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DFT calculations of 2,6-dimethylpyrazine (26DMP) and its complex with chloranilic acid (CLA): comparison to INS, IR and Raman vibration spectra.

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Streszczenie

The inelastic neutron scattering (INS), infrared and Raman spectra of crystalline 2,6-dimethylpyrazine (26DMP) and its complex with chloranilic acid (26DMP·CLA) were measured. Simultaneously the DFT calculations of the molecular structures and frequencies of the normal vibrations were performed by using various functionals. The INS spectra were simulated in the energy range up to 1200 cm^{-1}, on the basis of the calculated frequencies. A very good conformity was obtained between experimental and calculated data with respect to the structure as well as to frequencies, with exception, however, of the CH_3 torsional modes. The structural analysis based on the deviation from the sum of the van der Waals radii showed that the packing of the methyl groups in the 26DMP·CLA complex was markedly stronger than that in the neat 26DMP. However, the DFT calculations overestimated the role of this effect that may be due to a limitation of the applied methods. In addition the anharmonicity of the rotational potential led to the librational energies different from those obtained using a harmonic potential.

Słowa kluczowe

molecule, 6-Dimethylpyrazine, 6-Dimethylpyrazine–chloranilic acid complex, DFT calculation, INS, IR, Raman

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