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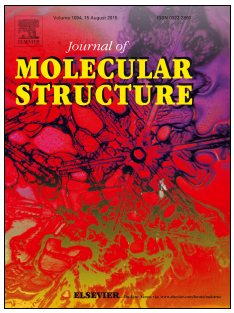

Experimental and theoretical investigations on spectroscopic properties of tropicamide

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Experimental and theoretical investigations on spectroscopic properties of Tropicamide

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Abstract

Spectroscopic properties of tropicamide have been characterized by FT-IR, FT-Raman, NMR and UV-Vis analytical techniques with the help of high level quantum chemical calculations. In addition to gain better insight on structural features of title molecule, some other interesting molecular properties such as potential energy surface, HOMO-LUMO energy, mulliken atomic charge distribution, molecular electrostatic potential energy surfaces and thermo dynamical parameters were calculated. The obtained experimental and theoretical results show an excellent correlation, which gives the structural contribution for the better understanding in the field of spectroscopy.

Keywords

Tropicamide, FT- IR, FT-Raman, NMR, UV-Vis, DFT