Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Exploration of the Potential Energy Surface of Small Ethanol Clusters

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SUPPLEMENTARY MATERIAL

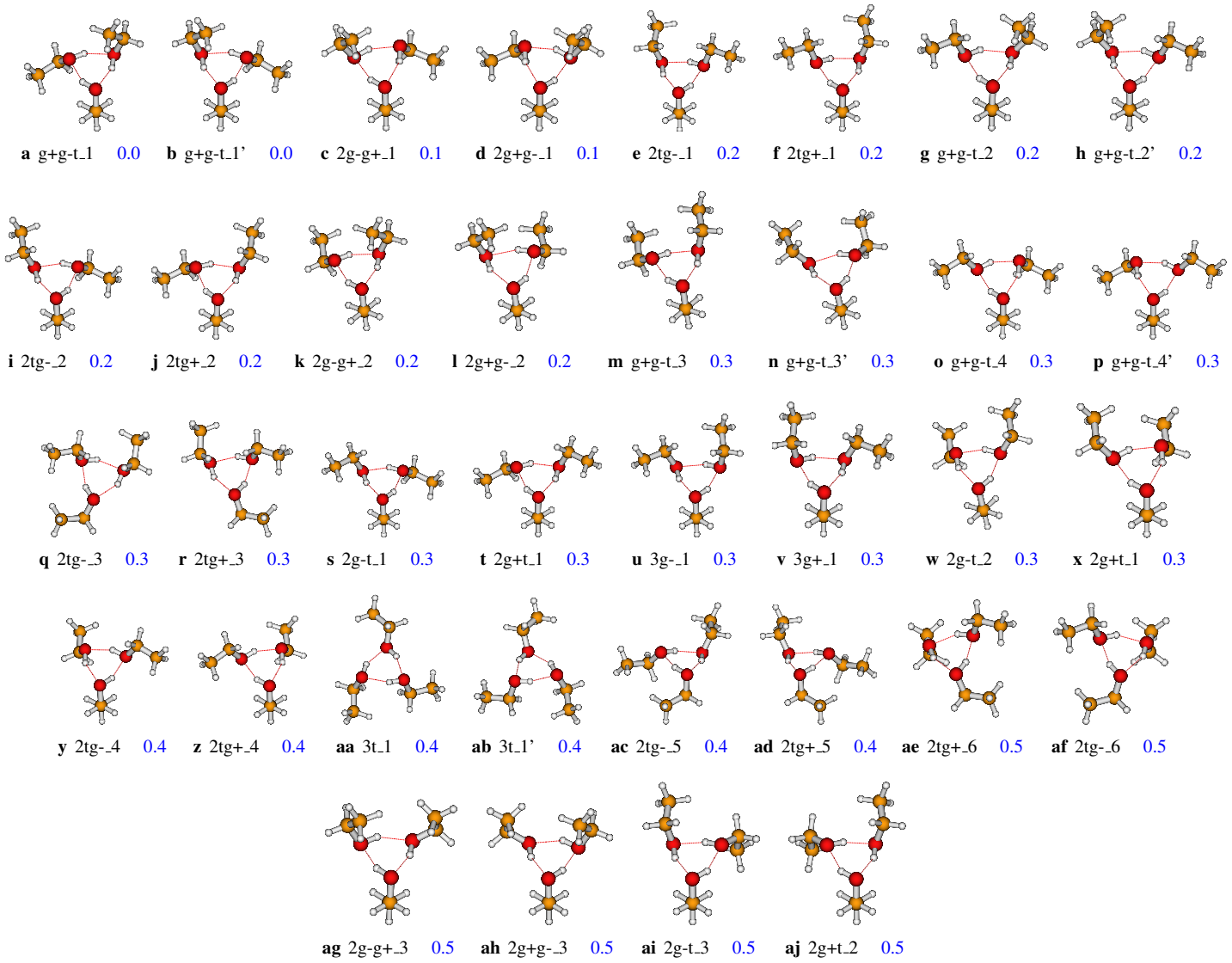

Fig. S 1 Structures of the ethanol trimer within 0.5 kcal/mol as optimized at the MP2/aug-cc-pVDZ level of theory. Structures are presented in enantiomeric pairs to highlight the symmetry of the PES of the ethanol trimer.

We have calculated the mean absolute deviation (MAD) by considering DLPNO-CCSD(T)/CBS binding energies as benchmarks. MAD_1 represents the mean absolute deviation using MP2/aug-cc-pVDZ ZPE corrected

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Tab. S 1 Binding energies (in kcal/mol) of neutral ethanol clusters computed at different levels of theory. The MAD is the mean absolute deviation calculated using the DLPNO-CCSD(T)/CBS//MP2/aug-cc-pVDZ results as benchmark. MAD1 and MAD2 use the ZPE corrected and the ZPE uncorrected MP2/aug-cc-pVDZ results as benchmark, respectively.

n	ΔE_n[a]	ΔE_n[b]	ΔE_n[c]	ΔE_n[d]	ΔE_n[e]	ΔE_n[f]	ΔE_n[g]	ΔE_n[h]	ΔE_n[i]	ΔE_n[j]	ΔE_n[k]	ΔE_n[l]	ΔE_n[m]
2	-6.2	-7.5	-6.3	-7.7	-4.9	-6.6	-5.9	-7.2	**-6.3**	-2.9	-5.8	-3.6	-5.1
3	-17.8	-20.8	-17.1	-20.3	-14.7	-18.1	-16.8	-20.0	**-17.5**	-16.9	-15.4	-11.6	-16.2
4	-33.3	-37.8	-31.1	-35.9	-26.5	-32.5	-30.5	-35.6	**-30.9**	-28.9	-27.3		
5	-45.9	-51.6	-42.6	-48.7	-36.3	-43.8	-41.7	-48.3	**-42.1**	-38.9			
6	-57.9	-65.1	-55.6	-63.5	-46.4	-55.2	-52.6	-61.3		-49.4			
MAD1	0.0	——	1.7	—-	6.5	—-	2.7	—-		3.1	——	4.4	——
MAD2	——	0.0	——	1.4	——	5.3	——	2.1	——	——	2.9	——	3.5
MAD	——	5.2	——	3.9	——	1.1	——	3.6	**0.0**	——	2.1	——	1.3

a This work at MP2/aug-cc-pVDZ level of theory with ZPE corrections
b This work at MP2/aug-cc-pVDZ level of theory without ZPE corrections
c This work at MN15/aug-cc-pVDZ level of theory with ZPE corrections
d This work at MN15/aug-cc-pVDZ level of theory without ZPE corrections
e This work at PW6B95D3/aug-cc-pVDZ level of theory with ZPE corrections
f This work at PW6B95D3/aug-cc-pVDZ level of theory without ZPE corrections
g This work at ωB97XD/aug-cc-pVDZ level of theory with ZPE corrections
h This work at ωB97XD/aug-cc-pVDZ level of theory without ZPE corrections
i This work at DLPNO-CCSD(T)/CBS//MP2/aug-cc-pVDZ level of theory without ZPE corrections
j Golub *et al.*[1] at M062X/aug-cc-pVDZ level of theory
k Sum *et al.*[2] at MP2/aug-cc-pVDZ without ZPE corrections
l Gonzalez *et al.*[3] at B3LYP/6-311+G(3df,2p) with ZPE corrections
m Lalanne *et al.*[4] at MP2/6-31G(d) level of theory

binding energies as references, while MAD_2 is the mean absolute deviation using MP2/aug-cc-pVDZ ZPE uncorrected binding energies as references. When MP2 is used as benchmark, we noted that the MN15 functionals yielded the smallest MAD1 and MAD2 as compared to other DFT functionals. The results show that the performance of the investigated functionals is in the following order: MN15 > ωB97XD > PW6B95D3. Besides, we have reported in Table S1 the binding energies from previous results in the literature (see the last four columns of Table S1). As compared to our MP2 results, all previously reported binding energies are underestimated.

References

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