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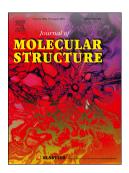
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ACCEPTED MANUSCRIPT

Synthesis, Crystal Structure, and Non-Covalent Interactions in Ethyl 4-Hydrazinobenzoate Hydrochloride.

Jelem Restrepo,^{1*} Christopher Glidewell,² Néstor Cubillán,³ Ysaias Alvarado,⁴ Necmi Dege,⁵ Miguel Morales-Toyo.^{1,6**}

¹Laboratory of Sustainable Synthesis of New Materials. Center for Research in Materials Technology (CITeMA), Venezuelan Institute of Scientific Research (IVIC), Bolivarian Republic of Venezuela.

²School of Chemistry, University of St Andrews, St Andrews, Fife KY16 9ST, UK. ³Programa de Química, Universidad del Atlántico, Barranquilla, Colombia.

⁴Laboratory of Molecular and Biomolecular Characterization, Center for Research in Materials Technology (CITeMA), Venezuelan Institute of Scientific Research (IVIC), Bolivarian Republic of Venezuela.

⁵Ondokuz Mayıs University, Arts and Sciences Faculty, Department of Physics, 55139 Samsun, Turkey.

⁶Facultad de Ciencias, Universidad Adventista Dominicana (UNAD), Autopista Duarte Km 74 ½, Villa Sonador, Provincial Monseñor Nouel, 42000, República Dominicana.

Emails: *jrestrep@ivic.gob.ve; **miguelmorales@unad.edu.do

ABSTRACT

The compound ethyl 4-hydrazinobenzoate hydrochloride (E-4HB), $C_9H_{13}N_2O_2Cl$, has been synthesized and characterized by FT-IR, 1H and ^{13}C NMR and X-ray diffraction. The compound crystallizes as colourless plates in the triclinic space group P-1, with Z' = 2 and cell parameters a = 5.9566 (4) Å, b = 7.4498 (6) Å, c = 23.5349 (17) Å, $\alpha = 84.323$ (3), $\beta = 84.521$ (3), $\gamma = 80.257$ (3), V = 1020.95 (13) Å 3 . The component ions are linked by two N-H...N hydrogen bonds and eight N-H...Cl hydrogen bonds to form complex sheets in which each of the chloride ions accepts hydrogen bonds from four different cations. Calculations on the Non-Covalent Interactions (NCI) amplify the crystallographic conclusions concerning the intermolecular hydrogen bonds.

Keywords: synthesis, crystal structure, molecular structure, hydrogen bonding, modelling of non-covalent interactions.

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