Photochemistry and Vibrational Spectra of Matrix Isolated Methyl 4-Chloro-5-Phenylisoxazole-3-Carboxylate

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Heterocyclic compounds such as isoxazoles and its derivatives are important building blocks of many compounds of biological interest. These heterocycles are involved directly or as intermediates in the synthesis of new compounds that are potentially useful in a variety of fields, with pharmaceutical and medicinal applications. On the other hand, the agricultural uses of isoxazole derivatives include herbicidal, insecticidal and soil fungicidal activities. Isoxazoles have also been used as semiconductors, as corrosion inhibitors in fuels and lubrificants and in the production of photographic and liquid crystalline materials [1].

In this study, methyl 4-chloro-5-phenylisoxazole-3-carboxylate (MCPIC) has been synthesized and its monomeric structure studied by DFT(B3LYP)/6-311++G(d,p) calculations. The DFT calculations predicted the existence of three different conformers with small energy differences in the ground state potential energy surface.

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 MCPIC monomer was investigated through *in situ* broadband irradiation using a standard Hg(Xe) lamp as UV-light ($\lambda > 235$ nm) source. The interpretation of the IR spectra of the compound isolated in the different matrices investigated and of those of the resulting photoproducts were supported by theoretical calculations undertaken at the DFT(B3LYP)/6-311++G(d,p) level of theory.

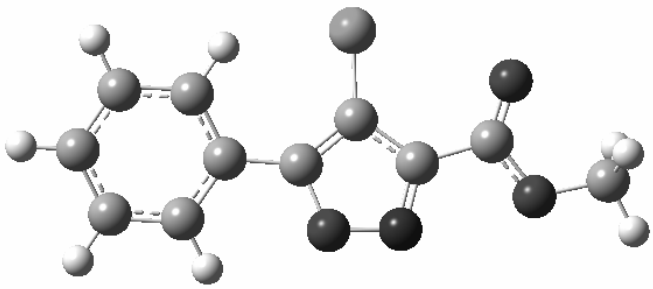

Fig. 1: Structure of the most stable conformer of MCPIC.

[1] S.A. Lang, Jr. and Y-I Lin, in A.R. Katristzky, C.W. Rees, (series Eds.), K.T. Potts (Ed.), Comprehensive Heterocyclic Chemistry, Vol. 6 Part 4B Pergamon, Oxford, 1984 (Chapter 4.16) page 1.

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