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Vibrational spectra and molecular dynamics of 1,2-di--p-XC6H4)ethanes (X=Br, NO2)

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Abstract

Infrared absorption spectra and internal rotation of 1,2-di-(p-XC6H4)ethanes (X=Br, NO2) have been investigated. The magnitude of the barrier to internal rotation of 1,2-di--p-bromophenyl)ethane has been estimated. The analysis of IR spectra of 1,2-di--p-nitrophenyl)ethane in liquid and crystalline states and its solutions has allowed to make conclusion about the presence of the dynamic equilibrium of the trans and gauche conformations. The division of the absorption bands into components and the factor analysis have been used in the interpretation of the IR spectra. The enthalpy and entropy differences of the trans and gauche conformations have been determined and besides these values are discovered to be anomalous large as compared with ones which are usually observed for the conformational equilibria.

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Keywords

Conformational equilibrium, Infrared spectra, Molecular dynamics