7-27-2011

Experimental and Theoretical Study of Vibrational Spectra of 3-Nitrofluoranthene [Abstract]

Kefa Karimu Onchoke
Stephen F Austin State University, onchokekk@sfasu.edu

Matthew Parks
Stephen F Austin State University

Experimental and Theoretical Study of Vibrational Spectra of 3-Nitrofluoranthene [Abstract]

The comparative studies of the infrared and Raman spectra of fluoranthene and 3-nitrofluoranthene (3-NF) were made via both FT-IR and density functional theory calculation with a triple ζ Gaussian basis set (B3LYP/6-311 + G(d,p)). The scaled theoretical vibrational frequencies show good agreement to experiment to within ~5 cm^{-1} for frequencies <1800 cm^{-1}. In addition, predictions of the DFT frequencies below 1800 cm^{-1} yielded an overall root mean square (RMS) of ±4.3 and ±27.4 cm^{-1} for fluoranthene and 3-NF, respectively. The vibrational assignments are proposed, with particular emphasis on the nitro group vibrations. This study shows the influence the geometrical distortions of the fluoranthene structure have upon nitro group substitution and provides vibrational spectral data useful for the development of spectroscopy-mutagenicity relationships in nitrated polycyclic aromatic hydrocarbons.