

## AN ANALYTIC THREE-DIMENSIONAL POTENTIAL ENERGY SURFACE FOR CO<sub>2</sub>-He, AND ITS PREDICTED INFRARED SPECTRUM

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A three-dimensional, analytic potential energy surface for CO<sub>2</sub>-He that explicitly incorporates its dependence on the  $Q_3$  asymmetric-stretch normal-mode coordinate of the CO<sub>2</sub> monomer, has been obtained by least-squares fitting new *ab initio* interaction energies to a new potential form. The potential energy values were obtained from a supermolecule calculation performed at the CCSD(T) level using an aug-cc-pVQZ basis set supplemented with bond functions, and the full counterpoise correction was applied. These points were fitted to a 3-dimensional generalization of the “Morse/Long-Range” potential function form<sup>a</sup> which incorporates theoretically known angle-dependent long-range inverse-power dispersion coefficients. The three-dimensional discrete-variable representation method was employed to calculate the rovibrational eigenvalues, without separating the inter- and intramolecular nuclear motions, and our simulated infrared spectra in  $\nu_3$  region of CO<sub>2</sub> is compared with experiment.<sup>b</sup> This three-dimensional surface will be used to predict the IR vibrational frequency shifts which have been observed for CO<sub>2</sub>-(He)<sub>N</sub> clusters with  $N$  up to 20.<sup>c</sup>

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<sup>a</sup> R.J. Le Roy and R.D.E. Henderson, *Mol. Phys.* (2007, in press).

<sup>b</sup> M.J. Weida, J.M. Sperhac and D.J. Nesbitt, *J. Chem. Phys.* **101**, 8351 (1994).

<sup>c</sup> J. Tang and A. R. W. McKellar, *J. Chem. Phys.* **121**, 181 (2004).