AXIAL AND EQUATORIAL HYDROGEN BONDS IN THIANE-HCl

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Despite the interest concerning hydrogen bond complexes in the gas phase
there have been no previous spectroscopic investigations of the dimers which are presumed to have both axial and equatorial conformations. The thiane-HCl complex falls into this type. Microwave spectroscopy provides
the advantage that the two forms can be separately studied since axial and equatorial forms exhibit individual rotational spectra. The proton acceptor molecule thiane carries two inequivalent non-bonding pairs at the sulfur atom and the conventional electronic models predict axial and
equatorial configurations with the electrophilic hydrogen atom of HCl pointing to the nucleophilic region of the non-bonding electron pairs.
Axial and equatorial conformers of thiane-HCl have been identified and characterized using molecular beam Fourier transform microwave spectroscopy. The spectra of several isotopic species have been analyzed. The determined rotational, centrifugal distortion and nuclear quadrupole coupling constants have been found to be consistent with a C_s symmetry for both forms. The structure of the hydrogen bond has been obtained from these spectroscopic constants.