MS32-P22

Structural determination of biological active N-phenyl-2-phthalimidoethanesulfonamide derivatives

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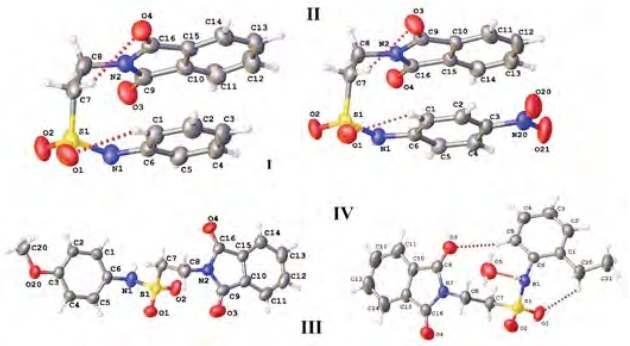
This study contains the structural characterization of unsubstituted N-phenyl-2-phthalimidoethanesulfonamide, $C_{16}H_{14}N_2O_4S$, (I), the N-(4- nitrophenyl)-, $C_{16}H_{13}N_3O6_S$, (II), N-(4-methoxyphenyl)-, $C_{16}H_{16}N_3O_6S$, (III), and N-(2-ethylphenyl)-, as the monohydrate, $C_{18}H_{18}N_2O_4S{\cdot}H_2O$, (IV), derivatives in order to determine the impact of different substituents and their positions on intermolecular interactions and ultimately on the crystal packing. Studies of the effects of substituents on aromatic systems are of critical importance in chemistry, biology and pharmaceutics. The π-electron delocalization brought about by the substituent affects the intermolecular interactions and the packing motifs of aromatic molecules in crystals. Changes in the positions of substituent groups can significantly alter the molecular configurations and crystal structures of isomers. A slight difference in molecular structure can lead to a profound impact on the crystal packing. X-ray structural studies were performed with Rigaku-Oxford Xcalibur diffractometer. Data collections and reductions along with absorption corrections were performed using CrysAlis^{Pro} software package [1]. Structure solutions and refinements were performed using SHELXT and SHELXL, respectively, embedded in the Olex2 [2-4].



References:

[1] CrysAlisPro Software System, Version 1.171.38.43, Rigaku Corporation, Oxford, UK, 2015.
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Keywords: crystal structure, substituent position effect, ethanesulfonamide

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Four 2-Hydroxyethyl substituted NHC iodide complexes: structural characterization and theoretical comparisons

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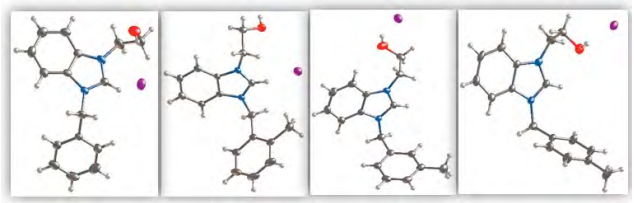
This study contains the structural characterization of four 2-Hydroxyethyl substituted N-heterocyclic carbene (NHC) iodide derivatives. Heterocyclic compounds are very important both industrially and biologically. These compounds are found in the vast majority of new drugs synthesized in the pharmaceutical industry. They are also used as ligands for the synthesis metal-N-heterocyclic carbene (NHC) complexes. In here, we report the molecular and crystal characterization of the NHC precursors. X-ray structural studies were performed with Rigaku-Oxford Xcalibur diffractometer. Data collections and reductions along with absorption corrections were performed using CrysAlis^{Pro} software package [1]. Structure solutions and refinements were performed using SHELXT and SHELXL, respectively, embedded in the Olex2 [2-4]. In the crystal structures, molecules are bonded to iodide anions through the O–H···I hydrogen bonds. Additionally, there are weak C–H···O interactions, which contribute to the stability of the crystal structures. One of the molecules is unsubstituted, and the others have methyl-substituents at the -ortho, -meta and -para positions on the benzene rings. We will also present the optimized geometries and the comparison of the frontier molecular orbital energy levels.



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[2] G. M. Sheldrick, Acta Crystallogr. A71, 3, 2015.
[3] G. M. Sheldrick, Acta Crystallogr. C71, 3, 2015.
[4] O. V. Dolomanov, L. J. Bourhis, R. J. Gildea, J. A. K. Howard, H. Puschmann, J Appl. Cryst. 42, 339, 2009.

Keywords: N-heterocyclic carbenes, iodide, crystal structure, DFT