Supplementary Material: The Performance of Dunning, Jensen and Karlsruhe Basis Sets on Computing Relative Energies and Geometries

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1 Supplementary Material

1.1 Structures

The MP2/AV5Z//MP2/AV5Z optimized structures are provided in the xyz-formatted files:

- buta13diene.xyz
- propan2ol.xyz
- waterdimer.xyz

1.2 Auxiliary Basis Sets

The following auxiliary basis sets, labeled using Psi4's file nomenclature, were used for each theory level indicated. These auxiliary basis sets were automatically assigned using Psi4's automatic basis selector algorithm based on the theory level and the standard basis set that was stated within each input file. The Jensen basis sets are indicated using the original notation (i.e. n=0–4).

HF/6-31G(d) df-scf = cc-pvdz-jkfit.gbs [1]

MP2/VDZ df-scf = cc-pvdz-jkfit.gbs [1]; df-mp2 = cc-pvdz-ri.gbs [2]

MP2/VTZ df-scf = cc-pvtz-jkfit.gbs [1]; df-mp2 = cc-pvtz-ri.gbs [2]

MP2/VQZ df-scf = cc-pvqz-jkfit.gbs [1]; df-mp2 = cc-pvqz-ri.gbs [2]

MP2/V5Z df-scf = cc-pv5z-jkfit.gbs [1]; df-mp2 = cc-pv5z-ri.gbs [2]

MP2/AVDZ df-scf = aug-cc-pvdz-jkfit.gbs [1]; df-mp2 = aug-cc-pvdz-ri.gbs [2]

MP2/AVTZ df-scf = aug-cc-pvtz-jkfit.gbs [1]; df-mp2 = aug-cc-pvtz-ri.gbs [2]

MP2/AVQZ df-scf = aug-cc-pvqz-jkfit.gbs [1]; df-mp2 = aug-cc-pvqz-ri.gbs [2]

MP2/AV5Z df-scf = aug-cc-pv5z-jkfit.gbs [1]; df-mp2 = aug-cc-pv5z-ri.gbs [3]

MP2/pc-0 df-scf = def2-qzvpp-jkfit.gbs [4, 5]; df-mp2 = def2-qzvpp-ri.gbs [4, 3]

MP2/pc-1 df-scf = def2-qzvpp-jkfit.gbs [4, 5]; df-mp2 = def2-qzvpp-ri.gbs [4, 3]

MP2/pc-2 df-scf = def2-qzvpp-jkfit.gbs [4, 5]; df-mp2 = def2-qzvpp-ri.gbs [4, 3]

MP2/pc-3 df-scf = def2-qzvpp-jkfit.gbs [4, 5]; df-mp2 = def2-qzvpp-ri.gbs [4, 3]

MP2/pc-4 df-scf = def2-qzvpp-jkfit.gbs [4, 5]; df-mp2 = def2-qzvpp-ri.gbs [4, 3]

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MP2/pcseg-0 df-scf = def2-sv_p_-jkfit.gbs [4, 5]; df-mp2 = sv_p_-ri.gbs [4, 3]

MP2/pcseg-1 df-scf = def2-svp-jkfit.gbs [4, 5]; df-mp2 = def2-svp-ri.gbs [4, 3]

MP2/pcseg-2 df-scf = def2-tzvpp-jkfit.gbs [4, 5]; df-mp2 = def2-tzvpp-ri.gbs [4, 3]

MP2/pcseg-3 df-scf = def2-qzvpp-jkfit.gbs [4, 5]; df-mp2 = def2-qzvpp-ri.gbs [4, 3]

MP2/pcseg-4 df-scf = cc-pv5z-jkfit.gbs [2]; df-mp2 = cc-pv5z-ri.gbs [2]

MP2/aug-pcseg-0 df-scf = def2-sv_p_-jkfit.gbs [4, 5]; df-mp2 = sv_p_-ri.gbs [4, 3]

MP2/aug-pcseg-1 df-scf = def2-svp-jkfit.gbs [4, 5]; df-mp2 = def2-svpd-ri.gbs [4, 3]

MP2/aug-pcseg-2 df-scf = def2-tzvpp-jkfit.gbs [4, 5]; df-mp2 = def2-tzvppd-ri.gbs [4, 3]

MP2/aug-pcseg-3 df-scf = def2-qzvpp-jkfit.gbs [4, 5]; df-mp2 = def2-qzvppd-ri.gbs [4, 3]

MP2/aug-pcseg-4 df-scf = aug-cc-pv5z-jkfit.gbs [2]; df-mp2 = aug-cc-pv5z-ri.gbs [3]

MP2/pcSseg-0 df-scf = def2-sv_p_-jkfit.gbs [4, 5]; df-mp2 = sv_p_-ri.gbs [4, 3]

MP2/pcSseg-1 df-scf = def2-svp-jkfit.gbs [4, 5]; df-mp2 = def2-svp-ri.gbs [4, 3]

MP2/pcSseg-2 df-scf = def2-tzvpp-jkfit.gbs [4, 5]; df-mp2 = def2-tzvpp-ri.gbs [4, 3]

MP2/pcSseg-3 df-scf = def2-qzvpp-jkfit.gbs [4, 5]; df-mp2 = def2-qzvpp-ri.gbs [4, 3]

MP2/pcSseg-4 df-scf = cc-pv5z-jkfit.gbs [2]; df-mp2 = cc-pwcv5z-ri.gbs [3]

MP2/aug-pcSseg-0 df-scf = def2-sv_p_-jkfit.gbs [4, 5]; df-mp2 = sv_p_-ri.gbs [4, 3]

MP2/aug-pcSseg-1 df-scf = def2-svp-jkfit.gbs [4, 5]; df-mp2 = def2-svpd-ri.gbs [4, 3]

MP2/aug-pcSseg-2 df-scf = def2-tzvpp-jkfit.gbs [4, 5]; df-mp2 = def2-tzvppd-ri.gbs [4, 3]

MP2/aug-pcSseg-3 df-scf = def2-qzvpp-jkfit.gbs [4, 5]; df-mp2 = def2-qzvppd-ri.gbs [4, 3]

MP2/aug-pcSseg-4 df-scf = aug-cc-pv5z-jkfit.gbs [2]; df-mp2 = aug-cc-pwcv5z-ri.gbs [3]

MP2/def2-sv(p) df-scf = def2-sv_p_-jkfit.gbs [4, 5]; df-mp2 = sv_p_-ri.gbs [4, 3]

MP2/def2-svp df-scf = def2-svp-jkfit.gbs [4, 5]; df-mp2 = def2-svp-ri.gbs [4, 3]

MP2/def2-TZVP df-scf = def2-tzvp-jkfit.gbs [4, 5]; df-mp2 = def2-tzvp-ri.gbs [4, 3]

MP2/def2-TZVPP df-scf = def2-tzvpp-jkfit.gbs [4, 5]; df-mp2 = def2-tzvppd-ri.gbs [4, 3]

MP2/def2-QZVPP df-scf = def2-qzvpp-jkfit.gbs [4, 5]; df-mp2 = def2-qzvppd-ri.gbs [4, 3]

MP2/def2-SVPD df-scf = def2-svp-jkfit.gbs [4, 5]; df-mp2 = def2-svpd-ri.gbs [4, 3]

MP2/def2-TZVPD df-scf = def2-tzvp-jkfit.gbs [4, 5]; df-mp2 = def2-tzvpd-ri.gbs [4, 3]

MP2/def2-TZVPPD df-scf = def2-tzvpp-jkfit.gbs [4, 5]; df-mp2 = def2-tzvppd-ri.gbs [4, 3]

MP2/def2-QZVPPD df-scf = def2-qzvpp-ri.gbs [4, 5]; df-mp2 = def2-qzvppd-ri.gbs [4, 3]

1.3 CBS Equations

The implementation of Feller's exponential equation [6] was done using the following:

$$E_{CBS} = E_{large\ bs} - \beta * exp(-1 * \alpha * \zeta_{large\ bs}) \tag{1}$$

$$\alpha = -1 * ln(ratio) \tag{2}$$

$$\beta = \frac{E_{large\ bs} - E_{medium\ bs}}{exp(-1 * \alpha * \zeta_{medium\ bs}) * (ratio - 1)} \tag{3}$$

$$ratio = \frac{E_{large\ bs} - E_{medium\ bs}}{E_{medium\ bs} - E_{small\ bs}} \tag{4}$$

The implementation of Halkier's power equation [7, 8] was done using the following:

$$E_{CBS} = \frac{E_{large\ bs} * (\zeta_{large\ bs})^{\alpha} - E_{medium\ bs} * (\zeta_{medium\ bs})^{\alpha}}{(\zeta_{large\ bs})^{\alpha} - (\zeta_{medium\ bs})^{\alpha}} \tag{5}$$

$$\alpha = 3.0 \tag{6}$$

In both equation "large bs," "medium bs" and "small bs" indicate values associated with the basis set sizes used in the triad sequence for extrapolation. "E" indicates an electronic energy and "ζ" is a cardinal number (i.e. 1, 2, 3, 4, 5). The form of both equations were taken from Psi4's "scf_xtpl_helgaker_3" and "corl_xtpl_helgaker_2" functions [9].

1.4 TZ2P(f,d)+diff Basis Set and Water Dimer 2 & 7

Following the methodology given in reference [10], we generated the TZ2P(f,d)+dif Cartesian basis set, whose contraction scheme, exponents and coefficients are given in Table S1. This basis set has a oxygen contraction scheme of (12s7p2d1f/6s5p2d1f) and a hydrogen contraction scheme of (6s2p1d/4s2p1d), resulting in 150 basis function for describing the orbital space of the water dimer. Note that the resulting basis set is slightly different than that reported in reference 7, which describes the oxygen contraction scheme as (11s7p2d1f/6s4p2d1f) and a total number of 130 basis functions describing the water dimer (see Table I in reference [10]).

A summary of the additional calculations, and if they resulted in a stationary point for water dimer **2** and **7**, is given in Table S2. None of the additional calculations resulted in identifing water dimer **2** and a stationary point.

Table S1: Contraction, exponents and coefficients for the TZ2P(f,d)+diff basis set implemented within this study.[a]

Hydrogen			Oxygen		
S	3	1.00	S	6	1.00
	33.64	0.025374		18050	0.000757
	5.058	0.189684		2660	0.006066
	1.147	0.852933		585.7	0.032782
S	1	1.00		160.9	0.132609
	0.3211	1.000000		51.16	0.396839
S	1	1.00		17.90	0.542572
	0.1013	1.000000	S	2	1.00
S	1	1.00		17.90	0.262490
	0.03016	1.000000		6.639	0.769828
P	1	1.00	S	1	1.00
	1.5	1.000000		2.077	1.000000
P	1	1.00	S	1	1.00
	0.375	1.000000		0.7736	1.000000
D	1	1.00	S	1	1.00
	1.0	1.000000		0.2558	1.000000
			S	1	1.00
				0.08993	1.000000
			P	3	1.00
				49.83	0.016358
				11.49	0.106453
				3.609	0.349302
			P	1	1.00
				1.321	0.657183
			P	1	1.00
				0.4821	1.000000
			P	1	1.00
				0.1651	1.000000
			P	1	1.00
				0.05840	1.000000
			D	1	1.00
				1.7	1.000000
			D	1	1.00
				0.425	1.000000
			F	1	1.00
				1.4	1.000000

[a] The black numbers come directly from reference [11], while the blue numbers were added according to reference [10].

Table S2: Additional theory levels that were used to fully optimized water dimer **2** and **7**. Electron correlation description and the found stationary points are also given.[a]

Theory	Electron Correlation	Stationary Point Found
CCSD(T)/TZ2P(f,d)+diff	full electrons	water dimer **7**
CCSD(T)/TZ2P(f,d)+diff	valence electrons	water dimer **7**
MP2/TZ2P(f,d)+diff	valence electrons	water dimer **7**
MP2/VTZ+diff	valence electrons	water dimer **7**
MP2/VTZ	valence electrons	–

[a] Optimizations were performed using C1 and Cs molecular symmetry for water dimer **2** and **7**, respectively. Convergence criteria were: a maximum force of 1.5E-5, an RMS force of 1.0E-5, a maximum displacement of 6.0E-5 and an RMS displacement of 4.0E-5 convergence criteria specified.

1.5 Additional Raw and Computed Data

Table S3: Electronic energies (Hartree) for all fully optimized conformations investigated herein. The SCF energies were extracted from the MP2 optimization calculations. The Jensen basis sets are indicated using the adjusted indexing (i.e. X=1–5).

Buta-1,3-diene

Conformation	HF/6-31G(d)	SCF/VDZ	SCF/VTZ	SCF/VQZ	SCF/V5Z
1	-154.919488609735	-154.932362747435	-154.977378461640	-154.987690667674	-154.990174264303
2	-154.914647397864	-154.927017807389	-154.971781589502	-154.982071663412	-154.984545203153
3	-154.909818509966	-154.922449672983	-154.967531728401	-154.977859871698	-154.980335585403
4	-154.913295405861	-154.925725851402	-154.970401430118	-154.980679430471	-154.983166952821
		SCF/AVDZ	**SCF/AVTZ**	**SCF/AVQZ**	**SCF/AV5Z**
1		-154.938143356847	-154.978707644772	-154.988085530946	-154.990209711097
2		-154.932611134325	-154.973127674395	-154.982452240892	-154.984570897390
3		-154.928401987971	-154.968860264688	-154.978249665191	-154.980362382324
4		-154.931149935656	-154.971712944012	-154.981072469443	-154.983199536134
	SCF/pc-1	**SCF/pc-2**	**SCF/pc-3**	**SCF/pc-4**	**HF/pc-5**
1	-154.497285502422	-154.884435787419	-154.977252320703	-154.988986817514	-154.990367321957
2	-154.492303440843	-154.879210970734	-154.971813460061	-154.983378615109	-154.984729006931
3	-154.487099508252	-154.874940334070	-154.967507209699	-154.979161668036	-154.980533550820
4	-154.491338778388	-154.877871512624	-154.970514480926	-154.981997477389	-154.983356070991
	SCF/pcseg-1	**SCF/pcseg-2**	**SCF/pcseg-3**	**SCF/pcseg-4**	**SCF/pcseg-5**
1	-154.491618983595	-154.881874777414	-154.972166101146	-154.987407244131	-154.989650083385
2	-154.486879066563	-154.876656067285	-154.966735830214	-154.981837694929	-154.984018028881
3	-154.481738919963	-154.872349173799	-154.962425587105	-154.977591561740	-154.979808333313
4	-154.486050487249	-154.875355293119	-154.965443278425	-154.980441264747	-154.982639657512
	SCF/aug-pcseg-1	**SCF/aug-pcseg-2**	**SCF/aug-pcseg-3**	**SCF/aug-pcseg-4**	**SCF/aug-pcseg-5**
1	-154.499978748033	-154.886229607521	-154.973934482471	-154.987622338568	-154.989675953059
2	-154.494464575904	-154.881864790598	-154.968212371382	-154.981993087652	-154.984036274728
3	-154.489673333339	-154.877964113657	-154.963943805445	-154.977778883144	-154.979835057686
4	-154.493839129281	-154.879645059065	-154.966880154682	-154.980615370202	-154.982666253911
	SCF/pcSseg-1	**SCF/pcSseg-2**	**SCF/pcSseg-3**	**SCF/pcSseg-4**	**SCF/pcSseg-5**
1	-154.533113485302	-154.895762801162	-154.974012824188	-154.987807687443	-154.989758754188
2	-154.528382570335	-154.890562743813	-154.968572604497	-154.982210048639	-154.984115301946
3	-154.523243659847	-154.886176032968	-154.964293057620	-154.977990722042	-154.979911756363
4	-154.527552558946	-154.889378369553	-154.967285410133	-154.980832374050	-154.982745268726
	SCF/aug-pcSseg-1	**SCF/aug-pcSseg-2**	**SCF/aug-pcSseg-3**	**SCF/aug-pcSseg-4**	**SCF/aug-pcSseg-5**
1	-154.541320211904	-154.898885786365	-154.975458193232	-154.987942461147	-154.989786562339
2	-154.535844551906	-154.894012653290	-154.969763438444	-154.982306520885	-154.984140246478
3	-154.531048423669	-154.889879149941	-154.965503431438	-154.978103804883	-154.979938790180
4	-154.535210586316	-154.892260305240	-154.968425029623	-154.980938759320	-154.982774336285
	SCF/def2-SV(P)	**SCF/def2-SVP**	**SCF/def2-TZVP**	**SCF/def2-TZVPP**	**SCF/def2-QZVPP**
1	-154.790033321673	-154.808479562342	-154.979842509355	-154.982073681063	-154.989339513912
2	-154.785006453888	-154.803454166156	-154.974302660765	-154.976502354011	-154.983723676817
3	-154.780360686151	-154.798731776288	-154.970057832549	-154.972274845807	-154.979521184091
4	-154.783987668027	-154.802410565570	-154.972877665174	-154.975108118142	-154.982335435010
		SCF/def2-SVPD	**SCF/def2-TZVPD**	**SCF/def2-TZVPPD**	**SCF/def2-QZVPPD**
1		-154.812886647704	-154.980123769935	-154.982310651091	-154.989364685787
2		-154.807535633783	-154.974543738836	-154.976718084015	-154.983735294598
3		-154.803385461532	-154.970305888652	-154.972495879285	-154.979532947180
4		-154.806246269789	-154.973146884548	-154.975326254057	-154.982357953334

	MP2/VDZ	MP2/VTZ	MP2/VQZ	MP2/V5Z
1	-155.469305303616	-155.627673059461	-155.678192217970	-155.695935085759
2	-155.464682433074	-155.623058020947	-155.673558346648	-155.691295186844
3	-155.459060474304	-155.617325046742	-155.667767042358	-155.685485384763
4	-155.463506913180	-155.621786588266	-155.672271623478	-155.690042379917
	MP2/AVDZ	**MP2/AVTZ**	**MP2/AVQZ**	**MP2/AV5Z**
1	-155.495192926811	-155.638274505550	-155.683080366331	-155.698347542624
2	-155.490395172727	-155.633771474322	-155.678443177063	-155.693697972912
3	-155.485000545744	-155.628018157632	-155.672629765378	-155.687878926865
4	-155.489091292396	-155.632364011250	-155.677184853034	-155.692463880022
MP2/pc-1	**MP2/pc-2**	**MP2/pc-3**	**MP2/pc-4**	**MP2/pc-5**
-154.825240069586	-155.419949104195	-155.619043370118	-155.680896381864	-155.696464743085
-154.821463723807	-155.415690382038	-155.614703787418	-155.676309106511	-155.691820542445
-154.816429353020	-155.410961054550	-155.609108341631	-155.670540447167	-155.686013745965
-154.820558954655	-155.414024044813	-155.613276181946	-155.674972545941	-155.690562010721
MP2/pcseg-1	**MP2/pcseg-2**	**MP2/pcseg-3**	**MP2/pcseg-4**	**MP2/pcseg-5**
-154.850640703600	-155.417224182059	-155.614359571517	-155.671970429290	-155.693438055672
-154.847292804631	-155.412938333949	-155.610054950344	-155.667454020800	-155.688820289290
-154.842802919663	-155.408213188723	-155.604517739081	-155.661711204283	-155.683060553306
-154.845878688498	-155.411271790550	-155.608569129459	-155.666086833472	-155.687533689099
MP2/aug-pcseg-1	**MP2/aug-pcseg-2**	**MP2/aug-pcseg-3**	**MP2/aug-pcseg-4**	**MP2/aug-pcseg-5**
-154.865233839827	-155.442461718975	-155.623432995413	-155.674273332288	-155.694123554597
-154.861869942150	-155.438912302056	-155.618659756220	-155.669675644634	-155.689485159904
-154.858067820504	-155.433754543018	-155.612891555308	-155.663894231139	-155.683711233549
-154.859771766602	-155.436800291318	-155.617356891319	-155.668396616761	-155.688207827503
MP2/pcSseg-1	**MP2/pcSseg-2**	**MP2/pcSseg-3**	**MP2/pcSseg-4**	**MP2/pcSseg-5**
-154.893758183990	-155.446203781133	-155.627057685504	-155.679837630824	-155.696371947446
-154.890416544866	-155.442005473461	-155.622784664582	-155.675257129042	-155.691710857319
-154.885931074309	-155.437189636558	-155.617265702939	-155.669475968988	-155.685895736169
-154.889011303924	-155.440348451840	-155.621266424108	-155.673931734791	-155.690463188629
MP2/aug-pcSseg-1	**MP2/aug-pcSseg-2**	**MP2/aug-pcSseg-3**	**MP2/aug-pcSseg-4**	**MP2/aug-pcSseg-5**
-154.908152667961	-155.468490645277	-155.634179138670	-155.681125499293	-155.696772526499
-154.904806996505	-155.464564655336	-155.629412299889	-155.676505563922	-155.692106547333
-154.901002526707	-155.459216195810	-155.623649148470	-155.670717913204	-155.686295080632
-154.902727435769	-155.462795533735	-155.628147051460	-155.675225177345	-155.690859207496
MP2/def2-SV(P)	**MP2/def2-SVP**	**MP2/def2-TZVP**	**MP2/def2-TZVPP**	**MP2/def2-QZVPP**
-155.283767315196	-155.343083406484	-155.612258634674	-155.630326231488	-155.678424248688
-155.279601628682	-155.338845286122	-155.607491750968	-155.625745774404	-155.673843579931
-155.274534406551	-155.333649424683	-155.601972769388	-155.620069542906	-155.668075610902
-155.278219570650	-155.337480538543	-155.606167110328	-155.624406976466	-155.672516012688
	MP2/def2-SVPD	**MP2/def2-TZVPD**	**MP2/def2-TZVPPD**	**MP2/def2-QZVPPD**
	-155.371175911027	-155.615958373906	-155.632947054988	-155.678915394321
	-155.366983323566	-155.611278514504	-155.628392787528	-155.674329709604
	-155.361516049726	-155.605696575819	-155.622770046484	-155.668566076033
	-155.365378014635	-155.609844299516	-155.627011982487	-155.673003399670

Table S3 – continued from previous page.

Propan-2-ol

Conformation	HF/6-31G(d)	SCF/VDZ	SCF/VTZ	SCF/VQZ	SCF/V5Z	MP2/VDZ	MP2/VTZ	MP2/VQZ	MP2/V5Z
1	-193.114966160166	-193.133260721900	-193.194448962755	-193.208705328385	-193.212333223040	-193.760468064608	-193.971916783335	-194.038501482325	-194.062368330456
2	-193.115327636627	-193.133390729657	-193.194901781381	-193.209206047210	-193.212845210048	-193.760253825591	-193.972294765228	-194.039048288588	-194.062942693656
3	-193.112733270816	-193.130892037875	-193.192731266017	-193.207083001297	-193.210738809647	-193.757816769025	-193.970242041782	-194.037068210929	-194.060998534208
4	-193.113117147415	-193.131290781343	-193.193049358639	-193.207381932196	-193.211016118834	-193.757630519198	-193.970057400963	-194.036860689853	-194.060780754743
5	-193.112733270778	-193.126894695248	-193.188766702149	-193.203049458790	-193.206679682310	-193.753734138181	-193.966323673982	-194.033166538214	-194.057065436792
6	-193.109071495977	-193.127479312469	-193.189157304472	-193.203420175938	-193.207051682264	-193.754630908094	-193.966943291364	-194.033725734711	-194.057624405290
7	-193.109471191854	-193.126812358425	-193.188322319684	-193.202552473663	-193.206177387623	-193.754070267410	-193.966009553979	-194.032659054839	-194.056529438024
		SCF/AVDZ	SCF/AVTZ	SCF/AVQZ	SCF/AV5Z	MP2/AVDZ	MP2/AVTZ	MP2/AVQZ	MP2/AV5Z
1		-193.147460566258	-193.197118319680	-193.209454026037	-193.212413583699	-193.806731905384	-193.988669184230	-194.045497755143	-194.065579929926
2		-193.147935400544	-193.197642694874	-193.209969287042	-193.212927412949	-193.807286111919	-193.989225432026	-194.046070329753	-194.066158925440
3		-193.145646691120	-193.195551186399	-193.207868991476	-193.210827716026	-193.805085325587	-193.987308977223	-194.044151681744	-194.064237490528
4		-193.145878380026	-193.195813059459	-193.208139404111	-193.211097080167	-193.805082721013	-193.987111138576	-194.043924261860	-194.064006080262
5		-193.141702415139	-193.191495848460	-193.203808880824	-193.206764137282	-193.801413901627	-193.983389266205	-194.040219656377	-194.060299237409
6		-193.142083480426	-193.191876408144	-193.204179985301	-193.207135011542	-193.802002200293	-193.983947012000	-194.040790390982	-194.060865401861
7		-193.141255066612	-193.190982963688	-193.203299262827	-193.206259385418	-193.800895032565	-193.982853102159	-194.039681954317	-194.059757710496
	SCF/pc-1	SCF/pc-2	SCF/pc-3	SCF/pc-4	HF/pc-5	MP2/pc-1	MP2/pc-2	MP2/pc-3	MP2/pc-4	MP2/pc-5
1	-192.555415027878	-193.070375270966	-193.197152158830	-193.211054771553	-193.212606658663	-192.916161309958	-193.698032102289	-193.963343765891	-194.043234251209	-194.063231026086
2	-192.554679054034	-193.070612280075	-193.197635252695	-193.211568389612	-193.213118106883	-192.914781317595	-193.698102045000	-193.963786914072	-194.043834183823	-194.063817673253
3	-192.553779887200	-193.068089660441	-193.195470501325	-193.209469615089	-193.211018484544	-192.914062840558	-193.695531498694	-193.961725750995	-194.041872439627	-194.061888153984
4	-192.552707746955	-193.068738604759	-193.195764255066	-193.209741998651	-193.211293980517	-192.912108784758	-193.695924722152	-193.961616524450	-194.041657324781	-194.061663883562
5	-192.549190321926	-193.064160513101	-193.191446095662	-193.205397638413	-193.206957050747	-192.908908408454	-193.691556663675	-193.957775675955	-194.037829786302	-194.057921941754
6	-192.550745538406	-193.064723501811	-193.191886331356	-193.205775821879	-193.207328884666	-192.911079507794	-193.692591494846	-193.958522474844	-194.038373761305	-194.058484171802
7	-192.550098069783	-193.063953641498	-193.190977812951	-193.204892654100	-193.206454340743	-192.910587116963	-193.691553993905	-193.957418487950	-194.037266153443	-194.057372260789
	SCF/pcseg-1	SCF/pcseg-2	SCF/pcseg-3	SCF/pcseg-4	SCF/pcseg-5	MP2/pcseg-1	MP2/pcseg-2	MP2/pcseg-3	MP2/pcseg-4	MP2/pcseg-5
1	-192.542145832988	-193.068002927886	-193.191666101124	-193.209287012830	-193.211673842239	-192.947844115626	-193.695402784474	-193.958973411370	-194.032720498303	-194.059482735018
2	-192.543586046920	-193.068353769175	-193.192165452615	-193.209802436458	-193.212187722412	-192.948916163181	-193.695604172165	-193.959443825568	-194.033323507113	-194.060077112506
3	-192.540528164353	-193.065757169024	-193.189980818627	-193.207712836375	-193.210088596213	-192.945325103881	-193.692932963791	-193.957374117717	-194.031383879892	-194.058155531268
4	-192.542156621061	-193.066474822974	-193.190279333062	-193.207979173927	-193.210359267347	-192.947130859823	-193.693448419919	-193.957264084510	-194.031162070527	-194.057921760927
5	-192.537748888306	-193.061895022423	-193.186006253854	-193.203637381530	-193.206028655110	-192.943001048733	-193.689034757286	-193.953440822810	-194.027353633427	-194.054207373665
6	-192.538108390755	-193.062425274250	-193.186433973070	-193.204009368526	-193.206401173307	-192.943233712654	-193.690012596559	-193.954150456904	-194.027907651485	-194.054767427192
7	-192.536303369548	-193.061573787287	-193.185521367633	-193.203131302476	-193.205523249094	-192.941943774787	-193.688893811851	-193.953061374007	-194.026781196331	-194.053648481667
	SCF/aug-pcseg-1	SCF/aug-pcseg-2	SCF/aug-pcseg-3	SCF/aug-pcseg-4	SCF/aug-pcseg-5	MP2/aug-pcseg-1	MP2/aug-pcseg-2	MP2/aug-pcseg-3	MP2/aug-pcseg-4	MP2/aug-pcseg-5
1	-192.562094331359	-193.083675055820	-193.193180054205	-193.209458803837	-193.211706914347	-192.981890618545	-193.735448401727	-193.968165846229	-194.034979296704	-194.060122389704
2	-192.563067403256	-193.084071191916	-193.193696682708	-193.209977840587	-193.212222853770	-192.982779695957	-193.735952670181	-193.968721503587	-194.035590375451	-194.060726810720
3	-192.560768440768	-193.081809808278	-193.191618133087	-193.207876610971	-193.210122866092	-192.980390484755	-193.733684355911	-193.966798417303	-194.033606073776	-194.058792187541
4	-192.561738206356	-193.082082136150	-193.191875076220	-193.208146320275	-193.210392414503	-192.981376683780	-193.733863913430	-193.966593795978	-194.033434025833	-194.058570405562
5	-192.557018632180	-193.077737306292	-193.187548318081	-193.203814956389	-193.206063432122	-192.976985975337	-193.729910326519	-193.962789879508	-194.029623807587	-194.054844260120
6	-192.557337865191	-193.078064940121	-193.187930256811	-193.204185995410	-193.206437582778	-192.977550990208	-193.730433496123	-193.963338063417	-194.030186944106	-194.055395865280
7	-192.556036963353	-193.077298235014	-193.187035409662	-193.203303099647	-193.205556276170	-192.976278392952	-193.729331662107	-193.962238983746	-194.029051351246	-194.054273850688
	SCF/pcSseg-1	SCF/pcSseg-2	SCF/pcSseg-3	SCF/pcSseg-4	SCF/pcSseg-5	MP2/pcSseg-1	MP2/pcSseg-2	MP2/pcSseg-3	MP2/pcSseg-4	MP2/pcSseg-5
1	-192.607540836540	-193.090912463093	-193.193753658484	-193.209846841176	-193.211836232060	-193.015111739767	-193.739106646230	-193.974115986416	-194.042137248924	-194.062790100258
2	-192.608965416833	-193.091228792343	-193.194252418949	-193.210357218260	-193.212348809946	-193.016191338139	-193.739277085422	-193.974601672540	-194.042717044097	-194.063377804731
3	-192.605972261096	-193.088642297831	-193.192063295879	-193.208261022501	-193.210250962246	-193.012652147803	-193.736632176865	-193.972458032532	-194.040771987925	-194.061454460041
4	-192.607557448899	-193.089271832967	-193.192383163562	-193.208535244541	-193.210520631970	-193.014419775630	-193.737044959941	-193.972398117471	-194.040555886804	-194.061223531138
5	-192.603044580986	-193.084876422744	-193.188072976253	-193.204192266852	-193.206185948459	-193.010190057213	-193.732840334017	-193.968536079107	-194.036722684792	-194.057491222125
6	-192.603408641375	-193.085404293090	-193.188495246531	-193.204566465036	-193.206558500141	-193.010439453668	-193.733822540222	-193.969235624739	-194.037265272276	-194.058051253251
7	-192.601612217110	-193.084597776652	-193.187586602031	-193.203689475577	-193.205682965033	-193.009123184010	-193.732736314535	-193.968143122758	-194.036175942653	-194.056939076150
	SCF/aug-pcSseg-1	SCF/aug-pcSseg-2	SCF/aug-pcSseg-3	SCF/aug-pcSseg-4	SCF/aug-pcSseg-5	MP2/aug-pcSseg-1	MP2/aug-pcSseg-2	MP2/aug-pcSseg-3	MP2/aug-pcSseg-4	MP2/aug-pcSseg-5
1	-192.627299470239	-193.102337017317	-193.195075182500	-193.209954793003	-193.211861723852	-193.048909306112	-193.773507833843	-193.981373372748	-194.043464518614	-194.063243789739
2	-192.628275870867	-193.102806547340	-193.195587027921	-193.210469333124	-193.212374852996	-193.049818157320	-193.774109244917	-193.981932983979	-194.044066369089	-194.063834422235
3	-192.626018466604	-193.100493002124	-193.193503509749	-193.208370608194	-193.210277897121	-193.047460147552	-193.771780117928	-193.979985681669	-194.042105708291	-194.061905820082
4	-192.626973944254	-193.100817725630	-193.193770419891	-193.208645343521	-193.210547253801	-193.048437900480	-193.772016637178	-193.979793756573	-194.041906385224	-194.061680215829
5	-192.622163498739	-193.096630827904	-193.189432629260	-193.204307727443	-193.206213757558	-193.043959456348	-193.768185023033	-193.975970911586	-194.038101757589	-194.057948906586
6	-192.622470191316	-193.096967266644	-193.189813816600	-193.204679932638	-193.206586203703	-193.044505359804	-193.768709652004	-193.976537642196	-194.038654819086	-194.058506332182
7	-192.621176387769	-193.096132554195	-193.188925614902	-193.203802693568	-193.205710309578	-193.043231838694	-193.767540593130	-193.975417295611	-194.037538257083	-194.057391635639

Table S3 – continued from previous page.

	SCF/def2-SV(P)	SCF/def2-SVP	SCF/def2-TZVP	SCF/def2-TZVPP	SCF/def2-QZVPP	MP2/def2-SV(P)	MP2/def2-SVP	MP2/def2-TZVP	MP2/def2-TZVPP	MP2/def2-QZVPP
1	-192.946276665537	-192.977695237619	-193.197614916389	-193.201773203579	-193.211347455148	-193.514392233759	-193.602424108078	-193.950534939048	-193.977011456306	-194.039510231184
2	-192.946783575249	-192.978148630564	-193.198080976119	-193.202268387922	-193.211855677696	-193.514768963155	-193.602679407075	-193.951016216882	-193.977467351566	-194.040075344452
3	-192.944095586781	-192.975524047694	-193.195874006654	-193.200114776477	-193.209750871259	-193.511868479261	-193.599927176555	-193.948825688151	-193.975444929890	-194.038109872938
4	-192.944568271462	-192.976111857365	-193.196179712481	-193.200411613396	-193.210030060686	-193.512113099561	-193.600246638828	-193.948719795438	-193.975220232942	-194.037908937573
5	-192.940101987065	-192.971555168152	-193.191900977929	-193.196114480887	-193.205686987455	-193.507739436356	-193.595800225890	-193.944916361077	-193.971545636006	-194.034146594270
6	-192.940645957832	-192.972024829054	-193.192294185178	-193.196490901378	-193.206066093667	-193.508602398603	-193.596607645000	-193.945600320719	-193.972155693262	-194.034700191409
7	-192.939689747481	-192.971149850466	-193.191428533119	-193.195625999051	-193.205191379248	-193.507559489085	-193.595638608637	-193.944534878156	-193.971126879970	-194.033628317185
		SCF/def2-SVPD	SCF/def2-TZVPD	SCF/def2-TZVPPD	SCF/def2-QZVPPD		MP2/def2-SVPD	MP2/def2-TZVPD	MP2/def2-TZVPPD	MP2/def2-QZVPPD
1		-192.990298353240	-193.198766055149	-193.202651630153	-193.211453445140		-193.645492582147	-193.957874414285	-193.981815364508	-194.040383625824
2		-192.990814339498	-193.199265553636	-193.203168323130	-193.211961858174		-193.645967908642	-193.958425631897	-193.982395018130	-194.040957222742
3		-192.988585021651	-193.197174197373	-193.201080626519	-193.209866008725		-193.643858872679	-193.956444013786	-193.980431963419	-194.039009259083
4		-192.988941090935	-193.197411049915	-193.201332169626	-193.210138249041		-193.644030150186	-193.956261754698	-193.980227034978	-194.038814666770
5		-192.984793847096	-193.193085239233	-193.197000227645	-193.205798365268		-193.640212233752	-193.952368223418	-193.976424992401	-194.035037263781
6		-192.985083134312	-193.193467851713	-193.197380711840	-193.206175530936		-193.640661061483	-193.952901012512	-193.976969929142	-194.035586036038
7		-192.984259976532	-193.192599819493	-193.196493410934	-193.205298084276		-193.639692007027	-193.951835183565	-193.975885534163	-194.034495248702
					Water dimer					
Conformation	HF/6-31G(d)	SCF/VDZ	SCF/VTZ	SCF/VQZ	SCF/V5Z		MP2/VDZ	MP2/VTZ	MP2/VQZ	MP2/V5Z
1	-152.030406296633	-152.061135808606	-152.120564238170	-152.135449406629	-152.139642976407		-152.469124170449	-152.646883482079	-152.703982629548	-152.725354018802
3	-152.029297036701	-152.060550603223	-152.120018598547	-152.135003089396	-152.139218057553		-152.467249403608	-152.645490041991	-152.702847754950	-152.724393424166
4	-152.029697259791	-152.060104113092	-152.119431240949	-152.134245475098	-152.138391965076		-152.469074208984	-152.646133607321	-152.702945274659	-152.724180752288
5	-152.028864066480	-152.059227982535	-152.118833958178	-152.133807603962	-152.138075286242		-152.468099776882	-152.645385409227	-152.702360762203	-152.723772463784
6	-152.028388064071	-152.059133564521	-152.118974807098	-152.133924886676	-152.138163660939		-152.465980895273	-152.644644419576	-152.702093742555	-152.723677023336
8	-152.025580928322	-152.056497457578	-152.116262038770	-152.131230040211	-152.135378073846		-152.464322578481	-152.641712948568	-152.698468145125	-152.719556491992
9	-152.028162112064	-152.059354045869	-152.118682656309	-152.133541978654	-152.137690469400		-152.466278821336	-152.643928908813	-152.700994754823	-152.722353668448
10	-152.026641460662	-152.057764615232	-152.117513846199	-152.132488432374	-152.136709042764		-152.464198906004	-152.642114290142	-152.699343835687	-152.720838624580
		SCF/AVDZ	SCF/AVTZ	SCF/AVQZ	SCF/AV5Z		MP2/AVDZ	MP2/AVTZ	MP2/AVQZ	MP2/AV5Z
1		-152.087390372073	-152.126096573124	-152.137228973979	-152.139917515687		-152.530131655237	-152.666137926241	-152.711914961685	-152.728460544505
3		-152.086917980123	-152.125693231014	-152.136822543132	-152.139512795947		-152.529073964971	-152.665165584472	-152.711001945734	-152.727571527151
4		-152.086321451369	-152.124892420779	-152.135994499867	-152.138685529722		-152.528717067474	-152.664811559587	-152.710663447505	-152.727233557963
5			-152.124583500067	-152.135702998935	-152.138400763293		-152.528470242964	-152.664411226457	-152.710302666296	-152.726886022796
6		-152.086336414442	-152.124714377900	-152.135781331480	-152.138473661950		-152.528470243123	-152.664345620008	-152.710242593835	-152.726828017530
8		-152.082921848151	-152.121760190178	-152.132931457602	-152.135645867705		-152.524109763248	-152.660066663601	-152.705936964786	-152.722512573862
9		-152.085437682740	-152.124126570628	-152.135253618977	-152.137956981094		-152.526994584281	-152.662946263674	-152.708820745192	-152.725400710743
10		-152.084384031184	-152.123147015825	-152.134278542723	-152.136992642683		-152.525473688348	-152.661469820648	-152.707348903558	-152.723933619918
	SCF/pc-1	SCF/pc-2	SCF/pc-3	SCF/pc-4	HF/pc-5	MP2/pc-1	MP2/pc-2	MP2/pc-3	MP2/pc-4	MP2/pc-5
1	-151.555546231858	-152.015392162065	-152.128278507607	-152.139166455818	-152.140146350927	-151.769665534306	-152.424050433305	-152.643176857519	-152.710625489762	-152.726898629377
3	-151.554794377176	-152.014672418900	-152.127818181892	-152.138734683578	-152.139739233401	-151.768838209428	-152.422646799184	-152.642164631378	-152.709715400480	-152.726021342638
4	-151.549192165455	-152.014061607937	-152.126956374371	-152.137931555923	-152.138907711623	-151.763303742298	-152.423206400854	-152.641935895517	-152.709340012916	-152.725699133085
5	-151.548430934072	-152.013409201724	-152.126645264478	-152.137627607294	-152.138619372255	-151.762124670517	-152.422362101802	-152.641506346291	-152.708978728188	-152.725350896208
6	-151.548805744582	-152.013432518348	-152.126798110258	-152.137716907404	-152.138695063857	-151.761875093865	-152.421704822803	-152.641350994698	-152.708897417983	-152.725290072400
8	-151.541301724685	-152.010810214798	-152.123831452747	-152.134889509933	-152.135880246891	-151.753619541905	-152.419020463195	-152.637402423789	-152.704745355689	-152.721029084778
9	-151.548183349392	-152.013693903010	-152.126387259377	-152.137211335493	-152.138185133999	-151.761134871811	-152.421772587813	-152.640435424585	-152.707577835198	-152.723892519293
10	-151.545320223817	-152.012281791322	-152.125349829982	-152.136239244688	-152.137219983684	-151.757697167720	-152.419890306587	-152.638810858864	-152.706134273072	-152.722446548829
	SCF/pcseg-1	SCF/pcseg-2	SCF/pcseg-3	SCF/pcseg-4	SCF/pcseg-5	MP2/pcseg-1	MP2/pcseg-2	MP2/pcseg-3	MP2/pcseg-4	MP2/pcseg-5
1	-151.563726604297	-152.014082091310	-152.124317846550	-152.137737284963	-152.139304567747	-151.823337007427	-152.422888513250	-152.641372886883	-152.701284259365	-152.723073359232
3	-151.563254373567	-152.013395838651	-152.123867213489	-152.137305411956	-152.138896537208	-151.820628351880	-152.421471834895	-152.640379397348	-152.700419692435	-152.722194120188
4	-151.562791276089	-152.012828465072	-152.123021466300	-152.136457104401	-152.138080202364	-151.823724269932	-152.422188596411	-152.640159044378	-152.699901706866	-152.721828112276
5	-151.561448393559	-152.012182494838	-152.122712759359	-152.136165077782	-152.137785736717	-151.821910060285	-152.421336868198	-152.639734911982	-152.699537467883	-152.721475107594
6	-151.561875820622	-152.012228240566	-152.122879865909	-152.136242037994	-152.137862441444	-151.819851479347	-152.420682379037	-152.639576554954	-152.699484472713	-152.721407088698
8	-151.556152974828	-152.009609062328	-152.119865437982	-152.133446933320	-152.135029721724	-151.815480134650	-152.418057402910	-152.635761471172	-152.695208999748	-152.717132679904
9	-151.560088938370	-152.012428161762	-152.122420062897	-152.135749600778	-152.137347390016	-151.817630300400	-152.420630423370	-152.638677102099	-152.698107029049	-152.720027080537
10	-151.557785348152	-152.011035160118	-152.121385518203	-152.134788249487	-152.136378733613	-151.814958762160	-152.418773537395	-152.637049119971	-152.696631589606	-152.718560426008

Table S3 – continued from previous page.

	SCF/aug-pcseg-1	SCF/aug-pcseg-2	SCF/aug-pcseg-3	SCF/aug-pcseg-4	SCF/aug-pcseg-5	MP2/aug-pcseg-1	MP2/aug-pcseg-2	MP2/aug-pcseg-3	MP2/aug-pcseg-4	MP2/aug-pcseg-5
1	-151.601621489422	-152.028764059876	-152.125539583852	-152.137856705900	-152.139338394741	-151.883590877799	-152.461391606785	-152.647992886245	-152.702824828668	-152.723470149876
3	-151.601112333720	-152.028180934400	-152.125132514047	-152.137440584776	-152.138926225246	-151.882879353333	-152.460236583368	-152.647082943172	-152.701994486766	-152.722600584564
4	-151.598763722132	-152.027428387744	-152.124298972868	-152.136608543593	-152.138114417103	-151.880494389304	-152.459977464596	-152.646705802914	-152.701457860563	-152.722249571014
5			-152.124026453180		-152.137830328003			-152.646367139772		-152.721911333152
6	-151.598996559717	-152.027624113999	-152.124075908667	-152.136422317405	-152.137902618058	-151.880463931614	-152.459995812771	-152.646338317083	-152.701132002723	-152.721857584254
8	-151.591413570327	-152.023476171143	-152.121131513318	-152.133535827984	-152.135045109306	-151.872016668996	-152.454941499732	-152.642123691580	-152.696670337680	-152.717542815917
9	-151.596533921893	-152.026378090858	-152.123525522692	-152.135876922844	-152.137373917240	-151.878085631257	-152.458290468760	-152.644938344599	-152.699640576164	-152.720446262363
10	-151.594526965827	-152.025350669650	-152.122517112228	-152.134908271149	-152.136403012608	-151.875492857254	-152.456784965885	-152.643460933340	-152.698162507900	-152.718978786042
	SCF/pcSseg-1	**SCF/pcSseg-2**	**SCF/pcSseg-3**	**SCF/pcSseg-4**	**SCF/pcSseg-5**	**MP2/pcSseg-1**	**MP2/pcSseg-2**	**MP2/pcSseg-3**	**MP2/pcSseg-4**	**MP2/pcSseg-5**
1	-151.632456160681	-152.033354868134	-152.126545357743	-152.138454530188	-152.139526107627	-151.893697508305	-152.461204848386	-152.654451383128	-152.710503306715	-152.726189081349
3	-151.632068595257	-152.032672306026	-152.126089724167	-152.138022063768	-152.139114736145	-151.891188366750	-152.459825128899	-152.653487508130	-152.709569018182	-152.725312923296
4	-151.631485552493	-152.032110551610	-152.125221532614	-152.137202993239	-152.138291417462	-151.894077092116	-152.460551762209	-152.653235727220	-152.709200485712	-152.724998157085
5	-151.630184780703	-152.031447003289	-152.124917240506	-152.136902452554	-152.137999237601	-151.892274012206	-152.459681130178	-152.652823883412	-152.708832848982	-152.724648487830
6	-151.630704420584	-152.031476018033	-152.125076451331	-152.137000989375	-152.138076859284	-151.890453060611	-152.459016315705	-152.652665288151	-152.708756757097	-152.724583429874
8	-151.624670373732	-152.028934228420	-152.122104292091	-152.134171364419	-152.135249360446	-151.885664489708	-152.456431535443	-152.648892611614	-152.704605602183	-152.720322535861
9	-151.628744947255	-152.031714713047	-152.124648802902	-152.136491832733	-152.137562052552	-151.888019707790	-152.458943108336	-152.651771592075	-152.707428413930	-152.723192324380
10	-151.626428167929	-152.030324923257	-152.123621455117	-152.135522429190	-152.136593269982	-151.885327603134	-152.457102794699	-152.650169704619	-152.705987272999	-152.721738751979
	SCF/aug-pcSseg-1	**SCF/aug-pcSseg-2**	**SCF/aug-pcSseg-3**	**SCF/aug-pcSseg-4**	**SCF/aug-pcSseg-5**	**MP2/aug-pcSseg-1**	**MP2/aug-pcSseg-2**	**MP2/aug-pcSseg-3**	**MP2/aug-pcSseg-4**	**MP2/aug-pcSseg-5**
1	-151.670414076493	-152.049022465181	-152.127740576251	-152.138541565802	-152.139553985087	-151.954195879003	-152.499970463206	-152.660315958101	-152.711358723355	-152.726478371719
3	-151.669918356230	-152.048623643778	-152.127309966890	-152.138125951467	-152.139142036223	-151.953498448340	-152.499151680436	-152.659464021468	-152.710490393969	-152.725612109606
4	-151.667590161765		-152.126496853676	-152.137326732896	-152.138323541560	-151.951080009344		-152.659056927259	-152.710140457238	-152.725296222283
5			-152.126212940366	-152.137036085028	-152.138037435944			-152.658734648214	-152.709787454423	-152.724955741081
6	-151.667788715014	-152.048129208478	-152.126247087785	-152.137117111686	-152.138106458601	-151.951063011985	-152.498950603101	-152.658713539244	-152.709721742519	-152.724899796197
8	-151.659992132976	-152.043861426294	-152.123354313212	-152.134254627773	-152.135272809818	-151.942377244731	-152.493748911978	-152.654533707041	-152.705477635370	-152.720629507280
9	-151.665167192530	-152.046777334743	-152.125730069497	-152.136593071402	-152.137590395439	-151.948513101103	-152.497107969007	-152.657369307431	-152.708348950317	-152.723500015279
10	-151.663145462650	-152.045800617024	-152.124707564687	-152.135616088515	-152.136621309091	-151.945914340133	-152.495696080014	-152.655928171307	-152.706921438262	-152.722050833591
	SCF/def2-SV(P)	**SCF/def2-SVP**	**SCF/def2-TZVP**	**SCF/def2-TZVPP**	**SCF/def2-QZVPP**	**MP2/def2-SV(P)**	**MP2/def2-SVP**	**MP2/def2-TZVP**	**MP2/def2-TZVPP**	**MP2/def2-QZVPP**
1	-151.884867719499	-151.929881639382	-152.124007660745	-152.130797862552	-152.139029252272	-152.265229137820	-152.336180986242	-152.634983674685	-152.655487700996	-152.706730001205
3	-151.884091986930	-151.929331223678	-152.123438497895	-152.130329163454	-152.138609402159	-152.263531176542	-152.334212480143	-152.633880544971	-152.654376941800	-152.705745853650
4	-151.883938105434	-151.929007350018	-152.122744721733	-152.129623967997	-152.137788685236	-152.265175092748	-152.336212030284	-152.633993157432	-152.654488911459	-152.705498137552
5	-151.883060529943	-151.928142774454	-152.122347001231	-152.129202350423	-152.137470390851	-152.263996604378	-152.335114228696	-152.633381090511	-152.653940668688	-152.705088344415
6	-151.882973614969	-151.928157398905	-152.122473048439	-152.129370978174	-152.137565612855	-152.262832862859	-152.333309387710	-152.633221148215	-152.653646704155	-152.704970182351
8	-151.880220987061	-151.925320308858	-152.119409815334	-152.126510378046	-152.134777992985	-152.260100644685	-152.331512831772	-152.629451474849	-152.650250447809	-152.700948093135
9	-151.883167055653	-151.928059396352	-152.122064571521	-152.128899496420	-152.137116814091	-152.262390792126	-152.333080298857	-152.632420386608	-152.652635180934	-152.703740940256
10	-151.881548651918	-151.926511729539	-152.120910129676	-152.127863034210	-152.136133778065	-152.260256291327	-152.331080044428	-152.630659802686	-152.651056866646	-152.702225888386
		SCF/def2-SVPD	**SCF/def2-TZVPD**	**SCF/def2-TZVPPD**	**SCF/def2-QZVPPD**		**MP2/def2-SVPD**	**MP2/def2-TZVPD**	**MP2/def2-TZVPPD**	**MP2/def2-QZVPPD**
1		-151.953836785089	-152.127174358994	-152.132911185707	-152.139447121276		-152.388146897499	-152.646221542910	-152.662340246832	-152.708249339451
3		-151.953477048262	-152.126663485502	-152.132476330999	-152.139028565776		-152.387453936459	-152.645208992619	-152.661407800828	-152.707335562316
4			-152.125967304910	-152.131697528579	-152.138210962714			-152.644879957505	-152.660981137534	-152.706975856086
5			-152.125621018121	-152.131376900842	-152.137908619581			-152.644506279852	-152.660611832993	-152.706610994051
6		-151.952952292739	-152.125676607241	-152.131471159991	-152.137998441578		-152.386799663382	-152.644393195919	-152.660516714103	-152.706520319457
8		-151.948986213537	-152.122840173559	-152.128587183223	-152.135185010998		-152.381707333373	-152.640404549904	-152.656510494754	-152.702356887259
9		-151.951732113654	-152.125164910012	-152.130940012862	-152.137493311287		-152.385158382413	-152.643281496685	-152.659323369571	-152.705188502611
10		-151.950691340456	-152.124138066787	-152.129951036457	-152.136533070971		-152.383575522422	-152.641764094711	-152.657879985391	-152.703725087560

Table S4: Computed CBS MP2 relative energies (Scheme 2) for buta-1,3-diene, propan-2-ol and water dimer conformations for each basis set family (e.g. VXZ, AVXZ, pc-X). Absolute differences are included in comparison to CBS value computed by the [3,4,5] basis set triad. Also provided are the mean of the absolute differences for each molecule and computed overall all conformations for a give basis set family.

Conformation	CBS MP2 Rel. Energy	Abs. Difference to [3,4,5]	CBS MP2 Rel. Energy	Abs. Difference to [3,4,5]	CBS MP2 Rel. Energy
			VXZ		
			ζ=[D,T,Q]		**ζ=[T,Q,5]**
Buta-1,3-diene					
1			0.000		0.000
2			2.902	0.010	2.912
3			6.581	0.009	6.573
4			3.711	0.033	3.678
Mean				0.017	
Propan-2-ol					
1			0.401	0.028	0.373
2			0.000		0.000
3			1.229	0.027	1.202
4			1.365	0.024	1.341
5			3.670	0.012	3.682
6			3.335	0.005	3.330
7			4.055	0.023	4.033
Mean				0.020	
Water Dimer					
1			0.000		0.000
3			0.593	0.094	0.499
4			0.778	0.038	0.816
5			1.084	0.105	0.979
6			1.052	0.130	0.922
8			3.639	0.190	3.829
9			1.884	0.001	1.885
10			2.871	0.108	2.763
Mean				0.095	
Overall Mean				0.052	
			AVXZ		
			ζ=[D,T,Q]		**ζ=[T,Q,5]**
Buta-1,3-diene					
1			0.000		0.000
2			2.967	0.046	2.922
3			6.641	0.062	6.579
4			3.692	0.008	3.684
Mean				0.039	
Propan-2-ol					
1			0.363	0.005	0.368
2			0.000		0.000
3			1.219	0.011	1.207
4			1.377	0.021	1.355
5			3.684	0.003	3.682
6			3.320	0.008	3.329
7			4.018	0.007	4.025
Mean				0.009	
Water Dimer					
1			0.000		0.000
3			0.553	0.011	0.542
4			0.742	0.011	0.752
5					0.964
6			0.971	0.024	0.995
8			3.716	0.004	3.720
9			1.896	0.004	1.900
10			2.824	0.005	2.820
Mean				0.010	
Overall Mean				0.015	

Table S4 – continued from previous page.

	pc-X				
	ζ=[1,2,3]		ζ=[2,3,4]		ζ=[3,4,5]
Buta-1,3-diene					
1	0.000		0.000		0.000
2	2.771	0.165	2.944	0.009	2.935
3	6.575	0.040	6.667	0.051	6.616
4	3.572	0.104	3.720	0.043	3.677
Mean		0.103		0.034	
Propan-2-ol					
1	0.364	0.004	0.437	0.077	0.360
2	0.000		0.000		0.000
3	0.972	0.217	1.208	0.018	1.190
4	1.366	0.028	1.382	0.044	1.338
5	3.510	0.123	3.773	0.140	3.633
6	3.077	0.188	3.505	0.240	3.264
7	3.809	0.161	4.208	0.238	3.970
Mean		0.120		0.126	
Water Dimer					
1	0.000		0.000		0.000
3	0.479	0.063	0.535	0.007	0.542
4	1.211	0.516	0.855	0.160	0.695
5	1.308	0.395	1.055	0.142	0.913
6	1.224	0.294	1.053	0.123	0.930
8	4.418	0.735	3.793	0.110	3.683
9	2.252	0.396	2.031	0.176	1.855
10	3.221	0.452	2.877	0.109	2.768
Mean		0.407		0.118	
Overall Mean		0.243		0.105	

	pcseg-X				
	ζ=[1,2,3]		ζ=[2,3,4]		ζ=[3,4,5]
Buta-1,3-diene					
1	0.000		0.000		0.000
2	2.715	0.220	2.901	0.034	2.935
3	6.452	0.126	6.610	0.033	6.577
4	3.571	0.124	3.686	0.010	3.695
Mean		0.157		0.026	
Propan-2-ol					
1	0.458	0.090	0.433	0.065	0.368
2	0.000		0.000		0.000
3	1.092	0.099	1.187	0.004	1.191
4	1.349	0.001	1.362	0.015	1.347
5	3.525	0.095	3.735	0.115	3.620
6	3.180	0.084	3.444	0.180	3.264
7	3.924	0.038	4.175	0.213	3.962
Mean		0.068		0.099	
Water Dimer					
1	0.000		0.000		0.000
3	0.448	0.125	0.491	0.082	0.573
4	0.885	0.168	0.949	0.231	0.718
5	1.014	0.083	1.158	0.227	0.931
6	0.931	0.051	1.120	0.138	0.982
8	3.926	0.277	4.069	0.420	3.648
9	1.987	0.148	2.187	0.348	1.839
10	2.934	0.183	3.067	0.316	2.751
Mean		0.148		0.252	
Overall Mean		0.120		0.152	

Table S4 – continued from previous page.

	aug-pcseg-X				
	ζ=[1,2,3]		ζ=[2,3,4]		ζ=[3,4,5]
Buta-1,3-diene					
1	0.000		0.000		0.000
2	3.587	0.652	2.793	0.141	2.935
3	7.467	0.907	6.430	0.130	6.560
4	3.972	0.235	3.596	0.142	3.738
Mean		0.598		0.138	
Propan-2-ol					
1	0.402	0.025	0.406	0.030	0.376
2	0.000		0.000		0.000
3	1.096	0.085	1.272	0.090	1.181
4	1.297	0.057	1.367	0.014	1.354
5	3.659	0.021	3.760	0.123	3.637
6	3.302	0.002	3.399	0.099	3.300
7	4.030	0.034	4.128	0.132	3.996
Mean		0.038		0.081	
Water Dimer					
1	0.000		0.000		0.000
3	0.474	0.099	0.485	0.089	0.573
4	0.841	0.160	0.894	0.213	0.681
5	1.218	0.341	1.096	0.219	0.877
6	1.236	0.277	1.083	0.124	0.959
8	3.656	0.072	4.027	0.443	3.584
9	1.991	0.192	2.071	0.272	1.800
10	2.960	0.247	3.010	0.297	2.713
Mean		0.198		0.237	
Overall Mean		0.213		0.160	

	pcSseg-X				
	ζ=[1,2,3]		ζ=[2,3,4]		ζ=[3,4,5]
Buta-1,3-diene					
1	0.000		0.000		0.000
2	2.710	0.246	2.983	0.027	2.955
3	6.380	0.254	6.743	0.109	6.635
4	3.622	0.067	3.708	0.019	3.689
Mean		0.189		0.052	
Propan-2-ol					
1	0.461	0.089	0.401	0.028	0.373
2	0.000		0.000		0.000
3	1.182	0.011	1.157	0.036	1.193
4	1.339	0.006	1.348	0.003	1.345
5	3.667	0.043	3.736	0.111	3.624
6	3.323	0.063	3.455	0.195	3.260
7	4.069	0.095	4.141	0.167	3.974
Mean		0.051		0.090	
Water Dimer					
1	0.000		0.000		0.000
3	0.438	0.084	0.582	0.059	0.523
4	0.910	0.227	0.875	0.192	0.683
5	1.021	0.126	1.091	0.196	0.895
6	0.935	0.018	1.087	0.170	0.917
8	3.891	0.226	3.897	0.232	3.665
9	1.954	0.126	2.090	0.262	1.828
10	2.887	0.138	2.940	0.192	2.749
Mean		0.135		0.186	
Overall Mean		0.114		0.125	

Table S4 – continued from previous page.

	aug-pcSseg-X				
	ζ=[1,2,3]		ζ=[2,3,4]		ζ=[3,4,5]
Buta-1,3-diene					
1	0.000		0.000		0.000
2	3.340	0.385	2.823	0.132	2.955
3	7.111	0.492	6.473	0.146	6.619
4	3.901	0.184	3.638	0.078	3.716
Mean		0.354		0.119	
Propan-2-ol					
1	0.362	0.002	0.396	0.032	0.364
2	0.000		0.000		0.000
3	1.101	0.089	1.239	0.049	1.190
4	1.316	0.031	1.367	0.021	1.346
5	3.747	0.106	3.743	0.102	3.641
6	3.378	0.089	3.402	0.113	3.289
7	4.089	0.102	4.101	0.114	3.988
Mean		0.070		0.072	
Water Dimer					
1	0.000		0.000		0.000
3	0.551	0.007	0.556	0.011	0.544
4					0.710
5					0.918
6	1.296	0.356	1.050	0.109	0.940
8	3.655	0.003	3.772	0.119	3.653
9	1.975	0.134	1.936	0.096	1.841
10	2.936	0.168	2.836	0.067	2.769
Mean		0.133		0.081	
Overall Mean		0.153		0.085	

Table S5: The relative energies (kcal·mol^{-1}) of buta-1,3-diene, propan-2-ol and water dimer's conformations and configurations as computed using Dunning, Jensen and Karlruhe basis sets. All geometries were fully optimized at the theory levels specified for the relative energies (e.g. MP2/VDZ//MP2VDZ, MP2/pc-3//MP2/pc-3, MP2/def2-TZVPP//MP2/def2-TZVPP).

Conformation	**Pople Basis Set**	**Dunning Basis Sets**			
	HF/6-31G(d)	**MP2/VDZ**	**MP2/VTZ**	**MP2/VQZ**	**MP2/V5Z**
Buta-1,3-diene					
1	0.000	0.000	0.000	0.000	0.000
2	3.038	2.901	2.896	2.908	2.912
3	6.068	6.429	6.493	6.542	6.557
4	3.886	3.639	3.694	3.715	3.698
Propan-2-ol					
1	0.227	0.000	0.237	0.343	0.360
2	0.000	0.134	0.000	0.000	0.000
3	1.628	1.664	1.288	1.243	1.220
4	1.387	1.781	1.404	1.373	1.357
5	3.926	4.226	3.747	3.691	3.688
6	3.675	3.663	3.358	3.340	3.337
7	4.106	4.015	3.944	4.009	4.024
Water dimer					
1	0.000	0.000	0.000	0.000	0.000
3	0.696	1.176	0.874	0.712	0.603
4	0.445	0.031	0.471	0.651	0.736
5	0.968	0.643	0.940	1.018	0.992
6	1.266	1.972	1.405	1.185	1.052
8	3.028	3.013	3.245	3.460	3.638
9	1.408	1.785	1.854	1.875	1.883
10	2.362	3.091	2.993	2.911	2.833
		MP2/AVDZ	**MP2/AVTZ**	**MP2/AVQZ**	**MP2/AV5Z**
Buta-1,3-diene					
1		0.000	0.000	0.000	0.000
2		3.011	2.826	2.910	2.918
3		6.396	6.436	6.558	6.569
4		3.829	3.709	3.699	3.692
Propan-2-ol					
1		0.348	0.349	0.359	0.363

Table S5 – continued from previous page.

2	0.000	0.000	0.000	0.000
3	1.381	1.203	1.204	1.206
4	1.383	1.327	1.347	1.351
5	3.685	3.662	3.671	3.677
6	3.316	3.312	3.313	3.322
7	4.010	3.999	4.009	4.017
Water dimer				
1	0.000	0.000	0.000	0.000
3	0.664	0.610	0.573	0.558
4	0.888	0.832	0.785	0.770
5		1.084	1.012	0.988
6	1.043	1.125	1.049	1.024
8	3.779	3.810	3.751	3.732
9	1.969	2.003	1.942	1.920
10	2.923	2.929	2.865	2.841

Table S5 – continued from previous page.

	Jensen Basis Sets (with X=1–5)				
	MP2/pc-1	**MP2/pc-2**	**MP2/pc-3**	**MP2/pc-4**	**MP2/pc-5**
Buta-1,3-diene					
1	0.000	0.000	0.000	0.000	0.000
2	2.370	2.672	2.723	2.879	2.914
3	5.529	5.640	6.234	6.498	6.558
4	2.937	3.718	3.619	3.717	3.704
Propan-2-ol					
1	0.000	0.044	0.278	0.376	0.368
2	0.866	0.000	0.000	0.000	0.000
3	1.317	1.613	1.293	1.231	1.211
4	2.543	1.366	1.362	1.366	1.352
5	4.551	4.107	3.772	3.768	3.700
6	3.189	3.458	3.303	3.426	3.347
7	3.498	4.109	3.996	4.122	4.045
Water dimer					
1	0.000	0.000	0.000	0.000	0.000
3	0.519	0.881	0.635	0.571	0.551
4	3.992	0.530	0.779	0.807	0.753
5	4.732	1.059	1.048	1.033	0.971
6	4.889	1.472	1.146	1.084	1.009
8	10.069	3.156	3.624	3.690	3.683
9	5.353	1.429	1.720	1.912	1.886
10	7.510	2.611	2.740	2.818	2.794
	MP2/pcseg-1	**MP2/pcseg-2**	**MP2/pcseg-3**	**MP2/pcseg-4**	**MP2/pcseg-5**
Buta-1,3-diene					
1	0.000	0.000	0.000	0.000	0.000
2	2.101	2.689	2.701	2.834	2.898
3	4.918	5.654	6.176	6.438	6.512
4	2.988	3.735	3.634	3.692	3.705
Propan-2-ol					
1	0.673	0.126	0.295	0.378	0.373
2	0.000	0.000	0.000	0.000	0.000
3	2.253	1.676	1.299	1.217	1.206
4	1.120	1.353	1.368	1.356	1.353
5	3.712	4.122	3.767	3.746	3.683
6	3.566	3.509	3.322	3.399	3.332
7	4.375	4.211	4.005	4.105	4.034
Water dimer					
1	0.243	0.000	0.000	0.000	0.000
3	1.943	0.889	0.623	0.543	0.552
4	0.000	0.439	0.762	0.868	0.781
5	1.138	0.974	1.028	1.096	1.003
6	2.430	1.384	1.127	1.129	1.046
8	5.173	3.032	3.521	3.812	3.728
9	3.824	1.417	1.692	1.994	1.912
10	5.500	2.582	2.713	2.920	2.832
	MP2/aug-pcseg-1	**MP2/aug-pcseg-2**	**MP2/aug-pcseg-3**	**MP2/aug-pcseg-4**	**MP2/aug-pcseg-5**
Buta-1,3-diene					
1	0.000	0.000	0.000	0.000	0.000
2	2.111	2.227	2.995	2.885	2.911
3	4.497	5.464	6.615	6.513	6.534
4	3.428	3.553	3.813	3.688	3.712
Propan-2-ol					
1	0.558	0.316	0.349	0.383	0.379
2	0.000	0.000	0.000	0.000	0.000
3	1.499	1.423	1.207	1.245	1.214
4	0.880	1.311	1.335	1.353	1.353
5	3.636	3.792	3.722	3.744	3.691
6	3.281	3.463	3.378	3.391	3.345
7	4.080	4.155	4.068	4.103	4.049
Water dimer					
1	0.000	0.000	0.000	0.000	0.000
3	0.446	0.725	0.571	0.521	0.546
4	1.943	0.887	0.808	0.858	0.766
5			1.020		0.978
6	1.962	0.876	1.038	1.062	1.012
8	7.263	4.048	3.683	3.862	3.719
9	3.455	1.946	1.917	1.998	1.898
10	5.082	2.891	2.844	2.926	2.818

Table S5 – continued from previous page.

	MP2/pcSseg-1	MP2/pcSseg-2	MP2/pcSseg-3	MP2/pcSseg-4	MP2/pcSseg-5
Buta-1,3-diene					
1	0.000	0.000	0.000	0.000	0.000
2	2.097	2.634	2.681	2.874	2.925
3	4.912	5.656	6.145	6.502	6.574
4	2.979	3.674	3.634	3.706	3.708
Propan-2-ol					
1	0.677	0.107	0.305	0.364	0.369
2	0.000	0.000	0.000	0.000	0.000
3	2.221	1.660	1.345	1.221	1.207
4	1.112	1.401	1.383	1.356	1.352
5	3.766	4.039	3.806	3.762	3.694
6	3.609	3.423	3.367	3.421	3.342
7	4.435	4.104	4.053	4.105	4.040
Water dimer					
1	0.238	0.000	0.000	0.000	0.000
3	1.813	0.866	0.605	0.586	0.550
4	0.000	0.410	0.763	0.818	0.747
5	1.131	0.956	1.021	1.048	0.967
6	2.274	1.373	1.121	1.096	1.008
8	5.279	2.995	3.488	3.701	3.681
9	3.801	1.419	1.682	1.930	1.880
10	5.490	2.574	2.687	2.834	2.793

	MP2/aug-pcSseg-1	MP2/aug-pcSseg-2	MP2/aug-pcSseg-3	MP2/aug-pcSseg-4	MP2/aug-pcSseg-5
Buta-1,3-diene					
1	0.000	0.000	0.000	0.000	0.000
2	2.099	2.464	2.991	2.899	2.928
3	4.487	5.820	6.608	6.531	6.575
4	3.404	3.574	3.785	3.703	3.711
Propan-2-ol					
1	0.570	0.377	0.351	0.378	0.371
2	0.000	0.000	0.000	0.000	0.000
3	1.480	1.462	1.222	1.230	1.210
4	0.866	1.313	1.342	1.355	1.352
5	3.676	3.718	3.741	3.743	3.693
6	3.334	3.388	3.386	3.396	3.343
7	4.133	4.122	4.089	4.096	4.043
Water dimer					
1	0.000	0.000	0.000	0.000	0.000
3	0.438	0.514	0.535	0.545	0.544
4	1.955		0.790	0.764	0.742
5			0.992	0.986	0.955
6	1.966	0.640	1.006	1.027	0.991
8	7.416	3.904	3.628	3.690	3.670
9	3.566	1.796	1.849	1.889	1.869
10	5.197	2.682	2.753	2.784	2.778

			Karlsruhe Basis Sets		
	MP2/def2-SV(P)	**MP2/def2-SVP**	**MP2/def2-TZVP**	**MP2/def2-TZVPP**	**MP2/def2-QZVPP**
Buta-1,3-diene					
1	0.000	0.000	0.000	0.000	0.000
2	2.614	2.659	2.991	2.874	2.874
3	5.794	5.920	6.454	6.436	6.494
4	3.481	3.516	3.822	3.714	3.707
Propan-2-ol					
1	0.236	0.160	0.302	0.286	0.355
2	0.000	0.000	0.000	0.000	0.000
3	1.820	1.727	1.375	1.269	1.233
4	1.667	1.527	1.441	1.410	1.359
5	4.411	4.317	3.828	3.716	3.720
6	3.870	3.810	3.399	3.333	3.373
7	4.524	4.418	4.067	3.979	4.046
Water dimer					
1	0.000	0.019	0.000	0.000	0.000
3	1.065	1.255	0.692	0.697	0.618
4	0.034	0.000	0.622	0.627	0.773
5	0.773	0.689	1.006	0.971	1.030
6	1.504	1.821	1.106	1.155	1.104
8	3.218	2.949	3.472	3.286	3.628
9	1.781	1.965	1.608	1.790	1.876
10	3.121	3.220	2.713	2.780	2.826

Table S5 – continued from previous page.

	MP2/def2-SVPD	MP2/def2-TZVPD	MP2/def2-TZVPPD	MP2/def2-QZVPPD
Buta-1,3-diene				
1	0.000	0.000	0.000	0.000
2	2.631	2.937	2.858	2.878
3	6.062	6.439	6.386	6.494
4	3.638	3.837	3.724	3.710
Propan-2-ol				
1	0.298	0.346	0.364	0.360
2	0.000	0.000	0.000	0.000
3	1.323	1.243	1.232	1.222
4	1.216	1.358	1.360	1.344
5	3.612	3.801	3.746	3.715
6	3.330	3.467	3.404	3.370
7	3.938	4.136	4.085	4.055
Water dimer				
1	0.000	0.000	0.000	0.000
3	0.435	0.635	0.585	0.573
4		0.842	0.853	0.799
5		1.076	1.085	1.028
6	0.845	1.147	1.144	1.085
8	4.041	3.650	3.658	3.698
9	1.875	1.845	1.893	1.921
10	2.869	2.797	2.799	2.839

Table S6: Absolute error (kcal·mol^{-1}) in the relative energies for buta-1,3-diene, propan-2-ol, the water dimer. The mean absolute errors as computed for each molecule and for all conformations investigated are also provide. The relative energies computed by MP2/AV[T,Q,5//Q,5]Z//MP2/AV[T,Q,5]Z CBS extrapolation (see Table S4) were used as target reference values.

	Pople Basis Set	Dunning Basis Sets			
	HF/6-31G(d)	MP2/VDZ	MP2/VTZ	MP2/VQZ	MP2/V5Z
Buta-1,3-diene					
1	0.000	0.000	0.000	0.000	0.000
2	0.116	0.021	0.026	0.014	0.010
3	0.511	0.150	0.085	0.037	0.022
4	0.202	0.045	0.010	0.031	0.014
Mean	0.207	0.054	0.030	0.021	0.011
Propan-2-ol					
1	0.141	0.368	0.131	0.025	0.008
2	0.000	0.134	0.000	0.000	0.000
3	0.421	0.457	0.081	0.036	0.013
4	0.032	0.426	0.049	0.018	0.002
5	0.244	0.544	0.065	0.009	0.006
6	0.346	0.334	0.029	0.011	0.008
7	0.081	0.010	0.081	0.016	0.001
Mean	0.181	0.325	0.062	0.016	0.005
Water dimer					
1	0.000	0.000	0.000	0.000	0.000
3	0.154	0.634	0.332	0.170	0.061
4	0.307	0.721	0.282	0.101	0.016
5	0.004	0.321	0.024	0.054	0.028
6	0.272	0.978	0.410	0.191	0.058
8	0.692	0.707	0.476	0.260	0.082
9	0.492	0.114	0.046	0.025	0.017
10	0.457	0.271	0.173	0.091	0.014
Mean	0.297	0.468	0.218	0.111	0.034
Overall Mean	0.235	0.328	0.121	0.057	0.019
		MP2/AVDZ	**MP2/AVTZ**	**MP2/AVQZ**	**MP2/AV5Z**
Buta-1,3-diene					
1		0.000	0.000	0.000	0.000
2		0.089	0.096	0.012	0.004
3		0.183	0.143	0.021	0.010
4		0.145	0.025	0.016	0.008
Mean		0.104	0.066	0.012	0.005
Propan-2-ol					
1		0.020	0.019	0.009	0.005
2		0.000	0.000	0.000	0.000
3		0.174	0.004	0.003	0.001
4		0.028	0.028	0.008	0.004
5		0.003	0.020	0.011	0.005
6		0.013	0.017	0.016	0.007
7		0.015	0.026	0.016	0.008
Mean		0.036	0.016	0.009	0.004
Water dimer					
1		0.000	0.000	0.000	0.000
3		0.122	0.068	0.031	0.016
4		0.135	0.080	0.033	0.018
5			0.119	0.048	0.024
6		0.048	0.130	0.055	0.030
8		0.059	0.090	0.031	0.012
9		0.069	0.103	0.042	0.020
10		0.103	0.110	0.045	0.021
Mean		0.076	0.087	0.036	0.018
Overall Mean		0.067	0.057	0.021	0.010

Table S6 – continued from previous page.

	Jensen Basis Sets (with X=1–5)				
	MP2/pc-1	**MP2/pc-2**	**MP2/pc-3**	**MP2/pc-4**	**MP2/pc-5**
Buta-1,3-diene					
1	0.000	0.000	0.000	0.000	0.000
2	0.552	0.249	0.198	0.043	0.007
3	1.050	0.939	0.345	0.080	0.021
4	0.746	0.034	0.065	0.033	0.020
Mean	0.587	0.306	0.152	0.039	0.012
Propan-2-ol					
1	0.368	0.324	0.090	0.008	0.000
2	0.866	0.000	0.000	0.000	0.000
3	0.110	0.406	0.086	0.024	0.004
4	1.188	0.011	0.007	0.011	0.003
5	0.869	0.425	0.090	0.086	0.018
6	0.140	0.129	0.026	0.097	0.018
7	0.527	0.084	0.029	0.097	0.020
Mean	0.581	0.197	0.047	0.046	0.009
Water dimer					
1	0.000	0.000	0.000	0.000	0.000
3	0.023	0.339	0.093	0.029	0.008
4	3.240	0.223	0.026	0.054	0.000
5	3.768	0.095	0.084	0.069	0.007
6	3.894	0.477	0.151	0.090	0.015
8	6.349	0.564	0.097	0.030	0.037
9	3.453	0.471	0.180	0.012	0.014
10	4.690	0.209	0.080	0.001	0.026
Mean	3.177	0.297	0.089	0.036	0.013
Overall Mean	1.675	0.262	0.087	0.040	0.012
	MP2/pcseg-1	**MP2/pcseg-2**	**MP2/pcseg-3**	**MP2/pcseg-4**	**MP2/pcseg-5**
Buta-1,3-diene					
1	0.000	0.000	0.000	0.000	0.000
2	0.821	0.232	0.220	0.088	0.024
3	1.661	0.924	0.403	0.141	0.067
4	0.696	0.051	0.050	0.008	0.021
Mean	0.794	0.302	0.168	0.059	0.028
Propan-2-ol					
1	0.305	0.242	0.073	0.010	0.005
2	0.000	0.000	0.000	0.000	0.000
3	1.046	0.469	0.092	0.010	0.001
4	0.235	0.002	0.013	0.001	0.002
5	0.030	0.440	0.085	0.064	0.001
6	0.237	0.180	0.007	0.070	0.003
7	0.350	0.186	0.020	0.080	0.009
Mean	0.315	0.217	0.041	0.034	0.003
Water dimer					
1	0.243	0.000	0.000	0.000	0.000
3	1.401	0.347	0.081	0.000	0.010
4	0.752	0.313	0.009	0.115	0.029
5	0.174	0.010	0.064	0.132	0.039
6	1.435	0.390	0.132	0.135	0.051
8	1.453	0.689	0.199	0.092	0.008
9	1.924	0.483	0.208	0.094	0.012
10	2.681	0.238	0.107	0.100	0.012
Mean	1.258	0.309	0.100	0.083	0.020
Overall Mean	0.813	0.273	0.093	0.060	0.015

Table S6 – continued from previous page.

	MP2/aug-pcseg-1	MP2/aug-pcseg-2	MP2/aug-pcseg-3	MP2/aug-pcseg-4	MP2/aug-pcseg-5
Buta-1,3-diene					
1	0.000	0.000	0.000	0.000	0.000
2	0.811	0.694	0.074	0.037	0.011
3	2.082	1.115	0.036	0.066	0.045
4	0.256	0.131	0.129	0.004	0.028
Mean	0.787	0.485	0.060	0.027	0.021
Propan-2-ol					
1	0.190	0.052	0.019	0.015	0.011
2	0.000	0.000	0.000	0.000	0.000
3	0.292	0.216	0.000	0.038	0.007
4	0.475	0.044	0.020	0.002	0.002
5	0.046	0.110	0.040	0.062	0.009
6	0.048	0.134	0.049	0.062	0.016
7	0.055	0.130	0.043	0.078	0.024
Mean	0.158	0.098	0.025	0.037	0.010
Water dimer					
1	0.000	0.000	0.000	0.000	0.000
3	0.096	0.183	0.029	0.021	0.003
4	1.191	0.135	0.055	0.105	0.014
5			0.056	0.097	0.014
6	0.967	0.119	0.044	0.068	0.017
8	3.543	0.327	0.037	0.142	0.001
9	1.555	0.046	0.017	0.098	0.002
10	2.262	0.071	0.024	0.106	0.001
Mean	1.373	0.126	0.033	0.080	0.007
Overall Mean	0.770	0.195	0.035	0.053	0.011
	MP2/pcSseg-1	**MP2/pcSseg-2**	**MP2/pcSseg-3**	**MP2/pcSseg-4**	**MP2/pcSseg-5**
Buta-1,3-diene					
1	0.000	0.000	0.000	0.000	0.000
2	0.825	0.287	0.240	0.047	0.003
3	1.667	0.922	0.434	0.077	0.005
4	0.705	0.010	0.050	0.022	0.024
Mean	0.799	0.305	0.181	0.037	0.008
Propan-2-ol					
1	0.309	0.261	0.063	0.004	0.001
2	0.000	0.000	0.000	0.000	0.000
3	1.014	0.453	0.138	0.014	0.000
4	0.243	0.046	0.028	0.001	0.003
5	0.084	0.357	0.124	0.080	0.012
6	0.280	0.094	0.038	0.092	0.013
7	0.410	0.079	0.028	0.080	0.015
Mean	0.334	0.184	0.060	0.039	0.006
Water dimer					
1	0.238	0.000	0.000	0.000	0.000
3	1.270	0.324	0.063	0.044	0.008
4	0.752	0.343	0.010	0.065	0.005
5	0.167	0.008	0.057	0.084	0.003
6	1.279	0.379	0.126	0.101	0.013
8	1.559	0.725	0.232	0.019	0.039
9	1.901	0.481	0.218	0.030	0.019
10	2.671	0.246	0.133	0.014	0.027
Mean	1.230	0.313	0.105	0.045	0.014
Overall Mean	0.809	0.264	0.104	0.041	0.010

Table S6 – continued from previous page.

	MP2/aug-pcSseg-1	MP2/aug-pcSseg-2	MP2/aug-pcSseg-3	MP2/aug-pcSseg-4	MP2/aug-pcSseg-5
Buta-1,3-diene					
1	0.000	0.000	0.000	0.000	0.000
2	0.822	0.458	0.070	0.023	0.006
3	2.092	0.759	0.029	0.048	0.004
4	0.280	0.110	0.101	0.019	0.027
Mean	0.798	0.332	0.050	0.022	0.009
Propan-2-ol					
1	0.202	0.009	0.017	0.010	0.003
2	0.000	0.000	0.000	0.000	0.000
3	0.273	0.255	0.015	0.023	0.003
4	0.489	0.042	0.013	0.000	0.003
5	0.006	0.036	0.059	0.061	0.011
6	0.005	0.059	0.057	0.067	0.014
7	0.108	0.097	0.064	0.071	0.018
Mean	0.155	0.071	0.032	0.033	0.008
Water dimer					
1	0.000	0.000	0.000	0.000	0.000
3	0.105	0.028	0.008	0.003	0.001
4	1.203		0.038	0.012	0.011
5			0.028	0.022	0.009
6			0.011	0.032	0.004
8	3.696	0.184	0.092	0.030	0.050
9	1.666	0.104	0.051	0.011	0.031
10	2.377	0.138	0.066	0.035	0.041
Mean	1.508	0.091	0.037	0.018	0.018
Overall Mean	0.784	0.142	0.038	0.025	0.012

			Karlsruhe Basis Sets		
	MP2/def2-SV(P)	MP2/def2-SVP	MP2/def2-TZVP	MP2/def2-TZVPP	MP2/def2-QZVPP
Buta-1,3-diene					
1	0.000	0.000	0.000	0.000	0.000
2	0.308	0.262	0.070	0.047	0.047
3	0.785	0.659	0.124	0.143	0.085
4	0.203	0.168	0.139	0.030	0.024
Mean	0.324	0.272	0.083	0.055	0.039
Propan-2-ol					
1	0.132	0.208	0.066	0.082	0.013
2	0.000	0.000	0.000	0.000	0.000
3	0.613	0.520	0.168	0.062	0.026
4	0.312	0.172	0.086	0.055	0.004
5	0.729	0.635	0.146	0.034	0.038
6	0.541	0.481	0.070	0.004	0.044
7	0.499	0.393	0.042	0.046	0.021
Mean	0.404	0.344	0.082	0.040	0.021
Water dimer					
1	0.000	0.019	0.000	0.000	0.000
3	0.523	0.713	0.150	0.155	0.075
4	0.718	0.752	0.131	0.126	0.021
5	0.191	0.275	0.042	0.007	0.066
6	0.509	0.827	0.111	0.161	0.110
8	0.502	0.771	0.249	0.434	0.092
9	0.119	0.065	0.291	0.110	0.024
10	0.301	0.401	0.106	0.039	0.007
Mean	0.358	0.478	0.135	0.129	0.049
Overall Mean	0.368	0.385	0.105	0.081	0.037

Table S6 – continued from previous page.

	MP2/def2-SVPD	MP2/def2-TZVPD	MP2/def2-TZVPPD	MP2/def2-QZVPPD
Buta-1,3-diene				
1	0.000	0.000	0.000	0.000
2	0.291	0.015	0.064	0.044
3	0.517	0.140	0.193	0.085
4	0.046	0.153	0.040	0.026
Mean	0.213	0.077	0.074	0.039
Propan-2-ol				
1	0.070	0.022	0.004	0.008
2	0.000	0.000	0.000	0.000
3	0.116	0.036	0.025	0.015
4	0.139	0.003	0.005	0.011
5	0.070	0.119	0.064	0.033
6	0.001	0.138	0.075	0.041
7	0.087	0.111	0.060	0.030
Mean	0.069	0.061	0.033	0.020
Water dimer				
1	0.000	0.000	0.000	0.000
3	0.107	0.093	0.043	0.031
4		0.090	0.101	0.047
5		0.112	0.120	0.064
6	0.149	0.153	0.150	0.090
8	0.321	0.070	0.062	0.023
9	0.025	0.055	0.007	0.021
10	0.0488	0.023	0.021	0.019
Mean	0.108	0.074	0.063	0.037
Overall Mean	0.117	0.070	0.054	0.031

Table S7: RMSD (Å) values for buta-1,3-diene, propan-2-ol and water dimer conformations and configurations, using the MP2/aV5Z geometries as the target values. The RMSD values within parentheses were computed using only the heavy atoms (i.e. nonhydrogen atoms). The Jensen basis sets are with the adjusted indexing values (i.e. X=1–5).

	Pople Basis Set		Dunning Basis Sets		
Conf.	**HF/6-31G(d)**	**MP2/VDZ**	**MP2/VTZ**	**MP2/VQZ**	**MP2/V5Z**
Buta-1,3-diene					
1	0.012 (0.009)	0.024 (0.016)	0.004 (0.003)	0.001 (0.000)	0.001 (0.000)
2	0.043 (0.026)	0.024 (0.015)	0.004 (0.003)	0.001 (0.001)	0.001 (0.001)
3	0.018 (0.011)	0.022 (0.014)	0.004 (0.003)	0.001 (0.001)	0.001 (0.000)
4	0.029 (0.018)	0.025 (0.016)	0.004 (0.003)	0.002 (0.001)	0.001 (0.001)
Mean	0.025 (0.016)	0.024 (0.015)	0.004 (0.003)	0.001 (0.001)	0.001 (0.001)
Propan-2-ol					
1	0.018 (0.011)	0.020 (0.008)	0.004 (0.002)	0.002 (0.000)	0.001 (0.001)
2	0.023 (0.010)	0.020 (0.008)	0.004 (0.001)	0.001 (0.001)	0.001 (0.000)
3	0.021 (0.010)	0.023 (0.008)	0.005 (0.002)	0.001 (0.001)	0.001 (0.000)
4	0.019 (0.011)	0.021 (0.009)	0.005 (0.002)	0.002 (0.001)	0.001 (0.000)
5	0.020 (0.011)	0.020 (0.008)	0.005 (0.002)	0.002 (0.000)	0.001 (0.000)
6	0.020 (0.010)	0.019 (0.007)	0.005 (0.002)	0.001 (0.001)	0.001 (0.000)
7	0.017 (0.011)	0.021 (0.008)	0.006 (0.002)	0.002 (0.000)	0.001 (0.000)
Mean	0.020 (0.011)	0.021 (0.008)	0.005 (0.002)	0.002 (0.001)	0.001 (0.000)
Water dimer					
1	0.030 (0.034)	0.074 (0.003)	0.035 (0.002)	0.022 (0.001)	0.005 (0.000)
3	0.064 (0.043)	0.120 (0.004)	0.060 (0.004)	0.027 (0.000)	0.008 (0.000)
4	0.105 (0.039)	0.204 (0.009)	0.104 (0.008)	0.058 (0.006)	0.013 (0.002)
5	0.209 (0.055)	0.398 (0.027)	0.205 (0.020)	0.103 (0.010)	0.022 (0.002)
6	0.024 (0.028)	0.036 (0.018)	0.020 (0.009)	0.013 (0.005)	0.004 (0.001)
8	0.109 (0.125)	0.217 (0.199)	0.112 (0.101)	0.050 (0.045)	0.009 (0.009)
9	0.008 (0.003)	0.070 (0.067)	0.029 (0.028)	0.012 (0.011)	0.002 (0.002)
10	0.025 (0.023)	0.100 (0.097)	0.030 (0.030)	0.014 (0.013)	0.002 (0.002)
Mean	0.072 (0.044)	0.152 (0.053)	0.074 (0.025)	0.037 (0.011)	0.008 (0.002)
Overall Mean	0.043 (0.026)	0.077 (0.028)	0.034 (0.012)	0.017 (0.005)	0.004 (0.001)

	MP2/AVDZ	**MP2/AVTZ**	**MP2/AVQZ**
Buta-1,3-diene			
1	0.025 (0.017)	0.005 (0.004)	0.001 (0.001)
2	0.029 (0.018)	0.008 (0.005)	0.001 (0.001)
3	0.024 (0.016)	0.005 (0.004)	0.001 (0.001)
4	0.026 (0.018)	0.006 (0.004)	0.001 (0.001)
Mean	0.026 (0.017)	0.006 (0.004)	0.001 (0.001)
Propan-2-ol			
1	0.018 (0.012)	0.003 (0.003)	0.001 (0.001)
2	0.019 (0.012)	0.004 (0.003)	0.001 (0.001)
3	0.020 (0.012)	0.003 (0.003)	0.001 (0.001)
4	0.018 (0.012)	0.004 (0.003)	0.001 (0.001)
5	0.018 (0.011)	0.004 (0.003)	0.001 (0.001)
6	0.018 (0.011)	0.004 (0.003)	0.001 (0.001)
7	0.018 (0.012)	0.004 (0.003)	0.001 (0.001)
Mean	0.018 (0.012)	0.004 (0.003)	0.001 (0.001)
Water dimer			
1	0.010 (0.006)	0.005 (0.002)	0.002 (0.000)
3	0.017 (0.008)	0.008 (0.003)	0.001 (0.000)
4	0.018 (0.014)	0.016 (0.009)	0.003 (0.001)
5		0.026 (0.009)	0.006 (0.002)
6	0.018 (0.015)	0.006 (0.006)	0.001 (0.001)
8	0.011 (0.001)	0.011 (0.007)	0.004 (0.002)
9	0.006 (0.005)	0.003 (0.002)	0.001 (0.001)
10	0.004 (0.001)	0.003 (0.001)	0.002 (0.001)
Mean	0.012 (0.007)	0.010 (0.005)	0.003 (0.001)
Overall Mean	0.018 (0.011)	0.007 (0.004)	0.002 (0.001)

Table S7 – continued from previous page.

	MP2/pc-1	MP2/pc-2	MP2/pc-3	MP2/pc-4	MP2/pc-5
Buta-1,3-diene					
1	0.037 (0.028)	0.013 (0.008)	0.003 (0.002)	0.001 (0.001)	0.001 (0.001)
2	0.035 (0.026)	0.037 (0.016)	0.007 (0.003)	0.003 (0.001)	0.001 (0.001)
3	0.033 (0.025)	0.012 (0.006)	0.004 (0.001)	0.002 (0.001)	0.001 (0.001)
4	0.032 (0.025)	0.017 (0.010)	0.004 (0.002)	0.001 (0.001)	0.001 (0.001)
Mean	0.034 (0.026)	0.020 (0.010)	0.004 (0.002)	0.002 (0.001)	0.001 (0.001)
Propan-2-ol					
1	0.058 (0.028)	0.014 (0.006)	0.002 (0.001)	0.001 (0.001)	0.001 (0.000)
2	0.063 (0.027)	0.019 (0.006)	0.007 (0.001)	0.001 (0.001)	0.001 (0.001)
3	0.059 (0.028)	0.018 (0.006)	0.003 (0.001)	0.001 (0.000)	0.001 (0.000)
4	0.058 (0.027)	0.016 (0.008)	0.003 (0.002)	0.001 (0.001)	0.001 (0.000)
5	0.063 (0.028)	0.019 (0.003)	0.006 (0.001)	0.001 (0.000)	0.001 (0.000)
6	0.058 (0.027)	0.014 (0.004)	0.006 (0.001)	0.001 (0.001)	0.001 (0.000)
7	0.072 (0.028)	0.012 (0.004)	0.003 (0.001)	0.001 (0.000)	0.001 (0.000)
Mean	0.062 (0.028)	0.016 (0.005)	0.004 (0.001)	0.001 (0.001)	0.001 (0.000)
Water dimer					
1	0.177 (0.124)	0.035 (0.009)	0.031 (0.000)	0.006 (0.001)	0.003 (0.002)
3	0.211 (0.123)	0.100 (0.017)	0.025 (0.004)	0.006 (0.002)	0.002 (0.002)
4	0.142 (0.102)	0.114 (0.023)	0.004 (0.002)	0.004 (0.005)	0.002 (0.003)
5	0.199 (0.094)	0.245 (0.039)	0.027 (0.003)	0.008 (0.006)	0.003 (0.003)
6	0.131 (0.111)	0.014 (0.004)	0.007 (0.002)	0.005 (0.006)	0.003 (0.003)
8	0.230 (0.245)	0.135 (0.128)	0.016 (0.020)	0.012 (0.010)	0.008 (0.007)
9	0.179 (0.165)	0.046 (0.043)	0.007 (0.006)	0.007 (0.007)	0.004 (0.004)
10	0.223 (0.212)	0.068 (0.066)	0.001 (0.001)	0.009 (0.009)	0.005 (0.004)
Mean	0.187 (0.147)	0.095 (0.041)	0.015 (0.005)	0.007 (0.006)	0.004 (0.004)
Overall Mean	0.108 (0.078)	0.050 (0.021)	0.009 (0.003)	0.004 (0.003)	0.002 (0.002)

	MP2/pcseg-1	MP2/pcseg-2	MP2/pcseg-3	MP2/pcseg-4	MP2/pcseg-5
Buta-1,3-diene					
1	0.032 (0.021)	0.014 (0.008)	0.003 (0.002)	0.002 (0.001)	0.001 (0.001)
2	0.040 (0.024)	0.037 (0.017)	0.008 (0.003)	0.006 (0.002)	0.003 (0.001)
3	0.030 (0.019)	0.012 (0.006)	0.005 (0.002)	0.003 (0.001)	0.002 (0.001)
4	0.030 (0.020)	0.018 (0.011)	0.005 (0.004)	0.003 (0.001)	0.001 (0.001)
Mean	0.033 (0.021)	0.020 (0.011)	0.005 (0.003)	0.003 (0.001)	0.002 (0.001)
Propan-2-ol					
1	0.042 (0.034)	0.014 (0.006)	0.002 (0.001)	0.002 (0.001)	0.001 (0.001)
2	0.052 (0.031)	0.020 (0.006)	0.007 (0.001)	0.002 (0.001)	0.001 (0.001)
3	0.042 (0.034)	0.018 (0.007)	0.003 (0.001)	0.002 (0.001)	0.001 (0.001)
4	0.042 (0.031)	0.016 (0.008)	0.004 (0.002)	0.002 (0.001)	0.001 (0.001)
5	0.060 (0.033)	0.020 (0.004)	0.005 (0.002)	0.002 (0.000)	0.001 (0.000)
6	0.049 (0.032)	0.014 (0.004)	0.005 (0.001)	0.002 (0.001)	0.001 (0.001)
7	0.047 (0.036)	0.012 (0.005)	0.002 (0.001)	0.002 (0.000)	0.001 (0.001)
Mean	0.048 (0.033)	0.016 (0.006)	0.004 (0.001)	0.002 (0.001)	0.001 (0.001)
Water dimer					
1	0.138 (0.021)	0.028 (0.011)	0.026 (0.001)	0.008 (0.003)	0.002 (0.001)
3	0.082 (0.028)	0.088 (0.017)	0.013 (0.003)	0.011 (0.002)	0.001 (0.001)
4	0.198 (0.047)	0.115 (0.024)	0.002 (0.001)	0.004 (0.001)	0.002 (0.002)
5	0.347 (0.034)	0.244 (0.040)	0.028 (0.006)	0.003 (0.001)	0.006 (0.003)
6	0.093 (0.072)	0.014 (0.003)	0.007 (0.006)	0.002 (0.001)	0.002 (0.002)
8	0.259 (0.270)	0.135 (0.131)	0.022 (0.026)	0.009 (0.008)	0.005 (0.005)
9	0.105 (0.092)	0.043 (0.041)	0.006 (0.006)	0.001 (0.001)	0.002 (0.002)
10	0.127 (0.116)	0.065 (0.063)	0.002 (0.001)	0.005 (0.004)	0.004 (0.004)
Mean	0.169 (0.085)	0.091 (0.041)	0.013 (0.006)	0.005 (0.003)	0.003 (0.003)
Overall Mean	0.096 (0.052)	0.049 (0.022)	0.008 (0.004)	0.004 (0.002)	0.002 (0.002)

Table S7 – continued from previous page.

	MP2/aug-pcseg-1	MP2/aug-pcseg-2	MP2/aug-pcseg-3	MP2/aug-pcseg-4	MP2/aug-pcseg-5
Buta-1,3-diene					
1	0.034 (0.023)	0.017 (0.011)	0.003 (0.002)	0.001 (0.000)	0.001 (0.001)
2	0.070 (0.034)	0.039 (0.020)	0.007 (0.004)	0.002 (0.001)	0.002 (0.001)
3	0.034 (0.023)	0.021 (0.013)	0.004 (0.002)	0.002 (0.001)	0.001 (0.001)
4	0.034 (0.023)	0.022 (0.014)	0.007 (0.004)	0.002 (0.001)	0.001 (0.001)
Mean	0.043 (0.026)	0.025 (0.014)	0.005 (0.003)	0.002 (0.001)	0.001 (0.001)
Propan-2-ol					
1	0.051 (0.039)	0.013 (0.008)	0.003 (0.002)	0.002 (0.000)	0.001 (0.000)
2	0.058 (0.036)	0.016 (0.007)	0.004 (0.002)	0.002 (0.001)	0.001 (0.001)
3	0.052 (0.039)	0.015 (0.008)	0.004 (0.002)	0.002 (0.000)	0.001 (0.001)
4	0.051 (0.035)	0.012 (0.008)	0.003 (0.002)	0.001 (0.001)	0.001 (0.001)
5	0.062 (0.038)	0.013 (0.008)	0.003 (0.002)	0.002 (0.000)	0.001 (0.000)
6	0.056 (0.038)	0.013 (0.008)	0.003 (0.002)	0.002 (0.000)	0.001 (0.001)
7	0.053 (0.040)	0.014 (0.008)	0.003 (0.002)	0.002 (0.000)	0.001 (0.000)
Mean	0.055 (0.038)	0.014 (0.008)	0.003 (0.002)	0.002 (0.000)	0.001 (0.001)
Water dimer					
1	0.114 (0.056)	0.019 (0.014)	0.003 (0.003)	0.008 (0.002)	0.004 (0.001)
3	0.082 (0.063)	0.033 (0.028)	0.010 (0.002)	0.002 (0.001)	0.002 (0.000)
4	0.157 (0.079)	0.038 (0.008)	0.008 (0.008)	0.005 (0.001)	0.004 (0.001)
5			0.018 (0.005)	0.036 (0.000)	0.002 (0.002)
6	0.076 (0.056)	0.023 (0.007)	0.007 (0.006)	0.004 (0.003)	0.001 (0.001)
8	0.063 (0.033)	0.037 (0.018)	0.007 (0.007)	0.002 (0.001)	0.003 (0.002)
9	0.075 (0.054)	0.008 (0.006)	0.003 (0.003)	0.002 (0.002)	0.002 (0.001)
10	0.069 (0.047)	0.018 (0.017)	0.001 (0.001)	0.003 (0.003)	0.002 (0.001)
Mean	0.091 (0.055)	0.025 (0.014)	0.007 (0.004)	0.008 (0.002)	0.003 (0.001)
Overall Mean	0.066 (0.042)	0.021 (0.012)	0.005 (0.003)	0.004 (0.001)	0.002 (0.001)

	MP2/pcSseg-1	MP2/pcSseg-2	MP2/pcSseg-3	MP2/pcSseg-4	MP2/pcSseg-5
Buta-1,3-diene					
1	0.028 (0.018)	0.012 (0.007)	0.002 (0.001)	0.002 (0.001)	0.001 (0.001)
2	0.037 (0.021)	0.033 (0.015)	0.008 (0.003)	0.004 (0.002)	0.001 (0.001)
3	0.026 (0.017)	0.010 (0.005)	0.004 (0.001)	0.002 (0.002)	0.001 (0.001)
4	0.026 (0.018)	0.016 (0.009)	0.004 (0.002)	0.002 (0.001)	0.001 (0.001)
Mean	0.029 (0.019)	0.018 (0.009)	0.005 (0.002)	0.003 (0.002)	0.001 (0.001)
Propan-2-ol					
1	0.039 (0.030)	0.013 (0.006)	0.002 (0.001)	0.001 (0.001)	0.001 (0.001)
2	0.049 (0.027)	0.018 (0.005)	0.006 (0.001)	0.002 (0.001)	0.001 (0.001)
3	0.039 (0.030)	0.016 (0.006)	0.003 (0.001)	0.002 (0.001)	0.001 (0.000)
4	0.039 (0.027)	0.014 (0.007)	0.003 (0.002)	0.001 (0.001)	0.001 (0.001)
5	0.057 (0.029)	0.018 (0.003)	0.005 (0.001)	0.002 (0.001)	0.001 (0.001)
6	0.046 (0.028)	0.013 (0.003)	0.005 (0.001)	0.002 (0.001)	0.001 (0.001)
7	0.044 (0.032)	0.012 (0.004)	0.002 (0.001)	0.001 (0.000)	0.001 (0.001)
Mean	0.045 (0.029)	0.015 (0.005)	0.004 (0.001)	0.002 (0.001)	0.001 (0.001)
Water dimer					
1	0.132 (0.026)	0.028 (0.008)	0.027 (0.004)	0.006 (0.001)	0.002 (0.001)
3	0.083 (0.034)	0.089 (0.013)	0.010 (0.005)	0.007 (0.003)	0.003 (0.002)
4	0.193 (0.053)	0.120 (0.022)	0.005 (0.002)	0.005 (0.005)	0.002 (0.002)
5	0.335 (0.039)	0.253 (0.038)	0.027 (0.008)	0.010 (0.006)	0.004 (0.003)
6	0.098 (0.076)	0.016 (0.006)	0.008 (0.008)	0.005 (0.006)	0.002 (0.002)
8	0.259 (0.273)	0.141 (0.136)	0.019 (0.022)	0.010 (0.009)	0.006 (0.006)
9	0.109 (0.096)	0.045 (0.042)	0.004 (0.003)	0.006 (0.006)	0.003 (0.003)
10	0.132 (0.121)	0.068 (0.065)	0.003 (0.003)	0.010 (0.009)	0.004 (0.004)
Mean	0.168 (0.090)	0.095 (0.041)	0.013 (0.007)	0.007 (0.006)	0.003 (0.003)
Overall Mean	0.093 (0.052)	0.049 (0.021)	0.008 (0.004)	0.004 (0.003)	0.002 (0.002)

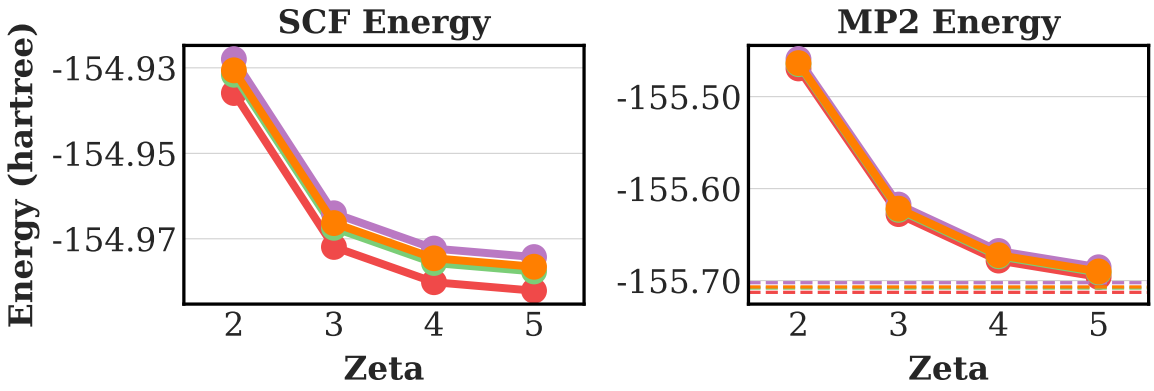
Table S7 – continued from previous page.

	MP2/aug-pcSseg-1	MP2/aug-pcSseg-2	MP2/aug-pcSseg-3	MP2/aug-pcSseg-4	MP2/aug-pcSseg-5
Buta-1,3-diene					
1	0.031 (0.020)	0.015 (0.011)	0.003 (0.002)	0.001 (0.001)	0.001 (0.001)
2	0.068 (0.032)	0.029 (0.016)	0.006 (0.004)	0.002 (0.001)	0.001 (0.001)
3	0.030 (0.020)	0.016 (0.010)	0.003 (0.001)	0.002 (0.001)	0.001 (0.001)
4	0.030 (0.020)	0.019 (0.013)	0.006 (0.004)	0.001 (0.001)	0.001 (0.001)
Mean	0.040 (0.023)	0.020 (0.013)	0.005 (0.003)	0.002 (0.001)	0.001 (0.001)
Propan-2-ol					
1	0.049 (0.035)	0.011 (0.006)	0.002 (0.001)	0.001 (0.000)	0.001 (0.000)
2	0.055 (0.033)	0.015 (0.006)	0.002 (0.001)	0.001 (0.001)	0.001 (0.001)
3	0.049 (0.035)	0.013 (0.007)	0.003 (0.001)	0.002 (0.000)	0.001 (0.000)
4	0.048 (0.031)	0.011 (0.006)	0.002 (0.001)	0.001 (0.001)	0.001 (0.001)
5	0.060 (0.034)	0.013 (0.007)	0.002 (0.001)	0.001 (0.000)	0.001 (0.000)
6	0.053 (0.034)	0.013 (0.006)	0.003 (0.001)	0.001 (0.000)	0.001 (0.001)
7	0.050 (0.036)	0.012 (0.007)	0.002 (0.001)	0.001 (0.000)	0.001 (0.000)
Mean	0.052 (0.034)	0.013 (0.006)	0.002 (0.001)	0.001 (0.000)	0.001 (0.000)
Water dimer					
1	0.115 (0.061)	0.015 (0.018)	0.009 (0.005)	0.003 (0.002)	0.003 (0.002)
3	0.086 (0.068)	0.032 (0.026)	0.008 (0.006)	0.003 (0.002)	0.003 (0.002)
4	0.166 (0.083)		0.013 (0.010)	0.006 (0.005)	0.003 (0.002)
5			0.027 (0.008)	0.011 (0.008)	0.003 (0.002)
6			0.011 (0.009)	0.006 (0.006)	0.002 (0.002)
8	0.065 (0.035)	0.028 (0.017)	0.009 (0.009)	0.008 (0.008)	0.004 (0.004)
9	0.077 (0.056)	0.005 (0.001)	0.010 (0.010)	0.008 (0.008)	0.003 (0.003)
10	0.071 (0.049)	0.018 (0.017)	0.007 (0.007)	0.008 (0.008)	0.004 (0.004)
Mean	0.097 (0.059)	0.020 (0.016)	0.012 (0.008)	0.007 (0.006)	0.003 (0.003)
Overall Mean	0.065 (0.040)	0.017 (0.011)	0.007 (0.004)	0.004 (0.003)	0.002 (0.001)

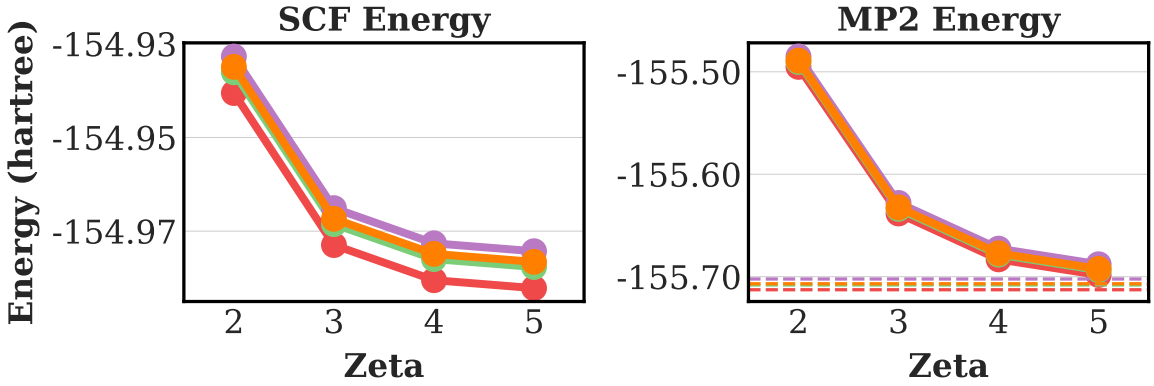
	MP2/def2-SV(P)	MP2/def2-SVP	MP2/def2-TZVP	MP2/def2-TZVPP	MP2/def2-QZVPP
Buta-1,3-diene					
1	0.024 (0.013)	0.020 (0.012)	0.005 (0.003)	0.004 (0.003)	0.001 (0.001)
2	0.029 (0.015)	0.022 (0.013)	0.012 (0.006)	0.005 (0.003)	0.002 (0.001)
3	0.024 (0.011)	0.021 (0.009)	0.005 (0.002)	0.004 (0.003)	0.002 (0.001)
4	0.027 (0.015)	0.021 (0.013)	0.008 (0.005)	0.004 (0.004)	0.002 (0.001)
Mean	0.026 (0.013)	0.021 (0.012)	0.008 (0.004)	0.004 (0.003)	0.002 (0.001)
Propan-2-ol					
1	0.021 (0.008)	0.017 (0.007)	0.005 (0.002)	0.003 (0.002)	0.001 (0.001)
2	0.021 (0.008)	0.018 (0.006)	0.008 (0.002)	0.004 (0.002)	0.001 (0.000)
3	0.023 (0.008)	0.018 (0.006)	0.008 (0.002)	0.003 (0.002)	0.002 (0.001)
4	0.021 (0.009)	0.019 (0.008)	0.007 (0.002)	0.005 (0.002)	0.001 (0.001)
5	0.021 (0.006)	0.018 (0.006)	0.007 (0.002)	0.004 (0.002)	0.001 (0.000)
6	0.019 (0.007)	0.016 (0.006)	0.008 (0.002)	0.004 (0.002)	0.001 (0.001)
7	0.020 (0.007)	0.017 (0.006)	0.012 (0.002)	0.003 (0.002)	0.001 (0.000)
Mean	0.021 (0.008)	0.018 (0.006)	0.008 (0.002)	0.004 (0.002)	0.001 (0.001)
Water dimer					
1	0.063 (0.002)	0.100 (0.000)	0.012 (0.003)	0.010 (0.005)	0.006 (0.000)
3	0.079 (0.001)	0.088 (0.003)	0.006 (0.004)	0.024 (0.008)	0.009 (0.001)
4	0.152 (0.000)	0.198 (0.009)	0.031 (0.001)	0.042 (0.008)	0.012 (0.003)
5	0.297 (0.017)	0.372 (0.026)	0.065 (0.008)	0.089 (0.014)	0.025 (0.004)
6	0.035 (0.023)	0.037 (0.014)	0.004 (0.001)	0.010 (0.004)	0.005 (0.001)
8	0.198 (0.195)	0.219 (0.207)	0.065 (0.062)	0.056 (0.051)	0.008 (0.008)
9	0.072 (0.068)	0.064 (0.061)	0.025 (0.023)	0.008 (0.008)	0.001 (0.001)
10	0.097 (0.093)	0.091 (0.088)	0.025 (0.024)	0.007 (0.006)	0.002 (0.001)
Mean	0.124 (0.050)	0.146 (0.051)	0.029 (0.016)	0.031 (0.013)	0.009 (0.002)
Overall Mean	0.065 (0.027)	0.072 (0.026)	0.017 (0.008)	0.015 (0.007)	0.004 (0.001)

Table S7 – continued from previous page.

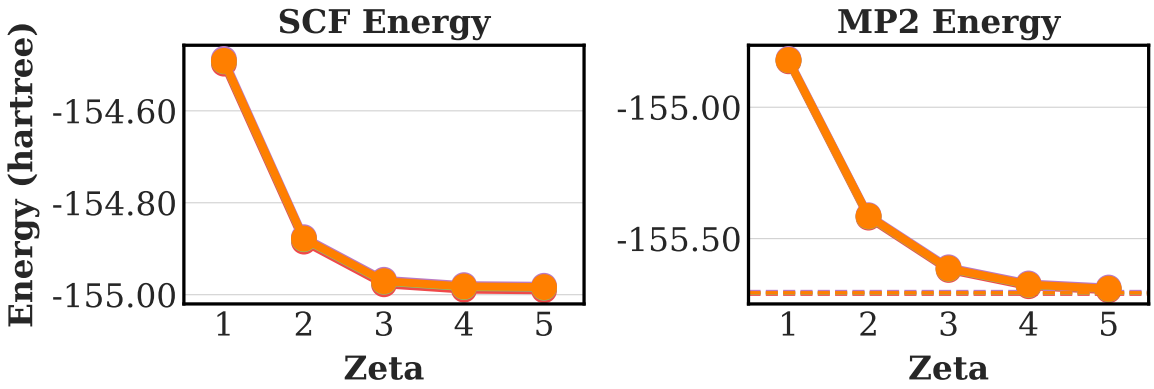
	MP2/def2-SVPD	MP2/def2-TZVPD	MP2/def2-TZVPPD	MP2/def2-QZVPPD
Buta-1,3-diene				
1	0.021 (0.014)	0.006 (0.003)	0.004 (0.004)	0.001 (0.001)
2	0.031 (0.016)	0.014 (0.007)	0.009 (0.005)	0.003 (0.001)
3	0.021 (0.014)	0.006 (0.003)	0.005 (0.004)	0.001 (0.001)
4	0.022 (0.015)	0.009 (0.005)	0.006 (0.004)	0.002 (0.001)
Mean	0.024 (0.015)	0.009 (0.004)	0.006 (0.004)	0.002 (0.001)
Propan-2-ol				
1	0.016 (0.008)	0.006 (0.003)	0.003 (0.003)	0.001 (0.000)
2	0.019 (0.008)	0.007 (0.003)	0.004 (0.003)	0.001 (0.000)
3	0.018 (0.008)	0.006 (0.003)	0.004 (0.003)	0.001 (0.001)
4	0.015 (0.008)	0.006 (0.003)	0.004 (0.003)	0.001 (0.001)
5	0.018 (0.008)	0.006 (0.003)	0.004 (0.003)	0.001 (0.001)
6	0.017 (0.008)	0.007 (0.003)	0.004 (0.003)	0.001 (0.001)
7	0.016 (0.008)	0.006 (0.003)	0.003 (0.003)	0.001 (0.001)
Mean	0.017 (0.008)	0.006 (0.003)	0.004 (0.003)	0.001 (0.001)
Water dimer				
1	0.041 (0.010)	0.015 (0.012)	0.011 (0.007)	0.002 (0.001)
3	0.021 (0.007)	0.017 (0.015)	0.014 (0.009)	0.005 (0.001)
4		0.021 (0.020)	0.012 (0.013)	0.006 (0.005)
5		0.035 (0.022)	0.024 (0.015)	0.018 (0.007)
6	0.014 (0.008)	0.022 (0.017)	0.013 (0.013)	0.004 (0.005)
8	0.019 (0.018)	0.007 (0.005)	0.009 (0.011)	0.009 (0.009)
9	0.013 (0.011)	0.015 (0.014)	0.011 (0.011)	0.005 (0.005)
10	0.029 (0.027)	0.017 (0.017)	0.014 (0.013)	0.008 (0.008)
Mean	0.023 (0.014)	0.019 (0.015)	0.014 (0.011)	0.007 (0.005)
Overall Mean	0.021 (0.012)	0.012 (0.008)	0.008 (0.007)	0.004 (0.003)



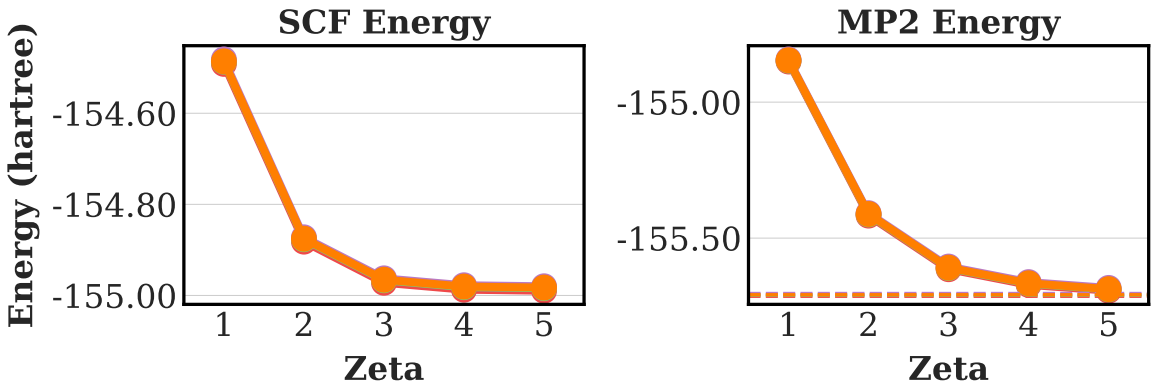
(a) VXZ



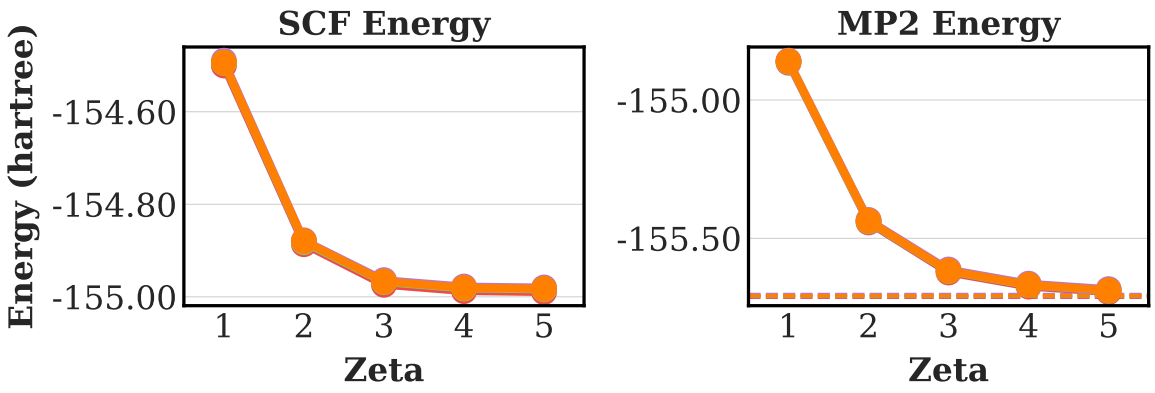
(b) AVXZ



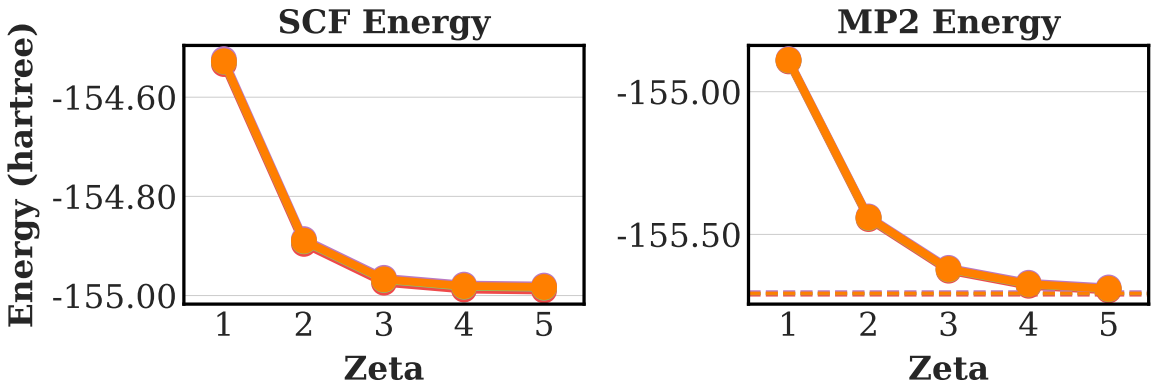
(c) pc-X



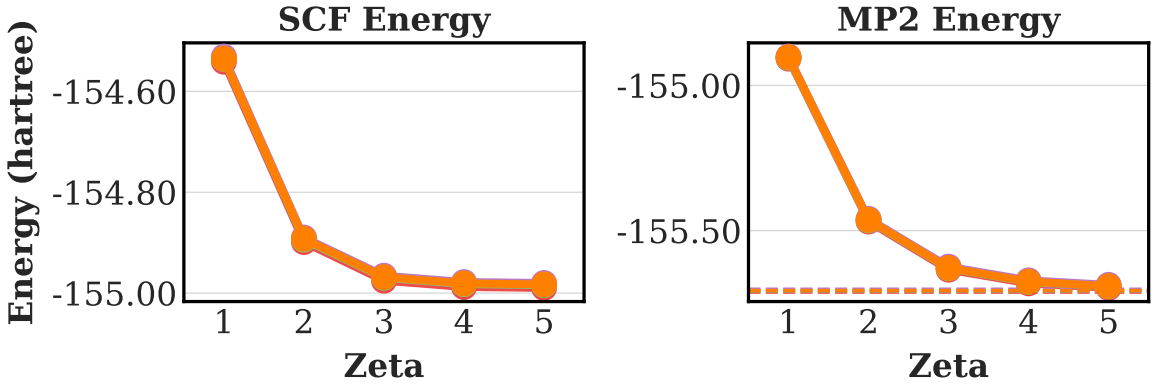
(d) pcseg-X



(a) aug-pcseg-X

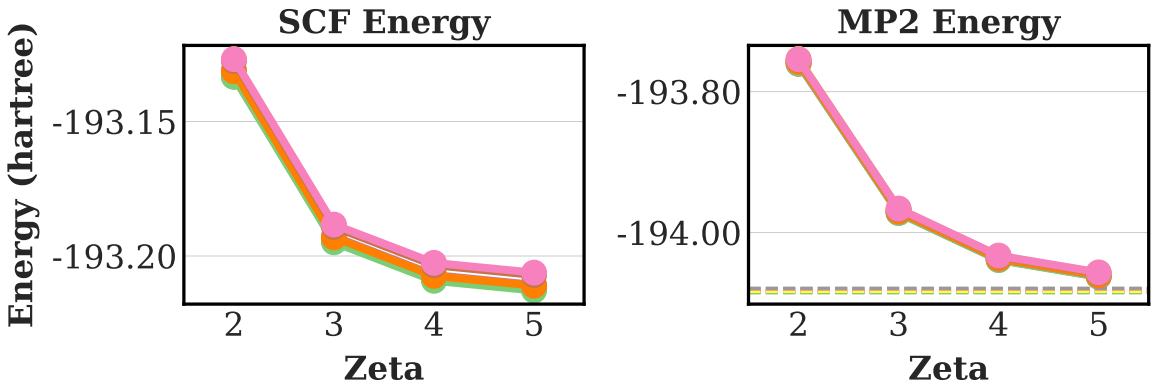


(b) pcSseg-X

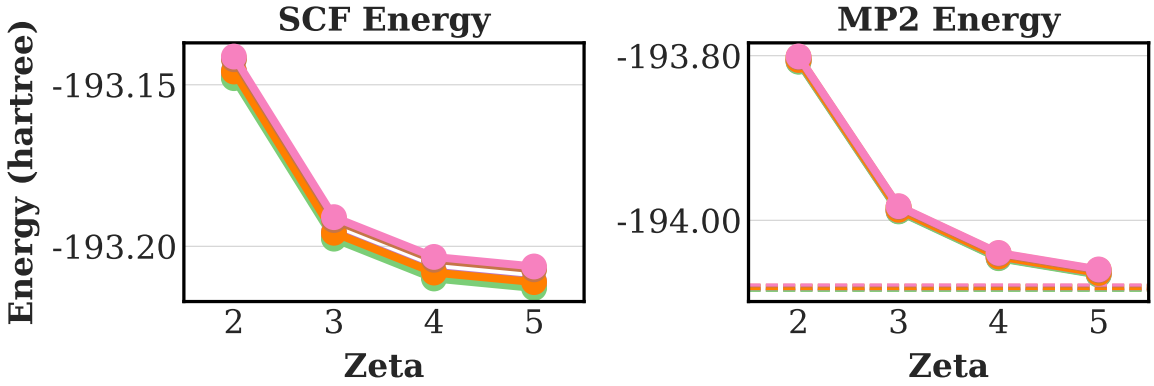


(c) aug-pcSseg-X

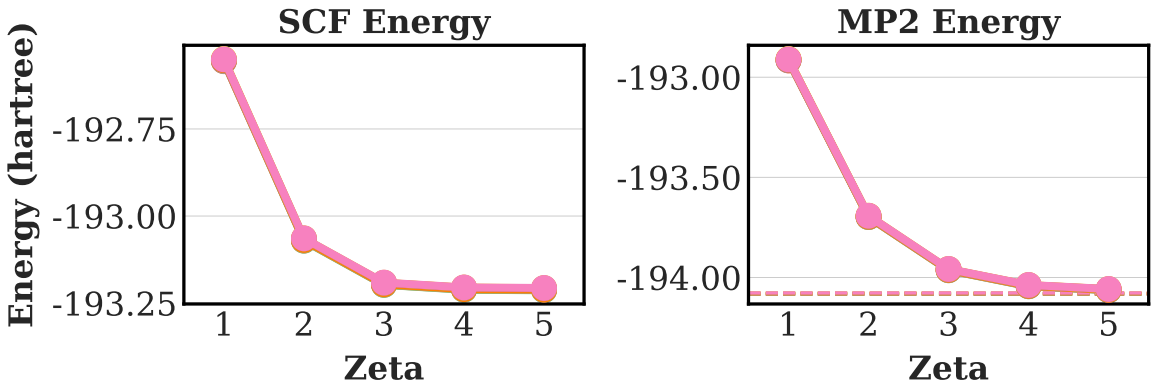
Figure S1: The SCF and MP2 electronic energies computed using Dunning and Jensen basis sets for buta-1,3-diene conformations. The MP2 CBS extrapolations are displayed using horizontal dashed lines, computed using Scheme 2 and the [3,4,5] triad in each basis set family. The SCF energies was extracted from the MP2 optimization calculations. Note that there is significant data overlap in many of the graphs due to the large y-axis scale compared to the small differences between the energies computed at each cardinal (i.e. zeta) number. For the legend, please see Figure 2 within the main text.



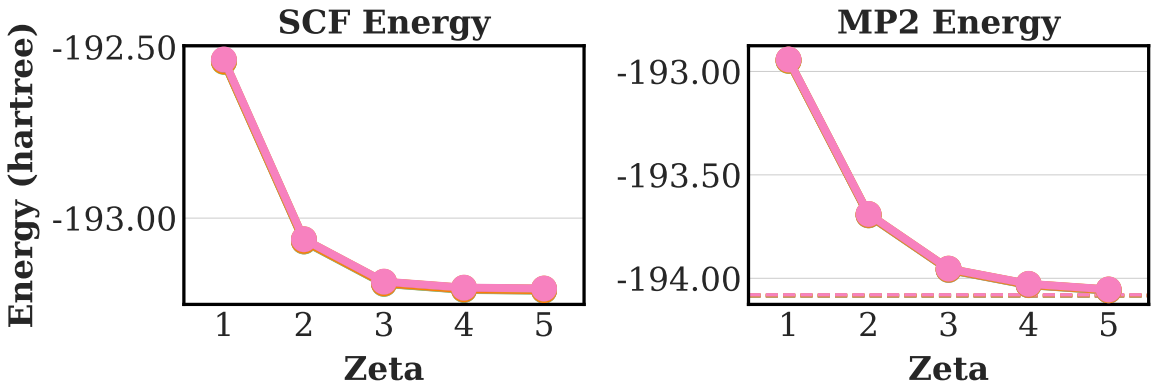
(a) VXZ



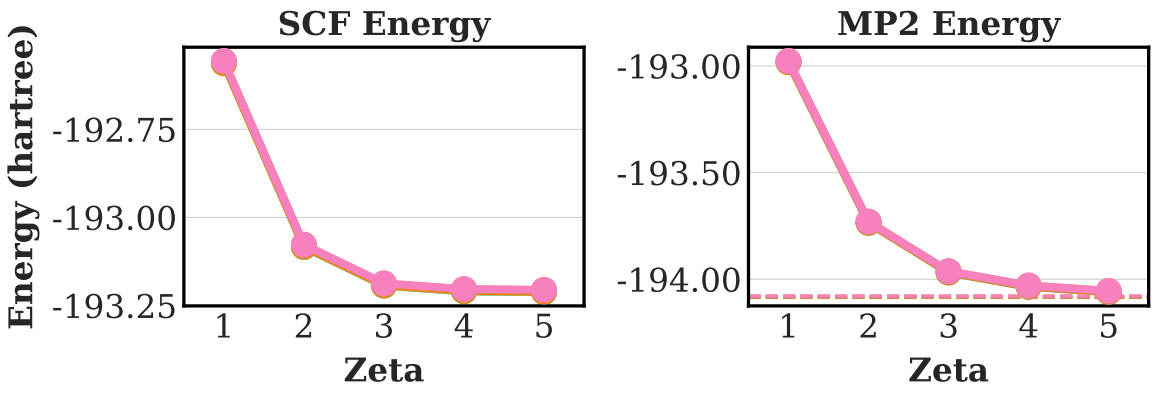
(b) AVXZ



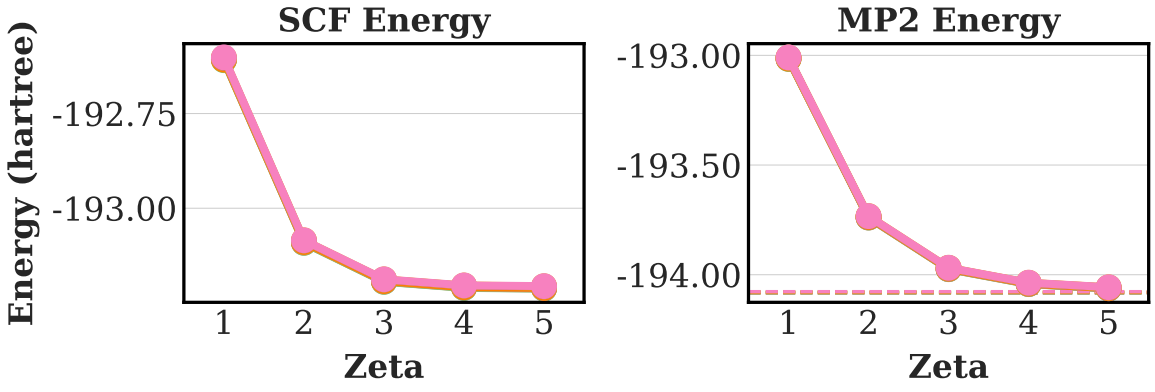
(c) pc-X



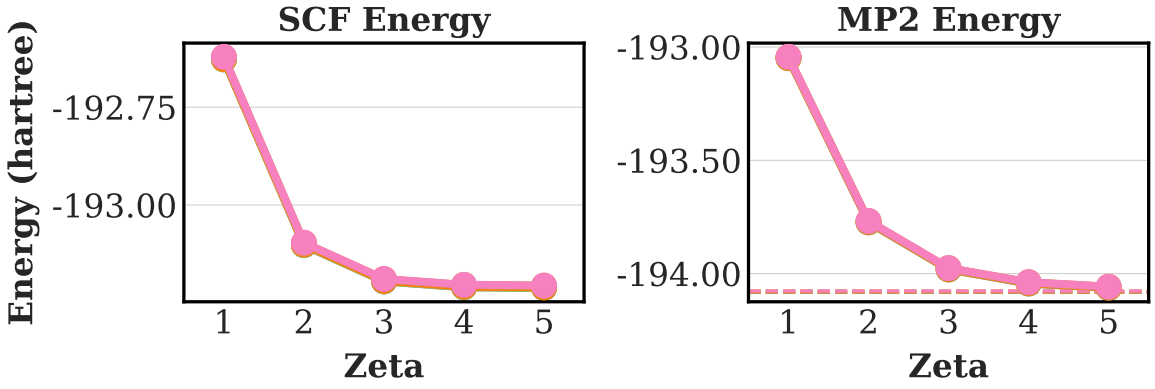
(d) pcseg-X



(a) aug-pcseg-X

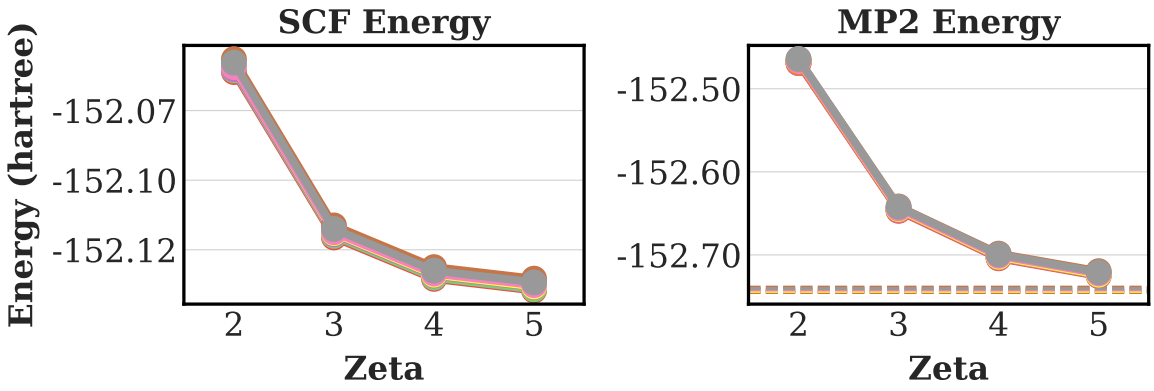


(b) pcSseg-X

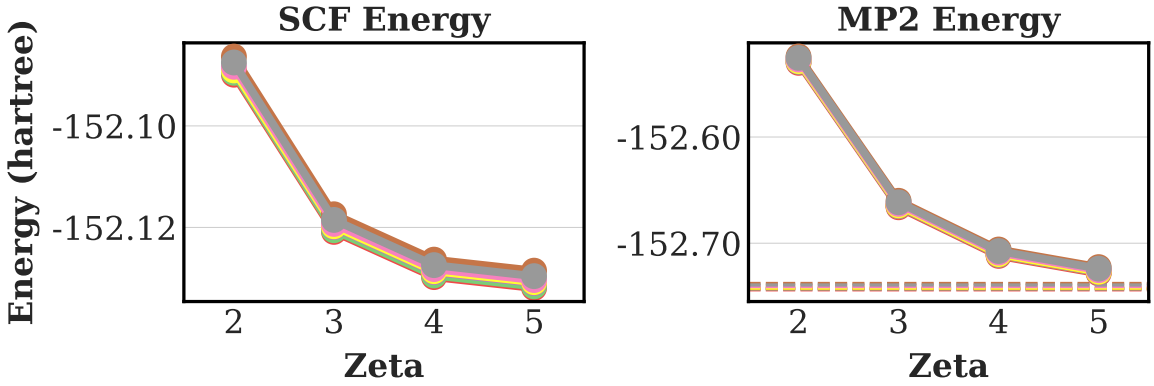


(c) aug-pcSseg-X

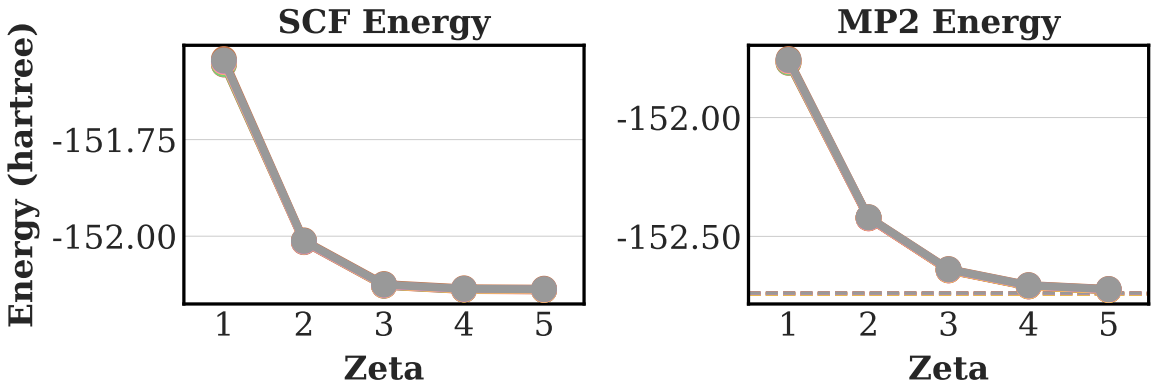
Figure S2: The SCF and MP2 electronic energies computed using Dunning and Jensen basis sets for different propan-2-ol conformations. Additional information can be found in Figure S1's caption. For the legend, please see Figure 3 within the main text.



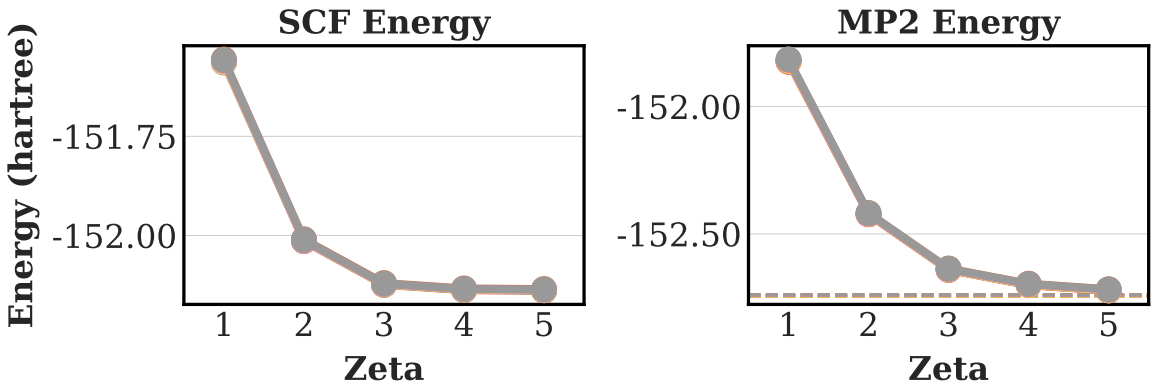
(a) VXZ



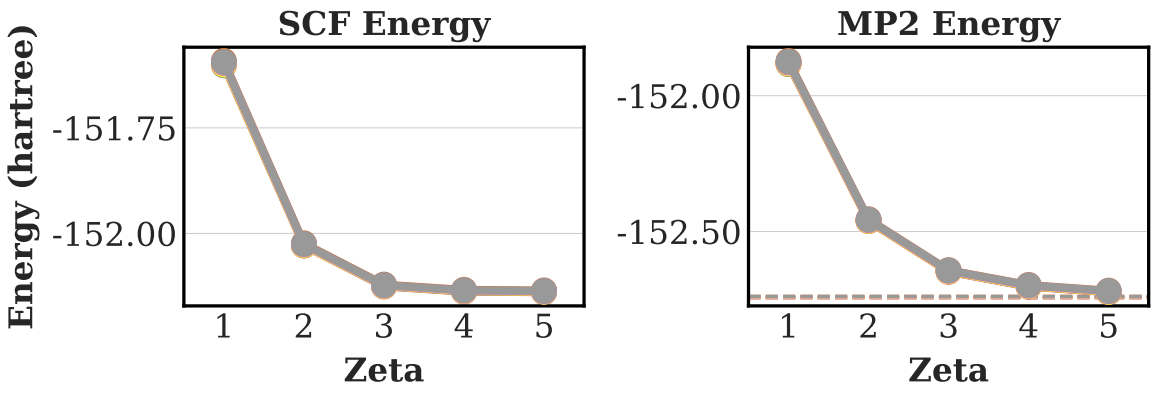
(b) AVXZ



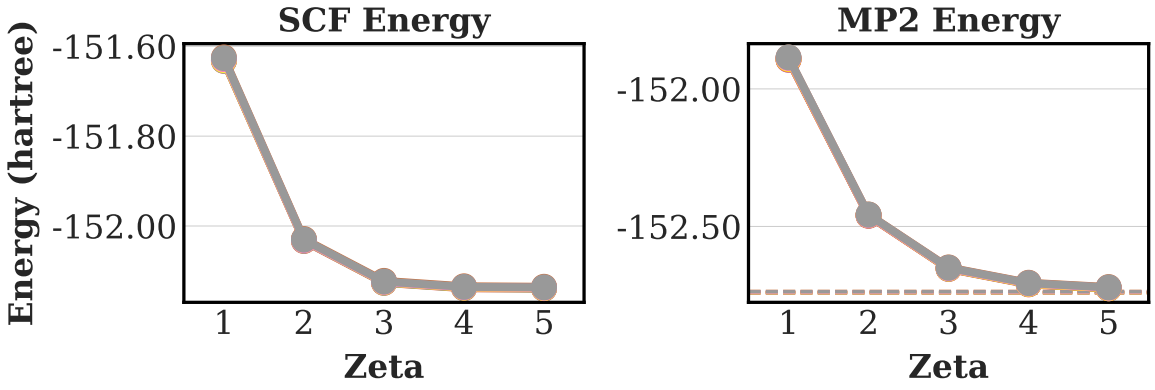
(c) pc-X



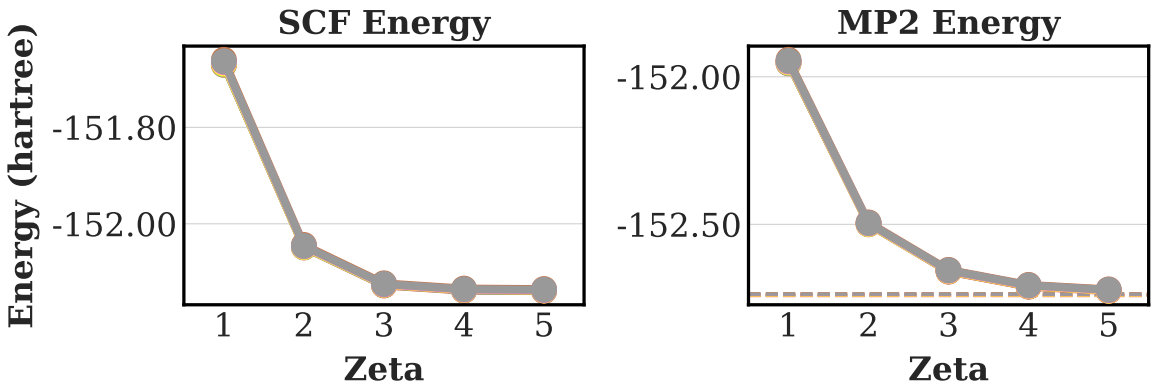
(d) pcseg-X



(a) aug-pcseg-X

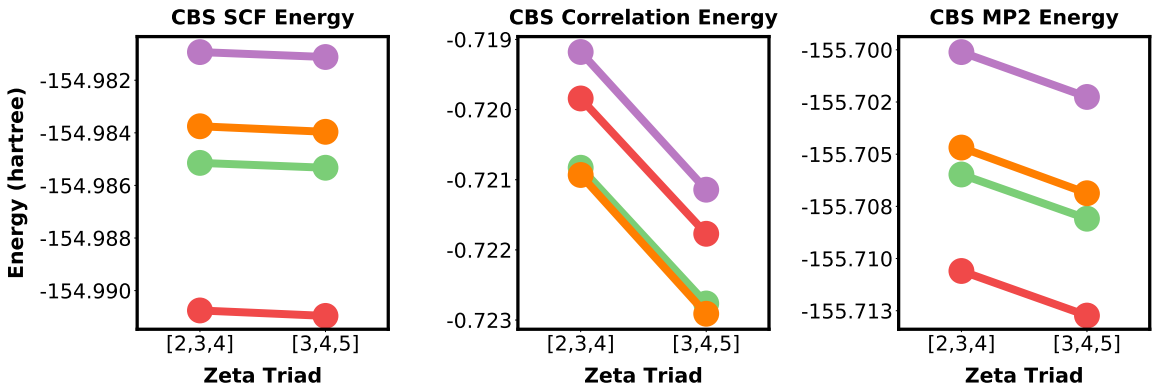


(b) pcSseg-X

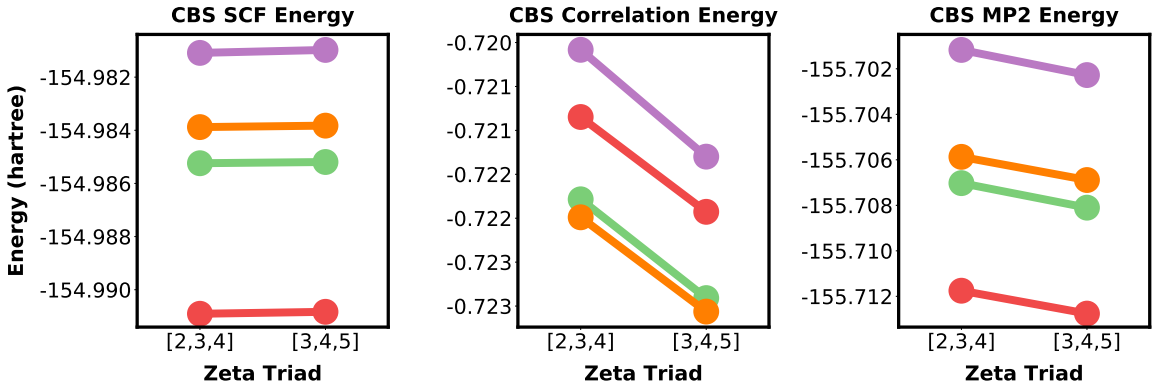


(c) aug-pcSseg-X

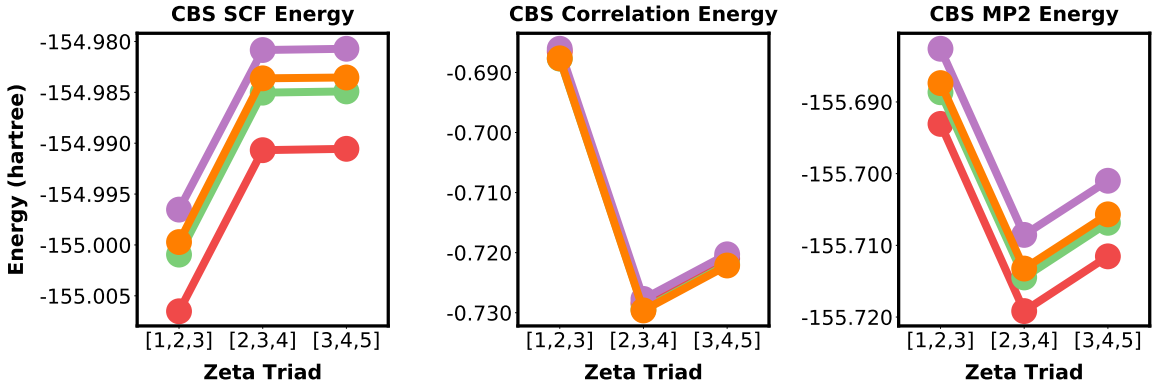
Figure S3: The SCF and MP2 electronic energies computed using Dunning and Jensen basis sets for different water dimer configurations. Additional information can be found in Figure S1's caption. For the legend, please see Figure 4 in the main text.



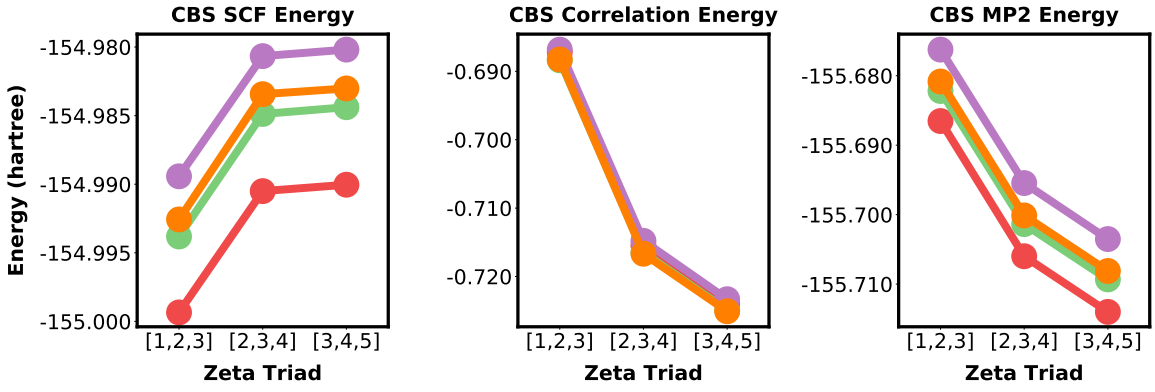
(a) VXZ



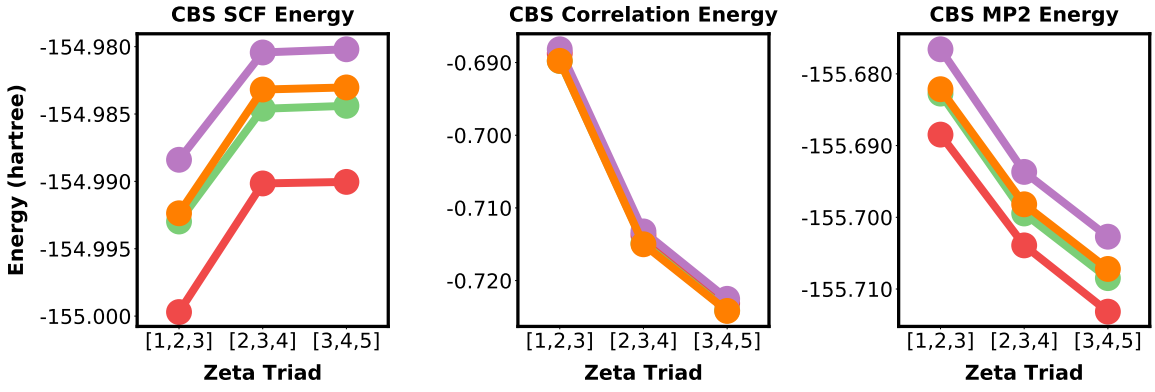
(b) AVXZ



(c) pc-X



(d) pcseg-X



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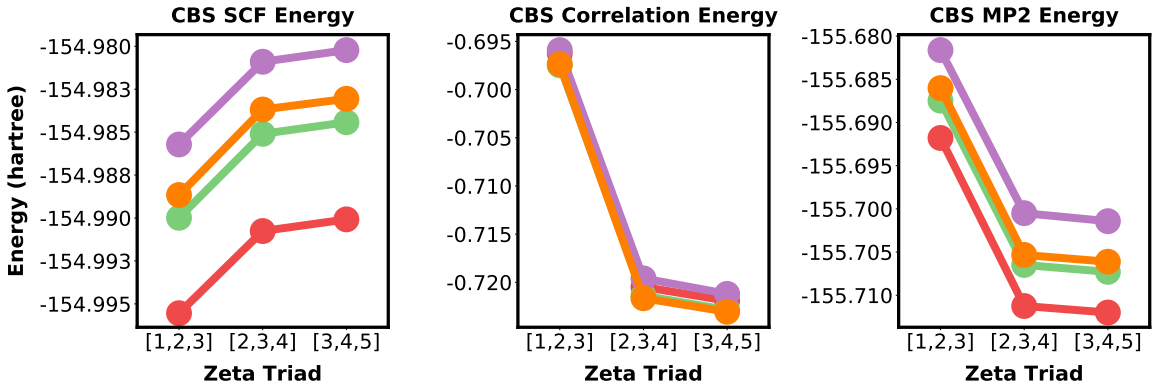
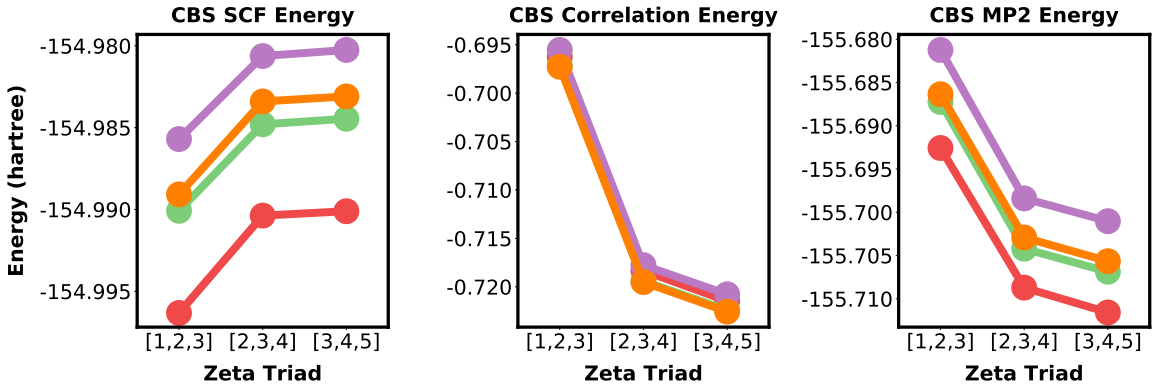
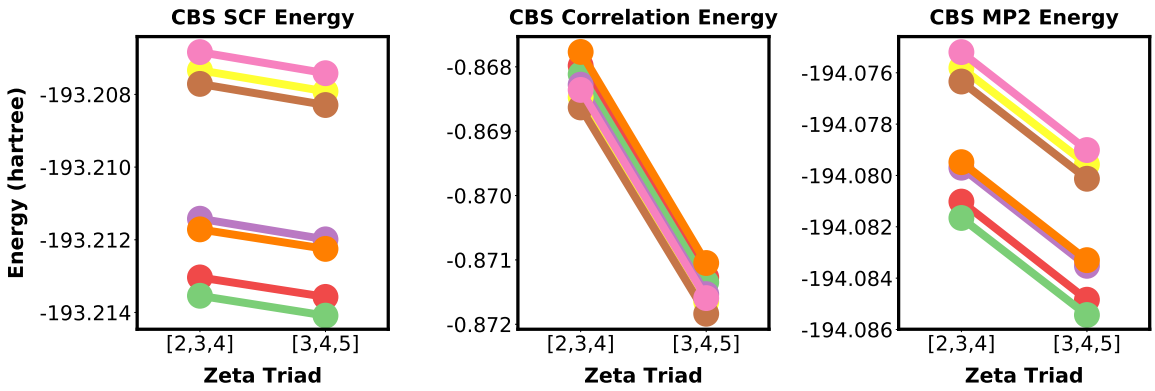


(b) pcSseg-X

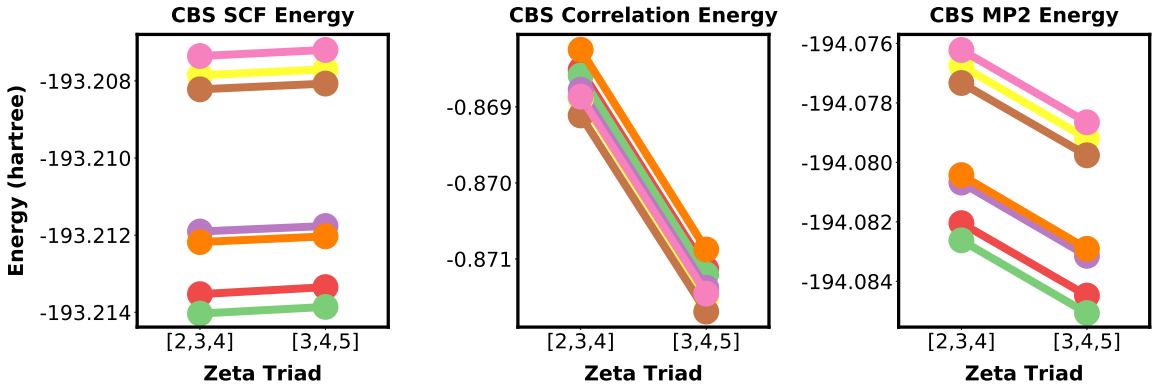


(c) aug-pcSseg-X

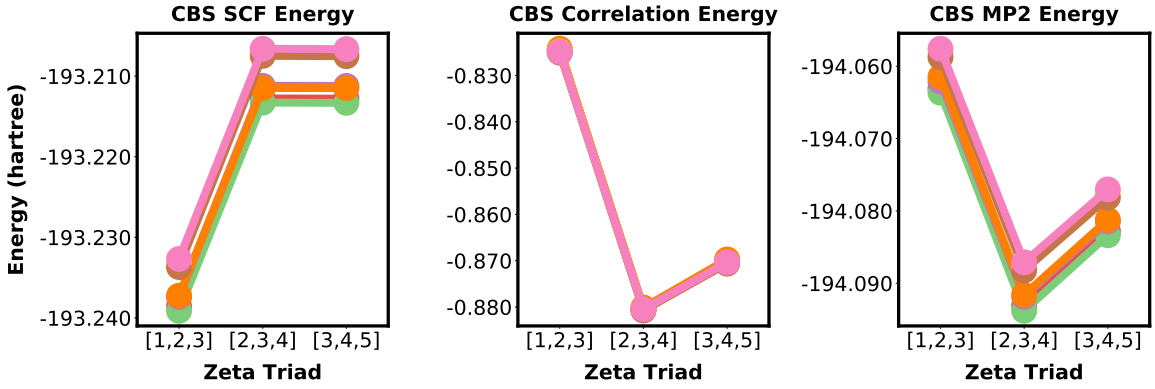
Figure S4: Plots of the CBS extrapolation energies for buta-1,3-diene conformations, as computed using Scheme 2. Separately shown are the extrapolations for the correlation energy (left), SCF energy (middle) and the total energy (right).



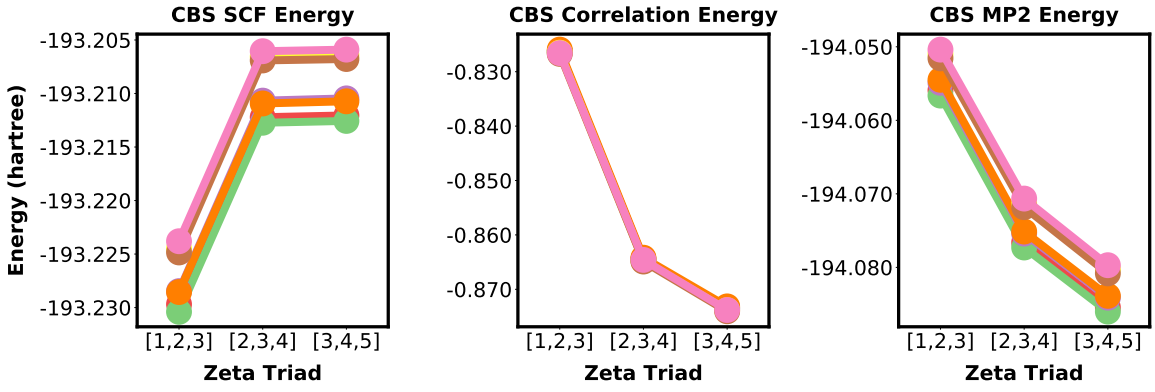
(a) VXZ



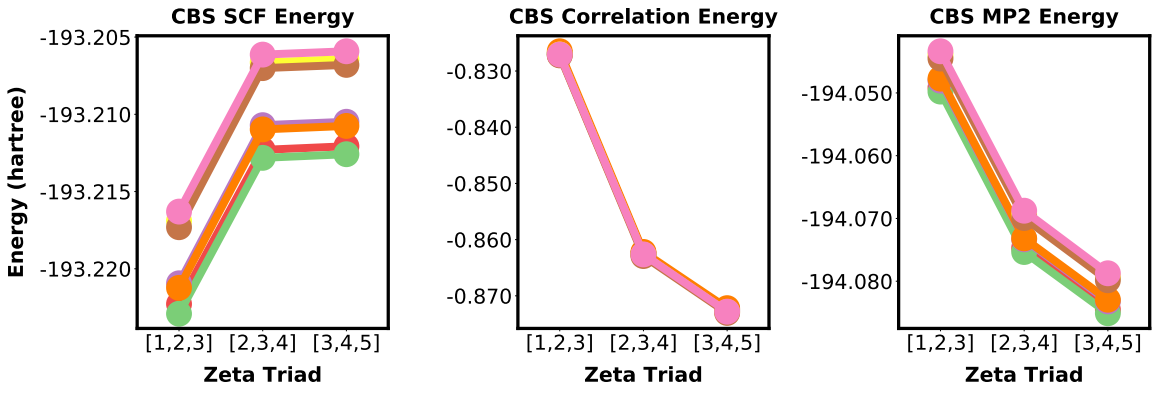
(b) AVXZ



(c) pc-X



(d) pcseg-X



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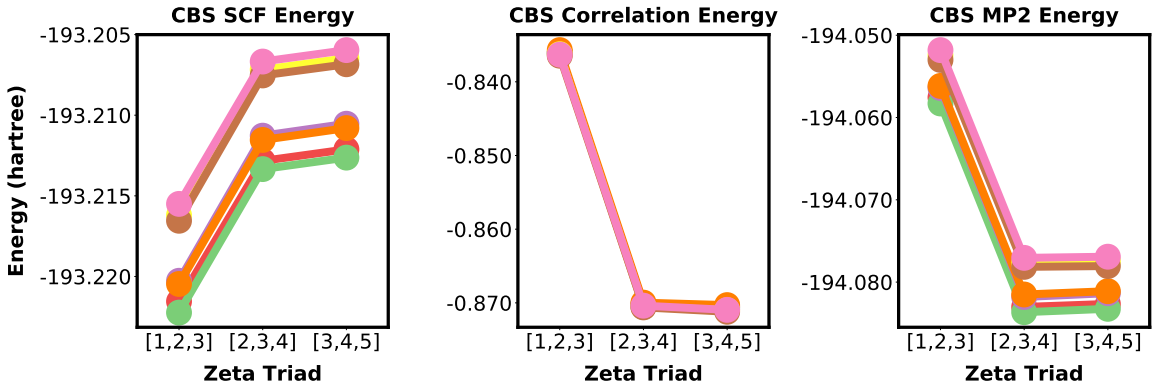
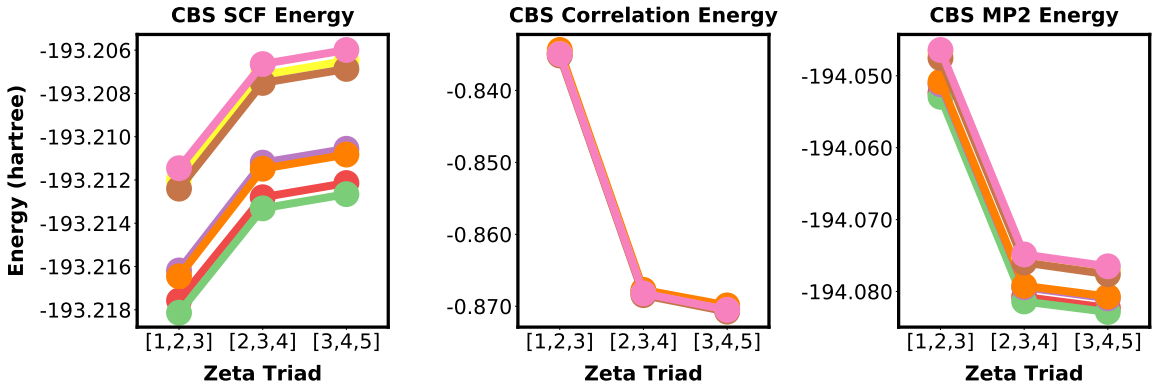
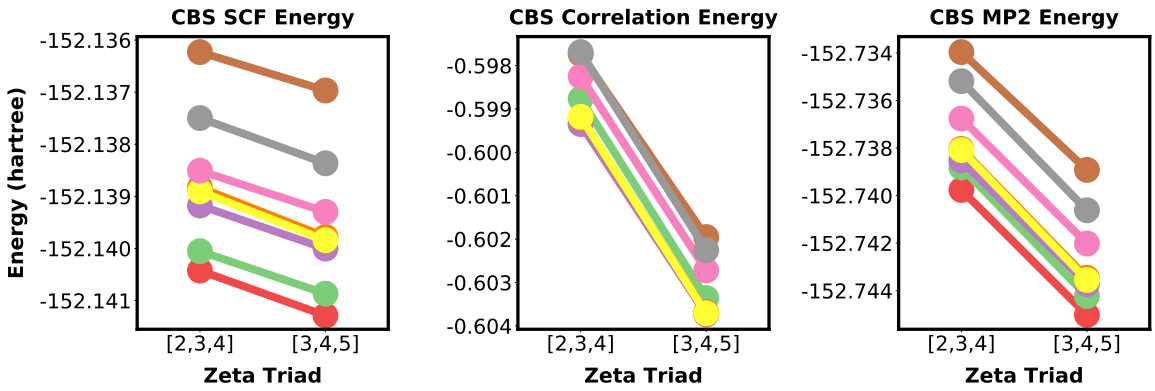


(b) pcSseg-X

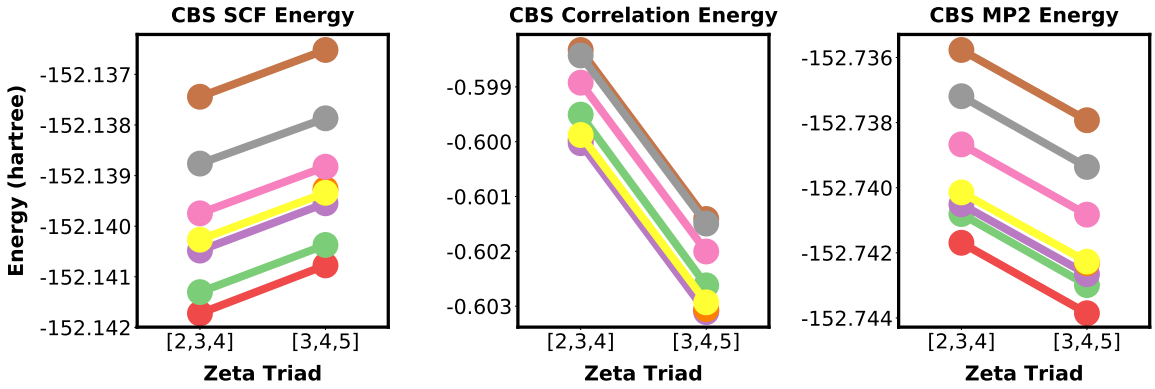


(c) aug-pcSseg-X

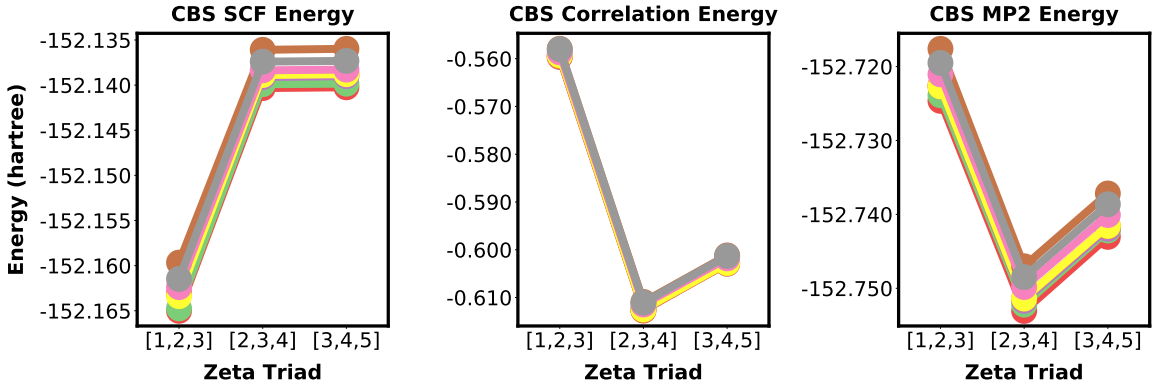
Figure S5: Plots of the CBS extrapolation energies for propan-2-ol conformations, as computed using Scheme 2. Separately shown are the extrapolations for the correlation energy (left), SCF energy (middle) and the total energy (right).



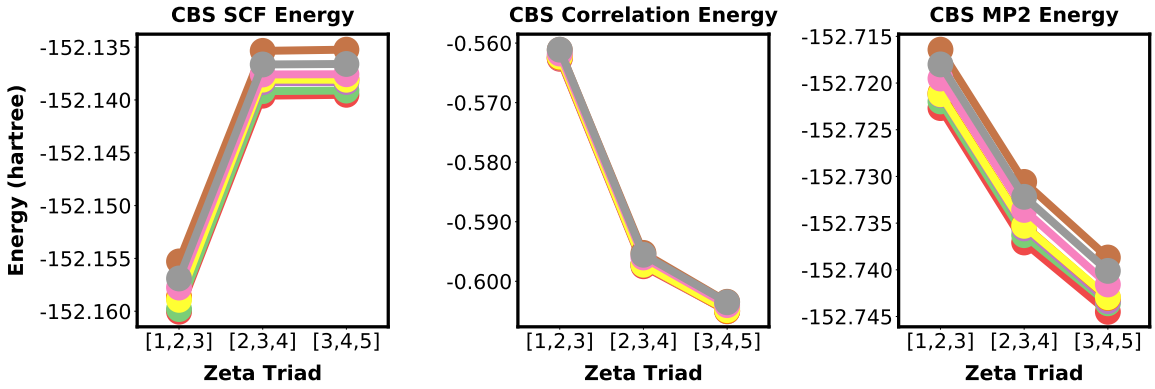
(a) VXZ



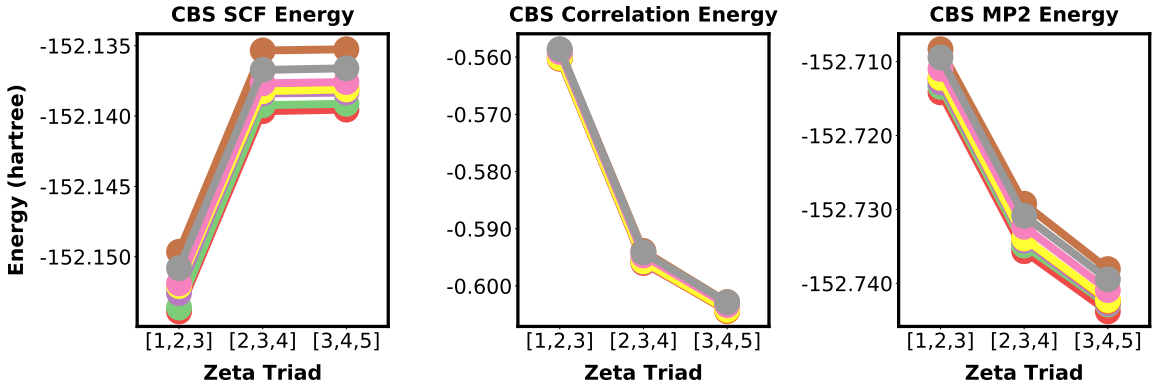
(b) AVXZ



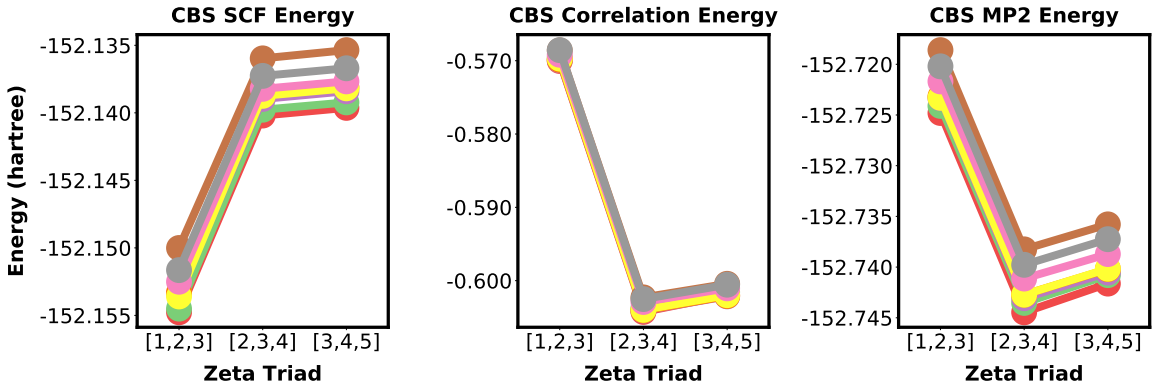
(c) pc-X



(d) pcseg-X



(a) aug-pcseg-X



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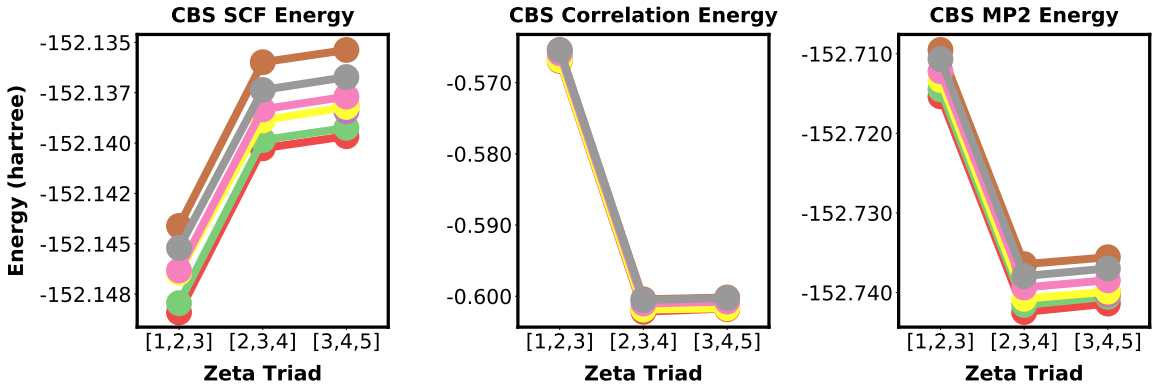
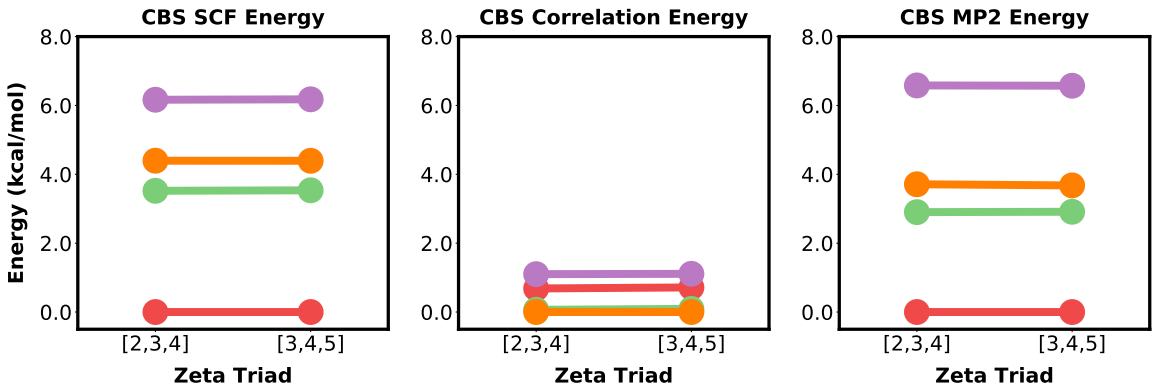
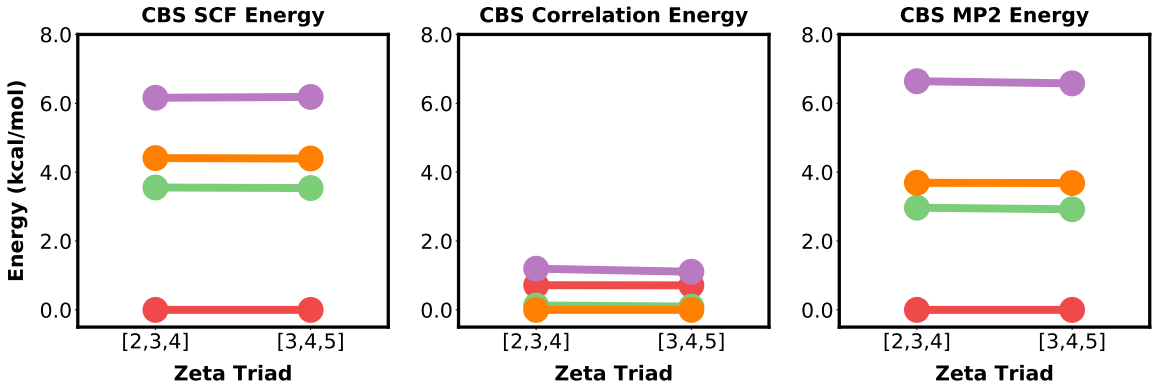


(c) aug-pcSseg-X

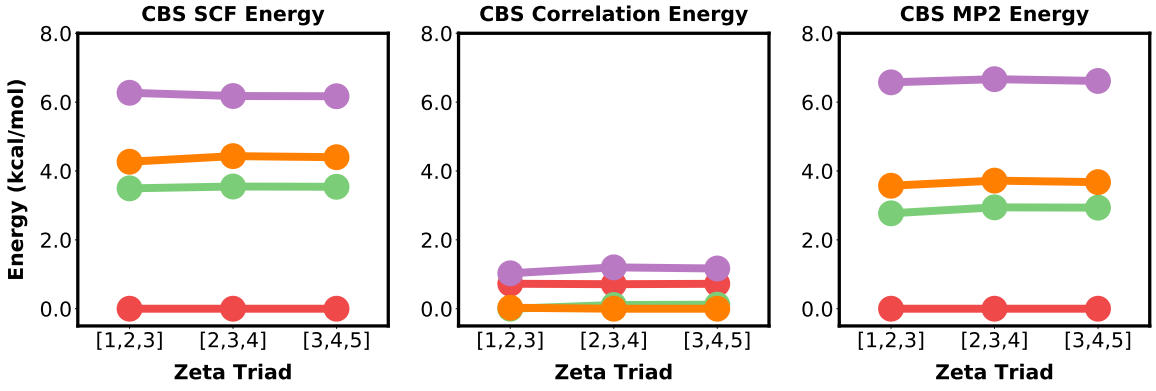
Figure S6: Plots of the CBS extrapolation energies for water dimer configurations, as computed using Scheme 2. Separately shown are the extrapolations for the correlation energy (left), SCF energy (middle) and the total energy (right).



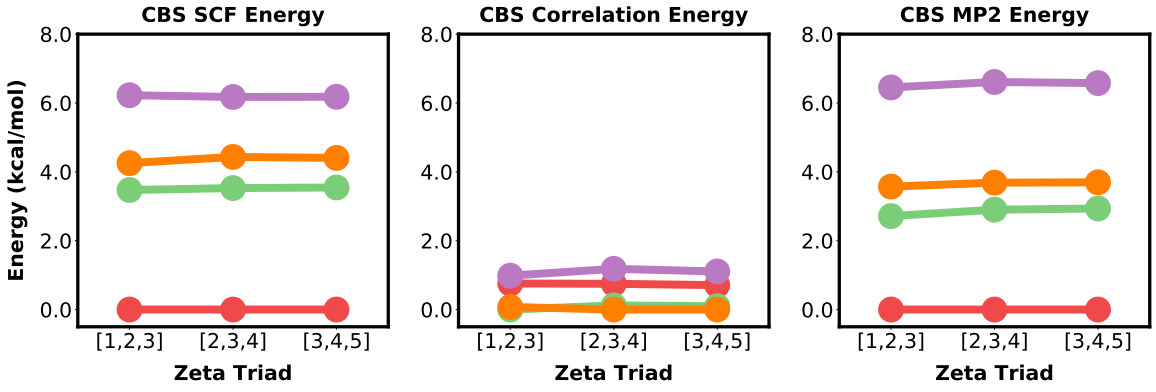
(a) VXZ



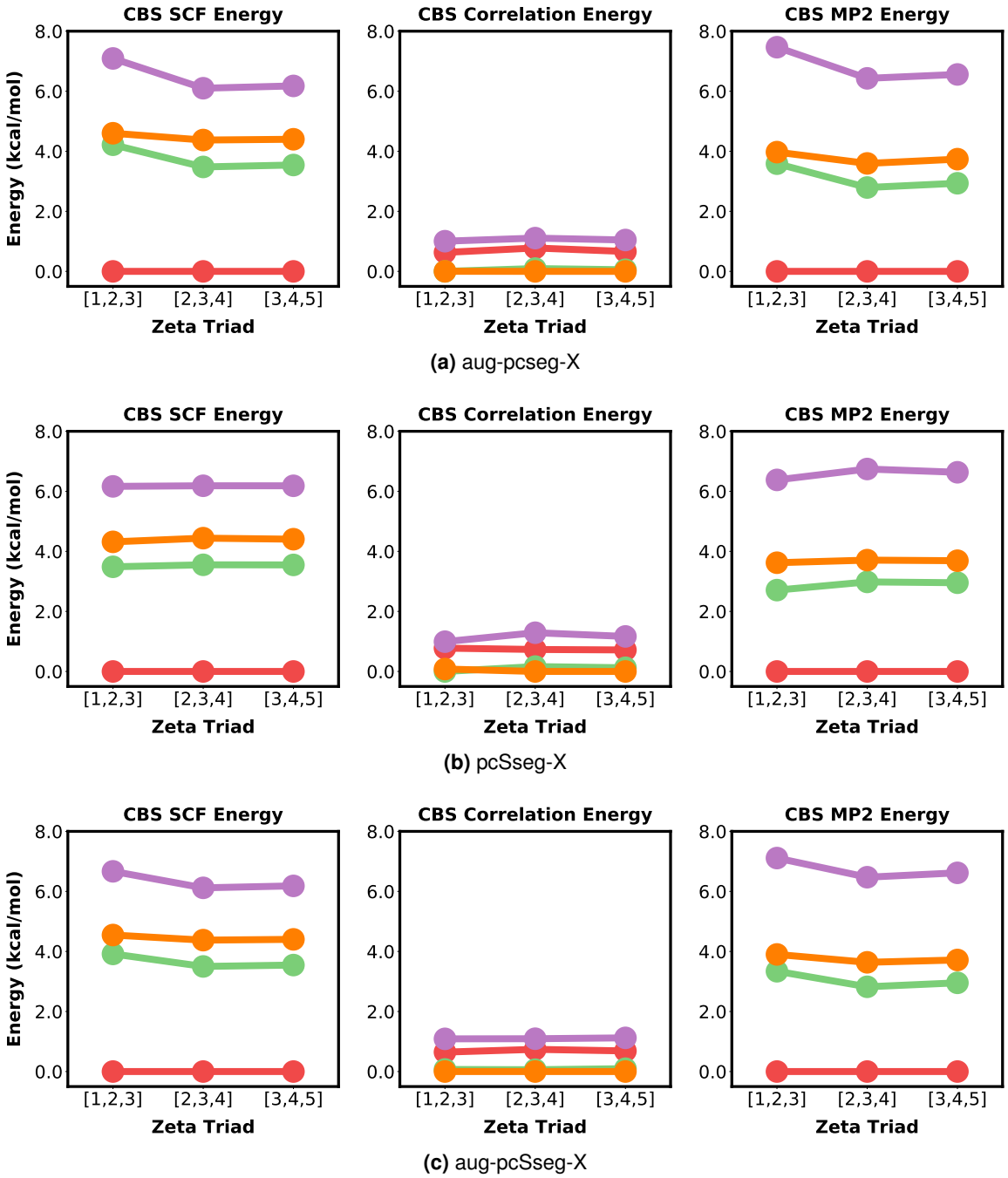
(b) AVXZ



(c) pc-X



(d) pcseg-X

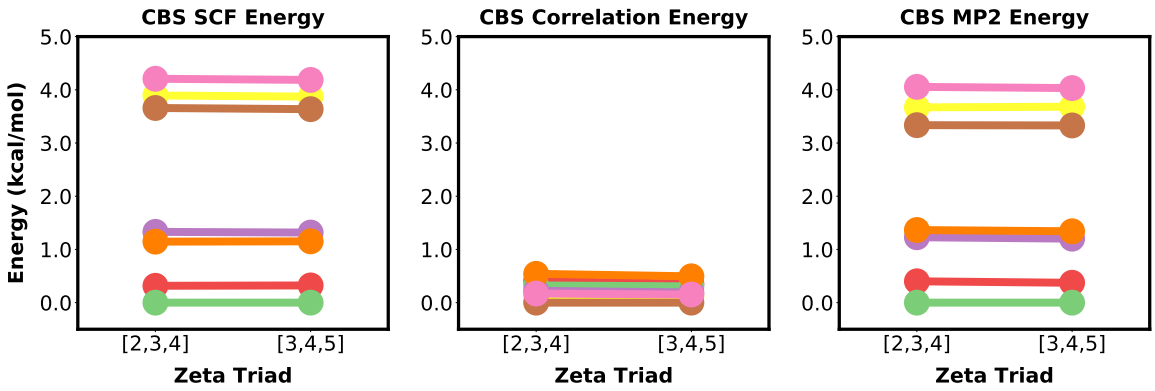


(a) aug-pcseg-X

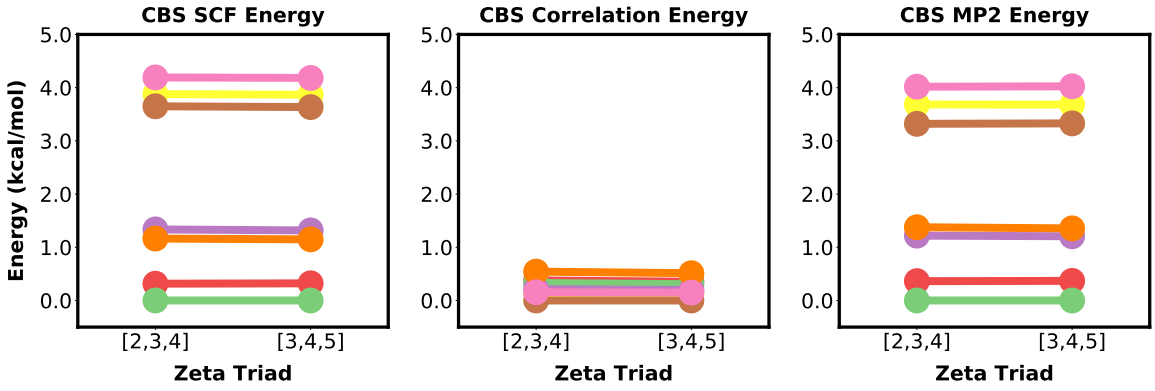
(b) pcSseg-X

(c) aug-pcSseg-X

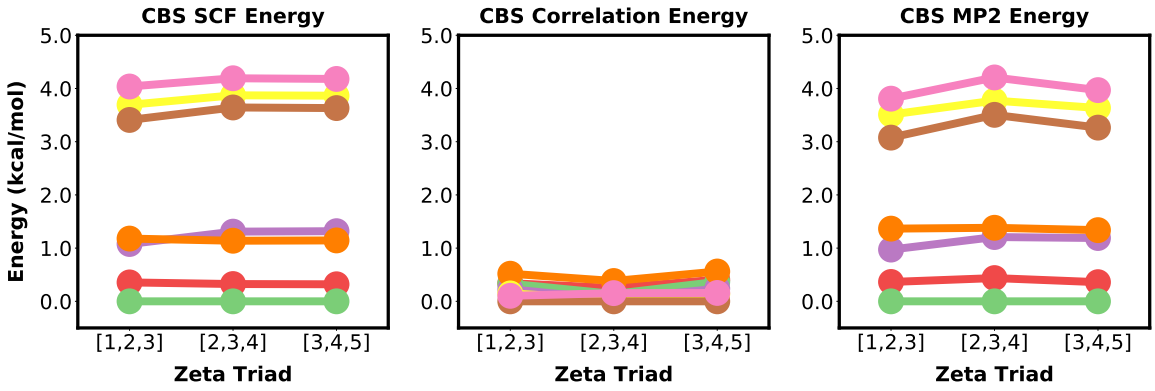
Figure S7: Plots of the relative CBS extrapolation energies for buta-1,3-diene conformations, as computed using Scheme 2. Separately shown are the extrapolations for the correlation energy (left), SCF energy (middle) and the total energy (right)



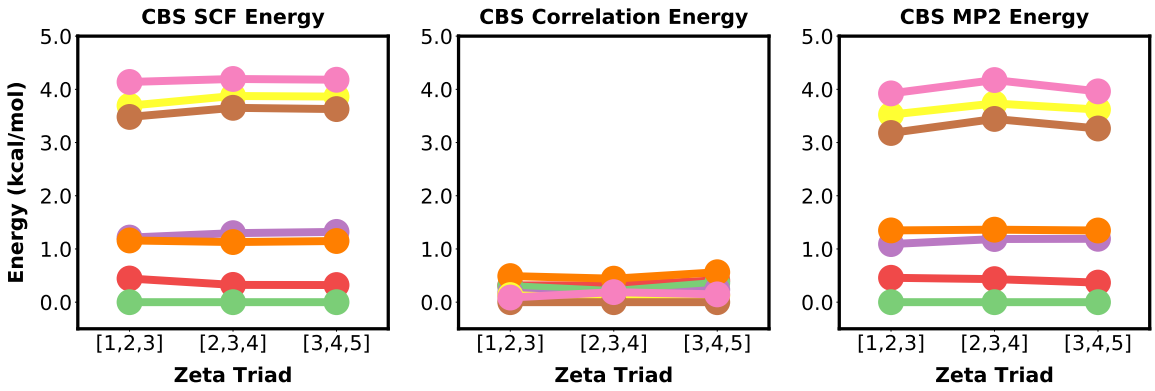
(a) VXZ



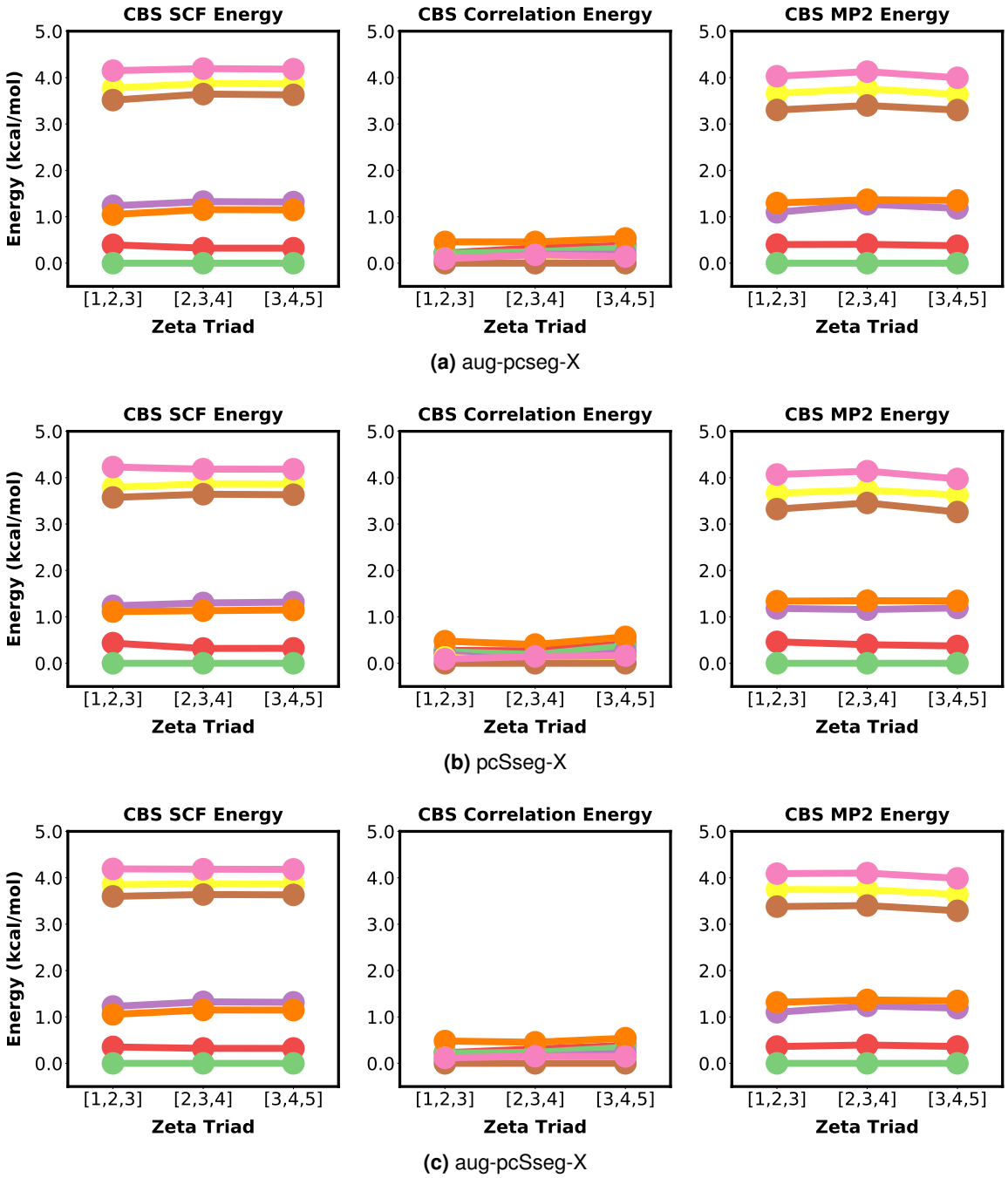
(b) AVXZ



(c) pc-X



(d) pcseg-X

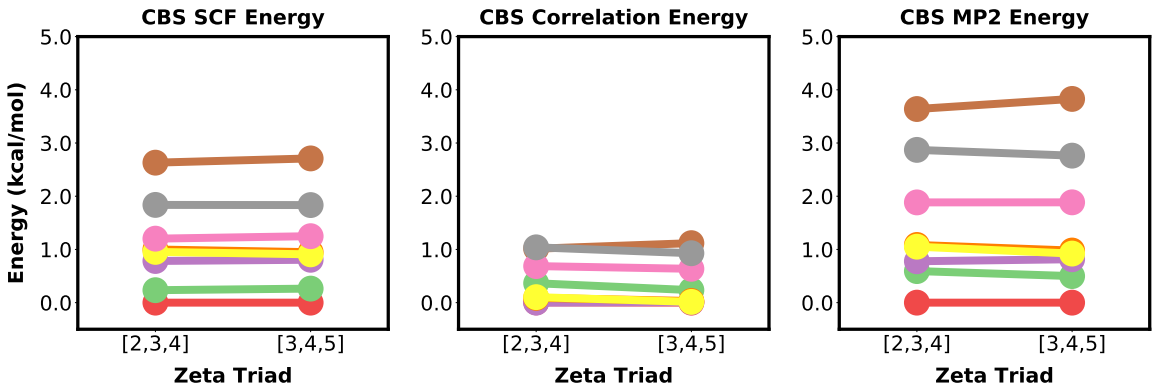


(a) aug-pcseg-X

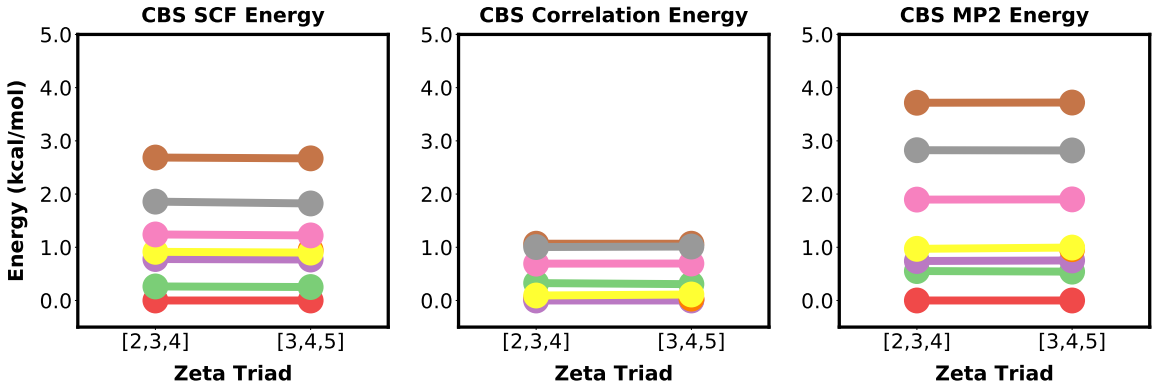
(b) pcSseg-X

(c) aug-pcSseg-X

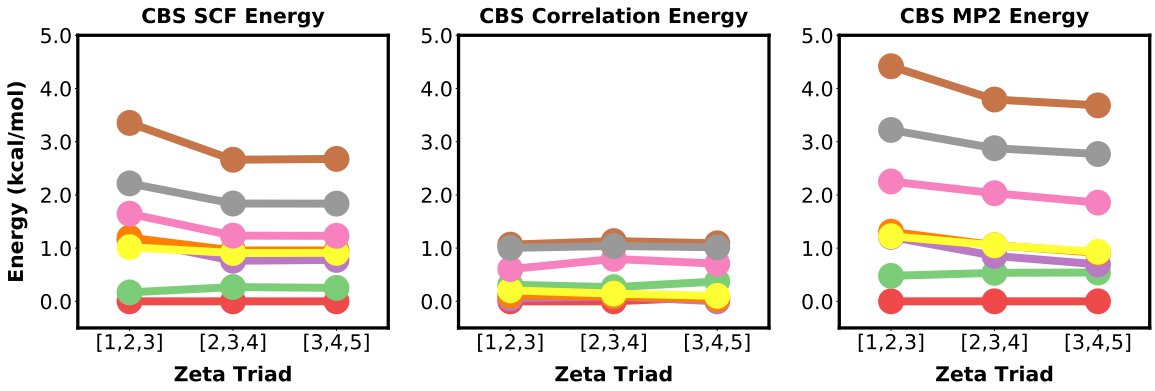
Figure S8: Plots of the relative CBS extrapolation energies for propan-2-ol conformations, as computed using Scheme 2. Separately shown are the extrapolations for the correlation energy (left), SCF energy (middle) and the total energy (right)



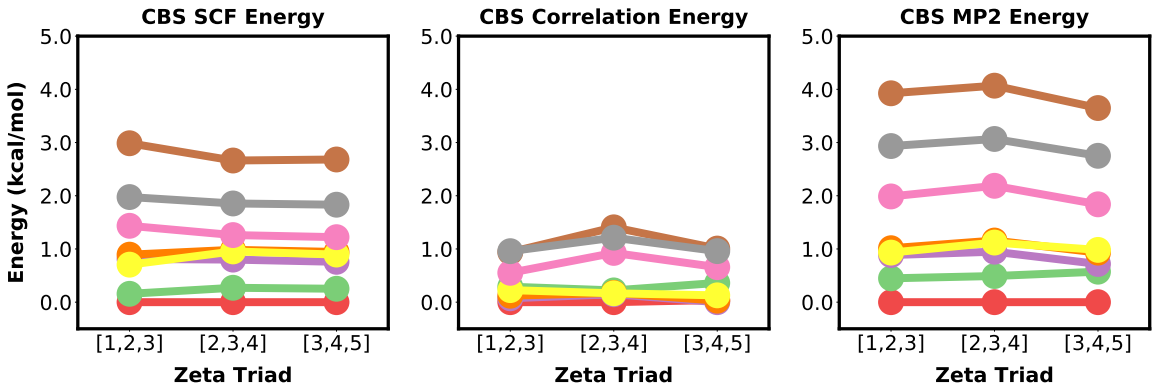
(a) VXZ



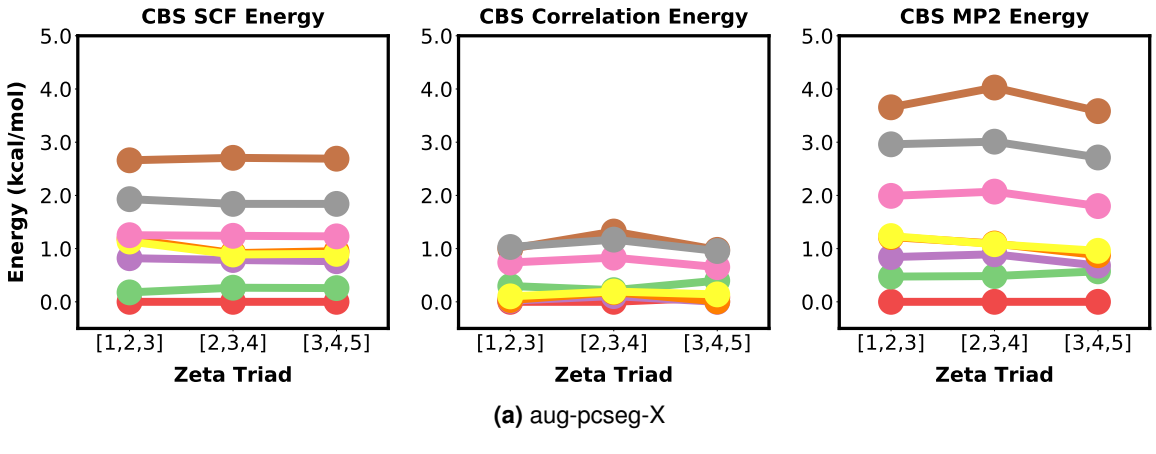
(b) AVXZ



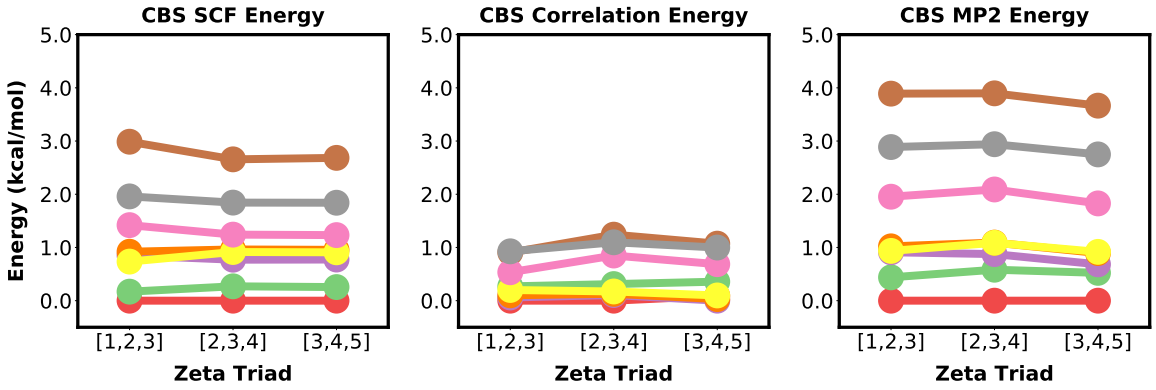
(c) pc-X



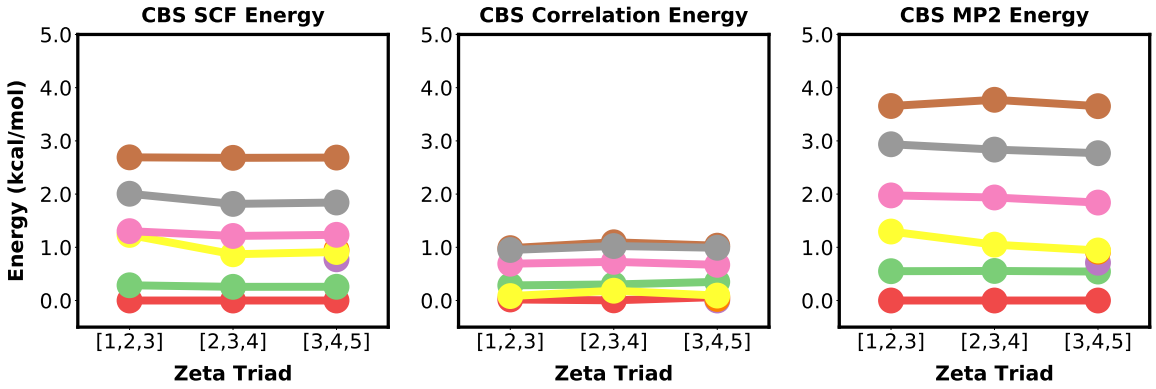
(d) pcseg-X



(a) aug-pcseg-X



(b) pcSseg-X



(c) aug-pcSseg-X

Figure S9: Plots of the relative CBS extrapolation energies for water dimer configurations, as computed using Scheme 2. Separately shown are the extrapolations for the correlation energy (left), SCF energy (middle) and the total energy (right)

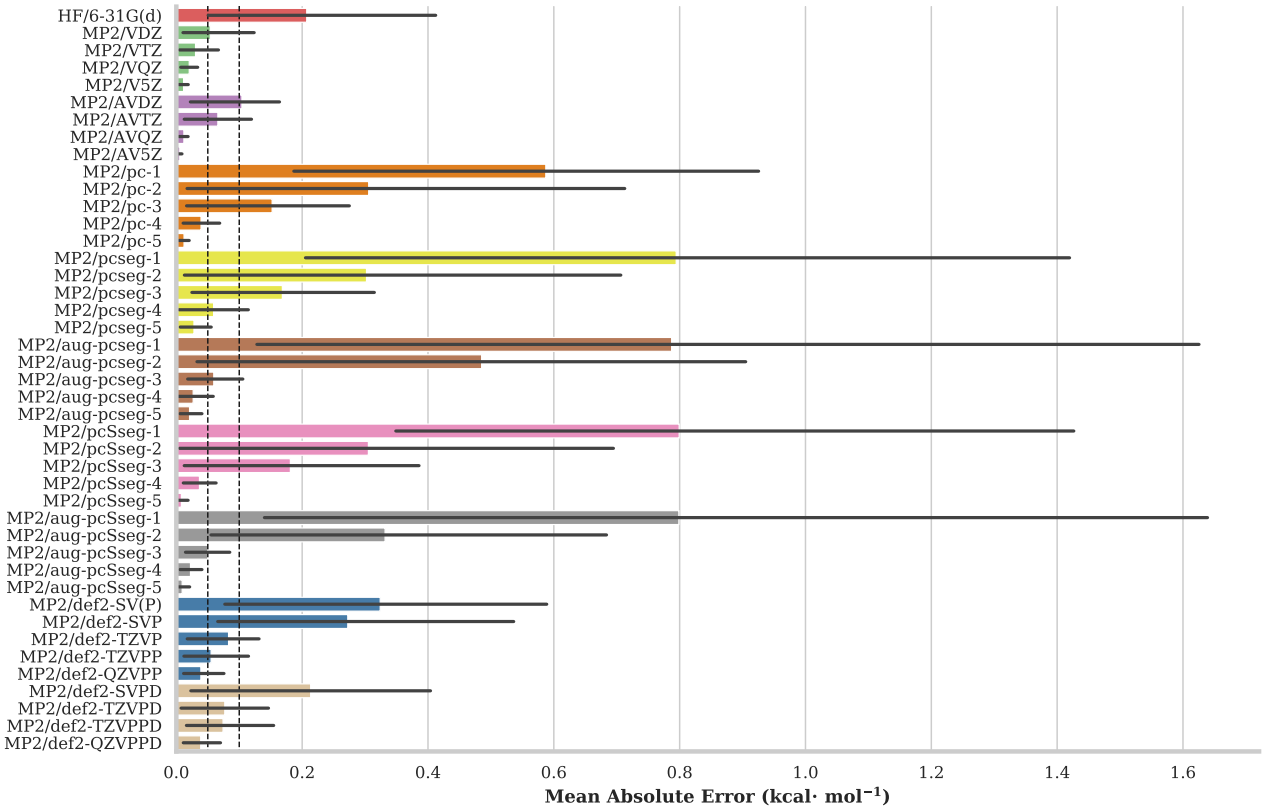


Figure S10: The mean absolute error (kcal·mol^{-1}) in the relative energies of the buta-1,3-diene conformations, using MP2/CBS (i.e. MP2/AV[T,Q,5//Q,5]Z//MP2/AV[T,Q,5]Z, Scheme 2) energies as reference values. The solid line indicates the standard error of the mean. The two dashed lines indicate values at 0.05 and 0.10 kcal·mol^{-1}. The Jensen basis sets are with the adjusted indexing values (i.e. X=1–5).

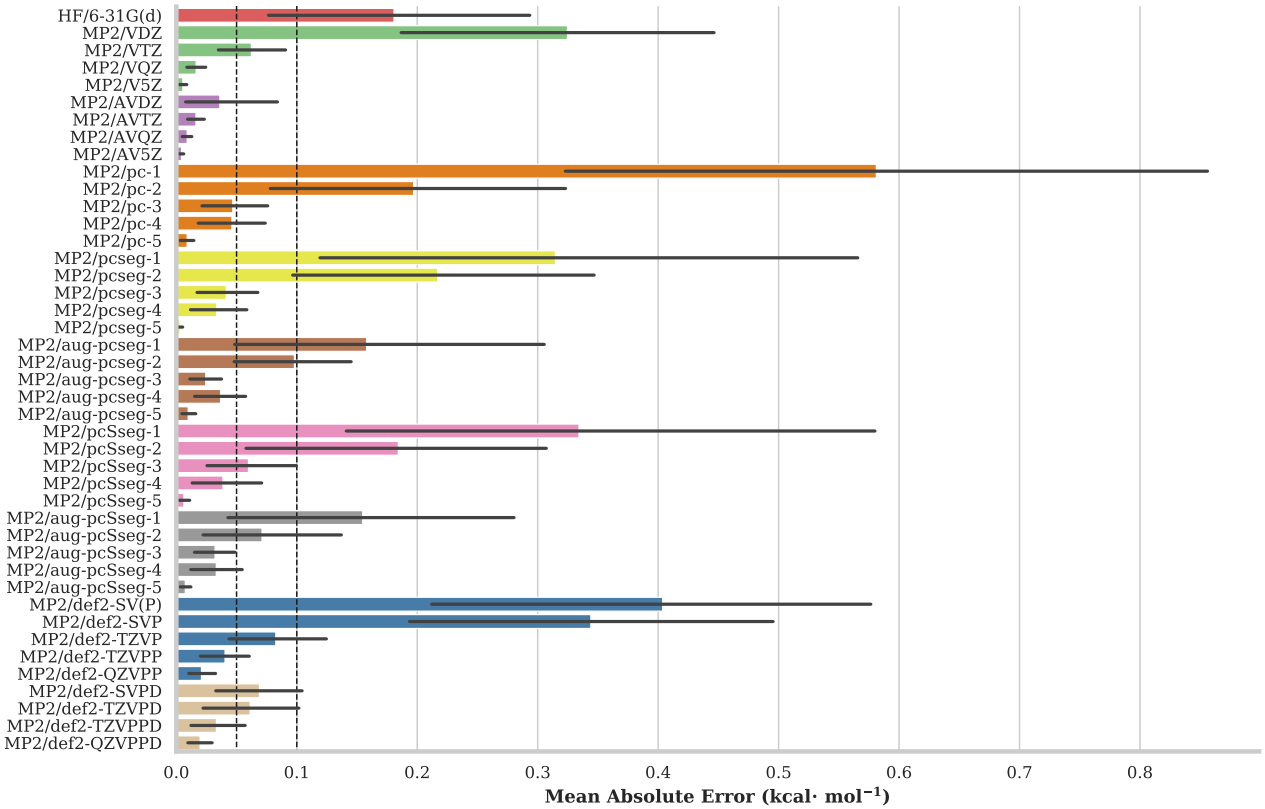


Figure S11: The mean absolute error (kcal·mol^{-1}) in the relative energies of the propan-2-ol conformations, using MP2/CBS (i.e. MP2/AV[T,Q,5//Q,5]Z//MP2/AV[T,Q,5]Z, Scheme 2) energies as reference values. The solid line indicates the standard error of the mean. The two dashed lines indicate values at 0.05 and 0.10 kcal·mol^{-1}. The Jensen basis sets are with the adjusted indexing values (i.e. X=1–5).

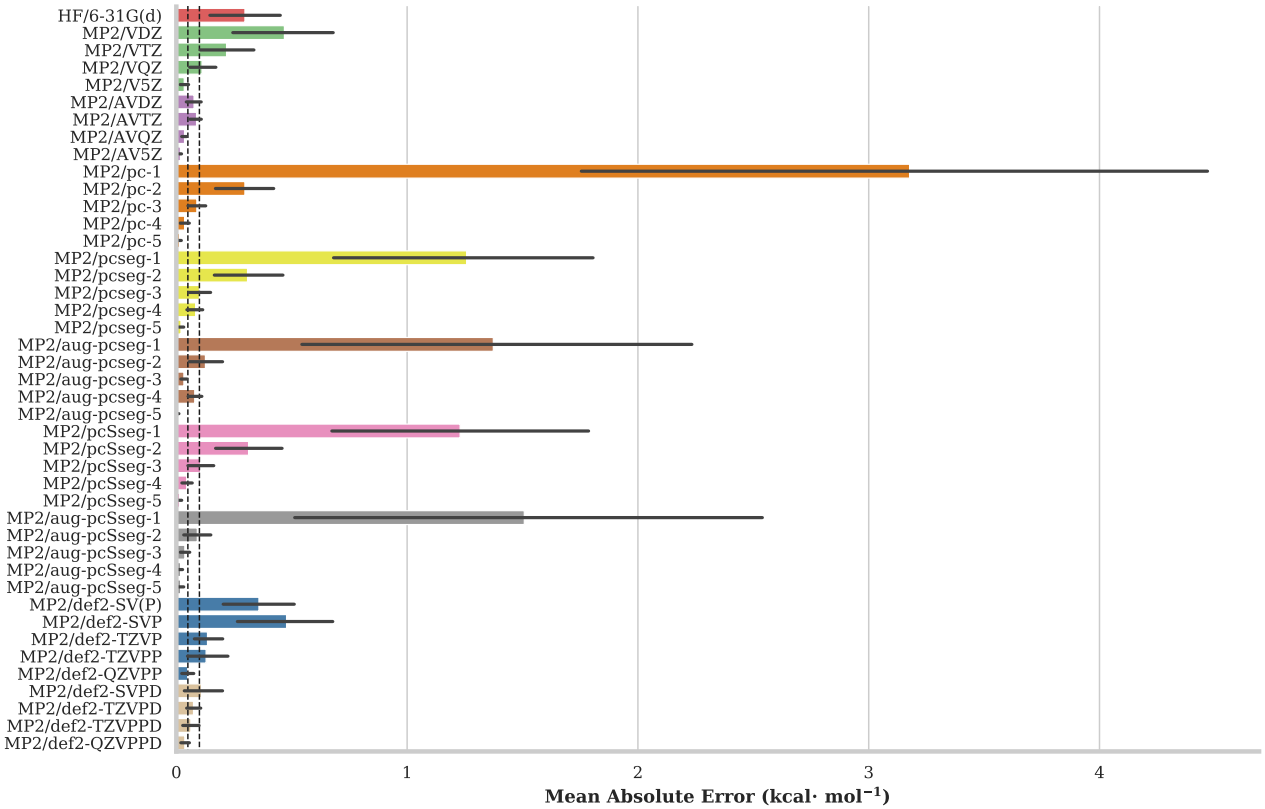


Figure S12: The mean absolute error (kcal·mol^{-1}) in the relative energies of the water dimer configurations, using MP2/CBS (i.e. MP2/AV[T,Q,5//Q,5]Z//MP2/AV[T,Q,5]Z, Scheme 2) energies as reference values. The solid line indicates the standard error of the mean. The two dashed lines indicate values at 0.05 and 0.10 kcal·mol^{-1}. The Jensen basis sets are with the adjusted indexing values (i.e. X=1–5).

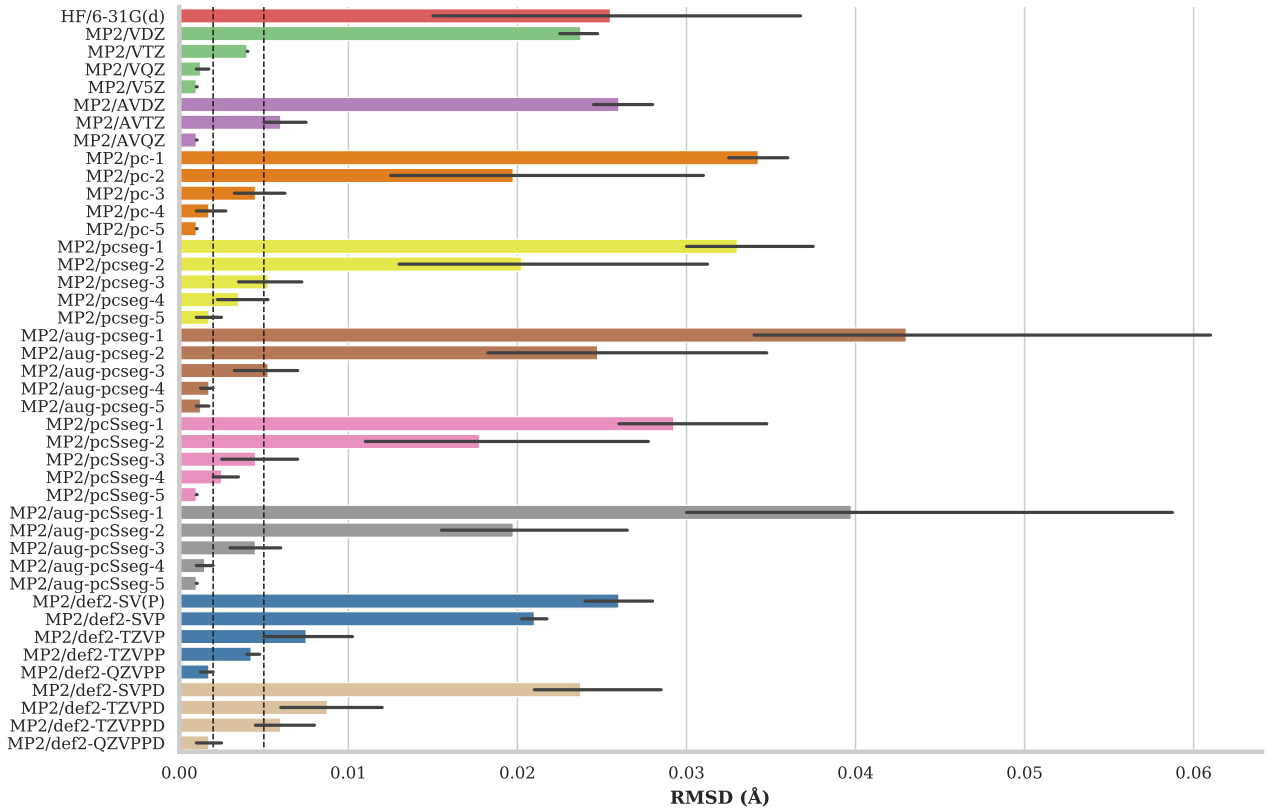


Figure S13: The mean all-atom RMSD (Å) the buta-1,3-diene conformations in comparison to MP2/aV5Z geometries. All atoms were used in computing the RMSD values. The two dashed lines indicate values at 0.002 and 0.005 Å. The Jensen basis sets are with the adjusted indexing values (i.e. X=1–5).

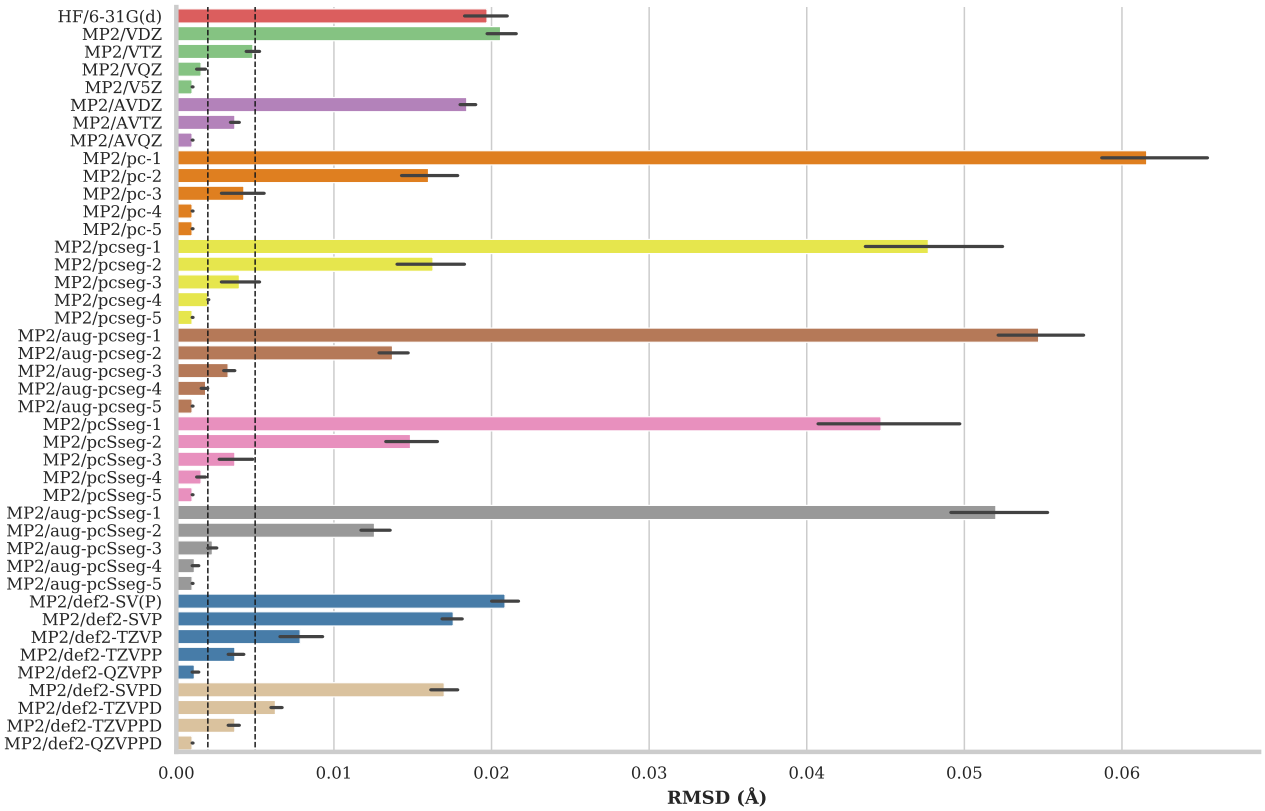


Figure S14: The mean all-atom RMSD (Å) the propan-2-ol conformations in comparison to MP2/aV5Z geometries. All atoms were used in computing the RMSD values. The two dashed lines indicate values at 0.002 and 0.0005 Å. The Jensen basis sets are with the adjusted indexing values (i.e. X=1–5).

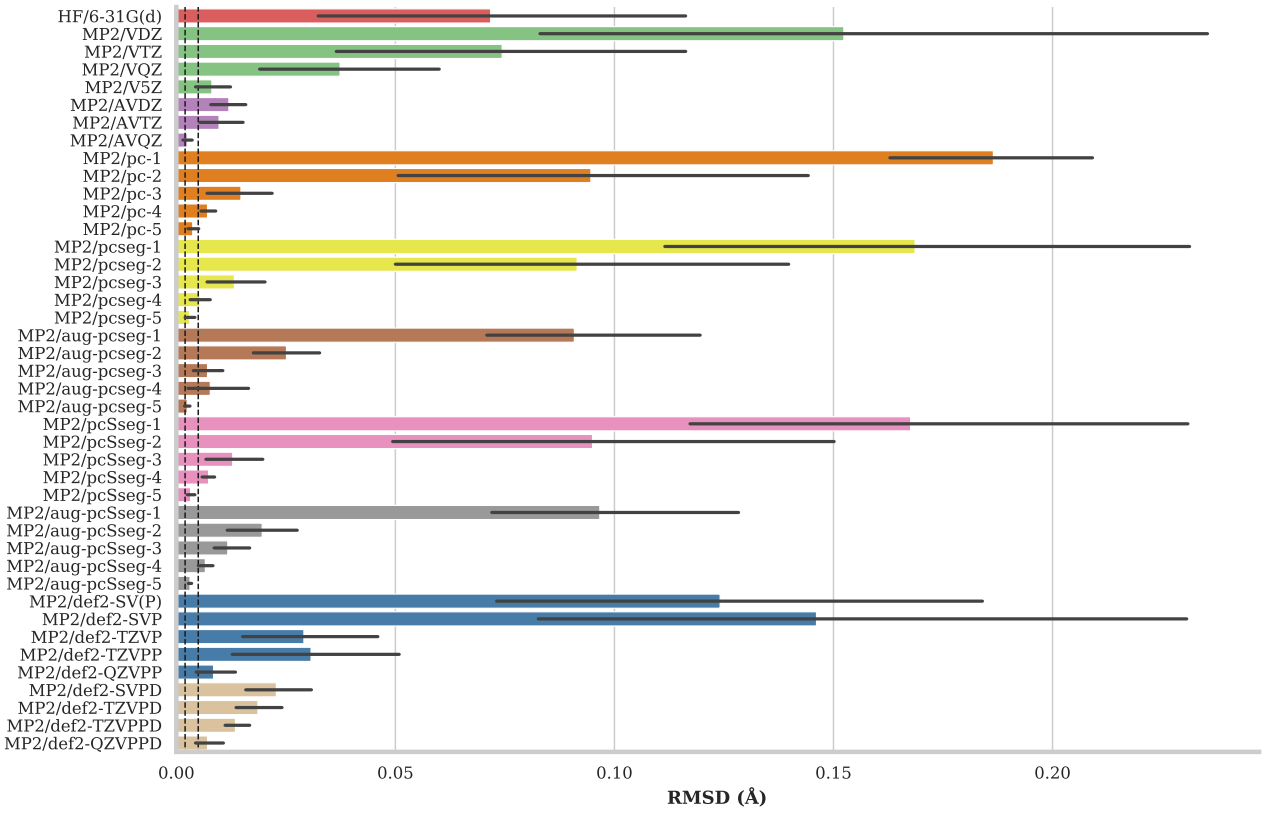


Figure S15: The mean all-atom RMSD (Å) the water dimer configurations in comparison to MP2/aV5Z geometries. All atoms were used in computing the RMSD values. The two dashed lines indicate values at 0.002 and 0.005 Å. The Jensen basis sets are with the adjusted indexing values (i.e. X=1–5).

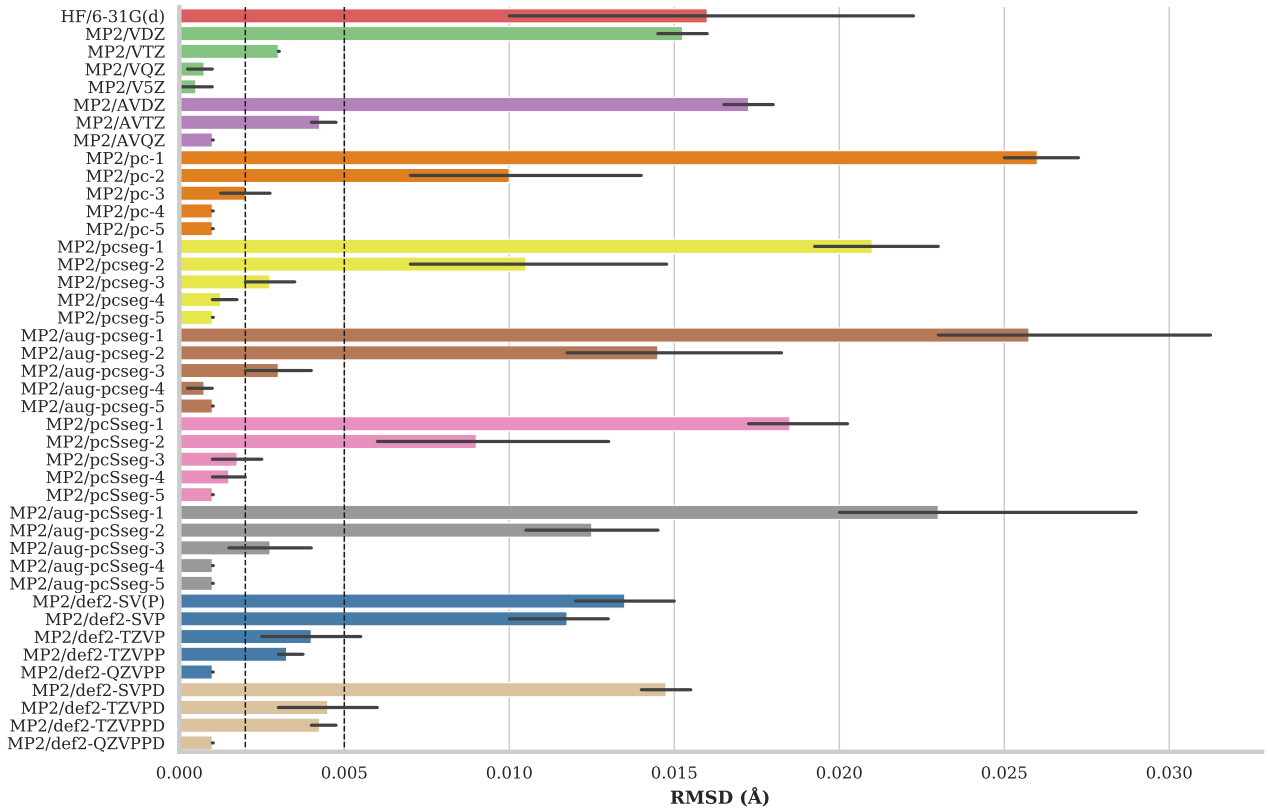


Figure S16: The mean heavy-atom RMSD (Å) the buta-1,3-diene conformations in comparison to MP2/aV5Z geometries. All hydrogen atoms were excluded in calculating the RMSD values. The two dashed lines indicate values at 0.002 and 0.005 Å. The Jensen basis sets are with the adjusted indexing values (i.e. X=1–5).

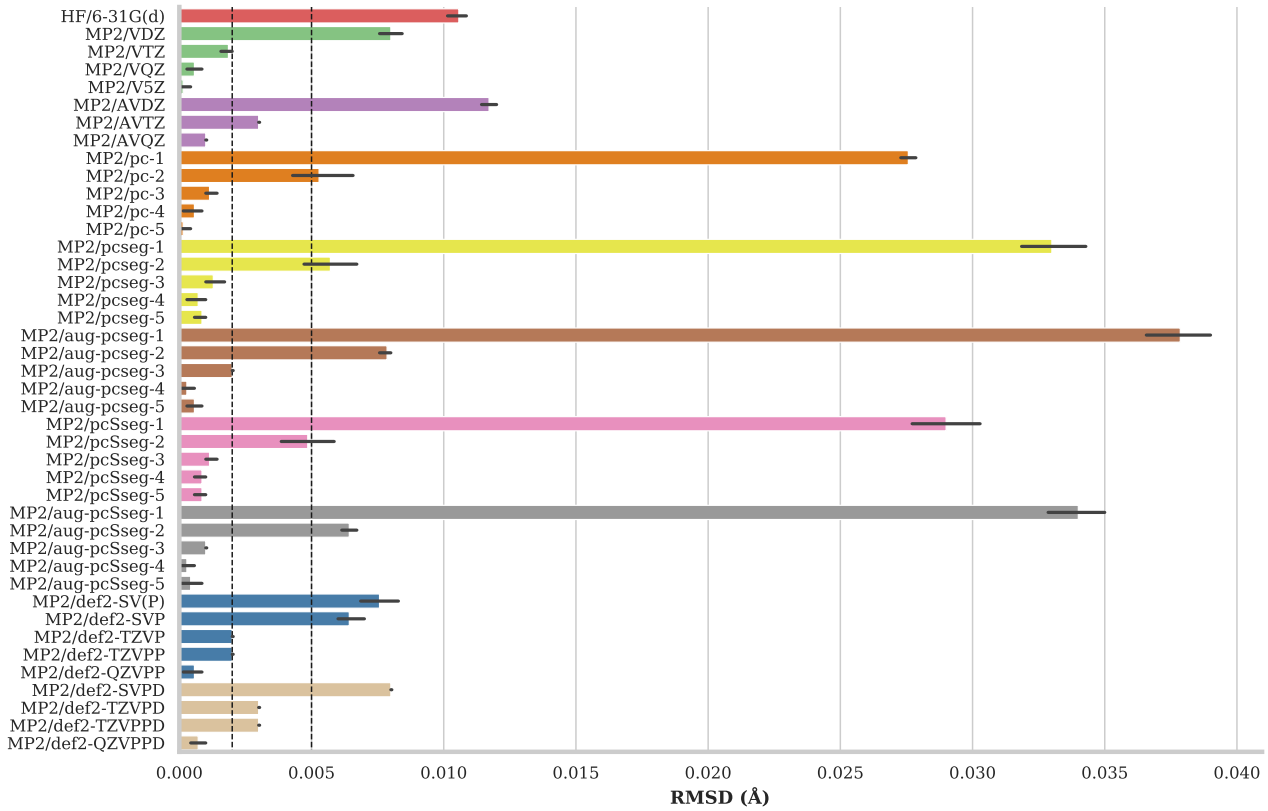


Figure S17: The mean heavy-atom RMSD (Å) the propan-2-ol conformations in comparison to MP2/aV5Z geometries. All hydrogen atoms were excluded in calculating the RMSD values. The two dashed lines indicate values at 0.002 and 0.005 Å. The Jensen basis sets are with the adjusted indexing values (i.e. X=1–5).

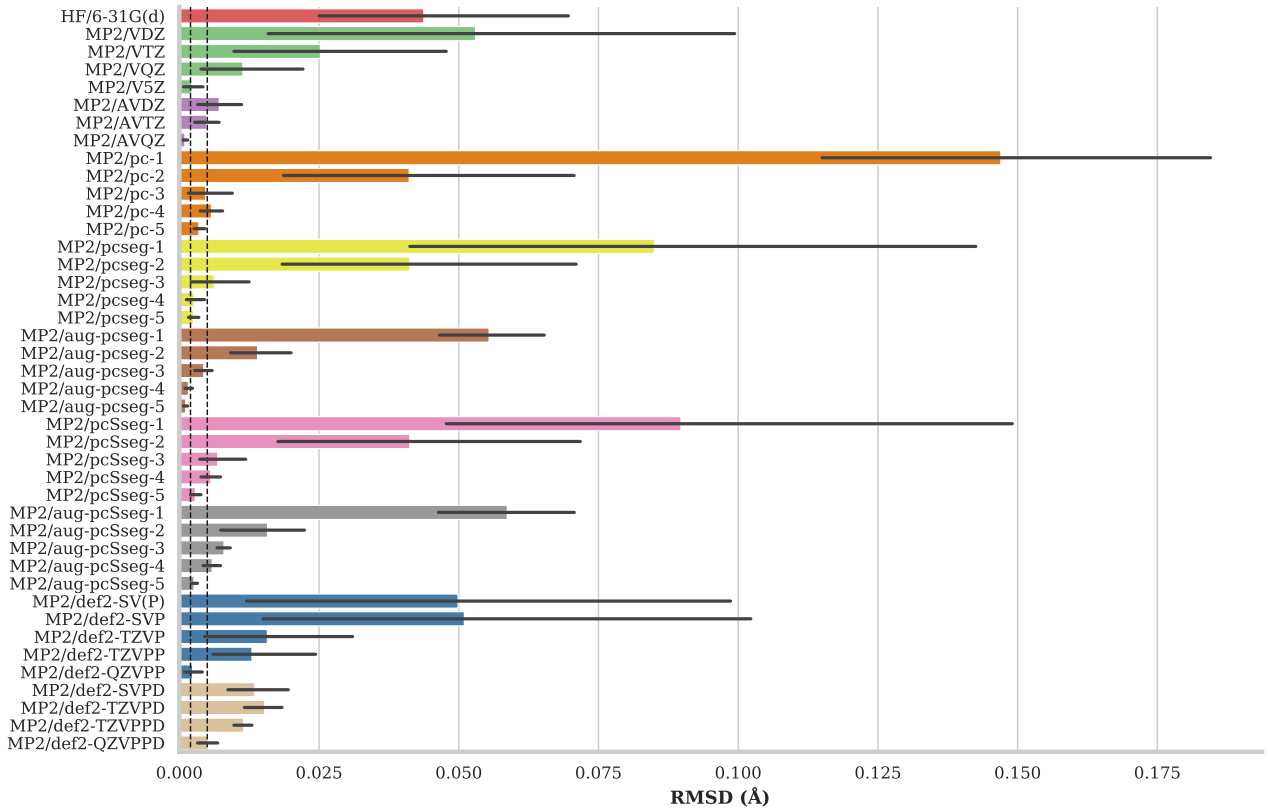


Figure S18: The mean heavy-atom RMSD (Å) the water dimer configurations in comparison to MP2/aV5Z geometries. All hydrogen atoms were excluded in calculating the RMSD values. The two dashed lines indicate values at 0.002 and 0.005 Å. The Jensen basis sets are with the adjusted indexing values (i.e. X=1–5).

Table S8. Raw calculation times (seconds) for computing a single self-consistent-field (SCF) calculation of propan-2-ol.[a,b]

Pople Basis Set	**Dunning Basis Sets**			
HF/6-31G(d)	**MP2/VDZ**	**MP2/VTZ**	**MP2/VQZ**	**MP2/V5Z**
1.8	3.0	11.1	60.4	299.1
	MP2/AVDZ	**MP2/AVTZ**	**MP2/AVQZ**	**MP2/AV5Z**
	6.6	34.9	209.4	895.7
	Jensen Basis Sets[c]			
MP2/pc-1	**MP2/pc-2**	**MP2/pc-3**	**MP2/pc-4**	**MP2/pc-5**
3.5	5.0	12.4	51.2	160.0
MP2/pcseg-1	**MP2/pcseg-2**	**MP2/pcseg-3**	**MP2/pcseg-4**	**MP2/pcseg-5**
1.8	2.8	9.0	46.7	360.7
MP2/aug-pceg-1	**MP2/aug-pceg-2**	**MP2/aug-pceg-3**	**MP2/aug-pceg-4**	**MP2/aug-pceg-5**
2.2	5.2	22.0	103.3	992.3
MP2/pcSseg-1	**MP2/pcSseg-2**	**MP2/pcSseg-3**	**MP2/pcSseg-4**	**MP2/pcSseg-5**
1.8	3.1	12.6	54.3	426.6
MP2/aug-pcSseg-1	**MP2/aug-pcSseg-2**	**MP2/aug-pcSseg-3**	**MP2/aug-pcSseg-4**	**MP2/aug-pcSseg-5**
2.3	5.8	24.5	116.6	1099.2
	Karlsruhe Basis Sets			
MP2/def2-SV(P)	**MP2/def2-SVP**	**MP2/def2-TZVP**	**MP2/def2-TZVPP**	**MP2/def2-QZVPP**
2.2	2.8	5.9	10.0	40.9
	MP2/def2-SVPD	**MP2/def2-TZVPD**	**MP2/def2-TZVPPD**	**MP2/def2-QZVPPD**
	4.5	8.8	14.0	53.0

[a] A total of six independent SCF calculations were performed using the same propan-2-ol input geometry to generate the average values.
[b] All calculations were performed using one core of an AMD FX-8350 processor within a Linux Mint 17.1 desktop computer that contained 31.5 GB of RAM.
[c] The Jensen basis sets are with the adjusted indexing values (i.e. X=1–5).

Table S9: Top five theory levels ranked by Equation 4 (main text) as a function of the scaling factor used. Two sets of ranking are presented, based on the mean absolute energy error and either the use of relative mean time or the number of uncontracted Cartesian functions. The Jensen basis sets are with the adjusted indexing values (i.e. X=1–5).

	nC = Relative Mean Time				nC = Number of Cartesian Functions				
f	Theory	Relative Mean Time	Cartesian Functions	Mean Absolute Energy Error	Score	Theory	Relative Mean Time	Cartesian Functions	Mean Absolute Energy Error	Score
0.00	MP2/pcseg-5	200.4	1160	0.003	0.000	MP2/pcseg-5	200.4	1160	0.003	0.000
	MP2/AV5Z	497.6	1568	0.004	0.002	MP2/AV5Z	497.6	1568	0.004	0.002
	MP2/V5Z	166.1	1064	0.005	0.004	MP2/V5Z	166.1	1064	0.005	0.004
	MP2/pcSseg-5	237.0	1208	0.006	0.006	MP2/pcSseg-5	237.0	1208	0.006	0.006
	MP2/aug-pcSseg-5	610.7	1712	0.008	0.008	MP2/aug-pcSseg-5	610.7	1712	0.008	0.008
0.10	MP2/pc-5	88.9	1208	0.009	0.023	MP2/AVTZ	19.4	420	0.016	0.043
	MP2/AVTZ	19.4	420	0.016	0.024	MP2/VQZ	33.6	560	0.016	0.051
	MP2/VQZ	33.6	560	0.016	0.026	MP2/aug-pcseg-3	12.2	420	0.025	0.055
	MP2/AVQZ	116.3	860	0.009	0.028	MP2/AVQZ	116.3	860	0.009	0.058
	MP2/V5Z	166.1	1064	0.005	0.030	MP2/AVDZ	3.7	172	0.036	0.059
0.20	MP2/AVTZ	19.4	420	0.016	0.024	MP2/AVDZ	3.7	172	0.036	0.060
	MP2/VQZ	33.6	560	0.016	0.029	MP2/AVTZ	19.4	420	0.016	0.063
	MP2/def2-QZVPP	22.7	568	0.021	0.032	MP2/aug-pcseg-3	12.2	420	0.025	0.074
	MP2/def2-QZVPPD	29.4	623	0.020	0.032	MP2/def2-TZVPPD	7.8	319	0.033	0.074
	MP2/aug-pcseg-3	12.2	420	0.025	0.033	MP2/def2-TZVPP	5.6	264	0.040	0.077
0.25	MP2/AVTZ	19.4	420	0.016	0.025	MP2/AVDZ	3.7	172	0.036	0.061
	MP2/VQZ	33.6	560	0.016	0.030	MP2/AVTZ	19.4	420	0.016	0.073
	MP2/def2-QZVPP	22.7	568	0.021	0.032	MP2/def2-TZVPPD	7.8	319	0.033	0.079
	MP2/aug-pcseg-3	12.2	420	0.025	0.032	MP2/def2-TZVPP	5.6	264	0.040	0.080
	MP2/def2-QZVPPD	29.4	623	0.020	0.033	MP2/pcseg-3	5.0	260	0.041	0.081
0.30	MP2/AVTZ	19.4	420	0.016	0.025	MP2/AVDZ	3.7	172	0.036	0.062
	MP2/aug-pcseg-3	12.2	420	0.025	0.031	MP2/AVTZ	19.4	420	0.016	0.083
	MP2/VQZ	33.6	560	0.016	0.032	MP2/def2-TZVPP	5.6	264	0.040	0.084
	MP2/def2-QZVPP	22.7	568	0.021	0.032	MP2/pcseg-3	5.0	260	0.041	0.084
	MP2/def2-QZVPPD	29.4	623	0.020	0.034	MP2/def2-TZVPPD	7.8	319	0.033	0.085
0.40	MP2/AVTZ	19.4	420	0.016	0.026	MP2/AVDZ	3.7	172	0.036	0.063
	MP2/aug-pcseg-3	12.2	420	0.025	0.030	MP2/pcseg-3	5.0	260	0.041	0.090
	MP2/def2-QZVPP	22.7	568	0.021	0.033	MP2/def2-TZVPP	5.6	264	0.040	0.090
	MP2/VQZ	33.6	560	0.016	0.035	MP2/def2-SVPD	2.5	155	0.069	0.093
	MP2/def2-TZVPPD	7.8	319	0.033	0.036	MP2/pc-3	6.9	260	0.047	0.095
0.50	MP2/AVTZ	19.4	420	0.016	0.027	MP2/AVDZ	3.7	172	0.036	0.065
	MP2/aug-pcseg-3	12.2	420	0.025	0.028	MP2/def2-SVPD	2.5	155	0.069	0.088
	MP2/AVDZ	3.7	172	0.036	0.031	MP2/pcseg-3	5.0	260	0.041	0.096
	MP2/def2-TZVPPD	7.8	319	0.033	0.032	MP2/def2-TZVPP	5.6	264	0.040	0.096
	MP2/def2-QZVPP	22.7	568	0.021	0.033	MP2/aug-pcSseg-2	3.2	184	0.071	0.099

Table S9 – continued from previous page.

0.60	MP2/AVDZ	3.7	172	0.036	0.025	MP2/AVDZ	3.7	172	0.036	0.066
	MP2/aug-pcseg-3	12.2	420	0.025	0.026	MP2/def2-SVPD	2.5	155	0.069	0.083
	MP2/AVTZ	19.4	420	0.016	0.027	MP2/aug-pcSseg-2	3.2	184	0.071	0.095
	MP2/def2-TZVPPD	7.8	319	0.033	0.028	MP2/pcseg-3	5.0	260	0.041	0.102
	MP2/def2-TZVPP	5.6	264	0.040	0.030	MP2/def2-TZVPP	5.6	264	0.040	0.102
0.70	MP2/AVDZ	3.7	172	0.036	0.020	MP2/AVDZ	3.7	172	0.036	0.068
	MP2/def2-TZVPPD	7.8	319	0.033	0.023	MP2/def2-SVPD	2.5	155	0.069	0.078
	MP2/aug-pcseg-3	12.2	420	0.025	0.024	MP2/aug-pcSseg-1	1.3	76	0.155	0.089
	MP2/pcseg-3	5.0	260	0.041	0.024	MP2/aug-pcseg-1	1.2	76	0.158	0.090
	MP2/def2-TZVPP	5.6	264	0.040	0.025	MP2/aug-pcSseg-2	3.2	184	0.071	0.091
0.75	MP2/AVDZ	3.7	172	0.036	0.018	MP2/AVDZ	3.7	172	0.036	0.068
	MP2/def2-TZVPPD	7.8	319	0.033	0.021	MP2/def2-SVPD	2.5	155	0.069	0.075
	MP2/pcseg-3	5.0	260	0.041	0.021	MP2/aug-pcSseg-1	1.3	76	0.155	0.076
	MP2/def2-TZVPP	5.6	264	0.040	0.022	MP2/aug-pcseg-1	1.2	76	0.158	0.078
	MP2/aug-pcseg-3	12.2	420	0.025	0.023	HF/6-31G(d)	1.0	76	0.181	0.088
0.80	MP2/AVDZ	3.7	172	0.036	0.015	MP2/aug-pcSseg-1	1.3	76	0.155	0.064
	MP2/pcseg-3	5.0	260	0.041	0.018	MP2/aug-pcseg-1	1.2	76	0.158	0.065
	MP2/def2-TZVPP	5.6	264	0.040	0.019	MP2/AVDZ	3.7	172	0.036	0.069
	MP2/def2-TZVPPD	7.8	319	0.033	0.019	MP2/def2-SVPD	2.5	155	0.069	0.072
	MP2/aug-pcseg-3	12.2	420	0.025	0.022	HF/6-31G(d)	1.0	76	0.181	0.073
0.90	MP2/AVDZ	3.7	172	0.036	0.010	MP2/aug-pcSseg-1	1.3	76	0.155	0.039
	MP2/pcseg-3	5.0	260	0.041	0.013	MP2/aug-pcseg-1	1.2	76	0.158	0.040
	MP2/def2-TZVPP	5.6	264	0.040	0.013	HF/6-31G(d)	1.0	76	0.181	0.044
	MP2/def2-SVPD	2.5	155	0.069	0.014	MP2/pcseg-1	1.0	52	0.315	0.054
	MP2/aug-pcSseg-2	3.2	184	0.071	0.015	MP2/pcSseg-1	1.0	52	0.334	0.057
1.00	HF/6-31G(d)	1.0	76	0.181	0.000	MP2/pc-1	1.9	52	0.581	0.000
	MP2/pcseg-1	1.0	52	0.315	0.000	MP2/pcseg-1	1.0	52	0.315	0.000
	MP2/pcSseg-1	1.0	52	0.334	0.000	MP2/pcSseg-1	1.0	52	0.334	0.000
	MP2/aug-pcseg-1	1.2	76	0.158	0.000	HF/6-31G(d)	1.0	76	0.181	0.014
	MP2/def2-SV(P)	1.2	76	0.404	0.000	MP2/aug-pcseg-1	1.2	76	0.158	0.014

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