The ifluence of steric and polar effects on hydrogen bonding in 2(N,N-diethylamino)-methyl)-4-NO_2-phenols.

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Streszczenie

Two crystal structures consisting of 2-(N,N-diethylamino)-methyl-4-NO3-Phenol molecules were determined. In the triclinic crystals (with a = 9.527(2) A, h = I 1.268{3) A, c = I 1.408(3)A, c~ = 87.80(3) ~ [3 = 69.62(3) ~ "y = 81.82(3) ~ z = 4, space group P/) asymmetric cyclic dimers were found, formed by two nonequivalent O ""H.-N + hydrogen bonds of 2.614(3) and 2.660(3) ,~ len.,,ths. In the complex of 2-(N,N-diethylamino)-methvl-4-NO~-phenol with 4-NO2-phenol(orthorhombiccrystalswitha = 20.732(4) A,h = 16.618(2) A, c = 10.452(2)A, Z = 8, space group Phca) an intermolecular O ".H-O (2.525(2) A) hydrogen bond between 4-NO2-phenol and zwitterionic 2-(N,N-diethylamino)-methyl-4-NO2-phenol ,.,,'as found. In the latter molecule the intramolecuiar O-"-H-N + (2.760(2) ,,~) bridge is formed. The zwitterionic molecules form chains along the crystallographic b axis by NH .... O (3. 105(2) ,~) hydrogen bridges. The N-H + groups participate in bifurcated hydrogen bonds. The influence of the steric strain caused by N-alkyl chains and polar interactions of the NO2 group on the character of the hydrogen bond and the structure of cyclic dimers is discussed. The IR and UV spectra determined show the full agreement in description of the hydrogen bonding schemes, simultaneously demonstrating a drastic rearrangement of these schemes upon going to CCla solutions.

Słowa kluczowe

Hydrogen bond, crystal structure, FT-IR spectra, 2-(N, N-diethylamino)-methyl-4-NOzphenol, cyclic dimers

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