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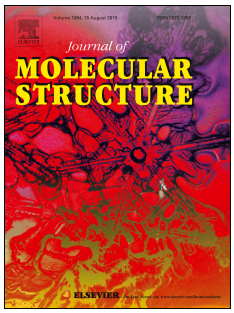

Experimental and theoretical vibrational study of *N*-carbamoyl-L-proline

L.E. Fernández, G.E. Delgado, L.V. Maturano, R.M. Tótaro, E.L. Varetti

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

L. E. Fernández [a], G. E. Delgado [b], L. V. Maturano [a], R. M. Tótaro [c] and E. L. Varetti [d, *]

[a] Instituto de Química Física, Facultad de Bioquímica, Química y Farmacia, Universidad Nacional de Tucumán, San Lorenzo 456, 4000 S. M. de Tucumán, Argentina.

[b] Laboratorio de Cristalografía, Facultad de Ciencias, Departamento de Química, Universidad de Los Andes, Mérida 5101, Venezuela.

[c] Facultad de Agronomía y Zootecnia, Universidad Nacional de Tucumán, Avda. Roca 1900, 4000 S. M. de Tucumán, Argentina.

[d] Centro de Química Inorgánica (CEQUINOR, CONICET-UNLP), Facultad de Ciencias Exactas, Universidad Nacional de La Plata, C. Correo 962, 1900 La Plata, Argentina.

Abstract

The infrared and Raman spectra of *N*-carbamoyl-L-proline, $C_6H_{10}N_2O_3$ [(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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[*] Author to whom correspondence should be sent (e-mail address: varetti@quimica.unlp.edu.ar).