Anomalous strengthening of the intramolecular hydrogen bond by steric repulsion.

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Streszczenie

The crystal structures of two ortho-aminomethylphenols, the 4,5-dimethyl- and 3,5,6-trimethyl-2(*N*,*N*-dimethylaminomethyl) phenols, were determined. The stronger intramolecular hydrogen bond was found in the compound with the higher number of methyl substituents. This result was supported by IR spectra. The atomic charge distribution calculated by the MNDO-PM3 method predicts higher strengths of the hydrogen bond in 4,5-dimethyl-2(*N*,*N*-dimethylaminomethyl) phenol molecules. Both theoretical calculations and crystallographic results explain the observed effects with reference to the steric interaction of the ortho methyl group which squeezes the O□Htctdot;N hydrogen bridge.

Słowa kluczowe

Hydrogen bonding, Ortho-aminophenols, Steric repulsion, X-ray crystallography

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