



Modelling the spectroscopic behaviour of hot molecules

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At elevated temperatures the molecules absorb and emit light in a very complicated fashion which is hard to characterise on the basis of laboratory measurement. Computed line lists of molecule transitions therefore provide a vital input for models of hot atmospheres. I will describe the calculation and use of such line lists including the BT2 water line list [1], which contains some 500 million distinct rotation-vibration transitions. This linelist proved crucial in the detection of water in extrasolar planet HD189733b and has been used extensively in atmospheric modelling. Illustrations will be given at the meeting. A new linelist for the ammonia molecule has just been completed [2] which shows that standard compilations for this molecule need to be improved. Progress on a more extensive linelist for hot ammonia and linelists for other molecules will be discussed at the meeting.

[1] R.J. Barber, J. Tennyson, G.J. Harris and R.N. Tolchenov, Mon. Not. R. Astr. Soc., 368, 1087-1094 (2006)

[2] S.N. Yurchenko, R.J. Barber, A. Yachmenev, W. Theil, P. Jensen and J. Tennyson, J. Phys. Chem. A, 113, 11845-11855 (2009).