PROGRESS IN COMPUTING ACCURATE INFRARED LINELISTS FOR CO$_2$

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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 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.