THE STRUCTURE OF CO$_2$-N$_2$O DETERMINED BY FOURIER TRANSFORM MICROWAVE SPECTROSCOPY OF THE $^{15}$N$^{14}$NO-CONTAINING ISOTOPOMER

MARK D. MARSHALL, Department of Chemistry-2243, Amherst College, P.O. Box 5000, Amherst, MA 01002-5000; and HELEN O. LEUNG, Department of Chemistry, Mount Holyoke College, South Hadley, MA 01075-6407.

In both the infrared $^a$ and previous microwave $^b$ studies of the van der Waals molecule CO$_2$—N$_2$O, it was impossible to resolve experimentally the structural ambiguity concerning the orientation of the N$_2$O subunit in this approximately slipped parallel complex. Isotopic substitution of the outer nitrogen in the N$_2$O results in a microwave spectrum that is consistent with a structure in which the terminal oxygen of the N$_2$O is closer to the central carbon of the CO$_2$. Substitution coordinates derived from Kraitchman’s equations support this conclusion. This experimentally determined structure is in agreement with the conclusion reached on the basis of $ab$ $initio$ results used in conjunction with the earlier infrared work.$^a$