MICROWAVE SPECTRA AND MOLECULAR GEOMETRIES OF BENZONITRILE AND PENTAFLUOROBENZONITRILE

MAHDI KAMAEE, JENNIFER VAN WIJNGAARDEN, Department of Chemistry, University of Manitoba, Winnipeg, MB, Canada.

The ground state rotational spectra of benzonitrile (BN) and pentafluorobenzonitrile (PFBN) were investigated using Balle-Flygare Fourier transform microwave (FTMW) spectroscopy in the region between 5 and 25 GHz. In addition to the parent species, transitions due to the five $^{13}$C isotopologues were measured in natural abundance and used to calculate relevant geometric parameters of the ring backbone of the two compounds. The experimental results compare well with the equilibrium structure determined via ab initio theory (MP2/6-311++G(2d,2p)). To better understand the effect of fluorination on the ring moiety, the electronic environments around the nitrogen atom in both species were compared through a Townes-Dailey-type analysis of the observed $^{14}$N quadrupole hyperfine structure.