The structure, methyl rotation reflected in inelastic and quasielastic neutron scattering and vibrational spectra of 1,2,3,5-tetramethoxybenzene and its 2:1 complex with 1,2,4,5-tetracyanobenzene.

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Kolekcja

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Streszczenie

X-raydiffractionstudiesshowthatmoleculesofthe1,2,3,5-tetramethoxybenzeneTMOB2·1,2,4,5-tetracyanobenzene complex form¯CCDCCDCC¯columns with the shortdistances between molecular planes of C and D molecules equal to 3.186 Å. The vibrational spectrarecorded by using the inelastic neutron scattering, Raman, IR, and quasielastic neutron scatteringQENStechniques aided by density functional theory calculations for the isolated molecules andthe crystalline state enabled all four inequivalent librational modes, ascribed to the methoxy groups,to be analyzed. A rather good consistency was found between the experimental frequencies andthose calculated for the crystal. The consistency was also achieved between the experimentalstructure of molecules and the theoretically reproduced one. A close similarity of the structures ofthe TMOB molecule isolated and in the complex is taken as a sign of dominating intramolecularinteraction. The QENS spectra contain three Lorentzians of relative intensities of 1:1:2. Thus thetwo most strongly hindered of the four inequivalent methoxy groups in the crystalline lattice arecharacterized by rather similar barrier heights in good agreement with the packing analysis.

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