Supplementary Material for "Symmetry-adapted perturbation theory with Kohn-Sham orbitals using non-empirically tuned, long-range-corrected density functionals"

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1. RANGE SEPARATION PARAMETERS

Tables S1 and S2 list the "tuned" value of the range separation parameter, ω, for each of the monomers considered in this work. These values were tuned using the aug-cc-pV6Z basis set for He, the aug-cc-pV5Z basis set for Ne, the aug-cc-pVQZ basis set for the SS41 data set, and the aug-cc-pVTZ basis set for both the S22 and S66 data sets. Optimized values are computed separately for the LRC-ωPBE functional[1] and the LRC-ωPBEh functional.[2]

2. BENCHMARK ENERGY COMPONENTS FOR THE SS41 DATA SET

Energy components for SS41computed at the SAPT2+(3)/aug-cc-pVQZ level are listed in Table S3 and energy components for S22computed at the SAPT2+(3)/aug-cc-pVTZ level are listed in Table S4. The SAPT2+(3) is defined as follows:[3]

$$\begin{aligned} E_{\text{SAPT2+(3)}} = {} & E_{\text{elst}}^{(10)} + E_{\text{elst,resp}}^{(12)} + E_{\text{elst,resp}}^{(13)} \\ & + E_{\text{exch}}^{(10)} + E_{\text{exch}}^{(11)} + E_{\text{exch}}^{(12)} \\ & + E_{\text{ind,resp}}^{(20)} + E_{\text{exch-ind,resp}}^{(20)} + {}^{t}E_{\text{ind}}^{(22)} + {}^{t}E_{\text{exch-ind}}^{(22)} + \delta E_{\text{int,resp}}^{\text{HF}} \\ & + E_{\text{disp}}^{(20)} + E_{\text{exch-disp}}^{(20)} + E_{\text{disp}}^{(21)} + E_{\text{disp}}^{(22)} + E_{\text{disp}}^{(30)} \, . \end{aligned} \tag{S1}$$

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The energy components are grouped as follows:[4]

$$E_{\text{electrostatic}} = E^{(10)}_{\text{elst}} + E^{(12)}_{\text{elst,resp}} + E^{(13)}_{\text{elst,resp}} \ , \tag{S2}$$

$$E_{\text{exchange}} = E^{(10)}_{\text{exch}} + E^{(11)}_{\text{exch}} + E^{(12)}_{\text{exch}} \ , \tag{S3}$$

$$E_{\text{induction}} = E^{(20)}_{\text{ind,resp}} + E^{(20)}_{\text{exch-ind,resp}} + {}^{t}E^{(22)}_{\text{ind}} + {}^{t}E^{(22)}_{\text{exch-ind}} + \delta E^{\text{HF}}_{\text{int,resp}} \ , \tag{S4}$$

$$E_{\text{dispersion}} = E^{(20)}_{\text{disp}} + E^{(20)}_{\text{exch-disp}} + E^{(21)}_{\text{disp}} + E^{(22)}_{\text{disp}} + E^{(30)}_{\text{disp}} \ . \tag{S5}$$

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[1] A. W. Lange and J. M. Herbert, J. Am. Chem. Soc. **131**, 3913 (2009).

[2] M. A. Rohrdanz, K. M. Martins, and J. M. Herbert, J. Chem. Phys. **130**, 054112 (2009).

[3] E. G. Hohenstein and C. D. Sherrill, WIREs Comput. Mol. Sci. **2**, 304 (2012).

[4] J. C. Flick, D. Kosenkov, E. G. Hohenstein, C. D. Sherrill, and L. V. Slipchenko, J. Chem. Theory Comput. **8**, 2835 (2012).

	ω/bohr^{-1}	
Monomer	LRC-ωPBE	LRC-ωPBEh
—He_2 and Ne_2—		
He	1.025	0.900
Ne	0.800	0.650
—SS41 molecules—		
Ar	0.550	0.475
ethene	0.375	0.300
methane	0.450	0.400
borane	0.475	0.425
ethyne	0.400	0.350
water	0.500	0.400
methanol	0.425	0.350
CH_3F	0.500	0.425
ethane	0.425	0.375
F_2	0.675	0.550
formaldehyde	0.450	0.350
formamide	0.375	0.300
formic acid	0.400	0.325
CH_3NH_2	0.400	0.325
ammonia	0.450	0.350
HCN	0.450	0.400
HF	0.600	0.500

TABLE S1: Tuned range separation parameters for various monomers in He_2, Ne_2, and SS41 data set. The basis sets used are aug-cc-pV6Z basis set for He, aug-cc-pV5Z for Ne, and aug-cc-pVQZ basis set for the monomers in the SS41 data set.

	ω/bohr^{-1}	
Monomer	LRC-ωPBE	LRC-ωPBEh
—S22 molecules—		
adenine	0.275	0.225
2-aminopyridine	0.300	0.225
benzene	0.275	0.225
ethyne	0.400	0.350
ethene	0.350	0.300
methane	0.450	0.400
formamide	0.375	0.300
formic acid	0.425	0.325
water	0.500	0.400
HCN	0.550	0.500
indole	0.275	0.225
ammonia	0.450	0.350
phenol	0.300	0.250
pyrazine	0.375	0.300
2-pyridoxine	0.300	0.250
thymine	0.625	0.525
uracil	0.475	0.375
—S66 molecules—		
methylamine	0.400	0.325
methanol	0.425	0.350
$AcNH_2$	0.350	0.275
AcOH	0.375	0.300
cyclopentane	0.425	0.375
neopentane	0.300	0.250
pentane	0.300	0.250
peptide	0.325	0.250
pyridine	0.300	0.225

TABLE S2: Tuned range separation parameters for various monomers. The aug-cc-pVTZ basis set in each case.

system	Elst.	Exch.-Rep.	Ind.	Disp.	Total
	—A24 dimers—				
H_2O-NH_3	-10.99	11.25	-3.76	-3.06	-6.57
H_2O dimer	-7.90	7.59	-2.35	-2.37	-5.03
HCN dimer	-5.91	4.10	-1.54	-1.74	-5.10
HF dimer	-6.41	6.04	-2.36	-1.83	-4.56
NH_3 dimer	-4.75	4.48	-0.86	-2.04	-3.17
HF-CH_4	-1.39	2.51	-1.25	-1.50	-1.62
NH_3-CH_4	-0.95	1.42	-0.38	-0.93	-0.83
H_2O-CH_4	-0.70	1.06	-0.27	-0.80	-0.71
CH_2O dimer	-6.57	8.43	-2.37	-4.28	-4.78
H_2O-C_2H_4	-3.45	4.38	-1.28	-2.08	-2.42
CH_2O-C_2H_4	-1.70	2.55	-0.49	-2.09	-1.73
C_2H_2 dimer (TS)	-1.83	2.06	-0.54	-1.31	-1.62
NH_3-C_2H_4	-1.67	2.35	-0.48	-1.51	-1.31
C_2H_4 dimer (TS)	-0.84	2.11	-0.30	-2.02	-1.06
CH_4-C_2H_4	-0.42	0.92	-0.13	-0.87	-0.50
BH_3-CH_4	-1.50	3.88	-1.08	-2.68	-1.38
CH_4-C_2H_6 (non-linear)	-0.36	1.22	-0.07	-1.66	-0.86
CH_4-C_2H_6 (linear)	-0.23	0.87	-0.05	-1.23	-0.64
CH_4-dimer	-0.20	0.77	-0.04	-1.09	-0.56
Ar-CH_4	-0.17	0.59	-0.03	-0.79	-0.41
Ar-C_2H_4	-0.23	0.72	-0.05	-0.74	-0.31
C_2H_4-C_2H_2	-0.32	3.68	-0.25	-2.11	1.00
C_2H_4 dimer (PS)	-0.52	4.45	-0.28	-2.40	1.25
C_2H_2 dimer (PS)	0.23	3.04	-0.21	-1.89	1.17
	—S22 dimers—				
HCOOH dimer	-32.23	40.78	-18.90	-10.04	-20.38
$HCONH_2$ dimer	-25.39	27.79	-11.25	-8.10	-16.95
	—S66 dimers—				
H_2O-CH_3OH	-8.82	9.15	-2.88	-3.11	-5.65
H_2O-CH_3NH2	-12.07	12.84	-4.31	-3.53	-7.06
CH_3OH dimer	-8.92	9.67	-3.04	-3.53	-5.84
CH_3OH-CH_3NH2	-12.69	14.41	-4.81	-4.66	-7.74
CH_3OH-H_2O	-7.78	7.78	-2.45	-2.66	-5.11
CH_3NH2-CH_3OH	-4.12	4.85	-1.11	-2.77	-3.15
CH_3NH2 dimer	-5.82	7.04	-1.65	-3.85	-4.28
CH_3NH2-H_2O	-12.21	13.25	-4.44	-4.00	-7.40
C_2H_2-H_2O	-3.93	3.37	-1.01	-1.54	-3.11
	—X40 dimers—				
CH_4-F_2	-0.37	0.93	-0.13	-0.91	-0.48
CH_3F-CH_4	-0.37	1.09	-0.11	-1.42	-0.80
CH_3F dimer	-1.45	1.29	-0.23	-1.33	-1.72
HF-CH_3OH	-13.85	14.04	-6.34	-3.58	-9.74
HF-CH_3NH_2	-23.29	25.65	-11.82	-5.23	-14.69
CH_3F-CH_3OH	-5.18	5.36	-1.39	-2.65	-3.86

system	Elst.	Exch.-Rep.	Ind.	Disp.	Total
Adenine thymine Watson-Crick complex	-26.58	31.77	-11.90	-10.63	-17.33
Adenine thymine stacking complex	-10.66	18.30	-2.49	-18.28	-13.12
Ammonia dimer	-4.89	4.82	-0.91	-2.09	-3.07
Water dimer	-8.10	8.15	-2.45	-2.42	-4.83
Methane dimer	-0.15	0.59	-0.03	-0.94	-0.53
Ethene dimer	-1.13	2.37	-0.23	-2.48	-1.46
Ethene ethyne complex	-1.77	2.21	-0.57	-1.36	-1.48
Formic acid dimer	-32.22	41.28	-18.97	-9.93	-19.84
Formamide dimer	-25.36	28.14	-11.27	-8.03	-16.52
Benzene water complex	-2.71	3.32	-1.00	-2.91	-3.30
Benzene ammonia complex	-1.74	2.76	-0.53	-2.82	-2.34
Benzene methane complex	-0.96	2.61	-0.31	-2.79	-1.46
Benzene dimer T-shaped	-2.00	4.58	-0.70	-4.78	-2.91
Benzene dimer parallel displaced	-2.54	9.04	-0.93	-8.24	-2.68
Indole benzene T-shape complex	-4.25	7.10	-1.95	-6.70	-5.80
Indole benzene stacking complex	-4.31	13.36	-1.48	-12.40	-4.84
Pyrazine dimer	-4.27	9.71	-1.02	-8.90	-4.47
2-pyridoxine 2-aminopyridine complex	-26.91	32.33	-12.67	-10.21	-17.46
Phenol dimer	-8.57	11.37	-3.22	-6.80	-7.22
Uracil dimer stack	-8.52	11.72	-1.75	-12.17	-10.72
Uracil dimer h-bonded	-29.79	32.00	-14.03	-9.66	-21.47
Benzene HCN complex	-3.84	4.55	-1.91	-3.67	-4.87

TABLE S4: The energy components and total binding energies calculated by SAPT2+(3)/aug-cc-pVTZ method for S22 data set.