Crystallographic and quantum-chemical study of stacking interactions of resonance-assisted hydrogen-bridged rings

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Mutual contacts between resonance-assisted hydrogen-bridged (RAHB) rings,[1] as well as contacts between RAHB rings and C_6-aromatic rings[2] are systematically analyzed by searching Cambridge Structural Database (CSD) (Fig. 1) It is observed that the tendency of forming stacking interactions is very high in RAHB/RAHB contacts, since 91% of them corresponds to stacked arrangement. At the other side, the tendency of forming stacked contacts is not so pronounced in RAHB/C_6-aromatic contacts, although the majority of them (59%) corresponds also to stacking. The high level quantum-chemical calculations (CCSD(T)/CBS) are performed on model systems that are based on abundance in CSD. The energies of the strongest calculated RAHB/RAHB stacking interactions can reach -4.7 kcal/mol. The strongest calculated RAHB/benzene stacking interactions are weaker (-3.7 kcal/mol), but they can be also stronger than the corresponding RAHB/RAHB stacking interactions, depending on the RAHB system considered.

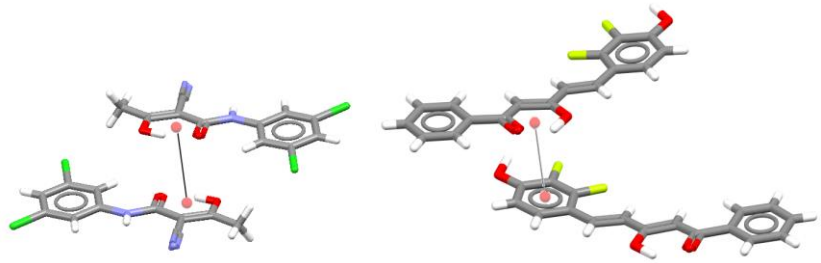

Figure 1. Fragments found in CSD a) RAHB/RAHB contacts; b) RAHB/C_6-aromatic contacts.

References

1. J. P. Blagojević Filipović, M. B. Hall, S. D. Zarić, *Cryst. Growth Des*, **2019**, *19* (10), 5619.
2. J. P. Blagojević Filipović, M. B. Hall, S. D. Zarić, Stacking Interactions of Resonance-Assisted Hydrogen-Bridged Rings and C_6-Aromatic Rings, *submitted*.

Acknowledgments

This work was supported by the Serbian Ministry of Education, Science and Technological Development [Grant number 172065] and an NPRP grant from the Qatar National Research Fund (a member of the Qatar Foundation) [Grant number NPRP8-425-1-087].