Chemistry Central Journal

Poster presentation

Open Access

Crystallographic and theoretical investigation of interactions of water molecule with aryl ring

SD Zarić*, GV Janjić and BD Ostojić

Address: Department of Chemistry, University of Belgrade, Studentski trg 16, 11 000 Belgrade, Serbia
* Corresponding author

from 4th German Conference on Chemoinformatics
Goslar, Germany. 9–11 November 2008

Published: 5 June 2009

Chemistry Central Journal 2009, **3**(Suppl 1):P43 doi:10.1186/1752-153X-3-S1-P43

This abstract is available from: http://www.journal.chemistrycentral.com/content/3/S1/P43

The OH/π interactions of water molecule with the π-electron cloud of aromatic groups can play important role enabling interactions of non-polar groups with polar solvent. These interactions were observed in various molecular systems [1][2][3][4]. The study of OH/π interactions between water molecule and aromatic groups of amino acids in proteins confirmed the relatively frequent occurrence of aromatic OH/π hydrogen bonding in protein crystal structures [2][3]. Besides XH/π aromatic interactions, there are abundant aromatic interactions such as π-π stacking that also play important role for protein structure and protein-ligand recognition. The Protein Data Bank studies revealed that the NH/π interactions are outnumbered by the aromatic-amide stacked structures.

In this paper we present the intermolecular interactions of water molecule with the C6 aromatic rings. The results were obtained by analyzing the interactions in crystal structures from the Cambridge Structural Database (CSD) and by *ab initio* calculations of the benzene-water dimer model systems including the CCSD(T) level of electron correlation correction. The crystal structures satisfying the geometric criteria were selected and screened for short intermolecular contacts between the water molecule and the aryl group. The analysis of data shows that there is substantial number of interactions with short distances between water molecule and aromatic ring. We observed a few types of the interactions.

The model systems of the water-benzene dimers were made based on the geometries observed in crystal structures. *Ab initio* calculations on the model systems of the dimers were performed and the geometries and energies of the interactions were obtained. The calculated interaction energies revealed that weak interactions coexists or are in competition with stronger interactions. The results of calculations were compared with the analysis of crystal structures from the CSD. The calculated distances and other geometrical features were in agreement with the geometries observed in the similar interactions in the crystal structures.

References

1. Milčić M, Zarić SD: *Eur J Inorg Chem* 2001:2143-2150.
2. Steiner T: *Biophys Chem* 2002, **95:**195-201.
3. Malone JF, Murray CM, Charlton MH, Docherty R, Lavery AJ: *J Chem Soc, Farad Trans* 1997, **93:**3429-3436.
4. Tsuzuki S, Honda K, Uchimaru T, Mikami M, Tanabe K: *J Am Chem Soc* 2000, **122:**11450-11458.