Elastic, quasielastic, and inelastic neutron-scattering studies on the charge-transfer hexamethylbenzene-tetracyanoquinodimethane complex.

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Rok wydania

2005

Czasopismo

Journal of Chemical Physics

Numer woluminu

123

Strony

124305-124309

DOI

10.1063/1.2035077

Streszczenie

The 1:1 hexamethylbenzene -tetracyanoquinodimethane complex shows a first-order phase transition at (heating/cooling) with no change of the space group. The neutron-diffraction studies reveal that this transition is related to a freezing of the rotation of methyl groups. The results for enabled precise determination of configuration of complexes. The planes of and molecules from small angle (6°) so that the dicyanomethylene group approaches the molecule to a distance of . The conformation of methyl groups was exactly determined. The quasielastic neutron-scattering spectra can be interpreted in terms of 120° jumps with different activation barrier in low- and high-temperature phases, equal to 3.7 and , respectively. These values are lower than that for neat . The conclusion can be drawn that the methyl groups can reorient more freely in the complex. This conclusion is in agreement with the results of inelastic neutron-scattering studies of low-frequency modes assigned to torsional vibrations of methyl groups. These frequencies are lower than those for neat . The analyzed increase of frequencies of these modes as compared with free molecules can be interpreted as due to formation of unconventional hydrogen bonds which are more pronounced in crystals of neat than in those of . The low-frequency librational modes can be treated as a sensitive measure of unconventional hydrogen bonds formed by the groups.I

Adres publiczny

https://doi.org/10.1063/1.2035077

Strona internetowa wydawcy

https://www.aip.org/

Kolekcja

Naukowa

Język

Angielski

Typ publikacji

Artykuł