

Matrix Isolation FTIR Spectroscopic and Theoretical Study of Dimethyl 2,2-Dioxo-1*H*,3*H*-Pyrazolo[1,5-*c*][1,3]Thiazole-6,7-Dicarboxylate

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Heterocyclic compounds play a central role in chemistry. They have a wide range of applications and represent about half of the known organic compounds. The discovery of new heterocyclic systems and the understanding of their properties and structure are important research topics. Our efforts have been focussed on the study of pericyclic reactions of extended dipoles such as azafulvenium methides and diazafulvenium methides in order to develop new routes to heterocyclic compounds [1, 2]. The diazafulvenium methides can be generated from the thermal extrusion of sulfur dioxide from 2,2-dioxo-1*H*,3*H*-pyrazolo[1,5-*c*][1,3]thiazoles making relevant the gathering of information on the chemistry and structure of 2,2-dioxo-1*H*,3*H*-pyrazolo[1,5-*c*][1,3]thiazoles.

In this study, dimethyl 2,2-dioxo-1*H*,3*H*-pyrazolo[1,5-*c*][1,3]thiazole-6,7-dicarboxylate (DPTD) has been synthesized and its monomeric structure studied by DFT calculations. A systematic search of the preferred conformations of DPTD on the ground state potential energy surface and their vibrational spectra was performed using the Gaussian 03 program at the DFT(B3LYP)/6-31+G(p) and DFT(B3LYP)/6-311++G(p,d) levels of theory.

The compound has also been studied by Matrix Isolation FTIR spectroscopy (in both argon and xenon matrices) and in the condensed phases: neat amorphous and crystalline solid states. Finally, the photochemical behaviour of the matrix isolated DPTD monomer was investigated through *in situ* broadband irradiation using a standard Hg(Xe) lamp as UV-light ($\lambda > 235$ nm) source.

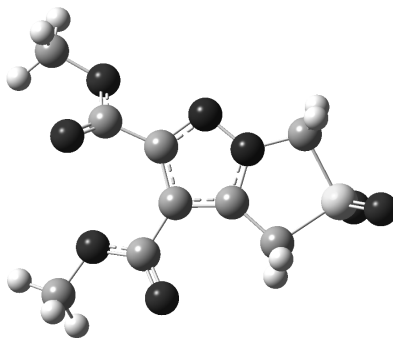


Fig. 1: Structure of the most stable conformer of DPTD.

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Acknowledgements

This work was funded by FCT (Projects POCTI/QUI/58937/2004 and POCTI/QUI/59019/2004), and the Instituto de Investigação Interdisciplinar of the University of Coimbra (Project III/BIO/40/2005). C.M. Nunes acknowledges FCT the Ph.D. grant (SFRH/BD/28844/2006).