The structure and vibrational spectra of the 2,5-dimethylpyrazine (2,5-DMP) 1: 1 adduct with 2,5-dichloro-3,6-dihydroxy-p-benzoquinone (CLA).

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Streszczenie

The complexation of 2,5-dimethylpyrazine (2,5-DMP) with 2,5-dichloro-3,6-dihydroxy-p-benzoquinone (CLA) leads to the formation of the hydrogen bonded OH···N infinite chains without any proton transfer. In the high and medium frequency region of the IR spectra a characteristic Hadži's trio with maxima at ca. 2400, 1800 and 1150 cm−1 is observed. The infrared, Raman and inelastic neutron scattering (INS) spectra are compared with those calculated by using the DFT methods applied to the crystalline state. The optimization of the structure by using this theoretical approach is also performed. Very good conformity of the experimental and theoretical structures is visible. The reproduction of vibrational spectra is also good except for the low frequency bands related to the CH3 torsional modes. One gets relatively good agreement by using PWC(dnp) approach. Applications of other theoretical models leads to much higher values of CH3 torsional frequency.

Słowa kluczowe

hydrogen bonds, molecule, 5-dimethylpyrazine, Chloranilic acid, Hadži's trio, Torsional modes of methyl groups, Inelastic neutron scattering

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