

WEAKLY BOUND CLUSTERS OF ATMOSPHERIC MOLECULES: INFRARED SPECTRA AND STRUCTURAL CALCULATIONS OF $(\text{CO}_2)_n\text{-(CO)}_m\text{-(N}_2)_p$, $(n,m,p) = (2,1,0), (2,0,1), (1,2,0), (1,0,2), (1,1,1), (1,3,0), (1,0,3), (1,2,1), (1,1,2)$

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Structural calculations and high-resolution infrared spectra are reported for trimers and tetramers containing CO_2 together with CO and/or N_2 . Among the 9 clusters studied here, only $(\text{CO}_2)_2\text{-CO}$ was previously observed by high-resolution spectroscopy. The spectra, which occur in the region of the ν_3 fundamental of CO_2 ($\sim 2350\text{ cm}^{-1}$), were recorded using a tunable optical parametric oscillator source to probe a pulsed supersonic slit jet expansion. The trimers $(\text{CO}_2)_2\text{-CO}$ and $(\text{CO}_2)_2\text{-N}_2$ have structures in which the CO or N_2 is aligned along the symmetry axis of a staggered side-by-side CO_2 dimer unit. The observation of two fundamental bands for $(\text{CO}_2)_2\text{-CO}$ and $(\text{CO}_2)_2\text{-N}_2$ shows that this CO_2 dimer unit is non-planar, unlike $(\text{CO}_2)_2$ itself. For the trimers $\text{CO}_2\text{-(CO)}_2$ and $\text{CO}_2\text{-(N}_2)_2$, the CO or N_2 monomers occupy equivalent positions in the 'equatorial plane' of the CO_2 , pointing toward its C atom. To form the tetramers $\text{CO}_2\text{-(CO)}_3$ and $\text{CO}_2\text{-(N}_2)_3$, a third CO or N_2 monomer is then added off to the 'side' of the first two. In the mixed tetramers $\text{CO}_2\text{-(CO)}_2\text{-N}_2$ and $\text{CO}_2\text{-CO-(N}_2)_2$, this 'side' position is taken by N_2 and not CO. In addition to the fundamental bands, combination bands are also observed for $(\text{CO}_2)_2\text{-CO}$, $\text{CO}_2\text{-(CO)}_2$, and $\text{CO}_2\text{-(N}_2)_2$, yielding some information about their low-frequency intermolecular vibrations.