

X-ray diffraction, inelastic neutron scattering (INS) and infrared (IR) studies on 2:1 hexamethylbenzene (HMB)-tetracyanoethylene (TCNE) complex.

Autorzy

Andrzej Pawlukoć

Wanda Sawka-Dobrowolska

Grażyna Bator

Lucjan Sobczyk

Eugeniusz Grech

J. Nowicka-Scheibe

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Streszczenie

The structure of the 2:1 hexamethylbenzene (HMB)–tetracyanoethylene (TCNE) complex was determined at 100 K. In the crystalline lattice the molecules of HMB (D) and TCNE (A) are arranged in DDADDADD stacks along the *b*-axis. Based on the red shift of the $\nu(\text{CN})$ IR frequencies the charge transfer (CT) degree (*Z*) was estimated to be equal to 0.14. It is markedly higher than that for the complex of HMB with tetracyanoquinodimethane (TCNQ) for which $Z = 0.06$. The analysis of vibrational modes connected with torsional motion in the low frequency region was performed based on the inelastic neutron scattering (INS) experiments and DFT theoretical calculations. The correlation between $\nu_{\text{exp}}/\nu_{\text{calc}}$ and ν_{calc} shows a deviation of experimental values from calculated ones. It is the higher the lower is the frequency of the analysed mode. The comparison of correlations for neat HMB and its complexes with TCNQ and TCNE suggests that some role in decreasing the barrier to rotation can be played by the charge transfer between D and A molecules.

Słowa kluczowe

CT complex, Hexamethylbenzene, Tetracyanoethylene, Crystal structure, INS, DFT, IR

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