THE ROTATIONAL SPECTRUM AND NUCLEAR QUADRUPOLE HYPERFINE STRUCTURE OF CO_2-N_2O

HELEN O. LEUNG, *Department of Chemistry, Mount Holyoke College, South Hadley, MA 01075*.

The rotational spectrum of $\mathrm{CO_2}$-$\mathrm{N_2O}$ has been recorded in the 7-19 GHz region using a pulsed molecular beam, Fourier transform microwave spectrometer of the Balle-Flygare type. Our work was facilitated by the spectroscopic constants obtained in an infrared study. [a] The hyperfine structure due to the two quadrupolar ^{14}N nuclei in the 24 transitions (9 a type and 15 b type) have been analyzed using the Watson S-reduced Hamiltonian with the inclusion of hyperfine interactions to yield rotational constants, centrifugal distortion constants, and the diagonal components of the nuclear quadrupole coupling tensor for each nitrogen nucleus. The rotational constants are consistent with a planar structure with the centers of mass of the subunits separated by 3.472 Å. Because of the planarity of the complex, the angles formed by each subunit to the line connecting the centers of mass (R) cannot be uniquely determined. However, if the structure is assumed to be similar to the slipped parallel structures of the isoelectronic $\mathrm{CO_2}$ dimer and $\mathrm{N_2O}$ dimer, then the angle between each subunit and R is about $56°$. χ_{bb} for each nitrogen nucleus indicates that the angle between the b-axis of the complex and the $\mathrm{N_2O}$ molecular axis ($cos^{-1}\sqrt{\langle cos^2\theta_b\rangle}$) is approximately $40°$.

[a] C. Dutton, A. Sazonov, and R. A. Beaudet, The 51st Ohio State University International Symposium on Molecular Spectroscopy, Talk FB08 (1996).