

Conjugation in hydrogen-bonded systems

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Analysis of the electron density distribution in clusters composed of hydrogen fluoride, water, and ammonia molecules, especially within the hydrogen-bond domains, reveals the existence of both σ - and π -binding between molecules. The σ -kind density distribution determines the mutual orientation of molecules. A π -system may be delocalized conjugated, which provides additional stabilization of molecular clusters. In those clusters where the sequence of hydrogen bonds is not planar, a peculiar kind of π -conjugation exists. HF anion and H₅O₂ cation are characterized by quasi-triple bonds between the electronegative atoms. The most long-lived species stabilized by delocalized π -binding are rings and open or closed hoops composed of fused rings. It is conjugated π -system that determines cooperativity phenomenon.

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