Crystal X-Ray Structures, Characterization, DFT Studies and Hirshfeld Surface Analysis Of "Zn" Complexes With N, N-Bis(Salicylidene)1,2-Ethylenediamine.

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Résumé :

In recent years, there has been notable attention among academic researchers on Schiff base ligands due to their diverse structural characteristics and wide range of physicochemical properties. This has led to the exploration of various applications for these ligands. The interest in Schiff base stems from their structural versatility, which allows them to be effectively employed as asymmetric and stabilizing agents for various complexes in different oxidation states. [1], [2]

In the study of the effects of steric strain on coordination compounds involving multidentate ligands, compounds of zinc are of interest as the absence of crystal field directive effects. [3], [4] should permit the ligand to adopt what might be considered its natural configuration. [5]

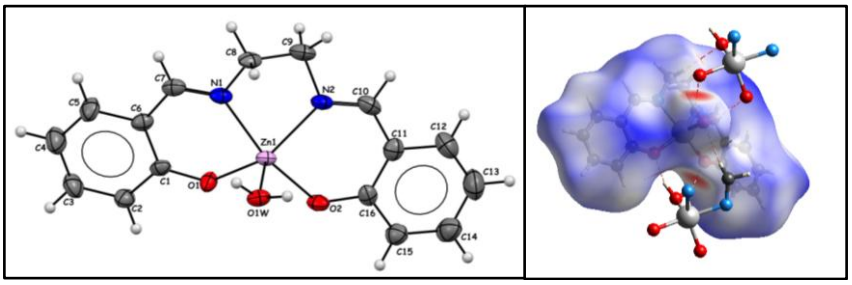
As part of our investigation, we successfully obtained two novel compounds derived from a salen-type Schiff base ligand. The synthesis was carried out under reflux conditions, and the resulting compounds were structurally characterized using single-crystal X-ray diffraction, crystal structure, FT-IR and DFT analysis.

An exhaustive investigation of the diverse intermolecular interactions via Hirshfeld surface analysis enables contributions to the crystal packing of the title complex to be quantified.

The crystal structure was stabilized by an extensive network of C—H···O and O—H···O hydrogen bonds for the first complex, and C—H···O interactions for the second, as well as

π–π stacking interactions.

Hirshfeld surface analysis indicates that the most significant contacts in the crystal packing are H···H (46.4%), C···H/H···C (18.5% / 13.5%) for the first compound, and H···H (57.5%), C···H/H···C (14.7% / 12.3%) for the second, respectively.



Figures :Ortep representation of the complex ,d norm of Hirshfeld surface.

Références :

[1] M.T.H. Tarafder, M.A. Ali, M.S. Elias, K.A. Crouse, S. Silong, Transition Met. Chem. 25 (2000) 706.

[2] N. Manav; N. Gandhi; N.K. Kaushik. J. Therm. Anal. Calorim. 61 (2000) 117-127.

[3] N.V. Tverdova, E.D. Pelevina, N.I. Giricheva, G.V. Girichev, N.P. Kuzmina, O.V. Kotova. J. Mol. Str., 1012 (2012) 151-161.

[4] C. Anitha, C.D. Sheela, P. Tharmaraj, S. Sumathi. Spectrochim. Acta (Part A) 96 (2012) 493-500.

[5] Bibhesh K. Singh, Hemant K. Rajour, Anant Prakash. Spectrochim. Acta (Part A) 94 (2012) 143-151.