SOME EFFECTS OF SUCCESSIVE FLUORINATION ON 1-IODOPROPANE

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Fourier transform radiofrequency and microwave spectroscopies have been used to record the pure rotational spectra of 1-iodo-3,3,3-trifluoropropane (I3FP) and 1-iodo-2,2,3,3,3-pentafluoropropane (I5FP). In both cases the compound of interest was seeded in a supersonic expansion of argon gas issued from a pulsed solenoid valve. Several hundred transitions have been recorded for both species. Using the same instrumentation we have also remeasured several rotational transitions for 1-iodopropane for which gauche and trans conformers are visible; previous workers have shown that the gauche conformer of 1-iodopropane is the most stable. The substitution of three fluorines for the hydrogens on C_3 of 1-iodopropane has the effect of locking the CCCI dihedral angle into the trans conformer for the fluorinated species in our experiments. Further observations have shown that the largest component of the dipole moment lies along the a-axis for trans-1-iodopropane, but lies along the b-axis for trans-15FP, switching back along the a-axis for trans-I3FP (but presumeably in the opposite direction than in 1-iodopropane). Spectroscopic constants will be presented and discussed.