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FTIR spectroscopic investigations of internal rotation of nitrosubstituted 1,2-diphenylethanes

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Abstract

Infrared absorption spectra and internal rotation of 1,2-di-(3,4- dinitrophenyl)ethane in crystalline phase, solutions in various temperatures have been investigated. The thermodynamic parameters of the conformational equilibrium have been determined. Quantum chemical ab initio energy calculations are carried out. The obtained data on the free energy, enthalpy and entropy differences of the conformations are discussed in terms of the reaction field model and compared with responsible results for 1,2-di(paranitrophenyl)ethane and 1,2-di(phenyl)ethane. The presence of the compensation effect (enthalpy-entropy compensation) in thermodynamics of conformational equilibria is confirmed.

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Keywords

Conformational equilibrium, Infrared spectra, Internal rotation