

H \cdots H Dihydrogen Bonding in Alkylsilane–Fluoromethane Complexes Observed by Microwave Spectroscopy

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Dihydrogen bonds (DHBs) are non-covalent interactions characterized by the X–H δ^+ ... δ^- H–Y motif, where X is an electronegative atom and Y an electropositive center (e.g. transition metals). In this work, we investigate DHB formation in clusters of multifluoromethanes (acting as proton donors) with trimethylsilane (TMS) and triethylsilane (TES) as hydrogen bond acceptors. Using chirped-pulse Fourier transform microwave (CP-FTMW) spectroscopy, we unambiguously identified DHBs via rotational transitions. Notably, spectral splittings reveal quantum tunneling dynamics in these complexes, indicating coherent interconversion between degenerate configurations.

Keywords

dihydrogen bonds · cluster chemistry · rotational spectra · quantum tunneling · silane

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