

Supramolecular assemblies driven by N-H...O and O-H...O hydrogen bonding interactions: Experimental and theoretical investigation into the supramolecular architectures of dihydropyrimidin-2(1H)-ones

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Introduction

Non-covalent interactions including hydrogen bonding, π - π stacking, and hydrophobic interactions have been widely used to design and manufacture crystal structures. The present study focus on the theoretical study of dihydropyrimidin-2(1H)-ones compare with the experimental data reported in the literature. The geometry of the compounds (DHP1, DHP2 and DHP3) herein has been fully optimized using density function theory (DFT) with hybrid functional B3LYP with basis set 6-31+G (d, p).

Method

Calculation using density functional theory with the hybrid functional B3LYP and the 6-31G+ basis set.

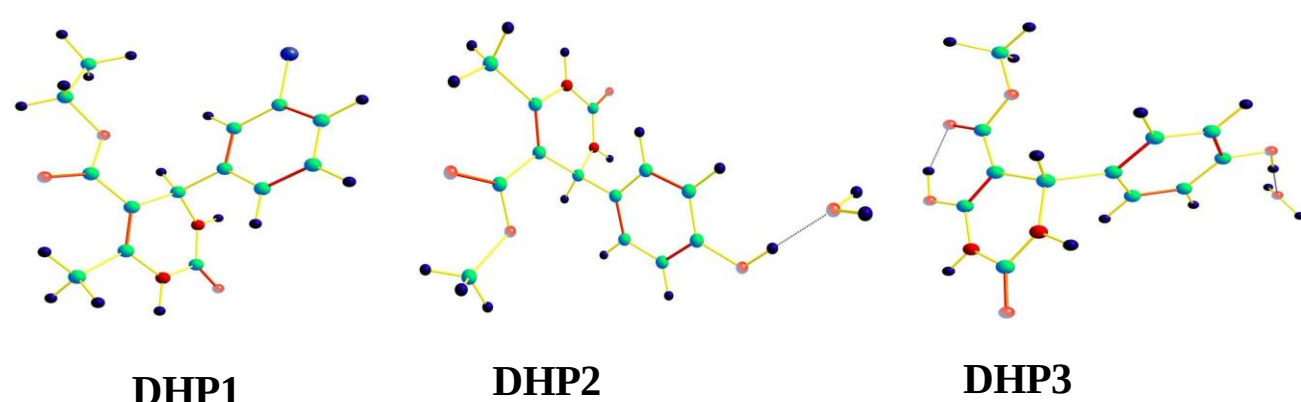


Figure 1. Optimized geometrical structure of **DHP1**, **DHP2** and **DHP3**

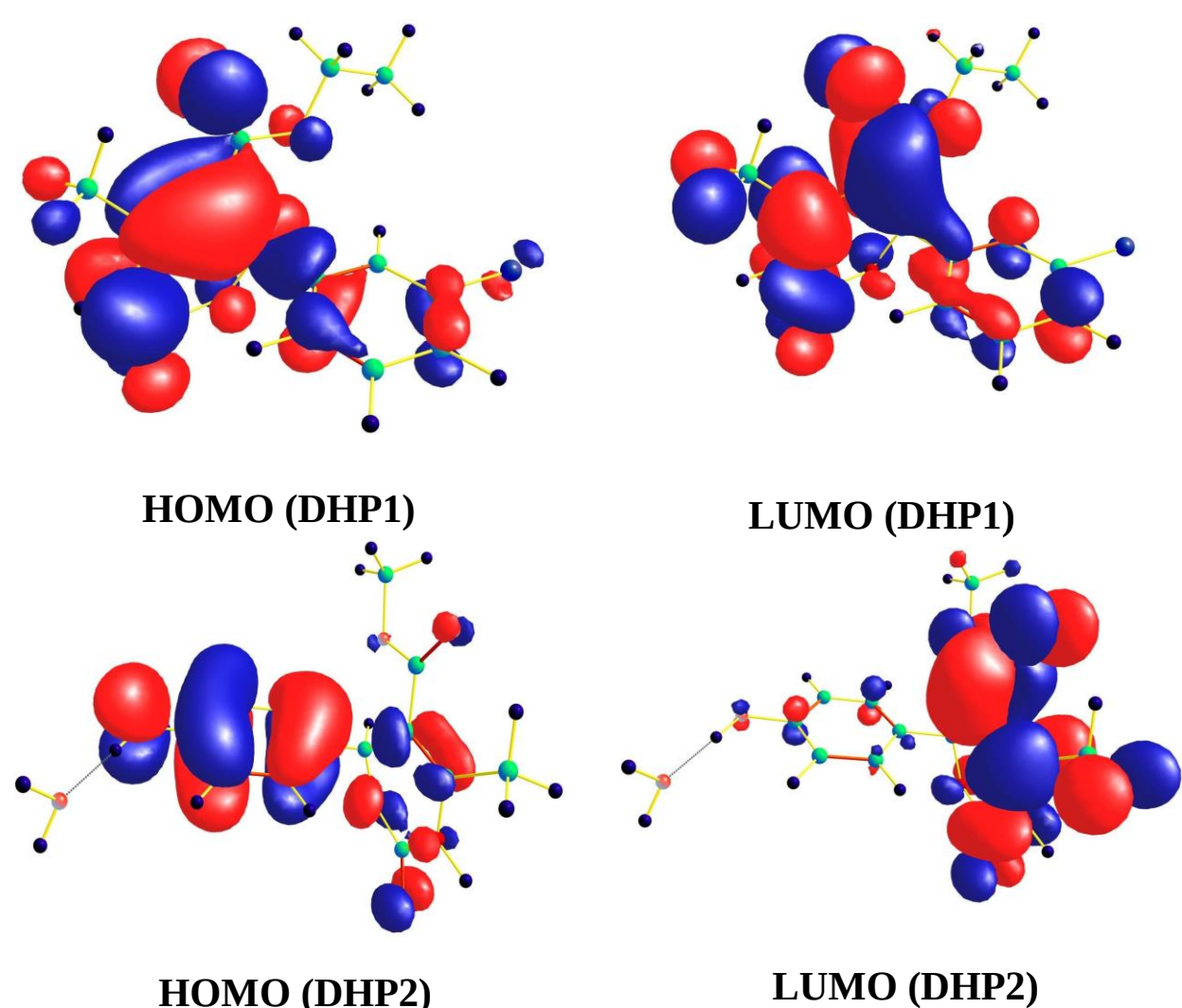


Figure 2. The HOMO-LUMO of **DHP1** and **DHP2**

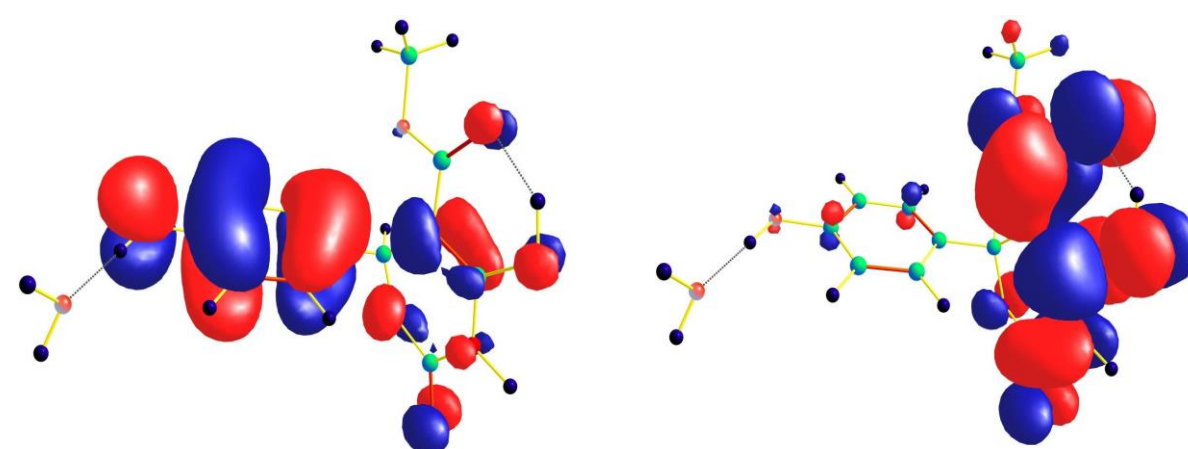


Figure 3. The HOMO-LUMO of **DHP3**

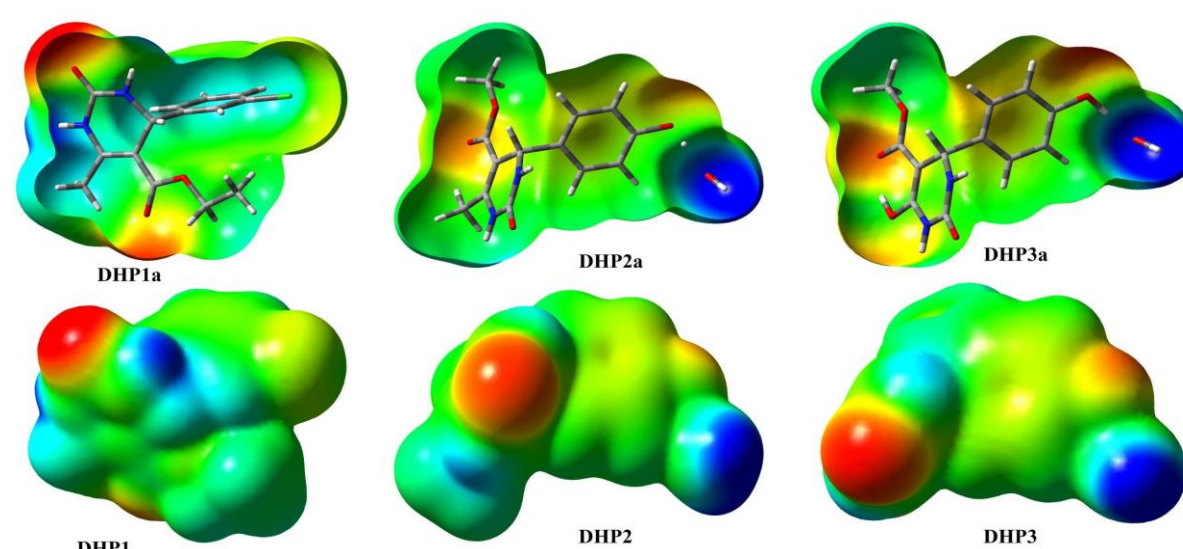


Figure 4. MEP surfaces of compounds (**DHP1**, **DHP2** and **DHP3**)

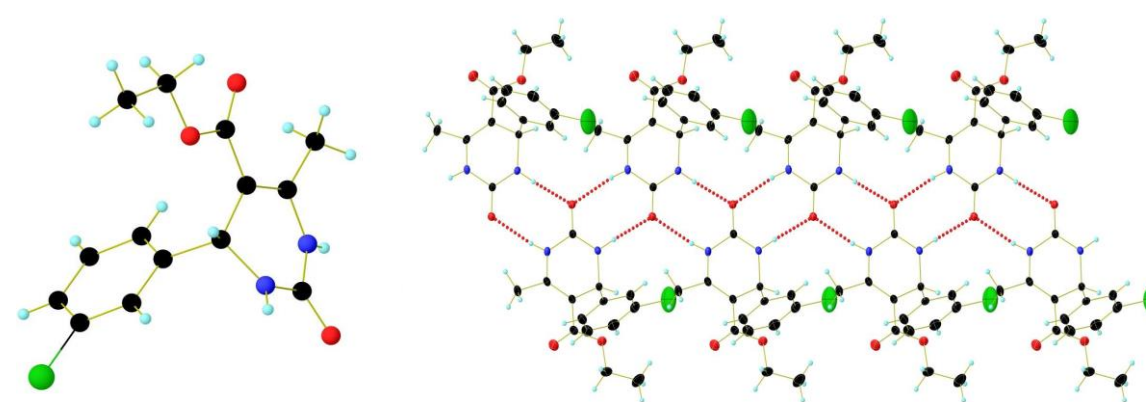


Figure 5. The experimental structure of **DHP1** (CCDC-1455903) showing supramolecular interaction

Conclusion

In conclusion, the results obtained from theoretical calculation was compared with the available data obtained from CSD. The theoretical studies shows a close correlation with the experimental data, slight different was expected because the theoretical studies were performed in gas phase, in which the intermolecular interactions was absent

References

- Schneider, H.J. Binding mechanisms in supramolecular complexes. *Angew. Chem. Int. Ed.* 2009, 48, 3924-3977.
- Schneider, H.J.; Yatsimirski, A. Principles and Methods in Supramolecular Chemistry; Wiley: Chichester, UK, 2000.