

Thermodynamic and UV-Visible Optical Characterization of the Deltic, Squaric and Croconic Cyclic Oxo-carbon Acids

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The croconic acid has been proposed as a contaminant in the sulfuric acid cloud droplets in the Venus clouds and may represent the absorber responsible for the ultraviolet cloud features and the pale-yellow color of the Venus clouds [1]. The influence of the presence of small organic acids in the optical characteristics of the atmospheres [1], its relevance in the description of Earth's global atmospheric chemistry [2] and the use of compounds related to the cyclic oxo-carbon acids as dyes [3], which may be employed as optical sensors, underlines the importance of the precise knowledge of their optical properties. Furthermore, the use of these compounds in a wide range of scientific and technological applications [4-5] emphasizes the need of determining the thermodynamic data of the cyclic oxo-carbon acids required to optimize their production and to investigate their chemical behavior in the presence of different reagents.

Since our current knowledge of the thermodynamic and optical properties of these compounds is relatively poor, a complete thermodynamic and ultraviolet-visible optical characterization of the deltic, squaric and croconic cyclic oxo-carbon acids was carried out using first principles methods employing very demanding calculation parameters [5]. Fig. 1 shows the calculated UV-Vis absorption spectrum of the croconic acid and its reflectivity, optical conductivity and refractive index optical functions [6]. Of these functions only the UV-Vis absorption spectrum is known from experiment and, as it can be appreciated in Fig. 1, the agreement with the computed spectra is very good. Furthermore, the origin of the peaks in the absorption spectra was unveiled by examining the inter-band electronic transitions in these materials.

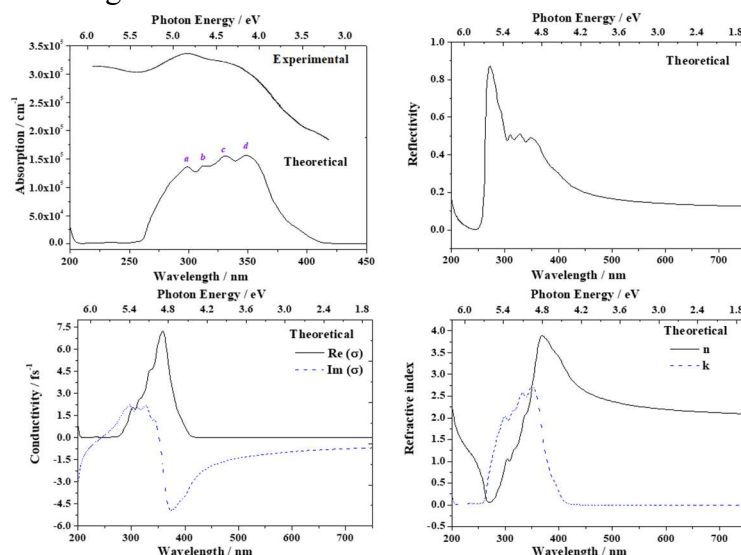


Figure 1: Calculated UV-Vis absorption spectrum and reflectivity, optical conductivity and refractive index optical functions of croconic acid. The computed UV-Vis absorption is compared with the experimental one [1].

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References

- [1] K. K. Hartley, A. R. Woff, L. D. Travis, *Icarus* 1989, 77, 382–390.
- [2] J. Chen, S. Jiang, Y. R. Liu, T. Huang, C. Y. Wang, *et al. RSC Adv.* 2017, 7, 6374–6388.
- [3] C. Encinas, E. Otazo, L. Rivera, S. Miltsova, J. Alonso, *Tetrahedron Lett.* 2002, 43, 8391–8393.
- [4] F. Colmenero, *Mat. Res. Express* 2019, 6, 045610.
- [5] F. Colmenero, R. Escribano, *J. Phys. Chem. A*, under review.
- [6] M. S. Dresselhaus, *Solid State Physics. II. Optical Properties of Solids*. Vol. 6 (MIT Press, New York, 2001).