

Triple Trouble: Hydrogen Bonding at the C≡N Bond

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Fourier-Transform Infrared (FTIR) spectroscopy, particularly in combination with supersonic jet cooling, offers precise insight into hydrogen bonds (HBs) in small molecular clusters, providing valuable benchmarks for theory and minimal models of binary mixture behavior.

Nitriles play key roles in synthetic and polymer chemistry –as oxidized and essential building blocks or as aprotic solvents such as acetonitrile (MeCN). By forming weak hydrogen bonds, nitriles serve as molecular reporters of how local chemical environments shape noncovalent interactions. Due to their low nitrogen basicity, linear HBs to the lone pair are energetically comparable to side-on interactions at the π -system, where dispersion forces contribute to the binding energy.

Besides acetonitrile^[1], this study investigates pivalonitrile (*t*-BuCN) and *tert*-butyl isocyanide (*t*-BuNC) as HB acceptors, with water (H₂O), methanol (MeOH) and *tert*-butyl alcohol (*t*-BuOH) as donors. Notably, the hydrogen bonds to pivalonitrile and *tert*-butyl isocyanide were examined in supersonic jet expansions for the first time.

Beyond hetero-dimers, larger hydrogen-bonded clusters such as trimers and tetramers were observed, offering insight into non-additive interactions and microsolvation. Mixed tetramers, in particular, serve as the smallest systems capable of modeling macroscopic miscibility.

[1] M. Bödecker, D. Mihrin, M. A. Suhm, R. Wugt Larsen, *J. Phys.Chem. A* **2024**, 128, 7124–7136.

Keywords

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