HIGH RESOLUTION SPECTRA OF CARBON DIOXIDE CLUSTERS IN THE ν_3 BAND REGION

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There is widespread interest in carbon dioxide clusters from a variety of experimental and theoretical perspectives. But in terms of high resolution spectroscopy, the only definitive information concerns $(CO_2)_2$ and $(CO_2)_3$. The dimer has a planar slipped parallel geometry with C_{2h} symmetry.^{*a*} Two isomers are known for the trimer: a planar cyclic form with C_{3h} symmetry.^{*b*} and a sort of "barrel-shaped" form with C_2 symmetry.^{*c*}

Here we analyze two new bands in the CO₂ ν_3 region. The first is a dimer combination band near 2382 cm⁻¹ whose assignment raises interesting questions about the intermolecular vibrations of (CO₂)₂.^d The second band is a trimer band near 2370 cm⁻¹ which is very similar to one we observed previously near 2364 cm⁻¹.^e We assign it to a combination involving another out-of-plane vibration of the cyclic trimer. In addition to these newly assigned bands, we also discuss a number of clear and (mostly) well-resolved bands which apparently must belong to (CO₂)_N clusters with N in the range 6 ~ 15. Although they cannot be precisely assigned at this time, these bands offer intriguing future prospects for learning more about the structures and vibrational dynamics of CO₂ clusters in a challenging and important size range.

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