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Structure–Mutagenicity Relationships and Energies of 1-, and 2-Nitrotriphenylenes [Abstract]

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The isomers 1- and 2-nitrotriphenylene are present in respirable matter, in combustion and diesel exhaust particulates, and exhibit mutagenic and carcinogenic properties. The structural and electronic properties of triphenylene, 1-, and 2-nitrotriphenylene were investigated with the density functional B3LYP calculations using the 6-311 + G** basis set. The geometrical bond length agreements were noted between the calculated and experimental geometry for triphenylene (TRP), and predictions of the structural data for 1- and 2-nitrotriphenylene are made in the absence of experimental crystal structures. The geometrical distortions of the triphenylene structure upon nitro group substitution, and structural–mutagenicity relationships of this important class of polycyclic aromatic hydrocarbons are discussed. The energy and molecular orbital energies (E_{LUMO}) were also investigated and found to yield predictive electrophilic reactivity of the isomers. The study of the structure-mutagenic relationships of nitrated polycyclic aromatic hydrocarbons (nitro-PAHs) is important in gaining insights into reasons underlying the differential mutagenic potencies of isomers of specific PAHs.