NON-ADIABATIC EFFECTS IN THE $\text{H}_3^+$ SPECTRUM

A. ALIJAH, Groupe de Spectrométrie Moléculaire et Atmosphérique, UMR CNRS 7331, University of Reims Champagne-Ardenne, 51100 Reims, France; P. H. R. AMARAL, L. G. DINIZ, J. R. MOHALLEM, Department of Physics, Federal University of Minas Gerais, CEP 31270-901 Belo Horizonte, Brazil

For accurate calculations of the rovibrational energy levels of $\text{H}_3^+$ and other light molecules, correction terms to the Born-Oppenheimer potential energy surface need to be considered, such as the diagonal adiabatic correction, the relativistic correction and the QED correction. The effect of non-adiabatic coupling to further electronic states, which results in shifts of the vibrational energies of about $1 \text{ cm}^{-1}$, is more difficult to describe, as it is dynamical in nature; the nuclei move simultaneously on several potential energy surfaces. However, for isolated electronic states, it can be simulated to a good approximation by employing vibrational and rotational reduced masses that are not constant but depend on the nuclear configuration. Bunker and Moss have derived explicit formulae to compute these masses, but they are difficult to apply in practice. Empirical approaches have therefore been developed in our group, for both polar and non-polar molecules, and first been applied to $\text{H}_2$, $\text{H}_3^+$ and $\text{LiH}_2$. A recent generalization based on the concept of Atoms in Molecules works for polar and non-polar molecules alike. The performance of this method for $\text{H}_3^+$ and $\text{D}_3^+$ will be demonstrated.