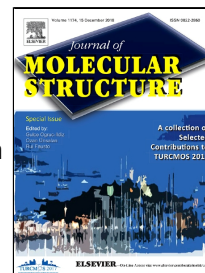


Accepted Manuscript

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PII: S0022-2860(18)31170-0
DOI: 10.1016/j.molstruc.2018.09.089
Reference: MOLSTR 25723
To appear in: *Journal of Molecular Structure*
Received Date: 23 July 2018
Accepted Date: 28 September 2018

Please cite this article as: Anelio J. Dugarte-Dugarte, Jacco van de Streek, Antonio M. dos Santos, Luke L. Daemen, Alexander A. Puretzky, Graciela Díaz de Delgado, José Miguel Delgado, Structure Determination of Oxamic Acid from Laboratory Powder X-Ray Diffraction Data and Energy minimization by DFT-D, *Journal of Molecular Structure* (2018), doi: 10.1016/j.molstruc.2018.09.089

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Structure Determination of Oxamic Acid from Laboratory Powder X-Ray Diffraction Data and Energy minimization by DFT-D

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Abstract

The structure determination from laboratory X-ray powder diffraction data of oxamic acid, a derivative of the biologically active oxalic acid and the simplest organic acid containing an amide group, is presented in this contribution. An energy minimization analysis by DFT-D was carried out. The structure was determined with the program TALP and refined by the Rietveld method with GSAS-II in space group *Cc* (No. 9). The final unit-cell parameters are $a = 9.4989(6)$, $b = 5.43796(9)$, $c = 6.8637(9)$ Å, $\beta = 107.152(5)^\circ$, $V = 338.772(10)$ Å³, $Z = 4$. The refinement converged to the figures of merit: $R_e = 0.01674$, $R_p = 0.03270$, $R_{wp} = 0.05652$ and $GoF = 3.378$ with a good fit between the calculated pattern of the structural model and the experimental pattern. The DFT-D calculations show an excellent reproduction of the experimental structure, validating the correctness of the structure. The non-centrosymmetric nature of the structure was confirmed by SHG measurements. In the crystal structure, the molecules are close to planar and form a complex infinite 2D hydrogen-bonding pattern based on the cyclic amide-acid heterosynthon.

Keywords: oxamic acid, structure determination, TALP, GSAS-II, DFT-D calculations, SHG measurements.

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