INFRARED SPECTRA OF $(CO_2)_2$-OCS COMPLEX: INFRARED OBSERVATION OF TWO DISTINCT BARREL-SHAPED ISOMERS

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Spectra of $(CO_2)_2$-OCS complex in the region of the OCS ν_1 fundamental ($\sim$2062 cm^{-1}) are observed using a tunable diode laser to probe a pulsed supersonic slit jet expansion. A previous microwave study of the complex by Peebles and Kuczkowskia [a] gave a distorted triangular cylinder. The geometerical disposition of the three dimer faces of this trimer are quite similar to the slipped CO_2 dimer, the lowest energy form of OCS-CO_2 (isomer a), also observed and analyzed in the microwave region, [b] and the higher energy form of OCS-CO_2 (isomer b), first observed by our group in the infrared region. [c]
Here we report the observation and analysis of two infrared bands, corresponding to two distinct isomers of the $(CO_2)_2$-OCS complex. A band around 2058.8 cm^{-1} was assigned to isomer I, which is the same as that studied previously by microwave spectroscopy. A second band around 2051.7 cm^{-1} was assigned to a higher energy isomer of the complex, isomer II, has not been observed previously, but expected on the basis of *ab initio* calculations. [d] Approximate structural parameters for this new isomer were obtained by means of isotopic substitution. In contrast to isomer I, the geometerical disposition of the faces containing OCS and CO_2 in isomer II are similar to isomer b of the OCS-CO_2 complex.

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[d] H. Valdés and J. A. Sordo, Int. J. Comput. Chem. 23, 444 (2002).