ANALYSIS OF HOT MOLECULAR SPECTRA

OLEG L. POLYANSKY, *Department of Physics and Astronomy, University College London, London WC1E 6BT, UK.*

Recent increases in accuracy of triatomic molecular energy level calculations for high rotational quantum numbers J is reviewed. Variational calculations which use exact kinetic energy operators can treat all vibrational states simultaneously. These calculations can use high quality *ab initio* and fitted potential energy surfaces. For spectroscopic accuracy on hydrogen containing molecules, it is necessary to include adiabatic and nonadiabatic corrections to the Born-Oppenheimer approximation. Relativistic corrections can also be important.

Application of the resulting calculations of energy levels and spectra to the analysis of seemingly unassignable spectra of water and H_3^+ is described. Spectra of water in sunspot ($T \sim 3200$K), laboratory ($T \sim 1600$K) and even room temperature contain hundreds or thousands of lines which remained unassigned for more than a decade (see for example Polyansky *et al.*, *Science* , v. 277, N5324, pp.346-348 (1997)). We present here the results of the assignments of these water lines. H_3^+ line assignment is also considered as well as progress on H_2S, NO_2, O_3 and the analysis of the spectra of other triatomic molecules.