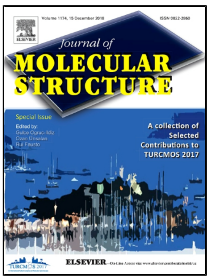
Accepted Manuscript



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Analio J. Dugarte-Dugarte, Jacco van de Streek, Antonio M. dos Santos, Luke L. Daemen, Alexander A. Puretzky, Graciela Díaz de Delgado, José Miguel Delgado

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: Analio 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

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

Analio J. Dugarte-Dugarte[1], Jacco van de Streek[2], Antonio M. dos Santos[3], Luke L. Daemen[3], Alexander A. Puretzky[4], Graciela Díaz de Delgado[1], José Miguel Delgado[1].

[1] *Laboratorio de Cristalografía-LNDRX, Departamento de Química, Facultad de Ciencias, Universidad de Los Andes, Mérida 5101, Venezuela.*
email: migueld@ula.ve

[2] *Institute of Inorganic and Analytical Chemistry, Goethe-University, Frankfurt am Main, Germany.*

[3] *Neutron Sciences Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee 37831, USA.*

[4] *Center for Nanophase Materials Science, Oak Ridge National Laboratory, Oak Ridge, Tennessee 37831, USA.*

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, β = 107.152(5)°, V = 338.772(10) Å^3, 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.