

ASSIGNMENT OF INFRARED AMMONIA SPECTRA

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Global ammonia emissions have more than doubled during the period of industrialisation, largely due to widespread use of intensive agricultural techniques and in particular the use of fertilisers and are set to double again by 2050. However the ammonia data in the present version of HITRAN is not only missing at key wavelengths, but also have significant problems. HITRAN contains 28 057 $^{14}\text{NH}_3$ lines of which some 10 % lack full quantum number assignments. Furthermore 1190 of the assigned lines have demonstrably incorrect assignments (for example are parity forbidden); others have incorrect lower state energies or symmetries leading to incorrect predictions of temperature-dependent spectra.

We have undertaken a systematic (re-)analysis of the data in HITRAN. This has been done using both lower state and upper state combination differences starting from a consistent set of lower state energy levels [P. Chen *et al*, *J. Mol. Spectrosc.*, **236**, 116 (2006)] and by using the newly computed variational line list BYTe [S. N. Yurchenko, R. J. Barber, and J. Tennyson, *Mon. Not. R. Astron. Soc.*, *in press*, (2011)]. Previous errors and misassignments have been corrected and significant progress is being made in making new assignments. Comparisons with the BYTe line list suggest that HITRAN is also missing a significant number of important transitions, particularly at frequencies above 5000 cm^{-1} .