CARBON DIOXIDE CLUSTERS: $(CO_2)_6$ TO $(CO_2)_{13}$

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We recenty reported[a] assignments of specific infrared bands in the CO_2 ν_3 region ($\sim$2350 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.[b] $(CO_2)_6$ 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[c] 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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[a] J. Norooz Oliaee, M. Dehgany, N. Moazzen-Ahmadi, and A.R.W. McKellar, *Phys. Chem. Chem. Phys.* **13**, 1297 (2011).

[b] H. Takeuchi, *J. Phys. Chem. A* **107**, 5703 (2008); C.S. Murthy, S.F. O'Shea, and I.R. McDonald, *Mol. Phys.* **50**, 531 (1983).

[c] R. Bukowski, J. Sadlej, B. Jeziorski, P. Jankowski, K. Szalewicz, S.A. Kucharski, H.L. Williams, and B.M. Rice, *J. Chem. Phys.* **110**, 3785 (1999).