2014

A TD-DFT Study of the Absorption Spectra of Mono-Nitrated Fluoranthenes [Abstract]

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The singlet electronic excited state properties of 1-, 2-, 3-, 7-, and 8-nitrofluoranthene (1-, 2-, 3-, 7-, 8-NF) were investigated using the time-dependent density functional method (TD-DFT) at the B3LYP/6-311+G(d,p)//TD-B3LYP/6-311(d,p) level of theory. The simulated and experimental UV/Vis spectra are in good agreement, thus enabling assignments and interpretation of the observed absorption bands. The influence of the nitro group upon electronic spectra, and structure–spectroscopic–mutagenicity correlations are made. The absorption λ_{max} (S_1 excitation energy) for the nitrated fluoranthenes are red-shifted by ~10–30 nm vis-à-vis fluoranthene: with wavelength shifts dependent on the planarity of the nitro group relative to the aryl moiety. The chemical hardness and HOMO–LUMO energy gaps for the nitro-fluoranthenes are predicted in the range 3.5–3.8 eV and follow the order: fluoranthene (3.99 eV) > 7-NF (3.81 eV) > 2-NF (3.72 eV) ≈ 8-NF (3.71 eV) > 1-NF (3.52 eV) > 3-NF (3.50 eV).