FUNDAMENTALS AND TORSIONAL COMBINATION BANDS OF TWO ISOMERS OF THE OCS-CO_2 COMPLEX

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Infrared spectra of two isomers of the weakly bound OCS-CO_2 complex were observed using a tunable diode laser to probe a pulsed supersonic slit-jet. Spectra were recorded in the regions of OCS ν_1 ($\sim$2060 cm^{-1}) and CO_2 ν_3 ($\sim$2349 cm^{-1}) fundamental stretching vibrations. The lowest energy isomer (isomer *a*) was previously studied by microwave spectroscopy.[a] Here we report the first infrared observation of isomer *a* and also detection of a new higher energy form (isomer *b*). Structures were determined with the help of isotopic substitution. Both isomers are planar, with slipped near-parallel geometries. In isomer *a*, the intermolecular (centre of mass) separation is 3.55 Å and the C atom of the CO_2 is closer to the S atom of the OCS. In isomer *b*, the C atom of CO_2 slides closer to the O atom of OCS and the center of mass separation increases to 3.99 Å.[b] Three combination bands involving the intermolecular torsional (out-of-plane bend) vibrations were also analyzed. The out-of-plane torsional frequencies were measured to be 18.8 cm^{-1} and 15.9 cm^{-1} for isomers *a* and *b*, respectively, indicating that isomer *a* is indeed more bound than isomer *b*.

[a] Stewart E. Novick, R. D. Seunram and F. J. Lovas, *J. Chem. Phys.* **88**, 687-690 (1988).

[b] M. Dehghany, J. Norooz Oliaee, Mahin Afshari, N. Moazzen-Ahmadi and A. R. W. McKellar, *J. Chem. Phys.* **130**, 224310 (2009).