



Laboratoire CIMAP

Centre de recherche sur les Ions, les Matériaux et la Photonique

UMR 6252 – CEA – CNRS – ENSICAEN – UNICAEN

6 Boulevard Maréchal Juin

14050 Caen Cedex 4

✓ Proposition de sujet de stage M2

Titre : Theoretical study of vibrational spectrum the KAr diatomic molecule

Contact : Benoit Gervais – gervais@ganil.fr – 02 31 45 47 93

Julie Douady – julie.douady@ensicaen.fr – 02 31 45 25 77

The alkali-rare gas diatomics form a class of simple molecules, whose electronic structure can be described as an electron on top of two closed shell cores. As such, we can model the molecular interaction quite accurately by means of ab initio core-polarisation potential (AICPP). In the case of KAr molecule, a large amount of experimental measurement provides us information about the vibrational levels of several electronic levels associated to different potassium electronic configurations $K(4s)$, $K(4p)$, $K(5d)$ and $K(7s)$.

Our aim is to calculate the series of rotational and vibrational levels for all the potential energy curves associated with the potassium electronic configurations mentioned above, in order to probe the quality of the AICPP model. We have already calculated the potential energy curves and the student will use them to find the ro-vibrational levels associated with the motion of the nuclei. To do this, the student will first learn the literature associated with molecular vibration and the specific literature dedicated to the KAr molecule. Then, the student will solve the corresponding Schrödinger equation using a collocation method. For this, the student will have to adapt a numerical code (developed at CIMAP) to take into account the couplings between the different angular moments, which determine the characteristics of the rotational spectrum. In particular, the student will consider the coupling between the electronic orbital moment associated with the electronic motion around the nuclei, the molecular moment associated with the rotation of the nuclei around the center of mass and the electronic spin. The latter is responsible for lambda-doubling, a specific feature of the doublet term associated with an open-shell molecule with an unpaired electron. Depending on the time available, the student will study the RbHe molecule by the same means. It differs from the KAr molecule in the extent of spin-orbit coupling, which significantly modifies the ro-vibrational spectrum.

The placement constitutes an excellent introduction to molecular quantum mechanics. It will offer the student an excellent revision of angular momentum coupling, which is a cornerstone of quantum mechanics necessary for nuclear, atomic and molecular physics.