ROTATIONAL SPECTRUM OF THE CO_2–CO_2–N_2O TRIMER

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The rotational spectrum of a trimer containing CO_2 and N_2O has been assigned using a pulsed supersonic nozzle Fourier transform microwave spectrometer. 43 transitions of the normal species have been fit to a Watson A-reduction Hamiltonian to give the following constants: $A = 1597.4630(29)\mathrm{MHz}, B = 1232.9673(15)\mathrm{MHz}, C = 831.1002(11)\mathrm{MHz}, \Delta_J = 2.610(33)\mathrm{kHz}, \Delta_{JK} = -3.63(14)\mathrm{kHz}, \Delta_K = 7.30(36)\mathrm{kHz}, \delta_J = 0.830(15)\mathrm{kHz}, \mathrm{and}\ \delta_K = 0.71(10)\mathrm{kHz}$. These constants are consistent with predicted spectra of both CO_2–CO_2–N_2O and CO_2–N_2O–N_2O, but dipole moment data and preliminary isotopic work indicate that the observed spectrum probably belongs to the first species. The structure is believed to be barrel-like, with the three monomer units roughly parallel to each other. Theoretical modeling of the complex, including atom-atom electrostatic, dispersion and repulsion terms, gives minimum energy forms consistent with the observed rotational constants.