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Calculated linelists for spectra of hot molecules

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Abstract

At elevated temperatures even small molecules such as water or ammonia absorb and emit light in a very complicated fashion which is hard to characterise on the basis of laboraroty measurement alone. Computed line lists of molecule transitions therefore provide a vital input for models of hot atmospheres [1].

The calculation of reliable linelists is best done using a first principles quantum mechanical approach, possibly tuned to available laboratory data. This involves starting from a high accuracy, *ab initio* potential energy and dipole surfaces. While purely *ab initio* dipoles have been shown to be the most reliable [2], it is normally necessary to tune the potential energy surface using transition frequencies from laboratory measurements. These surfaces then form the input to variational nuclear motion calculations. Hot spectra require the treatment of many energy levels and, in particular, highly excited rotational states. This makes such calculations computionally very demanding.

My group has produced a number of rotation-vibration linelists using this approach. For example, the BT2 water line list [3] contains some 500 million distinct rotation-vibration transitions. This linelist proved crucial in the detection of water in extrasolar planet HD189733b [4]. It has been used extensively in modelling a variety of atmospheres.

New linelists for the ammonia molecule have been computed. The initial low-temperature linelist showed that standard compilations for this molecule need improving [5]. The much more extensive linelist for hot ammonia contains over a billion lines [6]; it is currently being used in models of a variety of objects. Progress on this work will be described at the meeting. The situation regarding other linelists will also be discussed.

References

[1] Tennyson, J., Harris, G.J., Barber, R.J., La Delfa, S., Voronin B.A., and Pavlenko, Y.V. Mol. Phys., Vol. 105, pp. 701-714, 2007.

[2] Lynas-Gray, A.E., Miller, S. and Tennyson, J. J. Mol. Spectrosc., Vol. 169, pp. 458-467, 1995.

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

[4] Tinetti, G. et al, Nature Vol. 448, pp. 169-171, 2007.

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

[6] Yurchenko, S.N., Barber, R.J., and Tennyson, J. Mon. Not. R. Astr. Soc., to be submitted.