Supplementary Information – HyDRA challenge

Tobias Henkes [ORCID: 0000-0002-7924-8302, email: tohe00001@stud.uni-saarland.de][1] and
Diego M. Andrada [ORCID: 0000-0003-2515-7859, email: diego.andrada@uni-saarland.de][2]

[1]Institute for Physical Chemistry, Saarland University, D-66123 Saarbrücken, Germany
[2]Institute for Inorganic Chemistry, Saarland University, D-66123 Saarbrücken, Germany

1 Computational Details

Firstly, we have explored the conformational space of all species of the training set. Up to five potential poses for each species were generated placing the water molecules with judicious orientation and pre-optimizing with a PM7 semi-empirical method.[9] Those with the lowest energy (within 5 kcal/mol threshold) have taken for a full optimization using a series of KS-DFT functionals, namely B3LYP,[1, 6] M06-2X,[11] and wB97xD.[2] The geometries have been evaluated at the KS-DFT/def2-TZVP level.[10] Dispersion corrections were included to the appropriate functionals with the Grimme formalism D3,[4] and the Becke-Jonson damping function, when possible.[5] The stationary points were located with the Berny algorithm [8] using redundant internal coordinates with a the cutoffs on forces (Maximum 0.000450) and step size (Maximum Displacement 0.001800) to determine convergence. Analytical Hessians were computed first only to determine the nature of stationary points.[7] For the calculations of the frequencies numerical differentiation along modes for anharmonic corrections were considered. The atomic average masses were used for vibrational calculations. Our calculations suggests a better performance at the wB97xD/def2-TZVP level of theory. Thus, all the calculations for the blind set have been performed at this level of theory. The search for the optimal geometry of the monohydrates from the blind set was analogous to the procedure described above for the training set. All the calculations have been performed with the Gaussian16.C01 package.[3]
The output files can be found free of charges at (https://doi.org/10.5281/zenodo.6005927).

2 Additional computed data (optional)

2.1 OH-stretching fundamentals for test set

Code	CAS	fundamentals (cm^{-1})	description
CON	502-49-8	3077	Only modes 70, 71, 72 were treated anharmonically.
		—	
DMI	80-73-9	3472	
		—	
FAH	50-0-0	3785	
		—	
MLA	547-64-8	3536	Geometry optimization with keyword ”tight”.
		—	
		—	
PCD	125132-75-4	3905	
		—	
		—	
		—	
PYR	110-86-1	3532	
		—	
THF	109-99-9	3706	
		—	
THT	110-01-0	3710	Geometry optimization with keyword ”tight”.
		—	
TPH	434-45-7	3914	
		—	
TFE	75-89-8	3569	
		—	
		—	

2.2 IR intensites and Raman scattering activities

No further information has been made available.

2.3 Isotopolog information

No further information has been made available.

2.4 Relative energies for local minima and spectral properties

No further information has been made available.

2.5 Other computed quantities for the training and test sets

No further information has been made available.

References

[1] BECKE, A. D. Density-functional thermochemistry. iii. the role of exact exchange. *J. Chem. Phys. 98*, 7 (1993), 5648–5652.

[2] CHAI, J.-D., AND HEAD-GORDON, M. Systematic optimization of long-range corrected hybrid density functionals. *J. Chem. Phys. 128*, 8 (2008), 084106.

[3] FRISCH, M. J., TRUCKS, G. W., SCHLEGEL, H. B., SCUSERIA, G. E., ROBB, M. A., CHEESEMAN, J. R., SCALMANI, G., BARONE, V., PETERSSON, G. A., NAKATSUJI, H., LI, X., CARICATO, M., MARENICH, A. V., BLOINO, J., JANESKO, B. G., GOMPERTS, R., MENNUCCI, B., HRATCHIAN, H. P., ORTIZ, J. V., IZMAYLOV, A. F., SONNENBERG, J. L., WILLIAMS-YOUNG, D., DING, F., LIPPARINI, F., EGIDI, F., GOINGS, J., PENG, B., PETRONE, A., HENDERSON, T., RANASINGHE, D., ZAKRZEWSKI, V. G., GAO, J., REGA, N., ZHENG, G., LIANG, W., HADA, M., EHARA, M., TOYOTA, K., FUKUDA, R., HASEGAWA, J., ISHIDA, M., NAKAJIMA, T., HONDA, Y., KITAO, O., NAKAI, H., VREVEN, T., THROSSELL, K., MONTGOMERY, JR., J. A., PERALTA, J. E., OGLIARO, F., BEARPARK, M. J., HEYD, J. J., BROTHERS, E. N., KUDIN, K. N., STAROVEROV, V. N., KEITH, T. A., KOBAYASHI, R., NORMAND, J., RAGHAVACHARI, K., RENDELL, A. P., BURANT, J. C., IYENGAR, S. S., TOMASI, J., COSSI, M., MILLAM, J. M., KLENE, M., ADAMO, C., CAMMI, R., OCHTERSKI, J. W., MARTIN, R. L., MOROKUMA, K., FARKAS, O., FORESMAN, J. B., AND FOX, D. J. Gaussian˜16 Revision C.01, 2016. Gaussian Inc. Wallingford CT.

[4] GRIMME, S., ANTONY, J., EHRLICH, S., AND KRIEG, H. A consistent and accurate ab initio parametrization of density functional dispersion correction (dft-d) for the 94 elements h-pu. *J. Chem. Phys. 132*, 15 (2010), 154104.

[5] GRIMME, S., EHRLICH, S., AND GOERIGK, L. Effect of the damping function in dispersion corrected density functional theory. *J. Comput. Chem. 32*, 7 (2011), 1456–1465.

[6] LEE, C., YANG, W., AND PARR, R. G. Development of the colle-salvetti correlation-energy formula into a functional of the electron density. *Phys. Rev. B 37* (Jan 1988), 785–789.

[7] MCIVER, J. W., AND KOMORNICKI, A. Structure of transition states in organic reactions. general theory and an application to the cyclobutene-butadiene isomerization using a semiempirical molecular orbital method. *J. Amer. Chem. Soc. 94*, 8 (1972), 2625–2633.

[8] PENG, C., AYALA, P. Y., SCHLEGEL, H. B., AND FRISCH, M. J. Using redundant internal coordinates to optimize equilibrium geometries and transition states. *J. Comput. Chem. 17*, 1 (1996), 49–56.

[9] STEWART, J. J. P. Optimization of parameters for semiempirical methods VI: more modifications to the NDDO approximations and re-optimization of parameters. *J. Mol. Model. 19*, 1 (JAN 2013), 1–32.

[10] WEIGEND, F., AND AHLRICHS, R. Balanced basis sets of split valence, triple zeta valence and quadruple zeta valence quality for h to rn: Design and assessment of accuracy. *Phys. Chem. Chem. Phys. 7* (2005), 3297–3305.

[11] ZHAO, Y., AND TRUHLAR, D. G. The M06 suite of density functionals for main group thermochemistry, thermochemical kinetics, noncovalent interactions, excited states, and transition elements: two new functionals and systematic testing of four M06-class functionals and 12 other functionals. *Theor. Chem. Acc 120*, 1-3 (MAY 2008), 215–241. Meeting on Practicing Chemistry with Theoretical Tools, Maui, HI, JAN 15-18, 2007.