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Antiparallel interactions as a mode of hydrogen bonding: Case of water in solid state

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Water is one of the most important molecules; it is clear that life on Earth depends on its anomalous properties derived from its unique structure: small size and high polarity [1] as well as flexibility [2]. A fundamental ability of water is hydrogen bonding.

Hydrogen bonds are generally considered strong when the H···Y distance is 2.2 to 2.5 Å and the X—H···Y angle is 170 to 180°, whereas for weak hydrogen-bond interactions, the H···Y distance is larger than 3.2 Å and the bond angle is less than 130°. Between strong and weak interactions are those ones of the moderate strength [3].

In this work [4], we analyzed geometries of all water–water interactions in the Cambridge Structural Database (CSD). We found 9928 water-water contacts and for all of them we calculated interaction energies at the accurate CCSD(T)/CBS level. Our results indicate two types of attractive water–water interactions; the first type involves the classical hydrogen bonds (d_{OH} < 3.0 Å and α > 120°), whereas the second type involves antiparallel O—H bond interactions (Figure 1). Namely, c.a. 70% of attractive water–water contacts are classical hydrogen bonds with most being stronger than -3.3 kcal/mol, while c.a. 19% of attractive water–water contacts are antiparallel dipolar interactions with interaction energies up to -4.7 kcal/mol.

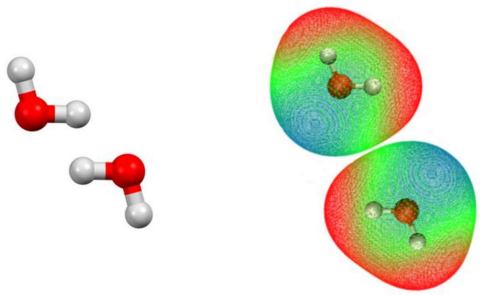

Figure 1: Antiparallel water-water interactions.

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[2] M. R. Milovanović, I. M. Stanković, J. M. Živković, D. B. Ninković, M. B. Hall, S. D. Zarić, *IUCrJ*, **9**, 639 (2022).