Structure and vibrational spectra of 1,3,5-trimethoxybenzene.

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Streszczenie

Inelastic neutron scattering infrared and Raman spectra of the crys-talline 1,3,5-trimethoxybenzene were measured and compared with simulated ones by using the Gaussian 98 and DMol3 programs at density functional theory methods. Application of the double numerical plus polarization ba-sis set for the crystalline state within the local density Perdew and Wang (PWC functionals) approximation quite well reproduces the low frequency bands related to the methyl group librational modes, which are very sen-sitive to molecular interactions. Infrared spectra for the crystalline sample and CCl 4 solution show spectacularly the change of low frequency modes by going from the symmetric D 3h molecules in the gas phase to asymmetric ones in the crystal.

Adres publiczny

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