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Stacking Interactions of Planar Hydrogen-Bridged Rings

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The arrangement corresponding to stacking interactions is observed in crystal structures of six-membered resonance-assisted hydrogen-bridged rings (RAHB) [1] and five-membered saturated hydrogen-bridged rings [2] - 91% and 86% of all contacts in Cambridge Structural Database (CSD), respectively, with preferentially antiparallel orientation (Figure 1). Stacking arrangement is also observed in crystal structures between six-membered RAHB and C_6-aromatic rings (59% of all contacts in CSD) and between five-membered saturated hydrogen-bridged rings and C_6-aromatic rings [3] (45% of all contacts in CSD).

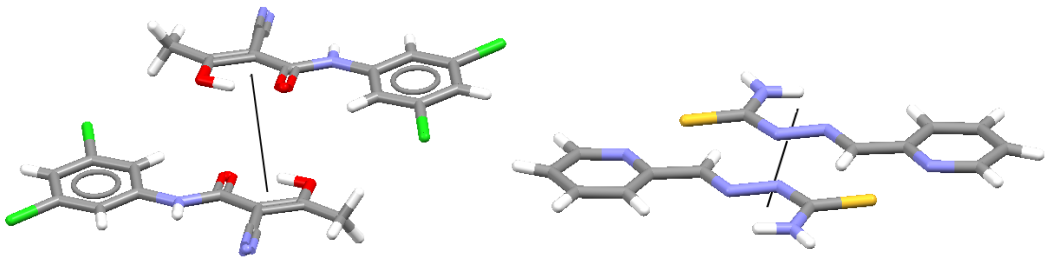

Figure 1. Fragments of crystal structures, found in CSD, where there are contacts between a) RAHB rings; b) saturated hydrogen-bridged rings

Interaction energies, calculated on dimer model systems in the gas phase at CCSD(T)/CBS level, are relatively strong. They are similar for RAHB/RAHB dimers [1] and saturated hydrogen-bridged ring dimers [2] (up to -4.7 kcal/mol and -4.9 kcal/mol, respectively). Difference is larger between interaction energies of RAHB/benzene and saturated hydrogen-bridged ring/benzene dimers [3] (up to -3.5 kcal/mol and -4.4 kcal/mol, respectively). These findings can be usefull for widening the concept of stacking interactions, since stacking interactions of saturated hydrogen-bridged systems were recently observed [2,3] and also in the design of supramolecular structures involving hydrogen-bridged rings.

References

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