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Quantum IR line list of NH_3 and isotopologues for ISM and dwarf studies

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Abstract. Ammonia (NH_3) was the first polyatomic molecule observed in the ISM. Its importance in interstellar molecules is only second to CO because its rovibrational spectroscopic signature can be used very effectively at deducing the conditions of the interstellar environment such as temperature and density, and because it is found in so many different interstellar objects in a wide temperature range. However, experimental determination of NH_3 IR spectra is extremely difficult due to the large-amplutide inversion vibration, and the existing HITRAN2008 database for NH_3 is limited in temperature, coverage, completeness, and accuracy. With rapid progress in theoretical chemistry and computational resources, now we are able to generate a highly reliable/accurate IR line list of NH_3 (and its isotopologues) for astronomical studies. Exact quantum rovibrational computations on an empirically refined potential energy surface (with nonadiabatic corrections included) have achieved accuracies of 0.02-0.05 cm^{-1} (for line position) and better than 85-95% (for line intensity) for both NH_3 and $^{15}NH_3$ spectra. The unique feature of our work is that our predictions are essentially as accurate as reproducing existing measurements, suitable for synthetic simulation of various astrophysical environments or objects. The reliabilty and accuracy of our predictions for missing bands and higher energies computed on HSL-2 (Fig. 1) have been proved by the most recent high-resolution experiments and extended up to 7000 cm^{-1}. See Huang *et al.* 2008, Huang *et al.* 2011, & Sung *et al.* 2012 for more details.

Keywords. radio lines: ISM — ISM: molecules — molecular data — astrochemistry

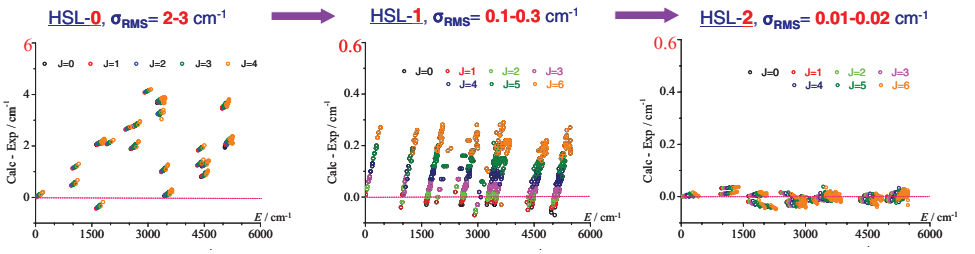

Figure 1. Accuracy evolution of our computed NH_3 rovibrational energy levels.

References

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