THEORETICAL NH_3 SPECTRA IN 5800-7000 CM^{-1} REGION AND CO_2 IR INTENSITY: UPDATES

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Recently we have successfully applied the "Best Theory + High-resolution Experimental Data" strategy to NH_3 [a] and CO_2. [b] The essential strategy is to refine a high quality, purely ab initio potential energy surface (PES) with reliable high resolution experimental data, so the IR line lists computed on the refined PES and dipole moment surface (DMS) can go beyond simple data reproduction. The goal is to make reliable predictions for higher J/K/energy rovibrational transitions with similar accuracies, i.e. 0.01-0.03 cm^{-1}. The reliability and accuracy of data included in the refinement largely determines the quality of predictions and the ultimate merit of our work. With recent $^{14}NH_3$ experiments in 5800 - 7000 cm^{-1}, the effective coverage (with 0.01-0.03 cm^{-1} accuracy) of our NH_3 PES has extended to this complex spectral region. Excellent agreement between current experiment analysis and our primitive HSL-3 PES refinement will be presented, and source of discrepancies will be discussed. The synergy between the experiments and theory is of great value. For CO_2, we have updated the theoretical IR intensity of the $^{12}C^{16}O_2$ line list with a more reliable DMS, then carried out very detailed comparisons with both pure experimental data and HITRAN/CDSD models. Results suggest that our line lists should be useful for the astronomical or earth-based detection of CO_2 isotopologues.

[a] X. Huang, D.W. Schwenke, and T.J. Lee, *J. Chem. Phys.* **129**, 214304 (2008); *J. Chem. Phys.* **134**, 044320/044321 (2011).
[b] X. Huang, D.W. Schwenke, S.A. Tashkun, and T.J. Lee *J. Chem. Phys.* **136**, ,submitted (2012).