ROTATIONAL SPECTRUM OF THE CO_2–CO_2–OCS TRIMER

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The rotational spectrum of the CO_2–CO_2–OCS trimer has been observed for the first time by pulsed supersonic nozzle Fourier-transform microwave spectroscopy. 52 observed transitions for the normal species were fit to a Watson A-reduction Hamiltonian to obtain the following spectroscopic constants: $A = 1299.1386(4)\mathrm{MHz}, B = 973.7411(3)\mathrm{MHz}, C = 648.6719(3)\mathrm{MHz}, \Delta_J = 1.270(5)\mathrm{kHz}, \Delta_{JK} = 2.41(2)\mathrm{kHz}, \delta_J = 0.336(2)\mathrm{kHz}, \delta_K = 1.95(1)\mathrm{kHz}$.

Measurements of the rotational spectra of a further eight isotopic species are consistent with a non-planar, barrel-like structure for the trimer which aligns the three monomer axes roughly parallel to one another. An analysis of the spectroscopic data will be presented and compared with results obtained from theoretical modeling of this system using atom-atom parameters.