INFRARED SPECTRA OF CO_2 - H_2 COMPLEXES

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Infrared spectra of weakly-bound CO_2-H_2 complexes have been studied in the region of the CO_2 ν_3 asymmetric stretch, using a tunable diode laser probe and a pulsed supersonic jet expansion. For CO_2-$para H_2$, results were obtained for three isotopic species, $^{12}C^{16}O_2$, $^{13}C^{16}O_2$, and $^{12}C^{18}O_2$. These spectra were analyzed using an asymmetric rotor Hamiltonian, with results that resembled those obtained previously for OCS- and N_2O-$para H_2$ [1], except that half the rotational levels were missing due to the symmetry of CO_2 and the spin statistics of the ^{16}O or ^{18}O nuclei (as in the similar case of CO_2-He [2]). The CO_2-$para H_2$ complex has a T-shaped structure with an intermolecular distance of about 3.5 Å, and the CO_2 ν_3 vibration exhibits a small red shift (-0.20 cm^{-1}) in the complex. For CO_2-$ortho H_2$, more complicated spectra were observed which could not be assigned, in contrast to OCS- and N_2O-H_2 where the $para H_2$ and $ortho H_2$ spectra were similar, though distinct.

[1] J. Tang and A.R.W. McKellar, *J. Chem. Phys.* **116**, 646 (2002); **117**, 8308 (2002).
[2] M.J. Weida, J.M. Sperhac, D.J. Nesbitt, and J.M. Hutson, *J. Chem. Phys.* **101**, 8351 (1994).