Theoretical Study of low electron scattering from molecules: Extension of the use of a separable form of the exchange potential to non linear polyatomics

The first step of the extension of the existing code to collisions involving non linear molecules was achieved. As a matter of fact such calculations require to first generate the linear combinations of symmetrised spherical harmonics with belong to each of the irreductible representation of the symmetry group of the molecule. The continuation of this work will be the subject of a new visit. On the other side, a complete study of the collisions of electrons with the NCCCCN molecule using the separable exchange Bordeaux code was achieved during this period. This study was motivated by a recent publication dedicated to the experimental evidence for radiative attachment from electron to this molecule in Astrochemistry. As a matter of fact the formation of anions in astrophysical environments has been predicted in chemical models for some time by radiative attachment. The issue of such calculations is to predict the shape resonances which may allow electron attachment to the considered molecule. The SCF electronic wave function of the fundamental $^1\Sigma$ state of the molecule was calculated in a 6-311G** Gaussian basis set for the experimental geometry and the polarisability estimated.

Figure 1: Computed partial elastic cross sections associated with the different symmetries for the collsions of electrons with NCCCCN($^1\Sigma$)

The quadrupole moment id found to be quite large (14 a.u) and because of the size of the molecule the single centre expansion of the static potential around the centre of mass needs to be calculated up to 15 Bohr. The six partial cross sections associated with the six s ymmetries considered in the calculations are represented in **Figure 1** . They show several shape resonances which are under analysis. The first resonance of Δg symmetry is situated around the position of the experimental peak of formation of both CCN^- and CN^-.The Π_g and Σ_u resonances between 8 and 10 eV are also in good correspondence with the experimental peak associated with the CCN^- formation. These results will be compared to some performed in Roma using a Hara free electron gaz exchange potential and submitted soon to publication. During my stay a publication which is a result of my last visit was published [1] and the final form of a common publication with a PhD student from the group of Roma who visited me in Bordeaux was also achieved and submitted [2].

---

1. Scattering of electron by gaseous CS(1S) : The role of short-range forces on the very-low energy $^2\Pi$ resonance. F. Sebatianelli, F. A. Gianturco, T. Stoecklin, I. Baccarelli, Chem. Phys. Letters. (2009) pulished online
2. The ionic patways of Lithium chemistry in the early universe : Quantum calculations for LiH+ reacting with H, S. Bovino, T. Stoecklin and F. A. Gianturco (submitted)