

# INFRARED SPECTRA OF $(\text{CO}_2)_n - (\text{RARE GAS})_m$ TRIMERS AND TETRAMER, $(n, m) = (1, 2), (1, 3), (2, 1)$

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**$(n, m) = (1, 2)$ .**  $\text{CO}_2\text{-Ar}_2$  has previously been studied in the microwave<sup>a</sup> and infrared.<sup>b</sup> Its structure has two Ar atoms occupying equivalent positions around the 'equator' of the  $\text{CO}_2$ , giving  $C_{2v}$  symmetry. Here we report observation of analogous infrared spectra of  $\text{CO}_2\text{-Ne}_2$  and  $\text{CO}_2\text{-Xe}_2$ . Meanwhile, for  $\text{CO}_2\text{-Ar}_2$  we observe a new  $a$ -type combination band giving an intermolecular bending frequency of  $32.2\text{ cm}^{-1}$ . Unlike the fundamental band, the combination band is free of interference from stronger  $\text{CO}_2\text{-Ar}$  transitions. Also, we observe  $\text{CO}_2\text{-Ar}_2$  in the  $\text{CO}_2$   $(01^11) - (01^10)$  hot band region, as well as weak fundamental band spectra of the mixed trimers  $\text{CO}_2\text{-Rg-He}$ , with  $\text{Rg} = \text{Ne, Ar, Xe}$ .

**$(n, m) = (1, 3)$ .** An interesting band near  $2345.2\text{ cm}^{-1}$  is assigned to  $\text{CO}_2\text{-Xe}_3$ , whose structure appears to have  $C_s$  symmetry containing a xenon trimer (near equilateral triangle) and a  $\text{CO}_2$  positioned so that two of the Xe atoms are in equivalent near equatorial positions.

**$(n, m) = (2, 1)$ .** We have assigned spectra of new trimers,  $(\text{CO}_2)_2\text{-Rg}$ . The Xe-containing species was noticed first, and this led us to identify weaker spectra with Ar and (even weaker) Ne. Their structures resemble having a  $\text{CO}_2$  dimer (planar slipped parallel) with the Rg atom located 'above' the dimer plane on (or close to) the dimer symmetry axis, analogous to  $(\text{CO}_2)_2\text{-CO}$ .<sup>c</sup> In the future, it should be possible to assign the various Kr clusters and to optimize each cluster by varying the expansion gas mixtures.

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<sup>a</sup>Y. Xu, W. Jäger, and M.C.L. Gerry, *J. Mol. Spectrosc.* **157**, 132 (1993).

<sup>b</sup>J.M. Sperhac, M.J. Weida, and D.J. Nesbitt, *J. Chem. Phys.* **104** 2202 (1996).

<sup>c</sup>A.J. Barclay, A.R.W. McKellar, and N. Moazzen-Ahmadi, *Chem. Phys. Lett.* **677**, 127 (2017).