

## THE 4.2 MICRON SPECTRA OF CO<sub>2</sub>-CO DIMER FOR BOTH THE C- AND O-BONDED ISOMERS, INCLUDING SPLITTING OF THE DEGENERATE $\nu_2$ BEND IN THE PRESENCE OF CO

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CO<sub>2</sub>-CO dimer was previously observed by high-resolution microwave and infrared spectroscopy in the form of a planar T-shaped C-bonded structure.<sup>a,b</sup> More recently, spectra of a second isomer were observed in the stretching region of carbon monoxide.<sup>c</sup> This isomer has also a planar T-shaped structure, but with the CO flipped by 180°. Moreover, two intermolecular frequencies were measured for each isomer. These are in very good agreement with recent high level theoretical calculations.

Here, CO<sub>2</sub>-CO dimer is observed in the carbon dioxide  $\nu_3$  asymmetric stretch region ( $\sim 2350$  cm<sup>-1</sup>). Both C-bonded and O-bonded isomers are analyzed for the normal isotopologue as well as for <sup>13</sup>CO<sub>2</sub>-CO and <sup>16</sup>O<sup>13</sup>C<sup>18</sup>O-CO, the latter being the first observation of an asymmetrically substituted form for which all values of  $K_a$  are allowed. Combination bands involving the lowest in-plane intermolecular mode are also observed yielding frequencies of 24.51 cm<sup>-1</sup> for the C-bonded form and 14.37 cm<sup>-1</sup> for the O-bonded form. In addition, two weak bands near 2337 cm<sup>-1</sup> are assigned to CO<sub>2</sub> hot band transitions (01<sup>1</sup>1) - (01<sup>1</sup>0), yielding the splitting of the degenerate CO<sub>2</sub> bend into in-plane and out-of-plane components due to the presence of the CO. This splitting has rather different values for the C- and O- bonded isomers, 4.56 and 1.59 cm<sup>-1</sup>, respectively, with the out-of-plane mode higher in energy than the in-plane for both cases.

<sup>a</sup>A.C. Legon, A.P. Suckley, *Journal of Chemical Physics* **91** 4440 (1989).

<sup>b</sup>R.W. Randall, J.P.L. Summersgill, B.J. Howard, *Journal Chemical Society Faraday Transactions* 86 1943 (1990).

<sup>c</sup>S. Sheybani-Deloui, A.J. Barclay, K.H. Michaelian, A.R.W. McKellar, N. Moazzen-Ahmadi, *Journal of Chemical Physics* **143** 121101 (2015).