PROGRESS IN COMPUTING ACCURATE INFRARED LINELISTS FOR CO_2

XINCHUAN HUANG, *SETI Institute, 515 N. Whisman Road, Mountain View, CA, 94043*; DAVID W. SCHWENKE, *MS T27B-1, NASA Ames Research Center, Moffett Field, CA, 94035*; and TIMOTHY J. LEE, *MS 245-1, NASA Ames Research Center, Moffett Field, CA, 94035*.

Following the "Best Theory + High-resolution Experimental Data" strategy, we have made progress on computing a reliable CO_2 infrared (IR) line list. A procedure that is similar to the one used for ammonia[a] is adopted to generate a global potential energy surface (PES), including various small corrections such as relativistic correction, basis-set extrapolation and a higher-order correlation correction, which will be followed by refinements using accurate high-resolution laboratory data. The purely *ab initio* PES includes a long-range Morse-potential part and a short-range local interaction part. Finite-Field approximations were adopted in dipole moment calculations using the CCSD(T)/aug-cc-pVQZ level of theory. Quadruple moment terms were computed and included. Exact variational rovibrational calculations on the purely *ab initio* PES and dipole surface have led to our first set of an IR line list. A comparison with HITRAN data will be discussed.

---

[a] X. Huang, D.W. Schwenke, and T.J. Lee, *J. Chem. Phys.* **129**, 214304 (2008); *J. Chem. Phys.* **132**, *submitted*, (2010).