

THE CHALCOGEN-BONDED COMPLEX $\text{H}_3\text{N}\cdots\text{S}=\text{C}=\text{S}$ CHARACTERIZED BY CHIRPED-PULSE BROADBAND MICROWAVE SPECTROSCOPY

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Ground-state rotational spectra were observed for a complex of ammonia and carbon disulphide in the 2.0-18.0 GHz frequency range by Chirped Pulse Fourier Transform Microwave Spectroscopy. The complex was generated through supersonic expansion of a dilute mixture of NH_3 (1%) and CS_2 (1%) in argon. Ten symmetric-top and four asymmetric-top isotopologues of $\text{H}_3\text{N}\cdots\text{CS}_2$ were isolated while using samples either in natural isotopic abundance or with isotopically enriched $^{15}\text{NH}_3$ or ND_3 . The complex has C_{3v} symmetry, with the connectivity of the atoms being $\text{H}_3\text{N}\cdots\text{S}=\text{C}=\text{S}$, thereby establishing that the non-covalent interaction is a chalcogen bond involving the non-bonding electron pair of NH_3 as the nucleophile and the axial region of one of the S atoms of CS_2 as the electrophile. It is assumed that the subunit geometries are unchanged upon complex formation which is consistent with small values determined for the intermolecular force constant ($k\sigma$). A simple model was used to account for the contribution of the subunit angular oscillations to the zero-point motions and thus obtain the intermolecular bond length, $r(\text{N}\cdots\text{S})$.