

INS spectroscopic study of the 1:1 tetramethylpyrazine (TMP) squaric acid (H₂SQ) complex.

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Streszczenie

Two tunneling bands in INS spectra are resolved at 1.55 and 4.20 μeV representing one methyl group each. Estimation based on the librational modes shows that two other methyl groups are characterized by the tunnel splittings located at 0.13 and 0.05 μeV thus overlapped by the elastic line. Corresponding librational modes in the vibrational density of states are consistent with pure $\cos(3\phi)$ rotational potentials. The INS spectra of the TMP · H₂SQ complex well agree with the X-ray diffraction structure at 100 K which shows four methyl groups of different environment strongly affected by unconventional C–H ... O hydrogen bonds. There is an interplay of the charge transfer and inter-molecular interaction in shaping the rotational potential.

Słowa kluczowe

CT complex, Squaric acid, Tetramethylpyrazine, INS, IR, Raman

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