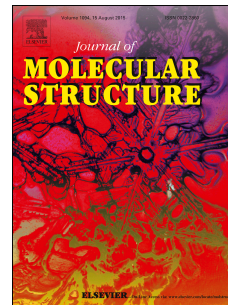


Accepted Manuscript

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PII: S0022-2860(18)30562-3

DOI: [10.1016/j.molstruc.2018.05.006](https://doi.org/10.1016/j.molstruc.2018.05.006)

Reference: MOLSTR 25178

To appear in: *Journal of Molecular Structure*

Received Date: 13 December 2017

Revised Date: 2 May 2018

Accepted Date: 3 May 2018

Please cite this article as: L.E. Fernández, G.E. Delgado, L.V. Maturano, R.M. Tótaró, E.L. Varetti, Experimental and theoretical vibrational study of *N*-carbamoyl-L-proline, *Journal of Molecular Structure* (2018), doi: 10.1016/j.molstruc.2018.05.006.

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Experimental and theoretical vibrational study of *N*-carbamoyl-L-proline

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Abstract

The infrared and Raman spectra of *N*-carbamoyl-L-proline, C₆H₁₀N₂O₃ [(2*S*)-1-carbamoylpyrrolidine-2-carboxylic acid] were obtained and interpreted with the help of DFT calculations. Six relatively stable molecular conformers were predicted by theory, being one of these similar to the conformer present in the crystal whose X-ray study was already known. The vibrational study was based in that conformer. The experimental vibrational data and assignments were used as basis for the definition of the Scaled Quantum Mechanics (SQM) force field for the molecule. The Potential Energy Distribution (P.E.D.), which revealed the complex nature of many molecular vibrations, and a set of internal force constants were calculated from this SQM force field.

Keywords: N-carbamoyl-L-proline; molecular structure; vibrational spectra; force field; DFT calculation

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