

INTERNAL ROTATION IN $\text{CF}_3\text{I} \cdots \text{NH}_3$ AND $\text{CF}_3\text{I} \cdots \text{N}(\text{CH}_3)_3$ PROBED BY CP-FTMW SPECTROSCOPY

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The pure rotational spectra of $\text{CF}_3\text{I} \cdots \text{NH}_3$ and $\text{CF}_3\text{I} \cdots \text{N}(\text{CH}_3)_3$ have been measured by chirped-pulse, Fourier transform microwave (CP-FTMW) spectroscopy between 7 and 18.5 GHz. Both molecules are generated by supersonic expansion of a gas sample containing a small percentage of each precursor in a balance of argon. The spectra of both complexes are consistent with C_{3v} prolate symmetric top structures. The observed spectrum of $\text{CF}_3\text{I} \cdots \text{NH}_3$ displays evidence for internal rotation of NH_3 about the principal axis. More than one hundred transitions of $\text{CF}_3\text{I} \cdots \text{NH}_3$ have been assigned to the internal rotor A state allowing rotational, centrifugal distortion constants and a nuclear quadrupole coupling constant for the iodine atom to be determined for this state. Measurements performed using a Balle-Flygare FTMW spectrometer further allow determination of a nuclear quadrupole coupling constant for the ^{14}N nucleus. Many transitions in the spectrum of the $\text{CF}_3\text{I} \cdots ^{15}\text{NH}_3$ isotopologue have also been measured and the length of the halogen bond between the iodine and nitrogen atoms has been determined. Measurements of hyperfine components in nine different $J'' \leftarrow J'$ transitions of $\text{CF}_3\text{I} \cdots \text{N}(\text{CH}_3)_3$ have allowed assignment of the spectrum of this complex to determine rotational, centrifugal distortion and nuclear quadrupole coupling constants.