Poster Presentation

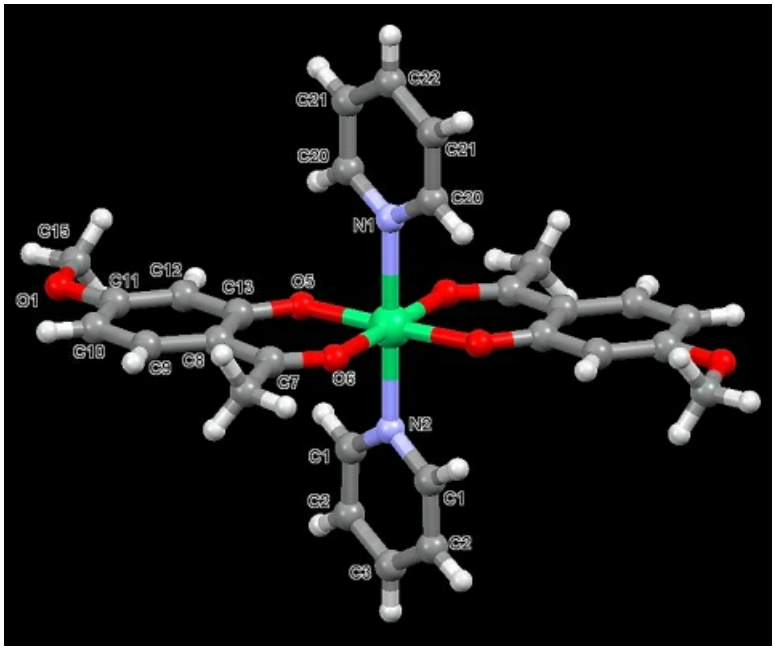
MS030.P08

Solvent effect on molecular structures: X-ray and DFT studeis

Urmila H Patel[1], Vijay M Barot[2], Sahaj A Gandhi[3], Bharatkumar D Patel[4], Mahesh K PATEL[1], BHAVESH SOCHA[1], Jatin G Jayswal[2]
[1]Physics Sardar Patel University, V.v.nagar, India, [2]S M Panchal Science, Commerce and Arts College, Talod, India, [3]Bhavan's Shri I. L. Pandya Arts, Science and Jashodaben Shah Commerce College, Dakor, India, [4]M B Patel Science College, Anand, India
E-mail: u_h_patel@yahoo.com

The presence of solvent in the molecular structures facilitates the intra and intermolecular interactions. The intermolecular interactions due to solvent play both explicit and implicit roles in the stability of molecular structures especially in the coordination of metallic structures. Sulfamethazine, one of the constituents of the triple sulfa drugs- sulfamethazine, sulfadiazine and sulfamerazine possesses wider biological spectrum [1]. Metal complexes of sulfonamides modify the pharmacology and toxicology of the sulfonamide based ligands. Another significant acetophenol and aromatic amine derivatives have also been found wider use as antibacterial agents. Biological activity of metal complexes differs from those of either ligands or the metal ions and an increased and/ or decreased biological activity have been reported for several transition metallic complexes [2]. To elucidate the role of solvent in the stability of these transition metallic complexes, we have investigated three dimensional structures of silver sulfamethazine in the presence of secondary ligand picoline, Ni complexes of cyclohexa-2,4 dienol derivatives and also its three dimensional structures in the presence of secondary ligand pyridine by X-ray diffraction technique. Hirshfeld surface analysis [3] carried out to establish the contribution of intermolecular interactions as confirmed by X-ray data. To have a detailed understanding of the modifications in the molecular structures, in the electronic properties and in the hydrogen bond interactions in the presence of solvent, theoretical investigations are performed by calculations of natural bond orbital (NBO), molecular electrostatic potential (MEP) and frontier molecular orbital (FMO) analysis.

[1] Nitya Anand (1979) Burger's Medicinal Chemistry, Part II, edited by M. E. Wolff, 1-40, New York, John Wiley.
[2] K. K. Narang, J. K. Gupta (1977), Transition Metal Chemistry, 2, 181-183.
[3] J. J. McKinnon, M. A. Spackman, A. S. Mitchell (2004), Acta Crystallographica B60, 627-668.



Keywords: Solvent, X-ray diffraction, DFT