Assembly of protonated tetramethylpyrazine (TMP) in triiodide. Vibrational spectra and DFT simulations.

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Streszczenie

In the complex of tetramethylpyrazine (TMP) with HI3 two protonated molecules of TMP form the assembly of composition (TMP×H+)2TMP(I3 -)2. The X-ray structure, determined at 100 K, shows the +N-H×××N hydrogen bonds markedly shorter than those found previously [13] at room temperature (2.828 ni s. 2.894 A). The DFT calculations for isolated cation yield the value of 3.038 capital A, ring that reflects the soft ness of the hydroen bond potential. The calculations of vibrational frequencies for crystalline state reflect very well the IR spectra. This relates particularly to the ni (NH+) mode. A remark able discrepancy is observed when calculations are performed for isolated assemblies.

Słowa kluczowe

protonated tetramethylpyrazine, complexation, vibrational spectra, DFT calculations