Microwave spectrum and geometry of cyanogen N-oxide, NCCNO

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The microwave spectrum of cyanogen N-oxide (NCCNO) has been measured using a new pulsed jet cavity Fourier transform microwave spectrometer, which incorporates automated frequency scanning. The sample was synthesized by gas phase thermolysis of dicyanofuroxan at 550°C[c], and subsequently diluted to ∼ 1 % in the Ne backing gas. The spectrum is that of a linear top; it is complicated by hyperfine splittings due to the two ^{14}N nuclei. Several isotopomers have been observed in natural abundance, and accurate rotational, centrifugal distortion and ^{14}N nuclear quadrupole coupling constants have been obtained. Several geometries (r_0, r_s, $r_{I,\varepsilon}$) have been determined.
Several molecules related to NCCNO have been found to exhibit quasi-linearity to a greater or lesser extent. These include HCNO, NCNCS, and NCNCO. It was thus conceivable, that NCCNO also might exhibit effects of quasi-linearity. To resolve the issue, the substitution geometry and the ^{14}N nuclear quadrupole coupling constants have been used to compare NCCNO to related molecules. To date the results indicate NCCNO to be truly linear. However, no conclusive answer is possible, since data on excited vibrational states are not available.

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