BOOK OF ABSTRACTS

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New aspects of Hydrogen Bonding: Antiparallel OH/OH Interactions. Cases of Water/Water, Water/Alcohol and Alcohol/Alcohol Dimers.

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According to IUPAC definition, the hydrogen bond 'is an attractive interaction' usually presented as X—H Y—Z, where the electropositive hydrogen atom is located between two electronegative species X and Y.[1] The stability of hydrogen bonds varies in the range from -0.2 to -40 kcal/mol depending on the nature of the X and Y species and the geometry of the hydrogen bond.

In this presentation, new modes of hydrogen bonding will be discussed. Namely, it was found that nearly 20% of all crystal structures, from Cambridge Structural Database, containing water-water or alcohol dimers, possess, so far, unusual antiparallel OH/OH interactions. The interaction energies of this type of hydrogen bonding (Figure 1.) are systematically calculated at CCSD(T)/CBS level of theory.[2] It was shown that the strength of the antiparallel interactions can be similar as the strength of classical hydrogen bonds, i.e. up to – 4.7 kcal/mol. The geometric parameters describing the antiparallel interactions were suggested, as well.

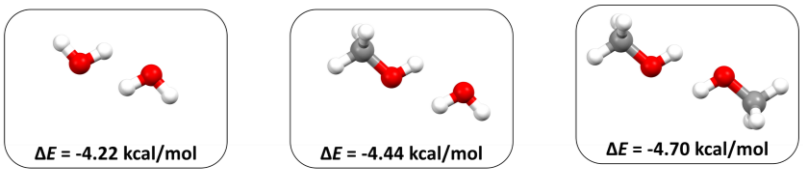

Figure 1. CCSD(T)/CBS energies of antiparallel: a) water dimer; b) water/methanol dimer and c) methanol/methanol dimer.

References

[1] Arunan, E.; Desiraju, G.; Klein, R.; Sadlej, J.; Scheiner, S.; Alkorta, I.; Clary, D.; Crabtree, R.; Dannenberg, J.; Hobza, P.; Kjaergaard, H.; Legon, A.; Mennucci, B.; Nesbitt, D., *Pure Appl. Chem.* **2011**, *83*, 1637−1641.

[2] a) Milovanović, M.R.; Stanković, I.M.; Živković, J. M.; Ninković, D.B.; Hall, M.B.; Zarić, S.D., *IUCrJ* **2022**, *9*, 639–647; b) Milovanović, M.R.; Živković, J. M.; Ninković, D.B.; Zarić, S.D., *J. Mol. Liq*. **2023**, *389*, 122758; c) Milovanović, M.R.; Zarić, S.D., J. *Phy. Chem. Lett*. **2024**, *15*, 1294−1304.

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