The (2:1) complex of picric acid with tetramethylpyrazine: the structure, IR spectra and tunnel splitting of methyl groups.

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Streszczenie

The crystal structure of 2:1 picric acid (PAH) with tetramethylpyrazine (TMP) was determined by using X-ray diffraction studies. Two equivalent $^{+}NH\cdots O^{-}$ hydrogen bonds are formed with the length of 2.601 Å (calculated 2.640 Å). In the IR spectra very broad doublet at *ca*. 2000 and 2400 cm^{-1} is observed, which can be interpreted as due to symmetric and asymmetric ^{+}NH vibrations. In neutron backscattering two tunnel splittings are observed, in agreement with the symmetry of 2:1 assemblies. At 4 K the tunnel peaks are located at 3.17 and 4.24 μeV.

Słowa kluczowe

Tetramethylpyrazine–picric acid complex, Hydrogen bond Infra-red spectra, Tunneling splitting

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