Poster

Crystal Structure, Hirshfeld Surface Analysis and Spectroscopic Studies of Newly Synthesized Dithiocarbazate Pyrazole Compound

Gustavo J. Lima[1*] and Claudia C. Gatto[1]

[1]*University of Brasilia, Institute of Chemistry, Laboratory of Inorganic Synthesis and Crystallography, Brasília-DF, Brazil.*

gustavojoneslima@gmail.com and ccgatto@unb.br

Diketones and their related derivatives represent a significant class of organic compounds due to their ability to coordinate with several transition metal ions and main group metal centers. Additionally, metal complexes with pyrazole ligands have garnered substantial interest because of their unique coordination properties and their relevance in biological and biochemical contexts [1]. Dithiocarbazates are an important class of biologically active organic compounds that have gained significant attention for their diverse pharmacological properties. They are promising candidates to obtain metal complexes with diverse biological applications, including antibacterial, antimicrobial, and antifungal activities [2,3].

The present study describes newly synthesized dithicarbazate derived from a pyrazole organic group (L). The compound was investigated by single crystal X-ray analysis, Hirshfeld surface, physicochemical and spectroscopic methods. The 3D Hirshfeld surface and the 2D fingerprint plots of L were analyzed quantitatively to verify the presence of intra- and intermolecular interactions. The d_{norm} surface shows regions with red, blue, and white colors, which indicate contacts with smaller, larger, and closer distances to the sum of van der Waals radii, respectively. Red spots are observed in the d_{norm} surfaces of HL indicating the presence of non-classical interactions (Figure 1).

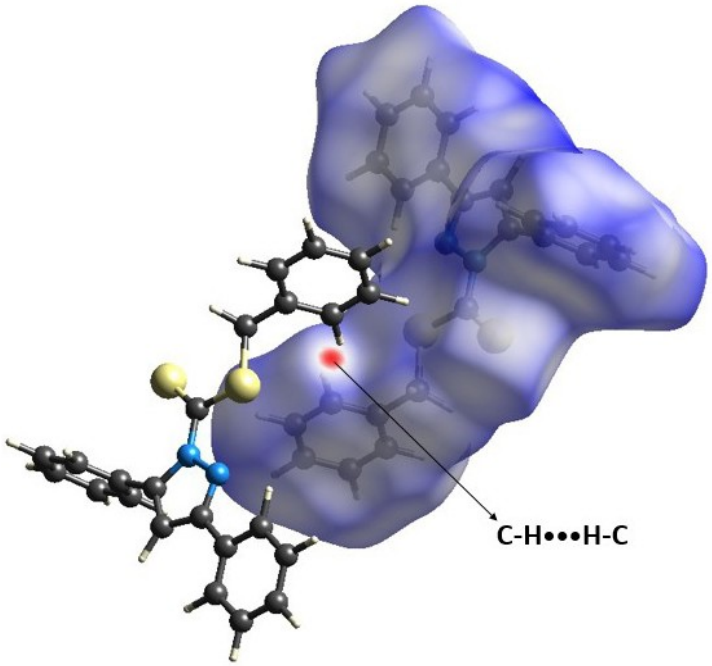

Figure 1. Hirshfeld surface mapped in d_{norm} for L.

[1] Evans IR, Howard JAK, Szécsényi KM, Leovac VM, Jacimovic ZK (2004) J Coord Chem 57:469.

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[3] Cavalcante, C. de Q. O.; da Mota, T. H. A.; de Oliveira, D. M.; Nascimento, É. C. M.; Martins, J. B. L.; Pittella-Silva, F.; Gatto, C. C.; *Front. Mol. Biosci.* (2023), *10*, 1.

This work was supported by UnB, FAPDF (Process: 00193-00001849/2023-49), CNPq, and CAPES.