

Thermodynamic Studies of Polycyclic Aromatic Compounds

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Available data for heats of combustion and vapor pressures of polycyclic aromatic compounds will be presented and evaluated. Special attention will be directed toward cases where large strain energies are involved and toward heterocyclic systems.

Electronic Interactions in Paramagnetic Polycyclic Substances

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All odd electron polycyclic substances and some even electron ones are paramagnetic. The paramagnetism permits detailed investigation of electronic interactions by magnetic resonance spectroscopy. The following properties will be discussed: spin distribution, rate of spin migration, spin-spin interactions, and inter-electron correlations.

The phenomena are illustrated by the behavior of hydrocarbon radicals, ketyls, and chelate compounds.

ESR Examination of the Electronic Distribution in Polycyclic Triplets

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The parameters describing the magnetic dipole interaction of the unpaired electrons in a triplet state are easily obtained using randomly oriented samples. The values of D and E are sensitive measures of an averaged distance between the electrons. In the metastable $\pi-\pi^*$ triplets responsible for the phosphorescence of aromatic hydrocarbons, both electrons are delocalized over the π -system. In many ground state triplets one electron may be effectively localized at one atom and serve as a probe of the density of the other electron at that center. Applications are made to determine the effect of substituents on delocalization in nitrenes and methylenes.