ANALYSIS OF THE ROTATIONAL SPECTRA OF 2,3,4,5,6-PENTAFLUOROTOLUENE AND 1-CHLORO-2,3,4,5,6-PENTAFLUOROBENZENE

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The microwave spectra of two substituted pentafluorobenzenes have been obtained. 2,3,4,5,6-Pentafluorotoluene was measured using the FTMW spectrometer at Eastern Illinois University and the chirped-pulse FTMW spectrometer at University of North Texas. The heavy atom structure has been obtained from the assigned ^{13}C transitions and is in reasonable agreement with *ab initio* calculations at the MP2/6-311++G(2d, 2p) level. The ground state rotational constants are $A = 1036.61253(10)$ MHz, $B = 1030.94126(10)$ MHz, and $C = 516.92062(9)$ MHz, and the single dipole moment component is $\mu_b = 1.98(17)$ D. Very small splittings for many of the assigned transitions and multiple, as yet unassigned, lines were presumably due to excited torsional states of the methyl group. In a related study, the microwave spectrum of 1-chloro-2,3,4,5,6-pentafluorobenzene was obtained for both the ^{35}Cl and the ^{37}Cl isotopologues using the chirped-pulse microwave spectrometer at University of Virginia. The preliminary ground state rotational constants for this compound are $A = 1028.5403(14)$ MHz, $B = 751.8198(3)$ MHz and $C = 434.3533(4)$ MHz for ^{35}Cl and $A = 1028.5435(7)$ MHz, $B = 734.4786(2)$ MHz and $C = 428.5082(2)$ MHz for ^{37}Cl. Initial fits of the nuclear quadrupole coupling constants give $\chi_{aa} = -79.512(15)$ MHz, $\chi_{bb} = 43.593(8)$ MHz, $\chi_{cc} = 35.92(2)$ MHz for the ^{35}Cl species and $\chi_{aa} = -62.68(2)$ MHz, $\chi_{bb} = 34.38(4)$ MHz, $\chi_{cc} = 28.29(17)$ MHz for the ^{37}Cl species. These results will be compared with pentafluorotoluene to observe the effects on the structure of the benzene ring when substituting a chlorine atom for a methyl group.