An approach to estimate the energy of the intramolecular hydrogen bond.

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Streszczenie

The problem of the energy of the intramolecular hydrogen bond is widely discussed in the literature, but it has not found an unequivocal univocal solution yet. The partition of the energy of the intramolecular hydrogen bond (ΔE_T) in chloro-derivatives of 2-(*N*-dimethylaminomethyl)-phenols calculated by ab initio and DFT methods was proposed and `pure' ΔE_T values were estimated. These values correlate well with those of r(H⋯N) and electron density $\rho(r)$ obtained by the AIM method.

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