VIBRATIONAL SPECTRA OF BERBERINE AND THEIR INTERPRETATION BY MEANS OF DFT QUANTUM-MECHANICAL CALCULATIONS

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S u m m a r y

Experimental vibrational spectra (Raman and infrared absorption) of berberine are obtained at room temperature. The vibrational spectra of berberine are calculated by the DFT method at the B3LYP/6-311++G(d,p) level. Based on the correlation between experimental and calculated data, the vibrational spectrum is interpreted in the frequency range of 800–1700 cm^{-1} in detail. The experimental and calculated spectra of intramolecular vibrations are found to correlate closely.