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H-bonded complexes between pyrazines containing methyl groups and strong proton donors: structure and dynamics.

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Streszczenie

Pyrazine belongs to an interesting class of heterocyclic compounds of moderate basicity that are capable of forming various molecular complexes of intriguing architecture, particularly from the crystallo-chemical point of view. The presence of methyl (-CH_3) groups in the pyrazine molecule is of interest to researchers because of the effect of the charge transfer phenomenon on the rotational barrier of the -CH_3 group. In the present review we analyzed the structures of various molecular complexes containing proton donors such as *p*-nitrophenol, picric acid, squaric acid, triiodo hydride, nitric acid and, in particular, chloranilic and bromanilic acids. The interactions, mainly via hydrogen bonds, lead to a variety of crystal structures mostly due to proton transfer to the nitrogen atoms in pyrazine. In this review, the structures of complexes and their crystal-lattice packing studied using X-ray diffraction are discussed. The variety of hydrogen bonds in the complexes studied is best reflected in their infrared absorption spectra. In many cases the absorption continua typical of the strong hydrogen bonds are present. Inelastic neutron scattering (INS) spectra were used to analyze dynamics. The results of tunneling splitting ascribed to methyl groups were also found interesting. This aspect is given focus in this work. One of the main observations from these studies was that methyl groups in the solid state of the molecular complexes rotated more freely than those in pure methyl derivatives of pyrazine.

Słowa kluczowe

molecular complexes, pyrazine, organic acid, proton donor, proton acceptor, methyl group dynamics, infrared, inelastic neutron scattering, hydrogen bond, proton transfer

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