CAN ORTHO-PARA TRANSITIONS FOR WATER BE OBSERVED ?

ANDREA MIANI, JONATHAN TENNYSON, *Department of Physics and Astronomy, University College London, Gower Street, WC1E 6BT, London, UK*.

The whole of the water spectrum can be considered as the juxtaposition of the spectrum of two different molecules, with different total nuclear spin: ortho-H_2O, and para-H_2O. No transitions have ever been observed between the two different nuclear-spin isotopomers, and it is widely assumed that interconversion is forbidden without some other intervention. However weak nuclear spin/rotation interaction occurs and this can drive ortho to para transitions. More than 12000 experimental vibrational rotational levels for water have been assigned so far. In this work we explore the whole of the vibrational-rotational spectrum of water, calculate *ab initio* values for the nuclear spin/rotational constants, and predict in which part of the spectrum the strongest transitions between ortho and para levels of water could be experimentally observed.