X-ray and neutron diffraction, IR and INS spectroscopic and DFT theoretical studies on the tetramethylpyrazine-1,2,4,5-tetracyanobenzene complex.

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Streszczenie

Elastic and inelastic neutron scattering as well as IR spectroscopic and DFT theoretical studies on tetramethylpyrazine (TMP)–1,2,4,5-tetracyanobenzene (TCNB) complex have shown that decisive in crystal packing are C–H⋯N hydrogen bonds, although in the H-bonding scale they should be treated as rather weak. In contrast to the other charge transfer (CT) complexes, like this in TCNB–durene, there is no alternation of molecules in stacking. INS spectra have shown a marked decrease of the CH_3 torsional frequencies that can be discussed in terms of the charge transfer from TMP toward TCNB counterpart. The role of such a phenomenon was confirmed by calculations of frequencies for ionized molecule of TMP which show a giant effect of ionization on the rotational potential of CH_3 groups. Theoretical analyses of various orientations of interacting molecules have shown that a deepest energy minimum is reached for perpendicular arrangement with C–H⋯N hydrogen bonding of the H⋯N distance equal to 2.31 Å (experimental value 2.37 Å).

Słowa kluczowe

CT complex, Tetramethylpyrazine, atom, molecule, lanthanides, 5-Tetracyanobenzene, Inelastic neutron scattering, IR, DFT theoretical study

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