TOWARDS AN ACCURATE INFRARED LINELIST FOR CO_2 AND ISOTOPOLOGUES

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Following the "Best Theory + High-resolution Experimental Data" strategy, we have completed an initial CO_2 infrared (IR) line list, denoted Ames-1. A procedure similar to the one used for ammonia[a] is adopted to generate a global potential energy surface (PES), including various small corrections such as scalar relativity, extrapolation to the one-particle basis-set limit, and a higher-order correlation correction, followed by refinement using accurate high-resolution laboratory data. We will discuss limitations in the use of HITRAN data for the refinement step. The current PES yields uncertainties of 0.01-0.02 $cm^{-1}$for J=0-117 $^{12}C^{16}O_2$ energy levels up to 13,845 cm^{-1} above the zero-point level. Comparisons between Ames-1, HITRAN, and CDSD will be presented for room temperature as well as selected higher temperatures. Results for ^{13}C, ^{14}C, ^{17}O, and ^{18}O isotopologues will be presented, and the accuracy for isotopologues will be discussed. Limitations of the current PES and the Ames-1 line list together with strategies to improve these will be discussed.

[a] X. Huang, D.W. Schwenke, and T.J. Lee, *J. Chem. Phys.* **129**, 214304 (2008); *J. Chem. Phys.* **134**, 044320/044321 (2011).