

# BOOK OF ABSTRACTS



## ICNI - III

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## Can the Benzene-Benzene and Water-Water Interactions be Similar?

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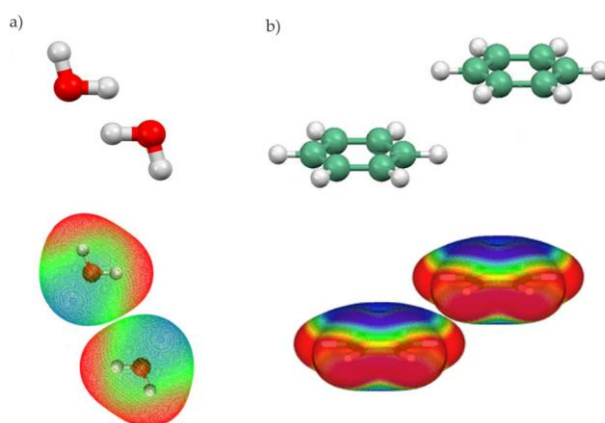
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Benzene and water are quite different by nature, benzene molecule does not have a dipole moment, while water molecule does. Considering these properties of water and benzene molecules, one can expect very different benzene/benzene and water/water interactions. We have analyzed the benzene/benzene and water/water interactions found in crystal structures from CSD and we found that both benzene/benzene and water/water can form antiparallel interactions.

Data from crystal structures in CSD shows that most benzene/benzene interactions are stacking interactions with large horizontal displacements, not the geometries that are minima on benzene/benzene potential surface. In these antiparallel interactions, the dipole moment of the C-H bond plays an important role. Also, in water/water interactions, there are a significant number of antiparallel interactions. Antiparallel interactions account for 20% of all attractive water/water contacts in the CSD. These antiparallel interactions result from the interaction of two O-H bonds in which dipoles are in antiparallel orientation.

This shows that although these two molecules are very different, they can have similar interactions concerning the local dipole moment. The deciding factor for these two important interactions is antiparallel dipole moments of the O-H and C-H bonds.



### References

- [1] Milovanović, M. R.; Stanković, I. M.; Živković, J. M.; Ninković, D. B.; Hall, M. B.; Zarić, S. D., *IUCrJ*, **2022**, *9*, 639-647.
- [2] Ninković, D. B.; Blagojević Filipović, J. P.; Hall, M. B.; Brothers, E. N.; Zarić, S. D., *ACS Central Science*, **2020**, *6*, 420-425.
- [3] Janjić, G. V.; Veljković, D. Ž.; Zarić, S. D.; *Crystal Growth & Design*, **2011**, *11*, 2680-2683.

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