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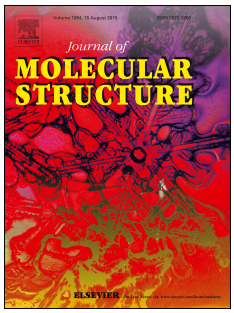

Structural and spectroscopic properties of itraconazole and ketoconazole – Experimental and theoretical studies

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Structural and spectroscopic properties of Itraconazole and Ketoconazole – Experimental and theoretical studies

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Abstract

The paper compares the experimental FT-IR and UV-Vis spectra of itraconazole and ketoconazole with the DFT calculations using four different functionals. The highest conformity of the geometry of the optimized rotamer of itraconazole with the experimental data was obtained by applying the CAM-B3LYP/6-31G(d,p) level of theory whereas the M06L/6-31G(d,p) method was the most suitable for ketoconazole. The best compatibility between the experimental and theoretical UV spectra was observed with the use of CAM-B3LYP/6-31G(d,p) method for both conazoles. The reason for the difference in the UV-Vis spectra of itraconazole and ketoconazole was discussed on the basis of time-dependent DFT and natural bond orbital methods.

Keywords: Itraconazole; Ketoconazole; Density Functional Theory, Infrared spectrum, Ultraviolet-Visible spectrum, Natural Bond Orbital

Highlights

- Experimental FT-IR, UV-Vis spectra of itraconazole and ketoconazole are compared with results of theoretical calculations.
- Spectral properties are estimated by DFT formalism and NBO calculations.

Graphical abstract