CARBON DIOXIDE CLUSTERS: (CO$_2$)$_6$ TO (CO$_2$)$_{13}$

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We recently reported assignments of specific infrared bands in the CO$_2$ $\nu_3$ region (\(\sim 2350 \text{ cm}^{-1}\)) to (CO$_2$)$_6$, (CO$_2$)$_7$, (CO$_2$)$_9$, (CO$_2$)$_{10}$, (CO$_2$)$_{11}$, (CO$_2$)$_{12}$, and (CO$_2$)$_{13}$. Spectra are obtained by direct absorption using a rapid-scan tuneable diode laser spectrometer to probe a pulsed supersonic slit-jet expansion and assignments are facilitated by recent calculations of Takeuchi based on the Murthy potential. (CO$_2$)$_6$ is a symmetric top with $S_6$ point group symmetry which can be thought of as a stack of two planar cyclic trimers. (CO$_2$)$_{13}$ is also an $S_6$ symmetric top, and consists of a single CO$_2$ monomer surrounded by an slightly distorted icosahedral cage. The remaining clusters are asymmetric tops without symmetry.

Here we report additional CO$_2$ cluster results. Calculations based on the SAPT-s potential indicate that the structure of (CO$_2$)$_{10}$ may be slightly different from that given by Takeuchi/Murthy. An additional band is observed for each of (CO$_2$)$_{13}$ and (CO$_2$)$_{10}$. A feature observed at 2378.2 cm$^{-1}$ is assigned as a (CO$_2$)$_6$ parallel combination band involving the sum of a fundamental and a low-lying intermolecular vibration. Most significantly, two bands are assigned to a second isomer of (CO$_2$)$_6$. This is also a symmetric top, but now with $S_4$ symmetry. The two symmetric hexamer isomers observed spectroscopically correspond well with the lowest energy structures given by both the SAPT-s and Murthy intermolecular potentials.

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