

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  $^{13}\text{C}$  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  $^{35}\text{Cl}$  and the  $^{37}\text{Cl}$  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  $^{35}\text{Cl}$  and  $A = 1028.5435(7)$  MHz,  $B = 734.4786(2)$  MHz and  $C = 428.5082(2)$  MHz for  $^{37}\text{Cl}$ . 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  $^{35}\text{Cl}$  species and  $\chi_{aa} = -62.68(2)$  MHz,  $\chi_{bb} = 34.38(4)$  MHz,  $\chi_{cc} = 28.29(17)$  MHz for the  $^{37}\text{Cl}$  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.