THEORETICAL AND EXPERIMENTAL STUDY OF THE INFRARED SPECTRA OF CO_2-(*para*-H_2)$_2$ TRIMERS

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The infrared spectra of several isotopologues of the CO_2-(*para*-H_2)$_2$ trimer have been predicted by applying exact basis-set calculations to a global potential energy surface which is defined as a sum of the accurately known two-body *para*-H_2–CO_2 and *para*-H_2–*para*-H_2 potentials.[a] These results are compared with new spectroscopic measurements, for which sixteen transitions have been assigned. A reduced-dimension treatment of the *para*-H_2 rotation has been employed by performing an exact hindered-rotor average.[b] Three-body effects and the quality of the potential are discussed. We present a new technique for representing the three-dimensional *para*-H_2 density in the body-fixed frame. It shown the two *para*-H_2 molecules are localized much more closely together than is the case for the two He atoms in the analogous CO_2–(He)$_2$ system.

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[a] H. Li, P.-N. Roy and R.J. Le Roy, *J. Chem. Phys.* (2010, submitted); K. Patkowski, W. Cencek, P. Jankowski, K. Szalewicz, J.B. Mehl, G. Garberoglio and A.H. Harvey, *J. Chem. Phys.* **129**, 094304 (2010).

[b] H. Li, P.-N. Roy and R.J. Le Roy, *J. Chem. Phys.* (2010 submitted).