

A NEW HIGH ACCURACY WATER LINE LIST: COMPUTATION AND APPLICATIONS

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Water is the third most common molecule in the Universe. Its spectrum is particularly rich and H₂O lines have been detected in locations as diverse as: the ISM, comets, Mira variables, sun spots, brown dwarfs and red giants. Nevertheless, only a very small fraction of the lines in the water spectrum are known experimentally, and if for no other reason than sheer number, it seems inevitable that astronomers will continue to use theoretical data when exploring the nature of these objects.

All previous water line lists suffer from incompleteness and inaccuracy (particularly at higher energies). We have produced a new list, BT2, that addresses these shortcomings.

Our *ab initio* computation has employed the best available potential energy and dipole moment surfaces to perform quantum mechanical nuclear motion (rotation-vibration) calculations using the DVR3D suite of codes. The preliminary calculations which established the optimum parameters for the basis function and the ro-vibrational basis set were also fundamental in producing accurate line positions.

The BT2 water line list contains in excess of 500 million transitions. It will be published shortly[4], but it is already finding laboratory[2] and astronomical applications[1, 3].

References

- [1] N. Dello Russo *et al*, ApJ 621 (2005)
- [2] P.-F. Coheur *et al*, J. Chem. Phys. 122 (2005)
- [3] D. P. K. Banerjee, R. J. Barber *et al*, (in prep.)
- [4] R. J. Barber, J. Tennyson *et al*, (in prep.)