoh-uracil-0.95re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-22-acoh-uracil-1.00re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-22-acoh-uracil-1.05re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-22-acoh-uracil-1.10re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-22-acoh-uracil-1.25re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-22-acoh-uracil-1.50re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-22-acoh-uracil-2.00re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-23-acnh2-uracil-0.90re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-23-acnh2-uracil-0.95re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-23-acnh2-uracil-1.00re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-23-acnh2-uracil-1.05re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-23-acnh2-uracil-1.10re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-23-acnh2-uracil-1.25re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-23-acnh2-uracil-1.50re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-23-acnh2-uracil-2.00re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-24-benzene-benzene-0.90re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-24-benzene-benzene-0.95re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-24-benzene-benzene-1.00re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-24-benzene-benzene-1.05re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-24-benzene-benzene-1.10re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-24-benzene-benzene-1.25re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-24-benzene-benzene-1.50re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-24-benzene-benzene-2.00re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-25-pyridine-pyridine-0.90re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-25-pyridine-pyridine-0.95re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-25-pyridine-pyridine-1.00re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-25-pyridine-pyridine-1.05re / def2-svp	literature	interaction energy kcal mol	held

Table S21, continued.

Method	System / basis	Ref.	Quantity	|Δ|
RKS/pbe	s66x8-25-pyridine-pyridine-1.10re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-25-pyridine-pyridine-1.25re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-25-pyridine-pyridine-1.50re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-25-pyridine-pyridine-2.00re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-26-uracil-uracil-0.90re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-26-uracil-uracil-0.95re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-26-uracil-uracil-1.00re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-26-uracil-uracil-1.05re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-26-uracil-uracil-1.10re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-26-uracil-uracil-1.25re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-26-uracil-uracil-1.50re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-26-uracil-uracil-2.00re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-27-benzene-pyridine-0.90re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-27-benzene-pyridine-0.95re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-27-benzene-pyridine-1.00re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-27-benzene-pyridine-1.05re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-27-benzene-pyridine-1.10re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-27-benzene-pyridine-1.25re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-27-benzene-pyridine-1.50re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-27-benzene-pyridine-2.00re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-28-benzene-uracil-0.90re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-28-benzene-uracil-0.95re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-28-benzene-uracil-1.00re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-28-benzene-uracil-1.05re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-28-benzene-uracil-1.10re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-28-benzene-uracil-1.25re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-28-benzene-uracil-1.50re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-28-benzene-uracil-2.00re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-29-pyridine-uracil-0.90re / def2-svp	literature	interaction energy kcal mol	held

Table S21, continued.

Method	System / basis	Ref.	Quantity	|Δ|
RKS/pbe	s66x8-29-pyridine-uracil-0.95re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-29-pyridine-uracil-1.00re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-29-pyridine-uracil-1.05re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-29-pyridine-uracil-1.10re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-29-pyridine-uracil-1.25re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-29-pyridine-uracil-1.50re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-29-pyridine-uracil-2.00re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-30-benzene-ethene-0.90re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-30-benzene-ethene-0.95re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-30-benzene-ethene-1.00re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-30-benzene-ethene-1.05re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-30-benzene-ethene-1.10re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-30-benzene-ethene-1.25re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-30-benzene-ethene-1.50re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-30-benzene-ethene-2.00re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-31-uracil-ethene-0.90re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-31-uracil-ethene-0.95re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-31-uracil-ethene-1.00re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-31-uracil-ethene-1.05re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-31-uracil-ethene-1.10re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-31-uracil-ethene-1.25re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-31-uracil-ethene-1.50re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-31-uracil-ethene-2.00re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-32-uracil-ethyne-0.90re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-32-uracil-ethyne-0.95re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-32-uracil-ethyne-1.00re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-32-uracil-ethyne-1.05re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-32-uracil-ethyne-1.10re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-32-uracil-ethyne-1.25re / def2-svp	literature	interaction energy kcal mol	held

Table S21, continued.

Method	System / basis	Ref.	Quantity	|Δ|
RKS/pbe	s66x8-32-uracil-ethyne-1.50re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-32-uracil-ethyne-2.00re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-33-pyridine-ethene-0.90re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-33-pyridine-ethene-0.95re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-33-pyridine-ethene-1.00re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-33-pyridine-ethene-1.05re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-33-pyridine-ethene-1.10re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-33-pyridine-ethene-1.25re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-33-pyridine-ethene-1.50re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-33-pyridine-ethene-2.00re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-34-pentane-pentane-0.90re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-34-pentane-pentane-0.95re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-34-pentane-pentane-1.00re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-34-pentane-pentane-1.05re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-34-pentane-pentane-1.10re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-34-pentane-pentane-1.25re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-34-pentane-pentane-1.50re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-34-pentane-pentane-2.00re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-35-neopentane-pentane-0.90re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-35-neopentane-pentane-0.95re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-35-neopentane-pentane-1.00re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-35-neopentane-pentane-1.05re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-35-neopentane-pentane-1.10re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-35-neopentane-pentane-1.25re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-35-neopentane-pentane-1.50re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-35-neopentane-pentane-2.00re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-36-neopentane-neopentane-0.90re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-36-neopentane-neopentane-0.95re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-36-neopentane-neopentane-1.00re / def2-svp	literature	interaction energy kcal mol	held

Table S21, continued.

Method	System / basis	Ref.	Quantity	|Δ|
RKS/pbe	s66x8-36-neopentane-neopentane-1.05re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-36-neopentane-neopentane-1.10re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-36-neopentane-neopentane-1.25re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-36-neopentane-neopentane-1.50re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-36-neopentane-neopentane-2.00re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-37-cyclopentane-neopentane-0.90re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-37-cyclopentane-neopentane-0.95re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-37-cyclopentane-neopentane-1.00re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-37-cyclopentane-neopentane-1.05re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-37-cyclopentane-neopentane-1.10re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-37-cyclopentane-neopentane-1.25re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-37-cyclopentane-neopentane-1.50re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-37-cyclopentane-neopentane-2.00re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-38-cyclopentane-cyclopentane-0.90re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-38-cyclopentane-cyclopentane-0.95re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-38-cyclopentane-cyclopentane-1.00re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-38-cyclopentane-cyclopentane-1.05re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-38-cyclopentane-cyclopentane-1.10re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-38-cyclopentane-cyclopentane-1.25re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-38-cyclopentane-cyclopentane-1.50re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-38-cyclopentane-cyclopentane-2.00re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-39-benzene-cyclopentane-0.90re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-39-benzene-cyclopentane-0.95re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-39-benzene-cyclopentane-1.00re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-39-benzene-cyclopentane-1.05re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-39-benzene-cyclopentane-1.10re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-39-benzene-cyclopentane-1.25re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-39-benzene-cyclopentane-1.50re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-39-benzene-cyclopentane-2.00re / def2-svp	literature	interaction energy kcal mol	held

Table S21, continued.

Method	System / basis	Ref.	Quantity	|Δ|
RKS/pbe	s66x8-40-benzene-neopentane-0.90re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-40-benzene-neopentane-0.95re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-40-benzene-neopentane-1.00re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-40-benzene-neopentane-1.05re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-40-benzene-neopentane-1.10re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-40-benzene-neopentane-1.25re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-40-benzene-neopentane-1.50re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-40-benzene-neopentane-2.00re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-41-uracil-pentane-0.90re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-41-uracil-pentane-0.95re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-41-uracil-pentane-1.00re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-41-uracil-pentane-1.05re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-41-uracil-pentane-1.10re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-41-uracil-pentane-1.25re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-41-uracil-pentane-1.50re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-41-uracil-pentane-2.00re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-42-uracil-cyclopentane-0.90re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-42-uracil-cyclopentane-0.95re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-42-uracil-cyclopentane-1.00re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-42-uracil-cyclopentane-1.05re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-42-uracil-cyclopentane-1.10re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-42-uracil-cyclopentane-1.25re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-42-uracil-cyclopentane-1.50re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-42-uracil-cyclopentane-2.00re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-43-uracil-neopentane-0.90re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-43-uracil-neopentane-0.95re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-43-uracil-neopentane-1.00re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-43-uracil-neopentane-1.05re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-43-uracil-neopentane-1.10re / def2-svp	literature	interaction energy kcal mol	held

Table S21, continued.

Method	System / basis	Ref.	Quantity	|Δ|
RKS/pbe	s66x8-43-uracil-neopentane-1.25re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-43-uracil-neopentane-1.50re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-43-uracil-neopentane-2.00re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-44-ethene-pentane-0.90re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-44-ethene-pentane-0.95re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-44-ethene-pentane-1.00re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-44-ethene-pentane-1.05re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-44-ethene-pentane-1.10re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-44-ethene-pentane-1.25re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-44-ethene-pentane-1.50re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-44-ethene-pentane-2.00re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-45-ethyne-pentane-0.90re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-45-ethyne-pentane-0.95re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-45-ethyne-pentane-1.00re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-45-ethyne-pentane-1.05re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-45-ethyne-pentane-1.10re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-45-ethyne-pentane-1.25re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-45-ethyne-pentane-1.50re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-45-ethyne-pentane-2.00re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-46-peptide-pentane-0.90re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-46-peptide-pentane-0.95re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-46-peptide-pentane-1.00re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-46-peptide-pentane-1.05re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-46-peptide-pentane-1.10re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-46-peptide-pentane-1.25re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-46-peptide-pentane-1.50re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-46-peptide-pentane-2.00re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-47-benzene-benzene-ts-0.90re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-47-benzene-benzene-ts-0.95re / def2-svp	literature	interaction energy kcal mol	held

Table S21, continued.

Method	System / basis	Ref.	Quantity	|Δ|
RKS/pbe	s66x8-47-benzene-benzene-ts-1.00re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-47-benzene-benzene-ts-1.05re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-47-benzene-benzene-ts-1.10re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-47-benzene-benzene-ts-1.25re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-47-benzene-benzene-ts-1.50re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-47-benzene-benzene-ts-2.00re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-48-pyridine-pyridine-ts-0.90re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-48-pyridine-pyridine-ts-0.95re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-48-pyridine-pyridine-ts-1.00re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-48-pyridine-pyridine-ts-1.05re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-48-pyridine-pyridine-ts-1.10re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-48-pyridine-pyridine-ts-1.25re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-48-pyridine-pyridine-ts-1.50re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-48-pyridine-pyridine-ts-2.00re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-49-benzene-pyridine-ts-0.90re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-49-benzene-pyridine-ts-0.95re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-49-benzene-pyridine-ts-1.00re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-49-benzene-pyridine-ts-1.05re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-49-benzene-pyridine-ts-1.10re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-49-benzene-pyridine-ts-1.25re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-49-benzene-pyridine-ts-1.50re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-49-benzene-pyridine-ts-2.00re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-50-benzene-ethyne-ch-0.90re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-50-benzene-ethyne-ch-0.95re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-50-benzene-ethyne-ch-1.00re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-50-benzene-ethyne-ch-1.05re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-50-benzene-ethyne-ch-1.10re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-50-benzene-ethyne-ch-1.25re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-50-benzene-ethyne-ch-1.50re / def2-svp	literature	interaction energy kcal mol	held

Table S21, continued.

Method	System / basis	Ref.	Quantity	|Δ|
RKS/pbe	s66x8-50-benzene-ethyne-ch-2.00re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-51-ethyne-ethyne-ts-0.90re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-51-ethyne-ethyne-ts-0.95re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-51-ethyne-ethyne-ts-1.00re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-51-ethyne-ethyne-ts-1.05re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-51-ethyne-ethyne-ts-1.10re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-51-ethyne-ethyne-ts-1.25re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-51-ethyne-ethyne-ts-1.50re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-51-ethyne-ethyne-ts-2.00re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-52-benzene-acoh-oh-0.90re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-52-benzene-acoh-oh-0.95re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-52-benzene-acoh-oh-1.00re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-52-benzene-acoh-oh-1.05re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-52-benzene-acoh-oh-1.10re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-52-benzene-acoh-oh-1.25re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-52-benzene-acoh-oh-1.50re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-52-benzene-acoh-oh-2.00re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-53-benzene-acnh2-nh-0.90re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-53-benzene-acnh2-nh-0.95re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-53-benzene-acnh2-nh-1.00re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-53-benzene-acnh2-nh-1.05re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-53-benzene-acnh2-nh-1.10re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-53-benzene-acnh2-nh-1.25re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-53-benzene-acnh2-nh-1.50re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-53-benzene-acnh2-nh-2.00re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-54-benzene-water-oh-0.90re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-54-benzene-water-oh-0.95re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-54-benzene-water-oh-1.00re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-54-benzene-water-oh-1.05re / def2-svp	literature	interaction energy kcal mol	held

Table S21, continued.

Method	System / basis	Ref.	Quantity	|Δ|
RKS/pbe	s66x8-54-benzene-water-oh-1.10re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-54-benzene-water-oh-1.25re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-54-benzene-water-oh-1.50re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-54-benzene-water-oh-2.00re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-55-benzene-meoh-oh-0.90re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-55-benzene-meoh-oh-0.95re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-55-benzene-meoh-oh-1.00re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-55-benzene-meoh-oh-1.05re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-55-benzene-meoh-oh-1.10re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-55-benzene-meoh-oh-1.25re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-55-benzene-meoh-oh-1.50re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-55-benzene-meoh-oh-2.00re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-56-benzene-menh2-nh-0.90re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-56-benzene-menh2-nh-0.95re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-56-benzene-menh2-nh-1.00re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-56-benzene-menh2-nh-1.05re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-56-benzene-menh2-nh-1.10re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-56-benzene-menh2-nh-1.25re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-56-benzene-menh2-nh-1.50re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-56-benzene-menh2-nh-2.00re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-57-benzene-peptide-nh-0.90re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-57-benzene-peptide-nh-0.95re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-57-benzene-peptide-nh-1.00re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-57-benzene-peptide-nh-1.05re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-57-benzene-peptide-nh-1.10re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-57-benzene-peptide-nh-1.25re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-57-benzene-peptide-nh-1.50re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-57-benzene-peptide-nh-2.00re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-58-pyridine-pyridine-ch-n-0.90re / def2-svp	literature	interaction energy kcal mol	held

Table S21, continued.

Method	System / basis	Ref.	Quantity	|Δ|
RKS/pbe	s66x8-58-pyridine-pyridine-ch-n-0.95re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-58-pyridine-pyridine-ch-n-1.00re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-58-pyridine-pyridine-ch-n-1.05re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-58-pyridine-pyridine-ch-n-1.10re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-58-pyridine-pyridine-ch-n-1.25re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-58-pyridine-pyridine-ch-n-1.50re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-58-pyridine-pyridine-ch-n-2.00re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-59-ethyne-water-ch-o-0.90re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-59-ethyne-water-ch-o-0.95re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-59-ethyne-water-ch-o-1.00re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-59-ethyne-water-ch-o-1.05re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-59-ethyne-water-ch-o-1.10re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-59-ethyne-water-ch-o-1.25re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-59-ethyne-water-ch-o-1.50re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-59-ethyne-water-ch-o-2.00re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-60-ethyne-acoh-oh-0.90re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-60-ethyne-acoh-oh-0.95re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-60-ethyne-acoh-oh-1.00re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-60-ethyne-acoh-oh-1.05re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-60-ethyne-acoh-oh-1.10re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-60-ethyne-acoh-oh-1.25re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-60-ethyne-acoh-oh-1.50re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-60-ethyne-acoh-oh-2.00re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-61-pentane-acoh-0.90re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-61-pentane-acoh-0.95re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-61-pentane-acoh-1.00re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-61-pentane-acoh-1.05re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-61-pentane-acoh-1.10re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-61-pentane-acoh-1.25re / def2-svp	literature	interaction energy kcal mol	held

Table S21, continued.

Method	System / basis	Ref.	Quantity	|Δ|
RKS/pbe	s66x8-61-pentane-acoh-1.50re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-61-pentane-acoh-2.00re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-62-pentane-acnh2-0.90re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-62-pentane-acnh2-0.95re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-62-pentane-acnh2-1.00re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-62-pentane-acnh2-1.05re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-62-pentane-acnh2-1.10re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-62-pentane-acnh2-1.25re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-62-pentane-acnh2-1.50re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-62-pentane-acnh2-2.00re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-63-benzene-acoh-0.90re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-63-benzene-acoh-0.95re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-63-benzene-acoh-1.00re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-63-benzene-acoh-1.05re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-63-benzene-acoh-1.10re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-63-benzene-acoh-1.25re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-63-benzene-acoh-1.50re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-63-benzene-acoh-2.00re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-64-peptide-ethene-0.90re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-64-peptide-ethene-0.95re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-64-peptide-ethene-1.00re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-64-peptide-ethene-1.05re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-64-peptide-ethene-1.10re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-64-peptide-ethene-1.25re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-64-peptide-ethene-1.50re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-64-peptide-ethene-2.00re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-65-pyridine-ethyne-0.90re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-65-pyridine-ethyne-0.95re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-65-pyridine-ethyne-1.00re / def2-svp	literature	interaction energy kcal mol	held

Table S21, continued.

Method	System / basis	Ref.	Quantity	|Δ|
RKS/pbe	s66x8-65-pyridine-ethyne-1.05re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-65-pyridine-ethyne-1.10re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-65-pyridine-ethyne-1.25re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-65-pyridine-ethyne-1.50re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-65-pyridine-ethyne-2.00re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-66-menh2-pyridine-0.90re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-66-menh2-pyridine-0.95re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-66-menh2-pyridine-1.00re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-66-menh2-pyridine-1.05re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-66-menh2-pyridine-1.10re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-66-menh2-pyridine-1.25re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-66-menh2-pyridine-1.50re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s66x8-66-menh2-pyridine-2.00re / def2-svp	literature	interaction energy kcal mol	held
RKS/pbe	s22-07-adenine-thymine-wc / def2-svp	orca	total energy ha	1.10×10^{-3}
RKS/pbe	s22-13-uracil-dimer-stack / def2-svp	orca	total energy ha	1.02×10^{-3}
RKS/pbe	s22-15-adenine-thymine-stack / def2-svp	orca	total energy ha	1.13×10^{-3}
RKS/pbe0	benzene-dimer / def2-svp	orca	total energy ha	incomplete
RKS/pbe0	benzene-dimer / def2-svp	orca	dispersion d3bj ha	incomplete
RKS/pbe	s22-01-ammonia-dimer / def2-svp	orca	interaction energy kcal mol	artifact-incomplete
RKS/pbe	s22-01-ammonia-dimer / def2-svp	orca	interaction energy kcal mol	artifact-incomplete
RKS/pbe	s22-02-water-dimer / def2-svp	orca	interaction energy kcal mol	artifact-incomplete
RKS/pbe	s22-02-water-dimer / def2-svp	orca	interaction energy kcal mol	artifact-incomplete
RKS/pbe	s22-03-formic-acid-dimer / def2-svp	orca	interaction energy kcal mol	artifact-incomplete
RKS/pbe	s22-03-formic-acid-dimer / def2-svp	orca	interaction energy kcal mol	artifact-incomplete
RKS/pbe	s22-04-formamide-dimer / def2-svp	orca	interaction energy kcal mol	artifact-incomplete
RKS/pbe	s22-04-formamide-dimer / def2-svp	orca	interaction energy kcal mol	artifact-incomplete
RKS/pbe	s22-05-uracil-dimer-hb / def2-svp	orca	interaction energy kcal mol	artifact-incomplete
RKS/pbe	s22-05-uracil-dimer-hb / def2-svp	orca	interaction energy kcal mol	artifact-incomplete
RKS/pbe	s22-06-2-pyridone-2-aminopyridine / def2-svp	orca	interaction energy kcal mol	artifact-incomplete
RKS/pbe	s22-06-2-pyridone-2-aminopyridine / def2-svp	orca	interaction energy kcal mol	artifact-incomplete
RKS/pbe	s22-07-adenine-thymine-wc / def2-svp	orca	interaction energy kcal mol	artifact-incomplete
RKS/pbe	s22-07-adenine-thymine-wc / def2-svp	orca	interaction energy kcal mol	artifact-incomplete
RKS/pbe	s22-08-methane-dimer / def2-svp	orca	interaction energy kcal mol	artifact-incomplete
RKS/pbe	s22-08-methane-dimer / def2-svp	orca	interaction energy kcal mol	artifact-incomplete
RKS/pbe	s22-09-ethene-dimer / def2-svp	orca	interaction energy kcal mol	artifact-incomplete
RKS/pbe	s22-09-ethene-dimer / def2-svp	orca	interaction energy kcal mol	artifact-incomplete
RKS/pbe	s22-10-benzene-ch4 / def2-svp	orca	interaction energy kcal mol	artifact-incomplete
RKS/pbe	s22-10-benzene-ch4 / def2-svp	orca	interaction energy kcal mol	artifact-incomplete

Table S21, continued.

Method	System / basis	Ref.	Quantity	|Δ|
RKS/pbe	s22-11-benzene-dimer-stack / def2-svp	orca	interaction energy kcal mol	artifact-incomplete
RKS/pbe	s22-11-benzene-dimer-stack / def2-svp	orca	interaction energy kcal mol	artifact-incomplete
RKS/pbe	s22-12-pyrazine-dimer / def2-svp	orca	interaction energy kcal mol	artifact-incomplete
RKS/pbe	s22-12-pyrazine-dimer / def2-svp	orca	interaction energy kcal mol	artifact-incomplete
RKS/pbe	s22-13-uracil-dimer-stack / def2-svp	orca	interaction energy kcal mol	artifact-incomplete
RKS/pbe	s22-13-uracil-dimer-stack / def2-svp	orca	interaction energy kcal mol	artifact-incomplete
RKS/pbe	s22-14-indole-benzene-stack / def2-svp	orca	interaction energy kcal mol	artifact-incomplete
RKS/pbe	s22-14-indole-benzene-stack / def2-svp	orca	interaction energy kcal mol	artifact-incomplete
RKS/pbe	s22-15-adenine-thymine-stack / def2-svp	orca	interaction energy kcal mol	artifact-incomplete
RKS/pbe	s22-15-adenine-thymine-stack / def2-svp	orca	interaction energy kcal mol	artifact-incomplete
RKS/pbe	s22-16-ethene-ethyne / def2-svp	orca	interaction energy kcal mol	artifact-incomplete
RKS/pbe	s22-16-ethene-ethyne / def2-svp	orca	interaction energy kcal mol	artifact-incomplete
RKS/pbe	s22-17-benzene-h2o / def2-svp	orca	interaction energy kcal mol	artifact-incomplete
RKS/pbe	s22-17-benzene-h2o / def2-svp	orca	interaction energy kcal mol	artifact-incomplete
RKS/pbe	s22-18-benzene-nh3 / def2-svp	orca	interaction energy kcal mol	artifact-incomplete
RKS/pbe	s22-18-benzene-nh3 / def2-svp	orca	interaction energy kcal mol	artifact-incomplete
RKS/pbe	s22-19-benzene-hcn / def2-svp	orca	interaction energy kcal mol	artifact-incomplete
RKS/pbe	s22-19-benzene-hcn / def2-svp	orca	interaction energy kcal mol	artifact-incomplete
RKS/pbe	s22-20-benzene-dimer-t / def2-svp	orca	interaction energy kcal mol	artifact-incomplete
RKS/pbe	s22-20-benzene-dimer-t / def2-svp	orca	interaction energy kcal mol	artifact-incomplete
RKS/pbe	s22-21-indole-benzene-t / def2-svp	orca	interaction energy kcal mol	artifact-incomplete
RKS/pbe	s22-21-indole-benzene-t / def2-svp	orca	interaction energy kcal mol	artifact-incomplete
RKS/pbe	s22-22-phenol-dimer / def2-svp	orca	interaction energy kcal mol	artifact-incomplete
RKS/pbe	s22-22-phenol-dimer / def2-svp	orca	interaction energy kcal mol	artifact-incomplete
RKS/pbe	s22-01-ammonia-dimer / def2-svp	orca	interaction energy kcal mol	queued
RKS/pbe	s22-02-water-dimer / def2-svp	orca	interaction energy kcal mol	queued
RKS/pbe	s22-03-formic-acid-dimer / def2-svp	orca	interaction energy kcal mol	queued
RKS/pbe	s22-04-formamide-dimer / def2-svp	orca	interaction energy kcal mol	queued
RKS/pbe	s22-05-uracil-dimer-hb / def2-svp	orca	interaction energy kcal mol	queued
RKS/pbe	s22-06-2-pyridone-2-aminopyridine / def2-svp	orca	interaction energy kcal mol	queued
RKS/pbe	s22-07-adenine-thymine-wc / def2-svp	orca	interaction energy kcal mol	queued
RKS/pbe	s22-08-methane-dimer / def2-svp	orca	interaction energy kcal mol	queued
RKS/pbe	s22-09-ethene-dimer / def2-svp	orca	interaction energy kcal mol	queued
RKS/pbe	s22-10-benzene-ch4 / def2-svp	orca	interaction energy kcal mol	queued
RKS/pbe	s22-11-benzene-dimer-stack / def2-svp	orca	interaction energy kcal mol	queued
RKS/pbe	s22-12-pyrazine-dimer / def2-svp	orca	interaction energy kcal mol	queued
RKS/pbe	s22-13-uracil-dimer-stack / def2-svp	orca	interaction energy kcal mol	queued
RKS/pbe	s22-14-indole-benzene-stack / def2-svp	orca	interaction energy kcal mol	queued
RKS/pbe	s22-15-adenine-thymine-stack / def2-svp	orca	interaction energy kcal mol	queued
RKS/pbe	s22-16-ethene-ethyne / def2-svp	orca	interaction energy kcal mol	queued
RKS/pbe	s22-17-benzene-h2o / def2-svp	orca	interaction energy kcal mol	queued
RKS/pbe	s22-18-benzene-nh3 / def2-svp	orca	interaction energy kcal mol	queued
RKS/pbe	s22-19-benzene-hcn / def2-svp	orca	interaction energy kcal mol	queued
RKS/pbe	s22-20-benzene-dimer-t / def2-svp	orca	interaction energy kcal mol	queued
RKS/pbe	s22-21-indole-benzene-t / def2-svp	orca	interaction energy kcal mol	queued
RKS/pbe	s22-22-phenol-dimer / def2-svp	orca	interaction energy kcal mol	queued

Table S21, continued.

Method	System / basis	Ref.	Quantity	$\lvert\Delta\rvert$
Dispersion-corrected DFT				
3 pass, 2 fail, 1 blocked. Median $\lvert\Delta E\rvert$ 2.9×10^{-4}, max 2.9×10^{-4} E_h.				
RKS/pbe0	h2o-dimer / def2-tzvp	orca	total energy ha	2.88×10^{-4}
RKS/pbe0	h2o-dimer / def2-tzvp	orca	scf energy ha	2.88×10^{-4}
RKS/pbe0	h2o-dimer / def2-tzvp	orca	dispersion d4 ha	2.00×10^{-9}
RKS/b3lyp	methane-dimer / def2-tzvp	orca	dispersion energy ha	7.20×10^{-3}
RKS/b3lyp	methane-dimer / def2-tzvp	orca	total energy ha	6.96×10^{-3}
RKS/b3lyp	methane-dimer / def2-tzvp	orca	scf energy ha	blocked
Double hybrids				
3 pass, 3 fail, 24 artifact-incomplete, 8 blocked. Median $\lvert\Delta E\rvert$ 1.3×10^{-6}, max 1.4×10^{-6} E_h.				
B2PLYP	h2o / cc-pvtz	orca	total energy ha	1.41×10^{-6}
B2PLYP	h2o / cc-pvtz	orca	scf energy ha	1.33×10^{-6}
B2PLYP	h2o / cc-pvtz	orca	mp2 correlation ha	7.70×10^{-8}
B2PLYP/b2plyp	h2o / def2-svp	orca	total energy ha	6.32×10^{-4}
DSD-PBEP86/ dsd-pbep86	h2o / def2-svp	orca	total energy ha	2.75×10^{-3}
PWPB95/pwpb95	h2o / def2-svp	orca	total energy ha	3.88×10^{-4}
B2PLYP/b2plyp	h2o / def2-svp	orca	total energy ha	artifact-incomplete
B2PLYP/b2plyp	h2o / def2-svp	orca	total energy ha	artifact-incomplete
B2PLYP/b2plyp	h2o / def2-svp	orca	total energy ha	artifact-incomplete
DSD-PBEP86/ dsd-pbep86	h2o / def2-svp	orca	total energy ha	artifact-incomplete
DSD-PBEP86/ dsd-pbep86	h2o / def2-svp	orca	total energy ha	artifact-incomplete
DSD-PBEP86/ dsd-pbep86	h2o / def2-svp	orca	total energy ha	artifact-incomplete
PWPB95/pwpb95	h2o / def2-svp	orca	total energy ha	artifact-incomplete
PWPB95/pwpb95	h2o / def2-svp	orca	total energy ha	artifact-incomplete
PWPB95/pwpb95	h2o / def2-svp	orca	total energy ha	artifact-incomplete
B2PLYP/b2plyp	h2o / sto-3g	orca	total energy ha	artifact-incomplete
B2PLYP/b2plyp	h2o / sto-3g	orca	total energy ha	artifact-incomplete
DSD-PBEP86/ dsd-pbep86	h2o / sto-3g	orca	total energy ha	artifact-incomplete
DSD-PBEP86/ dsd-pbep86	h2o / sto-3g	orca	total energy ha	artifact-incomplete
PWPB95/pwpb95	h2o / sto-3g	orca	total energy ha	artifact-incomplete
PWPB95/pwpb95	h2o / sto-3g	orca	total energy ha	artifact-incomplete
B2PLYP/b2plyp	h2o / def2-svp	orca	total energy ha	artifact-incomplete
B2PLYP/b2plyp	h2o / sto-3g	orca	total energy ha	artifact-incomplete
B2PLYP/b2plyp	h2o / def2-tzvp	orca	total energy ha	artifact-incomplete
DSD-PBEP86/ dsd-pbep86	h2o / def2-svp	orca	total energy ha	artifact-incomplete
DSD-PBEP86/ dsd-pbep86	h2o / sto-3g	orca	total energy ha	artifact-incomplete
DSD-PBEP86/ dsd-pbep86	h2o / def2-tzvp	orca	total energy ha	artifact-incomplete
PWPB95/pwpb95	h2o / def2-svp	orca	total energy ha	artifact-incomplete
PWPB95/pwpb95	h2o / sto-3g	orca	total energy ha	artifact-incomplete
PWPB95/pwpb95	h2o / def2-tzvp	orca	total energy ha	artifact-incomplete
B2PLYP/b2plyp	h2o / def2-svp	orca	total energy ha	blocked
B2PLYP/b2plyp	h2o / def2-svp	orca	total energy ha	blocked
DSD-PBEP86/ dsd-pbep86	h2o / def2-svp	orca	total energy ha	blocked
PWPB95/pwpb95	h2o / def2-svp	orca	total energy ha	blocked
PWPB95/pwpb95	h2o / def2-svp	orca	total energy ha	blocked
B2PLYP/b2plyp	h2o / sto-3g	orca	total energy ha	blocked

Table S21, continued.

Method	System / basis	Ref.	Quantity	$\lvert\Delta\rvert$
DSD-PBEP86/ dsd-pbep86	h2o / sto-3g	orca	total energy ha	blocked
PWPB95/pwpb95	h2o / sto-3g	orca	total energy ha	blocked
Møller–Plesset				
246 pass, 22 held, 43 fail, 46 artifact-incomplete, 14 reference-missing, 6 blocked. Median $\lvert\Delta E\rvert$ 3.4×10^{-8}, max 1.4×10^{-4} E_h.				
MP2	h2o / cc-pvqz	orca	mp2 total energy ha	9.02×10^{-9}
MP2	h2o / cc-pv5z	orca	mp2 total energy ha	1.30×10^{-10}
MP2	ch4 / cc-pvqz	orca	mp2 total energy ha	3.25×10^{-9}
MP2	co / cc-pvqz	orca	mp2 total energy ha	8.03×10^{-8}
MP2	co / cc-pv5z	orca	mp2 total energy ha	7.12×10^{-8}
MP2	h2 / cc-pvdz	orca	mp2 total energy ha	6.60×10^{-10}
MP2	h2 / cc-pvdz	orca	mp2 total energy ha	6.01×10^{-9}
MP2	h2 / cc-pvdz	orca	mp2 total energy ha	8.70×10^{-11}
MP2	h2 / cc-pvdz	orca	mp2 total energy ha	3.15×10^{-10}
MP2	h2 / cc-pvdz	orca	mp2 total energy ha	7.90×10^{-11}
MP2	h2 / cc-pvdz	orca	mp2 total energy ha	1.56×10^{-9}
MP2	s22-01-ammonia-dimer-monoA / cc-pvdz	internal	density fitting error ha	3.92×10^{-5}
MP2	s22-01-ammonia-dimer-monoA / cc-pvdz	internal	density fitting error total energy kcal mol	3.92×10^{-5}
MP2	s22-01-ammonia-dimer-monoB / cc-pvdz	internal	density fitting error ha	3.92×10^{-5}
MP2	s22-01-ammonia-dimer-monoB / cc-pvdz	internal	density fitting error total energy kcal mol	3.92×10^{-5}
MP2	s22-01-ammonia-dimer / cc-pvdz	internal	density fitting error ha	8.13×10^{-5}
MP2	s22-01-ammonia-dimer / cc-pvdz	internal	density fitting error total energy kcal mol	8.13×10^{-5}
MP2	s22-02-water-dimer-monoA / cc-pvdz	internal	density fitting error ha	1.52×10^{-5}
MP2	s22-02-water-dimer-monoA / cc-pvdz	internal	density fitting error total energy kcal mol	1.52×10^{-5}
MP2	s22-02-water-dimer-monoB / cc-pvdz	internal	density fitting error ha	1.53×10^{-5}
MP2	s22-02-water-dimer-monoB / cc-pvdz	internal	density fitting error total energy kcal mol	1.53×10^{-5}
MP2	s22-02-water-dimer / cc-pvdz	internal	density fitting error ha	3.43×10^{-5}
MP2	s22-02-water-dimer / cc-pvdz	internal	density fitting error total energy kcal mol	3.43×10^{-5}
MP2	s22-03-formic-acid-dimer-monoA / cc-pvdz	internal	density fitting error ha	6.09×10^{-5}
MP2	s22-03-formic-acid-dimer-monoA / cc-pvdz	internal	density fitting error total energy kcal mol	6.09×10^{-5}
MP2	s22-03-formic-acid-dimer-monoB / cc-pvdz	internal	density fitting error ha	6.09×10^{-5}
MP2	s22-03-formic-acid-dimer-monoB / cc-pvdz	internal	density fitting error total energy kcal mol	6.09×10^{-5}
MP2	s22-04-formamide-dimer-monoA / cc-pvdz	internal	density fitting error ha	4.78×10^{-6}
MP2	s22-04-formamide-dimer-monoA / cc-pvdz	internal	density fitting error total energy kcal mol	4.78×10^{-6}
MP2	s22-04-formamide-dimer-monoB / cc-pvdz	internal	density fitting error ha	4.78×10^{-6}
MP2	s22-04-formamide-dimer-monoB / cc-pvdz	internal	density fitting error total energy kcal mol	4.78×10^{-6}
MP2	s22-08-methane-dimer-monoA / cc-pvdz	internal	density fitting error ha	4.99×10^{-5}

Table S21, continued.

Method	System / basis	Ref.	Quantity	$\lvert\Delta\rvert$
MP2	s22-08-methane-dimer-monoA / cc-pvdz	internal	density fitting error total energy kcal mol	4.99×10^{-5}
MP2	s22-08-methane-dimer-monoB / cc-pvdz	internal	density fitting error ha	4.99×10^{-5}
MP2	s22-08-methane-dimer-monoB / cc-pvdz	internal	density fitting error total energy kcal mol	4.99×10^{-5}
MP2	s22-08-methane-dimer / cc-pvdz	internal	density fitting error ha	9.73×10^{-5}
MP2	s22-08-methane-dimer / cc-pvdz	internal	density fitting error total energy kcal mol	9.73×10^{-5}
MP2	s22-09-ethene-dimer-monoA / cc-pvdz	internal	density fitting error ha	7.22×10^{-5}
MP2	s22-09-ethene-dimer-monoA / cc-pvdz	internal	density fitting error total energy kcal mol	7.22×10^{-5}
MP2	s22-09-ethene-dimer-monoB / cc-pvdz	internal	density fitting error ha	7.22×10^{-5}
MP2	s22-09-ethene-dimer-monoB / cc-pvdz	internal	density fitting error total energy kcal mol	7.22×10^{-5}
MP2	s22-09-ethene-dimer / cc-pvdz	internal	density fitting error ha	1.40×10^{-4}
MP2	s22-09-ethene-dimer / cc-pvdz	internal	density fitting error total energy kcal mol	1.40×10^{-4}
MP2	s22-10-benzene-ch4-monoB / cc-pvdz	internal	density fitting error ha	4.94×10^{-5}
MP2	s22-10-benzene-ch4-monoB / cc-pvdz	internal	density fitting error total energy kcal mol	4.94×10^{-5}
MP2	s22-16-ethene-ethyne-monoA / cc-pvdz	internal	density fitting error total energy kcal mol	7.22×10^{-5}
MP2	s22-16-ethene-ethyne-monoB / cc-pvdz	internal	density fitting error total energy kcal mol	1.59×10^{-5}
MP2	s22-16-ethene-ethyne / cc-pvdz	internal	density fitting error ha	5.79×10^{-5}
MP2	s22-16-ethene-ethyne / cc-pvdz	internal	density fitting error total energy kcal mol	5.79×10^{-5}
MP2	s22-17-benzene-h2o-monoB / cc-pvdz	internal	density fitting error total energy kcal mol	1.42×10^{-5}
MP2	s22-18-benzene-nh3-monoB / cc-pvdz	internal	density fitting error total energy kcal mol	3.77×10^{-5}
MP2	s22-19-benzene-hcn-monoB / cc-pvdz	internal	density fitting error total energy kcal mol	7.18×10^{-5}
MP2	h2o / cc-pvtz	orca	total energy ha	2.52×10^{-5}
SCS-MP2	h2o / cc-pvtz	orca	total energy ha	5.19×10^{-5}
SOS-MP2	h2o / cc-pvtz	orca	total energy ha	6.52×10^{-5}
MP2	oh-radical / def2-svp	orca	total energy ha	2.22×10^{-9}
MP2	oh-radical / def2-svp	orca	total energy ha	2.22×10^{-9}
DLPNO-MP2	h2o / def2-svp	orca	total energy ha	1.66×10^{-8}
DLPNO-MP2	h2o / def2-svp	orca	total energy ha	1.66×10^{-8}
DLPNO-MP2	oh-radical / def2-svp	orca	total energy ha	2.22×10^{-9}
DLPNO-MP2	oh-radical / def2-svp	orca	total energy ha	2.22×10^{-9}
MP2	oh-radical / sto-3g	orca	total energy ha	7.73×10^{-9}
MP2	acetic-acid / def2-svp	orca	total energy ha	6.44×10^{-8}
MP2	acetic-acid / def2-svp	orca	correlation energy ha	6.14×10^{-8}
MP2	acetic-acid / def2-tzvp	orca	total energy ha	7.39×10^{-8}
MP2	acetic-acid / def2-tzvp	orca	correlation energy ha	7.64×10^{-8}
MP2	acetic-acid / sto-3g	orca	total energy ha	4.27×10^{-8}
MP2	acetic-acid / sto-3g	orca	correlation energy ha	3.87×10^{-8}
MP2	acetic-acid / def2-svp	orca	total energy ha	6.47×10^{-8}
MP2	acetic-acid / def2-svp	orca	correlation energy ha	6.22×10^{-8}
MP2	acetic-acid / def2-tzvp	orca	total energy ha	7.39×10^{-8}
MP2	acetic-acid / def2-tzvp	orca	correlation energy ha	7.59×10^{-8}
SCS-MP2	acetic-acid / def2-svp	orca	total energy ha	4.75×10^{-8}

Table S21, continued.

Method	System / basis	Ref.	Quantity	$\lvert\Delta\rvert$
SCS-MP2	acetic-acid / def2-svp	orca	correlation energy ha	4.49×10^{-8}
SCS-MP2	acetic-acid / def2-tzvp	orca	total energy ha	6.88×10^{-8}
SCS-MP2	acetic-acid / def2-tzvp	orca	correlation energy ha	7.12×10^{-8}
SCS-MP2	acetic-acid / sto-3g	orca	total energy ha	2.25×10^{-8}
SCS-MP2	acetic-acid / sto-3g	orca	correlation energy ha	1.81×10^{-8}
SOS-MP2	acetic-acid / def2-svp	orca	total energy ha	3.90×10^{-8}
SOS-MP2	acetic-acid / def2-svp	orca	correlation energy ha	3.66×10^{-8}
SOS-MP2	acetic-acid / def2-tzvp	orca	total energy ha	6.62×10^{-8}
SOS-MP2	acetic-acid / def2-tzvp	orca	correlation energy ha	6.81×10^{-8}
SOS-MP2	acetic-acid / sto-3g	orca	total energy ha	1.24×10^{-8}
SOS-MP2	acetic-acid / sto-3g	orca	correlation energy ha	7.80×10^{-9}
MP2	c2h4 / def2-svp	orca	total energy ha	3.96×10^{-8}
MP2	c2h4 / def2-svp	orca	correlation energy ha	3.93×10^{-8}
MP2	c2h4 / def2-tzvp	orca	total energy ha	4.93×10^{-10}
MP2	c2h4 / def2-tzvp	orca	correlation energy ha	1.40×10^{-9}
MP2	c2h4 / sto-3g	orca	total energy ha	1.04×10^{-8}
MP2	c2h4 / sto-3g	orca	correlation energy ha	9.70×10^{-9}
MP2	c2h4 / def2-svp	orca	total energy ha	3.98×10^{-8}
MP2	c2h4 / def2-svp	orca	correlation energy ha	3.94×10^{-8}
MP2	c2h4 / def2-tzvp	orca	total energy ha	3.59×10^{-10}
MP2	c2h4 / def2-tzvp	orca	correlation energy ha	1.10×10^{-9}
SCS-MP2	c2h4 / def2-svp	orca	total energy ha	3.47×10^{-8}
SCS-MP2	c2h4 / def2-svp	orca	correlation energy ha	3.42×10^{-8}
SCS-MP2	c2h4 / def2-tzvp	orca	total energy ha	4.63×10^{-9}
SCS-MP2	c2h4 / def2-tzvp	orca	correlation energy ha	5.00×10^{-9}
SCS-MP2	c2h4 / sto-3g	orca	total energy ha	5.86×10^{-9}
SCS-MP2	c2h4 / sto-3g	orca	correlation energy ha	5.20×10^{-9}
SOS-MP2	c2h4 / def2-svp	orca	total energy ha	3.22×10^{-8}
SOS-MP2	c2h4 / def2-svp	orca	correlation energy ha	3.17×10^{-8}
SOS-MP2	c2h4 / def2-tzvp	orca	total energy ha	6.69×10^{-9}
SOS-MP2	c2h4 / def2-tzvp	orca	correlation energy ha	7.30×10^{-9}
SOS-MP2	c2h4 / sto-3g	orca	total energy ha	3.63×10^{-9}
SOS-MP2	c2h4 / sto-3g	orca	correlation energy ha	2.50×10^{-9}
MP2	ch2o / def2-svp	orca	total energy ha	8.19×10^{-8}
MP2	ch2o / def2-svp	orca	correlation energy ha	8.05×10^{-8}
MP2	ch2o / def2-tzvp	orca	total energy ha	3.32×10^{-8}
MP2	ch2o / def2-tzvp	orca	correlation energy ha	3.24×10^{-8}
MP2	ch2o / sto-3g	orca	total energy ha	7.85×10^{-8}
MP2	ch2o / sto-3g	orca	correlation energy ha	7.82×10^{-8}
MP2	ch2o / def2-svp	orca	total energy ha	8.23×10^{-8}
MP2	ch2o / def2-svp	orca	correlation energy ha	8.16×10^{-8}
MP2	ch2o / def2-tzvp	orca	total energy ha	3.33×10^{-8}
MP2	ch2o / def2-tzvp	orca	correlation energy ha	3.22×10^{-8}
SCS-MP2	ch2o / def2-svp	orca	total energy ha	7.07×10^{-8}
SCS-MP2	ch2o / def2-svp	orca	correlation energy ha	6.94×10^{-8}
SCS-MP2	ch2o / def2-tzvp	orca	total energy ha	3.02×10^{-8}
SCS-MP2	ch2o / def2-tzvp	orca	correlation energy ha	2.94×10^{-8}
SCS-MP2	ch2o / sto-3g	orca	total energy ha	6.24×10^{-8}
SCS-MP2	ch2o / sto-3g	orca	correlation energy ha	6.28×10^{-8}
SOS-MP2	ch2o / def2-svp	orca	total energy ha	6.50×10^{-8}
SOS-MP2	ch2o / def2-svp	orca	correlation energy ha	6.44×10^{-8}
SOS-MP2	ch2o / def2-tzvp	orca	total energy ha	2.88×10^{-8}
SOS-MP2	ch2o / def2-tzvp	orca	correlation energy ha	2.79×10^{-8}
SOS-MP2	ch2o / sto-3g	orca	total energy ha	5.44×10^{-8}
SOS-MP2	ch2o / sto-3g	orca	correlation energy ha	5.46×10^{-8}
MP2	ch4 / def2-svp	orca	total energy ha	2.56×10^{-9}
MP2	ch4 / def2-svp	orca	correlation energy ha	2.30×10^{-9}
MP2	ch4 / def2-tzvp	orca	total energy ha	1.77×10^{-8}

Table S21, continued.

Method	System / basis	Ref.	Quantity	$\lvert\Delta\rvert$
MP2	ch4 / def2-tzvp	orca	correlation energy ha	1.77×10^{-8}
MP2	ch4 / sto-3g	orca	total energy ha	3.36×10^{-10}
MP2	ch4 / sto-3g	orca	correlation energy ha	9.00×10^{-10}
MP2	ch4 / def2-svp	orca	total energy ha	2.65×10^{-9}
MP2	ch4 / def2-svp	orca	correlation energy ha	2.20×10^{-9}
MP2	ch4 / def2-tzvp	orca	total energy ha	1.78×10^{-8}
MP2	ch4 / def2-tzvp	orca	correlation energy ha	1.84×10^{-8}
SCS-MP2	ch4 / def2-svp	orca	total energy ha	3.33×10^{-9}
SCS-MP2	ch4 / def2-svp	orca	correlation energy ha	3.40×10^{-9}
SCS-MP2	ch4 / def2-tzvp	orca	total energy ha	1.48×10^{-8}
SCS-MP2	ch4 / def2-tzvp	orca	correlation energy ha	1.53×10^{-8}
SCS-MP2	ch4 / sto-3g	orca	total energy ha	4.12×10^{-10}
SCS-MP2	ch4 / sto-3g	orca	correlation energy ha	1.00×10^{-9}
SOS-MP2	ch4 / def2-svp	orca	total energy ha	3.67×10^{-9}
SOS-MP2	ch4 / def2-svp	orca	correlation energy ha	3.40×10^{-9}
SOS-MP2	ch4 / def2-tzvp	orca	total energy ha	1.34×10^{-8}
SOS-MP2	ch4 / def2-tzvp	orca	correlation energy ha	1.41×10^{-8}
SOS-MP2	ch4 / sto-3g	orca	total energy ha	4.51×10^{-10}
SOS-MP2	ch4 / sto-3g	orca	correlation energy ha	1.10×10^{-9}
MP2	co / def2-svp	orca	total energy ha	9.63×10^{-8}
MP2	co / def2-svp	orca	correlation energy ha	9.55×10^{-8}
MP2	co / def2-tzvp	orca	total energy ha	8.29×10^{-8}
MP2	co / def2-tzvp	orca	correlation energy ha	8.39×10^{-8}
MP2	co / sto-3g	orca	total energy ha	4.36×10^{-9}
MP2	co / sto-3g	orca	correlation energy ha	4.40×10^{-9}
MP2	co / def2-svp	orca	total energy ha	9.57×10^{-8}
MP2	co / def2-svp	orca	correlation energy ha	9.45×10^{-8}
MP2	co / def2-tzvp	orca	total energy ha	8.30×10^{-8}
MP2	co / def2-tzvp	orca	correlation energy ha	8.43×10^{-8}
SCS-MP2	co / def2-svp	orca	total energy ha	8.91×10^{-8}
SCS-MP2	co / def2-svp	orca	correlation energy ha	8.81×10^{-8}
SCS-MP2	co / def2-tzvp	orca	total energy ha	7.49×10^{-8}
SCS-MP2	co / def2-tzvp	orca	correlation energy ha	7.61×10^{-8}
SCS-MP2	co / sto-3g	orca	total energy ha	4.85×10^{-9}
SCS-MP2	co / sto-3g	orca	correlation energy ha	4.80×10^{-9}
SOS-MP2	co / def2-svp	orca	total energy ha	8.55×10^{-8}
SOS-MP2	co / def2-svp	orca	correlation energy ha	8.44×10^{-8}
SOS-MP2	co / def2-tzvp	orca	total energy ha	7.10×10^{-8}
SOS-MP2	co / def2-tzvp	orca	correlation energy ha	7.17×10^{-8}
SOS-MP2	co / sto-3g	orca	total energy ha	5.00×10^{-9}
SOS-MP2	co / sto-3g	orca	correlation energy ha	4.90×10^{-9}
MP2	ethanol / def2-svp	orca	total energy ha	1.17×10^{-7}
MP2	ethanol / def2-svp	orca	correlation energy ha	1.16×10^{-7}
MP2	ethanol / def2-tzvp	orca	total energy ha	8.62×10^{-8}
MP2	ethanol / def2-tzvp	orca	correlation energy ha	8.69×10^{-8}
MP2	ethanol / sto-3g	orca	total energy ha	2.76×10^{-8}
MP2	ethanol / sto-3g	orca	correlation energy ha	2.73×10^{-8}
MP2	ethanol / def2-svp	orca	total energy ha	1.17×10^{-7}
MP2	ethanol / def2-svp	orca	correlation energy ha	1.16×10^{-7}
MP2	ethanol / def2-tzvp	orca	total energy ha	8.61×10^{-8}
MP2	ethanol / def2-tzvp	orca	correlation energy ha	8.64×10^{-8}
SCS-MP2	ethanol / def2-svp	orca	total energy ha	1.29×10^{-7}
SCS-MP2	ethanol / def2-svp	orca	correlation energy ha	1.28×10^{-7}
SCS-MP2	ethanol / def2-tzvp	orca	total energy ha	6.94×10^{-8}
SCS-MP2	ethanol / def2-tzvp	orca	correlation energy ha	6.96×10^{-8}
SCS-MP2	ethanol / sto-3g	orca	total energy ha	2.73×10^{-8}
SCS-MP2	ethanol / sto-3g	orca	correlation energy ha	2.73×10^{-8}
SOS-MP2	ethanol / def2-svp	orca	total energy ha	1.35×10^{-7}

Table S21, continued.

Method	System / basis	Ref.	Quantity	$\lvert\Delta\rvert$
SOS-MP2	ethanol / def2-svp	orca	correlation energy ha	1.34×10^{-7}
SOS-MP2	ethanol / def2-tzvp	orca	total energy ha	6.09×10^{-8}
SOS-MP2	ethanol / def2-tzvp	orca	correlation energy ha	6.19×10^{-8}
SOS-MP2	ethanol / sto-3g	orca	total energy ha	2.71×10^{-8}
SOS-MP2	ethanol / sto-3g	orca	correlation energy ha	2.68×10^{-8}
MP2	h2o / def2-svp	orca	total energy ha	2.41×10^{-8}
MP2	h2o / def2-svp	orca	correlation energy ha	2.41×10^{-8}
MP2	h2o / def2-tzvp	orca	total energy ha	2.72×10^{-8}
MP2	h2o / def2-tzvp	orca	correlation energy ha	2.64×10^{-8}
MP2	h2o / sto-3g	orca	total energy ha	6.45×10^{-9}
MP2	h2o / sto-3g	orca	correlation energy ha	6.30×10^{-9}
MP2	h2o / def2-svp	orca	total energy ha	2.40×10^{-8}
MP2	h2o / def2-svp	orca	correlation energy ha	2.38×10^{-8}
MP2	h2o / def2-tzvp	orca	total energy ha	2.73×10^{-8}
MP2	h2o / def2-tzvp	orca	correlation energy ha	2.68×10^{-8}
SCS-MP2	h2o / def2-svp	orca	total energy ha	1.04×10^{-8}
SCS-MP2	h2o / def2-svp	orca	correlation energy ha	9.90×10^{-9}
SCS-MP2	h2o / def2-tzvp	orca	total energy ha	1.74×10^{-8}
SCS-MP2	h2o / def2-tzvp	orca	correlation energy ha	1.73×10^{-8}
SCS-MP2	h2o / sto-3g	orca	total energy ha	7.35×10^{-9}
SCS-MP2	h2o / sto-3g	orca	correlation energy ha	6.40×10^{-9}
SOS-MP2	h2o / def2-svp	orca	total energy ha	3.51×10^{-9}
SOS-MP2	h2o / def2-svp	orca	correlation energy ha	3.30×10^{-9}
SOS-MP2	h2o / def2-tzvp	orca	total energy ha	1.25×10^{-8}
SOS-MP2	h2o / def2-tzvp	orca	correlation energy ha	1.18×10^{-8}
SOS-MP2	h2o / sto-3g	orca	total energy ha	7.79×10^{-9}
SOS-MP2	h2o / sto-3g	orca	correlation energy ha	6.90×10^{-9}
MP2	nh3 / def2-svp	orca	total energy ha	1.35×10^{-8}
MP2	nh3 / def2-svp	orca	correlation energy ha	1.42×10^{-8}
MP2	nh3 / def2-tzvp	orca	total energy ha	3.02×10^{-8}
MP2	nh3 / def2-tzvp	orca	correlation energy ha	3.02×10^{-8}
MP2	nh3 / sto-3g	orca	total energy ha	9.56×10^{-10}
MP2	nh3 / sto-3g	orca	correlation energy ha	9.00×10^{-10}
MP2	nh3 / def2-svp	orca	total energy ha	1.38×10^{-8}
MP2	nh3 / def2-svp	orca	correlation energy ha	1.43×10^{-8}
MP2	nh3 / def2-tzvp	orca	total energy ha	3.02×10^{-8}
MP2	nh3 / def2-tzvp	orca	correlation energy ha	2.93×10^{-8}
SCS-MP2	nh3 / def2-svp	orca	total energy ha	2.73×10^{-9}
SCS-MP2	nh3 / def2-svp	orca	correlation energy ha	3.60×10^{-9}
SCS-MP2	nh3 / def2-tzvp	orca	total energy ha	1.97×10^{-8}
SCS-MP2	nh3 / def2-tzvp	orca	correlation energy ha	1.88×10^{-8}
SCS-MP2	nh3 / sto-3g	orca	total energy ha	9.57×10^{-10}
SCS-MP2	nh3 / sto-3g	orca	correlation energy ha	1.00×10^{-9}
SOS-MP2	nh3 / def2-svp	orca	total energy ha	2.58×10^{-9}
SOS-MP2	nh3 / def2-svp	orca	correlation energy ha	2.70×10^{-9}
SOS-MP2	nh3 / def2-tzvp	orca	total energy ha	1.45×10^{-8}
SOS-MP2	nh3 / def2-tzvp	orca	correlation energy ha	1.36×10^{-8}
SOS-MP2	nh3 / sto-3g	orca	total energy ha	9.08×10^{-10}
SOS-MP2	nh3 / sto-3g	orca	correlation energy ha	1.10×10^{-9}
MP2	phenol / def2-svp	orca	total energy ha	2.21×10^{-7}
MP2	phenol / def2-svp	orca	correlation energy ha	2.24×10^{-7}
MP2	phenol / def2-tzvp	orca	total energy ha	1.38×10^{-7}
MP2	phenol / def2-tzvp	orca	correlation energy ha	1.16×10^{-7}
MP2	pyridine / def2-svp	orca	total energy ha	5.04×10^{-8}
MP2	pyridine / def2-svp	orca	correlation energy ha	5.49×10^{-8}
MP2	pyridine / def2-tzvp	orca	total energy ha	7.81×10^{-7}
MP2	pyridine / def2-tzvp	orca	correlation energy ha	7.77×10^{-7}
MP2	s22-01-ammonia-dimer / cc-pvdz	literature	interaction energy kcal mol	held

Table S21, continued.

Method	System / basis	Ref.	Quantity	$\lvert\Delta\rvert$
MP2	s22-02-water-dimer / cc-pvdz	literature	interaction energy kcal mol	held
MP2	s22-03-formic-acid-dimer / cc-pvdz	literature	interaction energy kcal mol	held
MP2	s22-04-formamide-dimer / cc-pvdz	literature	interaction energy kcal mol	held
MP2	s22-05-uracil-dimer-hb / cc-pvdz	literature	interaction energy kcal mol	held
MP2	s22-06-2-pyridone-2-aminopyridine / cc-pvdz	literature	interaction energy kcal mol	held
MP2	s22-07-adenine-thymine-wc / cc-pvdz	literature	interaction energy kcal mol	held
MP2	s22-08-methane-dimer / cc-pvdz	literature	interaction energy kcal mol	held
MP2	s22-09-ethene-dimer / cc-pvdz	literature	interaction energy kcal mol	held
MP2	s22-10-benzene-ch4 / cc-pvdz	literature	interaction energy kcal mol	held
MP2	s22-11-benzene-dimer-stack / cc-pvdz	literature	interaction energy kcal mol	held
MP2	s22-12-pyrazine-dimer / cc-pvdz	literature	interaction energy kcal mol	held
MP2	s22-13-uracil-dimer-stack / cc-pvdz	literature	interaction energy kcal mol	held
MP2	s22-14-indole-benzene-stack / cc-pvdz	literature	interaction energy kcal mol	held
MP2	s22-15-adenine-thymine-stack / cc-pvdz	literature	interaction energy kcal mol	held
MP2	s22-16-ethene-ethyne / cc-pvdz	literature	interaction energy kcal mol	held
MP2	s22-17-benzene-h2o / cc-pvdz	literature	interaction energy kcal mol	held
MP2	s22-18-benzene-nh3 / cc-pvdz	literature	interaction energy kcal mol	held
MP2	s22-19-benzene-hcn / cc-pvdz	literature	interaction energy kcal mol	held
MP2	s22-20-benzene-dimer-t / cc-pvdz	literature	interaction energy kcal mol	held
MP2	s22-21-indole-benzene-t / cc-pvdz	literature	interaction energy kcal mol	held
MP2	s22-22-phenol-dimer / cc-pvdz	literature	interaction energy kcal mol	held
MP2	h2o / def2-svp	orca	total energy ha	2.04×10^{-1}
MP2	h2o / def2-svp	orca	total energy ha	2.36×10^{-3}
MP2	oh-radical / def2-svp	orca	total energy ha	2.10×10^{-3}
MP2	oh-radical / def2-svp	orca	method total energy ha	2.10×10^{-3}
MP2	oh-radical / def2-svp	orca	method total energy ha	2.10×10^{-3}
MP2	nh2-radical / def2-svp	orca	total energy ha	1.48×10^{-1}
MP2	nh2-radical / def2-svp	orca	total energy ha	2.55×10^{-3}
SCS-MP2	h2o / def2-svp	orca	total energy ha	2.01×10^{-1}
SCS-MP2	h2o / def2-svp	orca	total energy ha	2.15×10^{-3}
SOS-MP2	h2o / def2-svp	orca	total energy ha	1.99×10^{-1}
SOS-MP2	h2o / def2-svp	orca	total energy ha	2.05×10^{-3}
DLPNO-MP2	h2o / def2-svp	orca	total energy ha	2.27×10^{-3}
DLPNO-MP2	h2o / def2-svp	orca	method total energy ha	2.27×10^{-3}
DLPNO-MP2	h2o / def2-svp	orca	method total energy ha	2.27×10^{-3}
DLPNO-MP2	oh-radical / def2-svp	orca	total energy ha	2.19×10^{-3}
DLPNO-MP2	oh-radical / def2-svp	orca	method total energy ha	2.19×10^{-3}
DLPNO-MP2	oh-radical / def2-svp	orca	method total energy ha	2.19×10^{-3}
MP2	oh-radical / sto-3g	orca	method total energy ha	4.15×10^{-5}
MP2	h2o / cc-pvdz	orca	total energy ha	2.25×10^{-3}
MP2	h2o / def2-svp	orca	total energy ha	2.36×10^{-3}
MP2	h2o / def2-svp	orca	total energy ha	2.36×10^{-3}
MP2	h2o / sto-3g	orca	total energy ha	9.57×10^{-5}
MP2	oh-radical / cc-pvdz	orca	total energy ha	2.02×10^{-3}
MP2	oh-radical / def2-svp	orca	total energy ha	2.10×10^{-3}
MP2	oh-radical / def2-svp	orca	total energy ha	2.10×10^{-3}
MP2	oh-radical / sto-3g	orca	total energy ha	4.15×10^{-5}
MP2	nh2-radical / cc-pvdz	orca	total energy ha	2.32×10^{-3}
MP2	nh2-radical / def2-svp	orca	total energy ha	2.55×10^{-3}
MP2	nh2-radical / def2-svp	orca	total energy ha	2.55×10^{-3}
SCS-MP2	h2o / cc-pvdz	orca	total energy ha	2.03×10^{-3}
SCS-MP2	h2o / def2-svp	orca	total energy ha	2.15×10^{-3}
SCS-MP2	h2o / def2-svp	orca	total energy ha	2.15×10^{-3}

Table S21, continued.

Method	System / basis	Ref.	Quantity	$\lvert\Delta\rvert$
SCS-MP2	h2o / sto-3g	orca	total energy ha	1.07×10^{-4}
SOS-MP2	h2o / cc-pvdz	orca	total energy ha	1.92×10^{-3}
SOS-MP2	h2o / def2-svp	orca	total energy ha	2.05×10^{-3}
SOS-MP2	h2o / def2-svp	orca	total energy ha	2.05×10^{-3}
SOS-MP2	h2o / sto-3g	orca	total energy ha	1.12×10^{-4}
DLPNO-MP2	h2o / cc-pvdz	orca	total energy ha	2.23×10^{-3}
DLPNO-MP2	h2o / def2-svp	orca	total energy ha	2.27×10^{-3}
DLPNO-MP2	h2o / def2-svp	orca	total energy ha	2.27×10^{-3}
DLPNO-MP2	oh-radical / cc-pvdz	orca	total energy ha	2.21×10^{-3}
DLPNO-MP2	oh-radical / def2-svp	orca	total energy ha	2.19×10^{-3}
DLPNO-MP2	oh-radical / def2-svp	orca	total energy ha	2.19×10^{-3}
MP2	h2o / def2-tzvp	orca	total energy ha	artifact-incomplete
MP2	co / def2-tzvp	orca	total energy ha	artifact-incomplete
MP2	n2 / def2-tzvp	orca	total energy ha	artifact-incomplete
MP2	hf / def2-tzvp	orca	total energy ha	artifact-incomplete
MP2	h2o / def2-svp	orca	total energy ha	artifact-incomplete
MP2	oh-radical / def2-svp	orca	total energy ha	artifact-incomplete
MP2	nh2-radical / def2-svp	orca	total energy ha	artifact-incomplete
SCS-MP2	h2o / def2-svp	orca	total energy ha	artifact-incomplete
SOS-MP2	h2o / def2-svp	orca	total energy ha	artifact-incomplete
DLPNO-MP2	h2o / def2-svp	orca	total energy ha	artifact-incomplete
DLPNO-MP2	oh-radical / def2-svp	orca	total energy ha	artifact-incomplete
MP2	h2o / sto-3g	orca	total energy ha	artifact-incomplete
MP2	h2o / sto-3g	orca	total energy ha	artifact-incomplete
MP2	oh-radical / sto-3g	orca	total energy ha	artifact-incomplete
MP2	oh-radical / sto-3g	orca	total energy ha	artifact-incomplete
MP2	nh2-radical / sto-3g	orca	total energy ha	artifact-incomplete
MP2	nh2-radical / sto-3g	orca	total energy ha	artifact-incomplete
SCS-MP2	h2o / sto-3g	orca	total energy ha	artifact-incomplete
SCS-MP2	h2o / sto-3g	orca	total energy ha	artifact-incomplete
SOS-MP2	h2o / sto-3g	orca	total energy ha	artifact-incomplete
SOS-MP2	h2o / sto-3g	orca	total energy ha	artifact-incomplete
DLPNO-MP2	h2o / sto-3g	orca	total energy ha	artifact-incomplete
DLPNO-MP2	h2o / sto-3g	orca	total energy ha	artifact-incomplete
DLPNO-MP2	oh-radical / sto-3g	orca	total energy ha	artifact-incomplete
DLPNO-MP2	oh-radical / sto-3g	orca	total energy ha	artifact-incomplete
MP2	h2o / cc-pvdz	orca	total energy ha	artifact-incomplete
MP2	h2o / def2-svp	orca	total energy ha	artifact-incomplete
MP2	h2o / sto-3g	orca	total energy ha	artifact-incomplete
MP2	oh-radical / cc-pvdz	orca	total energy ha	artifact-incomplete
MP2	oh-radical / def2-svp	orca	total energy ha	artifact-incomplete
MP2	oh-radical / sto-3g	orca	total energy ha	artifact-incomplete
MP2	nh2-radical / cc-pvdz	orca	total energy ha	artifact-incomplete
MP2	nh2-radical / def2-svp	orca	total energy ha	artifact-incomplete
MP2	nh2-radical / sto-3g	orca	total energy ha	artifact-incomplete
SCS-MP2	h2o / cc-pvdz	orca	total energy ha	artifact-incomplete
SCS-MP2	h2o / def2-svp	orca	total energy ha	artifact-incomplete
SCS-MP2	h2o / sto-3g	orca	total energy ha	artifact-incomplete
SOS-MP2	h2o / cc-pvdz	orca	total energy ha	artifact-incomplete
SOS-MP2	h2o / def2-svp	orca	total energy ha	artifact-incomplete
SOS-MP2	h2o / sto-3g	orca	total energy ha	artifact-incomplete
DLPNO-MP2	h2o / cc-pvdz	orca	total energy ha	artifact-incomplete
DLPNO-MP2	h2o / def2-svp	orca	total energy ha	artifact-incomplete
DLPNO-MP2	h2o / sto-3g	orca	total energy ha	artifact-incomplete
DLPNO-MP2	oh-radical / cc-pvdz	orca	total energy ha	artifact-incomplete
DLPNO-MP2	oh-radical / def2-svp	orca	total energy ha	artifact-incomplete
DLPNO-MP2	oh-radical / sto-3g	orca	total energy ha	artifact-incomplete
MP2	h2o / def2-svp	orca	total energy ha	reference-missing

Table S21, continued.

Method	System / basis	Ref.	Quantity	$\lvert\Delta\rvert$
MP2	oh-radical / def2-svp	orca	total energy ha	reference-missing
MP2	oh-radical / def2-svp	orca	total energy ha	reference-missing
MP2	nh2-radical / def2-svp	orca	total energy ha	reference-missing
SCS-MP2	h2o / def2-svp	orca	total energy ha	reference-missing
SOS-MP2	h2o / def2-svp	orca	total energy ha	reference-missing
DLPNO-MP2	h2o / def2-svp	orca	total energy ha	reference-missing
DLPNO-MP2	h2o / def2-svp	orca	total energy ha	reference-missing
DLPNO-MP2	oh-radical / def2-svp	orca	total energy ha	reference-missing
DLPNO-MP2	oh-radical / def2-svp	orca	total energy ha	reference-missing
MP2	h2o / sto-3g	orca	total energy ha	reference-missing
MP2	oh-radical / sto-3g	orca	total energy ha	reference-missing
SCS-MP2	h2o / sto-3g	orca	total energy ha	reference-missing
SOS-MP2	h2o / sto-3g	orca	total energy ha	reference-missing
MP2	nh2-radical / sto-3g	orca	total energy ha	blocked
DLPNO-MP2	h2o / sto-3g	orca	total energy ha	blocked
DLPNO-MP2	oh-radical / sto-3g	orca	total energy ha	blocked
MP2	nh2-radical / sto-3g	orca	total energy ha	blocked
DLPNO-MP2	h2o / sto-3g	orca	total energy ha	blocked
DLPNO-MP2	oh-radical / sto-3g	orca	total energy ha	blocked
Coupled cluster				
90 pass, 5 held, 105 fail, 114 artifact-incomplete, 35 reference-missing, 42 blocked. Median $\lvert\Delta E\rvert$ 2.7×10^{-5}, max 9.5×10^{-4} E_h.				
CCSD	h2 / cc-pvdz	orca	ccsd total energy ha	4.52×10^{-8}
CCSD	h2 / cc-pvdz	orca	ccsd total energy ha	5.17×10^{-8}
CCSD	h2 / cc-pvdz	orca	ccsd total energy ha	1.07×10^{-7}
CCSD	h2 / cc-pvdz	orca	ccsd total energy ha	1.05×10^{-6}
CCSD	h2 / cc-pvdz	orca	ccsd total energy ha	2.62×10^{-6}
CCSD	h2 / cc-pvdz	orca	ccsd total energy ha	3.51×10^{-8}
CCSD	n2 / cc-pvdz	orca	ccsd total energy ha	1.36×10^{-7}
CCSD	n2 / cc-pvdz	orca	ccsd total energy ha	3.29×10^{-7}
CCSD	n2 / cc-pvdz	orca	ccsd total energy ha	3.27×10^{-6}
CCSD	n2 / cc-pvdz	orca	ccsd total energy ha	8.20×10^{-6}
CCSD	c2h4-twisted / cc-pvdz	orca	ccsd total energy ha	1.33×10^{-7}
CCSD	h2o / cc-pvdz	orca	total energy ha	1.37×10^{-4}
CCSD	oh-radical / def2-svp	orca	total energy ha	2.22×10^{-9}
CCSD	oh-radical / def2-svp	orca	total energy ha	2.22×10^{-9}
CCSD(T)	oh-radical / def2-svp	orca	total energy ha	2.22×10^{-9}
CCSD(T)	oh-radical / def2-svp	orca	total energy ha	2.22×10^{-9}
CCSD(T)	h2o / def2-svp	orca	total energy ha	1.66×10^{-8}
CCSD(T)	h2o / def2-svp	orca	total energy ha	1.66×10^{-8}
CI	h2 / cc-pvdz	orca	total energy ha	5.46×10^{-10}
CI	h2 / cc-pvdz	orca	total energy ha	5.46×10^{-10}
CI	h2 / cc-pvdz	orca	total energy ha	5.46×10^{-10}
CI	h2 / cc-pvdz	orca	total energy ha	5.46×10^{-10}
CI	h2 / cc-pvdz	orca	total energy ha	5.46×10^{-10}
CI	h2 / cc-pvdz	orca	total energy ha	5.46×10^{-10}
CI	h2 / cc-pvdz	orca	total energy ha	5.46×10^{-10}
CI	h2 / cc-pvdz	orca	total energy ha	5.46×10^{-10}
CI	h2 / cc-pvdz	orca	total energy ha	5.46×10^{-10}
CI	h2 / cc-pvdz	orca	total energy ha	5.46×10^{-10}
CI	h2 / cc-pvdz	orca	total energy ha	5.46×10^{-10}
CI	h2 / cc-pvdz	orca	total energy ha	5.46×10^{-10}
DLPNO-CCSD	h2 / cc-pvdz	orca	total energy ha	5.46×10^{-10}
DLPNO-CCSD	h2 / cc-pvdz	orca	total energy ha	5.46×10^{-10}
dlpno-ccsd(t)	h2 / cc-pvdz	orca	total energy ha	5.46×10^{-10}
dlpno-ccsd(t)	h2 / cc-pvdz	orca	total energy ha	5.46×10^{-10}
DLPNO-CCSD	oh-radical / def2-svp	orca	total energy ha	2.22×10^{-9}

Table S21, continued.

Method	System / basis	Ref.	Quantity	$\lvert\Delta\rvert$
DLPNO-CCSD	oh-radical / def2-svp	orca	total energy ha	2.22×10^{-9}
dlpno-ccsd(t)	oh-radical / def2-svp	orca	total energy ha	2.22×10^{-9}
dlpno-ccsd(t)	oh-radical / def2-svp	orca	total energy ha	2.22×10^{-9}
DLPNO-CCSD(T)	h2o-dimer / cc-pvdz	orca	total energy ha	1.35×10^{-4}
DLPNO-CCSD(T)	h2o-dimer / cc-pvtz	orca	total energy ha	4.32×10^{-4}
DLPNO-CCSD(T)	h2o2 / def2-svp	orca	total energy ha	6.83×10^{-4}
DLPNO-CCSD(T)	h2o2 / def2-tzvp	orca	total energy ha	9.35×10^{-4}
DLPNO-CCSD(T)	h2o2 / cc-pvdz	orca	total energy ha	4.88×10^{-4}
DLPNO-CCSD(T)	h2o2 / cc-pvtz	orca	total energy ha	9.02×10^{-4}
DLPNO-CCSD(T)	lih / def2-svp	orca	total energy ha	7.99×10^{-6}
DLPNO-CCSD(T)	lih / def2-tzvp	orca	total energy ha	1.41×10^{-5}
DLPNO-CCSD(T)	lih / cc-pvdz	orca	total energy ha	3.48×10^{-5}
DLPNO-CCSD(T)	lih / cc-pvtz	orca	total energy ha	2.79×10^{-5}
DLPNO-CCSD(T)	lih / cc-pvqz	orca	total energy ha	3.18×10^{-5}
DLPNO-CCSD(T)	o2-triplet / def2-svp	orca	total energy ha	9.49×10^{-4}
DLPNO-CCSD(T)	o2-triplet / cc-pvdz	orca	total energy ha	5.44×10^{-4}
CCSD(T)	co2 / def2-svp	orca	total energy ha	3.51×10^{-4}
CCSD(T)	co2 / cc-pvdz	orca	total energy ha	4.33×10^{-4}
CCSD(T)	h2o-dimer / cc-pvdz	orca	total energy ha	2.76×10^{-4}
CCSD(T)	h2o-dimer / cc-pvtz	orca	total energy ha	3.63×10^{-4}
DLPNO-CCSD(T)	h2o-dimer / cc-pvdz	orca	total energy ha	1.35×10^{-4}
DLPNO-CCSD(T)	h2o-dimer / cc-pvtz	orca	total energy ha	4.32×10^{-4}
CCSD(T)	h2o2 / def2-svp	orca	total energy ha	1.76×10^{-4}
CCSD(T)	h2o2 / cc-pvdz	orca	total energy ha	2.81×10^{-4}
DLPNO-CCSD(T)	h2o2 / def2-svp	orca	total energy ha	6.83×10^{-4}
DLPNO-CCSD(T)	h2o2 / def2-tzvp	orca	total energy ha	9.35×10^{-4}
DLPNO-CCSD(T)	h2o2 / cc-pvdz	orca	total energy ha	4.88×10^{-4}
DLPNO-CCSD(T)	h2o2 / cc-pvtz	orca	total energy ha	9.02×10^{-4}
CCSD(T)	lih / cc-pvdz	orca	total energy ha	3.64×10^{-5}
CCSD(T)	lih / cc-pvtz	orca	total energy ha	2.22×10^{-6}
CCSD(T)	lih / cc-pvqz	orca	total energy ha	2.63×10^{-5}
DLPNO-CCSD(T)	lih / def2-svp	orca	total energy ha	7.99×10^{-6}
DLPNO-CCSD(T)	lih / def2-tzvp	orca	total energy ha	1.41×10^{-5}
DLPNO-CCSD(T)	lih / cc-pvdz	orca	total energy ha	3.48×10^{-5}
DLPNO-CCSD(T)	lih / cc-pvtz	orca	total energy ha	2.79×10^{-5}
DLPNO-CCSD(T)	lih / cc-pvqz	orca	total energy ha	3.18×10^{-5}
CCSD(T)	o2-triplet / def2-svp	orca	total energy ha	2.18×10^{-4}
CCSD(T)	o2-triplet / cc-pvdz	orca	total energy ha	3.17×10^{-4}
DLPNO-CCSD(T)	o2-triplet / def2-svp	orca	total energy ha	9.49×10^{-4}
DLPNO-CCSD(T)	o2-triplet / cc-pvdz	orca	total energy ha	5.44×10^{-4}
CCSD(T)	cyclopropene / def2-svp	orca	total energy ha	3.51×10^{-4}
DLPNO-CCSD(T)	h2o-dimer / def2-tzvp	orca	total energy ha	7.92×10^{-5}
DLPNO-CCSD(T)	h2o-dimer / cc-pvdz	orca	total energy ha	1.35×10^{-4}
DLPNO-CCSD(T)	h2o-dimer / cc-pvtz	orca	total energy ha	4.32×10^{-4}
DLPNO-CCSD(T)	h2o2 / def2-svp	orca	total energy ha	6.83×10^{-4}
DLPNO-CCSD(T)	h2o2 / cc-pvdz	orca	total energy ha	4.88×10^{-4}
DLPNO-CCSD(T)	h2o2 / cc-pvtz	orca	total energy ha	9.02×10^{-4}
DLPNO-CCSD(T)	lih / def2-svp	orca	total energy ha	7.99×10^{-6}
DLPNO-CCSD(T)	lih / def2-tzvp	orca	total energy ha	1.41×10^{-5}
DLPNO-CCSD(T)	lih / cc-pvdz	orca	total energy ha	3.48×10^{-5}
DLPNO-CCSD(T)	lih / cc-pvtz	orca	total energy ha	2.79×10^{-5}
DLPNO-CCSD(T)	lih / cc-pvqz	orca	total energy ha	3.18×10^{-5}
CCSD(T)	nitromethane / def2-svp	orca	total energy ha	4.45×10^{-4}
DLPNO-CCSD(T)	o2-triplet / def2-svp	orca	total energy ha	9.49×10^{-4}
DLPNO-CCSD(T)	o2-triplet / cc-pvdz	orca	total energy ha	5.44×10^{-4}
CCSD(T)	s22-01-ammonia-dimer / cc-pvdz	literature	interaction energy kcal mol	held
CCSD(T)	s22-02-water-dimer / cc-pvdz	literature	interaction energy kcal mol	held
CCSD(T)	s22-08-methane-dimer / cc-pvdz	literature	interaction energy kcal mol	held

Table S21, continued.

Method	System / basis	Ref.	Quantity	$\lvert\Delta\rvert$
CCSD(T)	s22-09-ethene-dimer / cc-pvdz	literature	interaction energy kcal mol	held
CCSD(T)	s22-16-ethene-ethyne / cc-pvdz	literature	interaction energy kcal mol	held
CCSD	c2h4-twisted / cc-pvdz	orca	ccsd total energy ha	7.35×10^{-2}
CCSD	h2 / cc-pvdz	orca	total energy ha	3.47×10^{-2}
CCSD	h2 / cc-pvdz	orca	total energy ha	4.41×10^{-5}
CCSD(T)	h2 / cc-pvdz	orca	total energy ha	3.47×10^{-2}
CCSD(T)	h2 / cc-pvdz	orca	total energy ha	4.41×10^{-5}
CCSD	oh-radical / def2-svp	orca	total energy ha	4.62×10^{-5}
CCSD	oh-radical / def2-svp	orca	method total energy ha	4.62×10^{-5}
CCSD	oh-radical / def2-svp	orca	method total energy ha	4.62×10^{-5}
CCSD(T)	oh-radical / def2-svp	orca	total energy ha	4.71×10^{-5}
CCSD(T)	oh-radical / def2-svp	orca	method total energy ha	4.71×10^{-5}
CCSD(T)	oh-radical / def2-svp	orca	method total energy ha	4.71×10^{-5}
CCSD	nh2-radical / def2-svp	orca	total energy ha	1.67×10^{-1}
CCSD	nh2-radical / def2-svp	orca	total energy ha	1.55×10^{-5}
CCSD(T)	nh2-radical / def2-svp	orca	total energy ha	1.69×10^{-1}
CCSD(T)	nh2-radical / def2-svp	orca	total energy ha	2.54×10^{-5}
CCSD(T)	h2o / def2-svp	orca	total energy ha	7.40×10^{-5}
CCSD(T)	h2o / def2-svp	orca	method total energy ha	7.40×10^{-5}
CCSD(T)	h2o / def2-svp	orca	method total energy ha	7.40×10^{-5}
CI	h2 / cc-pvdz	orca	total energy ha	3.46×10^{-2}
CI	h2 / cc-pvdz	orca	total energy ha	4.42×10^{-5}
CI	h2 / cc-pvdz	orca	total energy ha	4.66×10^{-5}
CI	h2 / cc-pvdz	orca	method total energy ha	4.66×10^{-5}
CI	h2 / cc-pvdz	orca	method total energy ha	4.66×10^{-5}
CI	h2 / cc-pvdz	orca	total energy ha	4.64×10^{-5}
CI	h2 / cc-pvdz	orca	method total energy ha	4.64×10^{-5}
CI	h2 / cc-pvdz	orca	method total energy ha	4.64×10^{-5}
CI	h2 / cc-pvdz	orca	total energy ha	4.64×10^{-5}
CI	h2 / cc-pvdz	orca	method total energy ha	4.64×10^{-5}
CI	h2 / cc-pvdz	orca	method total energy ha	4.64×10^{-5}
CI	h2 / cc-pvdz	orca	total energy ha	4.41×10^{-5}
CI	h2 / cc-pvdz	orca	method total energy ha	4.41×10^{-5}
CI	h2 / cc-pvdz	orca	method total energy ha	4.41×10^{-5}
CI	h2 / cc-pvdz	orca	total energy ha	4.41×10^{-5}
CI	h2 / cc-pvdz	orca	method total energy ha	4.41×10^{-5}
CI	h2 / cc-pvdz	orca	method total energy ha	4.41×10^{-5}
CI	h2 / cc-pvdz	orca	total energy ha	4.41×10^{-5}
CI	h2 / cc-pvdz	orca	method total energy ha	4.41×10^{-5}
CI	h2 / cc-pvdz	orca	method total energy ha	4.41×10^{-5}
CI	h2 / cc-pvdz	orca	total energy ha	3.47×10^{-2}
CI	h2 / cc-pvdz	orca	total energy ha	4.48×10^{-5}
CI	h2 / cc-pvdz	orca	total energy ha	3.47×10^{-2}
CI	h2 / cc-pvdz	orca	total energy ha	4.48×10^{-5}
DLPNO-CCSD	h2 / cc-pvdz	orca	total energy ha	3.75×10^{-5}
DLPNO-CCSD	h2 / cc-pvdz	orca	method total energy ha	3.75×10^{-5}
DLPNO-CCSD	h2 / cc-pvdz	orca	method total energy ha	3.75×10^{-5}
dlpno-ccsd(t)	h2 / cc-pvdz	orca	total energy ha	3.75×10^{-5}
dlpno-ccsd(t)	h2 / cc-pvdz	orca	method total energy ha	3.75×10^{-5}
dlpno-ccsd(t)	h2 / cc-pvdz	orca	method total energy ha	3.75×10^{-5}
DLPNO-CCSD	oh-radical / def2-svp	orca	total energy ha	1.86×10^{-3}
DLPNO-CCSD	oh-radical / def2-svp	orca	method total energy ha	1.86×10^{-3}
DLPNO-CCSD	oh-radical / def2-svp	orca	method total energy ha	1.86×10^{-3}
dlpno-ccsd(t)	oh-radical / def2-svp	orca	total energy ha	1.92×10^{-3}
dlpno-ccsd(t)	oh-radical / def2-svp	orca	method total energy ha	1.92×10^{-3}
dlpno-ccsd(t)	oh-radical / def2-svp	orca	method total energy ha	1.92×10^{-3}
CCSD	h2 / cc-pvdz	orca	total energy ha	4.41×10^{-5}
CCSD	h2 / cc-pvtz	orca	total energy ha	3.54×10^{-5}

Table S21, continued.

Method	System / basis	Ref.	Quantity	$\lvert\Delta\rvert$
CCSD(T)	h2 / cc-pvdz	orca	total energy ha	4.41×10^{-5}
CCSD(T)	h2 / cc-pvtz	orca	total energy ha	3.54×10^{-5}
CCSD	oh-radical / def2-svp	orca	total energy ha	4.62×10^{-5}
CCSD	oh-radical / def2-svp	orca	total energy ha	4.62×10^{-5}
CCSD(T)	oh-radical / def2-svp	orca	total energy ha	4.71×10^{-5}
CCSD(T)	oh-radical / def2-svp	orca	total energy ha	4.71×10^{-5}
CCSD	nh2-radical / def2-svp	orca	total energy ha	1.55×10^{-5}
CCSD	nh2-radical / def2-svp	orca	total energy ha	1.55×10^{-5}
CCSD(T)	nh2-radical / def2-svp	orca	total energy ha	2.54×10^{-5}
CCSD(T)	nh2-radical / def2-svp	orca	total energy ha	2.54×10^{-5}
CCSD(T)	h2o / def2-svp	orca	total energy ha	7.40×10^{-5}
CCSD(T)	h2o / def2-svp	orca	total energy ha	7.40×10^{-5}
CI	h2 / cc-pvdz	orca	total energy ha	4.42×10^{-5}
CI	h2 / cc-pvtz	orca	total energy ha	3.53×10^{-5}
CI	h2 / cc-pvdz	orca	total energy ha	4.66×10^{-5}
CI	h2 / cc-pvtz	orca	total energy ha	3.64×10^{-5}
CI	h2 / cc-pvdz	orca	total energy ha	4.64×10^{-5}
CI	h2 / cc-pvtz	orca	total energy ha	3.64×10^{-5}
CI	h2 / cc-pvdz	orca	total energy ha	4.64×10^{-5}
CI	h2 / cc-pvtz	orca	total energy ha	3.64×10^{-5}
CI	h2 / cc-pvdz	orca	total energy ha	4.41×10^{-5}
CI	h2 / cc-pvtz	orca	total energy ha	3.54×10^{-5}
CI	h2 / cc-pvdz	orca	total energy ha	4.41×10^{-5}
CI	h2 / cc-pvtz	orca	total energy ha	3.54×10^{-5}
CI	h2 / cc-pvdz	orca	total energy ha	4.41×10^{-5}
CI	h2 / cc-pvtz	orca	total energy ha	3.54×10^{-5}
CI	h2 / cc-pvdz	orca	total energy ha	4.48×10^{-5}
CI	h2 / cc-pvtz	orca	total energy ha	3.60×10^{-5}
CI	h2 / cc-pvdz	orca	total energy ha	4.48×10^{-5}
CI	h2 / cc-pvtz	orca	total energy ha	3.60×10^{-5}
DLPNO-CCSD	h2 / cc-pvdz	orca	total energy ha	3.75×10^{-5}
DLPNO-CCSD	h2 / cc-pvtz	orca	total energy ha	2.47×10^{-5}
dlpno-ccsd(t)	h2 / cc-pvdz	orca	total energy ha	3.75×10^{-5}
dlpno-ccsd(t)	h2 / cc-pvtz	orca	total energy ha	2.47×10^{-5}
DLPNO-CCSD	oh-radical / def2-svp	orca	total energy ha	1.86×10^{-3}
DLPNO-CCSD	oh-radical / def2-svp	orca	total energy ha	1.86×10^{-3}
dlpno-ccsd(t)	oh-radical / def2-svp	orca	total energy ha	1.92×10^{-3}
dlpno-ccsd(t)	oh-radical / def2-svp	orca	total energy ha	1.92×10^{-3}
DLPNO-CCSD(T)	co2 / cc-pvdz	orca	total energy ha	1.18×10^{-3}
DLPNO-CCSD(T)	co2 / def2-svp	orca	total energy ha	1.18×10^{-3}
DLPNO-CCSD(T)	co2 / cc-pvdz	orca	total energy ha	1.18×10^{-3}
CCSD(T)	lih / def2-svp	orca	total energy ha	2.81×10^{-3}
CCSD(T)	lih / def2-tzvp	orca	total energy ha	3.54×10^{-2}
DLPNO-CCSD(T)	co2 / def2-svp	orca	total energy ha	1.18×10^{-3}
DLPNO-CCSD(T)	co2 / cc-pvdz	orca	total energy ha	1.18×10^{-3}
DLPNO-CCSD(T)	cyclopropene / cc-pvdz	orca	total energy ha	1.32×10^{-2}
CCSD(T)	nitromethane / cc-pvdz	orca	total energy ha	5.85×10^{-4}
DLPNO-CCSD(T)	nitromethane / def2-svp	orca	total energy ha	6.43×10^{-3}
DLPNO-CCSD(T)	nitromethane / cc-pvdz	orca	total energy ha	6.14×10^{-3}
CCSD(T)	h2 / cc-pvdz	orca	total energy ha	artifact-incomplete
CCSD	h2 / cc-pvdz	orca	total energy ha	artifact-incomplete
CCSD(T)	h2 / cc-pvdz	orca	total energy ha	artifact-incomplete
CCSD	oh-radical / def2-svp	orca	total energy ha	artifact-incomplete
CCSD(T)	oh-radical / def2-svp	orca	total energy ha	artifact-incomplete
CCSD	nh2-radical / def2-svp	orca	total energy ha	artifact-incomplete
CCSD(T)	nh2-radical / def2-svp	orca	total energy ha	artifact-incomplete
CCSD(T)	h2o / def2-svp	orca	total energy ha	artifact-incomplete
CI	h2 / cc-pvdz	orca	total energy ha	artifact-incomplete

Table S21, continued.

Method	System / basis	Ref.	Quantity	|Δ|
CI	h2 / cc-pvdz	orca	total energy ha	artifact-incomplete
CI	h2 / cc-pvdz	orca	total energy ha	artifact-incomplete
CI	h2 / cc-pvdz	orca	total energy ha	artifact-incomplete
CI	h2 / cc-pvdz	orca	total energy ha	artifact-incomplete
CI	h2 / cc-pvdz	orca	total energy ha	artifact-incomplete
CI	h2 / cc-pvdz	orca	total energy ha	artifact-incomplete
CI	h2 / cc-pvdz	orca	total energy ha	artifact-incomplete
CI	h2 / cc-pvdz	orca	total energy ha	artifact-incomplete
DLPNO-CCSD	h2 / cc-pvdz	orca	total energy ha	artifact-incomplete
dlpno-ccsd(t)	h2 / cc-pvdz	orca	total energy ha	artifact-incomplete
DLPNO-CCSD	oh-radical / def2-svp	orca	total energy ha	artifact-incomplete
dlpno-ccsd(t)	oh-radical / def2-svp	orca	total energy ha	artifact-incomplete
CCSD	h2 / sto-3g	orca	total energy ha	artifact-incomplete
CCSD	h2 / sto-3g	orca	total energy ha	artifact-incomplete
CCSD(T)	h2 / sto-3g	orca	total energy ha	artifact-incomplete
CCSD(T)	h2 / sto-3g	orca	total energy ha	artifact-incomplete
CCSD	oh-radical / sto-3g	orca	total energy ha	artifact-incomplete
CCSD	oh-radical / sto-3g	orca	total energy ha	artifact-incomplete
CCSD(T)	oh-radical / sto-3g	orca	total energy ha	artifact-incomplete
CCSD(T)	oh-radical / sto-3g	orca	total energy ha	artifact-incomplete
CCSD	nh2-radical / sto-3g	orca	total energy ha	artifact-incomplete
CCSD	nh2-radical / sto-3g	orca	total energy ha	artifact-incomplete
CCSD(T)	nh2-radical / sto-3g	orca	total energy ha	artifact-incomplete
CCSD(T)	nh2-radical / sto-3g	orca	total energy ha	artifact-incomplete
CCSD(T)	h2o / sto-3g	orca	total energy ha	artifact-incomplete
CCSD(T)	h2o / sto-3g	orca	total energy ha	artifact-incomplete
CI	h2 / sto-3g	orca	total energy ha	artifact-incomplete
CI	h2 / sto-3g	orca	total energy ha	artifact-incomplete
CI	h2 / sto-3g	orca	total energy ha	artifact-incomplete
CI	h2 / sto-3g	orca	total energy ha	artifact-incomplete
CI	h2 / sto-3g	orca	total energy ha	artifact-incomplete
CI	h2 / sto-3g	orca	total energy ha	artifact-incomplete
CI	h2 / sto-3g	orca	total energy ha	artifact-incomplete
CI	h2 / sto-3g	orca	total energy ha	artifact-incomplete
CI	h2 / sto-3g	orca	total energy ha	artifact-incomplete
CI	h2 / sto-3g	orca	total energy ha	artifact-incomplete
CI	h2 / sto-3g	orca	total energy ha	artifact-incomplete
CI	h2 / sto-3g	orca	total energy ha	artifact-incomplete
CI	h2 / sto-3g	orca	total energy ha	artifact-incomplete
CI	h2 / sto-3g	orca	total energy ha	artifact-incomplete
CI	h2 / sto-3g	orca	total energy ha	artifact-incomplete
CI	h2 / sto-3g	orca	total energy ha	artifact-incomplete
CI	h2 / sto-3g	orca	total energy ha	artifact-incomplete
CI	h2 / sto-3g	orca	total energy ha	artifact-incomplete
CI	h2 / sto-3g	orca	total energy ha	artifact-incomplete
CI	h2 / sto-3g	orca	total energy ha	artifact-incomplete
DLPNO-CCSD	h2 / sto-3g	orca	total energy ha	artifact-incomplete
DLPNO-CCSD	h2 / sto-3g	orca	total energy ha	artifact-incomplete
dlpno-ccsd(t)	h2 / sto-3g	orca	total energy ha	artifact-incomplete
dlpno-ccsd(t)	h2 / sto-3g	orca	total energy ha	artifact-incomplete
DLPNO-CCSD	oh-radical / sto-3g	orca	total energy ha	artifact-incomplete
DLPNO-CCSD	oh-radical / sto-3g	orca	total energy ha	artifact-incomplete
dlpno-ccsd(t)	oh-radical / sto-3g	orca	total energy ha	artifact-incomplete
dlpno-ccsd(t)	oh-radical / sto-3g	orca	total energy ha	artifact-incomplete
CCSD	h2 / cc-pvdz	orca	total energy ha	artifact-incomplete
CCSD	h2 / sto-3g	orca	total energy ha	artifact-incomplete
CCSD	h2 / cc-pvtz	orca	total energy ha	artifact-incomplete
CCSD(T)	h2 / cc-pvdz	orca	total energy ha	artifact-incomplete
CCSD(T)	h2 / sto-3g	orca	total energy ha	artifact-incomplete
CCSD(T)	h2 / cc-pvtz	orca	total energy ha	artifact-incomplete

Table S21, continued.

Method	System / basis	Ref.	Quantity	|Δ|
CCSD	oh-radical / def2-svp	orca	total energy ha	artifact-incomplete
CCSD	oh-radical / sto-3g	orca	total energy ha	artifact-incomplete
CCSD(T)	oh-radical / def2-svp	orca	total energy ha	artifact-incomplete
CCSD(T)	oh-radical / sto-3g	orca	total energy ha	artifact-incomplete
CCSD	nh2-radical / def2-svp	orca	total energy ha	artifact-incomplete
CCSD	nh2-radical / sto-3g	orca	total energy ha	artifact-incomplete
CCSD(T)	nh2-radical / def2-svp	orca	total energy ha	artifact-incomplete
CCSD(T)	nh2-radical / sto-3g	orca	total energy ha	artifact-incomplete
CCSD(T)	h2o / def2-svp	orca	total energy ha	artifact-incomplete
CCSD(T)	h2o / sto-3g	orca	total energy ha	artifact-incomplete
CI	h2 / cc-pvdz	orca	total energy ha	artifact-incomplete
CI	h2 / sto-3g	orca	total energy ha	artifact-incomplete
CI	h2 / cc-pvtz	orca	total energy ha	artifact-incomplete
CI	h2 / cc-pvdz	orca	total energy ha	artifact-incomplete
CI	h2 / sto-3g	orca	total energy ha	artifact-incomplete
CI	h2 / cc-pvtz	orca	total energy ha	artifact-incomplete
CI	h2 / cc-pvdz	orca	total energy ha	artifact-incomplete
CI	h2 / sto-3g	orca	total energy ha	artifact-incomplete
CI	h2 / cc-pvtz	orca	total energy ha	artifact-incomplete
CI	h2 / cc-pvdz	orca	total energy ha	artifact-incomplete
CI	h2 / sto-3g	orca	total energy ha	artifact-incomplete
CI	h2 / cc-pvtz	orca	total energy ha	artifact-incomplete
CI	h2 / cc-pvdz	orca	total energy ha	artifact-incomplete
CI	h2 / sto-3g	orca	total energy ha	artifact-incomplete
CI	h2 / cc-pvtz	orca	total energy ha	artifact-incomplete
CI	h2 / cc-pvdz	orca	total energy ha	artifact-incomplete
CI	h2 / sto-3g	orca	total energy ha	artifact-incomplete
CI	h2 / cc-pvtz	orca	total energy ha	artifact-incomplete
CI	h2 / cc-pvdz	orca	total energy ha	artifact-incomplete
CI	h2 / sto-3g	orca	total energy ha	artifact-incomplete
CI	h2 / cc-pvtz	orca	total energy ha	artifact-incomplete
CI	h2 / cc-pvdz	orca	total energy ha	artifact-incomplete
CI	h2 / sto-3g	orca	total energy ha	artifact-incomplete
CI	h2 / cc-pvtz	orca	total energy ha	artifact-incomplete
DLPNO-CCSD	h2 / cc-pvdz	orca	total energy ha	artifact-incomplete
DLPNO-CCSD	h2 / sto-3g	orca	total energy ha	artifact-incomplete
DLPNO-CCSD	h2 / cc-pvtz	orca	total energy ha	artifact-incomplete
dlpno-ccsd(t)	h2 / cc-pvdz	orca	total energy ha	artifact-incomplete
dlpno-ccsd(t)	h2 / sto-3g	orca	total energy ha	artifact-incomplete
dlpno-ccsd(t)	h2 / cc-pvtz	orca	total energy ha	artifact-incomplete
DLPNO-CCSD	oh-radical / def2-svp	orca	total energy ha	artifact-incomplete
DLPNO-CCSD	oh-radical / sto-3g	orca	total energy ha	artifact-incomplete
dlpno-ccsd(t)	oh-radical / def2-svp	orca	total energy ha	artifact-incomplete
dlpno-ccsd(t)	oh-radical / sto-3g	orca	total energy ha	artifact-incomplete
CCSD	h2 / cc-pvdz	orca	total energy ha	reference-missing
CCSD(T)	h2 / cc-pvdz	orca	total energy ha	reference-missing
CCSD	oh-radical / def2-svp	orca	total energy ha	reference-missing
CCSD	oh-radical / def2-svp	orca	total energy ha	reference-missing
CCSD(T)	oh-radical / def2-svp	orca	total energy ha	reference-missing
CCSD(T)	oh-radical / def2-svp	orca	total energy ha	reference-missing
CCSD	nh2-radical / def2-svp	orca	total energy ha	reference-missing
CCSD(T)	nh2-radical / def2-svp	orca	total energy ha	reference-missing
CCSD(T)	h2o / def2-svp	orca	total energy ha	reference-missing
CCSD(T)	h2o / def2-svp	orca	total energy ha	reference-missing
CI	h2 / cc-pvdz	orca	total energy ha	reference-missing

Table S21, continued.

Method	System / basis	Ref.	Quantity	|Δ|
CI	h2 / cc-pvdz	orca	total energy ha	reference-missing
CI	h2 / cc-pvdz	orca	total energy ha	reference-missing
CI	h2 / cc-pvdz	orca	total energy ha	reference-missing
CI	h2 / cc-pvdz	orca	total energy ha	reference-missing
CI	h2 / cc-pvdz	orca	total energy ha	reference-missing
CI	h2 / cc-pvdz	orca	total energy ha	reference-missing
CI	h2 / cc-pvdz	orca	total energy ha	reference-missing
CI	h2 / cc-pvdz	orca	total energy ha	reference-missing
CI	h2 / cc-pvdz	orca	total energy ha	reference-missing
CI	h2 / cc-pvdz	orca	total energy ha	reference-missing
CI	h2 / cc-pvdz	orca	total energy ha	reference-missing
CI	h2 / cc-pvdz	orca	total energy ha	reference-missing
CI	h2 / cc-pvdz	orca	total energy ha	reference-missing
DLPNO-CCSD	h2 / cc-pvdz	orca	total energy ha	reference-missing
DLPNO-CCSD	h2 / cc-pvdz	orca	total energy ha	reference-missing
dlpno-ccsd(t)	h2 / cc-pvdz	orca	total energy ha	reference-missing
dlpno-ccsd(t)	h2 / cc-pvdz	orca	total energy ha	reference-missing
DLPNO-CCSD	oh-radical / def2-svp	orca	total energy ha	reference-missing
DLPNO-CCSD	oh-radical / def2-svp	orca	total energy ha	reference-missing
dlpno-ccsd(t)	oh-radical / def2-svp	orca	total energy ha	reference-missing
dlpno-ccsd(t)	oh-radical / def2-svp	orca	total energy ha	reference-missing
CCSD	h2 / def2-svp	orca	total energy ha	reference-missing
CCSD(T)	h2 / def2-svp	orca	total energy ha	reference-missing
CCSD(T)	h2 / 3-21g	orca	energy total ha	blocked
CCSD	h2 / sto-3g	orca	total energy ha	blocked
CCSD(T)	h2 / sto-3g	orca	total energy ha	blocked
CCSD	oh-radical / sto-3g	orca	total energy ha	blocked
CCSD(T)	oh-radical / sto-3g	orca	total energy ha	blocked
CCSD	nh2-radical / sto-3g	orca	total energy ha	blocked
CCSD(T)	nh2-radical / sto-3g	orca	total energy ha	blocked
CCSD(T)	h2o / sto-3g	orca	total energy ha	blocked
CI	h2 / sto-3g	orca	total energy ha	blocked
CI	h2 / sto-3g	orca	total energy ha	blocked
CI	h2 / sto-3g	orca	total energy ha	blocked
CI	h2 / sto-3g	orca	total energy ha	blocked
CI	h2 / sto-3g	orca	total energy ha	blocked
CI	h2 / sto-3g	orca	total energy ha	blocked
CI	h2 / sto-3g	orca	total energy ha	blocked
CI	h2 / sto-3g	orca	total energy ha	blocked
CI	h2 / sto-3g	orca	total energy ha	blocked
DLPNO-CCSD	h2 / sto-3g	orca	total energy ha	blocked
dlpno-ccsd(t)	h2 / sto-3g	orca	total energy ha	blocked
DLPNO-CCSD	oh-radical / sto-3g	orca	total energy ha	blocked
dlpno-ccsd(t)	oh-radical / sto-3g	orca	total energy ha	blocked
CCSD	h2 / sto-3g	orca	total energy ha	blocked
CCSD(T)	h2 / sto-3g	orca	total energy ha	blocked
CCSD	oh-radical / sto-3g	orca	total energy ha	blocked
CCSD(T)	oh-radical / sto-3g	orca	total energy ha	blocked
CCSD	nh2-radical / sto-3g	orca	total energy ha	blocked
CCSD(T)	nh2-radical / sto-3g	orca	total energy ha	blocked
CCSD(T)	h2o / sto-3g	orca	total energy ha	blocked
CI	h2 / sto-3g	orca	total energy ha	blocked
CI	h2 / sto-3g	orca	total energy ha	blocked
CI	h2 / sto-3g	orca	total energy ha	blocked
CI	h2 / sto-3g	orca	total energy ha	blocked
CI	h2 / sto-3g	orca	total energy ha	blocked
CI	h2 / sto-3g	orca	total energy ha	blocked

Table S21, continued.

Method	System / basis	Ref.	Quantity	$\lvert\Delta\rvert$
CI	h2 / sto-3g	orca	total energy ha	blocked
CI	h2 / sto-3g	orca	total energy ha	blocked
CI	h2 / sto-3g	orca	total energy ha	blocked
DLPNO-CCSD	h2 / sto-3g	orca	total energy ha	blocked
dlpno-ccsd(t)	h2 / sto-3g	orca	total energy ha	blocked
DLPNO-CCSD	oh-radical / sto-3g	orca	total energy ha	blocked
dlpno-ccsd(t)	oh-radical / sto-3g	orca	total energy ha	blocked
CCSD(T)	cyclopropene / cc-pvdz	orca	total energy ha	blocked
Local correlation (DLPNO)				
186 pass, 267 held, 173 fail, 2 reference-missing, 35 blocked. Median $\lvert\Delta E\rvert$ 8.2×10^{-4}, max 4.7×10^{-3} E_h.				
dlpno-ccsd(t)	s22-01-ammonia-dimer / cc-pvdz	internal	local correlation energy ha	3.88×10^{-4}
dlpno-ccsd(t)	s22-01-ammonia-dimer / cc-pvdz	internal	interaction energy kcalmol	5.05×10^{-4}
dlpno-ccsd(t)	s22-01-ammonia-dimer / cc-pvdz	internal	local correlation energy ha	7.48×10^{-4}
dlpno-ccsd(t)	s22-01-ammonia-dimer / cc-pvdz	internal	interaction energy kcalmol	8.94×10^{-4}
dlpno-ccsd(t)	s22-01-ammonia-dimer / cc-pvdz	internal	local correlation energy ha	1.32×10^{-3}
dlpno-ccsd(t)	s22-01-ammonia-dimer / cc-pvdz	internal	interaction energy kcalmol	7.38×10^{-4}
DLPNO-MP2	s22-01-ammonia-dimer / cc-pvdz	internal	local truncation error interaction energy kcal mol	3.15×10^{-4}
DLPNO-MP2	s22-01-ammonia-dimer / cc-pvdz	internal	local truncation error interaction energy kcal mol	4.45×10^{-4}
DLPNO-MP2	s22-01-ammonia-dimer / cc-pvdz	internal	local truncation error interaction energy kcal mol	4.72×10^{-4}
DLPNO-MP2	s22-01-ammonia-dimer / cc-pvdz	internal	local correlation energy ha	3.05×10^{-3}
DLPNO-MP2	s22-01-ammonia-dimer / cc-pvdz	internal	interaction energy kcalmol	3.15×10^{-4}
DLPNO-MP2	s22-01-ammonia-dimer / cc-pvdz	internal	local correlation energy ha	1.99×10^{-3}
DLPNO-MP2	s22-01-ammonia-dimer / cc-pvdz	internal	interaction energy kcalmol	4.45×10^{-4}
dlpno-ccsd(t)	s22-01-ammonia-dimer-monoA / cc-pvdz	internal	local correlation energy ha	4.46×10^{-4}
dlpno-ccsd(t)	s22-01-ammonia-dimer-monoA / cc-pvdz	internal	local correlation energy ha	8.21×10^{-4}
dlpno-ccsd(t)	s22-01-ammonia-dimer-monoA / cc-pvdz	internal	local correlation energy ha	1.03×10^{-3}
DLPNO-MP2	s22-01-ammonia-dimer-monoA / cc-pvdz	internal	local correlation energy ha	1.68×10^{-3}
DLPNO-MP2	s22-01-ammonia-dimer-monoA / cc-pvdz	internal	local correlation energy ha	1.22×10^{-3}
DLPNO-MP2	s22-01-ammonia-dimer-monoA / cc-pvdz	internal	local correlation energy ha	9.51×10^{-4}
dlpno-ccsd(t)	s22-01-ammonia-dimer-monoB / cc-pvdz	internal	local correlation energy ha	4.46×10^{-4}
dlpno-ccsd(t)	s22-01-ammonia-dimer-monoB / cc-pvdz	internal	local correlation energy ha	8.21×10^{-4}
dlpno-ccsd(t)	s22-01-ammonia-dimer-monoB / cc-pvdz	internal	local correlation energy ha	1.03×10^{-3}
DLPNO-MP2	s22-01-ammonia-dimer-monoB / cc-pvdz	internal	local correlation energy ha	1.68×10^{-3}
DLPNO-MP2	s22-01-ammonia-dimer-monoB / cc-pvdz	internal	local correlation energy ha	1.22×10^{-3}
DLPNO-MP2	s22-01-ammonia-dimer-monoB / cc-pvdz	internal	local correlation energy ha	9.51×10^{-4}
DLPNO-MP2	s22-01-ammonia-dimer / cc-pvdz	internal	local correlation energy ha	1.43×10^{-3}
DLPNO-MP2	s22-01-ammonia-dimer / cc-pvdz	internal	interaction energy kcalmol	4.72×10^{-4}
dlpno-ccsd(t)	s22-02-water-dimer / cc-pvdz	internal	local correlation energy ha	9.41×10^{-4}
dlpno-ccsd(t)	s22-02-water-dimer / cc-pvdz	internal	interaction energy kcalmol	8.80×10^{-4}
dlpno-ccsd(t)	s22-02-water-dimer / cc-pvdz	internal	local correlation energy ha	8.40×10^{-5}
dlpno-ccsd(t)	s22-02-water-dimer / cc-pvdz	internal	interaction energy kcalmol	2.06×10^{-4}
dlpno-ccsd(t)	s22-02-water-dimer / cc-pvdz	internal	local correlation energy ha	8.17×10^{-4}

Table S21, continued.

Method	System / basis	Ref.	Quantity	$\lvert\Delta\rvert$
dlpno-ccsd(t)	s22-02-water-dimer / cc-pvdz	internal	interaction energy kcalmol	1.61×10^{-4}
dlpno-ccsd(t)	s22-02-water-dimer / cc-pvdz	internal	local truncation error interaction energy kcal mol	2.06×10^{-4}
dlpno-ccsd(t)	s22-02-water-dimer / cc-pvdz	internal	local truncation error interaction energy kcal mol	1.61×10^{-4}
DLPNO-MP2	s22-02-water-dimer / cc-pvdz	internal	local truncation error interaction energy kcal mol	4.45×10^{-4}
DLPNO-MP2	s22-02-water-dimer / cc-pvdz	internal	local truncation error interaction energy kcal mol	3.39×10^{-4}
DLPNO-MP2	s22-02-water-dimer / cc-pvdz	internal	local truncation error interaction energy kcal mol	3.21×10^{-4}
DLPNO-MP2	s22-02-water-dimer / cc-pvdz	internal	local correlation energy ha	2.51×10^{-3}
DLPNO-MP2	s22-02-water-dimer / cc-pvdz	internal	interaction energy kcalmol	4.45×10^{-4}
DLPNO-MP2	s22-02-water-dimer / cc-pvdz	internal	local correlation energy ha	1.22×10^{-3}
DLPNO-MP2	s22-02-water-dimer / cc-pvdz	internal	interaction energy kcalmol	3.39×10^{-4}
dlpno-ccsd(t)	s22-02-water-dimer-monoA / cc-pvdz	internal	local correlation energy ha	9.12×10^{-4}
dlpno-ccsd(t)	s22-02-water-dimer-monoA / cc-pvdz	internal	local correlation energy ha	1.45×10^{-4}
dlpno-ccsd(t)	s22-02-water-dimer-monoA / cc-pvdz	internal	local correlation energy ha	3.28×10^{-4}
DLPNO-MP2	s22-02-water-dimer-monoA / cc-pvdz	internal	local correlation energy ha	1.03×10^{-3}
DLPNO-MP2	s22-02-water-dimer-monoA / cc-pvdz	internal	local correlation energy ha	4.39×10^{-4}
DLPNO-MP2	s22-02-water-dimer-monoA / cc-pvdz	internal	local correlation energy ha	2.89×10^{-4}
dlpno-ccsd(t)	s22-02-water-dimer-monoB / cc-pvdz	internal	local correlation energy ha	9.09×10^{-4}
dlpno-ccsd(t)	s22-02-water-dimer-monoB / cc-pvdz	internal	local correlation energy ha	1.45×10^{-4}
dlpno-ccsd(t)	s22-02-water-dimer-monoB / cc-pvdz	internal	local correlation energy ha	3.28×10^{-4}
DLPNO-MP2	s22-02-water-dimer-monoB / cc-pvdz	internal	local correlation energy ha	1.03×10^{-3}
DLPNO-MP2	s22-02-water-dimer-monoB / cc-pvdz	internal	local correlation energy ha	4.40×10^{-4}
DLPNO-MP2	s22-02-water-dimer-monoB / cc-pvdz	internal	local correlation energy ha	2.90×10^{-4}
DLPNO-MP2	s22-02-water-dimer / cc-pvdz	internal	local correlation energy ha	9.00×10^{-4}
DLPNO-MP2	s22-02-water-dimer / cc-pvdz	internal	interaction energy kcalmol	3.21×10^{-4}
DLPNO-MP2	s22-03-formic-acid-dimer / cc-pvdz	internal	interaction energy kcalmol	1.41×10^{-3}
DLPNO-MP2	s22-03-formic-acid-dimer / cc-pvdz	internal	local correlation energy ha	4.44×10^{-3}
DLPNO-MP2	s22-03-formic-acid-dimer / cc-pvdz	internal	interaction energy kcalmol	8.57×10^{-4}
dlpno-ccsd(t)	s22-03-formic-acid-dimer-monoA / cc-pvdz	internal	local correlation energy ha	1.61×10^{-3}
dlpno-ccsd(t)	s22-03-formic-acid-dimer-monoA / cc-pvdz	internal	local correlation energy ha	1.61×10^{-4}
DLPNO-MP2	s22-03-formic-acid-dimer-monoA / cc-pvdz	internal	local correlation energy ha	3.90×10^{-3}
DLPNO-MP2	s22-03-formic-acid-dimer-monoA / cc-pvdz	internal	local correlation energy ha	1.79×10^{-3}
DLPNO-MP2	s22-03-formic-acid-dimer-monoA / cc-pvdz	internal	local correlation energy ha	1.19×10^{-3}
dlpno-ccsd(t)	s22-03-formic-acid-dimer-monoB / cc-pvdz	internal	local correlation energy ha	1.61×10^{-3}
dlpno-ccsd(t)	s22-03-formic-acid-dimer-monoB / cc-pvdz	internal	local correlation energy ha	1.61×10^{-4}

Table S21, continued.

Method	System / basis	Ref.	Quantity	$\lvert\Delta\rvert$
DLPNO-MP2	s22-03-formic-acid-dimer-monoB / cc-pvdz	internal	local correlation energy ha	3.90×10^{-3}
DLPNO-MP2	s22-03-formic-acid-dimer-monoB / cc-pvdz	internal	local correlation energy ha	1.79×10^{-3}
DLPNO-MP2	s22-03-formic-acid-dimer-monoB / cc-pvdz	internal	local correlation energy ha	1.19×10^{-3}
DLPNO-MP2	s22-03-formic-acid-dimer / cc-pvdz	internal	local correlation energy ha	2.98×10^{-3}
DLPNO-MP2	s22-03-formic-acid-dimer / cc-pvdz	internal	interaction energy kcalmol	6.04×10^{-4}
DLPNO-MP2	s22-04-formamide-dimer / cc-pvdz	internal	interaction energy kcalmol	1.31×10^{-3}
dlpno-ccsd(t)	s22-04-formamide-dimer-monoA / cc-pvdz	internal	local correlation energy ha	1.51×10^{-3}
dlpno-ccsd(t)	s22-04-formamide-dimer-monoA / cc-pvdz	internal	local correlation energy ha	1.57×10^{-4}
DLPNO-MP2	s22-04-formamide-dimer-monoA / cc-pvdz	internal	local correlation energy ha	3.98×10^{-3}
DLPNO-MP2	s22-04-formamide-dimer-monoA / cc-pvdz	internal	local correlation energy ha	1.94×10^{-3}
DLPNO-MP2	s22-04-formamide-dimer-monoA / cc-pvdz	internal	local correlation energy ha	1.19×10^{-3}
dlpno-ccsd(t)	s22-04-formamide-dimer-monoB / cc-pvdz	internal	local correlation energy ha	1.51×10^{-3}
dlpno-ccsd(t)	s22-04-formamide-dimer-monoB / cc-pvdz	internal	local correlation energy ha	1.57×10^{-4}
DLPNO-MP2	s22-04-formamide-dimer-monoB / cc-pvdz	internal	local correlation energy ha	3.98×10^{-3}
DLPNO-MP2	s22-04-formamide-dimer-monoB / cc-pvdz	internal	local correlation energy ha	1.94×10^{-3}
DLPNO-MP2	s22-04-formamide-dimer-monoB / cc-pvdz	internal	local correlation energy ha	1.19×10^{-3}
DLPNO-MP2	s22-04-formamide-dimer / cc-pvdz	internal	local correlation energy ha	3.54×10^{-3}
DLPNO-MP2	s22-04-formamide-dimer / cc-pvdz	internal	interaction energy kcalmol	1.17×10^{-3}
DLPNO-MP2	s22-05-uracil-dimer-hb / cc-pvdz	internal	local truncation error interaction energy kcal mol	3.01×10^{-4}
DLPNO-MP2	s22-05-uracil-dimer-hb / cc-pvdz	internal	local truncation error interaction energy kcal mol	2.40×10^{-4}
DLPNO-MP2	s22-05-uracil-dimer-hb / cc-pvdz	internal	interaction energy kcalmol	3.01×10^{-4}
DLPNO-MP2	s22-05-uracil-dimer-hb / cc-pvdz	internal	interaction energy kcalmol	2.40×10^{-4}
DLPNO-MP2	s22-05-uracil-dimer-hb / cc-pvdz	internal	interaction energy kcalmol	1.09×10^{-3}
DLPNO-MP2	s22-06-2-pyridone-2-aminopyridine / cc-pvdz	internal	interaction energy kcalmol	1.35×10^{-3}
DLPNO-MP2	s22-06-2-pyridone-2-aminopyridine / cc-pvdz	internal	interaction energy kcalmol	1.09×10^{-3}
DLPNO-MP2	s22-06-2-pyridone-2-aminopyridine-monoB / cc-pvdz	internal	local correlation energy ha	4.73×10^{-3}
DLPNO-MP2	s22-06-2-pyridone-2-aminopyridine / cc-pvdz	internal	interaction energy kcalmol	1.14×10^{-3}
DLPNO-MP2	s22-07-adenine-thymine-wc / cc-pvdz	internal	interaction energy kcalmol	1.52×10^{-3}
DLPNO-MP2	s22-07-adenine-thymine-wc / cc-pvdz	internal	interaction energy kcalmol	1.34×10^{-3}
DLPNO-MP2	s22-07-adenine-thymine-wc / cc-pvdz	internal	interaction energy kcalmol	1.49×10^{-3}
dlpno-ccsd(t)	s22-08-methane-dimer / cc-pvdz	internal	local correlation energy ha	6.28×10^{-4}
dlpno-ccsd(t)	s22-08-methane-dimer / cc-pvdz	internal	interaction energy kcalmol	8.79×10^{-5}
dlpno-ccsd(t)	s22-08-methane-dimer / cc-pvdz	internal	local correlation energy ha	5.45×10^{-4}
dlpno-ccsd(t)	s22-08-methane-dimer / cc-pvdz	internal	interaction energy kcalmol	9.94×10^{-6}
dlpno-ccsd(t)	s22-08-methane-dimer / cc-pvdz	internal	local correlation energy ha	5.91×10^{-4}
dlpno-ccsd(t)	s22-08-methane-dimer / cc-pvdz	internal	interaction energy kcalmol	2.21×10^{-5}

Table S21, continued.

Method	System / basis	Ref.	Quantity	$\lvert\Delta\rvert$
dlpno-ccsd(t)	s22-08-methane-dimer / cc-pvdz	internal	local truncation error interaction energy kcal mol	8.79×10^{-5}
dlpno-ccsd(t)	s22-08-methane-dimer / cc-pvdz	internal	local truncation error interaction energy kcal mol	9.95×10^{-6}
dlpno-ccsd(t)	s22-08-methane-dimer / cc-pvdz	internal	local truncation error interaction energy kcal mol	2.21×10^{-5}
DLPNO-MP2	s22-08-methane-dimer / cc-pvdz	internal	local truncation error interaction energy kcal mol	1.83×10^{-4}
DLPNO-MP2	s22-08-methane-dimer / cc-pvdz	internal	local truncation error interaction energy kcal mol	1.77×10^{-4}
DLPNO-MP2	s22-08-methane-dimer / cc-pvdz	internal	local truncation error interaction energy kcal mol	1.73×10^{-4}
DLPNO-MP2	s22-08-methane-dimer / cc-pvdz	internal	local correlation energy ha	2.25×10^{-3}
DLPNO-MP2	s22-08-methane-dimer / cc-pvdz	internal	interaction energy kcalmol	1.83×10^{-4}
DLPNO-MP2	s22-08-methane-dimer / cc-pvdz	internal	local correlation energy ha	1.63×10^{-3}
DLPNO-MP2	s22-08-methane-dimer / cc-pvdz	internal	interaction energy kcalmol	1.77×10^{-4}
dlpno-ccsd(t)	s22-08-methane-dimer-monoA / cc-pvdz	internal	local correlation energy ha	2.70×10^{-4}
dlpno-ccsd(t)	s22-08-methane-dimer-monoA / cc-pvdz	internal	local correlation energy ha	2.77×10^{-4}
dlpno-ccsd(t)	s22-08-methane-dimer-monoA / cc-pvdz	internal	local correlation energy ha	3.07×10^{-4}
DLPNO-MP2	s22-08-methane-dimer-monoA / cc-pvdz	internal	local correlation energy ha	1.03×10^{-3}
DLPNO-MP2	s22-08-methane-dimer-monoA / cc-pvdz	internal	local correlation energy ha	7.26×10^{-4}
DLPNO-MP2	s22-08-methane-dimer-monoA / cc-pvdz	internal	local correlation energy ha	4.82×10^{-4}
dlpno-ccsd(t)	s22-08-methane-dimer-monoB / cc-pvdz	internal	local correlation energy ha	2.70×10^{-4}
dlpno-ccsd(t)	s22-08-methane-dimer-monoB / cc-pvdz	internal	local correlation energy ha	2.77×10^{-4}
dlpno-ccsd(t)	s22-08-methane-dimer-monoB / cc-pvdz	internal	local correlation energy ha	3.07×10^{-4}
DLPNO-MP2	s22-08-methane-dimer-monoB / cc-pvdz	internal	local correlation energy ha	1.03×10^{-3}
DLPNO-MP2	s22-08-methane-dimer-monoB / cc-pvdz	internal	local correlation energy ha	7.26×10^{-4}
DLPNO-MP2	s22-08-methane-dimer-monoB / cc-pvdz	internal	local correlation energy ha	4.82×10^{-4}
DLPNO-MP2	s22-08-methane-dimer / cc-pvdz	internal	local correlation energy ha	1.14×10^{-3}
DLPNO-MP2	s22-08-methane-dimer / cc-pvdz	internal	interaction energy kcalmol	1.73×10^{-4}
dlpno-ccsd(t)	s22-09-ethene-dimer / cc-pvdz	internal	interaction energy kcalmol	8.47×10^{-4}
dlpno-ccsd(t)	s22-09-ethene-dimer / cc-pvdz	internal	local correlation energy ha	1.49×10^{-3}
dlpno-ccsd(t)	s22-09-ethene-dimer / cc-pvdz	internal	interaction energy kcalmol	7.81×10^{-4}
dlpno-ccsd(t)	s22-09-ethene-dimer / cc-pvdz	internal	local correlation energy ha	1.27×10^{-3}
dlpno-ccsd(t)	s22-09-ethene-dimer / cc-pvdz	internal	interaction energy kcalmol	3.11×10^{-4}
dlpno-ccsd(t)	s22-09-ethene-dimer / cc-pvdz	internal	local truncation error interaction energy kcal mol	3.11×10^{-4}
DLPNO-MP2	s22-09-ethene-dimer / cc-pvdz	internal	interaction energy kcalmol	9.24×10^{-4}
DLPNO-MP2	s22-09-ethene-dimer / cc-pvdz	internal	local correlation energy ha	3.51×10^{-3}
DLPNO-MP2	s22-09-ethene-dimer / cc-pvdz	internal	interaction energy kcalmol	8.57×10^{-4}
dlpno-ccsd(t)	s22-09-ethene-dimer-monoA / cc-pvdz	internal	local correlation energy ha	2.97×10^{-3}
dlpno-ccsd(t)	s22-09-ethene-dimer-monoA / cc-pvdz	internal	local correlation energy ha	1.13×10^{-3}
dlpno-ccsd(t)	s22-09-ethene-dimer-monoA / cc-pvdz	internal	local correlation energy ha	4.77×10^{-4}

Table S21, continued.

Method	System / basis	Ref.	Quantity	$\lvert\Delta\rvert$
DLPNO-MP2	s22-09-ethene-dimer-monoA / cc-pvdz	internal	local correlation energy ha	2.13×10^{-3}
DLPNO-MP2	s22-09-ethene-dimer-monoA / cc-pvdz	internal	local correlation energy ha	1.33×10^{-3}
DLPNO-MP2	s22-09-ethene-dimer-monoA / cc-pvdz	internal	local correlation energy ha	7.85×10^{-4}
dlpno-ccsd(t)	s22-09-ethene-dimer-monoB / cc-pvdz	internal	local correlation energy ha	2.97×10^{-3}
dlpno-ccsd(t)	s22-09-ethene-dimer-monoB / cc-pvdz	internal	local correlation energy ha	1.13×10^{-3}
dlpno-ccsd(t)	s22-09-ethene-dimer-monoB / cc-pvdz	internal	local correlation energy ha	4.77×10^{-4}
DLPNO-MP2	s22-09-ethene-dimer-monoB / cc-pvdz	internal	local correlation energy ha	2.13×10^{-3}
DLPNO-MP2	s22-09-ethene-dimer-monoB / cc-pvdz	internal	local correlation energy ha	1.33×10^{-3}
DLPNO-MP2	s22-09-ethene-dimer-monoB / cc-pvdz	internal	local correlation energy ha	7.85×10^{-4}
DLPNO-MP2	s22-09-ethene-dimer / cc-pvdz	internal	local correlation energy ha	2.41×10^{-3}
DLPNO-MP2	s22-09-ethene-dimer / cc-pvdz	internal	interaction energy kcalmol	8.43×10^{-4}
DLPNO-MP2	s22-10-benzene-ch4 / cc-pvdz	internal	local truncation error interaction energy kcal mol	3.66×10^{-4}
DLPNO-MP2	s22-10-benzene-ch4 / cc-pvdz	internal	local truncation error interaction energy kcal mol	3.09×10^{-4}
DLPNO-MP2	s22-10-benzene-ch4 / cc-pvdz	internal	local truncation error interaction energy kcal mol	2.65×10^{-4}
DLPNO-MP2	s22-10-benzene-ch4 / cc-pvdz	internal	interaction energy kcalmol	3.66×10^{-4}
DLPNO-MP2	s22-10-benzene-ch4 / cc-pvdz	internal	interaction energy kcalmol	3.09×10^{-4}
DLPNO-MP2	s22-10-benzene-ch4-monoA / cc-pvdz	internal	local correlation energy ha	3.70×10^{-3}
dlpno-ccsd(t)	s22-10-benzene-ch4-monoB / cc-pvdz	internal	local correlation energy ha	2.82×10^{-4}
dlpno-ccsd(t)	s22-10-benzene-ch4-monoB / cc-pvdz	internal	local correlation energy ha	2.74×10^{-4}
dlpno-ccsd(t)	s22-10-benzene-ch4-monoB / cc-pvdz	internal	local correlation energy ha	3.14×10^{-4}
DLPNO-MP2	s22-10-benzene-ch4-monoB / cc-pvdz	internal	local correlation energy ha	1.04×10^{-3}
DLPNO-MP2	s22-10-benzene-ch4-monoB / cc-pvdz	internal	local correlation energy ha	7.32×10^{-4}
DLPNO-MP2	s22-10-benzene-ch4-monoB / cc-pvdz	internal	local correlation energy ha	4.88×10^{-4}
DLPNO-MP2	s22-10-benzene-ch4 / cc-pvdz	internal	local correlation energy ha	4.45×10^{-3}
DLPNO-MP2	s22-10-benzene-ch4 / cc-pvdz	internal	interaction energy kcalmol	2.65×10^{-4}
DLPNO-MP2	s22-11-benzene-dimer-stack-monoA / cc-pvdz	internal	local correlation energy ha	3.70×10^{-3}
DLPNO-MP2	s22-11-benzene-dimer-stack-monoB / cc-pvdz	internal	local correlation energy ha	3.70×10^{-3}
DLPNO-MP2	s22-11-benzene-dimer-stack / cc-pvdz	internal	interaction energy kcalmol	1.30×10^{-3}
DLPNO-MP2	s22-12-pyrazine-dimer-monoA / cc-pvdz	internal	local correlation energy ha	3.19×10^{-3}
DLPNO-MP2	s22-12-pyrazine-dimer-monoB / cc-pvdz	internal	local correlation energy ha	3.19×10^{-3}
DLPNO-MP2	s22-12-pyrazine-dimer / cc-pvdz	internal	interaction energy kcalmol	1.52×10^{-3}
DLPNO-MP2	s22-14-indole-benzene-stack-monoA / cc-pvdz	internal	local correlation energy ha	3.70×10^{-3}
dlpno-ccsd(t)	s22-16-ethene-ethyne / cc-pvdz	internal	local correlation energy ha	3.64×10^{-3}

Table S21, continued.

Method	System / basis	Ref.	Quantity	|Δ|
dlpno-ccsd(t)	s22-16-ethene-ethyne / cc-pvdz	internal	local correlation energy ha	1.23×10^{-4}
dlpno-ccsd(t)	s22-16-ethene-ethyne / cc-pvdz	internal	local correlation energy ha	1.35×10^{-3}
dlpno-ccsd(t)	s22-16-ethene-ethyne / cc-pvdz	internal	local truncation error interaction energy kcal mol	3.05×10^{-4}
dlpno-ccsd(t)	s22-16-ethene-ethyne / cc-pvdz	internal	local truncation error interaction energy kcal mol	1.37×10^{-4}
DLPNO-MP2	s22-16-ethene-ethyne / cc-pvdz	internal	local correlation energy ha	4.45×10^{-3}
DLPNO-MP2	s22-16-ethene-ethyne / cc-pvdz	internal	local correlation energy ha	3.23×10^{-3}
DLPNO-MP2	s22-16-ethene-ethyne-monoA / cc-pvdz	internal	local correlation energy ha	2.13×10^{-3}
DLPNO-MP2	s22-16-ethene-ethyne-monoA / cc-pvdz	internal	local correlation energy ha	1.33×10^{-3}
DLPNO-MP2	s22-16-ethene-ethyne / cc-pvdz	internal	local correlation energy ha	2.23×10^{-3}
DLPNO-MP2	s22-17-benzene-h2o / cc-pvdz	internal	local truncation error interaction energy kcal mol	3.31×10^{-4}
DLPNO-MP2	s22-17-benzene-h2o / cc-pvdz	internal	local truncation error interaction energy kcal mol	2.76×10^{-4}
DLPNO-MP2	s22-18-benzene-nh3 / cc-pvdz	internal	local truncation error interaction energy kcal mol	1.93×10^{-4}
DLPNO-MP2	s22-18-benzene-nh3 / cc-pvdz	internal	local truncation error interaction energy kcal mol	8.32×10^{-5}
DLPNO-MP2	s22-18-benzene-nh3 / cc-pvdz	internal	local truncation error interaction energy kcal mol	2.04×10^{-5}
dlpno-ccsd(t)	water-dimer / def2-svp	orca	hf energy	7.49×10^{-9}
dlpno-ccsd(t)	s22-01-ammonia-dimer / cc-pvdz	internal	local truncation error total energy kcal mol	held
dlpno-ccsd(t)	s22-01-ammonia-dimer / cc-pvdz	internal	local truncation error total energy kcal mol	held
dlpno-ccsd(t)	s22-01-ammonia-dimer / cc-pvdz	internal	local truncation error total energy kcal mol	held
DLPNO-MP2	s22-01-ammonia-dimer / cc-pvdz	internal	local truncation error total energy kcal mol	held
DLPNO-MP2	s22-01-ammonia-dimer / cc-pvdz	internal	local truncation error total energy kcal mol	held
DLPNO-MP2	s22-01-ammonia-dimer / cc-pvdz	internal	local truncation error total energy kcal mol	held
dlpno-ccsd(t)	s22-01-ammonia-dimer-monoA / cc-pvdz	internal	local truncation error total energy kcal mol	held
dlpno-ccsd(t)	s22-01-ammonia-dimer-monoA / cc-pvdz	internal	local truncation error total energy kcal mol	held
dlpno-ccsd(t)	s22-01-ammonia-dimer-monoA / cc-pvdz	internal	local truncation error total energy kcal mol	held
DLPNO-MP2	s22-01-ammonia-dimer-monoA / cc-pvdz	internal	local truncation error total energy kcal mol	held
DLPNO-MP2	s22-01-ammonia-dimer-monoA / cc-pvdz	internal	local truncation error total energy kcal mol	held
DLPNO-MP2	s22-01-ammonia-dimer-monoA / cc-pvdz	internal	local truncation error total energy kcal mol	held
dlpno-ccsd(t)	s22-01-ammonia-dimer-monoB / cc-pvdz	internal	local truncation error total energy kcal mol	held
dlpno-ccsd(t)	s22-01-ammonia-dimer-monoB / cc-pvdz	internal	local truncation error total energy kcal mol	held
dlpno-ccsd(t)	s22-01-ammonia-dimer-monoB / cc-pvdz	internal	local truncation error total energy kcal mol	held
DLPNO-MP2	s22-01-ammonia-dimer-monoB / cc-pvdz	internal	local truncation error total energy kcal mol	held
DLPNO-MP2	s22-01-ammonia-dimer-monoB / cc-pvdz	internal	local truncation error total energy kcal mol	held

Table S21, continued.

Method	System / basis	Ref.	Quantity	|Δ|
DLPNO-MP2	s22-01-ammonia-dimer-monoB / cc-pvdz	internal	local truncation error total energy kcal mol	held
dlpno-ccsd(t)	s22-02-water-dimer / cc-pvdz	internal	local truncation error total energy kcal mol	held
dlpno-ccsd(t)	s22-02-water-dimer / cc-pvdz	internal	local truncation error total energy kcal mol	held
dlpno-ccsd(t)	s22-02-water-dimer / cc-pvdz	internal	local truncation error total energy kcal mol	held
DLPNO-MP2	s22-02-water-dimer / cc-pvdz	internal	local truncation error total energy kcal mol	held
DLPNO-MP2	s22-02-water-dimer / cc-pvdz	internal	local truncation error total energy kcal mol	held
DLPNO-MP2	s22-02-water-dimer / cc-pvdz	internal	local truncation error total energy kcal mol	held
dlpno-ccsd(t)	s22-02-water-dimer-monoA / cc-pvdz	internal	local truncation error total energy kcal mol	held
dlpno-ccsd(t)	s22-02-water-dimer-monoA / cc-pvdz	internal	local truncation error total energy kcal mol	held
dlpno-ccsd(t)	s22-02-water-dimer-monoA / cc-pvdz	internal	local truncation error total energy kcal mol	held
DLPNO-MP2	s22-02-water-dimer-monoA / cc-pvdz	internal	local truncation error total energy kcal mol	held
DLPNO-MP2	s22-02-water-dimer-monoA / cc-pvdz	internal	local truncation error total energy kcal mol	held
DLPNO-MP2	s22-02-water-dimer-monoA / cc-pvdz	internal	local truncation error total energy kcal mol	held
dlpno-ccsd(t)	s22-02-water-dimer-monoB / cc-pvdz	internal	local truncation error total energy kcal mol	held
dlpno-ccsd(t)	s22-02-water-dimer-monoB / cc-pvdz	internal	local truncation error total energy kcal mol	held
dlpno-ccsd(t)	s22-02-water-dimer-monoB / cc-pvdz	internal	local truncation error total energy kcal mol	held
DLPNO-MP2	s22-02-water-dimer-monoB / cc-pvdz	internal	local truncation error total energy kcal mol	held
DLPNO-MP2	s22-02-water-dimer-monoB / cc-pvdz	internal	local truncation error total energy kcal mol	held
DLPNO-MP2	s22-02-water-dimer-monoB / cc-pvdz	internal	local truncation error total energy kcal mol	held
DLPNO-MP2	s22-03-formic-acid-dimer / cc-pvdz	internal	local truncation error total energy kcal mol	held
DLPNO-MP2	s22-03-formic-acid-dimer / cc-pvdz	internal	local truncation error total energy kcal mol	held
DLPNO-MP2	s22-03-formic-acid-dimer / cc-pvdz	internal	local truncation error total energy kcal mol	held
dlpno-ccsd(t)	s22-03-formic-acid-dimer-monoA / cc-pvdz	internal	local truncation error total energy kcal mol	held
dlpno-ccsd(t)	s22-03-formic-acid-dimer-monoA / cc-pvdz	internal	local truncation error total energy kcal mol	held
dlpno-ccsd(t)	s22-03-formic-acid-dimer-monoA / cc-pvdz	internal	local truncation error total energy kcal mol	held
DLPNO-MP2	s22-03-formic-acid-dimer-monoA / cc-pvdz	internal	local truncation error total energy kcal mol	held
DLPNO-MP2	s22-03-formic-acid-dimer-monoA / cc-pvdz	internal	local truncation error total energy kcal mol	held
DLPNO-MP2	s22-03-formic-acid-dimer-monoA / cc-pvdz	internal	local truncation error total energy kcal mol	held
dlpno-ccsd(t)	s22-03-formic-acid-dimer-monoB / cc-pvdz	internal	local truncation error total energy kcal mol	held

Table S21, continued.

Method	System / basis	Ref.	Quantity	|Δ|
dlpno-ccsd(t)	s22-03-formic-acid-dimer-monoB / cc-pvdz	internal	local truncation error total energy kcal mol	held
dlpno-ccsd(t)	s22-03-formic-acid-dimer-monoB / cc-pvdz	internal	local truncation error total energy kcal mol	held
DLPNO-MP2	s22-03-formic-acid-dimer-monoB / cc-pvdz	internal	local truncation error total energy kcal mol	held
DLPNO-MP2	s22-03-formic-acid-dimer-monoB / cc-pvdz	internal	local truncation error total energy kcal mol	held
DLPNO-MP2	s22-03-formic-acid-dimer-monoB / cc-pvdz	internal	local truncation error total energy kcal mol	held
DLPNO-MP2	s22-04-formamide-dimer / cc-pvdz	internal	local truncation error total energy kcal mol	held
DLPNO-MP2	s22-04-formamide-dimer / cc-pvdz	internal	local truncation error total energy kcal mol	held
DLPNO-MP2	s22-04-formamide-dimer / cc-pvdz	internal	local truncation error total energy kcal mol	held
dlpno-ccsd(t)	s22-04-formamide-dimer-monoA / cc-pvdz	internal	local truncation error total energy kcal mol	held
dlpno-ccsd(t)	s22-04-formamide-dimer-monoA / cc-pvdz	internal	local truncation error total energy kcal mol	held
dlpno-ccsd(t)	s22-04-formamide-dimer-monoA / cc-pvdz	internal	local truncation error total energy kcal mol	held
DLPNO-MP2	s22-04-formamide-dimer-monoA / cc-pvdz	internal	local truncation error total energy kcal mol	held
DLPNO-MP2	s22-04-formamide-dimer-monoA / cc-pvdz	internal	local truncation error total energy kcal mol	held
DLPNO-MP2	s22-04-formamide-dimer-monoA / cc-pvdz	internal	local truncation error total energy kcal mol	held
dlpno-ccsd(t)	s22-04-formamide-dimer-monoB / cc-pvdz	internal	local truncation error total energy kcal mol	held
dlpno-ccsd(t)	s22-04-formamide-dimer-monoB / cc-pvdz	internal	local truncation error total energy kcal mol	held
dlpno-ccsd(t)	s22-04-formamide-dimer-monoB / cc-pvdz	internal	local truncation error total energy kcal mol	held
DLPNO-MP2	s22-04-formamide-dimer-monoB / cc-pvdz	internal	local truncation error total energy kcal mol	held
DLPNO-MP2	s22-04-formamide-dimer-monoB / cc-pvdz	internal	local truncation error total energy kcal mol	held
DLPNO-MP2	s22-04-formamide-dimer-monoB / cc-pvdz	internal	local truncation error total energy kcal mol	held
DLPNO-MP2	s22-05-uracil-dimer-hb / cc-pvdz	internal	local truncation error total energy kcal mol	held
DLPNO-MP2	s22-05-uracil-dimer-hb / cc-pvdz	internal	local truncation error total energy kcal mol	held
DLPNO-MP2	s22-05-uracil-dimer-hb / cc-pvdz	internal	local truncation error total energy kcal mol	held
DLPNO-MP2	s22-05-uracil-dimer-hb-monoA / cc-pvdz	internal	local truncation error total energy kcal mol	held
DLPNO-MP2	s22-05-uracil-dimer-hb-monoA / cc-pvdz	internal	local truncation error total energy kcal mol	held
DLPNO-MP2	s22-05-uracil-dimer-hb-monoA / cc-pvdz	internal	local truncation error total energy kcal mol	held
DLPNO-MP2	s22-05-uracil-dimer-hb-monoB / cc-pvdz	internal	local truncation error total energy kcal mol	held
DLPNO-MP2	s22-05-uracil-dimer-hb-monoB / cc-pvdz	internal	local truncation error total energy kcal mol	held
DLPNO-MP2	s22-05-uracil-dimer-hb-monoB / cc-pvdz	internal	local truncation error total energy kcal mol	held

Table S21, continued.

Method	System / basis	Ref.	Quantity	|Δ|
DLPNO-MP2	s22-06-2-pyridone-2-aminopyridine / cc-pvdz	internal	local truncation error total energy kcal mol	held
DLPNO-MP2	s22-06-2-pyridone-2-aminopyridine / cc-pvdz	internal	local truncation error total energy kcal mol	held
DLPNO-MP2	s22-06-2-pyridone-2-aminopyridine / cc-pvdz	internal	local truncation error total energy kcal mol	held
DLPNO-MP2	s22-06-2-pyridone-2-aminopyridine-monoA / cc-pvdz	internal	local truncation error total energy kcal mol	held
DLPNO-MP2	s22-06-2-pyridone-2-aminopyridine-monoA / cc-pvdz	internal	local truncation error total energy kcal mol	held
DLPNO-MP2	s22-06-2-pyridone-2-aminopyridine-monoA / cc-pvdz	internal	local truncation error total energy kcal mol	held
DLPNO-MP2	s22-06-2-pyridone-2-aminopyridine-monoB / cc-pvdz	internal	local truncation error total energy kcal mol	held
DLPNO-MP2	s22-06-2-pyridone-2-aminopyridine-monoB / cc-pvdz	internal	local truncation error total energy kcal mol	held
DLPNO-MP2	s22-06-2-pyridone-2-aminopyridine-monoB / cc-pvdz	internal	local truncation error total energy kcal mol	held
DLPNO-MP2	s22-07-adenine-thymine-wc / cc-pvdz	internal	local truncation error total energy kcal mol	held
DLPNO-MP2	s22-07-adenine-thymine-wc / cc-pvdz	internal	local truncation error total energy kcal mol	held
DLPNO-MP2	s22-07-adenine-thymine-wc / cc-pvdz	internal	local truncation error total energy kcal mol	held
DLPNO-MP2	s22-07-adenine-thymine-wc-monoA / cc-pvdz	internal	local truncation error total energy kcal mol	held
DLPNO-MP2	s22-07-adenine-thymine-wc-monoA / cc-pvdz	internal	local truncation error total energy kcal mol	held
DLPNO-MP2	s22-07-adenine-thymine-wc-monoA / cc-pvdz	internal	local truncation error total energy kcal mol	held
DLPNO-MP2	s22-07-adenine-thymine-wc-monoB / cc-pvdz	internal	local truncation error total energy kcal mol	held
DLPNO-MP2	s22-07-adenine-thymine-wc-monoB / cc-pvdz	internal	local truncation error total energy kcal mol	held
DLPNO-MP2	s22-07-adenine-thymine-wc-monoB / cc-pvdz	internal	local truncation error total energy kcal mol	held
dlpno-ccsd(t)	s22-08-methane-dimer / cc-pvdz	internal	local truncation error total energy kcal mol	held
dlpno-ccsd(t)	s22-08-methane-dimer / cc-pvdz	internal	local truncation error total energy kcal mol	held
dlpno-ccsd(t)	s22-08-methane-dimer / cc-pvdz	internal	local truncation error total energy kcal mol	held
DLPNO-MP2	s22-08-methane-dimer / cc-pvdz	internal	local truncation error total energy kcal mol	held
DLPNO-MP2	s22-08-methane-dimer / cc-pvdz	internal	local truncation error total energy kcal mol	held
DLPNO-MP2	s22-08-methane-dimer / cc-pvdz	internal	local truncation error total energy kcal mol	held
dlpno-ccsd(t)	s22-08-methane-dimer-monoA / cc-pvdz	internal	local truncation error total energy kcal mol	held
dlpno-ccsd(t)	s22-08-methane-dimer-monoA / cc-pvdz	internal	local truncation error total energy kcal mol	held
dlpno-ccsd(t)	s22-08-methane-dimer-monoA / cc-pvdz	internal	local truncation error total energy kcal mol	held
DLPNO-MP2	s22-08-methane-dimer-monoA / cc-pvdz	internal	local truncation error total energy kcal mol	held
DLPNO-MP2	s22-08-methane-dimer-monoA / cc-pvdz	internal	local truncation error total energy kcal mol	held

Table S21, continued.

Method	System / basis	Ref.	Quantity	|Δ|
DLPNO-MP2	s22-08-methane-dimer-monoA / cc-pvdz	internal	local truncation error total energy kcal mol	held
dlpno-ccsd(t)	s22-08-methane-dimer-monoB / cc-pvdz	internal	local truncation error total energy kcal mol	held
dlpno-ccsd(t)	s22-08-methane-dimer-monoB / cc-pvdz	internal	local truncation error total energy kcal mol	held
dlpno-ccsd(t)	s22-08-methane-dimer-monoB / cc-pvdz	internal	local truncation error total energy kcal mol	held
DLPNO-MP2	s22-08-methane-dimer-monoB / cc-pvdz	internal	local truncation error total energy kcal mol	held
DLPNO-MP2	s22-08-methane-dimer-monoB / cc-pvdz	internal	local truncation error total energy kcal mol	held
DLPNO-MP2	s22-08-methane-dimer-monoB / cc-pvdz	internal	local truncation error total energy kcal mol	held
dlpno-ccsd(t)	s22-09-ethene-dimer / cc-pvdz	internal	local truncation error total energy kcal mol	held
dlpno-ccsd(t)	s22-09-ethene-dimer / cc-pvdz	internal	local truncation error total energy kcal mol	held
dlpno-ccsd(t)	s22-09-ethene-dimer / cc-pvdz	internal	local truncation error total energy kcal mol	held
DLPNO-MP2	s22-09-ethene-dimer / cc-pvdz	internal	local truncation error total energy kcal mol	held
DLPNO-MP2	s22-09-ethene-dimer / cc-pvdz	internal	local truncation error total energy kcal mol	held
DLPNO-MP2	s22-09-ethene-dimer / cc-pvdz	internal	local truncation error total energy kcal mol	held
dlpno-ccsd(t)	s22-09-ethene-dimer-monoA / cc-pvdz	internal	local truncation error total energy kcal mol	held
dlpno-ccsd(t)	s22-09-ethene-dimer-monoA / cc-pvdz	internal	local truncation error total energy kcal mol	held
dlpno-ccsd(t)	s22-09-ethene-dimer-monoA / cc-pvdz	internal	local truncation error total energy kcal mol	held
DLPNO-MP2	s22-09-ethene-dimer-monoA / cc-pvdz	internal	local truncation error total energy kcal mol	held
DLPNO-MP2	s22-09-ethene-dimer-monoA / cc-pvdz	internal	local truncation error total energy kcal mol	held
DLPNO-MP2	s22-09-ethene-dimer-monoA / cc-pvdz	internal	local truncation error total energy kcal mol	held
dlpno-ccsd(t)	s22-09-ethene-dimer-monoB / cc-pvdz	internal	local truncation error total energy kcal mol	held
dlpno-ccsd(t)	s22-09-ethene-dimer-monoB / cc-pvdz	internal	local truncation error total energy kcal mol	held
dlpno-ccsd(t)	s22-09-ethene-dimer-monoB / cc-pvdz	internal	local truncation error total energy kcal mol	held
DLPNO-MP2	s22-09-ethene-dimer-monoB / cc-pvdz	internal	local truncation error total energy kcal mol	held
DLPNO-MP2	s22-09-ethene-dimer-monoB / cc-pvdz	internal	local truncation error total energy kcal mol	held
DLPNO-MP2	s22-09-ethene-dimer-monoB / cc-pvdz	internal	local truncation error total energy kcal mol	held
DLPNO-MP2	s22-10-benzene-ch4 / cc-pvdz	internal	local truncation error total energy kcal mol	held
DLPNO-MP2	s22-10-benzene-ch4 / cc-pvdz	internal	local truncation error total energy kcal mol	held
DLPNO-MP2	s22-10-benzene-ch4 / cc-pvdz	internal	local truncation error total energy kcal mol	held
DLPNO-MP2	s22-10-benzene-ch4-monoA / cc-pvdz	internal	local truncation error total energy kcal mol	held

Table S21, continued.

Method	System / basis	Ref.	Quantity	|Δ|
DLPNO-MP2	s22-10-benzene-ch4-monoA / cc-pvdz	internal	local truncation error total energy kcal mol	held
DLPNO-MP2	s22-10-benzene-ch4-monoA / cc-pvdz	internal	local truncation error total energy kcal mol	held
dlpno-ccsd(t)	s22-10-benzene-ch4-monoB / cc-pvdz	internal	local truncation error total energy kcal mol	held
dlpno-ccsd(t)	s22-10-benzene-ch4-monoB / cc-pvdz	internal	local truncation error total energy kcal mol	held
dlpno-ccsd(t)	s22-10-benzene-ch4-monoB / cc-pvdz	internal	local truncation error total energy kcal mol	held
DLPNO-MP2	s22-10-benzene-ch4-monoB / cc-pvdz	internal	local truncation error total energy kcal mol	held
DLPNO-MP2	s22-10-benzene-ch4-monoB / cc-pvdz	internal	local truncation error total energy kcal mol	held
DLPNO-MP2	s22-10-benzene-ch4-monoB / cc-pvdz	internal	local truncation error total energy kcal mol	held
DLPNO-MP2	s22-11-benzene-dimer-stack / cc-pvdz	internal	local truncation error total energy kcal mol	held
DLPNO-MP2	s22-11-benzene-dimer-stack / cc-pvdz	internal	local truncation error total energy kcal mol	held
DLPNO-MP2	s22-11-benzene-dimer-stack / cc-pvdz	internal	local truncation error total energy kcal mol	held
DLPNO-MP2	s22-11-benzene-dimer-stack-monoA / cc-pvdz	internal	local truncation error total energy kcal mol	held
DLPNO-MP2	s22-11-benzene-dimer-stack-monoA / cc-pvdz	internal	local truncation error total energy kcal mol	held
DLPNO-MP2	s22-11-benzene-dimer-stack-monoA / cc-pvdz	internal	local truncation error total energy kcal mol	held
DLPNO-MP2	s22-11-benzene-dimer-stack-monoB / cc-pvdz	internal	local truncation error total energy kcal mol	held
DLPNO-MP2	s22-11-benzene-dimer-stack-monoB / cc-pvdz	internal	local truncation error total energy kcal mol	held
DLPNO-MP2	s22-11-benzene-dimer-stack-monoB / cc-pvdz	internal	local truncation error total energy kcal mol	held
DLPNO-MP2	s22-12-pyrazine-dimer / cc-pvdz	internal	local truncation error total energy kcal mol	held
DLPNO-MP2	s22-12-pyrazine-dimer / cc-pvdz	internal	local truncation error total energy kcal mol	held
DLPNO-MP2	s22-12-pyrazine-dimer / cc-pvdz	internal	local truncation error total energy kcal mol	held
DLPNO-MP2	s22-12-pyrazine-dimer-monoA / cc-pvdz	internal	local truncation error total energy kcal mol	held
DLPNO-MP2	s22-12-pyrazine-dimer-monoA / cc-pvdz	internal	local truncation error total energy kcal mol	held
DLPNO-MP2	s22-12-pyrazine-dimer-monoA / cc-pvdz	internal	local truncation error total energy kcal mol	held
DLPNO-MP2	s22-12-pyrazine-dimer-monoB / cc-pvdz	internal	local truncation error total energy kcal mol	held
DLPNO-MP2	s22-12-pyrazine-dimer-monoB / cc-pvdz	internal	local truncation error total energy kcal mol	held
DLPNO-MP2	s22-12-pyrazine-dimer-monoB / cc-pvdz	internal	local truncation error total energy kcal mol	held
DLPNO-MP2	s22-13-uracil-dimer-stack / cc-pvdz	internal	local truncation error total energy kcal mol	held
DLPNO-MP2	s22-13-uracil-dimer-stack / cc-pvdz	internal	local truncation error total energy kcal mol	held
DLPNO-MP2	s22-13-uracil-dimer-stack / cc-pvdz	internal	local truncation error total energy kcal mol	held

Table S21, continued.

Method	System / basis	Ref.	Quantity	|Δ|
DLPNO-MP2	s22-13-uracil-dimer-stack-monoA / cc-pvdz	internal	local truncation error total energy kcal mol	held
DLPNO-MP2	s22-13-uracil-dimer-stack-monoA / cc-pvdz	internal	local truncation error total energy kcal mol	held
DLPNO-MP2	s22-13-uracil-dimer-stack-monoA / cc-pvdz	internal	local truncation error total energy kcal mol	held
DLPNO-MP2	s22-13-uracil-dimer-stack-monoB / cc-pvdz	internal	local truncation error total energy kcal mol	held
DLPNO-MP2	s22-13-uracil-dimer-stack-monoB / cc-pvdz	internal	local truncation error total energy kcal mol	held
DLPNO-MP2	s22-13-uracil-dimer-stack-monoB / cc-pvdz	internal	local truncation error total energy kcal mol	held
DLPNO-MP2	s22-14-indole-benzene-stack / cc-pvdz	internal	local truncation error total energy kcal mol	held
DLPNO-MP2	s22-14-indole-benzene-stack / cc-pvdz	internal	local truncation error total energy kcal mol	held
DLPNO-MP2	s22-14-indole-benzene-stack / cc-pvdz	internal	local truncation error total energy kcal mol	held
DLPNO-MP2	s22-14-indole-benzene-stack-monoA / cc-pvdz	internal	local truncation error total energy kcal mol	held
DLPNO-MP2	s22-14-indole-benzene-stack-monoA / cc-pvdz	internal	local truncation error total energy kcal mol	held
DLPNO-MP2	s22-14-indole-benzene-stack-monoA / cc-pvdz	internal	local truncation error total energy kcal mol	held
DLPNO-MP2	s22-14-indole-benzene-stack-monoB / cc-pvdz	internal	local truncation error total energy kcal mol	held
DLPNO-MP2	s22-14-indole-benzene-stack-monoB / cc-pvdz	internal	local truncation error total energy kcal mol	held
DLPNO-MP2	s22-14-indole-benzene-stack-monoB / cc-pvdz	internal	local truncation error total energy kcal mol	held
DLPNO-MP2	s22-15-adenine-thymine-stack / cc-pvdz	internal	local truncation error total energy kcal mol	held
DLPNO-MP2	s22-15-adenine-thymine-stack / cc-pvdz	internal	local truncation error total energy kcal mol	held
DLPNO-MP2	s22-15-adenine-thymine-stack / cc-pvdz	internal	local truncation error total energy kcal mol	held
DLPNO-MP2	s22-15-adenine-thymine-stack-monoA / cc-pvdz	internal	local truncation error total energy kcal mol	held
DLPNO-MP2	s22-15-adenine-thymine-stack-monoA / cc-pvdz	internal	local truncation error total energy kcal mol	held
DLPNO-MP2	s22-15-adenine-thymine-stack-monoA / cc-pvdz	internal	local truncation error total energy kcal mol	held
DLPNO-MP2	s22-15-adenine-thymine-stack-monoB / cc-pvdz	internal	local truncation error total energy kcal mol	held
DLPNO-MP2	s22-15-adenine-thymine-stack-monoB / cc-pvdz	internal	local truncation error total energy kcal mol	held
DLPNO-MP2	s22-15-adenine-thymine-stack-monoB / cc-pvdz	internal	local truncation error total energy kcal mol	held
dlpno-ccsd(t)	s22-16-ethene-ethyne / cc-pvdz	internal	local truncation error total energy kcal mol	held
dlpno-ccsd(t)	s22-16-ethene-ethyne / cc-pvdz	internal	local truncation error total energy kcal mol	held
dlpno-ccsd(t)	s22-16-ethene-ethyne / cc-pvdz	internal	local truncation error total energy kcal mol	held
DLPNO-MP2	s22-16-ethene-ethyne / cc-pvdz	internal	local truncation error total energy kcal mol	held
DLPNO-MP2	s22-16-ethene-ethyne / cc-pvdz	internal	local truncation error total energy kcal mol	held

Table S21, continued.

Method	System / basis	Ref.	Quantity	|Δ|
DLPNO-MP2	s22-16-ethene-ethyne / cc-pvdz	internal	local truncation error total energy kcal mol	held
dlpno-ccsd(t)	s22-16-ethene-ethyne-monoA / cc-pvdz	internal	local truncation error total energy kcal mol	held
dlpno-ccsd(t)	s22-16-ethene-ethyne-monoA / cc-pvdz	internal	local truncation error total energy kcal mol	held
dlpno-ccsd(t)	s22-16-ethene-ethyne-monoA / cc-pvdz	internal	local truncation error total energy kcal mol	held
DLPNO-MP2	s22-16-ethene-ethyne-monoA / cc-pvdz	internal	local truncation error total energy kcal mol	held
DLPNO-MP2	s22-16-ethene-ethyne-monoA / cc-pvdz	internal	local truncation error total energy kcal mol	held
DLPNO-MP2	s22-16-ethene-ethyne-monoA / cc-pvdz	internal	local truncation error total energy kcal mol	held
dlpno-ccsd(t)	s22-16-ethene-ethyne-monoB / cc-pvdz	internal	local truncation error total energy kcal mol	held
dlpno-ccsd(t)	s22-16-ethene-ethyne-monoB / cc-pvdz	internal	local truncation error total energy kcal mol	held
dlpno-ccsd(t)	s22-16-ethene-ethyne-monoB / cc-pvdz	internal	local truncation error total energy kcal mol	held
DLPNO-MP2	s22-16-ethene-ethyne-monoB / cc-pvdz	internal	local truncation error total energy kcal mol	held
DLPNO-MP2	s22-16-ethene-ethyne-monoB / cc-pvdz	internal	local truncation error total energy kcal mol	held
DLPNO-MP2	s22-16-ethene-ethyne-monoB / cc-pvdz	internal	local truncation error total energy kcal mol	held
DLPNO-MP2	s22-17-benzene-h2o / cc-pvdz	internal	local truncation error total energy kcal mol	held
DLPNO-MP2	s22-17-benzene-h2o / cc-pvdz	internal	local truncation error total energy kcal mol	held
DLPNO-MP2	s22-17-benzene-h2o / cc-pvdz	internal	local truncation error total energy kcal mol	held
DLPNO-MP2	s22-17-benzene-h2o-monoA / cc-pvdz	internal	local truncation error total energy kcal mol	held
DLPNO-MP2	s22-17-benzene-h2o-monoA / cc-pvdz	internal	local truncation error total energy kcal mol	held
DLPNO-MP2	s22-17-benzene-h2o-monoA / cc-pvdz	internal	local truncation error total energy kcal mol	held
dlpno-ccsd(t)	s22-17-benzene-h2o-monoB / cc-pvdz	internal	local truncation error total energy kcal mol	held
dlpno-ccsd(t)	s22-17-benzene-h2o-monoB / cc-pvdz	internal	local truncation error total energy kcal mol	held
dlpno-ccsd(t)	s22-17-benzene-h2o-monoB / cc-pvdz	internal	local truncation error total energy kcal mol	held
DLPNO-MP2	s22-17-benzene-h2o-monoB / cc-pvdz	internal	local truncation error total energy kcal mol	held
DLPNO-MP2	s22-17-benzene-h2o-monoB / cc-pvdz	internal	local truncation error total energy kcal mol	held
DLPNO-MP2	s22-17-benzene-h2o-monoB / cc-pvdz	internal	local truncation error total energy kcal mol	held
DLPNO-MP2	s22-18-benzene-nh3 / cc-pvdz	internal	local truncation error total energy kcal mol	held
DLPNO-MP2	s22-18-benzene-nh3 / cc-pvdz	internal	local truncation error total energy kcal mol	held
DLPNO-MP2	s22-18-benzene-nh3 / cc-pvdz	internal	local truncation error total energy kcal mol	held
DLPNO-MP2	s22-18-benzene-nh3-monoA / cc-pvdz	internal	local truncation error total energy kcal mol	held

Table S21, continued.

Method	System / basis	Ref.	Quantity	|Δ|
DLPNO-MP2	s22-18-benzene-nh3-monoA / cc-pvdz	internal	local truncation error total energy kcal mol	held
DLPNO-MP2	s22-18-benzene-nh3-monoA / cc-pvdz	internal	local truncation error total energy kcal mol	held
dlpno-ccsd(t)	s22-18-benzene-nh3-monoB / cc-pvdz	internal	local truncation error total energy kcal mol	held
dlpno-ccsd(t)	s22-18-benzene-nh3-monoB / cc-pvdz	internal	local truncation error total energy kcal mol	held
dlpno-ccsd(t)	s22-18-benzene-nh3-monoB / cc-pvdz	internal	local truncation error total energy kcal mol	held
DLPNO-MP2	s22-18-benzene-nh3-monoB / cc-pvdz	internal	local truncation error total energy kcal mol	held
DLPNO-MP2	s22-18-benzene-nh3-monoB / cc-pvdz	internal	local truncation error total energy kcal mol	held
DLPNO-MP2	s22-18-benzene-nh3-monoB / cc-pvdz	internal	local truncation error total energy kcal mol	held
DLPNO-MP2	s22-19-benzene-hcn / cc-pvdz	internal	local truncation error total energy kcal mol	held
DLPNO-MP2	s22-19-benzene-hcn / cc-pvdz	internal	local truncation error total energy kcal mol	held
DLPNO-MP2	s22-19-benzene-hcn / cc-pvdz	internal	local truncation error total energy kcal mol	held
DLPNO-MP2	s22-19-benzene-hcn-monoA / cc-pvdz	internal	local truncation error total energy kcal mol	held
DLPNO-MP2	s22-19-benzene-hcn-monoA / cc-pvdz	internal	local truncation error total energy kcal mol	held
DLPNO-MP2	s22-19-benzene-hcn-monoA / cc-pvdz	internal	local truncation error total energy kcal mol	held
dlpno-ccsd(t)	s22-19-benzene-hcn-monoB / cc-pvdz	internal	local truncation error total energy kcal mol	held
dlpno-ccsd(t)	s22-19-benzene-hcn-monoB / cc-pvdz	internal	local truncation error total energy kcal mol	held
dlpno-ccsd(t)	s22-19-benzene-hcn-monoB / cc-pvdz	internal	local truncation error total energy kcal mol	held
DLPNO-MP2	s22-19-benzene-hcn-monoB / cc-pvdz	internal	local truncation error total energy kcal mol	held
DLPNO-MP2	s22-19-benzene-hcn-monoB / cc-pvdz	internal	local truncation error total energy kcal mol	held
DLPNO-MP2	s22-19-benzene-hcn-monoB / cc-pvdz	internal	local truncation error total energy kcal mol	held
DLPNO-MP2	s22-20-benzene-dimer-t / cc-pvdz	internal	local truncation error total energy kcal mol	held
DLPNO-MP2	s22-20-benzene-dimer-t / cc-pvdz	internal	local truncation error total energy kcal mol	held
DLPNO-MP2	s22-20-benzene-dimer-t / cc-pvdz	internal	local truncation error total energy kcal mol	held
DLPNO-MP2	s22-20-benzene-dimer-t-monoA / cc-pvdz	internal	local truncation error total energy kcal mol	held
DLPNO-MP2	s22-20-benzene-dimer-t-monoA / cc-pvdz	internal	local truncation error total energy kcal mol	held
DLPNO-MP2	s22-20-benzene-dimer-t-monoA / cc-pvdz	internal	local truncation error total energy kcal mol	held
DLPNO-MP2	s22-20-benzene-dimer-t-monoB / cc-pvdz	internal	local truncation error total energy kcal mol	held
DLPNO-MP2	s22-20-benzene-dimer-t-monoB / cc-pvdz	internal	local truncation error total energy kcal mol	held
DLPNO-MP2	s22-20-benzene-dimer-t-monoB / cc-pvdz	internal	local truncation error total energy kcal mol	held

Table S21, continued.

Method	System / basis	Ref.	Quantity	|Δ|
DLPNO-MP2	s22-21-indole-benzene-t / cc-pvdz	internal	local truncation error total energy kcal mol	held
DLPNO-MP2	s22-21-indole-benzene-t / cc-pvdz	internal	local truncation error total energy kcal mol	held
DLPNO-MP2	s22-21-indole-benzene-t / cc-pvdz	internal	local truncation error total energy kcal mol	held
DLPNO-MP2	s22-21-indole-benzene-t-monoA / cc-pvdz	internal	local truncation error total energy kcal mol	held
DLPNO-MP2	s22-21-indole-benzene-t-monoA / cc-pvdz	internal	local truncation error total energy kcal mol	held
DLPNO-MP2	s22-21-indole-benzene-t-monoA / cc-pvdz	internal	local truncation error total energy kcal mol	held
DLPNO-MP2	s22-21-indole-benzene-t-monoB / cc-pvdz	internal	local truncation error total energy kcal mol	held
DLPNO-MP2	s22-21-indole-benzene-t-monoB / cc-pvdz	internal	local truncation error total energy kcal mol	held
DLPNO-MP2	s22-21-indole-benzene-t-monoB / cc-pvdz	internal	local truncation error total energy kcal mol	held
DLPNO-MP2	s22-22-phenol-dimer / cc-pvdz	internal	local truncation error total energy kcal mol	held
DLPNO-MP2	s22-22-phenol-dimer / cc-pvdz	internal	local truncation error total energy kcal mol	held
DLPNO-MP2	s22-22-phenol-dimer / cc-pvdz	internal	local truncation error total energy kcal mol	held
DLPNO-MP2	s22-22-phenol-dimer-monoA / cc-pvdz	internal	local truncation error total energy kcal mol	held
DLPNO-MP2	s22-22-phenol-dimer-monoA / cc-pvdz	internal	local truncation error total energy kcal mol	held
DLPNO-MP2	s22-22-phenol-dimer-monoA / cc-pvdz	internal	local truncation error total energy kcal mol	held
DLPNO-MP2	s22-22-phenol-dimer-monoB / cc-pvdz	internal	local truncation error total energy kcal mol	held
DLPNO-MP2	s22-22-phenol-dimer-monoB / cc-pvdz	internal	local truncation error total energy kcal mol	held
DLPNO-MP2	s22-22-phenol-dimer-monoB / cc-pvdz	internal	local truncation error total energy kcal mol	held
DLPNO-CCSD	s22-01-ammonia-dimer / cc-pvdz	internal	dlpno ccsd correlation energy threshold monotonicity kcal mol	9.74×10^{-4}
dlpno-ccsd(t)	s22-01-ammonia-dimer / cc-pvdz	internal	local truncation error interaction energy kcal mol	5.05×10^{-4}
dlpno-ccsd(t)	s22-01-ammonia-dimer / cc-pvdz	internal	local truncation error interaction energy kcal mol	8.94×10^{-4}
dlpno-ccsd(t)	s22-01-ammonia-dimer / cc-pvdz	internal	local truncation error interaction energy kcal mol	7.38×10^{-4}
DLPNO-CCSD	s22-01-ammonia-dimer-monoA / cc-pvdz	internal	dlpno ccsd correlation energy threshold monotonicity kcal mol	5.31×10^{-4}
DLPNO-CCSD	s22-01-ammonia-dimer-monoB / cc-pvdz	internal	dlpno ccsd correlation energy threshold monotonicity kcal mol	5.31×10^{-4}
DLPNO-CCSD	s22-02-water-dimer / cc-pvdz	internal	dlpno ccsd correlation energy threshold monotonicity kcal mol	1.77×10^{-3}
dlpno-ccsd(t)	s22-02-water-dimer / cc-pvdz	internal	local truncation error interaction energy kcal mol	8.80×10^{-4}

Table S21, continued.

Method	System / basis	Ref.	Quantity	|Δ|
DLPNO-CCSD	s22-02-water-dimer-monoA / cc-pvdz	internal	dlpno ccsd correlation energy threshold monotonicity kcal mol	1.19×10^{-3}
DLPNO-CCSD	s22-02-water-dimer-monoB / cc-pvdz	internal	dlpno ccsd correlation energy threshold monotonicity kcal mol	1.19×10^{-3}
DLPNO-MP2	s22-03-formic-acid-dimer / cc-pvdz	internal	local truncation error interaction energy kcal mol	1.41×10^{-3}
DLPNO-MP2	s22-03-formic-acid-dimer / cc-pvdz	internal	local truncation error interaction energy kcal mol	8.57×10^{-4}
DLPNO-MP2	s22-03-formic-acid-dimer / cc-pvdz	internal	local truncation error interaction energy kcal mol	6.04×10^{-4}
DLPNO-MP2	s22-03-formic-acid-dimer / cc-pvdz	internal	local correlation energy ha	9.22×10^{-3}
dlpno-ccsd(t)	s22-03-formic-acid-dimer-monoA / cc-pvdz	internal	local correlation energy ha	5.97×10^{-3}
DLPNO-CCSD	s22-03-formic-acid-dimer-monoA / cc-pvdz	internal	dlpno ccsd correlation energy threshold monotonicity kcal mol	5.56×10^{-3}
dlpno-ccsd(t)	s22-03-formic-acid-dimer-monoB / cc-pvdz	internal	local correlation energy ha	5.97×10^{-3}
DLPNO-CCSD	s22-03-formic-acid-dimer-monoB / cc-pvdz	internal	dlpno ccsd correlation energy threshold monotonicity kcal mol	5.56×10^{-3}
DLPNO-MP2	s22-04-formamide-dimer / cc-pvdz	internal	local truncation error interaction energy kcal mol	1.63×10^{-3}
DLPNO-MP2	s22-04-formamide-dimer / cc-pvdz	internal	local truncation error interaction energy kcal mol	1.31×10^{-3}
DLPNO-MP2	s22-04-formamide-dimer / cc-pvdz	internal	local truncation error interaction energy kcal mol	1.17×10^{-3}
DLPNO-MP2	s22-04-formamide-dimer / cc-pvdz	internal	local correlation energy ha	9.58×10^{-3}
DLPNO-MP2	s22-04-formamide-dimer / cc-pvdz	internal	interaction energy kcalmol	1.63×10^{-3}
DLPNO-MP2	s22-04-formamide-dimer / cc-pvdz	internal	local correlation energy ha	5.20×10^{-3}
dlpno-ccsd(t)	s22-04-formamide-dimer-monoA / cc-pvdz	internal	local correlation energy ha	5.09×10^{-3}
DLPNO-CCSD	s22-04-formamide-dimer-monoA / cc-pvdz	internal	dlpno ccsd correlation energy threshold monotonicity kcal mol	4.82×10^{-3}
dlpno-ccsd(t)	s22-04-formamide-dimer-monoB / cc-pvdz	internal	local correlation energy ha	5.09×10^{-3}
DLPNO-CCSD	s22-04-formamide-dimer-monoB / cc-pvdz	internal	dlpno ccsd correlation energy threshold monotonicity kcal mol	4.82×10^{-3}
DLPNO-MP2	s22-05-uracil-dimer-hb / cc-pvdz	internal	local truncation error interaction energy kcal mol	1.09×10^{-3}
DLPNO-MP2	s22-05-uracil-dimer-hb / cc-pvdz	internal	local correlation energy ha	3.58×10^{-2}
DLPNO-MP2	s22-05-uracil-dimer-hb / cc-pvdz	internal	local correlation energy ha	2.23×10^{-2}
DLPNO-MP2	s22-05-uracil-dimer-hb-monoA / cc-pvdz	internal	local correlation energy ha	1.78×10^{-2}
DLPNO-MP2	s22-05-uracil-dimer-hb-monoA / cc-pvdz	internal	local correlation energy ha	1.11×10^{-2}
DLPNO-MP2	s22-05-uracil-dimer-hb-monoA / cc-pvdz	internal	local correlation energy ha	6.90×10^{-3}
DLPNO-MP2	s22-05-uracil-dimer-hb-monoB / cc-pvdz	internal	local correlation energy ha	1.78×10^{-2}
DLPNO-MP2	s22-05-uracil-dimer-hb-monoB / cc-pvdz	internal	local correlation energy ha	1.11×10^{-2}
DLPNO-MP2	s22-05-uracil-dimer-hb-monoB / cc-pvdz	internal	local correlation energy ha	6.90×10^{-3}

Table S21, continued.

Method	System / basis	Ref.	Quantity	$\lvert\Delta\rvert$
DLPNO-MP2	s22-05-uracil-dimer-hb / cc-pvdz	internal	local correlation energy ha	1.49×10^{-2}
DLPNO-MP2	s22-06-2-pyridone-2-aminopyridine / cc-pvdz	internal	local truncation error interaction energy kcal mol	1.35×10^{-3}
DLPNO-MP2	s22-06-2-pyridone-2-aminopyridine / cc-pvdz	internal	local truncation error interaction energy kcal mol	1.09×10^{-3}
DLPNO-MP2	s22-06-2-pyridone-2-aminopyridine / cc-pvdz	internal	local truncation error interaction energy kcal mol	1.14×10^{-3}
DLPNO-MP2	s22-06-2-pyridone-2-aminopyridine / cc-pvdz	internal	local correlation energy ha	2.70×10^{-2}
DLPNO-MP2	s22-06-2-pyridone-2-aminopyridine / cc-pvdz	internal	local correlation energy ha	1.68×10^{-2}
DLPNO-MP2	s22-06-2-pyridone-2-aminopyridine-monoA / cc-pvdz	internal	local correlation energy ha	1.34×10^{-2}
DLPNO-MP2	s22-06-2-pyridone-2-aminopyridine-monoA / cc-pvdz	internal	local correlation energy ha	8.35×10^{-3}
DLPNO-MP2	s22-06-2-pyridone-2-aminopyridine-monoA / cc-pvdz	internal	local correlation energy ha	5.73×10^{-3}
DLPNO-MP2	s22-06-2-pyridone-2-aminopyridine-monoB / cc-pvdz	internal	local correlation energy ha	1.22×10^{-2}
DLPNO-MP2	s22-06-2-pyridone-2-aminopyridine-monoB / cc-pvdz	internal	local correlation energy ha	7.35×10^{-3}
DLPNO-MP2	s22-06-2-pyridone-2-aminopyridine / cc-pvdz	internal	local correlation energy ha	1.16×10^{-2}
DLPNO-MP2	s22-07-adenine-thymine-wc / cc-pvdz	internal	local truncation error interaction energy kcal mol	1.52×10^{-3}
DLPNO-MP2	s22-07-adenine-thymine-wc / cc-pvdz	internal	local truncation error interaction energy kcal mol	1.34×10^{-3}
DLPNO-MP2	s22-07-adenine-thymine-wc / cc-pvdz	internal	local truncation error interaction energy kcal mol	1.49×10^{-3}
DLPNO-MP2	s22-07-adenine-thymine-wc / cc-pvdz	internal	local correlation energy ha	4.37×10^{-2}
DLPNO-MP2	s22-07-adenine-thymine-wc / cc-pvdz	internal	local correlation energy ha	2.77×10^{-2}
DLPNO-MP2	s22-07-adenine-thymine-wc-monoA / cc-pvdz	internal	local correlation energy ha	2.21×10^{-2}
DLPNO-MP2	s22-07-adenine-thymine-wc-monoA / cc-pvdz	internal	local correlation energy ha	1.37×10^{-2}
DLPNO-MP2	s22-07-adenine-thymine-wc-monoA / cc-pvdz	internal	local correlation energy ha	9.57×10^{-3}
DLPNO-MP2	s22-07-adenine-thymine-wc-monoB / cc-pvdz	internal	local correlation energy ha	2.00×10^{-2}
DLPNO-MP2	s22-07-adenine-thymine-wc-monoB / cc-pvdz	internal	local correlation energy ha	1.27×10^{-2}
DLPNO-MP2	s22-07-adenine-thymine-wc-monoB / cc-pvdz	internal	local correlation energy ha	8.17×10^{-3}
DLPNO-MP2	s22-07-adenine-thymine-wc / cc-pvdz	internal	local correlation energy ha	1.92×10^{-2}
DLPNO-CCSD	s22-08-methane-dimer / cc-pvdz	internal	dlpno ccsd correlation energy threshold monotonicity kcal mol	1.12×10^{-4}
DLPNO-CCSD	s22-08-methane-dimer-monoA / cc-pvdz	internal	dlpno ccsd correlation energy threshold monotonicity kcal mol	1.80×10^{-5}
DLPNO-CCSD	s22-08-methane-dimer-monoB / cc-pvdz	internal	dlpno ccsd correlation energy threshold monotonicity kcal mol	1.80×10^{-5}
dlpno-ccsd(t)	s22-09-ethene-dimer / cc-pvdz	internal	local correlation energy ha	5.09×10^{-3}

Table S21, continued.

Method	System / basis	Ref.	Quantity	$\lvert\Delta\rvert$
DLPNO-CCSD	s22-09-ethene-dimer / cc-pvdz	internal	dlpno ccsd correlation energy threshold monotonicity kcal mol	5.77×10^{-3}
dlpno-ccsd(t)	s22-09-ethene-dimer / cc-pvdz	internal	local truncation error interaction energy kcal mol	8.47×10^{-4}
dlpno-ccsd(t)	s22-09-ethene-dimer / cc-pvdz	internal	local truncation error interaction energy kcal mol	7.81×10^{-4}
DLPNO-MP2	s22-09-ethene-dimer / cc-pvdz	internal	local truncation error interaction energy kcal mol	9.24×10^{-4}
DLPNO-MP2	s22-09-ethene-dimer / cc-pvdz	internal	local truncation error interaction energy kcal mol	8.57×10^{-4}
DLPNO-MP2	s22-09-ethene-dimer / cc-pvdz	internal	local truncation error interaction energy kcal mol	8.43×10^{-4}
DLPNO-MP2	s22-09-ethene-dimer / cc-pvdz	internal	local correlation energy ha	5.18×10^{-3}
DLPNO-CCSD	s22-09-ethene-dimer-monoA / cc-pvdz	internal	dlpno ccsd correlation energy threshold monotonicity kcal mol	3.06×10^{-3}
DLPNO-CCSD	s22-09-ethene-dimer-monoB / cc-pvdz	internal	dlpno ccsd correlation energy threshold monotonicity kcal mol	3.06×10^{-3}
DLPNO-MP2	s22-10-benzene-ch4 / cc-pvdz	internal	local correlation energy ha	1.04×10^{-2}
DLPNO-MP2	s22-10-benzene-ch4 / cc-pvdz	internal	local correlation energy ha	6.63×10^{-3}
DLPNO-MP2	s22-10-benzene-ch4-monoA / cc-pvdz	internal	local correlation energy ha	9.02×10^{-3}
DLPNO-MP2	s22-10-benzene-ch4-monoA / cc-pvdz	internal	local correlation energy ha	5.59×10^{-3}
DLPNO-CCSD	s22-10-benzene-ch4-monoB / cc-pvdz	internal	dlpno ccsd correlation energy threshold monotonicity kcal mol	2.30×10^{-5}
DLPNO-MP2	s22-11-benzene-dimer-stack / cc-pvdz	internal	local truncation error interaction energy kcal mol	1.93×10^{-3}
DLPNO-MP2	s22-11-benzene-dimer-stack / cc-pvdz	internal	local truncation error interaction energy kcal mol	1.76×10^{-3}
DLPNO-MP2	s22-11-benzene-dimer-stack / cc-pvdz	internal	local truncation error interaction energy kcal mol	1.30×10^{-3}
DLPNO-MP2	s22-11-benzene-dimer-stack / cc-pvdz	internal	local correlation energy ha	2.00×10^{-2}
DLPNO-MP2	s22-11-benzene-dimer-stack / cc-pvdz	internal	interaction energy kcalmol	1.93×10^{-3}
DLPNO-MP2	s22-11-benzene-dimer-stack / cc-pvdz	internal	local correlation energy ha	1.30×10^{-2}
DLPNO-MP2	s22-11-benzene-dimer-stack / cc-pvdz	internal	interaction energy kcalmol	1.76×10^{-3}
DLPNO-MP2	s22-11-benzene-dimer-stack-monoA / cc-pvdz	internal	local correlation energy ha	9.02×10^{-3}
DLPNO-MP2	s22-11-benzene-dimer-stack-monoA / cc-pvdz	internal	local correlation energy ha	5.59×10^{-3}
DLPNO-MP2	s22-11-benzene-dimer-stack-monoB / cc-pvdz	internal	local correlation energy ha	9.02×10^{-3}
DLPNO-MP2	s22-11-benzene-dimer-stack-monoB / cc-pvdz	internal	local correlation energy ha	5.59×10^{-3}
DLPNO-MP2	s22-11-benzene-dimer-stack / cc-pvdz	internal	local correlation energy ha	8.70×10^{-3}
DLPNO-MP2	s22-12-pyrazine-dimer / cc-pvdz	internal	local truncation error interaction energy kcal mol	2.13×10^{-3}
DLPNO-MP2	s22-12-pyrazine-dimer / cc-pvdz	internal	local truncation error interaction energy kcal mol	1.85×10^{-3}

Table S21, continued.

Method	System / basis	Ref.	Quantity	$\lvert\Delta\rvert$
DLPNO-MP2	s22-12-pyrazine-dimer / cc-pvdz	internal	local truncation error interaction energy kcal mol	1.52×10^{-3}
DLPNO-MP2	s22-12-pyrazine-dimer / cc-pvdz	internal	local correlation energy ha	2.09×10^{-2}
DLPNO-MP2	s22-12-pyrazine-dimer / cc-pvdz	internal	interaction energy kcalmol	2.13×10^{-3}
DLPNO-MP2	s22-12-pyrazine-dimer / cc-pvdz	internal	local correlation energy ha	1.24×10^{-2}
DLPNO-MP2	s22-12-pyrazine-dimer / cc-pvdz	internal	interaction energy kcalmol	1.85×10^{-3}
DLPNO-MP2	s22-12-pyrazine-dimer-monoA / cc-pvdz	internal	local correlation energy ha	9.41×10^{-3}
DLPNO-MP2	s22-12-pyrazine-dimer-monoA / cc-pvdz	internal	local correlation energy ha	5.27×10^{-3}
DLPNO-MP2	s22-12-pyrazine-dimer-monoB / cc-pvdz	internal	local correlation energy ha	9.41×10^{-3}
DLPNO-MP2	s22-12-pyrazine-dimer-monoB / cc-pvdz	internal	local correlation energy ha	5.27×10^{-3}
DLPNO-MP2	s22-12-pyrazine-dimer / cc-pvdz	internal	local correlation energy ha	7.90×10^{-3}
DLPNO-MP2	s22-13-uracil-dimer-stack / cc-pvdz	internal	local truncation error interaction energy kcal mol	3.81×10^{-3}
DLPNO-MP2	s22-13-uracil-dimer-stack / cc-pvdz	internal	local truncation error interaction energy kcal mol	3.26×10^{-3}
DLPNO-MP2	s22-13-uracil-dimer-stack / cc-pvdz	internal	local truncation error interaction energy kcal mol	3.13×10^{-3}
DLPNO-MP2	s22-13-uracil-dimer-stack / cc-pvdz	internal	local correlation energy ha	3.76×10^{-2}
DLPNO-MP2	s22-13-uracil-dimer-stack / cc-pvdz	internal	interaction energy kcalmol	3.81×10^{-3}
DLPNO-MP2	s22-13-uracil-dimer-stack / cc-pvdz	internal	local correlation energy ha	2.37×10^{-2}
DLPNO-MP2	s22-13-uracil-dimer-stack / cc-pvdz	internal	interaction energy kcalmol	3.26×10^{-3}
DLPNO-MP2	s22-13-uracil-dimer-stack-monoA / cc-pvdz	internal	local correlation energy ha	1.69×10^{-2}
DLPNO-MP2	s22-13-uracil-dimer-stack-monoA / cc-pvdz	internal	local correlation energy ha	1.02×10^{-2}
DLPNO-MP2	s22-13-uracil-dimer-stack-monoA / cc-pvdz	internal	local correlation energy ha	6.52×10^{-3}
DLPNO-MP2	s22-13-uracil-dimer-stack-monoB / cc-pvdz	internal	local correlation energy ha	1.69×10^{-2}
DLPNO-MP2	s22-13-uracil-dimer-stack-monoB / cc-pvdz	internal	local correlation energy ha	1.02×10^{-2}
DLPNO-MP2	s22-13-uracil-dimer-stack-monoB / cc-pvdz	internal	local correlation energy ha	6.52×10^{-3}
DLPNO-MP2	s22-13-uracil-dimer-stack / cc-pvdz	internal	local correlation energy ha	1.62×10^{-2}
DLPNO-MP2	s22-13-uracil-dimer-stack / cc-pvdz	internal	interaction energy kcalmol	3.13×10^{-3}
DLPNO-MP2	s22-14-indole-benzene-stack / cc-pvdz	internal	local truncation error interaction energy kcal mol	3.04×10^{-3}
DLPNO-MP2	s22-14-indole-benzene-stack / cc-pvdz	internal	local truncation error interaction energy kcal mol	2.69×10^{-3}
DLPNO-MP2	s22-14-indole-benzene-stack / cc-pvdz	internal	local truncation error interaction energy kcal mol	2.35×10^{-3}
DLPNO-MP2	s22-14-indole-benzene-stack / cc-pvdz	internal	local correlation energy ha	3.05×10^{-2}
DLPNO-MP2	s22-14-indole-benzene-stack / cc-pvdz	internal	interaction energy kcalmol	3.04×10^{-3}
DLPNO-MP2	s22-14-indole-benzene-stack / cc-pvdz	internal	local correlation energy ha	2.04×10^{-2}
DLPNO-MP2	s22-14-indole-benzene-stack / cc-pvdz	internal	interaction energy kcalmol	2.69×10^{-3}
DLPNO-MP2	s22-14-indole-benzene-stack-monoA / cc-pvdz	internal	local correlation energy ha	9.02×10^{-3}
DLPNO-MP2	s22-14-indole-benzene-stack-monoA / cc-pvdz	internal	local correlation energy ha	5.59×10^{-3}

Table S21, continued.

Method	System / basis	Ref.	Quantity	$\lvert\Delta\rvert$
DLPNO-MP2	s22-14-indole-benzene-stack-monoB / cc-pvdz	internal	local correlation energy ha	1.85×10^{-2}
DLPNO-MP2	s22-14-indole-benzene-stack-monoB / cc-pvdz	internal	local correlation energy ha	1.21×10^{-2}
DLPNO-MP2	s22-14-indole-benzene-stack-monoB / cc-pvdz	internal	local correlation energy ha	8.54×10^{-3}
DLPNO-MP2	s22-14-indole-benzene-stack / cc-pvdz	internal	local correlation energy ha	1.46×10^{-2}
DLPNO-MP2	s22-14-indole-benzene-stack / cc-pvdz	internal	interaction energy kcalmol	2.35×10^{-3}
DLPNO-MP2	s22-15-adenine-thymine-stack / cc-pvdz	internal	local truncation error interaction energy kcal mol	5.37×10^{-3}
DLPNO-MP2	s22-15-adenine-thymine-stack / cc-pvdz	internal	local truncation error interaction energy kcal mol	4.63×10^{-3}
DLPNO-MP2	s22-15-adenine-thymine-stack / cc-pvdz	internal	local truncation error interaction energy kcal mol	4.40×10^{-3}
DLPNO-MP2	s22-15-adenine-thymine-stack / cc-pvdz	internal	local correlation energy ha	4.69×10^{-2}
DLPNO-MP2	s22-15-adenine-thymine-stack / cc-pvdz	internal	interaction energy kcalmol	5.37×10^{-3}
DLPNO-MP2	s22-15-adenine-thymine-stack / cc-pvdz	internal	local correlation energy ha	3.04×10^{-2}
DLPNO-MP2	s22-15-adenine-thymine-stack / cc-pvdz	internal	interaction energy kcalmol	4.63×10^{-3}
DLPNO-MP2	s22-15-adenine-thymine-stack-monoA / cc-pvdz	internal	local correlation energy ha	2.22×10^{-2}
DLPNO-MP2	s22-15-adenine-thymine-stack-monoA / cc-pvdz	internal	local correlation energy ha	1.37×10^{-2}
DLPNO-MP2	s22-15-adenine-thymine-stack-monoA / cc-pvdz	internal	local correlation energy ha	9.52×10^{-3}
DLPNO-MP2	s22-15-adenine-thymine-stack-monoB / cc-pvdz	internal	local correlation energy ha	1.94×10^{-2}
DLPNO-MP2	s22-15-adenine-thymine-stack-monoB / cc-pvdz	internal	local correlation energy ha	1.20×10^{-2}
DLPNO-MP2	s22-15-adenine-thymine-stack-monoB / cc-pvdz	internal	local correlation energy ha	7.82×10^{-3}
DLPNO-MP2	s22-15-adenine-thymine-stack / cc-pvdz	internal	local correlation energy ha	2.17×10^{-2}
DLPNO-MP2	s22-15-adenine-thymine-stack / cc-pvdz	internal	interaction energy kcalmol	4.40×10^{-3}
DLPNO-CCSD	s22-16-ethene-ethyne / cc-pvdz	internal	dlpno ccsd correlation energy threshold monotonicity kcal mol	4.43×10^{-3}
dlpno-ccsd(t)	s22-16-ethene-ethyne / cc-pvdz	internal	local truncation error interaction energy kcal mol	6.39×10^{-4}
DLPNO-MP2	s22-16-ethene-ethyne / cc-pvdz	internal	local truncation error interaction energy kcal mol	6.90×10^{-4}
DLPNO-MP2	s22-16-ethene-ethyne / cc-pvdz	internal	local truncation error interaction energy kcal mol	6.68×10^{-4}
DLPNO-MP2	s22-16-ethene-ethyne / cc-pvdz	internal	local truncation error interaction energy kcal mol	6.51×10^{-4}
DLPNO-CCSD	s22-16-ethene-ethyne-monoA / cc-pvdz	internal	dlpno ccsd correlation energy threshold monotonicity kcal mol	3.06×10^{-3}
DLPNO-CCSD	s22-16-ethene-ethyne-monoB / cc-pvdz	internal	dlpno ccsd correlation energy threshold monotonicity kcal mol	1.70×10^{-3}

Table S21, continued.

Method	System / basis	Ref.	Quantity	|Δ|
DLPNO-MP2	s22-17-benzene-h2o / cc-pvdz	internal	local truncation error interaction energy kcal mol	4.97×10^{-4}
DLPNO-CCSD	s22-17-benzene-h2o-monoB / cc-pvdz	internal	dlpno ccsd correlation energy threshold monotonicity kcal mol	1.22×10^{-3}
DLPNO-CCSD	s22-18-benzene-nh3-monoB / cc-pvdz	internal	dlpno ccsd correlation energy threshold monotonicity kcal mol	5.82×10^{-4}
DLPNO-MP2	s22-19-benzene-hcn / cc-pvdz	internal	local truncation error interaction energy kcal mol	8.98×10^{-4}
DLPNO-MP2	s22-19-benzene-hcn / cc-pvdz	internal	local truncation error interaction energy kcal mol	8.52×10^{-4}
DLPNO-MP2	s22-19-benzene-hcn / cc-pvdz	internal	local truncation error interaction energy kcal mol	7.79×10^{-4}
DLPNO-CCSD	s22-19-benzene-hcn-monoB / cc-pvdz	internal	dlpno ccsd correlation energy threshold monotonicity kcal mol	1.96×10^{-3}
DLPNO-MP2	s22-20-benzene-dimer-t / cc-pvdz	internal	local truncation error interaction energy kcal mol	8.18×10^{-4}
DLPNO-MP2	s22-20-benzene-dimer-t / cc-pvdz	internal	local truncation error interaction energy kcal mol	7.53×10^{-4}
DLPNO-MP2	s22-20-benzene-dimer-t / cc-pvdz	internal	local truncation error interaction energy kcal mol	6.29×10^{-4}
DLPNO-MP2	s22-21-indole-benzene-t / cc-pvdz	internal	local truncation error interaction energy kcal mol	1.47×10^{-3}
DLPNO-MP2	s22-21-indole-benzene-t / cc-pvdz	internal	local truncation error interaction energy kcal mol	1.31×10^{-3}
DLPNO-MP2	s22-21-indole-benzene-t / cc-pvdz	internal	local truncation error interaction energy kcal mol	1.25×10^{-3}
DLPNO-MP2	s22-22-phenol-dimer / cc-pvdz	internal	local truncation error interaction energy kcal mol	2.77×10^{-3}
DLPNO-MP2	s22-22-phenol-dimer / cc-pvdz	internal	local truncation error interaction energy kcal mol	2.53×10^{-3}
DLPNO-MP2	s22-22-phenol-dimer / cc-pvdz	internal	local truncation error interaction energy kcal mol	2.51×10^{-3}
dlpno-ccsd(t)	water-dimer / def2-svp	orca	ccsd correlation	2.65×10^{-4}
dlpno-ccsd(t)	water-dimer / def2-svp	orca	total energy ha	1.79×10^{-4}
dlpno-ccsd(t)	water-dimer / def2-svp	orca	triples correction	8.55×10^{-5}
DLPNO-CCSD	h2 / def2-svp	orca	total energy ha	reference-missing
dlpno-ccsd(t)	h2 / def2-svp	orca	total energy ha	reference-missing
dlpno-ccsd(t)	atom-al / sto-3g	orca	energy total ha	blocked
dlpno-ccsd(t)	atom-c / 3-21g	orca	energy total ha	blocked
dlpno-ccsd(t)	atom-c / sto-3g	orca	energy total ha	blocked
DLPNO-MP2	atom-c / sto-3g	orca	energy total ha	blocked
dlpno-ccsd(t)	atom-li / 3-21g	orca	energy total ha	blocked
dlpno-ccsd(t)	atom-li / sto-3g	orca	energy total ha	blocked
DLPNO-MP2	atom-li / sto-3g	orca	energy total ha	blocked
dlpno-ccsd(t)	atom-mg / sto-3g	orca	energy total ha	blocked
dlpno-ccsd(t)	atom-na / sto-3g	orca	energy total ha	blocked
dlpno-ccsd(t)	atom-o / 3-21g	orca	energy total ha	blocked
dlpno-ccsd(t)	atom-si / sto-3g	orca	energy total ha	blocked
dlpno-ccsd(t)	ch4 / sto-3g	orca	energy total ha	blocked
dlpno-ccsd(t)	h2 / 3-21g	orca	energy total ha	blocked
DLPNO-MP2	h2 / 3-21g	orca	energy total ha	blocked
DLPNO-MP2	h2 / sto-3g	orca	energy total ha	blocked
dlpno-ccsd(t)	h2o / sto-3g	orca	energy total ha	blocked
dlpno-ccsd(t)	hf / sto-3g	orca	energy total ha	blocked
dlpno-ccsd(t)	lih / sto-3g	orca	energy total ha	blocked

Table S21, continued.

Method	System / basis	Ref.	Quantity	$\lvert\Delta\rvert$
dlpno-ccsd(t)	nh3 / sto-3g	orca	energy total ha	blocked
dlpno-ccsd(t)	oh-radical / sto-3g	orca	energy total ha	blocked
dlpno-ccsd(t)	water-cluster:1 / sto-3g	orca	energy total ha	blocked
dlpno-ccsd(t)	water-dimer / def2-svp	orca	ccsd correlation ha	blocked
dlpno-ccsd(t)	water-dimer / def2-svp	orca	ccsd correlation ha	blocked
dlpno-ccsd(t)	water-dimer / def2-svp	orca	reference energy ha	blocked
dlpno-ccsd(t)	water-dimer / def2-svp	orca	reference energy ha	blocked
dlpno-ccsd(t)	water-dimer / def2-svp	orca	total energy ha	blocked
dlpno-ccsd(t)	water-dimer / def2-svp	orca	total energy ha	blocked
dlpno-ccsd(t)	water-dimer / def2-svp	orca	triples correction ha	blocked
dlpno-ccsd(t)	water-dimer / def2-svp	orca	triples correction ha	blocked
dlpno-ccsd(t)	water-dimer / def2-svp	orca	total energy ha	blocked
dlpno-ccsd(t)	water-dimer / def2-svp	orca	total energy ha	blocked
dlpno-ccsd(t)	water-dimer / def2-svp	orca	total energy ha	blocked
dlpno-ccsd(t)	water-dimer / def2-svp	orca	total energy ha	blocked
dlpno-ccsd(t)	water-dimer / def2-svp	orca	total energy ha	blocked
dlpno-ccsd(t)	water-dimer / def2-svp	orca	total energy ha	blocked
Active-space CI				
55 pass, 37 artifact-incomplete, 17 reference-missing, 17 blocked. Median $\lvert\Delta E\rvert$ 4.5×10^{-10}, max 4.8×10^{-8} E_h.				
CASCI	n2 / cc-pvdz	openmolcas	total energy ha	8.20×10^{-9}
CASCI	n2 / cc-pvdz	openmolcas	active natural occupation max abs deviation	n/a
CASCI	n2 / cc-pvdz	openmolcas	total energy ha	8.29×10^{-9}
CASSCF	n2 / cc-pvdz	openmolcas	total energy ha	0
CASSCF	n2 / cc-pvdz	openmolcas	total energy ha	3.00×10^{-10}
CASSCF	n2 / cc-pvdz	openmolcas	active natural occupation max abs deviation	n/a
CASSCF	n2 / cc-pvdz	openmolcas	active natural occupation max abs deviation	n/a
CASCI	n2 / cc-pvdz	openmolcas	total energy ha	8.20×10^{-9}
CASCI	n2 / cc-pvdz	openmolcas	active natural occupation max abs deviation	n/a
CASSCF	n2 / cc-pvdz	openmolcas	total energy ha	1.00×10^{-10}
CASSCF	n2 / cc-pvdz	openmolcas	total energy ha	7.00×10^{-10}
CASSCF	n2 / cc-pvdz	openmolcas	active natural occupation max abs deviation	n/a
CASSCF	n2 / cc-pvdz	openmolcas	active natural occupation max abs deviation	n/a
CASCI	n2 / cc-pvtz	openmolcas	total energy ha	1.14×10^{-8}
CASCI	n2 / cc-pvtz	openmolcas	active natural occupation max abs deviation	n/a
CASSCF	n2 / cc-pvtz	openmolcas	total energy ha	0
CASSCF	n2 / cc-pvtz	openmolcas	total energy ha	1.00×10^{-10}
CASSCF	n2 / cc-pvtz	openmolcas	active natural occupation max abs deviation	n/a
CASSCF	n2 / cc-pvtz	openmolcas	active natural occupation max abs deviation	n/a
CASCI	n2 / cc-pvdz	openmolcas	total energy ha	4.82×10^{-8}
CASCI	n2 / cc-pvdz	openmolcas	active natural occupation max abs deviation	n/a
CASSCF	n2 / cc-pvdz	openmolcas	total energy ha	0
CASSCF	n2 / cc-pvdz	openmolcas	total energy ha	3.00×10^{-10}
CASSCF	n2 / cc-pvdz	openmolcas	active natural occupation max abs deviation	n/a
CASSCF	n2 / cc-pvdz	openmolcas	active natural occupation max abs deviation	n/a
CASCI	n2 / cc-pvdz	openmolcas	total energy ha	7.00×10^{-10}

Table S21, continued.

Method	System / basis	Ref.	Quantity	$\lvert\Delta\rvert$
CASCI	n2 / cc-pvdz	openmolcas	active natural occupation max abs deviation	n/a
CASSCF	n2 / cc-pvdz	openmolcas	total energy ha	5.00×10^{-10}
CASSCF	n2 / cc-pvdz	openmolcas	total energy ha	6.00×10^{-10}
CASSCF	n2 / cc-pvdz	openmolcas	active natural occupation max abs deviation	n/a
CASSCF	n2 / cc-pvdz	openmolcas	active natural occupation max abs deviation	n/a
CASCI	hf-molecule / cc-pvdz	openmolcas	total energy ha	3.40×10^{-9}
CASCI	hf-molecule / cc-pvdz	openmolcas	active natural occupation max abs deviation	n/a
CASSCF	hf-molecule / cc-pvdz	openmolcas	total energy ha	0
CASSCF	hf-molecule / cc-pvdz	openmolcas	total energy ha	3.00×10^{-10}
CASSCF	hf-molecule / cc-pvdz	openmolcas	active natural occupation max abs deviation	n/a
CASSCF	hf-molecule / cc-pvdz	openmolcas	active natural occupation max abs deviation	n/a
CASCI	hf-molecule / cc-pvdz	openmolcas	total energy ha	6.10×10^{-9}
CASCI	hf-molecule / cc-pvdz	openmolcas	active natural occupation max abs deviation	n/a
CASSCF	hf-molecule / cc-pvdz	openmolcas	total energy ha	1.00×10^{-10}
CASSCF	hf-molecule / cc-pvdz	openmolcas	total energy ha	5.00×10^{-10}
CASSCF	hf-molecule / cc-pvdz	openmolcas	active natural occupation max abs deviation	n/a
CASSCF	hf-molecule / cc-pvdz	openmolcas	active natural occupation max abs deviation	n/a
CASCI	h2o / cc-pvdz	openmolcas	total energy ha	3.50×10^{-9}
CASCI	h2o / cc-pvdz	openmolcas	active natural occupation max abs deviation	n/a
CASSCF	h2o / cc-pvdz	openmolcas	total energy ha	1.00×10^{-10}
CASSCF	h2o / cc-pvdz	openmolcas	total energy ha	3.00×10^{-10}
CASSCF	h2o / cc-pvdz	openmolcas	active natural occupation max abs deviation	n/a
CASSCF	h2o / cc-pvdz	openmolcas	active natural occupation max abs deviation	n/a
CASCI	c2 / cc-pvdz	openmolcas	total energy ha	2.30×10^{-9}
CASCI	c2 / cc-pvdz	openmolcas	active natural occupation max abs deviation	n/a
CASSCF	c2 / cc-pvdz	openmolcas	total energy ha	2.00×10^{-10}
CASSCF	c2 / cc-pvdz	openmolcas	total energy ha	4.00×10^{-10}
CASSCF	c2 / cc-pvdz	openmolcas	active natural occupation max abs deviation	n/a
CASSCF	c2 / cc-pvdz	openmolcas	active natural occupation max abs deviation	n/a
DMRG	h2 / cc-pvdz	pyscf	total energy ha	artifact-incomplete
CISD	h2 / sto-3g	pyscf	total energy ha	artifact-incomplete
CISD	h2 / sto-3g	pyscf	total energy ha	artifact-incomplete
FCI	h2 / sto-3g	pyscf	total energy ha	artifact-incomplete
FCI	h2 / sto-3g	pyscf	total energy ha	artifact-incomplete
SELECTED_CI	h2 / sto-3g	pyscf	total energy ha	artifact-incomplete
SELECTED_CI	h2 / sto-3g	pyscf	total energy ha	artifact-incomplete
DMRG	h2 / sto-3g	pyscf	total energy ha	artifact-incomplete
DMRG	h2 / sto-3g	pyscf	total energy ha	artifact-incomplete
V2RDM	h2 / sto-3g	pyscf	total energy ha	artifact-incomplete
V2RDM	h2 / sto-3g	pyscf	total energy ha	artifact-incomplete
transcorrelated_ci	h2 / sto-3g	pyscf	total energy ha	artifact-incomplete
transcorrelated_ci	h2 / sto-3g	pyscf	total energy ha	artifact-incomplete
CASCI	h2 / sto-3g	openmolcas	total energy ha	artifact-incomplete

Table S21, continued.

Method	System / basis	Ref.	Quantity	|Δ|
CASCI	h2 / sto-3g	openmolcas	total energy ha	artifact-incomplete
MRCI	h2 / sto-3g	openmolcas	total energy ha	artifact-incomplete
MRCI	h2 / sto-3g	openmolcas	total energy ha	artifact-incomplete
CASSCF	h2 / sto-3g	openmolcas	total energy ha	artifact-incomplete
CASSCF	h2 / sto-3g	openmolcas	total energy ha	artifact-incomplete
CISD	h2 / cc-pvdz	pyscf	total energy ha	artifact-incomplete
CISD	h2 / sto-3g	pyscf	total energy ha	artifact-incomplete
FCI	h2 / cc-pvdz	pyscf	total energy ha	artifact-incomplete
FCI	h2 / sto-3g	pyscf	total energy ha	artifact-incomplete
SELECTED_CI	h2 / cc-pvdz	pyscf	total energy ha	artifact-incomplete
SELECTED_CI	h2 / sto-3g	pyscf	total energy ha	artifact-incomplete
DMRG	h2 / cc-pvdz	pyscf	total energy ha	artifact-incomplete
DMRG	h2 / sto-3g	pyscf	total energy ha	artifact-incomplete
V2RDM	h2 / cc-pvdz	pyscf	total energy ha	artifact-incomplete
V2RDM	h2 / sto-3g	pyscf	total energy ha	artifact-incomplete
transcorrelated_ci	h2 / cc-pvdz	pyscf	total energy ha	artifact-incomplete
transcorrelated_ci	h2 / sto-3g	pyscf	total energy ha	artifact-incomplete
CASCI	h2 / cc-pvdz	openmolcas	total energy ha	artifact-incomplete
CASCI	h2 / sto-3g	openmolcas	total energy ha	artifact-incomplete
MRCI	h2 / cc-pvdz	openmolcas	total energy ha	artifact-incomplete
MRCI	h2 / sto-3g	openmolcas	total energy ha	artifact-incomplete
CASSCF	h2 / cc-pvdz	openmolcas	total energy ha	artifact-incomplete
CASSCF	h2 / sto-3g	openmolcas	total energy ha	artifact-incomplete
CISD	h2 / cc-pvdz	pyscf	total energy ha	reference-missing
FCI	h2 / cc-pvdz	pyscf	total energy ha	reference-missing
SELECTED_CI	h2 / cc-pvdz	pyscf	total energy ha	reference-missing
V2RDM	h2 / cc-pvdz	pyscf	total energy ha	reference-missing
transcorrelated_ci	h2 / cc-pvdz	pyscf	total energy ha	reference-missing
CASCI	h2 / cc-pvdz	openmolcas	total energy ha	reference-missing
MRCI	h2 / cc-pvdz	openmolcas	total energy ha	reference-missing
CASSCF	h2 / cc-pvdz	openmolcas	total energy ha	reference-missing
CISD	h2 / sto-3g	pyscf	total energy ha	reference-missing
FCI	h2 / sto-3g	pyscf	total energy ha	reference-missing
SELECTED_CI	h2 / sto-3g	pyscf	total energy ha	reference-missing
DMRG	h2 / sto-3g	pyscf	total energy ha	reference-missing
V2RDM	h2 / sto-3g	pyscf	total energy ha	reference-missing
transcorrelated_ci	h2 / sto-3g	pyscf	total energy ha	reference-missing
CASCI	h2 / sto-3g	openmolcas	total energy ha	reference-missing
MRCI	h2 / sto-3g	openmolcas	total energy ha	reference-missing
CASSCF	h2 / sto-3g	openmolcas	total energy ha	reference-missing
FCI	h2 / sto-3g	orca	energy total ha	blocked
CISD	h2 / sto-3g	pyscf	total energy ha	blocked
FCI	h2 / sto-3g	pyscf	total energy ha	blocked
SELECTED_CI	h2 / sto-3g	pyscf	total energy ha	blocked
DMRG	h2 / sto-3g	pyscf	total energy ha	blocked
V2RDM	h2 / sto-3g	pyscf	total energy ha	blocked
transcorrelated_ci	h2 / sto-3g	pyscf	total energy ha	blocked
CASCI	h2 / sto-3g	openmolcas	total energy ha	blocked
MRCI	h2 / sto-3g	openmolcas	total energy ha	blocked
CASSCF	h2 / sto-3g	openmolcas	total energy ha	blocked
CASSCF	n2 / cc-pvdz	openmolcas	casscf nuclear gradient dEdz n1 ha per bohr	blocked
SELECTED_CI	n2 / cc-pvdz	vibeqc	correlation energy ha	blocked
SELECTED_CI	n2 / cc-pvdz	vibeqc	correlation energy ha	blocked
SELECTED_CI	n2 / cc-pvdz	vibeqc	correlation energy ha	blocked
SELECTED_CI	n2 / cc-pvdz	vibeqc	correlation energy ha	blocked
SELECTED_CI	n2 / cc-pvdz	vibeqc	correlation energy ha	blocked

Table S21, continued.

Method	System / basis	Ref.	Quantity	$\lvert\Delta\rvert$
SELECTED_CI	n2 / cc-pvdz	vibeqc	correlation energy ha	blocked
Multireference perturbation theory				
10 pass, 2 fail, 16 artifact-incomplete, 8 reference-missing, 4 blocked. Median $\lvert\Delta E\rvert$ 1.2×10^{-6}, max 9.1×10^{-6} E_h.				
NEVPT2	n2 / cc-pvdz	orca	total energy ha	2.04×10^{-6}
NEVPT2	n2 / cc-pvdz	orca	correlation energy ha	2.04×10^{-6}
CASPT2	hf-molecule / cc-pvdz	openmolcas	total energy ha	9.15×10^{-6}
CASPT2	hf-molecule / cc-pvdz	openmolcas	correlation energy ha	9.15×10^{-6}
NEVPT2	hf-molecule / cc-pvdz	orca	total energy ha	4.35×10^{-7}
NEVPT2	hf-molecule / cc-pvdz	orca	correlation energy ha	4.35×10^{-7}
CASPT2	h2o / cc-pvdz	openmolcas	total energy ha	1.20×10^{-6}
CASPT2	h2o / cc-pvdz	openmolcas	correlation energy ha	1.20×10^{-6}
NEVPT2	h2o / cc-pvdz	orca	total energy ha	3.64×10^{-7}
NEVPT2	h2o / cc-pvdz	orca	correlation energy ha	3.64×10^{-7}
CASPT2	n2 / cc-pvdz	openmolcas	total energy ha	8.85×10^{-5}
CASPT2	n2 / cc-pvdz	openmolcas	correlation energy ha	8.85×10^{-5}
CASPT2	h2 / sto-3g	openmolcas	total energy ha	artifact-incomplete
CASPT2	h2 / sto-3g	openmolcas	total energy ha	artifact-incomplete
CASPT2	lih / sto-3g	openmolcas	total energy ha	artifact-incomplete
CASPT2	lih / sto-3g	openmolcas	total energy ha	artifact-incomplete
CASPT2	lih / sto-3g	openmolcas	total energy ha	artifact-incomplete
CASPT2	lih / sto-3g	openmolcas	total energy ha	artifact-incomplete
NEVPT2	h2 / sto-3g	openmolcas	total energy ha	artifact-incomplete
NEVPT2	h2 / sto-3g	openmolcas	total energy ha	artifact-incomplete
CASPT2	h2 / cc-pvdz	openmolcas	total energy ha	artifact-incomplete
CASPT2	h2 / sto-3g	openmolcas	total energy ha	artifact-incomplete
CASPT2	lih / cc-pvdz	openmolcas	total energy ha	artifact-incomplete
CASPT2	lih / sto-3g	openmolcas	total energy ha	artifact-incomplete
CASPT2	lih / cc-pvdz	openmolcas	total energy ha	artifact-incomplete
CASPT2	lih / sto-3g	openmolcas	total energy ha	artifact-incomplete
NEVPT2	h2 / cc-pvdz	openmolcas	total energy ha	artifact-incomplete
NEVPT2	h2 / sto-3g	openmolcas	total energy ha	artifact-incomplete
CASPT2	h2 / cc-pvdz	openmolcas	total energy ha	reference-missing
CASPT2	lih / cc-pvdz	openmolcas	total energy ha	reference-missing
CASPT2	lih / cc-pvdz	openmolcas	total energy ha	reference-missing
NEVPT2	h2 / cc-pvdz	openmolcas	total energy ha	reference-missing
CASPT2	h2 / sto-3g	openmolcas	total energy ha	reference-missing
CASPT2	lih / sto-3g	openmolcas	total energy ha	reference-missing
CASPT2	lih / sto-3g	openmolcas	total energy ha	reference-missing
NEVPT2	h2 / sto-3g	openmolcas	total energy ha	reference-missing
CASPT2	h2 / sto-3g	openmolcas	total energy ha	blocked
CASPT2	lih / sto-3g	openmolcas	total energy ha	blocked
CASPT2	lih / sto-3g	openmolcas	total energy ha	blocked
NEVPT2	h2 / sto-3g	openmolcas	total energy ha	blocked
Other post-Hartree–Fock				
74 blocked.				
CCSD(T)	benzene / sto-3g	orca	total energy ha	blocked
dlpno-ccsd(t)	benzene / def2-svp	orca	total energy ha	blocked
dlpno-ccsd(t)	benzene / cc-pvdz	orca	total energy ha	blocked
MP2	butadiene / cc-pvtz	orca	total energy ha	blocked
MP2	crambin / cc-pvtz	orca	total energy ha	blocked
CCSD(T)	c2h4 / def2-svp	orca	ccsd correlation energy ha	blocked
CCSD(T)	c2h4 / def2-svp	orca	total energy ha	blocked
CCSD(T)	c2h4 / def2-svp	orca	triples energy ha	blocked
dlpno-ccsd(t)	ch2o / cc-pvdz	orca	ccsd correlation energy ha	blocked
dlpno-ccsd(t)	ch2o / cc-pvdz	orca	total energy ha	blocked
dlpno-ccsd(t)	ch2o / cc-pvdz	orca	triples energy ha	blocked

Table S21, continued.

Method	System / basis	Ref.	Quantity	|Δ|
MP2	cr-co6 / def2-svp	orca	total energy ha	blocked
MP2	cyclopentadiene / def2-svp	orca	total energy ha	blocked
MP2	cyclopentadiene / cc-pvdz	orca	total energy ha	blocked
dlpno-ccsd(t)	cyclopropene / def2-svp	orca	ccsd correlation energy ha	blocked
dlpno-ccsd(t)	cyclopropene / def2-svp	orca	total energy ha	blocked
dlpno-ccsd(t)	cyclopropene / def2-svp	orca	triples energy ha	blocked
dlpno-ccsd(t)	glycine / def2-svp	orca	ccsd correlation energy ha	blocked
dlpno-ccsd(t)	glycine / def2-svp	orca	total energy ha	blocked
dlpno-ccsd(t)	glycine / def2-svp	orca	triples energy ha	blocked
MP2	s22-formamide-dimer / def2-tzvp	orca	total energy ha	blocked
dlpno-ccsd(t)	h2o2 / def2-tzvp	orca	ccsd correlation energy ha	blocked
dlpno-ccsd(t)	h2o2 / def2-tzvp	orca	total energy ha	blocked
dlpno-ccsd(t)	h2o2 / def2-tzvp	orca	triples energy ha	blocked
MP2	hf / def2-tzvp	orca	correlation energy ha	blocked
MP2	hf / def2-tzvp	orca	opposite spin correlation energy ha	blocked
MP2	hf / def2-tzvp	orca	same spin correlation energy ha	blocked
MP2	hf / def2-tzvp	orca	total energy ha	blocked
CCSD(T)	imidazole / sto-3g	orca	total energy ha	blocked
MP2	naphthalene / sto-3g	orca	correlation energy ha	blocked
MP2	naphthalene / sto-3g	orca	opposite spin correlation energy ha	blocked
MP2	naphthalene / sto-3g	orca	same spin correlation energy ha	blocked
MP2	naphthalene / sto-3g	orca	total energy ha	blocked
MP2	ni-co4 / def2-svp	orca	correlation energy ha	blocked
MP2	ni-co4 / def2-svp	orca	opposite spin correlation energy ha	blocked
MP2	ni-co4 / def2-svp	orca	same spin correlation energy ha	blocked
MP2	ni-co4 / def2-svp	orca	total energy ha	blocked
MP2	norbornadiene / cc-pvdz	orca	correlation energy ha	blocked
MP2	norbornadiene / cc-pvdz	orca	opposite spin correlation energy ha	blocked
MP2	norbornadiene / cc-pvdz	orca	same spin correlation energy ha	blocked
MP2	norbornadiene / cc-pvdz	orca	total energy ha	blocked
CCSD(T)	oh-radical / def2-tzvp	orca	total energy ha	blocked
MP2	p-benzoquinone / cc-pvdz	orca	correlation energy ha	blocked
MP2	p-benzoquinone / cc-pvdz	orca	opposite spin correlation energy ha	blocked
MP2	p-benzoquinone / cc-pvdz	orca	same spin correlation energy ha	blocked
MP2	p-benzoquinone / cc-pvdz	orca	total energy ha	blocked
MP2	propanamide / cc-pvtz	orca	total energy ha	blocked
CCSD(T)	propanamide / sto-3g	orca	total energy ha	blocked
MP2	pyridazine / cc-pvtz	orca	total energy ha	blocked
CCSD(T)	pyridazine / sto-3g	orca	total energy ha	blocked
MP2	pyridine / sto-3g	orca	correlation energy ha	blocked
MP2	pyridine / sto-3g	orca	opposite spin correlation energy ha	blocked
MP2	pyridine / sto-3g	orca	same spin correlation energy ha	blocked
MP2	pyridine / sto-3g	orca	total energy ha	blocked
CCSD(T)	pyrimidine / cc-pvdz	orca	total energy ha	blocked
MP2	pyrrole / def2-tzvp	orca	total energy ha	blocked
MP2	s22-benzene-methane / def2-svp	orca	correlation energy ha	blocked

Table S21, continued.

Method	System / basis	Ref.	Quantity	$\lvert\Delta\rvert$
MP2	s22-benzene-methane / def2-svp	orca	opposite spin correlation energy ha	blocked
MP2	s22-benzene-methane / def2-svp	orca	same spin correlation energy ha	blocked
MP2	s22-benzene-methane / def2-svp	orca	total energy ha	blocked
MP2	s22-formamide-dimer / sto-3g	orca	correlation energy ha	blocked
MP2	s22-formamide-dimer / sto-3g	orca	opposite spin correlation energy ha	blocked
MP2	s22-formamide-dimer / sto-3g	orca	same spin correlation energy ha	blocked
MP2	s22-formamide-dimer / sto-3g	orca	total energy ha	blocked
CCSD(T)	s22-formic-acid-dimer / cc-pvtz	orca	total energy ha	blocked
dlpno-ccsd(t)	s22-water-dimer / cc-pvtz	orca	ccsd correlation energy ha	blocked
dlpno-ccsd(t)	s22-water-dimer / cc-pvtz	orca	total energy ha	blocked
dlpno-ccsd(t)	s22-water-dimer / cc-pvtz	orca	triples energy ha	blocked
MP2	tetrazine / sto-3g	orca	correlation energy ha	blocked
MP2	tetrazine / sto-3g	orca	opposite spin correlation energy ha	blocked
MP2	tetrazine / sto-3g	orca	same spin correlation energy ha	blocked
MP2	tetrazine / sto-3g	orca	total energy ha	blocked
MP2	uracil / def2-tzvp	orca	total energy ha	blocked
CCSD(T)	urea / cc-pvtz	orca	total energy ha	blocked

Excited states

342 pass, 244 held, 77 fail, 8 artifact-incomplete, 20 reference-missing. Median $\lvert\Delta E\rvert$ 5.5×10^{-7}, max 1.2×10^{-6} E_h.

RHF	h2co / def2-svp	orca	total energy ha	1.19×10^{-8}
RKS/pbe	h2 / def2-svp	orca	total energy ha	1.09×10^{-6}
RHF	h2co / sto-3g	orca	total energy ha	2.16×10^{-9}
RKS/pbe	h2 / sto-3g	orca	total energy ha	1.16×10^{-6}
RHF	h2co / def2-svp	orca	total energy ha	1.19×10^{-8}
RHF	h2co / sto-3g	orca	total energy ha	2.16×10^{-9}
RHF	h2co / def2-tzvp	orca	total energy ha	1.36×10^{-8}
RKS/pbe	h2 / def2-svp	orca	total energy ha	1.09×10^{-6}
RKS/pbe	h2 / sto-3g	orca	total energy ha	1.16×10^{-6}
RKS/pbe	h2 / def2-tzvp	orca	total energy ha	1.15×10^{-6}
RKS/pbe0	acetaldehyde / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/b3lyp	acetaldehyde / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/pbe	acetaldehyde / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/pbe0	acetaldehyde / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/b3lyp	acetaldehyde / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/pbe	acetaldehyde / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/pbe0	acetylene / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/b3lyp	acetylene / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/pbe	acetylene / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/pbe	acetylene / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/pbe0	acetylene / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/b3lyp	acetylene / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/pbe	acetylene / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/pbe	acetylene / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/pbe0	ammonia / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/b3lyp	ammonia / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/pbe0	ammonia / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/b3lyp	ammonia / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RHF	carbon-monoxide / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RHF	carbon-monoxide / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/pbe0	carbon-monoxide / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/pbe0	carbon-monoxide / aug-cc-pvtz	literature	vertical excitation energy ev	n/a

Table S21, continued.

Method	System / basis	Ref.	Quantity	|Δ|
RKS/pbe0	carbon-monoxide / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/pbe0	carbon-monoxide / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/pbe0	carbon-monoxide / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/b3lyp	carbon-monoxide / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/b3lyp	carbon-monoxide / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/b3lyp	carbon-monoxide / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/pbe	carbon-monoxide / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/pbe	carbon-monoxide / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/pbe	carbon-monoxide / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/pbe0	carbon-monoxide / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/pbe0	carbon-monoxide / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/pbe0	carbon-monoxide / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/pbe0	carbon-monoxide / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/pbe0	carbon-monoxide / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/b3lyp	carbon-monoxide / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/b3lyp	carbon-monoxide / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/b3lyp	carbon-monoxide / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/pbe	carbon-monoxide / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/pbe	carbon-monoxide / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/pbe	carbon-monoxide / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RHF	ccl2 / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/pbe0	ccl2 / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/pbe0	ccl2 / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/b3lyp	ccl2 / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/b3lyp	ccl2 / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/pbe	ccl2 / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/pbe0	ccl2 / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/pbe0	ccl2 / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/b3lyp	ccl2 / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/b3lyp	ccl2 / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/pbe	ccl2 / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RHF	cclf / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/pbe0	cclf / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/b3lyp	cclf / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/pbe	cclf / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/pbe0	cclf / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/b3lyp	cclf / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/pbe	cclf / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RHF	cf2 / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/pbe0	cf2 / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/b3lyp	cf2 / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/pbe	cf2 / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/pbe0	cf2 / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/b3lyp	cf2 / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/pbe	cf2 / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RHF	cyclopropene / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RHF	cyclopropene / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/pbe0	cyclopropene / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/b3lyp	cyclopropene / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/pbe0	cyclopropene / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/b3lyp	cyclopropene / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RHF	diazirine / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RHF	diazirine / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/pbe0	diazirine / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/pbe0	diazirine / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/pbe0	diazirine / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/b3lyp	diazirine / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/b3lyp	diazirine / aug-cc-pvtz	literature	vertical excitation energy ev	n/a

Table S21, continued.

Method	System / basis	Ref.	Quantity	|Δ|
RKS/b3lyp	diazirine / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/pbe	diazirine / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/pbe	diazirine / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/pbe	diazirine / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/pbe0	diazirine / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/pbe0	diazirine / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/b3lyp	diazirine / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/b3lyp	diazirine / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/b3lyp	diazirine / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/pbe	diazirine / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/pbe	diazirine / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/pbe	diazirine / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RHF	diazomethane / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RHF	diazomethane / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RHF	diazomethane / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/pbe0	diazomethane / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/pbe0	diazomethane / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/pbe0	diazomethane / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/b3lyp	diazomethane / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/b3lyp	diazomethane / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/b3lyp	diazomethane / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/pbe	diazomethane / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/pbe	diazomethane / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/pbe	diazomethane / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/pbe0	diazomethane / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/pbe0	diazomethane / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/pbe0	diazomethane / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/b3lyp	diazomethane / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/b3lyp	diazomethane / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/pbe	diazomethane / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/pbe	diazomethane / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RHF	dinitrogen / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/pbe0	dinitrogen / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/pbe0	dinitrogen / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/pbe0	dinitrogen / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/pbe0	dinitrogen / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/pbe0	dinitrogen / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/b3lyp	dinitrogen / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/b3lyp	dinitrogen / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/b3lyp	dinitrogen / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/pbe	dinitrogen / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/pbe	dinitrogen / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/pbe	dinitrogen / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/pbe	dinitrogen / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/pbe0	dinitrogen / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/pbe0	dinitrogen / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/pbe0	dinitrogen / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/pbe0	dinitrogen / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/b3lyp	dinitrogen / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/b3lyp	dinitrogen / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/pbe	dinitrogen / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/pbe	dinitrogen / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/pbe	dinitrogen / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/pbe	dinitrogen / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/pbe	dinitrogen / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RHF	ethylene / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RHF	ethylene / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RHF	ethylene / aug-cc-pvtz	literature	vertical excitation energy ev	n/a

Table S21, continued.

Method	System / basis	Ref.	Quantity	|Δ|
RKS/pbe0	ethylene / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/pbe0	ethylene / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/b3lyp	ethylene / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/pbe	ethylene / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/pbe	ethylene / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/pbe0	ethylene / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/pbe0	ethylene / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/b3lyp	ethylene / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/pbe	ethylene / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/pbe0	formaldehyde / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/pbe0	formaldehyde / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/pbe0	formaldehyde / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/b3lyp	formaldehyde / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/b3lyp	formaldehyde / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/b3lyp	formaldehyde / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/pbe	formaldehyde / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/pbe	formaldehyde / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/pbe	formaldehyde / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/pbe	formaldehyde / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/pbe	formaldehyde / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/pbe	formaldehyde / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/pbe0	formaldehyde / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/pbe0	formaldehyde / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/pbe0	formaldehyde / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/b3lyp	formaldehyde / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/b3lyp	formaldehyde / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/b3lyp	formaldehyde / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/b3lyp	formaldehyde / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/pbe	formaldehyde / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/pbe	formaldehyde / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/pbe	formaldehyde / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/pbe	formaldehyde / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/pbe	formaldehyde / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/pbe	formaldehyde / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/pbe	formaldehyde / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/pbe0	formamide / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/b3lyp	formamide / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/b3lyp	formamide / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/pbe	formamide / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/pbe0	formamide / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/pbe0	formamide / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/b3lyp	formamide / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/b3lyp	formamide / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/pbe	formamide / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/pbe0	formylfluoride / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/b3lyp	formylfluoride / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/pbe	formylfluoride / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/pbe0	formylfluoride / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/b3lyp	formylfluoride / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/pbe	formylfluoride / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RHF	hccl / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/pbe0	hccl / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/b3lyp	hccl / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/pbe	hccl / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/pbe0	hccl / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/b3lyp	hccl / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/pbe	hccl / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RHF	hcf / aug-cc-pvtz	literature	vertical excitation energy ev	n/a

Table S21, continued.

Method	System / basis	Ref.	Quantity	|Δ|
RKS/pbe0	hcf / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/b3lyp	hcf / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/pbe	hcf / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/pbe0	hcf / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/b3lyp	hcf / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/pbe	hcf / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/pbe0	hcp / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/pbe0	hcp / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/b3lyp	hcp / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/b3lyp	hcp / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/pbe	hcp / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/pbe	hcp / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/pbe0	hcp / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/pbe0	hcp / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/b3lyp	hcp / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/b3lyp	hcp / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/pbe	hcp / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/pbe	hcp / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RHF	hpo / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/pbe0	hpo / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/b3lyp	hpo / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/pbe	hpo / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/pbe0	hpo / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/b3lyp	hpo / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/pbe	hpo / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RHF	hps / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/pbe0	hps / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/b3lyp	hps / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/pbe	hps / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/pbe0	hps / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/b3lyp	hps / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/pbe	hps / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RHF	hsif / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/pbe0	hsif / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/b3lyp	hsif / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/pbe	hsif / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/pbe0	hsif / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/b3lyp	hsif / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/pbe	hsif / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RHF	hydrogen-chloride / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/pbe0	hydrogen-chloride / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/pbe0	hydrogen-chloride / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RHF	hydrogen-sulfide / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RHF	hydrogen-sulfide / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/pbe0	hydrogen-sulfide / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/b3lyp	hydrogen-sulfide / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/pbe	hydrogen-sulfide / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/pbe0	hydrogen-sulfide / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/b3lyp	hydrogen-sulfide / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/pbe	hydrogen-sulfide / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RHF	ketene / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RHF	ketene / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RHF	ketene / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/pbe0	ketene / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/pbe0	ketene / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/pbe0	ketene / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/b3lyp	ketene / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/b3lyp	ketene / aug-cc-pvtz	literature	vertical excitation energy ev	n/a

Table S21, continued.

Method	System / basis	Ref.	Quantity	|Δ|
RKS/b3lyp	ketene / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/pbe	ketene / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/pbe	ketene / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/pbe0	ketene / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/pbe0	ketene / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/pbe0	ketene / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/b3lyp	ketene / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/b3lyp	ketene / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/b3lyp	ketene / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/pbe	ketene / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/pbe	ketene / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/pbe0	methanimine / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/b3lyp	methanimine / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/pbe	methanimine / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/pbe0	methanimine / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/b3lyp	methanimine / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/pbe	methanimine / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RHF	nitrosomethane / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/pbe0	nitrosomethane / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/b3lyp	nitrosomethane / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/pbe	nitrosomethane / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/pbe0	nitrosomethane / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/b3lyp	nitrosomethane / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/pbe	nitrosomethane / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RHF	nitroxyl / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/pbe0	nitroxyl / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/pbe0	nitroxyl / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/b3lyp	nitroxyl / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/pbe	nitroxyl / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/pbe	nitroxyl / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/pbe0	nitroxyl / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/pbe0	nitroxyl / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/b3lyp	nitroxyl / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/pbe	nitroxyl / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/pbe	nitroxyl / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RHF	sicl2 / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/pbe0	sicl2 / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/b3lyp	sicl2 / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/pbe	sicl2 / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/pbe0	sicl2 / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/b3lyp	sicl2 / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/pbe	sicl2 / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RHF	silylidene / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/pbe0	silylidene / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/pbe0	silylidene / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/b3lyp	silylidene / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/b3lyp	silylidene / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/pbe	silylidene / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/pbe	silylidene / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/pbe0	silylidene / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/pbe0	silylidene / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/b3lyp	silylidene / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/b3lyp	silylidene / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/pbe	silylidene / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/pbe	silylidene / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/pbe0	streptocyanine-c1 / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/b3lyp	streptocyanine-c1 / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/pbe	streptocyanine-c1 / aug-cc-pvtz	literature	vertical excitation energy ev	n/a

Table S21, continued.

Method	System / basis	Ref.	Quantity	|Δ|
RHF	thioformaldehyde / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RHF	thioformaldehyde / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RHF	thioformaldehyde / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/pbe0	thioformaldehyde / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/b3lyp	thioformaldehyde / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/pbe	thioformaldehyde / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/pbe	thioformaldehyde / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/pbe0	thioformaldehyde / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/pbe0	thioformaldehyde / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/b3lyp	thioformaldehyde / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/b3lyp	thioformaldehyde / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/b3lyp	thioformaldehyde / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/pbe	thioformaldehyde / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/pbe	thioformaldehyde / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/pbe0	water / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/b3lyp	water / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/pbe	water / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/pbe0	water / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/b3lyp	water / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/pbe	water / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/pbe	h2co / def2-svp	orca	total energy ha	held
RKS/pbe	h2co / def2-svp	orca	total energy ha	held
RKS/pbe	h2co / sto-3g	orca	total energy ha	held
RKS/pbe	h2co / sto-3g	orca	total energy ha	held
RKS/pbe	h2co / def2-svp	orca	total energy ha	held
RKS/pbe	h2co / sto-3g	orca	total energy ha	held
RKS/pbe	h2co / def2-tzvp	orca	total energy ha	held
RKS/pbe	h2co / def2-svp	orca	total energy ha	held
RKS/pbe	h2co / sto-3g	orca	total energy ha	held
RKS/pbe	h2co / def2-tzvp	orca	total energy ha	held
RHF	acetylene / aug-cc-pvtz	literature	vertical excitation energy ev	held
RHF	acetylene / aug-cc-pvtz	literature	vertical excitation energy ev	held
RKS/pbe0	acetylene / aug-cc-pvtz	literature	vertical excitation energy ev	held
RKS/pbe0	acetylene / aug-cc-pvtz	literature	vertical excitation energy ev	held
RKS/pbe0	acetylene / aug-cc-pvtz	literature	vertical excitation energy ev	held
RKS/b3lyp	acetylene / aug-cc-pvtz	literature	vertical excitation energy ev	held
RKS/b3lyp	acetylene / aug-cc-pvtz	literature	vertical excitation energy ev	held
RKS/pbe	acetylene / aug-cc-pvtz	literature	vertical excitation energy ev	held
RKS/pbe	acetylene / aug-cc-pvtz	literature	vertical excitation energy ev	held
RKS/pbe0	acetylene / aug-cc-pvtz	literature	vertical excitation energy ev	held
RKS/pbe0	acetylene / aug-cc-pvtz	literature	vertical excitation energy ev	held
RKS/pbe0	acetylene / aug-cc-pvtz	literature	vertical excitation energy ev	held
RKS/b3lyp	acetylene / aug-cc-pvtz	literature	vertical excitation energy ev	held
RKS/b3lyp	acetylene / aug-cc-pvtz	literature	vertical excitation energy ev	held
RKS/pbe	acetylene / aug-cc-pvtz	literature	vertical excitation energy ev	held
RKS/pbe	acetylene / aug-cc-pvtz	literature	vertical excitation energy ev	held
RKS/b3lyp	ammonia / aug-cc-pvtz	literature	vertical excitation energy ev	held
RKS/b3lyp	ammonia / aug-cc-pvtz	literature	vertical excitation energy ev	held
RKS/pbe	ammonia / aug-cc-pvtz	literature	vertical excitation energy ev	held
RKS/pbe	ammonia / aug-cc-pvtz	literature	vertical excitation energy ev	held
RKS/b3lyp	ammonia / aug-cc-pvtz	literature	vertical excitation energy ev	held
RKS/b3lyp	ammonia / aug-cc-pvtz	literature	vertical excitation energy ev	held
RKS/pbe	ammonia / aug-cc-pvtz	literature	vertical excitation energy ev	held
RKS/pbe	ammonia / aug-cc-pvtz	literature	vertical excitation energy ev	held
RHF	beryllium / aug-cc-pvtz	literature	vertical excitation energy ev	held
RKS/pbe0	beryllium / aug-cc-pvtz	literature	vertical excitation energy ev	held
RKS/b3lyp	beryllium / aug-cc-pvtz	literature	vertical excitation energy ev	held
RKS/pbe	beryllium / aug-cc-pvtz	literature	vertical excitation energy ev	held

Table S21, continued.

Method	System / basis	Ref.	Quantity	|Δ|
RKS/pbe0	beryllium / aug-cc-pvtz	literature	vertical excitation energy ev	held
RKS/b3lyp	beryllium / aug-cc-pvtz	literature	vertical excitation energy ev	held
RKS/pbe	beryllium / aug-cc-pvtz	literature	vertical excitation energy ev	held
RHF	carbon-dimer / aug-cc-pvtz	literature	vertical excitation energy ev	held
RHF	carbon-dimer / aug-cc-pvtz	literature	vertical excitation energy ev	held
RHF	carbon-dimer / aug-cc-pvtz	literature	vertical excitation energy ev	held
RHF	carbon-dimer / aug-cc-pvtz	literature	vertical excitation energy ev	held
RKS/pbe0	carbon-dimer / aug-cc-pvtz	literature	vertical excitation energy ev	held
RKS/pbe0	carbon-dimer / aug-cc-pvtz	literature	vertical excitation energy ev	held
RKS/pbe0	carbon-dimer / aug-cc-pvtz	literature	vertical excitation energy ev	held
RKS/pbe0	carbon-dimer / aug-cc-pvtz	literature	vertical excitation energy ev	held
RKS/b3lyp	carbon-dimer / aug-cc-pvtz	literature	vertical excitation energy ev	held
RKS/b3lyp	carbon-dimer / aug-cc-pvtz	literature	vertical excitation energy ev	held
RKS/b3lyp	carbon-dimer / aug-cc-pvtz	literature	vertical excitation energy ev	held
RKS/b3lyp	carbon-dimer / aug-cc-pvtz	literature	vertical excitation energy ev	held
RKS/pbe0	carbon-dimer / aug-cc-pvtz	literature	vertical excitation energy ev	held
RKS/pbe0	carbon-dimer / aug-cc-pvtz	literature	vertical excitation energy ev	held
RKS/pbe0	carbon-dimer / aug-cc-pvtz	literature	vertical excitation energy ev	held
RKS/pbe0	carbon-dimer / aug-cc-pvtz	literature	vertical excitation energy ev	held
RKS/b3lyp	carbon-dimer / aug-cc-pvtz	literature	vertical excitation energy ev	held
RKS/b3lyp	carbon-dimer / aug-cc-pvtz	literature	vertical excitation energy ev	held
RKS/b3lyp	carbon-dimer / aug-cc-pvtz	literature	vertical excitation energy ev	held
RKS/b3lyp	carbon-dimer / aug-cc-pvtz	literature	vertical excitation energy ev	held
RHF	carbon-monoxide / aug-cc-pvtz	literature	vertical excitation energy ev	held
RHF	carbon-monoxide / aug-cc-pvtz	literature	vertical excitation energy ev	held
RHF	carbon-monoxide / aug-cc-pvtz	literature	vertical excitation energy ev	held
RKS/b3lyp	carbon-monoxide / aug-cc-pvtz	literature	vertical excitation energy ev	held
RKS/b3lyp	carbon-monoxide / aug-cc-pvtz	literature	vertical excitation energy ev	held
RHF	ccl2 / aug-cc-pvtz	literature	vertical excitation energy ev	held
RKS/pbe0	cyclopropene / aug-cc-pvtz	literature	vertical excitation energy ev	held
RKS/b3lyp	cyclopropene / aug-cc-pvtz	literature	vertical excitation energy ev	held
RKS/pbe	cyclopropene / aug-cc-pvtz	literature	vertical excitation energy ev	held
RKS/pbe	cyclopropene / aug-cc-pvtz	literature	vertical excitation energy ev	held
RKS/pbe0	cyclopropene / aug-cc-pvtz	literature	vertical excitation energy ev	held
RKS/b3lyp	cyclopropene / aug-cc-pvtz	literature	vertical excitation energy ev	held
RKS/pbe	cyclopropene / aug-cc-pvtz	literature	vertical excitation energy ev	held
RKS/pbe	cyclopropene / aug-cc-pvtz	literature	vertical excitation energy ev	held
RHF	diazirine / aug-cc-pvtz	literature	vertical excitation energy ev	held
RHF	diazirine / aug-cc-pvtz	literature	vertical excitation energy ev	held
RKS/pbe0	diazirine / aug-cc-pvtz	literature	vertical excitation energy ev	held
RKS/b3lyp	diazirine / aug-cc-pvtz	literature	vertical excitation energy ev	held
RKS/pbe	diazirine / aug-cc-pvtz	literature	vertical excitation energy ev	held
RKS/pbe0	diazirine / aug-cc-pvtz	literature	vertical excitation energy ev	held
RKS/pbe0	diazirine / aug-cc-pvtz	literature	vertical excitation energy ev	held
RKS/b3lyp	diazirine / aug-cc-pvtz	literature	vertical excitation energy ev	held
RKS/pbe	diazirine / aug-cc-pvtz	literature	vertical excitation energy ev	held
RHF	diazomethane / aug-cc-pvtz	literature	vertical excitation energy ev	held
RKS/pbe0	diazomethane / aug-cc-pvtz	literature	vertical excitation energy ev	held
RKS/b3lyp	diazomethane / aug-cc-pvtz	literature	vertical excitation energy ev	held
RKS/pbe	diazomethane / aug-cc-pvtz	literature	vertical excitation energy ev	held
RKS/pbe0	diazomethane / aug-cc-pvtz	literature	vertical excitation energy ev	held
RKS/b3lyp	diazomethane / aug-cc-pvtz	literature	vertical excitation energy ev	held
RKS/b3lyp	diazomethane / aug-cc-pvtz	literature	vertical excitation energy ev	held
RKS/pbe	diazomethane / aug-cc-pvtz	literature	vertical excitation energy ev	held
RKS/pbe	diazomethane / aug-cc-pvtz	literature	vertical excitation energy ev	held
RHF	dinitrogen / aug-cc-pvtz	literature	vertical excitation energy ev	held
RHF	dinitrogen / aug-cc-pvtz	literature	vertical excitation energy ev	held
RHF	dinitrogen / aug-cc-pvtz	literature	vertical excitation energy ev	held

Table S21, continued.

Method	System / basis	Ref.	Quantity	|Δ|
RHF	dinitrogen / aug-cc-pvtz	literature	vertical excitation energy ev	held
RHF	dinitrogen / aug-cc-pvtz	literature	vertical excitation energy ev	held
RHF	dinitrogen / aug-cc-pvtz	literature	vertical excitation energy ev	held
RKS/pbe0	dinitrogen / aug-cc-pvtz	literature	vertical excitation energy ev	held
RKS/b3lyp	dinitrogen / aug-cc-pvtz	literature	vertical excitation energy ev	held
RKS/b3lyp	dinitrogen / aug-cc-pvtz	literature	vertical excitation energy ev	held
RKS/pbe	dinitrogen / aug-cc-pvtz	literature	vertical excitation energy ev	held
RKS/pbe	dinitrogen / aug-cc-pvtz	literature	vertical excitation energy ev	held
RKS/pbe	dinitrogen / aug-cc-pvtz	literature	vertical excitation energy ev	held
RKS/pbe0	dinitrogen / aug-cc-pvtz	literature	vertical excitation energy ev	held
RKS/pbe0	dinitrogen / aug-cc-pvtz	literature	vertical excitation energy ev	held
RKS/pbe0	dinitrogen / aug-cc-pvtz	literature	vertical excitation energy ev	held
RKS/b3lyp	dinitrogen / aug-cc-pvtz	literature	vertical excitation energy ev	held
RKS/b3lyp	dinitrogen / aug-cc-pvtz	literature	vertical excitation energy ev	held
RKS/b3lyp	dinitrogen / aug-cc-pvtz	literature	vertical excitation energy ev	held
RKS/b3lyp	dinitrogen / aug-cc-pvtz	literature	vertical excitation energy ev	held
RKS/pbe	dinitrogen / aug-cc-pvtz	literature	vertical excitation energy ev	held
RKS/pbe	dinitrogen / aug-cc-pvtz	literature	vertical excitation energy ev	held
RHF	ethylene / aug-cc-pvtz	literature	vertical excitation energy ev	held
RKS/pbe0	ethylene / aug-cc-pvtz	literature	vertical excitation energy ev	held
RKS/b3lyp	ethylene / aug-cc-pvtz	literature	vertical excitation energy ev	held
RKS/b3lyp	ethylene / aug-cc-pvtz	literature	vertical excitation energy ev	held
RKS/pbe	ethylene / aug-cc-pvtz	literature	vertical excitation energy ev	held
RKS/pbe	ethylene / aug-cc-pvtz	literature	vertical excitation energy ev	held
RKS/pbe0	ethylene / aug-cc-pvtz	literature	vertical excitation energy ev	held
RKS/b3lyp	ethylene / aug-cc-pvtz	literature	vertical excitation energy ev	held
RKS/b3lyp	ethylene / aug-cc-pvtz	literature	vertical excitation energy ev	held
RKS/pbe	ethylene / aug-cc-pvtz	literature	vertical excitation energy ev	held
RKS/pbe	ethylene / aug-cc-pvtz	literature	vertical excitation energy ev	held
RKS/pbe	ethylene / aug-cc-pvtz	literature	vertical excitation energy ev	held
RHF	formaldehyde / aug-cc-pvtz	literature	vertical excitation energy ev	held
RHF	formaldehyde / aug-cc-pvtz	literature	vertical excitation energy ev	held
RHF	formaldehyde / aug-cc-pvtz	literature	vertical excitation energy ev	held
RHF	formaldehyde / aug-cc-pvtz	literature	vertical excitation energy ev	held
RHF	formaldehyde / aug-cc-pvtz	literature	vertical excitation energy ev	held
RHF	formaldehyde / aug-cc-pvtz	literature	vertical excitation energy ev	held
RHF	formaldehyde / aug-cc-pvtz	literature	vertical excitation energy ev	held
RHF	formaldehyde / aug-cc-pvtz	literature	vertical excitation energy ev	held
RKS/pbe0	formaldehyde / aug-cc-pvtz	literature	vertical excitation energy ev	held
RKS/pbe0	formaldehyde / aug-cc-pvtz	literature	vertical excitation energy ev	held
RKS/pbe0	formaldehyde / aug-cc-pvtz	literature	vertical excitation energy ev	held
RKS/pbe0	formaldehyde / aug-cc-pvtz	literature	vertical excitation energy ev	held
RKS/b3lyp	formaldehyde / aug-cc-pvtz	literature	vertical excitation energy ev	held
RKS/b3lyp	formaldehyde / aug-cc-pvtz	literature	vertical excitation energy ev	held
RKS/b3lyp	formaldehyde / aug-cc-pvtz	literature	vertical excitation energy ev	held
RKS/b3lyp	formaldehyde / aug-cc-pvtz	literature	vertical excitation energy ev	held
RKS/b3lyp	formaldehyde / aug-cc-pvtz	literature	vertical excitation energy ev	held
RKS/pbe	formaldehyde / aug-cc-pvtz	literature	vertical excitation energy ev	held
RKS/pbe	formaldehyde / aug-cc-pvtz	literature	vertical excitation energy ev	held
RKS/pbe	formaldehyde / aug-cc-pvtz	literature	vertical excitation energy ev	held
RKS/pbe0	formaldehyde / aug-cc-pvtz	literature	vertical excitation energy ev	held
RKS/pbe0	formaldehyde / aug-cc-pvtz	literature	vertical excitation energy ev	held
RKS/pbe0	formaldehyde / aug-cc-pvtz	literature	vertical excitation energy ev	held
RKS/pbe0	formaldehyde / aug-cc-pvtz	literature	vertical excitation energy ev	held
RKS/b3lyp	formaldehyde / aug-cc-pvtz	literature	vertical excitation energy ev	held
RKS/b3lyp	formaldehyde / aug-cc-pvtz	literature	vertical excitation energy ev	held
RKS/b3lyp	formaldehyde / aug-cc-pvtz	literature	vertical excitation energy ev	held
RKS/pbe	formaldehyde / aug-cc-pvtz	literature	vertical excitation energy ev	held

Table S21, continued.

Method	System / basis	Ref.	Quantity	|Δ|
RKS/pbe	formaldehyde / aug-cc-pvtz	literature	vertical excitation energy ev	held
RHF	formamide / aug-cc-pvtz	literature	vertical excitation energy ev	held
RHF	formamide / aug-cc-pvtz	literature	vertical excitation energy ev	held
RKS/pbe0	formamide / aug-cc-pvtz	literature	vertical excitation energy ev	held
RKS/pbe0	formamide / aug-cc-pvtz	literature	vertical excitation energy ev	held
RKS/pbe0	formamide / aug-cc-pvtz	literature	vertical excitation energy ev	held
RKS/b3lyp	formamide / aug-cc-pvtz	literature	vertical excitation energy ev	held
RKS/b3lyp	formamide / aug-cc-pvtz	literature	vertical excitation energy ev	held
RKS/pbe	formamide / aug-cc-pvtz	literature	vertical excitation energy ev	held
RKS/pbe	formamide / aug-cc-pvtz	literature	vertical excitation energy ev	held
RKS/pbe	formamide / aug-cc-pvtz	literature	vertical excitation energy ev	held
RKS/pbe0	formamide / aug-cc-pvtz	literature	vertical excitation energy ev	held
RKS/pbe0	formamide / aug-cc-pvtz	literature	vertical excitation energy ev	held
RKS/b3lyp	formamide / aug-cc-pvtz	literature	vertical excitation energy ev	held
RKS/b3lyp	formamide / aug-cc-pvtz	literature	vertical excitation energy ev	held
RKS/pbe	formamide / aug-cc-pvtz	literature	vertical excitation energy ev	held
RKS/pbe	formamide / aug-cc-pvtz	literature	vertical excitation energy ev	held
RKS/pbe	formamide / aug-cc-pvtz	literature	vertical excitation energy ev	held
RKS/pbe0	hydrogen-sulfide / aug-cc-pvtz	literature	vertical excitation energy ev	held
RKS/b3lyp	hydrogen-sulfide / aug-cc-pvtz	literature	vertical excitation energy ev	held
RKS/pbe	hydrogen-sulfide / aug-cc-pvtz	literature	vertical excitation energy ev	held
RKS/pbe0	hydrogen-sulfide / aug-cc-pvtz	literature	vertical excitation energy ev	held
RKS/b3lyp	hydrogen-sulfide / aug-cc-pvtz	literature	vertical excitation energy ev	held
RKS/pbe	hydrogen-sulfide / aug-cc-pvtz	literature	vertical excitation energy ev	held
RHF	ketene / aug-cc-pvtz	literature	vertical excitation energy ev	held
RHF	ketene / aug-cc-pvtz	literature	vertical excitation energy ev	held
RKS/pbe0	ketene / aug-cc-pvtz	literature	vertical excitation energy ev	held
RKS/pbe0	ketene / aug-cc-pvtz	literature	vertical excitation energy ev	held
RKS/b3lyp	ketene / aug-cc-pvtz	literature	vertical excitation energy ev	held
RKS/b3lyp	ketene / aug-cc-pvtz	literature	vertical excitation energy ev	held
RKS/pbe	ketene / aug-cc-pvtz	literature	vertical excitation energy ev	held
RKS/pbe	ketene / aug-cc-pvtz	literature	vertical excitation energy ev	held
RKS/pbe0	ketene / aug-cc-pvtz	literature	vertical excitation energy ev	held
RKS/pbe0	ketene / aug-cc-pvtz	literature	vertical excitation energy ev	held
RKS/b3lyp	ketene / aug-cc-pvtz	literature	vertical excitation energy ev	held
RKS/b3lyp	ketene / aug-cc-pvtz	literature	vertical excitation energy ev	held
RKS/pbe	ketene / aug-cc-pvtz	literature	vertical excitation energy ev	held
RKS/pbe	ketene / aug-cc-pvtz	literature	vertical excitation energy ev	held
RHF	nitrosomethane / aug-cc-pvtz	literature	vertical excitation energy ev	held
RHF	nitrosomethane / aug-cc-pvtz	literature	vertical excitation energy ev	held
RHF	nitrosomethane / aug-cc-pvtz	literature	vertical excitation energy ev	held
RKS/pbe0	nitrosomethane / aug-cc-pvtz	literature	vertical excitation energy ev	held
RKS/pbe0	nitrosomethane / aug-cc-pvtz	literature	vertical excitation energy ev	held
RKS/pbe0	nitrosomethane / aug-cc-pvtz	literature	vertical excitation energy ev	held
RKS/b3lyp	nitrosomethane / aug-cc-pvtz	literature	vertical excitation energy ev	held
RKS/b3lyp	nitrosomethane / aug-cc-pvtz	literature	vertical excitation energy ev	held
RKS/b3lyp	nitrosomethane / aug-cc-pvtz	literature	vertical excitation energy ev	held
RKS/pbe	nitrosomethane / aug-cc-pvtz	literature	vertical excitation energy ev	held
RKS/pbe	nitrosomethane / aug-cc-pvtz	literature	vertical excitation energy ev	held
RKS/pbe	nitrosomethane / aug-cc-pvtz	literature	vertical excitation energy ev	held
RKS/pbe0	nitrosomethane / aug-cc-pvtz	literature	vertical excitation energy ev	held
RKS/pbe0	nitrosomethane / aug-cc-pvtz	literature	vertical excitation energy ev	held
RKS/pbe0	nitrosomethane / aug-cc-pvtz	literature	vertical excitation energy ev	held
RKS/b3lyp	nitrosomethane / aug-cc-pvtz	literature	vertical excitation energy ev	held
RKS/b3lyp	nitrosomethane / aug-cc-pvtz	literature	vertical excitation energy ev	held
RKS/b3lyp	nitrosomethane / aug-cc-pvtz	literature	vertical excitation energy ev	held
RKS/pbe	nitrosomethane / aug-cc-pvtz	literature	vertical excitation energy ev	held
RKS/pbe	nitrosomethane / aug-cc-pvtz	literature	vertical excitation energy ev	held

Table S21, continued.

Method	System / basis	Ref.	Quantity	|Δ|
RKS/pbe	nitrosomethane / aug-cc-pvtz	literature	vertical excitation energy ev	held
RHF	nitroxyl / aug-cc-pvtz	literature	vertical excitation energy ev	held
RHF	nitroxyl / aug-cc-pvtz	literature	vertical excitation energy ev	held
RKS/pbe0	nitroxyl / aug-cc-pvtz	literature	vertical excitation energy ev	held
RKS/b3lyp	nitroxyl / aug-cc-pvtz	literature	vertical excitation energy ev	held
RKS/b3lyp	nitroxyl / aug-cc-pvtz	literature	vertical excitation energy ev	held
RKS/pbe	nitroxyl / aug-cc-pvtz	literature	vertical excitation energy ev	held
RKS/pbe0	nitroxyl / aug-cc-pvtz	literature	vertical excitation energy ev	held
RKS/b3lyp	nitroxyl / aug-cc-pvtz	literature	vertical excitation energy ev	held
RKS/pbe	nitroxyl / aug-cc-pvtz	literature	vertical excitation energy ev	held
RHF	streptocyanine-c1 / aug-cc-pvtz	literature	vertical excitation energy ev	held
RHF	thioformaldehyde / aug-cc-pvtz	literature	vertical excitation energy ev	held
RKS/pbe0	thioformaldehyde / aug-cc-pvtz	literature	vertical excitation energy ev	held
RKS/pbe0	thioformaldehyde / aug-cc-pvtz	literature	vertical excitation energy ev	held
RKS/pbe0	thioformaldehyde / aug-cc-pvtz	literature	vertical excitation energy ev	held
RKS/b3lyp	thioformaldehyde / aug-cc-pvtz	literature	vertical excitation energy ev	held
RKS/b3lyp	thioformaldehyde / aug-cc-pvtz	literature	vertical excitation energy ev	held
RKS/b3lyp	thioformaldehyde / aug-cc-pvtz	literature	vertical excitation energy ev	held
RKS/pbe	thioformaldehyde / aug-cc-pvtz	literature	vertical excitation energy ev	held
RKS/pbe	thioformaldehyde / aug-cc-pvtz	literature	vertical excitation energy ev	held
RKS/pbe0	thioformaldehyde / aug-cc-pvtz	literature	vertical excitation energy ev	held
RKS/pbe0	thioformaldehyde / aug-cc-pvtz	literature	vertical excitation energy ev	held
RKS/b3lyp	thioformaldehyde / aug-cc-pvtz	literature	vertical excitation energy ev	held
RKS/pbe	thioformaldehyde / aug-cc-pvtz	literature	vertical excitation energy ev	held
RKS/pbe	thioformaldehyde / aug-cc-pvtz	literature	vertical excitation energy ev	held
RHF	water / aug-cc-pvtz	literature	vertical excitation energy ev	held
RKS/pbe0	water / aug-cc-pvtz	literature	vertical excitation energy ev	held
RKS/b3lyp	water / aug-cc-pvtz	literature	vertical excitation energy ev	held
RKS/pbe	water / aug-cc-pvtz	literature	vertical excitation energy ev	held
RKS/pbe0	water / aug-cc-pvtz	literature	vertical excitation energy ev	held
RKS/b3lyp	water / aug-cc-pvtz	literature	vertical excitation energy ev	held
RKS/pbe	water / aug-cc-pvtz	literature	vertical excitation energy ev	held
RHF	acetaldehyde / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RHF	acetylene / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RHF	acetylene / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/b3lyp	acetylene / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/b3lyp	acetylene / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RHF	ammonia / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RHF	ammonia / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RHF	ammonia / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RHF	ammonia / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/pbe0	ammonia / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/pbe0	ammonia / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/pbe0	ammonia / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/b3lyp	ammonia / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/pbe	ammonia / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/pbe	ammonia / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/pbe0	ammonia / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/pbe0	ammonia / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/pbe0	ammonia / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/b3lyp	ammonia / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/pbe	ammonia / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/pbe	ammonia / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RHF	carbon-monoxide / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/pbe0	carbon-monoxide / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/b3lyp	carbon-monoxide / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/b3lyp	carbon-monoxide / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/pbe	carbon-monoxide / aug-cc-pvtz	literature	vertical excitation energy ev	n/a

Table S21, continued.

Method	System / basis	Ref.	Quantity	|Δ|
RKS/pbe	carbon-monoxide / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/pbe	carbon-monoxide / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/pbe0	carbon-monoxide / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/b3lyp	carbon-monoxide / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/b3lyp	carbon-monoxide / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/pbe	carbon-monoxide / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/pbe	carbon-monoxide / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/pbe	carbon-monoxide / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/pbe	ccl2 / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/pbe	ccl2 / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/pbe0	dinitrogen / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/b3lyp	dinitrogen / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/b3lyp	dinitrogen / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/b3lyp	dinitrogen / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/pbe0	ethylene / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/b3lyp	ethylene / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/pbe0	ethylene / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/b3lyp	ethylene / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RHF	formaldehyde / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/pbe0	formaldehyde / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/pbe0	formaldehyde / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/b3lyp	formaldehyde / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/pbe0	formaldehyde / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/pbe0	formaldehyde / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/b3lyp	formaldehyde / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/b3lyp	formaldehyde / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RHF	formamide / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RHF	formamide / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RHF	formylfluoride / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RHF	hcp / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RHF	hcp / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/b3lyp	hydrogen-chloride / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/pbe	hydrogen-chloride / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/b3lyp	hydrogen-chloride / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/pbe	hydrogen-chloride / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/pbe	ketene / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/pbe	ketene / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RHF	methanimine / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/b3lyp	nitroxyl / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RHF	silylidene / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/pbe0	streptocyanine-c1 / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/b3lyp	streptocyanine-c1 / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/pbe	streptocyanine-c1 / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RHF	water / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RHF	water / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/pbe0	water / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/b3lyp	water / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/pbe	water / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/pbe0	water / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/b3lyp	water / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RKS/pbe	water / aug-cc-pvtz	literature	vertical excitation energy ev	n/a
RHF	h2co / sto-3g	orca	total energy ha	artifact-incomplete
RHF	h2co / sto-3g	orca	total energy ha	artifact-incomplete
RKS/pbe	h2co / sto-3g	orca	total energy ha	artifact-incomplete
RKS/pbe	h2co / sto-3g	orca	total energy ha	artifact-incomplete
RKS/pbe	h2co / sto-3g	orca	total energy ha	artifact-incomplete
RKS/pbe	h2co / sto-3g	orca	total energy ha	artifact-incomplete
RKS/pbe	h2 / sto-3g	orca	total energy ha	artifact-incomplete

Table S21, continued.

Method	System / basis	Ref.	Quantity	|Δ|
RKS/pbe	h2 / sto-3g	orca	total energy ha	artifact-incomplete
RHF	h2co / def2-svp	orca	total energy ha	reference-missing
RKS/pbe	h2co / def2-svp	orca	total energy ha	reference-missing
RKS/pbe	h2co / def2-svp	orca	total energy ha	reference-missing
RKS/pbe	h2 / def2-svp	orca	total energy ha	reference-missing
RHF	h2co / sto-3g	orca	total energy ha	reference-missing
RKS/pbe	h2co / sto-3g	orca	total energy ha	reference-missing
RKS/pbe	h2co / sto-3g	orca	total energy ha	reference-missing
RKS/pbe	h2 / sto-3g	orca	total energy ha	reference-missing
RHF	h2co / def2-svp	orca	total energy ha	reference-missing
RHF	h2co / sto-3g	orca	total energy ha	reference-missing
RHF	h2co / def2-tzvp	orca	total energy ha	reference-missing
RKS/pbe	h2co / def2-svp	orca	total energy ha	reference-missing
RKS/pbe	h2co / sto-3g	orca	total energy ha	reference-missing
RKS/pbe	h2co / def2-tzvp	orca	total energy ha	reference-missing
RKS/pbe	h2co / def2-svp	orca	total energy ha	reference-missing
RKS/pbe	h2co / sto-3g	orca	total energy ha	reference-missing
RKS/pbe	h2co / def2-tzvp	orca	total energy ha	reference-missing
RKS/pbe	h2 / def2-svp	orca	total energy ha	reference-missing
RKS/pbe	h2 / sto-3g	orca	total energy ha	reference-missing
RKS/pbe	h2 / def2-tzvp	orca	total energy ha	reference-missing
Electron propagator				
93 pass, 19 fail, 4 artifact-incomplete, 10 reference-missing.				
OVGF	c2h4 / def2-svp	orca	orbital energy max abs deviation ev	n/a
OVGF	c2h4 / def2-svp	orca	ionization energy ev	n/a
OVGF	c2h4 / def2-svp	orca	ionization energy ev	n/a
OVGF	c2h4 / def2-svp	orca	ionization energy ev	n/a
OVGF	c2h4 / def2-tzvp	orca	orbital energy max abs deviation ev	n/a
OVGF	c2h4 / def2-tzvp	orca	ionization energy ev	n/a
OVGF	c2h4 / def2-tzvp	orca	ionization energy ev	n/a
OVGF	c2h4 / def2-tzvp	orca	ionization energy ev	n/a
OVGF	c2h4 / sto-3g	orca	orbital energy max abs deviation ev	n/a
OVGF	c2h4 / sto-3g	orca	ionization energy ev	n/a
OVGF	c2h4 / sto-3g	orca	ionization energy ev	n/a
OVGF	c2h4 / sto-3g	orca	ionization energy ev	n/a
OVGF	c2h4 / sto-3g	orca	ionization energy ev	n/a
OVGF	ch2o / def2-svp	orca	orbital energy max abs deviation ev	n/a
OVGF	ch2o / def2-svp	orca	ionization energy ev	n/a
OVGF	ch2o / def2-svp	orca	ionization energy ev	n/a
OVGF	ch2o / def2-svp	orca	ionization energy ev	n/a
OVGF	ch2o / def2-tzvp	orca	orbital energy max abs deviation ev	n/a
OVGF	ch2o / def2-tzvp	orca	ionization energy ev	n/a
OVGF	ch2o / def2-tzvp	orca	ionization energy ev	n/a
OVGF	ch2o / sto-3g	orca	orbital energy max abs deviation ev	n/a
OVGF	ch2o / sto-3g	orca	ionization energy ev	n/a
OVGF	ch2o / sto-3g	orca	ionization energy ev	n/a
OVGF	ch2o / sto-3g	orca	ionization energy ev	n/a
OVGF	ch2o / sto-3g	orca	ionization energy ev	n/a
OVGF	ch4 / def2-svp	orca	orbital energy max abs deviation ev	n/a
OVGF	ch4 / def2-svp	orca	ionization energy ev	n/a

Table S21, continued.

Method	System / basis	Ref.	Quantity	|Δ|
OVGF	ch4 / def2-tzvp	orca	orbital energy max abs deviation ev	n/a
OVGF	ch4 / def2-tzvp	orca	ionization energy ev	n/a
OVGF	ch4 / sto-3g	orca	orbital energy max abs deviation ev	n/a
OVGF	ch4 / sto-3g	orca	ionization energy ev	n/a
OVGF	ch4 / sto-3g	orca	ionization energy ev	n/a
OVGF	co / def2-svp	orca	orbital energy max abs deviation ev	n/a
OVGF	co / def2-svp	orca	ionization energy ev	n/a
OVGF	co / def2-svp	orca	ionization energy ev	n/a
OVGF	co / def2-svp	orca	ionization energy ev	n/a
OVGF	co / def2-tzvp	orca	orbital energy max abs deviation ev	n/a
OVGF	co / def2-tzvp	orca	ionization energy ev	n/a
OVGF	co / def2-tzvp	orca	ionization energy ev	n/a
OVGF	co / sto-3g	orca	orbital energy max abs deviation ev	n/a
OVGF	co / sto-3g	orca	ionization energy ev	n/a
OVGF	co / sto-3g	orca	ionization energy ev	n/a
OVGF	co / sto-3g	orca	ionization energy ev	n/a
OVGF	h2o / def2-svp	orca	orbital energy max abs deviation ev	n/a
OVGF	h2o / def2-svp	orca	ionization energy ev	n/a
OVGF	h2o / def2-svp	orca	ionization energy ev	n/a
OVGF	h2o / def2-svp	orca	ionization energy ev	n/a
OVGF	h2o / def2-svp	orca	ionization energy ev	n/a
OVGF	h2o / def2-tzvp	orca	orbital energy max abs deviation ev	n/a
OVGF	h2o / def2-tzvp	orca	ionization energy ev	n/a
OVGF	h2o / def2-tzvp	orca	ionization energy ev	n/a
OVGF	h2o / def2-tzvp	orca	ionization energy ev	n/a
OVGF	h2o / sto-3g	orca	orbital energy max abs deviation ev	n/a
OVGF	h2o / sto-3g	orca	ionization energy ev	n/a
OVGF	h2o / sto-3g	orca	ionization energy ev	n/a
OVGF	h2o / sto-3g	orca	ionization energy ev	n/a
OVGF	h2o / sto-3g	orca	ionization energy ev	n/a
OVGF	hf / def2-svp	orca	orbital energy max abs deviation ev	n/a
OVGF	hf / def2-svp	orca	ionization energy ev	n/a
OVGF	hf / def2-svp	orca	ionization energy ev	n/a
OVGF	hf / def2-svp	orca	ionization energy ev	n/a
OVGF	hf / def2-tzvp	orca	orbital energy max abs deviation ev	n/a
OVGF	hf / def2-tzvp	orca	ionization energy ev	n/a
OVGF	hf / sto-3g	orca	orbital energy max abs deviation ev	n/a
OVGF	n2 / def2-svp	orca	orbital energy max abs deviation ev	n/a
OVGF	n2 / def2-svp	orca	ionization energy ev	n/a
OVGF	n2 / def2-svp	orca	ionization energy ev	n/a
OVGF	n2 / def2-tzvp	orca	orbital energy max abs deviation ev	n/a
OVGF	n2 / def2-tzvp	orca	ionization energy ev	n/a
OVGF	n2 / def2-tzvp	orca	ionization energy ev	n/a
OVGF	n2 / sto-3g	orca	orbital energy max abs deviation ev	n/a

Table S21, continued.

Method	System / basis	Ref.	Quantity	|Δ|
OVGF	n2 / sto-3g	orca	ionization energy ev	n/a
OVGF	n2 / sto-3g	orca	ionization energy ev	n/a
OVGF	n2 / sto-3g	orca	ionization energy ev	n/a
OVGF	nh3 / def2-svp	orca	orbital energy max abs deviation ev	n/a
OVGF	nh3 / def2-svp	orca	ionization energy ev	n/a
OVGF	nh3 / def2-svp	orca	ionization energy ev	n/a
OVGF	nh3 / def2-svp	orca	ionization energy ev	n/a
OVGF	nh3 / def2-svp	orca	ionization energy ev	n/a
OVGF	nh3 / def2-tzvp	orca	orbital energy max abs deviation ev	n/a
OVGF	nh3 / def2-tzvp	orca	ionization energy ev	n/a
OVGF	nh3 / def2-tzvp	orca	ionization energy ev	n/a
OVGF	nh3 / def2-tzvp	orca	ionization energy ev	n/a
OVGF	nh3 / sto-3g	orca	orbital energy max abs deviation ev	n/a
OVGF	nh3 / sto-3g	orca	ionization energy ev	n/a
OVGF	nh3 / sto-3g	orca	ionization energy ev	n/a
OVGF	nh3 / sto-3g	orca	ionization energy ev	n/a
OVGF	nh3 / sto-3g	orca	ionization energy ev	n/a
OVGF	oh-radical / def2-svp	orca	orbital energy max abs deviation ev	n/a
OVGF	oh-radical / def2-svp	orca	ionization energy ev	n/a
OVGF	oh-radical / def2-tzvp	orca	orbital energy max abs deviation ev	n/a
OVGF	oh-radical / def2-tzvp	orca	ionization energy ev	n/a
OVGF	oh-radical / sto-3g	orca	orbital energy max abs deviation ev	n/a
OVGF	ch2o / def2-tzvp	orca	ionization energy ev	n/a
OVGF	ch4 / def2-svp	orca	ionization energy ev	n/a
OVGF	ch4 / def2-svp	orca	ionization energy ev	n/a
OVGF	ch4 / def2-tzvp	orca	ionization energy ev	n/a
OVGF	ch4 / def2-tzvp	orca	ionization energy ev	n/a
OVGF	ch4 / sto-3g	orca	ionization energy ev	n/a
OVGF	ch4 / sto-3g	orca	ionization energy ev	n/a
OVGF	co / def2-svp	orca	ionization energy ev	n/a
OVGF	co / def2-tzvp	orca	ionization energy ev	n/a
OVGF	co / sto-3g	orca	ionization energy ev	n/a
OVGF	hf / def2-svp	orca	ionization energy ev	n/a
OVGF	hf / def2-tzvp	orca	ionization energy ev	n/a
OVGF	hf / def2-tzvp	orca	ionization energy ev	n/a
OVGF	n2 / def2-svp	orca	ionization energy ev	n/a
OVGF	n2 / def2-svp	orca	ionization energy ev	n/a
OVGF	n2 / def2-tzvp	orca	ionization energy ev	n/a
OVGF	n2 / sto-3g	orca	ionization energy ev	n/a
OVGF	oh-radical / sto-3g	orca	ionization energy ev	n/a
OVGF	oh-radical / sto-3g	orca	ionization energy ev	n/a
OVGF	h2o / sto-3g	pyscf	total energy ha	artifact-incomplete
OVGF	h2o / sto-3g	pyscf	total energy ha	artifact-incomplete
OVGF	oh-radical / sto-3g	pyscf	total energy ha	artifact-incomplete
OVGF	oh-radical / sto-3g	pyscf	total energy ha	artifact-incomplete
OVGF	h2o / def2-svp	pyscf	total energy ha	reference-missing
OVGF	oh-radical / def2-svp	pyscf	total energy ha	reference-missing
OVGF	h2o / sto-3g	pyscf	total energy ha	reference-missing
OVGF	oh-radical / sto-3g	pyscf	total energy ha	reference-missing
OVGF	h2o / def2-svp	pyscf	total energy ha	reference-missing
OVGF	h2o / sto-3g	pyscf	total energy ha	reference-missing
OVGF	h2o / def2-tzvp	pyscf	total energy ha	reference-missing

Table S21, continued.

Method	System / basis	Ref.	Quantity	$\lvert\Delta\rvert$
OVGF	oh-radical / def2-svp	pyscf	total energy ha	reference-missing
OVGF	oh-radical / sto-3g	pyscf	total energy ha	reference-missing
OVGF	oh-radical / def2-tzvp	pyscf	total energy ha	reference-missing
Molecular properties				
213 pass, 1 held, 29 fail, 12 artifact-incomplete, 5 reference-missing, 5 blocked. Median $\lvert\Delta E\rvert$ 5.3×10^{-9}, max 3.5×10^{-3} E_h.				
RKS/pbe0	h2o-dimer / def2-tzvp	orca	optimized total energy ha	3.05×10^{-4}
RKS/pbe0	h2o-dimer / def2-tzvp	orca	optimized r oo angstrom	3.50×10^{-3}
RKS/pbe0	h2o-dimer / def2-tzvp	orca	optimized r oh donor angstrom	1.69×10^{-4}
RHF	h2o / sto-3g	orca	total energy ha	5.35×10^{-9}
UHF	oh-radical / sto-3g	orca	total energy ha	7.73×10^{-9}
RHF	oh-radical / sto-3g	orca	total energy ha	1.27×10^{-8}
RHF	h2o / sto-3g	orca	total energy ha	5.35×10^{-9}
RHF	h2o / sto-3g	orca	total energy ha	5.35×10^{-9}
RHF	h2o / sto-3g	orca	total energy ha	5.35×10^{-9}
RHF	h2o / sto-3g	orca	total energy ha	5.35×10^{-9}
RHF	h2o / sto-3g	orca	total energy ha	5.35×10^{-9}
RHF	h2o / sto-3g	orca	total energy ha	5.35×10^{-9}
RHF	h2o / sto-3g	orca	total energy ha	5.35×10^{-9}
RHF	h2 / sto-3g	orca	total energy ha	3.12×10^{-9}
RHF	h2o / sto-3g	orca	total energy ha	5.35×10^{-9}
RHF	c2h4 / def2-svp	orca	total energy ha	1.23×10^{-10}
RHF	c2h4 / def2-svp	orca	mulliken charge max abs deviation e	n/a
RHF	c2h4 / def2-svp	orca	loewdin charge max abs deviation e	n/a
RHF	c2h4 / def2-svp	orca	mayer bond order max abs deviation	n/a
RHF	c2h4 / def2-svp	orca	dipole moment au	n/a
RHF	c2h4 / def2-svp	orca	isotropic polarizability au	n/a
RHF	c2h4 / def2-svp	orca	orbital energy max abs deviation ha	7.70×10^{-7}
RHF	c2h4 / def2-tzvp	orca	total energy ha	4.49×10^{-10}
RHF	c2h4 / def2-tzvp	orca	mulliken charge max abs deviation e	n/a
RHF	c2h4 / def2-tzvp	orca	loewdin charge max abs deviation e	n/a
RHF	c2h4 / def2-tzvp	orca	mayer bond order max abs deviation	n/a
RHF	c2h4 / def2-tzvp	orca	dipole moment au	n/a
RHF	c2h4 / def2-tzvp	orca	isotropic polarizability au	n/a
RHF	c2h4 / def2-tzvp	orca	orbital energy max abs deviation ha	6.10×10^{-7}
RHF	c2h4 / sto-3g	orca	total energy ha	9.10×10^{-10}
RHF	c2h4 / sto-3g	orca	mulliken charge max abs deviation e	n/a
RHF	c2h4 / sto-3g	orca	loewdin charge max abs deviation e	n/a
RHF	c2h4 / sto-3g	orca	mayer bond order max abs deviation	n/a
RHF	c2h4 / sto-3g	orca	dipole moment au	n/a
RHF	c2h4 / sto-3g	orca	isotropic polarizability au	n/a
RHF	c2h4 / sto-3g	orca	orbital energy max abs deviation ha	4.70×10^{-7}
RHF	ch2o / def2-svp	orca	total energy ha	9.35×10^{-10}
RHF	ch2o / def2-svp	orca	mulliken charge max abs deviation e	n/a

Table S21, continued.

Method	System / basis	Ref.	Quantity	$\lvert\Delta\rvert$
RHF	ch2o / def2-svp	orca	loewdin charge max abs deviation e	n/a
RHF	ch2o / def2-svp	orca	mayer bond order max abs deviation	n/a
RHF	ch2o / def2-svp	orca	dipole moment au	n/a
RHF	ch2o / def2-svp	orca	isotropic polarizability au	n/a
RHF	ch2o / def2-svp	orca	orbital energy max abs deviation ha	1.54×10^{-6}
RHF	ch2o / def2-tzvp	orca	total energy ha	1.02×10^{-9}
RHF	ch2o / def2-tzvp	orca	mulliken charge max abs deviation e	n/a
RHF	ch2o / def2-tzvp	orca	loewdin charge max abs deviation e	n/a
RHF	ch2o / def2-tzvp	orca	mayer bond order max abs deviation	n/a
RHF	ch2o / def2-tzvp	orca	dipole moment au	n/a
RHF	ch2o / def2-tzvp	orca	isotropic polarizability au	n/a
RHF	ch2o / def2-tzvp	orca	orbital energy max abs deviation ha	3.51×10^{-6}
RHF	ch2o / sto-3g	orca	total energy ha	6.99×10^{-12}
RHF	ch2o / sto-3g	orca	mulliken charge max abs deviation e	n/a
RHF	ch2o / sto-3g	orca	loewdin charge max abs deviation e	n/a
RHF	ch2o / sto-3g	orca	mayer bond order max abs deviation	n/a
RHF	ch2o / sto-3g	orca	dipole moment au	n/a
RHF	ch2o / sto-3g	orca	isotropic polarizability au	n/a
RHF	ch2o / sto-3g	orca	orbital energy max abs deviation ha	1.09×10^{-6}
RHF	ch4 / def2-svp	orca	total energy ha	2.10×10^{-11}
RHF	ch4 / def2-svp	orca	mulliken charge max abs deviation e	n/a
RHF	ch4 / def2-svp	orca	loewdin charge max abs deviation e	n/a
RHF	ch4 / def2-svp	orca	mayer bond order max abs deviation	n/a
RHF	ch4 / def2-svp	orca	dipole moment au	n/a
RHF	ch4 / def2-svp	orca	isotropic polarizability au	n/a
RHF	ch4 / def2-svp	orca	orbital energy max abs deviation ha	3.90×10^{-7}
RHF	ch4 / def2-tzvp	orca	total energy ha	2.69×10^{-10}
RHF	ch4 / def2-tzvp	orca	mulliken charge max abs deviation e	n/a
RHF	ch4 / def2-tzvp	orca	loewdin charge max abs deviation e	n/a
RHF	ch4 / def2-tzvp	orca	mayer bond order max abs deviation	n/a
RHF	ch4 / def2-tzvp	orca	dipole moment au	n/a
RHF	ch4 / def2-tzvp	orca	isotropic polarizability au	n/a
RHF	ch4 / def2-tzvp	orca	orbital energy max abs deviation ha	5.30×10^{-7}
RHF	ch4 / sto-3g	orca	total energy ha	1.63×10^{-10}
RHF	ch4 / sto-3g	orca	mulliken charge max abs deviation e	n/a
RHF	ch4 / sto-3g	orca	loewdin charge max abs deviation e	n/a

Table S21, continued.

Method	System / basis	Ref.	Quantity	$\lvert\Delta\rvert$
RHF	ch4 / sto-3g	orca	mayer bond order max abs deviation	n/a
RHF	ch4 / sto-3g	orca	dipole moment au	n/a
RHF	ch4 / sto-3g	orca	isotropic polarizability au	n/a
RHF	ch4 / sto-3g	orca	orbital energy max abs deviation ha	4.90×10^{-7}
RHF	co / def2-svp	orca	total energy ha	9.43×10^{-10}
RHF	co / def2-svp	orca	mulliken charge max abs deviation e	n/a
RHF	co / def2-svp	orca	loewdin charge max abs deviation e	n/a
RHF	co / def2-svp	orca	hirshfeld charge max abs deviation e	n/a
RHF	co / def2-svp	orca	mayer bond order max abs deviation	n/a
RHF	co / def2-svp	orca	dipole moment au	n/a
RHF	co / def2-svp	orca	isotropic polarizability au	n/a
RHF	co / def2-svp	orca	orbital energy max abs deviation ha	3.37×10^{-6}
RHF	co / def2-tzvp	orca	total energy ha	8.81×10^{-10}
RHF	co / def2-tzvp	orca	mulliken charge max abs deviation e	n/a
RHF	co / def2-tzvp	orca	loewdin charge max abs deviation e	n/a
RHF	co / def2-tzvp	orca	hirshfeld charge max abs deviation e	n/a
RHF	co / def2-tzvp	orca	mayer bond order max abs deviation	n/a
RHF	co / def2-tzvp	orca	dipole moment au	n/a
RHF	co / def2-tzvp	orca	isotropic polarizability au	n/a
RHF	co / def2-tzvp	orca	orbital energy max abs deviation ha	8.20×10^{-7}
RHF	co / sto-3g	orca	total energy ha	3.86×10^{-10}
RHF	co / sto-3g	orca	mulliken charge max abs deviation e	n/a
RHF	co / sto-3g	orca	loewdin charge max abs deviation e	n/a
RHF	co / sto-3g	orca	mayer bond order max abs deviation	n/a
RHF	co / sto-3g	orca	dipole moment au	n/a
RHF	co / sto-3g	orca	isotropic polarizability au	n/a
RHF	co / sto-3g	orca	orbital energy max abs deviation ha	4.70×10^{-7}
RHF	ethanol / def2-svp	orca	total energy ha	1.09×10^{-9}
RHF	ethanol / def2-svp	orca	mulliken charge max abs deviation e	n/a
RHF	ethanol / def2-svp	orca	loewdin charge max abs deviation e	n/a
RHF	ethanol / def2-svp	orca	mayer bond order max abs deviation	n/a
RHF	ethanol / def2-svp	orca	dipole moment au	n/a
RHF	ethanol / def2-svp	orca	isotropic polarizability au	n/a
RHF	ethanol / def2-svp	orca	orbital energy max abs deviation ha	3.34×10^{-6}
RHF	ethanol / def2-tzvp	orca	total energy ha	6.29×10^{-10}
RHF	ethanol / def2-tzvp	orca	mulliken charge max abs deviation e	n/a

Table S21, continued.

Method	System / basis	Ref.	Quantity	$\lvert\Delta\rvert$
RHF	ethanol / def2-tzvp	orca	loewdin charge max abs deviation e	n/a
RHF	ethanol / def2-tzvp	orca	mayer bond order max abs deviation	n/a
RHF	ethanol / def2-tzvp	orca	dipole moment au	n/a
RHF	ethanol / def2-tzvp	orca	isotropic polarizability au	n/a
RHF	ethanol / def2-tzvp	orca	orbital energy max abs deviation ha	4.40×10^{-6}
RHF	ethanol / sto-3g	orca	total energy ha	2.27×10^{-10}
RHF	ethanol / sto-3g	orca	mulliken charge max abs deviation e	n/a
RHF	ethanol / sto-3g	orca	loewdin charge max abs deviation e	n/a
RHF	ethanol / sto-3g	orca	mayer bond order max abs deviation	n/a
RHF	ethanol / sto-3g	orca	dipole moment au	n/a
RHF	ethanol / sto-3g	orca	isotropic polarizability au	n/a
RHF	ethanol / sto-3g	orca	orbital energy max abs deviation ha	1.61×10^{-6}
RHF	h2o / def2-svp	orca	total energy ha	3.95×10^{-10}
RHF	h2o / def2-svp	orca	mulliken charge max abs deviation e	n/a
RHF	h2o / def2-svp	orca	loewdin charge max abs deviation e	n/a
RHF	h2o / def2-svp	orca	mayer bond order max abs deviation	n/a
RHF	h2o / def2-svp	orca	dipole moment au	n/a
RHF	h2o / def2-svp	orca	isotropic polarizability au	n/a
RHF	h2o / def2-svp	orca	orbital energy max abs deviation ha	1.64×10^{-6}
RHF	h2o / def2-tzvp	orca	total energy ha	4.59×10^{-10}
RHF	h2o / def2-tzvp	orca	mulliken charge max abs deviation e	n/a
RHF	h2o / def2-tzvp	orca	loewdin charge max abs deviation e	n/a
RHF	h2o / def2-tzvp	orca	mayer bond order max abs deviation	n/a
RHF	h2o / def2-tzvp	orca	dipole moment au	n/a
RHF	h2o / def2-tzvp	orca	isotropic polarizability au	n/a
RHF	h2o / def2-tzvp	orca	orbital energy max abs deviation ha	1.05×10^{-6}
RHF	h2o / sto-3g	orca	total energy ha	5.28×10^{-10}
RHF	h2o / sto-3g	orca	mulliken charge max abs deviation e	n/a
RHF	h2o / sto-3g	orca	loewdin charge max abs deviation e	n/a
RHF	h2o / sto-3g	orca	mayer bond order max abs deviation	n/a
RHF	h2o / sto-3g	orca	dipole moment au	n/a
RHF	h2o / sto-3g	orca	isotropic polarizability au	n/a
RHF	h2o / sto-3g	orca	orbital energy max abs deviation ha	4.70×10^{-7}
RHF	hf / def2-svp	orca	total energy ha	2.73×10^{-10}
RHF	hf / def2-svp	orca	mulliken charge max abs deviation e	n/a
RHF	hf / def2-svp	orca	loewdin charge max abs deviation e	n/a

Table S21, continued.

Method	System / basis	Ref.	Quantity	$\lvert\Delta\rvert$
RHF	hf / def2-svp	orca	mayer bond order max abs deviation	n/a
RHF	hf / def2-svp	orca	dipole moment au	n/a
RHF	hf / def2-svp	orca	isotropic polarizability au	n/a
RHF	hf / def2-svp	orca	orbital energy max abs deviation ha	6.50×10^{-7}
RHF	hf / def2-tzvp	orca	total energy ha	3.71×10^{-10}
RHF	hf / def2-tzvp	orca	mulliken charge max abs deviation e	n/a
RHF	hf / def2-tzvp	orca	loewdin charge max abs deviation e	n/a
RHF	hf / def2-tzvp	orca	mayer bond order max abs deviation	n/a
RHF	hf / def2-tzvp	orca	dipole moment au	n/a
RHF	hf / def2-tzvp	orca	isotropic polarizability au	n/a
RHF	hf / def2-tzvp	orca	orbital energy max abs deviation ha	7.60×10^{-7}
RHF	hf / sto-3g	orca	total energy ha	3.86×10^{-10}
RHF	hf / sto-3g	orca	mulliken charge max abs deviation e	n/a
RHF	hf / sto-3g	orca	loewdin charge max abs deviation e	n/a
RHF	hf / sto-3g	orca	mayer bond order max abs deviation	n/a
RHF	hf / sto-3g	orca	dipole moment au	n/a
RHF	hf / sto-3g	orca	isotropic polarizability au	n/a
RHF	hf / sto-3g	orca	orbital energy max abs deviation ha	4.10×10^{-7}
RHF	nh3 / def2-svp	orca	total energy ha	3.71×10^{-10}
RHF	nh3 / def2-svp	orca	mulliken charge max abs deviation e	n/a
RHF	nh3 / def2-svp	orca	loewdin charge max abs deviation e	n/a
RHF	nh3 / def2-svp	orca	mayer bond order max abs deviation	n/a
RHF	nh3 / def2-svp	orca	dipole moment au	n/a
RHF	nh3 / def2-svp	orca	isotropic polarizability au	n/a
RHF	nh3 / def2-svp	orca	orbital energy max abs deviation ha	6.30×10^{-7}
RHF	nh3 / def2-tzvp	orca	total energy ha	4.88×10^{-10}
RHF	nh3 / def2-tzvp	orca	mulliken charge max abs deviation e	n/a
RHF	nh3 / def2-tzvp	orca	loewdin charge max abs deviation e	n/a
RHF	nh3 / def2-tzvp	orca	mayer bond order max abs deviation	n/a
RHF	nh3 / def2-tzvp	orca	dipole moment au	n/a
RHF	nh3 / def2-tzvp	orca	isotropic polarizability au	n/a
RHF	nh3 / def2-tzvp	orca	orbital energy max abs deviation ha	2.41×10^{-6}
RHF	nh3 / sto-3g	orca	total energy ha	3.67×10^{-10}
RHF	nh3 / sto-3g	orca	mulliken charge max abs deviation e	n/a
RHF	nh3 / sto-3g	orca	loewdin charge max abs deviation e	n/a
RHF	nh3 / sto-3g	orca	mayer bond order max abs deviation	n/a
RHF	nh3 / sto-3g	orca	dipole moment au	n/a

Table S21, continued.

Method	System / basis	Ref.	Quantity	$\lvert\Delta\rvert$
RHF	nh3 / sto-3g	orca	isotropic polarizability au	n/a
RHF	nh3 / sto-3g	orca	orbital energy max abs deviation ha	6.50×10^{-7}
RHF	phenol / def2-svp	orca	total energy ha	3.45×10^{-9}
RHF	phenol / def2-svp	orca	mulliken charge max abs deviation e	n/a
RHF	phenol / def2-svp	orca	loewdin charge max abs deviation e	n/a
RHF	phenol / def2-svp	orca	mayer bond order max abs deviation	n/a
RHF	phenol / def2-svp	orca	dipole moment au	n/a
RHF	phenol / def2-svp	orca	isotropic polarizability au	n/a
RHF	phenol / def2-svp	orca	orbital energy max abs deviation ha	7.63×10^{-6}
RHF	phenol / sto-3g	orca	total energy ha	2.95×10^{-9}
RHF	phenol / sto-3g	orca	mulliken charge max abs deviation e	n/a
RHF	phenol / sto-3g	orca	loewdin charge max abs deviation e	n/a
RHF	phenol / sto-3g	orca	mayer bond order max abs deviation	n/a
RHF	phenol / sto-3g	orca	dipole moment au	n/a
RHF	phenol / sto-3g	orca	isotropic polarizability au	n/a
RHF	phenol / sto-3g	orca	orbital energy max abs deviation ha	1.89×10^{-6}
RHF	pyridine / def2-svp	orca	total energy ha	4.07×10^{-9}
RHF	pyridine / def2-svp	orca	mulliken charge max abs deviation e	n/a
RHF	pyridine / def2-svp	orca	loewdin charge max abs deviation e	n/a
RHF	pyridine / def2-svp	orca	mayer bond order max abs deviation	n/a
RHF	pyridine / def2-svp	orca	dipole moment au	n/a
RHF	pyridine / def2-svp	orca	isotropic polarizability au	n/a
RHF	pyridine / def2-svp	orca	orbital energy max abs deviation ha	1.15×10^{-6}
RHF	pyridine / sto-3g	orca	total energy ha	2.81×10^{-9}
RHF	pyridine / sto-3g	orca	mulliken charge max abs deviation e	n/a
RHF	pyridine / sto-3g	orca	loewdin charge max abs deviation e	n/a
RHF	pyridine / sto-3g	orca	mayer bond order max abs deviation	n/a
RHF	pyridine / sto-3g	orca	dipole moment au	n/a
RHF	pyridine / sto-3g	orca	isotropic polarizability au	n/a
RHF	pyridine / sto-3g	orca	orbital energy max abs deviation ha	1.37×10^{-6}
RKS/pbe	h2co / sto-3g	orca	total energy ha	held
RHF	h2 / sto-3g	orca	total energy ha	8.21×10^{-4}
RKS/pbe	h2co / sto-3g	orca	total energy ha	1.48×10^{-1}
MP2	h2o / sto-3g	orca	total energy ha	3.93×10^{-2}
RHF	c2h4 / def2-svp	orca	hirshfeld charge max abs deviation e	n/a
RHF	c2h4 / def2-tzvp	orca	hirshfeld charge max abs deviation e	n/a
RHF	c2h4 / sto-3g	orca	hirshfeld charge max abs deviation e	n/a

Table S21, continued.

Method	System / basis	Ref.	Quantity	|Δ|
RHF	ch2o / def2-svp	orca	hirshfeld charge max abs deviation e	n/a
RHF	ch2o / def2-tzvp	orca	hirshfeld charge max abs deviation e	n/a
RHF	ch2o / sto-3g	orca	hirshfeld charge max abs deviation e	n/a
RHF	ch4 / def2-svp	orca	hirshfeld charge max abs deviation e	n/a
RHF	ch4 / def2-tzvp	orca	hirshfeld charge max abs deviation e	n/a
RHF	ch4 / sto-3g	orca	hirshfeld charge max abs deviation e	n/a
RHF	co / sto-3g	orca	hirshfeld charge max abs deviation e	n/a
RHF	ethanol / def2-svp	orca	hirshfeld charge max abs deviation e	n/a
RHF	ethanol / def2-tzvp	orca	hirshfeld charge max abs deviation e	n/a
RHF	ethanol / sto-3g	orca	hirshfeld charge max abs deviation e	n/a
RHF	h2o / def2-svp	orca	hirshfeld charge max abs deviation e	n/a
RHF	h2o / def2-tzvp	orca	hirshfeld charge max abs deviation e	n/a
RHF	h2o / sto-3g	orca	hirshfeld charge max abs deviation e	n/a
RHF	hf / def2-svp	orca	hirshfeld charge max abs deviation e	n/a
RHF	hf / def2-tzvp	orca	hirshfeld charge max abs deviation e	n/a
RHF	hf / sto-3g	orca	hirshfeld charge max abs deviation e	n/a
RHF	nh3 / def2-svp	orca	hirshfeld charge max abs deviation e	n/a
RHF	nh3 / def2-tzvp	orca	hirshfeld charge max abs deviation e	n/a
RHF	nh3 / sto-3g	orca	hirshfeld charge max abs deviation e	n/a
RHF	phenol / def2-svp	orca	hirshfeld charge max abs deviation e	n/a
RHF	phenol / sto-3g	orca	hirshfeld charge max abs deviation e	n/a
RHF	pyridine / def2-svp	orca	hirshfeld charge max abs deviation e	n/a
RHF	pyridine / sto-3g	orca	hirshfeld charge max abs deviation e	n/a
RHF	h2o / sto-3g	orca	total energy ha	artifact-incomplete
RHF	h2o / sto-3g	orca	total energy ha	artifact-incomplete
RHF	h2o / sto-3g	orca	total energy ha	artifact-incomplete
RHF	h2o / sto-3g	orca	total energy ha	artifact-incomplete
RHF	h2o / sto-3g	orca	total energy ha	artifact-incomplete
RKS/pbe	h2co / sto-3g	orca	total energy ha	artifact-incomplete
OVGF	h2o / sto-3g	pyscf	total energy ha	artifact-incomplete
OVGF	oh-radical / sto-3g	pyscf	total energy ha	artifact-incomplete
CCSD(T)	h2 / sto-3g	orca	total energy ha	artifact-incomplete
dlpno-ccsd(t)	h2 / sto-3g	orca	total energy ha	artifact-incomplete
CASSCF	h2 / sto-3g	openmolcas	total energy ha	artifact-incomplete
CASPT2	h2 / sto-3g	openmolcas	total energy ha	artifact-incomplete

Table S21, continued.

Method	System / basis	Ref.	Quantity	$\lvert\Delta\rvert$
RKS/pbe	h2co / sto-3g	orca	total energy ha	reference-missing
OVGF	h2o / sto-3g	pyscf	total energy ha	reference-missing
OVGF	h2o / sto-3g	pyscf	total energy ha	reference-missing
OVGF	oh-radical / sto-3g	pyscf	total energy ha	reference-missing
OVGF	oh-radical / sto-3g	pyscf	total energy ha	reference-missing
MP2	h2o / sto-3g	orca	total energy ha	blocked
CCSD(T)	h2 / sto-3g	orca	total energy ha	blocked
dlpno-ccsd(t)	h2 / sto-3g	orca	total energy ha	blocked
CASSCF	h2 / sto-3g	openmolcas	total energy ha	blocked
CASPT2	h2 / sto-3g	openmolcas	total energy ha	blocked
Add-on corrections				
5 pass, 19 fail, 10 artifact-incomplete, 7 reference-missing, 5 blocked. Median $\lvert\Delta E\rvert$ 2.0×10^{-9}, max 4.0×10^{-9} E_h.				
HF-3C	h2o-dimer / minix	orca	total energy ha	1.70×10^{-9}
HF-3C	h2o-dimer / minix	orca	scf energy ha	9.24×10^{-10}
HF-3C	h2o-dimer / minix	orca	dispersion d3bj ha	2.68×10^{-9}
HF-3C	h2o-dimer / minix	orca	gcp plus srb ha	4.00×10^{-9}
R2SCAN-3C	h2o-dimer / def2-mtzvpp	orca	gcp ha	2.00×10^{-9}
R2SCAN-3C	h2o-dimer / def2-mtzvpp	orca	total energy ha	1.28×10^{-3}
R2SCAN-3C	h2o-dimer / def2-mtzvpp	orca	scf energy ha	1.22×10^{-3}
R2SCAN-3C	h2o-dimer / def2-mtzvpp	orca	dispersion d4 ha	6.04×10^{-5}
RKS/pbe	h2o / def2-svp	orca	total energy ha	4.59×10^{-4}
RKS/pbe	h2o / def2-svp	orca	total energy ha	3.01×10^{-4}
RKS/pbe	h2o / def2-svp	orca	total energy ha	4.00×10^{-2}
RHF	h2s / lanl2dz	orca	total energy ha	7.86×10^{1}
RKS/pbe	h2o / sto-3g	orca	total energy ha	2.24×10^{-2}
RHF	h2s / lanl2dz	orca	total energy ha	7.86×10^{1}
RKS/pbe	h2o / def2-svp	orca	total energy ha	4.59×10^{-4}
RKS/pbe	h2o / sto-3g	orca	total energy ha	1.15×10^{-3}
RKS/pbe	h2o / def2-tzvp	orca	total energy ha	5.04×10^{-4}
RKS/pbe	h2o / def2-svp	orca	total energy ha	3.01×10^{-4}
RKS/pbe	h2o / sto-3g	orca	total energy ha	9.93×10^{-4}
RKS/pbe	h2o / def2-tzvp	orca	total energy ha	3.45×10^{-4}
RKS/pbe	h2o / def2-svp	orca	total energy ha	4.00×10^{-2}
RKS/pbe	h2o / sto-3g	orca	total energy ha	2.24×10^{-2}
RKS/pbe	h2o / def2-tzvp	orca	total energy ha	2.81×10^{-2}
RHF	h2s / lanl2dz	orca	total energy ha	7.86×10^{1}
RKS/pbe	h2o / sto-3g	orca	total energy ha	artifact-incomplete
RKS/pbe	h2o / sto-3g	orca	total energy ha	artifact-incomplete
RKS/pbe	h2o / sto-3g	orca	total energy ha	artifact-incomplete
RKS/pbe	h2o / sto-3g	orca	total energy ha	artifact-incomplete
RKS/pbe	h2o / sto-3g	orca	total energy ha	artifact-incomplete
RKS/pbe	h2o / sto-3g	orca	total energy ha	artifact-incomplete
RHF	h2s / lanl2dz	orca	total energy ha	artifact-incomplete
RHF	h2s / lanl2dz	orca	total energy ha	artifact-incomplete
RHF	h2 / sto-3g	orca	total energy ha	artifact-incomplete
RHF	h2 / sto-3g	orca	total energy ha	artifact-incomplete
RHF	h2 / def2-svp	orca	total energy ha	reference-missing
RKS/pbe	h2o / sto-3g	orca	total energy ha	reference-missing
RKS/pbe	h2o / sto-3g	orca	total energy ha	reference-missing
RHF	h2 / sto-3g	orca	total energy ha	reference-missing
RHF	h2 / def2-svp	orca	total energy ha	reference-missing
RHF	h2 / sto-3g	orca	total energy ha	reference-missing
RHF	h2 / def2-tzvp	orca	total energy ha	reference-missing
RHF	h2 / def2-svp	orca	total energy ha	blocked
RHF	h2 / sto-3g	orca	total energy ha	blocked
RHF	h2 / def2-svp	orca	total energy ha	blocked
RHF	h2 / sto-3g	orca	total energy ha	blocked

Table S21, continued.

Method	System / basis	Ref.	Quantity	|Δ|
RHF	h2 / def2-tzvp	orca	total energy ha	blocked
Semiempirical				
31 artifact-incomplete, 18 reference-missing, 743 blocked.				
GFN2_XTB	h2	xtb	total energy ha	artifact-incomplete
MSINDO	h2o	msindo	total energy ha	artifact-incomplete
MSINDO	h2o	msindo	total energy ha	artifact-incomplete
MSINDO	hf	msindo	total energy ha	artifact-incomplete
MSINDO	hf	msindo	total energy ha	artifact-incomplete
MSINDO	hf	msindo	total energy ha	artifact-incomplete
MSINDO	hf	msindo	total energy ha	artifact-incomplete
GFN2_XTB	h2	xtb	total energy ha	artifact-incomplete
GFN2_XTB	h2	xtb	total energy ha	artifact-incomplete
OM1	h2o	internal	total energy ha	artifact-incomplete
OM1	h2o	internal	total energy ha	artifact-incomplete
OM2	h2o	internal	total energy ha	artifact-incomplete
OM2	h2o	internal	total energy ha	artifact-incomplete
OM3	h2o	internal	total energy ha	artifact-incomplete
OM3	h2o	internal	total energy ha	artifact-incomplete
PM6	h2o	internal	total energy ha	artifact-incomplete
PM6	h2o	internal	total energy ha	artifact-incomplete
DFTB0	h2o	internal	total energy ha	artifact-incomplete
DFTB0	h2o	internal	total energy ha	artifact-incomplete
SCC_DFTB	h2o	internal	total energy ha	artifact-incomplete
SCC_DFTB	h2o	internal	total energy ha	artifact-incomplete
MSINDO	h2o	msindo	total energy ha	artifact-incomplete
MSINDO	hf	msindo	total energy ha	artifact-incomplete
MSINDO	hf	msindo	total energy ha	artifact-incomplete
GFN2_XTB	h2	xtb	total energy ha	artifact-incomplete
OM1	h2o	internal	total energy ha	artifact-incomplete
OM2	h2o	internal	total energy ha	artifact-incomplete
OM3	h2o	internal	total energy ha	artifact-incomplete
PM6	h2o	internal	total energy ha	artifact-incomplete
DFTB0	h2o	internal	total energy ha	artifact-incomplete
SCC_DFTB	h2o	internal	total energy ha	artifact-incomplete
MSINDO	h2o	msindo	total energy ha	reference-missing
MSINDO	hf	msindo	total energy ha	reference-missing
MSINDO	hf	msindo	total energy ha	reference-missing
OM1	h2o	internal	total energy ha	reference-missing
OM2	h2o	internal	total energy ha	reference-missing
OM3	h2o	internal	total energy ha	reference-missing
PM6	h2o	internal	total energy ha	reference-missing
DFTB0	h2o	internal	total energy ha	reference-missing
SCC_DFTB	h2o	internal	total energy ha	reference-missing
MSINDO	h2o	msindo	total energy ha	reference-missing
MSINDO	hf	msindo	total energy ha	reference-missing
MSINDO	hf	msindo	total energy ha	reference-missing
OM1	h2o	internal	total energy ha	reference-missing
OM2	h2o	internal	total energy ha	reference-missing
OM3	h2o	internal	total energy ha	reference-missing
PM6	h2o	internal	total energy ha	reference-missing
DFTB0	h2o	internal	total energy ha	reference-missing
SCC_DFTB	h2o	internal	total energy ha	reference-missing
GFN2-XTB	atom-h	orca	energy total ha	blocked
GFN2_XTB	h2	xtb	total energy ha	blocked
DFTB0	acetamide	dftb+	total energy ha	blocked
DFTB0	acetamide	dftb+	total energy ha	blocked
DFTB0	acetamide	dftb+	total energy ha	blocked

Table S21, continued.

Method	System / basis	Ref.	Quantity	|Δ|
DFTB0	acetamide	dftb+	total energy ha	blocked
DFTB0	acetone	dftb+	total energy ha	blocked
DFTB0	acetone	dftb+	total energy ha	blocked
DFTB0	acetone	dftb+	total energy ha	blocked
DFTB0	acetone	dftb+	total energy ha	blocked
DFTB0	adenine	dftb+	total energy ha	blocked
DFTB0	adenine	dftb+	total energy ha	blocked
DFTB0	adenine	dftb+	total energy ha	blocked
DFTB0	adenine	dftb+	total energy ha	blocked
DFTB0	benzene	dftb+	total energy ha	blocked
DFTB0	benzene	dftb+	total energy ha	blocked
DFTB0	benzene	dftb+	total energy ha	blocked
DFTB0	benzene	dftb+	total energy ha	blocked
DFTB0	butadiene	dftb+	total energy ha	blocked
DFTB0	butadiene	dftb+	total energy ha	blocked
DFTB0	c2h4	dftb+	total energy ha	blocked
DFTB0	c2h4	dftb+	total energy ha	blocked
DFTB0	c2h4	dftb+	total energy ha	blocked
DFTB0	c2h4	dftb+	total energy ha	blocked
DFTB0	ch2o	dftb+	total energy ha	blocked
DFTB0	ch2o	dftb+	total energy ha	blocked
DFTB0	ch2o	dftb+	total energy ha	blocked
DFTB0	ch2o	dftb+	total energy ha	blocked
DFTB0	ch3oh	dftb+	total energy ha	blocked
DFTB0	ch3oh	dftb+	total energy ha	blocked
DFTB0	ch3oh	dftb+	total energy ha	blocked
DFTB0	ch4	dftb+	total energy ha	blocked
DFTB0	ch4	dftb+	total energy ha	blocked
DFTB0	ch4	dftb+	total energy ha	blocked
DFTB0	co2	dftb+	total energy ha	blocked
DFTB0	co2	dftb+	total energy ha	blocked
DFTB0	co2	dftb+	total energy ha	blocked
DFTB0	cyclopropene	dftb+	total energy ha	blocked
DFTB0	cyclopropene	dftb+	total energy ha	blocked
DFTB0	cyclopropene	dftb+	total energy ha	blocked
DFTB0	cyclopropene	dftb+	total energy ha	blocked
DFTB0	cytosine	dftb+	total energy ha	blocked
DFTB0	cytosine	dftb+	total energy ha	blocked
DFTB0	furan	dftb+	total energy ha	blocked
DFTB0	furan	dftb+	total energy ha	blocked
DFTB0	h2co	dftb+	total energy ha	blocked
DFTB0	h2co	dftb+	total energy ha	blocked
DFTB0	h2co	dftb+	total energy ha	blocked
DFTB0	h2o	dftb+	total energy ha	blocked
DFTB0	h2o	dftb+	total energy ha	blocked
DFTB0	h2o	dftb+	total energy ha	blocked
DFTB0	h2s	dftb+	total energy ha	blocked
DFTB0	h2s	dftb+	total energy ha	blocked
DFTB0	h2s	dftb+	total energy ha	blocked
DFTB0	hcooh	dftb+	total energy ha	blocked
DFTB0	hcooh	dftb+	total energy ha	blocked
DFTB0	hcooh	dftb+	total energy ha	blocked
DFTB0	hexatriene	dftb+	total energy ha	blocked
DFTB0	hexatriene	dftb+	total energy ha	blocked
DFTB0	imidazole	dftb+	total energy ha	blocked
DFTB0	imidazole	dftb+	total energy ha	blocked
DFTB0	naphthalene	dftb+	total energy ha	blocked
DFTB0	naphthalene	dftb+	total energy ha	blocked

Table S21, continued.

Method	System / basis	Ref.	Quantity	|Δ|
DFTB0	naphthalene	dftb+	total energy ha	blocked
DFTB0	nh3	dftb+	total energy ha	blocked
DFTB0	nh3	dftb+	total energy ha	blocked
DFTB0	nh3	dftb+	total energy ha	blocked
DFTB0	norbornadiene	dftb+	total energy ha	blocked
DFTB0	norbornadiene	dftb+	total energy ha	blocked
DFTB0	norbornadiene	dftb+	total energy ha	blocked
DFTB0	p-benzoquinone	dftb+	total energy ha	blocked
DFTB0	p-benzoquinone	dftb+	total energy ha	blocked
DFTB0	ph3	dftb+	total energy ha	blocked
DFTB0	ph3	dftb+	total energy ha	blocked
DFTB0	ph3	dftb+	total energy ha	blocked
DFTB0	propanamide	dftb+	total energy ha	blocked
DFTB0	propanamide	dftb+	total energy ha	blocked
DFTB0	pyridazine	dftb+	total energy ha	blocked
DFTB0	pyridazine	dftb+	total energy ha	blocked
DFTB0	pyridine	dftb+	total energy ha	blocked
DFTB0	pyridine	dftb+	total energy ha	blocked
DFTB0	pyrimidine	dftb+	total energy ha	blocked
DFTB0	pyrimidine	dftb+	total energy ha	blocked
DFTB0	pyrrole	dftb+	total energy ha	blocked
DFTB0	pyrrole	dftb+	total energy ha	blocked
DFTB0	s22-ammonia-dimer	dftb+	total energy ha	blocked
DFTB0	s22-ammonia-dimer	dftb+	total energy ha	blocked
DFTB0	s22-ammonia-dimer	dftb+	total energy ha	blocked
DFTB0	s22-benzene-methane	dftb+	total energy ha	blocked
DFTB0	s22-benzene-methane	dftb+	total energy ha	blocked
DFTB0	s22-benzene-methane	dftb+	total energy ha	blocked
DFTB0	s22-benzene-water	dftb+	total energy ha	blocked
DFTB0	s22-benzene-water	dftb+	total energy ha	blocked
DFTB0	s22-ethene-dimer	dftb+	total energy ha	blocked
DFTB0	s22-ethene-dimer	dftb+	total energy ha	blocked
DFTB0	s22-ethene-dimer	dftb+	total energy ha	blocked
DFTB0	s22-formamide-dimer	dftb+	total energy ha	blocked
DFTB0	s22-formamide-dimer	dftb+	total energy ha	blocked
DFTB0	s22-formamide-dimer	dftb+	total energy ha	blocked
DFTB0	s22-formamide-dimer	dftb+	total energy ha	blocked
DFTB0	s22-formic-acid-dimer	dftb+	total energy ha	blocked
DFTB0	s22-formic-acid-dimer	dftb+	total energy ha	blocked
DFTB0	s22-methane-dimer	dftb+	total energy ha	blocked
DFTB0	s22-methane-dimer	dftb+	total energy ha	blocked
DFTB0	s22-methane-dimer	dftb+	total energy ha	blocked
DFTB0	s22-water-dimer	dftb+	total energy ha	blocked
DFTB0	s22-water-dimer	dftb+	total energy ha	blocked
DFTB0	s22-water-dimer	dftb+	total energy ha	blocked
DFTB0	sih4	dftb+	total energy ha	blocked
DFTB0	sih4	dftb+	total energy ha	blocked
DFTB0	sih4	dftb+	total energy ha	blocked
DFTB0	tetrazine	dftb+	total energy ha	blocked
DFTB0	tetrazine	dftb+	total energy ha	blocked
DFTB0	thymine	dftb+	total energy ha	blocked
DFTB0	thymine	dftb+	total energy ha	blocked
DFTB0	triazine	dftb+	total energy ha	blocked
DFTB0	triazine	dftb+	total energy ha	blocked
GFN2-XTB	acetamide	xtb	total energy ha	blocked
GFN2-XTB	acetamide	xtb	total energy ha	blocked
GFN2-XTB	acetamide	xtb	total energy ha	blocked
GFN2-XTB	acetone	xtb	total energy ha	blocked

Table S21, continued.

Method	System / basis	Ref.	Quantity	|Δ|
GFN2-XTB	acetone	xtb	total energy ha	blocked
GFN2-XTB	adenine	xtb	total energy ha	blocked
GFN2-XTB	adenine	xtb	total energy ha	blocked
GFN2-XTB	adenine	xtb	total energy ha	blocked
GFN2-XTB	benzene	xtb	total energy ha	blocked
GFN2-XTB	benzene	xtb	total energy ha	blocked
GFN2-XTB	butadiene	xtb	total energy ha	blocked
GFN2-XTB	butadiene	xtb	total energy ha	blocked
GFN2-XTB	butadiene	xtb	total energy ha	blocked
GFN2-XTB	c2h4	xtb	total energy ha	blocked
GFN2-XTB	c2h4	xtb	total energy ha	blocked
GFN2-XTB	ch2o	xtb	total energy ha	blocked
GFN2-XTB	ch2o	xtb	total energy ha	blocked
GFN2-XTB	ch2o	xtb	total energy ha	blocked
GFN2-XTB	ch3oh	xtb	total energy ha	blocked
GFN2-XTB	ch3oh	xtb	total energy ha	blocked
GFN2-XTB	ch3oh	xtb	total energy ha	blocked
GFN2-XTB	ch4	xtb	total energy ha	blocked
GFN2-XTB	ch4	xtb	total energy ha	blocked
GFN2-XTB	ch4	xtb	total energy ha	blocked
GFN2-XTB	co2	xtb	total energy ha	blocked
GFN2-XTB	co2	xtb	total energy ha	blocked
GFN2-XTB	co2	xtb	total energy ha	blocked
GFN2-XTB	cyclopropene	xtb	total energy ha	blocked
GFN2-XTB	cyclopropene	xtb	total energy ha	blocked
GFN2-XTB	cytosine	xtb	total energy ha	blocked
GFN2-XTB	cytosine	xtb	total energy ha	blocked
GFN2-XTB	cytosine	xtb	total energy ha	blocked
GFN2-XTB	furan	xtb	total energy ha	blocked
GFN2-XTB	furan	xtb	total energy ha	blocked
GFN2-XTB	h2co	xtb	total energy ha	blocked
GFN2-XTB	h2co	xtb	total energy ha	blocked
GFN2-XTB	h2co	xtb	total energy ha	blocked
GFN2-XTB	h2o	xtb	total energy ha	blocked
GFN2-XTB	h2o	xtb	total energy ha	blocked
GFN2-XTB	h2o	xtb	total energy ha	blocked
GFN2-XTB	h2s	xtb	total energy ha	blocked
GFN2-XTB	h2s	xtb	total energy ha	blocked
GFN2-XTB	h2s	xtb	total energy ha	blocked
GFN2-XTB	hcooh	xtb	total energy ha	blocked
GFN2-XTB	hcooh	xtb	total energy ha	blocked
GFN2-XTB	hcooh	xtb	total energy ha	blocked
GFN2-XTB	hexatriene	xtb	total energy ha	blocked
GFN2-XTB	hexatriene	xtb	total energy ha	blocked
GFN2-XTB	hexatriene	xtb	total energy ha	blocked
GFN2-XTB	imidazole	xtb	total energy ha	blocked
GFN2-XTB	imidazole	xtb	total energy ha	blocked
GFN2-XTB	naphthalene	xtb	total energy ha	blocked
GFN2-XTB	naphthalene	xtb	total energy ha	blocked
GFN2-XTB	naphthalene	xtb	total energy ha	blocked
GFN2-XTB	naphthalene	xtb	total energy ha	blocked
GFN2-XTB	nh3	xtb	total energy ha	blocked
GFN2-XTB	nh3	xtb	total energy ha	blocked
GFN2-XTB	nh3	xtb	total energy ha	blocked
GFN2-XTB	norbornadiene	xtb	total energy ha	blocked
GFN2-XTB	norbornadiene	xtb	total energy ha	blocked
GFN2-XTB	norbornadiene	xtb	total energy ha	blocked
GFN2-XTB	p-benzoquinone	xtb	total energy ha	blocked

Table S21, continued.

Method	System / basis	Ref.	Quantity	|Δ|
GFN2-XTB	p-benzoquinone	xtb	total energy ha	blocked
GFN2-XTB	p-benzoquinone	xtb	total energy ha	blocked
GFN2-XTB	ph3	xtb	total energy ha	blocked
GFN2-XTB	ph3	xtb	total energy ha	blocked
GFN2-XTB	ph3	xtb	total energy ha	blocked
GFN2-XTB	propanamide	xtb	total energy ha	blocked
GFN2-XTB	propanamide	xtb	total energy ha	blocked
GFN2-XTB	pyridazine	xtb	total energy ha	blocked
GFN2-XTB	pyridazine	xtb	total energy ha	blocked
GFN2-XTB	pyridazine	xtb	total energy ha	blocked
GFN2-XTB	pyridine	xtb	total energy ha	blocked
GFN2-XTB	pyridine	xtb	total energy ha	blocked
GFN2-XTB	pyrimidine	xtb	total energy ha	blocked
GFN2-XTB	pyrimidine	xtb	total energy ha	blocked
GFN2-XTB	pyrimidine	xtb	total energy ha	blocked
GFN2-XTB	pyrrole	xtb	total energy ha	blocked
GFN2-XTB	pyrrole	xtb	total energy ha	blocked
GFN2-XTB	s22-ammonia-dimer	xtb	total energy ha	blocked
GFN2-XTB	s22-ammonia-dimer	xtb	total energy ha	blocked
GFN2-XTB	s22-benzene-methane	xtb	total energy ha	blocked
GFN2-XTB	s22-benzene-methane	xtb	total energy ha	blocked
GFN2-XTB	s22-benzene-methane	xtb	total energy ha	blocked
GFN2-XTB	s22-benzene-water	xtb	total energy ha	blocked
GFN2-XTB	s22-benzene-water	xtb	total energy ha	blocked
GFN2-XTB	s22-ethene-dimer	xtb	total energy ha	blocked
GFN2-XTB	s22-ethene-dimer	xtb	total energy ha	blocked
GFN2-XTB	s22-ethene-dimer	xtb	total energy ha	blocked
GFN2-XTB	s22-formamide-dimer	xtb	total energy ha	blocked
GFN2-XTB	s22-formamide-dimer	xtb	total energy ha	blocked
GFN2-XTB	s22-formic-acid-dimer	xtb	total energy ha	blocked
GFN2-XTB	s22-formic-acid-dimer	xtb	total energy ha	blocked
GFN2-XTB	s22-formic-acid-dimer	xtb	total energy ha	blocked
GFN2-XTB	s22-methane-dimer	xtb	total energy ha	blocked
GFN2-XTB	s22-methane-dimer	xtb	total energy ha	blocked
GFN2-XTB	s22-water-dimer	xtb	total energy ha	blocked
GFN2-XTB	s22-water-dimer	xtb	total energy ha	blocked
GFN2-XTB	s22-water-dimer	xtb	total energy ha	blocked
GFN2-XTB	sih4	xtb	total energy ha	blocked
GFN2-XTB	sih4	xtb	total energy ha	blocked
GFN2-XTB	sih4	xtb	total energy ha	blocked
GFN2-XTB	tetrazine	xtb	total energy ha	blocked
GFN2-XTB	tetrazine	xtb	total energy ha	blocked
GFN2-XTB	tetrazine	xtb	total energy ha	blocked
GFN2-XTB	thymine	xtb	total energy ha	blocked
GFN2-XTB	thymine	xtb	total energy ha	blocked
GFN2-XTB	triazine	xtb	total energy ha	blocked
GFN2-XTB	triazine	xtb	total energy ha	blocked
GFN2-XTB	triazine	xtb	total energy ha	blocked
MSINDO	acetamide	bonn-msindo	total energy ha	blocked
MSINDO	acetamide	bonn-msindo	total energy ha	blocked
MSINDO	acetone	bonn-msindo	total energy ha	blocked
MSINDO	acetone	bonn-msindo	total energy ha	blocked
MSINDO	adenine	bonn-msindo	total energy ha	blocked
MSINDO	benzene	bonn-msindo	total energy ha	blocked
MSINDO	benzene	bonn-msindo	total energy ha	blocked
MSINDO	butadiene	bonn-msindo	total energy ha	blocked
MSINDO	butadiene	bonn-msindo	total energy ha	blocked
MSINDO	c2h4	bonn-msindo	total energy ha	blocked

Table S21, continued.

Method	System / basis	Ref.	Quantity	|Δ|
MSINDO	ch2o	bonn-msindo	total energy ha	blocked
MSINDO	ch2o	bonn-msindo	total energy ha	blocked
MSINDO	ch3oh	bonn-msindo	total energy ha	blocked
MSINDO	ch3oh	bonn-msindo	total energy ha	blocked
MSINDO	ch3oh	bonn-msindo	total energy ha	blocked
MSINDO	ch4	bonn-msindo	total energy ha	blocked
MSINDO	ch4	bonn-msindo	total energy ha	blocked
MSINDO	ch4	bonn-msindo	total energy ha	blocked
MSINDO	co2	bonn-msindo	total energy ha	blocked
MSINDO	co2	bonn-msindo	total energy ha	blocked
MSINDO	co2	bonn-msindo	total energy ha	blocked
MSINDO	cyclopropene	bonn-msindo	total energy ha	blocked
MSINDO	cyclopropene	bonn-msindo	total energy ha	blocked
MSINDO	cytosine	bonn-msindo	total energy ha	blocked
MSINDO	furan	bonn-msindo	total energy ha	blocked
MSINDO	furan	bonn-msindo	total energy ha	blocked
MSINDO	h2co	bonn-msindo	total energy ha	blocked
MSINDO	h2co	bonn-msindo	total energy ha	blocked
MSINDO	h2co	bonn-msindo	total energy ha	blocked
MSINDO	h2o	bonn-msindo	total energy ha	blocked
MSINDO	h2o	bonn-msindo	total energy ha	blocked
MSINDO	h2o	bonn-msindo	total energy ha	blocked
MSINDO	h2s	bonn-msindo	total energy ha	blocked
MSINDO	h2s	bonn-msindo	total energy ha	blocked
MSINDO	h2s	bonn-msindo	total energy ha	blocked
MSINDO	hcooh	bonn-msindo	total energy ha	blocked
MSINDO	hcooh	bonn-msindo	total energy ha	blocked
MSINDO	hcooh	bonn-msindo	total energy ha	blocked
MSINDO	hexatriene	bonn-msindo	total energy ha	blocked
MSINDO	hexatriene	bonn-msindo	total energy ha	blocked
MSINDO	imidazole	bonn-msindo	total energy ha	blocked
MSINDO	imidazole	bonn-msindo	total energy ha	blocked
MSINDO	naphthalene	bonn-msindo	total energy ha	blocked
MSINDO	naphthalene	bonn-msindo	total energy ha	blocked
MSINDO	nh3	bonn-msindo	total energy ha	blocked
MSINDO	nh3	bonn-msindo	total energy ha	blocked
MSINDO	nh3	bonn-msindo	total energy ha	blocked
MSINDO	norbornadiene	bonn-msindo	total energy ha	blocked
MSINDO	norbornadiene	bonn-msindo	total energy ha	blocked
MSINDO	p-benzoquinone	bonn-msindo	total energy ha	blocked
MSINDO	ph3	bonn-msindo	total energy ha	blocked
MSINDO	ph3	bonn-msindo	total energy ha	blocked
MSINDO	ph3	bonn-msindo	total energy ha	blocked
MSINDO	propanamide	bonn-msindo	total energy ha	blocked
MSINDO	propanamide	bonn-msindo	total energy ha	blocked
MSINDO	pyridazine	bonn-msindo	total energy ha	blocked
MSINDO	pyridazine	bonn-msindo	total energy ha	blocked
MSINDO	pyridine	bonn-msindo	total energy ha	blocked
MSINDO	pyridine	bonn-msindo	total energy ha	blocked
MSINDO	pyrimidine	bonn-msindo	total energy ha	blocked
MSINDO	pyrimidine	bonn-msindo	total energy ha	blocked
MSINDO	pyrrole	bonn-msindo	total energy ha	blocked
MSINDO	s22-ammonia-dimer	bonn-msindo	total energy ha	blocked
MSINDO	s22-ammonia-dimer	bonn-msindo	total energy ha	blocked
MSINDO	s22-benzene-methane	bonn-msindo	total energy ha	blocked
MSINDO	s22-benzene-methane	bonn-msindo	total energy ha	blocked
MSINDO	s22-benzene-water	bonn-msindo	total energy ha	blocked
MSINDO	s22-benzene-water	bonn-msindo	total energy ha	blocked

Table S21, continued.

Method	System / basis	Ref.	Quantity	|Δ|
MSINDO	s22-ethene-dimer	bonn-msindo	total energy ha	blocked
MSINDO	s22-ethene-dimer	bonn-msindo	total energy ha	blocked
MSINDO	s22-ethene-dimer	bonn-msindo	total energy ha	blocked
MSINDO	s22-formamide-dimer	bonn-msindo	total energy ha	blocked
MSINDO	s22-formamide-dimer	bonn-msindo	total energy ha	blocked
MSINDO	s22-formic-acid-dimer	bonn-msindo	total energy ha	blocked
MSINDO	s22-formic-acid-dimer	bonn-msindo	total energy ha	blocked
MSINDO	s22-methane-dimer	bonn-msindo	total energy ha	blocked
MSINDO	s22-methane-dimer	bonn-msindo	total energy ha	blocked
MSINDO	s22-methane-dimer	bonn-msindo	total energy ha	blocked
MSINDO	s22-water-dimer	bonn-msindo	total energy ha	blocked
MSINDO	s22-water-dimer	bonn-msindo	total energy ha	blocked
MSINDO	sih4	bonn-msindo	total energy ha	blocked
MSINDO	sih4	bonn-msindo	total energy ha	blocked
MSINDO	sih4	bonn-msindo	total energy ha	blocked
MSINDO	tetrazine	bonn-msindo	total energy ha	blocked
MSINDO	tetrazine	bonn-msindo	total energy ha	blocked
MSINDO	thymine	bonn-msindo	total energy ha	blocked
MSINDO	thymine	bonn-msindo	total energy ha	blocked
MSINDO	triazine	bonn-msindo	total energy ha	blocked
MSINDO	triazine	bonn-msindo	total energy ha	blocked
OM2	acetamide	method-specific-not-staged	total energy ha	blocked
OM2	acetamide	method-specific-not-staged	total energy ha	blocked
OM2	acetone	method-specific-not-staged	total energy ha	blocked
OM2	acetone	method-specific-not-staged	total energy ha	blocked
OM2	adenine	method-specific-not-staged	total energy ha	blocked
OM2	benzene	method-specific-not-staged	total energy ha	blocked
OM2	benzene	method-specific-not-staged	total energy ha	blocked
OM2	butadiene	method-specific-not-staged	total energy ha	blocked
OM2	butadiene	method-specific-not-staged	total energy ha	blocked
OM2	c2h4	method-specific-not-staged	total energy ha	blocked
OM2	c2h4	method-specific-not-staged	total energy ha	blocked
OM2	ch2o	method-specific-not-staged	total energy ha	blocked

Table S21, continued.

Method	System / basis	Ref.	Quantity	|Δ|
OM2	cyclopropene	method-specific-not-staged	total energy ha	blocked
OM2	cyclopropene	method-specific-not-staged	total energy ha	blocked
OM2	cytosine	method-specific-not-staged	total energy ha	blocked
OM2	cytosine	method-specific-not-staged	total energy ha	blocked
OM2	furan	method-specific-not-staged	total energy ha	blocked
OM2	furan	method-specific-not-staged	total energy ha	blocked
OM2	furan	method-specific-not-staged	total energy ha	blocked
OM2	furan	method-specific-not-staged	total energy ha	blocked
OM2	furan	method-specific-not-staged	total energy ha	blocked
OM2	furan	method-specific-not-staged	total energy ha	blocked
OM2	hexatriene	method-specific-not-staged	total energy ha	blocked
OM2	hexatriene	method-specific-not-staged	total energy ha	blocked
OM2	imidazole	method-specific-not-staged	total energy ha	blocked
OM2	imidazole	method-specific-not-staged	total energy ha	blocked
OM2	naphthalene	method-specific-not-staged	total energy ha	blocked
OM2	norbornadiene	method-specific-not-staged	total energy ha	blocked
OM2	norbornadiene	method-specific-not-staged	total energy ha	blocked
OM2	p-benzoquinone	method-specific-not-staged	total energy ha	blocked
OM2	p-benzoquinone	method-specific-not-staged	total energy ha	blocked

Table S21, continued.

Method	System / basis	Ref.	Quantity	|Δ|
OM2	propanamide	method-specific-not-staged	total energy ha	blocked
OM2	pyridazine	method-specific-not-staged	total energy ha	blocked
OM2	pyridazine	method-specific-not-staged	total energy ha	blocked
OM2	pyridine	method-specific-not-staged	total energy ha	blocked
OM2	pyridine	method-specific-not-staged	total energy ha	blocked
OM2	pyrimidine	method-specific-not-staged	total energy ha	blocked
OM2	pyrrole	method-specific-not-staged	total energy ha	blocked
OM2	pyrrole	method-specific-not-staged	total energy ha	blocked
OM2	s22-ammonia-dimer	method-specific-not-staged	total energy ha	blocked
OM2	s22-ammonia-dimer	method-specific-not-staged	total energy ha	blocked
OM2	s22-ammonia-dimer	method-specific-not-staged	total energy ha	blocked
OM2	s22-benzene-methane	method-specific-not-staged	total energy ha	blocked
OM2	s22-benzene-methane	method-specific-not-staged	total energy ha	blocked
OM2	s22-benzene-water	method-specific-not-staged	total energy ha	blocked
OM2	s22-benzene-water	method-specific-not-staged	total energy ha	blocked
OM2	s22-ethene-dimer	method-specific-not-staged	total energy ha	blocked
OM2	s22-ethene-dimer	method-specific-not-staged	total energy ha	blocked
OM2	s22-ethene-dimer	method-specific-not-staged	total energy ha	blocked
OM2	s22-formamide-dimer	method-specific-not-staged	total energy ha	blocked

Table S21, continued.

Method	System / basis	Ref.	Quantity	|Δ|
OM2	s22-formamide-dimer	method-specific-not-staged	total energy ha	blocked
OM2	s22-formic-acid-dimer	method-specific-not-staged	total energy ha	blocked
OM2	s22-formic-acid-dimer	method-specific-not-staged	total energy ha	blocked
OM2	s22-methane-dimer	method-specific-not-staged	total energy ha	blocked
OM2	s22-methane-dimer	method-specific-not-staged	total energy ha	blocked
OM2	s22-water-dimer	method-specific-not-staged	total energy ha	blocked
OM2	s22-water-dimer	method-specific-not-staged	total energy ha	blocked
OM2	s22-water-dimer	method-specific-not-staged	total energy ha	blocked
OM2	tetrazine	method-specific-not-staged	total energy ha	blocked
OM2	tetrazine	method-specific-not-staged	total energy ha	blocked
OM2	thymine	method-specific-not-staged	total energy ha	blocked
OM2	thymine	method-specific-not-staged	total energy ha	blocked
OM2	thymine	method-specific-not-staged	total energy ha	blocked
OM2	thymine	method-specific-not-staged	total energy ha	blocked
OM2	thymine	method-specific-not-staged	total energy ha	blocked
OM2	thymine	method-specific-not-staged	total energy ha	blocked
OM2	triazine	method-specific-not-staged	total energy ha	blocked
OM2	triazine	method-specific-not-staged	total energy ha	blocked
OM3	acetamide	method-specific-not-staged	total energy ha	blocked

Table S21, continued.

Method	System / basis	Ref.	Quantity	|Δ|
OM3	acetamide	method-specific-not-staged	total energy ha	blocked
OM3	acetone	method-specific-not-staged	total energy ha	blocked
OM3	acetone	method-specific-not-staged	total energy ha	blocked
OM3	adenine	method-specific-not-staged	total energy ha	blocked
OM3	adenine	method-specific-not-staged	total energy ha	blocked
OM3	adenine	method-specific-not-staged	total energy ha	blocked
OM3	adenine	method-specific-not-staged	total energy ha	blocked
OM3	adenine	method-specific-not-staged	total energy ha	blocked
OM3	adenine	method-specific-not-staged	total energy ha	blocked
OM3	benzene	method-specific-not-staged	total energy ha	blocked
OM3	benzene	method-specific-not-staged	total energy ha	blocked
OM3	butadiene	method-specific-not-staged	total energy ha	blocked
OM3	butadiene	method-specific-not-staged	total energy ha	blocked
OM3	c2h4	method-specific-not-staged	total energy ha	blocked
OM3	ch2o	method-specific-not-staged	total energy ha	blocked
OM3	ch2o	method-specific-not-staged	total energy ha	blocked
OM3	cyclopropene	method-specific-not-staged	total energy ha	blocked
OM3	cyclopropene	method-specific-not-staged	total energy ha	blocked
OM3	cytosine	method-specific-not-staged	total energy ha	blocked

Table S21, continued.

Method	System / basis	Ref.	Quantity	|Δ|
OM3	furan	method-specific-not-staged	total energy ha	blocked
OM3	furan	method-specific-not-staged	total energy ha	blocked
OM3	hexatriene	method-specific-not-staged	total energy ha	blocked
OM3	hexatriene	method-specific-not-staged	total energy ha	blocked
OM3	imidazole	method-specific-not-staged	total energy ha	blocked
OM3	imidazole	method-specific-not-staged	total energy ha	blocked
OM3	imidazole	method-specific-not-staged	total energy ha	blocked
OM3	naphthalene	method-specific-not-staged	total energy ha	blocked
OM3	naphthalene	method-specific-not-staged	total energy ha	blocked
OM3	norbornadiene	method-specific-not-staged	total energy ha	blocked
OM3	norbornadiene	method-specific-not-staged	total energy ha	blocked
OM3	p-benzoquinone	method-specific-not-staged	total energy ha	blocked
OM3	propanamide	method-specific-not-staged	total energy ha	blocked
OM3	propanamide	method-specific-not-staged	total energy ha	blocked
OM3	pyridazine	method-specific-not-staged	total energy ha	blocked
OM3	pyridazine	method-specific-not-staged	total energy ha	blocked
OM3	pyridine	method-specific-not-staged	total energy ha	blocked
OM3	pyrimidine	method-specific-not-staged	total energy ha	blocked
OM3	pyrimidine	method-specific-not-staged	total energy ha	blocked

Table S21, continued.

Method	System / basis	Ref.	Quantity	|Δ|
OM3	pyrrole	method-specific-not-staged	total energy ha	blocked
OM3	pyrrole	method-specific-not-staged	total energy ha	blocked
OM3	pyrrole	method-specific-not-staged	total energy ha	blocked
OM3	pyrrole	method-specific-not-staged	total energy ha	blocked
OM3	pyrrole	method-specific-not-staged	total energy ha	blocked
OM3	pyrrole	method-specific-not-staged	total energy ha	blocked
OM3	pyrrole	method-specific-not-staged	total energy ha	blocked
OM3	s22-ammonia-dimer	method-specific-not-staged	total energy ha	blocked
OM3	s22-ammonia-dimer	method-specific-not-staged	total energy ha	blocked
OM3	s22-ammonia-dimer	method-specific-not-staged	total energy ha	blocked
OM3	s22-benzene-methane	method-specific-not-staged	total energy ha	blocked
OM3	s22-benzene-methane	method-specific-not-staged	total energy ha	blocked
OM3	s22-benzene-water	method-specific-not-staged	total energy ha	blocked
OM3	s22-benzene-water	method-specific-not-staged	total energy ha	blocked
OM3	s22-ethene-dimer	method-specific-not-staged	total energy ha	blocked
OM3	s22-ethene-dimer	method-specific-not-staged	total energy ha	blocked
OM3	s22-formamide-dimer	method-specific-not-staged	total energy ha	blocked
OM3	s22-formamide-dimer	method-specific-not-staged	total energy ha	blocked
OM3	s22-formic-acid-dimer	method-specific-not-staged	total energy ha	blocked

Table S21, continued.

Method	System / basis	Ref.	Quantity	|Δ|
OM3	s22-formic-acid-dimer	method-specific-not-staged	total energy ha	blocked
OM3	s22-methane-dimer	method-specific-not-staged	total energy ha	blocked
OM3	s22-methane-dimer	method-specific-not-staged	total energy ha	blocked
OM3	s22-methane-dimer	method-specific-not-staged	total energy ha	blocked
OM3	s22-water-dimer	method-specific-not-staged	total energy ha	blocked
OM3	s22-water-dimer	method-specific-not-staged	total energy ha	blocked
OM3	tetrazine	method-specific-not-staged	total energy ha	blocked
OM3	thymine	method-specific-not-staged	total energy ha	blocked
OM3	thymine	method-specific-not-staged	total energy ha	blocked
OM3	triazine	method-specific-not-staged	total energy ha	blocked
OM3	triazine	method-specific-not-staged	total energy ha	blocked
PM6	acetamide	mopac	total energy ha	blocked
PM6	acetamide	mopac	total energy ha	blocked
PM6	acetone	mopac	total energy ha	blocked
PM6	adenine	mopac	total energy ha	blocked
PM6	adenine	mopac	total energy ha	blocked
PM6	adenine	mopac	total energy ha	blocked
PM6	adenine	mopac	total energy ha	blocked
PM6	adenine	mopac	total energy ha	blocked
PM6	adenine	mopac	total energy ha	blocked
PM6	adenine	mopac	total energy ha	blocked
PM6	benzene	mopac	total energy ha	blocked
PM6	benzene	mopac	total energy ha	blocked
PM6	butadiene	mopac	total energy ha	blocked
PM6	butadiene	mopac	total energy ha	blocked
PM6	c2h4	mopac	total energy ha	blocked
PM6	ch2o	mopac	total energy ha	blocked
PM6	ch2o	mopac	total energy ha	blocked
PM6	ch3oh	mopac	total energy ha	blocked
PM6	ch3oh	mopac	total energy ha	blocked
PM6	ch3oh	mopac	total energy ha	blocked
PM6	ch3oh	mopac	total energy ha	blocked
PM6	ch4	mopac	total energy ha	blocked
PM6	ch4	mopac	total energy ha	blocked
PM6	ch4	mopac	total energy ha	blocked
PM6	ch4	mopac	total energy ha	blocked

Table S21, continued.

Method	System / basis	Ref.	Quantity	|Δ|
PM6	co2	mopac	total energy ha	blocked
PM6	co2	mopac	total energy ha	blocked
PM6	co2	mopac	total energy ha	blocked
PM6	co2	mopac	total energy ha	blocked
PM6	cyclopropene	mopac	total energy ha	blocked
PM6	cyclopropene	mopac	total energy ha	blocked
PM6	cytosine	mopac	total energy ha	blocked
PM6	furan	mopac	total energy ha	blocked
PM6	furan	mopac	total energy ha	blocked
PM6	h2co	mopac	total energy ha	blocked
PM6	h2co	mopac	total energy ha	blocked
PM6	h2co	mopac	total energy ha	blocked
PM6	h2co	mopac	total energy ha	blocked
PM6	h2o	mopac	total energy ha	blocked
PM6	h2o	mopac	total energy ha	blocked
PM6	h2o	mopac	total energy ha	blocked
PM6	h2o	mopac	total energy ha	blocked
PM6	h2s	mopac	total energy ha	blocked
PM6	h2s	mopac	total energy ha	blocked
PM6	h2s	mopac	total energy ha	blocked
PM6	h2s	mopac	total energy ha	blocked
PM6	hcooh	mopac	total energy ha	blocked
PM6	hcooh	mopac	total energy ha	blocked
PM6	hcooh	mopac	total energy ha	blocked
PM6	hcooh	mopac	total energy ha	blocked
PM6	hcooh	mopac	total energy ha	blocked
PM6	hcooh	mopac	total energy ha	blocked
PM6	hcooh	mopac	total energy ha	blocked
PM6	hcooh	mopac	total energy ha	blocked
PM6	hcooh	mopac	total energy ha	blocked
PM6	hcooh	mopac	total energy ha	blocked
PM6	hcooh	mopac	total energy ha	blocked
PM6	hcooh	mopac	total energy ha	blocked
PM6	hexatriene	mopac	total energy ha	blocked
PM6	hexatriene	mopac	total energy ha	blocked
PM6	imidazole	mopac	total energy ha	blocked
PM6	naphthalene	mopac	total energy ha	blocked
PM6	naphthalene	mopac	total energy ha	blocked
PM6	nh3	mopac	total energy ha	blocked
PM6	nh3	mopac	total energy ha	blocked
PM6	nh3	mopac	total energy ha	blocked
PM6	nh3	mopac	total energy ha	blocked
PM6	norbornadiene	mopac	total energy ha	blocked
PM6	norbornadiene	mopac	total energy ha	blocked
PM6	p-benzoquinone	mopac	total energy ha	blocked
PM6	ph3	mopac	total energy ha	blocked
PM6	ph3	mopac	total energy ha	blocked
PM6	ph3	mopac	total energy ha	blocked
PM6	ph3	mopac	total energy ha	blocked
PM6	propanamide	mopac	total energy ha	blocked
PM6	propanamide	mopac	total energy ha	blocked
PM6	pyridazine	mopac	total energy ha	blocked
PM6	pyridazine	mopac	total energy ha	blocked
PM6	pyridine	mopac	total energy ha	blocked
PM6	pyrimidine	mopac	total energy ha	blocked
PM6	pyrimidine	mopac	total energy ha	blocked
PM6	pyrrole	mopac	total energy ha	blocked
PM6	pyrrole	mopac	total energy ha	blocked

Table S21, continued.

Method	System / basis	Ref.	Quantity	|Δ|
PM6	s22-ammonia-dimer	mopac	total energy ha	blocked
PM6	s22-ammonia-dimer	mopac	total energy ha	blocked
PM6	s22-benzene-methane	mopac	total energy ha	blocked
PM6	s22-benzene-methane	mopac	total energy ha	blocked
PM6	s22-benzene-water	mopac	total energy ha	blocked
PM6	s22-benzene-water	mopac	total energy ha	blocked
PM6	s22-ethene-dimer	mopac	total energy ha	blocked
PM6	s22-ethene-dimer	mopac	total energy ha	blocked
PM6	s22-formamide-dimer	mopac	total energy ha	blocked
PM6	s22-formamide-dimer	mopac	total energy ha	blocked
PM6	s22-formic-acid-dimer	mopac	total energy ha	blocked
PM6	s22-formic-acid-dimer	mopac	total energy ha	blocked
PM6	s22-methane-dimer	mopac	total energy ha	blocked
PM6	s22-methane-dimer	mopac	total energy ha	blocked
PM6	s22-water-dimer	mopac	total energy ha	blocked
PM6	s22-water-dimer	mopac	total energy ha	blocked
PM6	sih4	mopac	total energy ha	blocked
PM6	sih4	mopac	total energy ha	blocked
PM6	sih4	mopac	total energy ha	blocked
PM6	sih4	mopac	total energy ha	blocked
PM6	tetrazine	mopac	total energy ha	blocked
PM6	thymine	mopac	total energy ha	blocked
PM6	thymine	mopac	total energy ha	blocked
PM6	triazine	mopac	total energy ha	blocked
PM6	triazine	mopac	total energy ha	blocked
SCC-DFTB	acetamide	dftb+	total energy ha	blocked
SCC-DFTB	acetamide	dftb+	total energy ha	blocked
SCC-DFTB	acetamide	dftb+	total energy ha	blocked
SCC-DFTB	acetamide	dftb+	total energy ha	blocked
SCC-DFTB	acetamide	dftb+	total energy ha	blocked
SCC-DFTB	acetamide	dftb+	total energy ha	blocked
SCC-DFTB	acetone	dftb+	total energy ha	blocked
SCC-DFTB	acetone	dftb+	total energy ha	blocked
SCC-DFTB	acetone	dftb+	total energy ha	blocked
SCC-DFTB	acetone	dftb+	total energy ha	blocked
SCC-DFTB	acetone	dftb+	total energy ha	blocked
SCC-DFTB	acetone	dftb+	total energy ha	blocked
SCC-DFTB	acetone	dftb+	total energy ha	blocked
SCC-DFTB	adenine	dftb+	total energy ha	blocked
SCC-DFTB	adenine	dftb+	total energy ha	blocked
SCC-DFTB	benzene	dftb+	total energy ha	blocked
SCC-DFTB	benzene	dftb+	total energy ha	blocked
SCC-DFTB	butadiene	dftb+	total energy ha	blocked
SCC-DFTB	butadiene	dftb+	total energy ha	blocked
SCC-DFTB	c2h4	dftb+	total energy ha	blocked
SCC-DFTB	ch2o	dftb+	total energy ha	blocked
SCC-DFTB	ch2o	dftb+	total energy ha	blocked
SCC-DFTB	ch2o	dftb+	total energy ha	blocked
SCC-DFTB	ch2o	dftb+	total energy ha	blocked
SCC-DFTB	ch2o	dftb+	total energy ha	blocked
SCC-DFTB	ch2o	dftb+	total energy ha	blocked
SCC-DFTB	ch2o	dftb+	total energy ha	blocked
SCC-DFTB	ch3oh	dftb+	total energy ha	blocked
SCC-DFTB	ch3oh	dftb+	total energy ha	blocked
SCC-DFTB	ch3oh	dftb+	total energy ha	blocked
SCC-DFTB	ch3oh	dftb+	total energy ha	blocked
SCC-DFTB	ch3oh	dftb+	total energy ha	blocked
SCC-DFTB	ch3oh	dftb+	total energy ha	blocked

Table S21, continued.

Method	System / basis	Ref.	Quantity	|Δ|
SCC-DFTB	ch3oh	dftb+	total energy ha	blocked
SCC-DFTB	ch3oh	dftb+	total energy ha	blocked
SCC-DFTB	ch3oh	dftb+	total energy ha	blocked
SCC-DFTB	ch3oh	dftb+	total energy ha	blocked
SCC-DFTB	ch3oh	dftb+	total energy ha	blocked
SCC-DFTB	ch3oh	dftb+	total energy ha	blocked
SCC-DFTB	ch4	dftb+	total energy ha	blocked
SCC-DFTB	ch4	dftb+	total energy ha	blocked
SCC-DFTB	ch4	dftb+	total energy ha	blocked
SCC-DFTB	co2	dftb+	total energy ha	blocked
SCC-DFTB	co2	dftb+	total energy ha	blocked
SCC-DFTB	co2	dftb+	total energy ha	blocked
SCC-DFTB	co2	dftb+	total energy ha	blocked
SCC-DFTB	co2	dftb+	total energy ha	blocked
SCC-DFTB	co2	dftb+	total energy ha	blocked
SCC-DFTB	co2	dftb+	total energy ha	blocked
SCC-DFTB	co2	dftb+	total energy ha	blocked
SCC-DFTB	co2	dftb+	total energy ha	blocked
SCC-DFTB	co2	dftb+	total energy ha	blocked
SCC-DFTB	co2	dftb+	total energy ha	blocked
SCC-DFTB	co2	dftb+	total energy ha	blocked
SCC-DFTB	cyclopropene	dftb+	total energy ha	blocked
SCC-DFTB	cyclopropene	dftb+	total energy ha	blocked
SCC-DFTB	cytosine	dftb+	total energy ha	blocked
SCC-DFTB	cytosine	dftb+	total energy ha	blocked
SCC-DFTB	cytosine	dftb+	total energy ha	blocked
SCC-DFTB	cytosine	dftb+	total energy ha	blocked
SCC-DFTB	cytosine	dftb+	total energy ha	blocked
SCC-DFTB	cytosine	dftb+	total energy ha	blocked
SCC-DFTB	furan	dftb+	total energy ha	blocked
SCC-DFTB	furan	dftb+	total energy ha	blocked
SCC-DFTB	furan	dftb+	total energy ha	blocked
SCC-DFTB	furan	dftb+	total energy ha	blocked
SCC-DFTB	furan	dftb+	total energy ha	blocked
SCC-DFTB	furan	dftb+	total energy ha	blocked
SCC-DFTB	furan	dftb+	total energy ha	blocked
SCC-DFTB	h2co	dftb+	total energy ha	blocked
SCC-DFTB	h2co	dftb+	total energy ha	blocked
SCC-DFTB	h2co	dftb+	total energy ha	blocked
SCC-DFTB	h2co	dftb+	total energy ha	blocked
SCC-DFTB	h2co	dftb+	total energy ha	blocked
SCC-DFTB	h2co	dftb+	total energy ha	blocked
SCC-DFTB	h2co	dftb+	total energy ha	blocked
SCC-DFTB	h2co	dftb+	total energy ha	blocked
SCC-DFTB	h2co	dftb+	total energy ha	blocked
SCC-DFTB	h2co	dftb+	total energy ha	blocked
SCC-DFTB	h2co	dftb+	total energy ha	blocked
SCC-DFTB	h2o	dftb+	total energy ha	blocked
SCC-DFTB	h2o	dftb+	total energy ha	blocked
SCC-DFTB	h2o	dftb+	total energy ha	blocked
SCC-DFTB	h2s	dftb+	total energy ha	blocked
SCC-DFTB	h2s	dftb+	total energy ha	blocked
SCC-DFTB	h2s	dftb+	total energy ha	blocked
SCC-DFTB	hcooh	dftb+	total energy ha	blocked
SCC-DFTB	hcooh	dftb+	total energy ha	blocked
SCC-DFTB	hcooh	dftb+	total energy ha	blocked
SCC-DFTB	hcooh	dftb+	total energy ha	blocked

Table S21, continued.

Method	System / basis	Ref.	Quantity	|Δ|
SCC-DFTB	hcooh	dftb+	total energy ha	blocked
SCC-DFTB	hcooh	dftb+	total energy ha	blocked
SCC-DFTB	hcooh	dftb+	total energy ha	blocked
SCC-DFTB	hcooh	dftb+	total energy ha	blocked
SCC-DFTB	hcooh	dftb+	total energy ha	blocked
SCC-DFTB	hcooh	dftb+	total energy ha	blocked
SCC-DFTB	hcooh	dftb+	total energy ha	blocked
SCC-DFTB	hcooh	dftb+	total energy ha	blocked
SCC-DFTB	hexatriene	dftb+	total energy ha	blocked
SCC-DFTB	hexatriene	dftb+	total energy ha	blocked
SCC-DFTB	imidazole	dftb+	total energy ha	blocked
SCC-DFTB	imidazole	dftb+	total energy ha	blocked
SCC-DFTB	imidazole	dftb+	total energy ha	blocked
SCC-DFTB	imidazole	dftb+	total energy ha	blocked
SCC-DFTB	imidazole	dftb+	total energy ha	blocked
SCC-DFTB	imidazole	dftb+	total energy ha	blocked
SCC-DFTB	imidazole	dftb+	total energy ha	blocked
SCC-DFTB	naphthalene	dftb+	total energy ha	blocked
SCC-DFTB	naphthalene	dftb+	total energy ha	blocked
SCC-DFTB	nh3	dftb+	total energy ha	blocked
SCC-DFTB	nh3	dftb+	total energy ha	blocked
SCC-DFTB	nh3	dftb+	total energy ha	blocked
SCC-DFTB	norbornadiene	dftb+	total energy ha	blocked
SCC-DFTB	norbornadiene	dftb+	total energy ha	blocked
SCC-DFTB	p-benzoquinone	dftb+	total energy ha	blocked
SCC-DFTB	p-benzoquinone	dftb+	total energy ha	blocked
SCC-DFTB	ph3	dftb+	total energy ha	blocked
SCC-DFTB	ph3	dftb+	total energy ha	blocked
SCC-DFTB	ph3	dftb+	total energy ha	blocked
SCC-DFTB	propanamide	dftb+	total energy ha	blocked
SCC-DFTB	propanamide	dftb+	total energy ha	blocked
SCC-DFTB	pyridazine	dftb+	total energy ha	blocked
SCC-DFTB	pyridazine	dftb+	total energy ha	blocked
SCC-DFTB	pyridine	dftb+	total energy ha	blocked
SCC-DFTB	pyridine	dftb+	total energy ha	blocked
SCC-DFTB	pyridine	dftb+	total energy ha	blocked
SCC-DFTB	pyridine	dftb+	total energy ha	blocked
SCC-DFTB	pyridine	dftb+	total energy ha	blocked
SCC-DFTB	pyridine	dftb+	total energy ha	blocked
SCC-DFTB	pyrimidine	dftb+	total energy ha	blocked
SCC-DFTB	pyrimidine	dftb+	total energy ha	blocked
SCC-DFTB	pyrimidine	dftb+	total energy ha	blocked
SCC-DFTB	pyrimidine	dftb+	total energy ha	blocked
SCC-DFTB	pyrimidine	dftb+	total energy ha	blocked
SCC-DFTB	pyrimidine	dftb+	total energy ha	blocked
SCC-DFTB	pyrimidine	dftb+	total energy ha	blocked
SCC-DFTB	pyrrole	dftb+	total energy ha	blocked
SCC-DFTB	pyrrole	dftb+	total energy ha	blocked
SCC-DFTB	pyrrole	dftb+	total energy ha	blocked
SCC-DFTB	pyrrole	dftb+	total energy ha	blocked
SCC-DFTB	pyrrole	dftb+	total energy ha	blocked
SCC-DFTB	pyrrole	dftb+	total energy ha	blocked
SCC-DFTB	pyrrole	dftb+	total energy ha	blocked
SCC-DFTB	s22-ammonia-dimer	dftb+	total energy ha	blocked
SCC-DFTB	s22-ammonia-dimer	dftb+	total energy ha	blocked
SCC-DFTB	s22-benzene-methane	dftb+	total energy ha	blocked
SCC-DFTB	s22-benzene-methane	dftb+	total energy ha	blocked
SCC-DFTB	s22-benzene-water	dftb+	total energy ha	blocked

Table S21, continued.

Method	System / basis	Ref.	Quantity	|Δ|
SCC-DFTB	s22-benzene-water	dftb+	total energy ha	blocked
SCC-DFTB	s22-ethene-dimer	dftb+	total energy ha	blocked
SCC-DFTB	s22-ethene-dimer	dftb+	total energy ha	blocked
SCC-DFTB	s22-formamide-dimer	dftb+	total energy ha	blocked
SCC-DFTB	s22-formamide-dimer	dftb+	total energy ha	blocked
SCC-DFTB	s22-formic-acid-dimer	dftb+	total energy ha	blocked
SCC-DFTB	s22-formic-acid-dimer	dftb+	total energy ha	blocked
SCC-DFTB	s22-methane-dimer	dftb+	total energy ha	blocked
SCC-DFTB	s22-methane-dimer	dftb+	total energy ha	blocked
SCC-DFTB	s22-water-dimer	dftb+	total energy ha	blocked
SCC-DFTB	s22-water-dimer	dftb+	total energy ha	blocked
SCC-DFTB	sih4	dftb+	total energy ha	blocked
SCC-DFTB	sih4	dftb+	total energy ha	blocked
SCC-DFTB	sih4	dftb+	total energy ha	blocked
SCC-DFTB	sih4	dftb+	total energy ha	blocked
SCC-DFTB	sih4	dftb+	total energy ha	blocked
SCC-DFTB	sih4	dftb+	total energy ha	blocked
SCC-DFTB	sih4	dftb+	total energy ha	blocked
SCC-DFTB	sih4	dftb+	total energy ha	blocked
SCC-DFTB	sih4	dftb+	total energy ha	blocked
SCC-DFTB	sih4	dftb+	total energy ha	blocked
SCC-DFTB	sih4	dftb+	total energy ha	blocked
SCC-DFTB	tetrazine	dftb+	total energy ha	blocked
SCC-DFTB	tetrazine	dftb+	total energy ha	blocked
SCC-DFTB	thymine	dftb+	total energy ha	blocked
SCC-DFTB	thymine	dftb+	total energy ha	blocked
SCC-DFTB	triazine	dftb+	total energy ha	blocked
SCC-DFTB	triazine	dftb+	total energy ha	blocked
SCC-DFTB	triazine	dftb+	total energy ha	blocked
SCC-DFTB	triazine	dftb+	total energy ha	blocked
SCC-DFTB	triazine	dftb+	total energy ha	blocked
SCC-DFTB	triazine	dftb+	total energy ha	blocked
Machine-learning potentials				
4 artifact-incomplete, 1 blocked.				
MACE	h2o	mace	total energy ha	artifact-incomplete
MACE	h2o	mace	total energy ha	artifact-incomplete
MACE	h2o	mace	total energy ha	artifact-incomplete
MACE	h2o	mace	total energy ha	artifact-incomplete
MACE	h2o	mace	total energy ha	blocked
Other				
483 pass, 14 pass-pending-tolerance, 1 held, 11 fail, 9 recorded-no-tolerance-class, 1 reference-missing, 1 blocked-reference-leg. Median $\|\Delta E\|$ 8.9×10^{-3}, max 3.5×10^{-2} E_h.				
see case id	bh9_01_33_bhfwd_rks_uks_pbe_def2qzvpp		barrier height forward kcal mol	5.46×10^{-3}
see case id	bh9_01_33_bhrev_rks_uks_pbe_def2qzvpp		barrier height reverse kcal mol	7.29×10^{-3}
see case id	bh9_01_33_re_rks_uks_pbe_def2qzvpp		reaction energy kcal mol	1.83×10^{-3}
see case id	bh9_01_34_bhfwd_rks_uks_pbe_def2qzvpp		barrier height forward kcal mol	1.13×10^{-2}
see case id	bh9_01_34_bhrev_rks_uks_pbe_def2qzvpp		barrier height reverse kcal mol	7.21×10^{-3}
see case id	bh9_01_34_re_rks_uks_pbe_def2qzvpp		reaction energy kcal mol	4.07×10^{-3}

Table S21, continued.

Method	System / basis	Ref.	Quantity	$\lvert\Delta\rvert$
see case id	bh9_01_35_bhfwd_rks_uks_pbe_def2qzvpp		barrier height forward kcal mol	4.27×10^{-3}
see case id	bh9_01_35_bhrev_rks_uks_pbe_def2qzvpp		barrier height reverse kcal mol	7.62×10^{-3}
see case id	bh9_01_35_re_rks_uks_pbe_def2qzvpp		reaction energy kcal mol	3.35×10^{-3}
see case id	bh9_01_36_bhfwd_rks_uks_pbe_def2qzvpp		barrier height forward kcal mol	4.00×10^{-3}
see case id	bh9_01_36_bhrev_rks_uks_pbe_def2qzvpp		barrier height reverse kcal mol	9.02×10^{-3}
see case id	bh9_01_36_re_rks_uks_pbe_def2qzvpp		reaction energy kcal mol	5.02×10^{-3}
see case id	bh9_01_44_bhfwd_rks_uks_pbe_def2qzvpp		barrier height forward kcal mol	4.70×10^{-3}
see case id	bh9_01_44_bhrev_rks_uks_pbe_def2qzvpp		barrier height reverse kcal mol	1.19×10^{-2}
see case id	bh9_01_44_re_rks_uks_pbe_def2qzvpp		reaction energy kcal mol	7.16×10^{-3}
see case id	bh9_01_45_re_rks_uks_pbe_def2qzvpp		reaction energy kcal mol	1.25×10^{-4}
see case id	bh9_01_46_bhfwd_rks_uks_pbe_def2qzvpp		barrier height forward kcal mol	3.54×10^{-3}
see case id	bh9_01_46_bhrev_rks_uks_pbe_def2qzvpp		barrier height reverse kcal mol	1.02×10^{-2}
see case id	bh9_01_46_re_rks_uks_pbe_def2qzvpp		reaction energy kcal mol	6.68×10^{-3}
see case id	bh9_01_47_bhfwd_rks_uks_pbe_def2qzvpp		barrier height forward kcal mol	3.50×10^{-3}
see case id	bh9_02_100_bhfwd_rks_uks_pbe_def2qzvpp		barrier height forward kcal mol	8.23×10^{-3}
see case id	bh9_02_100_bhrev_rks_uks_pbe_def2qzvpp		barrier height reverse kcal mol	6.77×10^{-3}
see case id	bh9_02_100_re_rks_uks_pbe_def2qzvpp		reaction energy kcal mol	1.46×10^{-3}
see case id	bh9_02_101_bhfwd_rks_uks_pbe_def2qzvpp		barrier height forward kcal mol	7.23×10^{-3}
see case id	bh9_02_101_bhrev_rks_uks_pbe_def2qzvpp		barrier height reverse kcal mol	7.07×10^{-3}
see case id	bh9_02_101_re_rks_uks_pbe_def2qzvpp		reaction energy kcal mol	1.59×10^{-4}
see case id	bh9_02_102_bhfwd_rks_uks_pbe_def2qzvpp		barrier height forward kcal mol	8.68×10^{-3}
see case id	bh9_02_102_bhrev_rks_uks_pbe_def2qzvpp		barrier height reverse kcal mol	8.07×10^{-3}
see case id	bh9_02_102_re_rks_uks_pbe_def2qzvpp		reaction energy kcal mol	6.11×10^{-4}
see case id	bh9_02_103_bhfwd_rks_uks_pbe_def2qzvpp		barrier height forward kcal mol	6.76×10^{-3}
see case id	bh9_02_103_bhrev_rks_uks_pbe_def2qzvpp		barrier height reverse kcal mol	7.65×10^{-3}
see case id	bh9_02_103_re_rks_uks_pbe_def2qzvpp		reaction energy kcal mol	8.85×10^{-4}
see case id	bh9_02_10_bhfwd_rks_uks_pbe_def2qzvpp		barrier height forward kcal mol	2.11×10^{-3}
see case id	bh9_02_10_bhrev_rks_uks_pbe_def2qzvpp		barrier height reverse kcal mol	2.54×10^{-2}
see case id	bh9_02_10_re_rks_uks_pbe_def2qzvpp		reaction energy kcal mol	2.33×10^{-2}

Table S21, continued.

Method	System / basis	Ref.	Quantity	$\lvert\Delta\rvert$
see case id	bh9_02_112_bhrev_rks_uks_pbe_def2qzvpp		barrier height reverse kcal mol	3.21×10^{-2}
see case id	bh9_02_113_bhrev_rks_uks_pbe_def2qzvpp		barrier height reverse kcal mol	3.34×10^{-2}
see case id	bh9_02_114_bhrev_rks_uks_pbe_def2qzvpp		barrier height reverse kcal mol	3.14×10^{-2}
see case id	bh9_02_115_bhrev_rks_uks_pbe_def2qzvpp		barrier height reverse kcal mol	3.08×10^{-2}
see case id	bh9_02_116_bhrev_rks_uks_pbe_def2qzvpp		barrier height reverse kcal mol	3.24×10^{-2}
see case id	bh9_02_117_bhfwd_rks_uks_pbe_def2qzvpp		barrier height forward kcal mol	3.54×10^{-3}
see case id	bh9_02_117_bhrev_rks_uks_pbe_def2qzvpp		barrier height reverse kcal mol	2.64×10^{-2}
see case id	bh9_02_117_re_rks_uks_pbe_def2qzvpp		reaction energy kcal mol	2.99×10^{-2}
see case id	bh9_02_118_bhfwd_rks_uks_pbe_def2qzvpp		barrier height forward kcal mol	9.87×10^{-3}
see case id	bh9_02_118_bhrev_rks_uks_pbe_def2qzvpp		barrier height reverse kcal mol	2.78×10^{-2}
see case id	bh9_02_118_re_rks_uks_pbe_def2qzvpp		reaction energy kcal mol	1.79×10^{-2}
see case id	bh9_02_119_bhfwd_rks_uks_pbe_def2qzvpp		barrier height forward kcal mol	8.86×10^{-3}
see case id	bh9_02_119_bhrev_rks_uks_pbe_def2qzvpp		barrier height reverse kcal mol	2.91×10^{-2}
see case id	bh9_02_119_re_rks_uks_pbe_def2qzvpp		reaction energy kcal mol	2.03×10^{-2}
see case id	bh9_02_11_bhfwd_rks_uks_pbe_def2qzvpp		barrier height forward kcal mol	9.90×10^{-4}
see case id	bh9_02_11_bhrev_rks_uks_pbe_def2qzvpp		barrier height reverse kcal mol	2.42×10^{-2}
see case id	bh9_02_11_re_rks_uks_pbe_def2qzvpp		reaction energy kcal mol	2.32×10^{-2}
see case id	bh9_02_120_bhfwd_rks_uks_pbe_def2qzvpp		barrier height forward kcal mol	1.02×10^{-2}
see case id	bh9_02_120_bhrev_rks_uks_pbe_def2qzvpp		barrier height reverse kcal mol	2.86×10^{-2}
see case id	bh9_02_120_re_rks_uks_pbe_def2qzvpp		reaction energy kcal mol	1.84×10^{-2}
see case id	bh9_02_121_bhfwd_rks_uks_pbe_def2qzvpp		barrier height forward kcal mol	1.02×10^{-2}
see case id	bh9_02_121_bhrev_rks_uks_pbe_def2qzvpp		barrier height reverse kcal mol	2.99×10^{-2}
see case id	bh9_02_121_re_rks_uks_pbe_def2qzvpp		reaction energy kcal mol	1.98×10^{-2}
see case id	bh9_02_122_bhfwd_rks_uks_pbe_def2qzvpp		barrier height forward kcal mol	1.47×10^{-2}
see case id	bh9_02_122_bhrev_rks_uks_pbe_def2qzvpp		barrier height reverse kcal mol	3.52×10^{-2}
see case id	bh9_02_122_re_rks_uks_pbe_def2qzvpp		reaction energy kcal mol	2.05×10^{-2}
see case id	bh9_02_123_bhfwd_rks_uks_pbe_def2qzvpp		barrier height forward kcal mol	1.47×10^{-2}
see case id	bh9_02_123_bhrev_rks_uks_pbe_def2qzvpp		barrier height reverse kcal mol	3.04×10^{-2}
see case id	bh9_02_123_re_rks_uks_pbe_def2qzvpp		reaction energy kcal mol	1.57×10^{-2}

Table S21, continued.

Method	System / basis	Ref.	Quantity	$\lvert\Delta\rvert$
see case id	bh9_02_126_bhfwd_rks_uks_pbe_def2qzvpp		barrier height forward kcal mol	1.43×10^{-2}
see case id	bh9_02_126_bhrev_rks_uks_pbe_def2qzvpp		barrier height reverse kcal mol	1.55×10^{-2}
see case id	bh9_02_126_re_rks_uks_pbe_def2qzvpp		reaction energy kcal mol	1.29×10^{-3}
see case id	bh9_02_127_bhfwd_rks_uks_pbe_def2qzvpp		barrier height forward kcal mol	1.52×10^{-2}
see case id	bh9_02_127_bhrev_rks_uks_pbe_def2qzvpp		barrier height reverse kcal mol	1.65×10^{-2}
see case id	bh9_02_127_re_rks_uks_pbe_def2qzvpp		reaction energy kcal mol	1.36×10^{-3}
see case id	bh9_02_129_bhfwd_rks_uks_pbe_def2qzvpp		barrier height forward kcal mol	1.81×10^{-2}
see case id	bh9_02_129_bhrev_rks_uks_pbe_def2qzvpp		barrier height reverse kcal mol	8.67×10^{-3}
see case id	bh9_02_129_re_rks_uks_pbe_def2qzvpp		reaction energy kcal mol	9.43×10^{-3}
see case id	bh9_02_12_bhfwd_rks_uks_pbe_def2qzvpp		barrier height forward kcal mol	4.46×10^{-3}
see case id	bh9_02_12_bhrev_rks_uks_pbe_def2qzvpp		barrier height reverse kcal mol	2.35×10^{-2}
see case id	bh9_02_12_re_rks_uks_pbe_def2qzvpp		reaction energy kcal mol	1.91×10^{-2}
see case id	bh9_02_131_bhfwd_rks_uks_pbe_def2qzvpp		barrier height forward kcal mol	2.01×10^{-2}
see case id	bh9_02_131_bhrev_rks_uks_pbe_def2qzvpp		barrier height reverse kcal mol	6.14×10^{-3}
see case id	bh9_02_131_re_rks_uks_pbe_def2qzvpp		reaction energy kcal mol	1.40×10^{-2}
see case id	bh9_02_132_bhfwd_rks_uks_pbe_def2qzvpp		barrier height forward kcal mol	1.76×10^{-2}
see case id	bh9_02_132_bhrev_rks_uks_pbe_def2qzvpp		barrier height reverse kcal mol	8.18×10^{-3}
see case id	bh9_02_132_re_rks_uks_pbe_def2qzvpp		reaction energy kcal mol	9.42×10^{-3}
see case id	bh9_02_137_bhfwd_rks_uks_pbe_def2qzvpp		barrier height forward kcal mol	1.43×10^{-2}
see case id	bh9_02_137_bhrev_rks_uks_pbe_def2qzvpp		barrier height reverse kcal mol	1.70×10^{-2}
see case id	bh9_02_137_re_rks_uks_pbe_def2qzvpp		reaction energy kcal mol	2.73×10^{-3}
see case id	bh9_02_138_bhfwd_rks_uks_pbe_def2qzvpp		barrier height forward kcal mol	1.56×10^{-2}
see case id	bh9_02_138_bhrev_rks_uks_pbe_def2qzvpp		barrier height reverse kcal mol	1.64×10^{-2}
see case id	bh9_02_138_re_rks_uks_pbe_def2qzvpp		reaction energy kcal mol	7.65×10^{-4}
see case id	bh9_02_13_bhfwd_rks_uks_pbe_def2qzvpp		barrier height forward kcal mol	4.63×10^{-3}
see case id	bh9_02_13_bhrev_rks_uks_pbe_def2qzvpp		barrier height reverse kcal mol	2.02×10^{-2}
see case id	bh9_02_13_re_rks_uks_pbe_def2qzvpp		reaction energy kcal mol	1.55×10^{-2}
see case id	bh9_02_14_bhfwd_rks_uks_pbe_def2qzvpp		barrier height forward kcal mol	3.00×10^{-3}
see case id	bh9_02_14_bhrev_rks_uks_pbe_def2qzvpp		barrier height reverse kcal mol	2.00×10^{-2}

Table S21, continued.

Method	System / basis	Ref.	Quantity	$\lvert\Delta\rvert$
see case id	bh9_02_14_re_rks_uks_pbe_def2qzvpp		reaction energy kcal mol	1.70×10^{-2}
see case id	bh9_02_15_bhfwd_rks_uks_pbe_def2qzvpp		barrier height forward kcal mol	3.69×10^{-3}
see case id	bh9_02_15_bhrev_rks_uks_pbe_def2qzvpp		barrier height reverse kcal mol	2.39×10^{-2}
see case id	bh9_02_15_re_rks_uks_pbe_def2qzvpp		reaction energy kcal mol	2.02×10^{-2}
see case id	bh9_02_16_bhfwd_rks_uks_pbe_def2qzvpp		barrier height forward kcal mol	8.12×10^{-3}
see case id	bh9_02_16_bhrev_rks_uks_pbe_def2qzvpp		barrier height reverse kcal mol	2.30×10^{-2}
see case id	bh9_02_16_re_rks_uks_pbe_def2qzvpp		reaction energy kcal mol	1.49×10^{-2}
see case id	bh9_02_17_bhfwd_rks_uks_pbe_def2qzvpp		barrier height forward kcal mol	8.59×10^{-3}
see case id	bh9_02_17_bhrev_rks_uks_pbe_def2qzvpp		barrier height reverse kcal mol	1.89×10^{-2}
see case id	bh9_02_17_re_rks_uks_pbe_def2qzvpp		reaction energy kcal mol	1.03×10^{-2}
see case id	bh9_02_18_bhfwd_rks_uks_pbe_def2qzvpp		barrier height forward kcal mol	9.01×10^{-3}
see case id	bh9_02_18_bhrev_rks_uks_pbe_def2qzvpp		barrier height reverse kcal mol	2.07×10^{-2}
see case id	bh9_02_18_re_rks_uks_pbe_def2qzvpp		reaction energy kcal mol	1.17×10^{-2}
see case id	bh9_02_19_bhfwd_rks_uks_pbe_def2qzvpp		barrier height forward kcal mol	9.95×10^{-3}
see case id	bh9_02_19_bhrev_rks_uks_pbe_def2qzvpp		barrier height reverse kcal mol	2.50×10^{-2}
see case id	bh9_02_19_re_rks_uks_pbe_def2qzvpp		reaction energy kcal mol	1.50×10^{-2}
see case id	bh9_02_20_bhfwd_rks_uks_pbe_def2qzvpp		barrier height forward kcal mol	8.02×10^{-3}
see case id	bh9_02_20_bhrev_rks_uks_pbe_def2qzvpp		barrier height reverse kcal mol	2.02×10^{-2}
see case id	bh9_02_20_re_rks_uks_pbe_def2qzvpp		reaction energy kcal mol	1.21×10^{-2}
see case id	bh9_02_22_bhfwd_rks_uks_pbe_def2qzvpp		barrier height forward kcal mol	1.24×10^{-2}
see case id	bh9_02_22_bhrev_rks_uks_pbe_def2qzvpp		barrier height reverse kcal mol	1.27×10^{-2}
see case id	bh9_02_22_re_rks_uks_pbe_def2qzvpp		reaction energy kcal mol	2.50×10^{-4}
see case id	bh9_02_23_bhfwd_rks_uks_pbe_def2qzvpp		barrier height forward kcal mol	8.72×10^{-3}
see case id	bh9_02_26_bhfwd_rks_uks_pbe_def2qzvpp		barrier height forward kcal mol	5.65×10^{-3}
see case id	bh9_02_26_bhrev_rks_uks_pbe_def2qzvpp		barrier height reverse kcal mol	1.82×10^{-2}
see case id	bh9_02_26_re_rks_uks_pbe_def2qzvpp		reaction energy kcal mol	1.25×10^{-2}
see case id	bh9_02_27_bhfwd_rks_uks_pbe_def2qzvpp		barrier height forward kcal mol	6.49×10^{-3}
see case id	bh9_02_27_bhrev_rks_uks_pbe_def2qzvpp		barrier height reverse kcal mol	1.97×10^{-2}
see case id	bh9_02_27_re_rks_uks_pbe_def2qzvpp		reaction energy kcal mol	1.32×10^{-2}

Table S21, continued.

Method	System / basis	Ref.	Quantity	$\lvert\Delta\rvert$
see case id	bh9_02_28_bhfwd_rks_uks_pbe_def2qzvpp		barrier height forward kcal mol	3.80×10^{-3}
see case id	bh9_02_28_bhrev_rks_uks_pbe_def2qzvpp		barrier height reverse kcal mol	1.93×10^{-2}
see case id	bh9_02_28_re_rks_uks_pbe_def2qzvpp		reaction energy kcal mol	1.55×10^{-2}
see case id	bh9_02_29_bhfwd_rks_uks_pbe_def2qzvpp		barrier height forward kcal mol	2.67×10^{-3}
see case id	bh9_02_29_bhrev_rks_uks_pbe_def2qzvpp		barrier height reverse kcal mol	1.38×10^{-2}
see case id	bh9_02_29_re_rks_uks_pbe_def2qzvpp		reaction energy kcal mol	1.65×10^{-2}
see case id	bh9_02_30_bhfwd_rks_uks_pbe_def2qzvpp		barrier height forward kcal mol	2.82×10^{-5}
see case id	bh9_02_30_bhrev_rks_uks_pbe_def2qzvpp		barrier height reverse kcal mol	8.60×10^{-3}
see case id	bh9_02_30_re_rks_uks_pbe_def2qzvpp		reaction energy kcal mol	8.57×10^{-3}
see case id	bh9_02_31_bhfwd_rks_uks_pbe_def2qzvpp		barrier height forward kcal mol	4.16×10^{-3}
see case id	bh9_02_31_bhrev_rks_uks_pbe_def2qzvpp		barrier height reverse kcal mol	8.15×10^{-3}
see case id	bh9_02_31_re_rks_uks_pbe_def2qzvpp		reaction energy kcal mol	1.23×10^{-2}
see case id	bh9_02_33_bhfwd_rks_uks_pbe_def2qzvpp		barrier height forward kcal mol	4.44×10^{-3}
see case id	bh9_02_33_bhrev_rks_uks_pbe_def2qzvpp		barrier height reverse kcal mol	2.38×10^{-2}
see case id	bh9_02_33_re_rks_uks_pbe_def2qzvpp		reaction energy kcal mol	1.94×10^{-2}
see case id	bh9_02_38_bhfwd_rks_uks_pbe_def2qzvpp		barrier height forward kcal mol	1.20×10^{-2}
see case id	bh9_02_38_bhrev_rks_uks_pbe_def2qzvpp		barrier height reverse kcal mol	1.65×10^{-2}
see case id	bh9_02_38_re_rks_uks_pbe_def2qzvpp		reaction energy kcal mol	4.53×10^{-3}
see case id	bh9_02_39_bhfwd_rks_uks_pbe_def2qzvpp		barrier height forward kcal mol	1.65×10^{-2}
see case id	bh9_02_39_bhrev_rks_uks_pbe_def2qzvpp		barrier height reverse kcal mol	2.02×10^{-2}
see case id	bh9_02_39_re_rks_uks_pbe_def2qzvpp		reaction energy kcal mol	3.68×10^{-3}
see case id	bh9_02_41_bhrev_rks_uks_pbe_def2qzvpp		barrier height reverse kcal mol	2.54×10^{-2}
see case id	bh9_02_48_bhrev_rks_uks_pbe_def2qzvpp		barrier height reverse kcal mol	1.51×10^{-2}
see case id	bh9_02_52_bhfwd_rks_uks_pbe_def2qzvpp		barrier height forward kcal mol	1.01×10^{-3}
see case id	bh9_02_52_bhrev_rks_uks_pbe_def2qzvpp		barrier height reverse kcal mol	2.09×10^{-2}
see case id	bh9_02_52_re_rks_uks_pbe_def2qzvpp		reaction energy kcal mol	2.19×10^{-2}
see case id	bh9_02_53_bhfwd_rks_uks_pbe_def2qzvpp		barrier height forward kcal mol	4.86×10^{-3}
see case id	bh9_02_53_bhrev_rks_uks_pbe_def2qzvpp		barrier height reverse kcal mol	2.06×10^{-2}
see case id	bh9_02_53_re_rks_uks_pbe_def2qzvpp		reaction energy kcal mol	2.55×10^{-2}

Table S21, continued.

Method	System / basis	Ref.	Quantity	$\lvert\Delta\rvert$
see case id	bh9_02_54_bhrev_rks_uks_pbe_def2qzvpp		barrier height reverse kcal mol	1.66×10^{-2}
see case id	bh9_02_55_bhfwd_rks_uks_pbe_def2qzvpp		barrier height forward kcal mol	3.89×10^{-3}
see case id	bh9_02_55_bhrev_rks_uks_pbe_def2qzvpp		barrier height reverse kcal mol	1.78×10^{-2}
see case id	bh9_02_55_re_rks_uks_pbe_def2qzvpp		reaction energy kcal mol	1.39×10^{-2}
see case id	bh9_02_60_bhfwd_rks_uks_pbe_def2qzvpp		barrier height forward kcal mol	1.37×10^{-3}
see case id	bh9_02_60_bhrev_rks_uks_pbe_def2qzvpp		barrier height reverse kcal mol	1.46×10^{-2}
see case id	bh9_02_60_re_rks_uks_pbe_def2qzvpp		reaction energy kcal mol	1.32×10^{-2}
see case id	bh9_02_61_bhrev_rks_uks_pbe_def2qzvpp		barrier height reverse kcal mol	2.35×10^{-2}
see case id	bh9_02_62_bhrev_rks_uks_pbe_def2qzvpp		barrier height reverse kcal mol	2.29×10^{-2}
see case id	bh9_02_63_bhfwd_rks_uks_pbe_def2qzvpp		barrier height forward kcal mol	4.17×10^{-3}
see case id	bh9_02_63_bhrev_rks_uks_pbe_def2qzvpp		barrier height reverse kcal mol	1.72×10^{-2}
see case id	bh9_02_63_re_rks_uks_pbe_def2qzvpp		reaction energy kcal mol	1.30×10^{-2}
see case id	bh9_02_64_bhfwd_rks_uks_pbe_def2qzvpp		barrier height forward kcal mol	3.21×10^{-3}
see case id	bh9_02_64_bhrev_rks_uks_pbe_def2qzvpp		barrier height reverse kcal mol	2.06×10^{-2}
see case id	bh9_02_64_re_rks_uks_pbe_def2qzvpp		reaction energy kcal mol	1.74×10^{-2}
see case id	bh9_02_65_bhfwd_rks_uks_pbe_def2qzvpp		barrier height forward kcal mol	3.09×10^{-3}
see case id	bh9_02_65_bhrev_rks_uks_pbe_def2qzvpp		barrier height reverse kcal mol	2.21×10^{-2}
see case id	bh9_02_65_re_rks_uks_pbe_def2qzvpp		reaction energy kcal mol	1.90×10^{-2}
see case id	bh9_02_66_bhfwd_rks_uks_pbe_def2qzvpp		barrier height forward kcal mol	1.02×10^{-3}
see case id	bh9_02_66_bhrev_rks_uks_pbe_def2qzvpp		barrier height reverse kcal mol	2.26×10^{-2}
see case id	bh9_02_66_re_rks_uks_pbe_def2qzvpp		reaction energy kcal mol	2.16×10^{-2}
see case id	bh9_02_67_bhrev_rks_uks_pbe_def2qzvpp		barrier height reverse kcal mol	2.74×10^{-2}
see case id	bh9_02_68_bhfwd_rks_uks_pbe_def2qzvpp		barrier height forward kcal mol	2.14×10^{-4}
see case id	bh9_02_68_bhrev_rks_uks_pbe_def2qzvpp		barrier height reverse kcal mol	2.81×10^{-2}
see case id	bh9_02_68_re_rks_uks_pbe_def2qzvpp		reaction energy kcal mol	2.83×10^{-2}
see case id	bh9_02_69_bhfwd_rks_uks_pbe_def2qzvpp		barrier height forward kcal mol	2.13×10^{-4}
see case id	bh9_02_69_bhrev_rks_uks_pbe_def2qzvpp		barrier height reverse kcal mol	2.62×10^{-2}
see case id	bh9_02_69_re_rks_uks_pbe_def2qzvpp		reaction energy kcal mol	2.60×10^{-2}
see case id	bh9_02_70_bhfwd_rks_uks_pbe_def2qzvpp		barrier height forward kcal mol	2.64×10^{-3}

Table S21, continued.

Method	System / basis	Ref.	Quantity	$\lvert\Delta\rvert$
see case id	bh9_02_70_bhrev_rks_uks_pbe_def2qzvpp		barrier height reverse kcal mol	1.99×10^{-2}
see case id	bh9_02_70_re_rks_uks_pbe_def2qzvpp		reaction energy kcal mol	2.26×10^{-2}
see case id	bh9_02_71_bhfwd_rks_uks_pbe_def2qzvpp		barrier height forward kcal mol	8.19×10^{-4}
see case id	bh9_02_71_bhrev_rks_uks_pbe_def2qzvpp		barrier height reverse kcal mol	2.05×10^{-2}
see case id	bh9_02_71_re_rks_uks_pbe_def2qzvpp		reaction energy kcal mol	2.13×10^{-2}
see case id	bh9_02_72_bhfwd_rks_uks_pbe_def2qzvpp		barrier height forward kcal mol	5.42×10^{-3}
see case id	bh9_02_72_bhrev_rks_uks_pbe_def2qzvpp		barrier height reverse kcal mol	2.00×10^{-2}
see case id	bh9_02_72_re_rks_uks_pbe_def2qzvpp		reaction energy kcal mol	1.46×10^{-2}
see case id	bh9_02_77_bhfwd_rks_uks_pbe_def2qzvpp		barrier height forward kcal mol	1.07×10^{-3}
see case id	bh9_02_77_bhrev_rks_uks_pbe_def2qzvpp		barrier height reverse kcal mol	2.36×10^{-2}
see case id	bh9_02_77_re_rks_uks_pbe_def2qzvpp		reaction energy kcal mol	2.47×10^{-2}
see case id	bh9_02_78_bhfwd_rks_uks_pbe_def2qzvpp		barrier height forward kcal mol	1.05×10^{-2}
see case id	bh9_02_78_bhrev_rks_uks_pbe_def2qzvpp		barrier height reverse kcal mol	2.44×10^{-2}
see case id	bh9_02_78_re_rks_uks_pbe_def2qzvpp		reaction energy kcal mol	1.39×10^{-2}
see case id	bh9_02_79_bhfwd_rks_uks_pbe_def2qzvpp		barrier height forward kcal mol	2.29×10^{-3}
see case id	bh9_02_79_bhrev_rks_uks_pbe_def2qzvpp		barrier height reverse kcal mol	2.25×10^{-2}
see case id	bh9_02_79_re_rks_uks_pbe_def2qzvpp		reaction energy kcal mol	2.48×10^{-2}
see case id	bh9_02_7_bhfwd_rks_uks_pbe_def2qzvpp		barrier height forward kcal mol	1.04×10^{-2}
see case id	bh9_02_7_bhrev_rks_uks_pbe_def2qzvpp		barrier height reverse kcal mol	2.77×10^{-2}
see case id	bh9_02_7_re_rks_uks_pbe_def2qzvpp		reaction energy kcal mol	1.73×10^{-2}
see case id	bh9_02_80_bhfwd_rks_uks_pbe_def2qzvpp		barrier height forward kcal mol	1.01×10^{-2}
see case id	bh9_02_80_bhrev_rks_uks_pbe_def2qzvpp		barrier height reverse kcal mol	2.34×10^{-2}
see case id	bh9_02_80_re_rks_uks_pbe_def2qzvpp		reaction energy kcal mol	1.34×10^{-2}
see case id	bh9_02_83_bhfwd_rks_uks_pbe_def2qzvpp		barrier height forward kcal mol	8.42×10^{-3}
see case id	bh9_02_83_bhrev_rks_uks_pbe_def2qzvpp		barrier height reverse kcal mol	4.54×10^{-3}
see case id	bh9_02_83_re_rks_uks_pbe_def2qzvpp		reaction energy kcal mol	3.88×10^{-3}
see case id	bh9_02_86_bhfwd_rks_uks_pbe_def2qzvpp		barrier height forward kcal mol	4.28×10^{-3}
see case id	bh9_02_86_bhrev_rks_uks_pbe_def2qzvpp		barrier height reverse kcal mol	1.02×10^{-2}
see case id	bh9_02_86_re_rks_uks_pbe_def2qzvpp		reaction energy kcal mol	5.90×10^{-3}

Table S21, continued.

Method	System / basis	Ref.	Quantity	$\lvert\Delta\rvert$
see case id	bh9_02_87_bhfwd_rks_uks_pbe_def2qzvpp		barrier height forward kcal mol	7.59×10^{-3}
see case id	bh9_02_87_bhrev_rks_uks_pbe_def2qzvpp		barrier height reverse kcal mol	1.33×10^{-2}
see case id	bh9_02_87_re_rks_uks_pbe_def2qzvpp		reaction energy kcal mol	5.69×10^{-3}
see case id	bh9_02_88_bhfwd_rks_uks_pbe_def2qzvpp		barrier height forward kcal mol	1.05×10^{-2}
see case id	bh9_02_88_bhrev_rks_uks_pbe_def2qzvpp		barrier height reverse kcal mol	1.46×10^{-2}
see case id	bh9_02_88_re_rks_uks_pbe_def2qzvpp		reaction energy kcal mol	4.13×10^{-3}
see case id	bh9_02_89_bhfwd_rks_uks_pbe_def2qzvpp		barrier height forward kcal mol	1.17×10^{-2}
see case id	bh9_02_89_bhrev_rks_uks_pbe_def2qzvpp		barrier height reverse kcal mol	1.52×10^{-2}
see case id	bh9_02_89_re_rks_uks_pbe_def2qzvpp		reaction energy kcal mol	3.43×10^{-3}
see case id	bh9_02_8_bhfwd_rks_uks_pbe_def2qzvpp		barrier height forward kcal mol	7.96×10^{-3}
see case id	bh9_02_8_bhrev_rks_uks_pbe_def2qzvpp		barrier height reverse kcal mol	2.41×10^{-2}
see case id	bh9_02_8_re_rks_uks_pbe_def2qzvpp		reaction energy kcal mol	1.61×10^{-2}
see case id	bh9_02_92_bhfwd_rks_uks_pbe_def2qzvpp		barrier height forward kcal mol	1.20×10^{-2}
see case id	bh9_02_92_bhrev_rks_uks_pbe_def2qzvpp		barrier height reverse kcal mol	1.41×10^{-2}
see case id	bh9_02_92_re_rks_uks_pbe_def2qzvpp		reaction energy kcal mol	2.08×10^{-3}
see case id	bh9_02_93_bhfwd_rks_uks_pbe_def2qzvpp		barrier height forward kcal mol	1.22×10^{-2}
see case id	bh9_02_93_bhrev_rks_uks_pbe_def2qzvpp		barrier height reverse kcal mol	1.40×10^{-2}
see case id	bh9_02_93_re_rks_uks_pbe_def2qzvpp		reaction energy kcal mol	1.83×10^{-3}
see case id	bh9_02_94_bhfwd_rks_uks_pbe_def2qzvpp		barrier height forward kcal mol	1.35×10^{-2}
see case id	bh9_02_94_bhrev_rks_uks_pbe_def2qzvpp		barrier height reverse kcal mol	1.52×10^{-2}
see case id	bh9_02_94_re_rks_uks_pbe_def2qzvpp		reaction energy kcal mol	1.73×10^{-3}
see case id	bh9_02_95_bhfwd_rks_uks_pbe_def2qzvpp		barrier height forward kcal mol	1.36×10^{-2}
see case id	bh9_02_95_bhrev_rks_uks_pbe_def2qzvpp		barrier height reverse kcal mol	1.54×10^{-2}
see case id	bh9_02_95_re_rks_uks_pbe_def2qzvpp		reaction energy kcal mol	1.76×10^{-3}
see case id	bh9_02_9_bhfwd_rks_uks_pbe_def2qzvpp		barrier height forward kcal mol	5.98×10^{-3}
see case id	bh9_02_9_bhrev_rks_uks_pbe_def2qzvpp		barrier height reverse kcal mol	2.49×10^{-2}
see case id	bh9_02_9_re_rks_uks_pbe_def2qzvpp		reaction energy kcal mol	1.90×10^{-2}
see case id	bh9_03_14_bhfwd_rks_uks_pbe_def2qzvpp		barrier height forward kcal mol	2.24×10^{-3}
see case id	bh9_03_14_bhrev_rks_uks_pbe_def2qzvpp		barrier height reverse kcal mol	1.61×10^{-2}

Table S21, continued.

Method	System / basis	Ref.	Quantity	$\lvert\Delta\rvert$
see case id	bh9_03_14_re_rks_uks_pbe_def2qzvpp		reaction energy kcal mol	1.39×10^{-2}
see case id	bh9_03_16_re_rks_uks_pbe_def2qzvpp		reaction energy kcal mol	1.26×10^{-2}
see case id	bh9_03_17_bhfwd_rks_uks_pbe_def2qzvpp		barrier height forward kcal mol	1.74×10^{-2}
see case id	bh9_03_17_bhrev_rks_uks_pbe_def2qzvpp		barrier height reverse kcal mol	1.51×10^{-2}
see case id	bh9_03_17_re_rks_uks_pbe_def2qzvpp		reaction energy kcal mol	2.26×10^{-3}
see case id	bh9_03_18_bhrev_rks_uks_pbe_def2qzvpp		barrier height reverse kcal mol	1.61×10^{-2}
see case id	bh9_03_19_bhfwd_rks_uks_pbe_def2qzvpp		barrier height forward kcal mol	8.37×10^{-3}
see case id	bh9_03_19_bhrev_rks_uks_pbe_def2qzvpp		barrier height reverse kcal mol	2.06×10^{-2}
see case id	bh9_03_19_re_rks_uks_pbe_def2qzvpp		reaction energy kcal mol	1.22×10^{-2}
see case id	bh9_03_20_bhfwd_rks_uks_pbe_def2qzvpp		barrier height forward kcal mol	4.01×10^{-3}
see case id	bh9_03_20_bhrev_rks_uks_pbe_def2qzvpp		barrier height reverse kcal mol	1.78×10^{-2}
see case id	bh9_03_20_re_rks_uks_pbe_def2qzvpp		reaction energy kcal mol	1.38×10^{-2}
see case id	bh9_03_21_bhfwd_rks_uks_pbe_def2qzvpp		barrier height forward kcal mol	1.99×10^{-2}
see case id	bh9_03_21_bhrev_rks_uks_pbe_def2qzvpp		barrier height reverse kcal mol	6.38×10^{-3}
see case id	bh9_03_21_re_rks_uks_pbe_def2qzvpp		reaction energy kcal mol	1.35×10^{-2}
see case id	bh9_03_22_bhrev_rks_uks_pbe_def2qzvpp		barrier height reverse kcal mol	1.11×10^{-2}
see case id	bh9_03_23_bhfwd_rks_uks_pbe_def2qzvpp		barrier height forward kcal mol	1.29×10^{-2}
see case id	bh9_03_25_bhfwd_rks_uks_pbe_def2qzvpp		barrier height forward kcal mol	2.39×10^{-2}
see case id	bh9_03_25_bhrev_rks_uks_pbe_def2qzvpp		barrier height reverse kcal mol	1.41×10^{-2}
see case id	bh9_03_25_re_rks_uks_pbe_def2qzvpp		reaction energy kcal mol	9.87×10^{-3}
see case id	bh9_03_29_re_rks_uks_pbe_def2qzvpp		reaction energy kcal mol	3.48×10^{-3}
see case id	bh9_03_40_re_rks_uks_pbe_def2qzvpp		reaction energy kcal mol	6.83×10^{-3}
see case id	bh9_04_40_re_rks_uks_pbe_def2qzvpp		reaction energy kcal mol	2.75×10^{-3}
see case id	bh9_04_41_bhfwd_rks_uks_pbe_def2qzvpp		barrier height forward kcal mol	4.90×10^{-3}
see case id	bh9_04_41_bhrev_rks_uks_pbe_def2qzvpp		barrier height reverse kcal mol	1.34×10^{-2}
see case id	bh9_04_41_re_rks_uks_pbe_def2qzvpp		reaction energy kcal mol	8.54×10^{-3}
see case id	bh9_04_42_bhfwd_rks_uks_pbe_def2qzvpp		barrier height forward kcal mol	4.37×10^{-3}
see case id	bh9_04_42_bhrev_rks_uks_pbe_def2qzvpp		barrier height reverse kcal mol	1.17×10^{-2}
see case id	bh9_04_42_re_rks_uks_pbe_def2qzvpp		reaction energy kcal mol	7.32×10^{-3}

Table S21, continued.

Method	System / basis	Ref.	Quantity	$\lvert\Delta\rvert$
see case id	bh9_04_43_bhfwd_rks_uks_pbe_def2qzvpp		barrier height forward kcal mol	1.23×10^{-2}
see case id	bh9_04_43_bhrev_rks_uks_pbe_def2qzvpp		barrier height reverse kcal mol	1.55×10^{-2}
see case id	bh9_04_43_re_rks_uks_pbe_def2qzvpp		reaction energy kcal mol	3.24×10^{-3}
see case id	bh9_04_44_bhrev_rks_uks_pbe_def2qzvpp		barrier height reverse kcal mol	3.30×10^{-2}
see case id	bh9_04_45_bhfwd_rks_uks_pbe_def2qzvpp		barrier height forward kcal mol	1.18×10^{-2}
see case id	bh9_04_45_bhrev_rks_uks_pbe_def2qzvpp		barrier height reverse kcal mol	1.57×10^{-2}
see case id	bh9_04_45_re_rks_uks_pbe_def2qzvpp		reaction energy kcal mol	3.98×10^{-3}
see case id	bh9_04_46_bhfwd_rks_uks_pbe_def2qzvpp		barrier height forward kcal mol	8.02×10^{-3}
see case id	bh9_04_46_bhrev_rks_uks_pbe_def2qzvpp		barrier height reverse kcal mol	5.44×10^{-3}
see case id	bh9_04_46_re_rks_uks_pbe_def2qzvpp		reaction energy kcal mol	2.58×10^{-3}
see case id	bh9_04_47_bhrev_rks_uks_pbe_def2qzvpp		barrier height reverse kcal mol	1.94×10^{-3}
see case id	bh9_04_48_bhfwd_rks_uks_pbe_def2qzvpp		barrier height forward kcal mol	1.06×10^{-2}
see case id	bh9_04_48_bhrev_rks_uks_pbe_def2qzvpp		barrier height reverse kcal mol	2.47×10^{-3}
see case id	bh9_04_48_re_rks_uks_pbe_def2qzvpp		reaction energy kcal mol	8.15×10^{-3}
see case id	bh9_04_49_bhfwd_rks_uks_pbe_def2qzvpp		barrier height forward kcal mol	2.17×10^{-2}
see case id	bh9_04_49_bhrev_rks_uks_pbe_def2qzvpp		barrier height reverse kcal mol	1.36×10^{-2}
see case id	bh9_04_49_re_rks_uks_pbe_def2qzvpp		reaction energy kcal mol	8.13×10^{-3}
see case id	bh9_04_51_bhfwd_rks_uks_pbe_def2qzvpp		barrier height forward kcal mol	1.86×10^{-2}
see case id	bh9_04_51_bhrev_rks_uks_pbe_def2qzvpp		barrier height reverse kcal mol	1.35×10^{-2}
see case id	bh9_04_51_re_rks_uks_pbe_def2qzvpp		reaction energy kcal mol	5.16×10^{-3}
see case id	bh9_04_52_re_rks_uks_pbe_def2qzvpp		reaction energy kcal mol	6.47×10^{-3}
see case id	bh9_04_56_bhfwd_rks_uks_pbe_def2qzvpp		barrier height forward kcal mol	1.01×10^{-2}
see case id	bh9_04_56_bhrev_rks_uks_pbe_def2qzvpp		barrier height reverse kcal mol	1.56×10^{-2}
see case id	bh9_04_56_re_rks_uks_pbe_def2qzvpp		reaction energy kcal mol	5.57×10^{-3}
see case id	bh9_04_57_bhfwd_rks_uks_pbe_def2qzvpp		barrier height forward kcal mol	2.37×10^{-2}
see case id	bh9_04_57_bhrev_rks_uks_pbe_def2qzvpp		barrier height reverse kcal mol	2.57×10^{-2}
see case id	bh9_04_57_re_rks_uks_pbe_def2qzvpp		reaction energy kcal mol	1.93×10^{-3}
see case id	bh9_04_59_re_rks_uks_pbe_def2qzvpp		reaction energy kcal mol	7.38×10^{-3}
see case id	bh9_04_60_re_rks_uks_pbe_def2qzvpp		reaction energy kcal mol	7.04×10^{-3}

Table S21, continued.

Method	System / basis	Ref.	Quantity	$\lvert\Delta\rvert$
see case id	bh9_04_61_bhfwd_rks_uks_pbe_def2qzvpp		barrier height forward kcal mol	1.03×10^{-2}
see case id	bh9_04_61_bhrev_rks_uks_pbe_def2qzvpp		barrier height reverse kcal mol	1.54×10^{-2}
see case id	bh9_04_61_re_rks_uks_pbe_def2qzvpp		reaction energy kcal mol	5.08×10^{-3}
see case id	bh9_04_63_bhrev_rks_uks_pbe_def2qzvpp		barrier height reverse kcal mol	5.46×10^{-3}
see case id	bh9_04_64_bhfwd_rks_uks_pbe_def2qzvpp		barrier height forward kcal mol	5.66×10^{-3}
see case id	bh9_04_64_bhrev_rks_uks_pbe_def2qzvpp		barrier height reverse kcal mol	8.57×10^{-3}
see case id	bh9_04_64_re_rks_uks_pbe_def2qzvpp		reaction energy kcal mol	2.90×10^{-3}
see case id	bh9_04_65_re_rks_uks_pbe_def2qzvpp		reaction energy kcal mol	3.18×10^{-3}
see case id	bh9_04_66_bhfwd_rks_uks_pbe_def2qzvpp		barrier height forward kcal mol	2.00×10^{-2}
see case id	bh9_04_66_bhrev_rks_uks_pbe_def2qzvpp		barrier height reverse kcal mol	1.66×10^{-2}
see case id	bh9_04_66_re_rks_uks_pbe_def2qzvpp		reaction energy kcal mol	3.41×10^{-3}
see case id	bh9_04_67_re_rks_uks_pbe_def2qzvpp		reaction energy kcal mol	4.74×10^{-3}
see case id	bh9_04_68_re_rks_uks_pbe_def2qzvpp		reaction energy kcal mol	3.10×10^{-3}
see case id	bh9_04_69_bhfwd_rks_uks_pbe_def2qzvpp		barrier height forward kcal mol	1.05×10^{-2}
see case id	bh9_04_69_bhrev_rks_uks_pbe_def2qzvpp		barrier height reverse kcal mol	1.58×10^{-2}
see case id	bh9_04_69_re_rks_uks_pbe_def2qzvpp		reaction energy kcal mol	5.31×10^{-3}
see case id	bh9_04_73_re_rks_uks_pbe_def2qzvpp		reaction energy kcal mol	3.39×10^{-3}
see case id	bh9_04_79_re_rks_uks_pbe_def2qzvpp		reaction energy kcal mol	1.35×10^{-3}
see case id	bh9_04_82_re_rks_uks_pbe_def2qzvpp		reaction energy kcal mol	2.77×10^{-3}
see case id	bh9_04_83_bhfwd_rks_uks_pbe_def2qzvpp		barrier height forward kcal mol	1.37×10^{-2}
see case id	bh9_04_83_bhrev_rks_uks_pbe_def2qzvpp		barrier height reverse kcal mol	1.03×10^{-2}
see case id	bh9_04_83_re_rks_uks_pbe_def2qzvpp		reaction energy kcal mol	3.38×10^{-3}
see case id	bh9_04_84_bhfwd_rks_uks_pbe_def2qzvpp		barrier height forward kcal mol	8.22×10^{-3}
see case id	bh9_04_84_bhrev_rks_uks_pbe_def2qzvpp		barrier height reverse kcal mol	1.42×10^{-2}
see case id	bh9_04_84_re_rks_uks_pbe_def2qzvpp		reaction energy kcal mol	5.98×10^{-3}
see case id	bh9_04_85_re_rks_uks_pbe_def2qzvpp		reaction energy kcal mol	4.20×10^{-3}
see case id	bh9_05_10_bhfwd_rks_uks_pbe_def2qzvpp		barrier height forward kcal mol	1.30×10^{-2}
see case id	bh9_05_10_bhrev_rks_uks_pbe_def2qzvpp		barrier height reverse kcal mol	1.04×10^{-2}
see case id	bh9_05_10_re_rks_uks_pbe_def2qzvpp		reaction energy kcal mol	2.58×10^{-3}

Table S21, continued.

Method	System / basis	Ref.	Quantity	$\lvert\Delta\rvert$
see case id	bh9_05_11_bhfwd_rks_uks_pbe_def2qzvpp		barrier height forward kcal mol	1.76×10^{-3}
see case id	bh9_05_11_bhrev_rks_uks_pbe_def2qzvpp		barrier height reverse kcal mol	2.33×10^{-3}
see case id	bh9_05_11_re_rks_uks_pbe_def2qzvpp		reaction energy kcal mol	5.74×10^{-4}
see case id	bh9_05_12_bhfwd_rks_uks_pbe_def2qzvpp		barrier height forward kcal mol	2.22×10^{-2}
see case id	bh9_05_12_bhrev_rks_uks_pbe_def2qzvpp		barrier height reverse kcal mol	2.91×10^{-2}
see case id	bh9_05_12_re_rks_uks_pbe_def2qzvpp		reaction energy kcal mol	6.91×10^{-3}
see case id	bh9_05_13_bhfwd_rks_uks_pbe_def2qzvpp		barrier height forward kcal mol	1.53×10^{-2}
see case id	bh9_05_13_bhrev_rks_uks_pbe_def2qzvpp		barrier height reverse kcal mol	2.36×10^{-2}
see case id	bh9_05_13_re_rks_uks_pbe_def2qzvpp		reaction energy kcal mol	8.38×10^{-3}
see case id	bh9_05_14_bhfwd_rks_uks_pbe_def2qzvpp		barrier height forward kcal mol	1.74×10^{-2}
see case id	bh9_05_14_bhrev_rks_uks_pbe_def2qzvpp		barrier height reverse kcal mol	3.12×10^{-2}
see case id	bh9_05_15_bhfwd_rks_uks_pbe_def2qzvpp		barrier height forward kcal mol	1.79×10^{-2}
see case id	bh9_05_15_bhrev_rks_uks_pbe_def2qzvpp		barrier height reverse kcal mol	2.19×10^{-2}
see case id	bh9_05_15_re_rks_uks_pbe_def2qzvpp		reaction energy kcal mol	4.00×10^{-3}
see case id	bh9_05_16_bhfwd_rks_uks_pbe_def2qzvpp		barrier height forward kcal mol	2.12×10^{-2}
see case id	bh9_05_16_bhrev_rks_uks_pbe_def2qzvpp		barrier height reverse kcal mol	2.20×10^{-2}
see case id	bh9_05_16_re_rks_uks_pbe_def2qzvpp		reaction energy kcal mol	7.54×10^{-4}
see case id	bh9_05_17_bhfwd_rks_uks_pbe_def2qzvpp		barrier height forward kcal mol	9.68×10^{-3}
see case id	bh9_05_17_bhrev_rks_uks_pbe_def2qzvpp		barrier height reverse kcal mol	6.75×10^{-3}
see case id	bh9_05_17_re_rks_uks_pbe_def2qzvpp		reaction energy kcal mol	2.92×10^{-3}
see case id	bh9_05_18_bhrev_rks_uks_pbe_def2qzvpp		barrier height reverse kcal mol	5.13×10^{-3}
see case id	bh9_05_20_bhfwd_rks_uks_pbe_def2qzvpp		barrier height forward kcal mol	1.75×10^{-2}
see case id	bh9_05_20_bhrev_rks_uks_pbe_def2qzvpp		barrier height reverse kcal mol	2.12×10^{-2}
see case id	bh9_05_20_re_rks_uks_pbe_def2qzvpp		reaction energy kcal mol	3.62×10^{-3}
see case id	bh9_05_21_bhrev_rks_uks_pbe_def2qzvpp		barrier height reverse kcal mol	3.02×10^{-2}
see case id	bh9_05_23_bhrev_rks_uks_pbe_def2qzvpp		barrier height reverse kcal mol	1.63×10^{-2}
see case id	bh9_05_24_bhfwd_rks_uks_pbe_def2qzvpp		barrier height forward kcal mol	1.57×10^{-2}
see case id	bh9_05_30_bhrev_rks_uks_pbe_def2qzvpp		barrier height reverse kcal mol	2.01×10^{-2}
see case id	bh9_05_31_bhfwd_rks_uks_pbe_def2qzvpp		barrier height forward kcal mol	1.64×10^{-2}

Table S21, continued.

Method	System / basis	Ref.	Quantity	$\lvert\Delta\rvert$
see case id	bh9_05_32_bhfwd_rks_uks_pbe_def2qzvpp		barrier height forward kcal mol	1.19×10^{-2}
see case id	bh9_05_34_bhfwd_rks_uks_pbe_def2qzvpp		barrier height forward kcal mol	1.84×10^{-2}
see case id	bh9_05_34_bhrev_rks_uks_pbe_def2qzvpp		barrier height reverse kcal mol	3.08×10^{-2}
see case id	bh9_05_36_bhfwd_rks_uks_pbe_def2qzvpp		barrier height forward kcal mol	3.41×10^{-4}
see case id	bh9_05_36_bhrev_rks_uks_pbe_def2qzvpp		barrier height reverse kcal mol	6.22×10^{-3}
see case id	bh9_05_36_re_rks_uks_pbe_def2qzvpp		reaction energy kcal mol	6.56×10^{-3}
see case id	bh9_05_39_bhrev_rks_uks_pbe_def2qzvpp		barrier height reverse kcal mol	2.08×10^{-2}
see case id	bh9_05_40_bhfwd_rks_uks_pbe_def2qzvpp		barrier height forward kcal mol	7.35×10^{-3}
see case id	bh9_05_40_bhrev_rks_uks_pbe_def2qzvpp		barrier height reverse kcal mol	1.54×10^{-3}
see case id	bh9_05_40_re_rks_uks_pbe_def2qzvpp		reaction energy kcal mol	8.89×10^{-3}
see case id	bh9_05_41_bhfwd_rks_uks_pbe_def2qzvpp		barrier height forward kcal mol	1.21×10^{-2}
see case id	bh9_05_41_bhrev_rks_uks_pbe_def2qzvpp		barrier height reverse kcal mol	1.53×10^{-2}
see case id	bh9_05_41_re_rks_uks_pbe_def2qzvpp		reaction energy kcal mol	3.15×10^{-3}
see case id	bh9_05_42_bhrev_rks_uks_pbe_def2qzvpp		barrier height reverse kcal mol	1.42×10^{-2}
see case id	bh9_05_8_bhfwd_rks_uks_pbe_def2qzvpp		barrier height forward kcal mol	2.30×10^{-3}
see case id	bh9_05_9_bhfwd_rks_uks_pbe_def2qzvpp		barrier height forward kcal mol	6.19×10^{-4}
see case id	bh9_05_9_bhrev_rks_uks_pbe_def2qzvpp		barrier height reverse kcal mol	9.22×10^{-4}
see case id	bh9_05_9_re_rks_uks_pbe_def2qzvpp		reaction energy kcal mol	3.04×10^{-4}
see case id	bh9_06_10_bhrev_rks_uks_pbe_def2qzvpp		barrier height reverse kcal mol	8.45×10^{-3}
see case id	bh9_06_11_bhrev_rks_uks_pbe_def2qzvpp		barrier height reverse kcal mol	1.17×10^{-2}
see case id	bh9_06_12_bhfwd_rks_uks_pbe_def2qzvpp		barrier height forward kcal mol	5.46×10^{-4}
see case id	bh9_06_12_bhrev_rks_uks_pbe_def2qzvpp		barrier height reverse kcal mol	3.02×10^{-3}
see case id	bh9_06_12_re_rks_uks_pbe_def2qzvpp		reaction energy kcal mol	2.49×10^{-3}
see case id	bh9_06_13_bhfwd_rks_uks_pbe_def2qzvpp		barrier height forward kcal mol	1.91×10^{-3}
see case id	bh9_06_13_bhrev_rks_uks_pbe_def2qzvpp		barrier height reverse kcal mol	4.61×10^{-3}
see case id	bh9_06_13_re_rks_uks_pbe_def2qzvpp		reaction energy kcal mol	2.72×10^{-3}
see case id	bh9_06_14_bhfwd_rks_uks_pbe_def2qzvpp		barrier height forward kcal mol	1.34×10^{-3}
see case id	bh9_06_14_bhrev_rks_uks_pbe_def2qzvpp		barrier height reverse kcal mol	4.08×10^{-3}
see case id	bh9_06_14_re_rks_uks_pbe_def2qzvpp		reaction energy kcal mol	2.75×10^{-3}

Table S21, continued.

Method	System / basis	Ref.	Quantity	$\lvert\Delta\rvert$
see case id	bh9_06_15_bhrev_rks_uks_pbe_def2qzvpp		barrier height reverse kcal mol	8.35×10^{-3}
see case id	bh9_06_16_bhfwd_rks_uks_pbe_def2qzvpp		barrier height forward kcal mol	1.64×10^{-2}
see case id	bh9_06_16_bhrev_rks_uks_pbe_def2qzvpp		barrier height reverse kcal mol	1.75×10^{-2}
see case id	bh9_06_16_re_rks_uks_pbe_def2qzvpp		reaction energy kcal mol	1.05×10^{-3}
see case id	bh9_06_17_bhfwd_rks_uks_pbe_def2qzvpp		barrier height forward kcal mol	1.16×10^{-2}
see case id	bh9_06_17_bhrev_rks_uks_pbe_def2qzvpp		barrier height reverse kcal mol	1.82×10^{-2}
see case id	bh9_06_17_re_rks_uks_pbe_def2qzvpp		reaction energy kcal mol	6.57×10^{-3}
see case id	bh9_06_18_bhfwd_rks_uks_pbe_def2qzvpp		barrier height forward kcal mol	3.46×10^{-3}
see case id	bh9_06_18_bhrev_rks_uks_pbe_def2qzvpp		barrier height reverse kcal mol	1.20×10^{-3}
see case id	bh9_06_18_re_rks_uks_pbe_def2qzvpp		reaction energy kcal mol	4.64×10^{-3}
see case id	bh9_06_19_bhrev_rks_uks_pbe_def2qzvpp		barrier height reverse kcal mol	8.25×10^{-3}
see case id	bh9_06_20_bhrev_rks_uks_pbe_def2qzvpp		barrier height reverse kcal mol	9.53×10^{-3}
see case id	bh9_06_21_bhfwd_rks_uks_pbe_def2qzvpp		barrier height forward kcal mol	7.24×10^{-3}
see case id	bh9_06_22_bhrev_rks_uks_pbe_def2qzvpp		barrier height reverse kcal mol	7.76×10^{-3}
see case id	bh9_06_23_bhrev_rks_uks_pbe_def2qzvpp		barrier height reverse kcal mol	4.01×10^{-3}
see case id	bh9_06_24_bhfwd_rks_uks_pbe_def2qzvpp		barrier height forward kcal mol	2.30×10^{-3}
see case id	bh9_06_24_bhrev_rks_uks_pbe_def2qzvpp		barrier height reverse kcal mol	1.64×10^{-2}
see case id	bh9_06_24_re_rks_uks_pbe_def2qzvpp		reaction energy kcal mol	1.41×10^{-2}
see case id	bh9_06_25_bhfwd_rks_uks_pbe_def2qzvpp		barrier height forward kcal mol	1.20×10^{-3}
see case id	bh9_06_25_bhrev_rks_uks_pbe_def2qzvpp		barrier height reverse kcal mol	1.15×10^{-2}
see case id	bh9_06_25_re_rks_uks_pbe_def2qzvpp		reaction energy kcal mol	1.27×10^{-2}
see case id	bh9_06_26_bhfwd_rks_uks_pbe_def2qzvpp		barrier height forward kcal mol	6.96×10^{-3}
see case id	bh9_06_26_bhrev_rks_uks_pbe_def2qzvpp		barrier height reverse kcal mol	1.10×10^{-2}
see case id	bh9_06_26_re_rks_uks_pbe_def2qzvpp		reaction energy kcal mol	1.79×10^{-2}
see case id	bh9_06_27_bhfwd_rks_uks_pbe_def2qzvpp		barrier height forward kcal mol	4.29×10^{-3}
see case id	bh9_06_27_bhrev_rks_uks_pbe_def2qzvpp		barrier height reverse kcal mol	2.96×10^{-3}
see case id	bh9_06_27_re_rks_uks_pbe_def2qzvpp		reaction energy kcal mol	1.32×10^{-3}
see case id	bh9_06_28_bhfwd_rks_uks_pbe_def2qzvpp		barrier height forward kcal mol	1.76×10^{-3}
see case id	bh9_06_28_bhrev_rks_uks_pbe_def2qzvpp		barrier height reverse kcal mol	5.36×10^{-3}

Table S21, continued.

Method	System / basis	Ref.	Quantity	$\lvert\Delta\rvert$
see case id	bh9_06_28_re_rks_uks_pbe_def2qzvpp		reaction energy kcal mol	3.60×10^{-3}
see case id	bh9_06_29_bhfwd_rks_uks_pbe_def2qzvpp		barrier height forward kcal mol	6.15×10^{-3}
see case id	bh9_06_29_bhrev_rks_uks_pbe_def2qzvpp		barrier height reverse kcal mol	1.06×10^{-3}
see case id	bh9_06_29_re_rks_uks_pbe_def2qzvpp		reaction energy kcal mol	5.09×10^{-3}
see case id	bh9_06_30_bhfwd_rks_uks_pbe_def2qzvpp		barrier height forward kcal mol	5.97×10^{-3}
see case id	bh9_06_30_bhrev_rks_uks_pbe_def2qzvpp		barrier height reverse kcal mol	9.95×10^{-4}
see case id	bh9_06_30_re_rks_uks_pbe_def2qzvpp		reaction energy kcal mol	6.96×10^{-3}
see case id	bh9_06_31_bhrev_rks_uks_pbe_def2qzvpp		barrier height reverse kcal mol	7.58×10^{-3}
see case id	bh9_06_32_bhrev_rks_uks_pbe_def2qzvpp		barrier height reverse kcal mol	9.68×10^{-3}
see case id	bh9_06_33_bhfwd_rks_uks_pbe_def2qzvpp		barrier height forward kcal mol	2.66×10^{-3}
see case id	bh9_06_34_bhrev_rks_uks_pbe_def2qzvpp		barrier height reverse kcal mol	5.29×10^{-3}
see case id	bh9_06_35_bhrev_rks_uks_pbe_def2qzvpp		barrier height reverse kcal mol	6.84×10^{-3}
see case id	bh9_06_8_bhfwd_rks_uks_pbe_def2qzvpp		barrier height forward kcal mol	1.94×10^{-3}
see case id	bh9_06_8_bhrev_rks_uks_pbe_def2qzvpp		barrier height reverse kcal mol	8.71×10^{-3}
see case id	bh9_06_8_re_rks_uks_pbe_def2qzvpp		reaction energy kcal mol	6.77×10^{-3}
see case id	bh9_06_9_bhfwd_rks_uks_pbe_def2qzvpp		barrier height forward kcal mol	1.49×10^{-3}
see case id	bh9_06_9_bhrev_rks_uks_pbe_def2qzvpp		barrier height reverse kcal mol	9.53×10^{-3}
see case id	bh9_06_9_re_rks_uks_pbe_def2qzvpp		reaction energy kcal mol	8.02×10^{-3}
see case id	bh9_07_6_bhfwd_rks_uks_pbe_def2qzvpp		barrier height forward kcal mol	1.14×10^{-2}
see case id	bh9_07_6_bhrev_rks_uks_pbe_def2qzvpp		barrier height reverse kcal mol	3.91×10^{-3}
see case id	bh9_07_6_re_rks_uks_pbe_def2qzvpp		reaction energy kcal mol	7.52×10^{-3}
see case id	bh9_07_7_bhfwd_rks_uks_pbe_def2qzvpp		barrier height forward kcal mol	4.11×10^{-3}
see case id	bh9_07_7_bhrev_rks_uks_pbe_def2qzvpp		barrier height reverse kcal mol	1.26×10^{-2}
see case id	bh9_07_7_re_rks_uks_pbe_def2qzvpp		reaction energy kcal mol	8.54×10^{-3}
see case id	bh9_08_10_re_rks_uks_pbe_def2qzvpp		reaction energy kcal mol	3.42×10^{-4}
see case id	bh9_08_11_bhfwd_rks_uks_pbe_def2qzvpp		barrier height forward kcal mol	3.39×10^{-3}
see case id	bh9_08_13_bhrev_rks_uks_pbe_def2qzvpp		barrier height reverse kcal mol	9.10×10^{-3}
see case id	bh9_08_15_bhrev_rks_uks_pbe_def2qzvpp		barrier height reverse kcal mol	6.32×10^{-3}
see case id	bh9_08_6_bhrev_rks_uks_pbe_def2qzvpp		barrier height reverse kcal mol	4.50×10^{-3}

Table S21, continued.

Method	System / basis	Ref.	Quantity	$\lvert\Delta\rvert$
see case id	bh9_08_9_bhfwd_rks_uks_pbe_def2qzvpp		barrier height forward kcal mol	3.98×10^{-3}
see case id	bh9_09_13_bhrev_rks_uks_pbe_def2qzvpp		barrier height reverse kcal mol	7.43×10^{-3}
see case id	bh9_09_14_bhfwd_rks_uks_pbe_def2qzvpp		barrier height forward kcal mol	1.03×10^{-2}
see case id	bh9_09_14_bhrev_rks_uks_pbe_def2qzvpp		barrier height reverse kcal mol	5.16×10^{-3}
see case id	bh9_09_14_re_rks_uks_pbe_def2qzvpp		reaction energy kcal mol	5.12×10^{-3}
see case id	bh9_09_15_bhfwd_rks_uks_pbe_def2qzvpp		barrier height forward kcal mol	4.35×10^{-3}
see case id	bh9_09_15_bhrev_rks_uks_pbe_def2qzvpp		barrier height reverse kcal mol	9.25×10^{-3}
see case id	bh9_09_15_re_rks_uks_pbe_def2qzvpp		reaction energy kcal mol	4.91×10^{-3}
see case id	bh9_09_16_bhfwd_rks_uks_pbe_def2qzvpp		barrier height forward kcal mol	7.70×10^{-3}
see case id	bh9_09_16_bhrev_rks_uks_pbe_def2qzvpp		barrier height reverse kcal mol	8.38×10^{-3}
see case id	bh9_09_16_re_rks_uks_pbe_def2qzvpp		reaction energy kcal mol	6.94×10^{-4}
see case id	bh9_09_17_bhfwd_rks_uks_pbe_def2qzvpp		barrier height forward kcal mol	7.15×10^{-3}
see case id	bh9_09_17_bhrev_rks_uks_pbe_def2qzvpp		barrier height reverse kcal mol	7.73×10^{-3}
see case id	bh9_09_17_re_rks_uks_pbe_def2qzvpp		reaction energy kcal mol	5.87×10^{-4}
see case id	bh9_09_18_bhfwd_rks_uks_pbe_def2qzvpp		barrier height forward kcal mol	1.06×10^{-3}
see case id	bh9_09_18_bhrev_rks_uks_pbe_def2qzvpp		barrier height reverse kcal mol	1.36×10^{-2}
see case id	bh9_09_18_re_rks_uks_pbe_def2qzvpp		reaction energy kcal mol	1.46×10^{-2}
see case id	bh9_09_19_bhfwd_rks_uks_pbe_def2qzvpp		barrier height forward kcal mol	4.41×10^{-3}
see case id	bh9_09_19_bhrev_rks_uks_pbe_def2qzvpp		barrier height reverse kcal mol	1.16×10^{-2}
see case id	bh9_09_19_re_rks_uks_pbe_def2qzvpp		reaction energy kcal mol	7.21×10^{-3}
see case id	bh9_09_20_bhfwd_rks_uks_pbe_def2qzvpp		barrier height forward kcal mol	3.28×10^{-3}
see case id	bh9_09_20_bhrev_rks_uks_pbe_def2qzvpp		barrier height reverse kcal mol	8.29×10^{-3}
see case id	bh9_09_20_re_rks_uks_pbe_def2qzvpp		reaction energy kcal mol	5.01×10^{-3}
see case id	bh9_09_21_bhfwd_rks_uks_pbe_def2qzvpp		barrier height forward kcal mol	9.79×10^{-3}
see case id	bh9_09_21_bhrev_rks_uks_pbe_def2qzvpp		barrier height reverse kcal mol	6.72×10^{-3}
see case id	bh9_09_21_re_rks_uks_pbe_def2qzvpp		reaction energy kcal mol	3.09×10^{-3}
see case id	bh9_09_22_bhfwd_rks_uks_pbe_def2qzvpp		barrier height forward kcal mol	3.20×10^{-3}
see case id	bh9_09_22_bhrev_rks_uks_pbe_def2qzvpp		barrier height reverse kcal mol	7.39×10^{-3}
see case id	bh9_09_22_re_rks_uks_pbe_def2qzvpp		reaction energy kcal mol	1.06×10^{-2}

Table S21, continued.

Method	System / basis	Ref.	Quantity	$\lvert\Delta\rvert$
see case id	bh9_09_23_bhfwd_rks_uks_pbe_def2qzvpp		barrier height forward kcal mol	8.52×10^{-3}
see case id	bh9_09_23_bhrev_rks_uks_pbe_def2qzvpp		barrier height reverse kcal mol	9.75×10^{-3}
see case id	bh9_09_23_re_rks_uks_pbe_def2qzvpp		reaction energy kcal mol	1.23×10^{-3}
see case id	bh9_09_25_bhfwd_rks_uks_pbe_def2qzvpp		barrier height forward kcal mol	1.49×10^{-3}
see case id	bh9_09_25_bhrev_rks_uks_pbe_def2qzvpp		barrier height reverse kcal mol	6.23×10^{-3}
see case id	bh9_09_25_re_rks_uks_pbe_def2qzvpp		reaction energy kcal mol	4.74×10^{-3}
see case id	bh9_09_26_bhfwd_rks_uks_pbe_def2qzvpp		barrier height forward kcal mol	7.49×10^{-3}
see case id	bh9_09_26_bhrev_rks_uks_pbe_def2qzvpp		barrier height reverse kcal mol	8.05×10^{-3}
see case id	bh9_09_26_re_rks_uks_pbe_def2qzvpp		reaction energy kcal mol	5.62×10^{-4}
FCI	h2 / 6-31g	vibeqc	total energy ha	0
FCI	h2 / 6-31g	vibeqc	total energy ha	0
FCI	h2 / 6-31g	vibeqc	total energy ha	2.00×10^{-15}
FCI	h2 / 6-31g	vibeqc	total energy ha	1.41×10^{-11}
see case id	c-diamond-pbe-pob-tzvp-rev2		total energy ha	pass-pending-tolerance
see case id	caf2-fluorite-pbe-pob-tzvp-rev2		total energy ha	pass-pending-tolerance
see case id	gaas-zincblende-pbe-pob-tzvp-rev2		total energy ha	pass-pending-tolerance
see case id	gaas-zincblende-rhf-sto-3g		total energy ha	pass-pending-tolerance
see case id	gap-zincblende-rhf-sto-3g		total energy ha	pass-pending-tolerance
see case id	ge-diamond-rhf-sto-3g		total energy ha	pass-pending-tolerance
see case id	ge-diamond-rks-pbe-sto-3g		total energy ha	pass-pending-tolerance
see case id	lif-rocksalt-pbe-pob-tzvp-rev2		total energy ha	pass-pending-tolerance
see case id	lih-rocksalt-rhf-sto-3g		total energy ha	pass-pending-tolerance
see case id	mgo-rocksalt-pbe-pob-tzvp-rev2		total energy ha	pass-pending-tolerance
see case id	nacl-rocksalt-pbe-pob-tzvp-rev2		total energy ha	pass-pending-tolerance
see case id	nacl-rocksalt-rhf-pob-tzvp-rev2		total energy ha	pass-pending-tolerance
see case id	sic-zincblende-pbe-pob-tzvp-rev2		total energy ha	pass-pending-tolerance
see case id	sic-zincblende-rhf-pob-tzvp-rev2		total energy ha	pass-pending-tolerance
see case id	pfeat_c_prim_rks_gdf_multik_pbe_pob_tzvp_rev2_222		band gap sampled kset ev	held
see case id	bh9_01_45_bhfwd_rks_uks_pbe_def2qzvpp		barrier height forward kcal mol	4.85×10^{-2}
see case id	bh9_01_45_bhrev_rks_uks_pbe_def2qzvpp		barrier height reverse kcal mol	4.86×10^{-2}
see case id	bh9_01_47_bhrev_rks_uks_pbe_def2qzvpp		barrier height reverse kcal mol	7.19×10^{-2}

Table S21, continued.

Method	System / basis	Ref.	Quantity	$\lvert\Delta\rvert$
see case id	bh9_01_47_re_rks_uks_pbe_def2qzvpp		reaction energy kcal mol	6.84×10^{-2}
see case id	bh9_03_16_bhfwd_rks_uks_pbe_def2qzvpp		barrier height forward kcal mol	1.32×10^{-1}
see case id	bh9_03_16_bhrev_rks_uks_pbe_def2qzvpp		barrier height reverse kcal mol	1.44×10^{-1}
see case id	bh9_04_40_bhfwd_rks_uks_pbe_def2qzvpp		barrier height forward kcal mol	4.21×10^{-2}
see case id	bh9_04_40_bhrev_rks_uks_pbe_def2qzvpp		barrier height reverse kcal mol	3.94×10^{-2}
see case id	bh9_05_14_re_rks_uks_pbe_def2qzvpp		reaction energy kcal mol	1.38×10^{-2}
see case id	bh9_05_34_re_rks_uks_pbe_def2qzvpp		reaction energy kcal mol	1.25×10^{-2}
see case id	pfeat_nacl_prim_rks_gapw_multik_pbe_pob_tzvp_rev2_222		band gap sampled kset ev	9.09×10^{-1}
see case id	c-pobdzvprev2-pbe-222-1p0-c300		frontier gap eV	recorded-no-tolerance-class
see case id	lif-pobdzvprev2-pbe-222-1p0-c150		frontier gap eV	recorded-no-tolerance-class
see case id	lif-pobdzvprev2-pbe-222-1p0-c300		frontier gap eV	recorded-no-tolerance-class
see case id	lif-pobtzvp-pbe-222-1p0-c300		frontier gap eV	recorded-no-tolerance-class
see case id	lif-pobtzvprev2-pbe-222-1p0-c300		frontier gap eV	recorded-no-tolerance-class
see case id	lif-sto3g-pbe-222-1p0-c300		frontier gap eV	recorded-no-tolerance-class
see case id	lif-sto3g-pbe-444-1p0-c150		frontier gap eV	recorded-no-tolerance-class
see case id	mgo-pobdzvprev2-pbe-222-1p0-c300		frontier gap eV	recorded-no-tolerance-class
see case id	si-pobtzvprev2-pbe-222-1p0-c150		frontier gap eV	recorded-no-tolerance-class
CI	h2 / def2-svp	orca	total energy ha	reference-missing
see case id	gap-zincblende-rks-pbe-sto-3g		total energy ha	blocked-reference-leg

Table S22: Complete periodic validation database, grouped by Fock-build route and property. $|\Delta|$ is in hartree unless the quantity names another unit. Conventions are stated in Section S4.

Method	System / basis	Ref.	Quantity	$\|\Delta\|$
Periodic: Gaussian density fitting				
1 held, 4 reference-missing, 20 blocked.				
RKS/pbe	lif-prim / pob-tzvp-rev2	gpaw	band gap sampled kset ev	held
RHF	mgo-prim / sto-3g	pyscf	total energy ha	reference-missing
RHF	lih-prim / sto-3g	pyscf	total energy ha	reference-missing
RKS/pbe	mgo-prim / sto-3g	pyscf	total energy ha	reference-missing
RKS/pbe0	mgo-prim / sto-3g	pyscf	total energy ha	reference-missing
RHF	mgo-prim / sto-3g	pyscf	total energy ha	blocked
RKS/pbe	mgo-prim / sto-3g	pyscf	total energy ha	blocked
RKS/pbe	mgo-prim / sto-3g	pyscf	total energy ha	blocked
RHF	lih-prim / sto-3g	pyscf	total energy ha	blocked
RKS/pbe	mgo-prim / sto-3g	pyscf	total energy ha	blocked
RKS/pbe0	mgo-prim / sto-3g	pyscf	total energy ha	blocked
RKS/pbe0	mgo-prim / sto-3g	pyscf	total energy ha	blocked
RKS/pbe0	mgo-prim / sto-3g	pyscf	total energy ha	blocked
UHF	o2-box / sto-3g	pyscf	total energy ha	blocked
UHF	o2-box / sto-3g	pyscf	total energy ha	blocked
UKS/pbe	o2-box / sto-3g	pyscf	total energy ha	blocked
UKS/pbe	o2-box / sto-3g	pyscf	total energy ha	blocked
RKS/r2scan	mgo-prim / sto-3g	pyscf	total energy ha	blocked
RKS/r2scan	mgo-prim / sto-3g	pyscf	total energy ha	blocked
RKS/pbe	mgo-prim / sto-3g	pyscf	total energy ha	blocked
RKS/pbe	mgo-prim / sto-3g	pyscf	total energy ha	blocked
RKS/pbe	mgo-prim / sto-3g	pyscf	total energy ha	blocked
RKS/pbe	mgo-prim / sto-3g	pyscf	total energy ha	blocked
RKS/pbe	h2o-box / sto-3g	pyscf	total energy ha	blocked
RKS/pbe	h2o-box / sto-3g	pyscf	total energy ha	blocked
Periodic: bipolar expansion				
26 pass-pending-tolerance, 4 recorded-no-tolerance-class, 19 reference-property-measured, 2 artifact-incomplete, 22 blocked.				
RHF	bn-zincblende / sto-3g	crystal23	total energy ha	pass-pending-tolerance
RHF	caf2-fluorite / sto-3g	crystal23	total energy ha	pass-pending-tolerance
RHF	gasb-zincblende / sto-3g	crystal23	total energy ha	pass-pending-tolerance
RHF	inas-zincblende / sto-3g	crystal23	total energy ha	pass-pending-tolerance
RKS/pbe	inas-zincblende / sto-3g	crystal23	total energy ha	pass-pending-tolerance
RHF	inp-zincblende / sto-3g	crystal23	total energy ha	pass-pending-tolerance
RKS/pbe	inp-zincblende / sto-3g	crystal23	total energy ha	pass-pending-tolerance
RHF	insb-zincblende / sto-3g	crystal23	total energy ha	pass-pending-tolerance
RKS/pbe	insb-zincblende / sto-3g	crystal23	total energy ha	pass-pending-tolerance
RHF	kbr-rocksalt / sto-3g	crystal23	total energy ha	pass-pending-tolerance
RKS/pbe	kbr-rocksalt / sto-3g	crystal23	total energy ha	pass-pending-tolerance
RHF	kcl-rocksalt / sto-3g	crystal23	total energy ha	pass-pending-tolerance

Table S22, continued.

Method	System / basis	Ref.	Quantity	|Δ|
RKS/pbe	kcl-rocksalt / sto-3g	crystal23	total energy ha	pass-pending-tolerance
RHF	ki-rocksalt / sto-3g	crystal23	total energy ha	pass-pending-tolerance
RKS/pbe	ki-rocksalt / sto-3g	crystal23	total energy ha	pass-pending-tolerance
RKS/pbe	lih-rocksalt / pob-tzvp-rev2	crystal23	total energy ha	pass-pending-tolerance
RHF	lih-rocksalt / pob-tzvp-rev2	crystal23	total energy ha	pass-pending-tolerance
RHF	mgo-rocksalt / sto-3g	crystal23	total energy ha	pass-pending-tolerance
RHF	naf-rocksalt / sto-3g	crystal23	total energy ha	pass-pending-tolerance
RKS/pbe	naf-rocksalt / sto-3g	crystal23	total energy ha	pass-pending-tolerance
RHF	rbcl-rocksalt / sto-3g	crystal23	total energy ha	pass-pending-tolerance
RKS/pbe	rbcl-rocksalt / sto-3g	crystal23	total energy ha	pass-pending-tolerance
RKS/pbe	si-diamond / pob-tzvp-rev2	crystal23	total energy ha	pass-pending-tolerance
RHF	si-diamond / pob-tzvp-rev2	crystal23	total energy ha	pass-pending-tolerance
RHF	sn-alpha / sto-3g	crystal23	total energy ha	pass-pending-tolerance
RKS/pbe	sn-alpha / sto-3g	crystal23	total energy ha	pass-pending-tolerance
RHF	lih-rocksalt / pob-tzvp	literature	total energy ha	recorded-no-tolerance-class
RKS/pw1pw-pob2013	lih-rocksalt / pob-tzvp	literature	total energy ha	recorded-no-tolerance-class
RHF	nacl-rocksalt / pob-tzvp	literature	total energy ha	recorded-no-tolerance-class
RKS/pw1pw-pob2013	nacl-rocksalt / pob-tzvp	literature	total energy ha	recorded-no-tolerance-class
RHF	caf2-fluorite / sto-3g	crystal23	crystal23 shrink2 minus shrink8 total energy mha	reference-property-measured
RHF	gasb-zincblende / sto-3g	crystal23	crystal23 shrink2 minus shrink8 total energy mha	reference-property-measured
RHF	inas-zincblende / sto-3g	crystal23	crystal23 shrink2 minus shrink8 total energy mha	reference-property-measured
RKS/pbe	inas-zincblende / sto-3g	crystal23	crystal23 shrink2 minus shrink8 total energy mha	reference-property-measured
RHF	inp-zincblende / sto-3g	crystal23	crystal23 shrink2 minus shrink8 total energy mha	reference-property-measured
RKS/pbe	inp-zincblende / sto-3g	crystal23	crystal23 shrink2 minus shrink8 total energy mha	reference-property-measured
RHF	insb-zincblende / sto-3g	crystal23	crystal23 shrink2 minus shrink8 total energy mha	reference-property-measured
RKS/pbe	insb-zincblende / sto-3g	crystal23	crystal23 shrink2 minus shrink8 total energy mha	reference-property-measured
RHF	kbr-rocksalt / sto-3g	crystal23	crystal23 shrink2 minus shrink8 total energy mha	reference-property-measured
RKS/pbe	kbr-rocksalt / sto-3g	crystal23	crystal23 shrink2 minus shrink8 total energy mha	reference-property-measured
RHF	kcl-rocksalt / sto-3g	crystal23	crystal23 shrink2 minus shrink8 total energy mha	reference-property-measured

Table S22, continued.

Method	System / basis	Ref.	Quantity	|Δ|
RKS/pbe	kcl-rocksalt / sto-3g	crystal23	crystal23 shrink2 minus shrink8 total energy mha	reference-property-measured
RHF	ki-rocksalt / sto-3g	crystal23	crystal23 shrink2 minus shrink8 total energy mha	reference-property-measured
RKS/pbe	ki-rocksalt / sto-3g	crystal23	crystal23 shrink2 minus shrink8 total energy mha	reference-property-measured
RHF	mgo-rocksalt / sto-3g	crystal23	crystal23 shrink2 minus shrink8 total energy mha	reference-property-measured
RHF	naf-rocksalt / sto-3g	crystal23	crystal23 shrink2 minus shrink8 total energy mha	reference-property-measured
RKS/pbe	naf-rocksalt / sto-3g	crystal23	crystal23 shrink2 minus shrink8 total energy mha	reference-property-measured
RHF	rbcl-rocksalt / sto-3g	crystal23	crystal23 shrink2 minus shrink8 total energy mha	reference-property-measured
RKS/pbe	rbcl-rocksalt / sto-3g	crystal23	crystal23 shrink2 minus shrink8 total energy mha	reference-property-measured
RHF	lih-prim / sto-3g	crystal23	total energy ha	artifact-incomplete
UHF	o2-box / sto-3g	crystal23	total energy ha	artifact-incomplete
RHF	lih-prim / sto-3g	crystal23	total energy ha	blocked
UHF	o2-box / sto-3g	crystal23	total energy ha	blocked
RKS/pbe	lih-prim / sto-3g	crystal23	total energy ha	blocked
RKS/pbe	lih-prim / sto-3g	crystal23	total energy ha	blocked
UKS/pbe	o2-box / sto-3g	crystal23	total energy ha	blocked
UKS/pbe	o2-box / sto-3g	crystal23	total energy ha	blocked
RHF	lih-prim / sto-3g	crystal23	total energy ha	blocked
RHF	lih-prim / sto-3g	crystal23	total energy ha	blocked
RKS/pbe	lih-prim / sto-3g	crystal23	total energy ha	blocked
RKS/pbe	lih-prim / sto-3g	crystal23	total energy ha	blocked
RKS/pbe0	lih-prim / sto-3g	crystal23	total energy ha	blocked
RKS/pbe0	lih-prim / sto-3g	crystal23	total energy ha	blocked
RKS/pbe0	lih-prim / sto-3g	crystal23	total energy ha	blocked
RKS/pbe0	lih-prim / sto-3g	crystal23	total energy ha	blocked
RKS/pbe	lih-prim / sto-3g	crystal23	total energy ha	blocked
RKS/pbe	lih-prim / sto-3g	crystal23	total energy ha	blocked
RKS/pbe	mgo-prim / sto-3g	crystal23	total energy ha	blocked
RKS/pbe	mgo-prim / sto-3g	crystal23	total energy ha	blocked
RKS/pbe	lif-prim / sto-3g	crystal23	total energy ha	blocked
RKS/pbe	lif-prim / sto-3g	crystal23	total energy ha	blocked
RKS/pbe	lih-prim / sto-3g	crystal23	total energy ha	blocked
RKS/pbe	lih-prim / sto-3g	crystal23	total energy ha	blocked

Periodic: Gaussian and plane waves

64 held, 67 fail, 2 incomplete, 1 artifact-incomplete, 4 reference-missing, 17 blocked.

RKS/pbe	c-prim / pob-dzvp-rev2	gpaw	band gap sampled kset ev	held
RKS/pbe	c-prim / pob-dzvp-rev2	gpaw	band gap sampled kset ev	held
RKS/pbe	c-prim / pob-dzvp-rev2	gpaw	band gap sampled kset ev	held
RKS/pbe	lif-prim / pob-dzvp-rev2	gpaw	band gap sampled kset ev	held
RKS/pbe	lif-prim / pob-dzvp-rev2	gpaw	band gap sampled kset ev	held
RKS/pbe	lif-prim / pob-dzvp-rev2	gpaw	band gap sampled kset ev	held
RKS/pbe	lif-prim / pob-dzvp-rev2	gpaw	band gap sampled kset ev	held
RKS/pbe	lif-prim / pob-dzvp-rev2	gpaw	band gap sampled kset ev	held
RKS/pbe	lif-prim / pob-tzvp	gpaw	band gap sampled kset ev	held
RKS/pbe	lif-prim / pob-tzvp-rev2	gpaw	band gap sampled kset ev	held
RKS/pbe	mgo-prim / pob-dzvp-rev2	gpaw	band gap sampled kset ev	held
RKS/pbe	mgo-prim / pob-dzvp-rev2	gpaw	band gap sampled kset ev	held
RKS/pbe	mgo-prim / pob-dzvp-rev2	gpaw	band gap sampled kset ev	held
RKS/pbe	nacl-prim / pob-dzvp-rev2	gpaw	band gap sampled kset ev	held
RKS/pbe	nacl-prim / pob-dzvp-rev2	gpaw	band gap sampled kset ev	held

Table S22, continued.

Method	System / basis	Ref.	Quantity	$\lvert\Delta\rvert$
RKS/pbe	nacl-prim / pob-dzvp-rev2	gpaw	band gap sampled kset ev	held
RKS/lda	si-prim / pob-tzvp-rev2	gpaw	band gap sampled kset ev	held
RKS/lda	si-prim / pob-tzvp-rev2	gpaw	band gap sampled kset ev	held
RKS/lda	si-prim / pob-tzvp-rev2	gpaw	band gap sampled kset ev	held
RKS/pbe	si-prim / pob-tzvp-rev2	gpaw	band gap sampled kset ev	held
RKS/pbe	si-prim / pob-tzvp-rev2	gpaw	band gap sampled kset ev	held
RKS/pbe	si-prim / pob-tzvp-rev2	gpaw	band gap sampled kset ev	held
RKS/pbe	si-prim / pob-tzvp-rev2	gpaw	band gap sampled kset ev	held
RKS/pbe	si-prim / pob-tzvp-rev2	gpaw	band gap sampled kset ev	held
RKS/pbe	si-prim / pob-tzvp-rev2	gpaw	band gap sampled kset ev	held
RKS/pbe	si-prim / pob-tzvp-rev2	gpaw	band gap sampled kset ev	held
RKS/pbe	si-prim / pob-tzvp-rev2	gpaw	band gap sampled kset ev	held
RKS/pbe	si-prim / pob-tzvp-rev2	gpaw	band gap sampled kset ev	held
RKS/pbe	si-prim / pob-tzvp-rev2	gpaw	band gap sampled kset ev	held
RKS/pbe	si-prim / pob-tzvp-rev2	gpaw	band gap sampled kset ev	held
RKS/pbe	c-prim / pob-dzvp-rev2	gpaw	band gap sampled kset ev	held
RKS/pbe	c-prim / pob-dzvp-rev2	gpaw	band gap sampled kset ev	held
RKS/pbe	c-prim / pob-tzvp	gpaw	band gap sampled kset ev	held
RKS/pbe	c-prim / pob-tzvp	gpaw	band gap sampled kset ev	held
RKS/pbe	c-prim / pob-tzvp	gpaw	band gap sampled kset ev	held
RKS/pbe	c-prim / pob-tzvp	gpaw	band gap sampled kset ev	held
RKS/pbe	lif-prim / pob-dzvp-rev2	gpaw	band gap sampled kset ev	held
RKS/pbe	lif-prim / pob-dzvp-rev2	gpaw	band gap sampled kset ev	held
RKS/pbe	lif-prim / pob-dzvp-rev2	gpaw	band gap sampled kset ev	held
RKS/pbe	lif-prim / pob-tzvp	gpaw	band gap sampled kset ev	held
RKS/pbe	lif-prim / pob-tzvp	gpaw	band gap sampled kset ev	held
RKS/pbe	lif-prim / pob-tzvp-rev2	gpaw	band gap sampled kset ev	held
RKS/pbe	lif-prim / pob-tzvp-rev2	gpaw	band gap sampled kset ev	held
RKS/pbe	mgo-prim / pob-dzvp-rev2	gpaw	band gap sampled kset ev	held
RKS/pbe	mgo-prim / pob-dzvp-rev2	gpaw	band gap sampled kset ev	held
RKS/pbe	mgo-prim / pob-tzvp-rev2	gpaw	band gap sampled kset ev	held
RKS/pbe	mgo-prim / pob-tzvp-rev2	gpaw	band gap sampled kset ev	held
RKS/pbe	mgo-prim / pob-tzvp-rev2	gpaw	band gap sampled kset ev	held
RKS/pbe	mgo-prim / pob-tzvp-rev2	gpaw	band gap sampled kset ev	held
RKS/pbe	nacl-prim / pob-dzvp-rev2	gpaw	band gap sampled kset ev	held
RKS/pbe	nacl-prim / pob-dzvp-rev2	gpaw	band gap sampled kset ev	held
RKS/pbe	nacl-prim / pob-tzvp	gpaw	band gap sampled kset ev	held
RKS/pbe	nacl-prim / pob-tzvp	gpaw	band gap sampled kset ev	held
RKS/pbe	nacl-prim / pob-tzvp-rev2	gpaw	band gap sampled kset ev	held
RKS/pbe	nacl-prim / pob-tzvp-rev2	gpaw	band gap sampled kset ev	held
RKS/lda	si-prim / pob-tzvp-rev2	gpaw	band gap sampled kset ev	held
RKS/pbe	si-prim / def2-sv(p)	gpaw	band gap sampled kset ev	held
RKS/pbe	si-prim / pob-tzvp	gpaw	band gap sampled kset ev	held
RKS/pbe	si-prim / pob-tzvp	gpaw	band gap sampled kset ev	held
RKS/pbe	si-prim / pob-tzvp-rev2	gpaw	band gap sampled kset ev	held
RKS/pbe	si-prim / pob-tzvp-rev2	gpaw	band gap sampled kset ev	held
RKS/pbe	si-prim / pob-tzvp-rev2	gpaw	band gap sampled kset ev	held
RKS/pbe	si-prim / pob-tzvp-rev2	gpaw	band gap sampled kset ev	held
RKS/pbe	si-prim / pob-tzvp-rev2	gpaw	band gap sampled kset ev	held
RKS/pbe	c-prim / pob-dzvp-rev2	gpaw	band gap sampled kset ev	5.53×10^{-1}
RKS/pbe	lif-prim / pob-dzvp-rev2	gpaw	band gap sampled kset ev	7.10×10^{-1}
RKS/pbe	lif-prim / sto-3g	gpaw	band gap sampled kset ev	6.04×10^{-1}
RKS/pbe	lif-prim / sto-3g	gpaw	band gap sampled kset ev	6.56×10^{-2}
RKS/pbe	lif-prim / sto-3g	gpaw	band gap sampled kset ev	5.84×10^{-2}
RKS/pbe	lif-prim / sto-3g	gpaw	band gap sampled kset ev	5.69×10^{-2}
RKS/pbe	mgo-prim / pob-dzvp-rev2	gpaw	band gap sampled kset ev	1.94×10^{-1}
RKS/pbe	nacl-prim / pob-dzvp-rev2	gpaw	band gap sampled kset ev	1.38×10^{-1}
RKS/lda	si-prim / pob-tzvp-rev2	gpaw	band gap sampled kset ev	3.24×10^{-1}

Table S22, continued.

Method	System / basis	Ref.	Quantity	$\lvert\Delta\rvert$
RKS/pbe	si-prim / pob-tzvp-rev2	gpaw	band gap sampled kset ev	2.92×10^{-1}
RKS/pbe	si-prim / sto-3g	gpaw	band gap sampled kset ev	3.97×10^{-1}
RKS/pbe	si-prim / pob-tzvp-rev2	gpaw	eos birch murnaghan a0 ang	n/a
RKS/pbe	si-prim / pob-tzvp-rev2	gpaw	eos birch murnaghan b0 gpa	n/a
RKS/pbe	si-prim / pob-tzvp-rev2	gpaw	eos relative energy span ev	n/a
RKS/pbe	si-prim / sto-3g	gpaw	band gap sampled kset ev	6.96×10^{-2}
RKS/pbe	si-prim / sto-3g	gpaw	band gap sampled kset ev	6.82×10^{-2}
RKS/pbe	si-prim / sto-3g	gpaw	band gap sampled kset ev	6.59×10^{-2}
RKS/pbe	c-prim / sto-3g	gpaw	band gap sampled kset ev	5.52×10^{-2}
RKS/pbe	c-prim / sto-3g	gpaw	band gap sampled kset ev	5.52×10^{-2}
RKS/pbe	c-prim / sto-3g	gpaw	band gap sampled kset ev	6.05×10^{-2}
RKS/pbe	c-prim / sto-3g	gpaw	band gap sampled kset ev	6.05×10^{-2}
RKS/pbe	lif-prim / sto-3g	gpaw	band gap sampled kset ev	5.28×10^{-2}
RKS/pbe	mgo-prim / pob-tzvp	gpaw	band gap sampled kset ev	1.13×10^{-1}
RKS/pbe	mgo-prim / pob-tzvp	gpaw	band gap sampled kset ev	1.13×10^{-1}
RKS/pbe	mgo-prim / pob-tzvp	gpaw	zone centre conduction level ev	1.32×10^{-1}
RKS/pbe	mgo-prim / pob-tzvp	gpaw	band gap sampled kset ev	9.93×10^{-2}
RKS/pbe	mgo-prim / pob-tzvp	gpaw	band gap sampled kset ev	9.93×10^{-2}
RKS/pbe	mgo-prim / pob-tzvp	gpaw	zone centre conduction level ev	1.33×10^{-1}
RKS/pbe	mgo-prim / sto-3g	gpaw	band gap sampled kset ev	7.26×10^{-2}
RKS/pbe	mgo-prim / sto-3g	gpaw	band gap sampled kset ev	7.26×10^{-2}
RKS/pbe	mgo-prim / sto-3g	gpaw	band gap sampled kset ev	5.87×10^{-2}
RKS/pbe	mgo-prim / sto-3g	gpaw	band gap sampled kset ev	5.87×10^{-2}
RKS/pbe	nacl-prim / sto-3g	gpaw	band gap sampled kset ev	1.67×10^{-1}
RKS/pbe	nacl-prim / sto-3g	gpaw	band gap sampled kset ev	1.67×10^{-1}
RKS/pbe	nacl-prim / sto-3g	gpaw	band gap sampled kset ev	1.28×10^{-1}
RKS/pbe	nacl-prim / sto-3g	gpaw	band gap sampled kset ev	1.68×10^{-1}
RKS/pbe	si-prim / pob-tzvp-rev2;sto-3g	vibeqc	cutoff ladder total energy move 150 to 600 ha	6.60
RKS/pbe	si-prim / sto-3g	gpaw	band gap sampled kset ev	7.19×10^{-2}
RKS/pbe	si-prim / sto-3g	gpaw	band gap sampled kset ev	6.96×10^{-2}
RKS/pbe	si-prim / sto-3g	gpaw	band gap sampled kset ev	6.96×10^{-2}
RKS/pbe	si-prim / sto-3g	gpaw	band gap sampled kset ev	1.26×10^{-1}
RKS/pbe	si-prim / sto-3g	gpaw	band gap sampled kset ev	1.01×10^{-1}
RKS/pbe	si-prim / sto-3g	gpaw	band gap sampled kset ev	5.48×10^{-2}
RKS/pbe	si-prim / sto-3g	gpaw	band gap sampled kset ev	4.05×10^{-2}
RKS/pbe	si-prim / sto-3g	gpaw	band gap sampled kset ev	1.32×10^{-2}
RKS/pbe	si-prim / sto-3g	gpaw	eos relative energy span ev	n/a
RKS/pbe	si-prim / sto-3g	gpaw	eos birch murnaghan a0 ang	n/a
RKS/pbe	si-prim / sto-3g	gpaw	eos birch murnaghan b0 prime	n/a
RKS/pbe	si-prim / sto-3g	gpaw	band gap sampled kset ev	6.96×10^{-2}
RKS/pbe	si-prim / sto-3g	gpaw	band gap sampled kset ev	6.99×10^{-2}
RKS/pbe	si-prim / sto-3g	gpaw	band gap sampled kset ev	6.82×10^{-2}
RKS/pbe	si-prim / sto-3g	gpaw	band gap sampled kset ev	6.82×10^{-2}
RKS/pbe	si-prim / sto-3g	gpaw	band gap sampled kset ev	1.20×10^{-1}
RKS/pbe	si-prim / sto-3g	gpaw	band gap sampled kset ev	1.16×10^{-1}
RKS/pbe	si-prim / sto-3g	gpaw	band gap sampled kset ev	5.41×10^{-2}
RKS/pbe	si-prim / sto-3g	gpaw	band gap sampled kset ev	4.05×10^{-2}
RKS/pbe	si-prim / sto-3g	gpaw	band gap sampled kset ev	1.47×10^{-2}
RKS/pbe	si-prim / sto-3g	gpaw	eos relative energy span ev	n/a
RKS/pbe	si-prim / sto-3g	gpaw	eos birch murnaghan a0 ang	n/a
RKS/pbe	si-prim / sto-3g	gpaw	eos birch murnaghan b0 prime	n/a
RKS/pbe	si-prim / sto-3g	gpaw	eos fft grid discontinuity ha	6.60
RKS/pbe	mgo-prim / def2-svp	gpaw	band gap sampled kset ev	2.35×10^{-1}

Table S22, continued.

Method	System / basis	Ref.	Quantity	$\lvert\Delta\rvert$
RKS/pbe	lif-prim / def2-svp	gpaw	band gap sampled kset ev	3.57×10^{-1}
RKS/pbe	si-prim / def2-svp	gpaw	band gap sampled kset ev	1.56×10^{-1}
RKS/pbe	si-prim / def2-svp	gpaw	band gap sampled kset ev	1.30×10^{-1}
RKS/pbe	si-prim / def2-svp	gpaw	band gap sampled kset ev	4.34×10^{-2}
RKS/pbe	si-prim / def2-svp	gpaw	band gap sampled kset ev	1.58×10^{-1}
RKS/pbe	si-prim / def2-svp	gpaw	lattice constant a0 angstrom	incomplete
RKS/pbe	si-prim / def2-svp	gpaw	bulk modulus b0 gpa	incomplete
UKS/pbe	o2-box / sto-3g	gpaw	total energy ha	artifact-incomplete
RHF	lif-prim / sto-3g	gpaw	total energy ha	reference-missing
UHF	o2-box / sto-3g	gpaw	total energy ha	reference-missing
UKS/pbe	o2-box / sto-3g	gpaw	total energy ha	reference-missing
RKS/pbe	si-prim / sto-3g	gpaw	total energy ha	reference-missing
RHF	lif-prim / sto-3g	gpaw	total energy ha	blocked
RKS/pbe	lif-prim / sto-3g	gpaw	total energy ha	blocked
RKS/pbe	lif-prim / sto-3g	gpaw	total energy ha	blocked
UHF	o2-box / sto-3g	gpaw	total energy ha	blocked
UKS/pbe	o2-box / sto-3g	gpaw	total energy ha	blocked
RKS/pbe	si-prim / sto-3g	gpaw	total energy ha	blocked
UKS/pbe	o2-box / sto-3g	gpaw	total energy ha	blocked
RKS/r2scan	lif-prim / sto-3g	gpaw	total energy ha	blocked
RKS/r2scan	lif-prim / sto-3g	gpaw	total energy ha	blocked
RKS/pbe	lif-prim / sto-3g	gpaw	total energy ha	blocked
RKS/pbe	lif-prim / sto-3g	gpaw	total energy ha	blocked
RKS/pbe	lif-prim / sto-3g	gpaw	total energy ha	blocked
RKS/pbe	lif-prim / sto-3g	gpaw	total energy ha	blocked
RKS/pbe	lif-prim / sto-3g	gpaw	total energy ha	blocked
RKS/pbe	lif-prim / sto-3g	gpaw	total energy ha	blocked
RKS/pbe	lif-prim / sto-3g	gpaw	total energy ha	blocked
RKS/pbe	lif-prim / sto-3g	gpaw	total energy ha	blocked

Periodic: GAPW

1 reference-missing, 5 blocked.

RHF	lif-prim / sto-3g	gpaw	total energy ha	reference-missing
RHF	lif-prim / sto-3g	gpaw	total energy ha	blocked
RKS/pbe	lif-prim / sto-3g	gpaw	total energy ha	blocked
RKS/pbe	lif-prim / sto-3g	gpaw	total energy ha	blocked
UKS/pbe	o2-box / sto-3g	gpaw	total energy ha	blocked
UKS/pbe	o2-box / sto-3g	gpaw	total energy ha	blocked

Periodic properties

11 artifact-incomplete, 1 blocked, 13 queued.

RHF	lih-prim / sto-3g	pyscf	total energy ha	artifact-incomplete
RHF	lih-prim / sto-3g	pyscf	total energy ha	artifact-incomplete
UKS/pbe	o2-box / sto-3g	pyscf	total energy ha	artifact-incomplete
UKS/pbe	o2-box / sto-3g	pyscf	total energy ha	artifact-incomplete
RKS/pbe	lif-prim / sto-3g	gpaw	total energy ha	artifact-incomplete
RKS/pbe	si-prim / sto-3g	gpaw	total energy ha	artifact-incomplete
RKS/pbe	si-prim / sto-3g	gpaw	total energy ha	artifact-incomplete
RKS/pbe	lih-prim / sto-3g	crystal23	total energy ha	artifact-incomplete
RKS/pbe	lih-prim / sto-3g	crystal23	total energy ha	artifact-incomplete
RKS/pbe	h2o-box / sto-3g	pyscf	total energy ha	artifact-incomplete
RKS/pbe	h2o-box / sto-3g	pyscf	total energy ha	artifact-incomplete
RKS/pbe	lif-prim / sto-3g	gpaw	total energy ha	blocked
RKS/pbe	lif-prim / sto-3g	gpaw	total energy ha	queued
RKS/pbe	si-prim / sto-3g	gpaw	total energy ha	queued
RKS/pbe	lih-prim / sto-3g	crystal23	total energy ha	queued
RKS/pbe	mgo-prim / sto-3g	crystal23	total energy ha	queued
RKS/pbe	mgo-prim / sto-3g	crystal23	total energy ha	queued

Table S22, continued.

Method	System / basis	Ref.	Quantity	|Δ|
RKS/pbe	lif-prim / sto-3g	gpaw	total energy ha	queued
RKS/pbe	lif-prim / sto-3g	gpaw	total energy ha	queued
RKS/pbe	lif-prim / sto-3g	gpaw	total energy ha	queued
RKS/pbe	lif-prim / sto-3g	gpaw	total energy ha	queued
RKS/pbe	lif-prim / sto-3g	crystal23	total energy ha	queued
RKS/pbe	lif-prim / sto-3g	crystal23	total energy ha	queued
RKS/pbe	lif-prim / sto-3g	gpaw	total energy ha	queued
RKS/pbe	lif-prim / sto-3g	gpaw	total energy ha	queued

References

[1] P. Jurečka, J. Šponer, J. Černý, and P. Hobza. "Benchmark database of accurate (MP2 and CCSD(T) complete basis set limit) interaction energies of small model complexes, DNA base pairs, and amino acid pairs". In: *Phys. Chem. Chem. Phys.* 8.17 (2006), pp. 1985–1993. DOI: 10.1039/B600027D.

[2] M. F. Peintinger, D. Vilela Oliveira, and T. Bredow. "Consistent Gaussian basis sets of triple-zeta valence with polarization quality for solid-state calculations". In: *Journal of Computational Chemistry* 34.6 (2013), pp. 451–459. DOI: 10.1002/jcc.23153.

[3] F. Weigend and R. Ahlrichs. "Balanced basis sets of split valence, triple zeta valence and quadruple zeta valence quality for H to Rn: design and assessment of accuracy". In: *Physical Chemistry Chemical Physics* 7.18 (2005), pp. 3297–3305. DOI: 10.1039/b508541a.

[4] C. Adamo and V. Barone. "Toward reliable density functional methods without adjustable parameters: the PBE0 model". In: *The Journal of Chemical Physics* 110.13 (1999), pp. 6158–6170. DOI: 10.1063/1.478522.

[5] J. P. Perdew, K. Burke, and M. Ernzerhof. "Generalized gradient approximation made simple". In: *Physical Review Letters* 77.18 (1996), pp. 3865–3868. DOI: 10.1103/PhysRevLett.77.3865.

[6] S. Grimme, J. Antony, S. Ehrlich, and H. Krieg. "A consistent and accurate ab initio parametrization of density functional dispersion correction (DFT-D) for the 94 elements H–Pu". In: *The Journal of Chemical Physics* 132.15 (2010), p. 154104. DOI: 10.1063/1.3382344.

[7] S. Grimme, S. Ehrlich, and L. Goerigk. "Effect of the damping function in dispersion corrected density functional theory". In: *Journal of Computational Chemistry* 32.7 (2011), pp. 1456–1465. DOI: 10.1002/jcc.21759.

[8] E. F. Valeev. *Libint: a library for the evaluation of molecular integrals of many-body operators over Gaussian functions*. https://github.com/evaleev/libint. Version 2.13.1. 2025.

[9] S. Lehtola, C. Steigemann, M. J. T. Oliveira, and M. A. L. Marques. "Recent developments in libxc — a comprehensive library of functionals for density functional theory". In: *SoftwareX* 7 (2018), pp. 1–5. DOI: 10.1016/j.softx.2017.11.002.