MILLIMETER/SUB-MILLIMETER SPECTROSCOPY OF CrCN ($X^6\Sigma^+$): A PREFERENCE FOR THE LINEAR CYANIDE STRUCTURE

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The pure rotational spectrum of CrCN has been recorded in the frequency range 450-530 GHz. This work is the first spectroscopic study of this molecule. Ten transitions of this radical, which was created by reacting chromium vapor with cyanogen gas, were recorded. The two isotopomers ^{52}CrCN and ^{53}CrCN have been observed in their natural abundance 9:1, and substitution of ^{13}C is currently underway. The spectrum clearly indicates that the electronic ground state is X $^6\Sigma^+$. Transitions arising from the excited v_2 bending mode were measured up to (05^50). The bending modes show *l*-type doubling in v_2 = 1 and v_2 = 2. The vibrational progression is extremely regular, indicating a rigid structure. While many sextets are present in the spectra, they are all accounted for by isotopomers and vibrational states. Therefore, we conclude that only one structure is present in our cell, that of the linear CrCN species. The data were analyzed using a Hund case (b) Hamiltonian and rotational, spin-spin, and spin-rotation constants were determined. Trends in 3d transition metal cyanide bonding will be discussed.