STACKING INTERACTIONS OF RESONANCE-ASSISTED HYDROGEN-BRIDGED RINGS

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Resonance-assisted hydrogen-bridged rings are often found in crystal structures in parallel alignment; 44% of all crystal structuresfound in Cambridge structural database, that contain this ring type, form parallel contacts. Distances between ring planes are typical for stacking (3.0-4.0 Å) and rings are in *anti* orientation.

Quantum chemical calculations of the stacking interaction energies are performed using different methods that are in good agreement with CCSD(T)/CBS methods, on model systems composed on dimers of molecules whose derivatives are the most common in crystal structures. The strongest calculated interactions (up to -5.1 kcal/mol) are comparable with stacking interactions of saturated hydrogen-bridged rings (-4.9 kcal/mol [1]) and stacking interactions between saturated hydrogen-bridged rings and C_6-aromatic rings (-4.4 kcal/mol [2]), as well as with hydrogen bonds between water molecules (-4.8 kcal/mol [3]).

Results indicate that energies of stacking interactions of resonance-assisted hydrogen-bridged rings are not substantially different than energies of stacking interactions between saturated hydrogen-bridged rings.

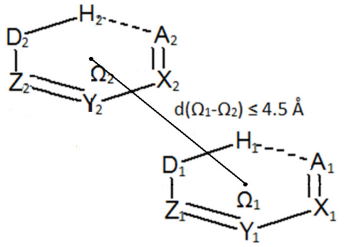

Figure 1. Structure used for the search of Cambridge Structural Database

[1] J. Blagojević,S. Zarić,*ChemCommun*, **51** (2015) 12989-12991.
[2] J. Blagojević, D. Veljković,S. Zarić, *CrystEngComm*, **19** (2017) 40-46.
[3] J. Andrić, G. Janjić,D. Ninković, S. Zarić, *PhysChemChemPhys*, **14** (2012) 10896-10898.