Electronically Excited States of the Trifluoroacetic Acid

Pietra Sautchuk Puppi[1*], N. C. Jones[2], S. V. Hoffmann[2], Paulo Limão-Vieira[3], Alessandra Souza Barbosa[1]

[1]*Departamento de Física, Universidade Federal do Paraná, Caixa Postal 19044, 81531-990 Curitiba, Paraná, Brazil.*

[2]*ISA, Department of Physics and Astronomy, Aarhus University, Ny Munkegade 120, DK-8000, Aarhus C, Denmark.*

[3]*Atomic and Molecular Collisions Laboratory, CEFITEC, Department of Physics, Universidade NOVA de Lisboa, 2829-516 Caparica, Portugal*

*email: pietrap@icloud.com

The Trifluoroacetic acid (TFA) has significant importance due to its frequent use in organic chemistry as a solvent for polymers and polymer processes, for both oxidation and reduction reactions and also for numerous acid-catalyzed reactions. In this work, we present a combined theoretical and experimental study on the electronically excited states of the Acetic acid derivative, Trifluoroacetic acid. The experimental absolute cross-sections were obtained employing high-resolution vacuum ultraviolet (VUV) photoabsorption measurements using synchrotron radiation [1], in the gas phase, for photon energies ranging from 4.0 up to 10.8 eV. The main purpose of this work is to perform a comprehensive electronic state spectroscopy investigation of TFA, as well as to provide absolute values for the photoabsorption cross-sections. To this end, we performed excited states calculations using Time-Dependent Density Functional Theory (TDDFT) with the aid of the B3LYP and CAM-B3LYP functional, alongside with the aug-cc-PVTZ basis set, as implemented in the package GAMESS [2]. We also compared the present results for the TFA with the data available from the literature about the parent molecule of Acetic acid [3], in particular, both the similarities and differences between the experimental spectra of these molecules and the present calculations were discussed.

References

1. M. H. Palmer *et al.*, J. Chem. Phys. **142**, 134302 (2015).
2. G.M.J. Barca *et al.*, J. Chem. Phys. **152**, 154102 (2020).
3. P. Limão-Vieira *et al.*, Chem. Phys. **324**, 339 (2006).