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A DFT Study of Vibrational Spectra and Mutagenicity Predictions of Mononitrated Fluoranthenes
[Abstract]

Predictions of Mononitrated Fluoranthenes The Raman and infrared (IR) spectra of the mononitrated fluoranthenes (1-, 2-, 3-, 7-, and 8-nitrofluoranthene), important environmental pollutants that induce mutagenic/carcinogenic effects upon mammalian and bacterial cells, were studied via density functional theory, using optimized geometries at the B3LYP/6-311+G(d,p) and PBE0/6-311+G(d,p) levels of theory. The predicted harmonic vibrational frequencies were used in normal mode assignments. To validate the spectra, experimental fluoranthene and 3-nitrofluoranthene were used to benchmark the predicted spectra. The scaled harmonic frequencies below 2000 cm^{-1} are in good agreement to experiment to $<5\text{ cm}^{-1}$ and 10 cm^{-1} or better at the B3LYP/6-311+G(d,p) and PBE0/6-311+G(d,p) levels, respectively. The high intensity nitro asymmetric/symmetric stretch modes ($\nu_{\text{asym}}/\nu_{\text{sym}}\text{NO}_2$), $\nu(\text{C}-\text{C})$ and $\nu(\text{C}-\text{H})$ stretch frequencies were then considered, and used in distinguishing nitrofluoranthene isomers. The $\nu_{\text{sym}}(\text{NO}_2)$ frequency shifts are correlated to the observed mutagenic potencies, thus shedding light on their relative reactivity. The observed differential mutagenic-vibrational correlations, and implications of the ν_{NO_2} shifts/biological mutagenic potencies between nitrofluoranthene isomers are then discussed.