

# Scientific Report

Trabelsi Tarek  
trabelsiitarek@gmail.com

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## 1 Introduction

This internship was done from 15/03/2016 to 30/04/2016 at : *Institut des Sciences Moléculaires(ISM)-Université Bordeaux*. My objectives were initially to calculate a model of potential energy surface for the  $\text{AlO}^+ - \text{He}$  collision, to learn how to fit this surface and to calculate the vibrational quenching of  $\text{AlO}^+$  colliding with He. However the first results showed that the well depth associated with the  $\text{He-AlO}^+$  complex was not deep enough to couple several vibrational states. It was then decided to test also the collisions of  $\text{AlO}^+$  with Ne and Ar and to perform the dynamics calculations in a second time.

## 2 Potential energy surfaces

The three PES were calculated using the explicitly correlated coupled-cluster method with single, double, and perturbative triple excitations (CCSD(T)-F12)<sup>1</sup> implemented in MOLPRO<sup>2</sup>. The atoms were described using the augmented correlation consistent aug-cc-pVTZ basis set<sup>3 4</sup> in connection with the corresponding auxiliary basis sets, density fitting functions and the complementary default basis sets.

The basis set superposition error (BSSE) was corrected at all geometries. We mapped these three potential energy surfaces using Jacobi coordinates for the  $\text{AlO}^+ - \text{X}$  ( $\text{X} = \text{Ar}, \text{Ne}, \text{He}$ ) molecular systems where :  
 $r$  is the  $\text{AlO}^+$  bound distance.

$R$  is the distance of ( $\text{X} = \text{Ar}, \text{Ne}, \text{He}$ ) from the  $\text{AlO}^+$  center of mass.

$\theta$  is the angle defined by X, center of mass and Oxygene atom (see Figure 1 right).

For all calculation the  $R$  and  $r$  distances were respectively varied from 3.0 to 50 bohrs and from 2.8 to 3.25 bohrs while  $\theta$  varied from 0 to 180 degree by step of 10. We present in this figure the potential energy curves for

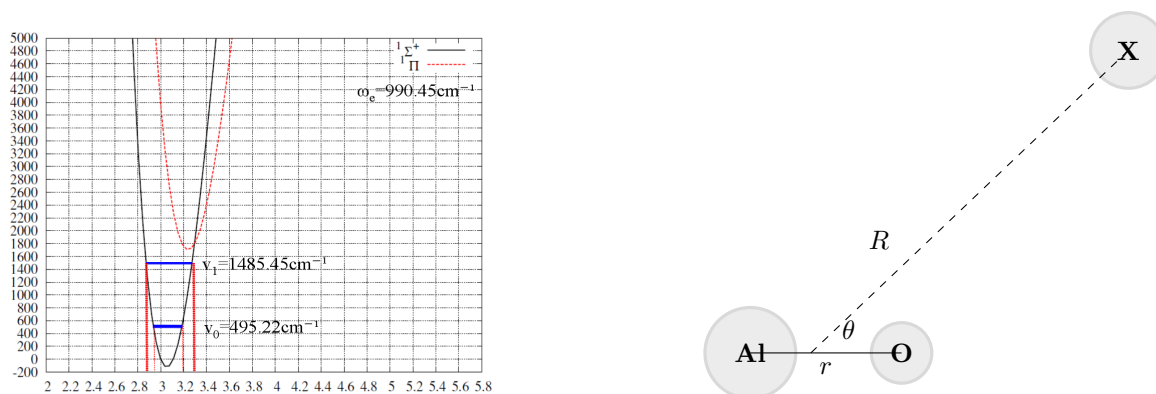


Figure 1: MRCI/aug-cc-pVQZ potential energy curves for  $\text{AlO}^+$  and Jacobi coordinate for  $\text{AlO}^+ - \text{X}$  (right)

$\text{AlO}^+$  of the ground ( $^1\Sigma^+$ ) and the first ( $^1\Pi$ ) excited electronics state. These curves calculated using the MRCI methode implemented in MOLPRO and the atoms are discribed using the augmented correlation consistent aug-cc-pVQZ. At this level the equilibrium geometry for  $\text{AlO}^+$  is  $r = 3.04$  bohr and the harmonic frequencies  $\Omega_e = 990 \text{ cm}^{-1}$  Fig. 1 (left)

<sup>1</sup>G. Rauhut, G. Knizia, and H.-J. Werner, J. Chem. Phys. 130, 054105 (2009).

<sup>2</sup><http://www.molpro.net>

<sup>3</sup>D. E. Woon and T. H. Dunning, Jr., J. Chem. Phys. 98, 1358 (1993)

<sup>4</sup>T. H. Dunning, Jr., J. Chem. Phys. 90, 1007 (1989).

## 2.1 $\text{AlO}^+ + \text{Ar}$

Before starting the calculation of the potential energy surface, some preliminary tests were performed on this system. First, we calculated the equilibrium geometry of the  $\text{AlO}^+ + \text{Ar}$  complex in the electronic ground state ( $^1A'$ ) using the CCSD(T)-F12 method and an aug-cc-pVTZ basis set. The minimum was obtained for  $\theta = 0$  degree,  $r = 3.04$  bohr and  $R = 7$  bohr. Then the full three dimensional potential energy surface was obtained

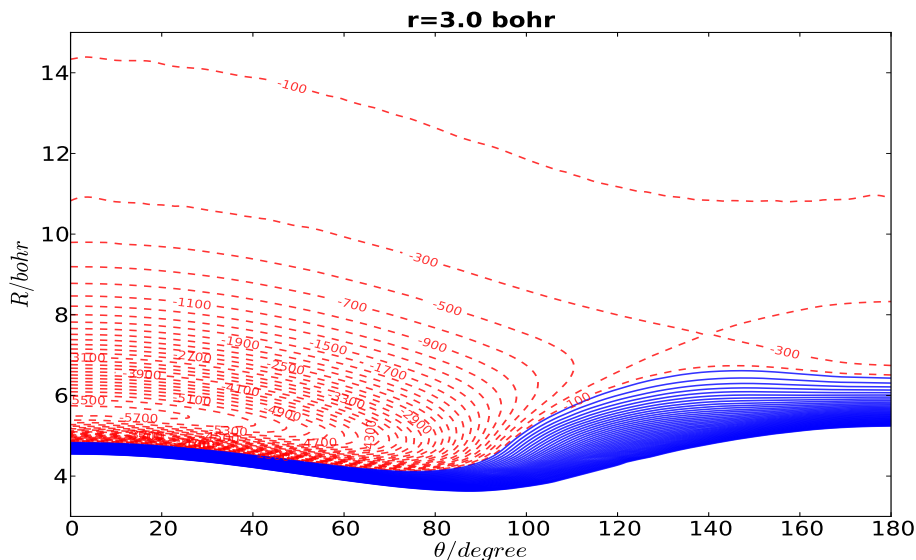


Figure 2: 2D-PES for  $\text{AlO}^+ - \text{Ar}$  calculated at equilibrium geometry for  $\text{AlO}^+$

from a total of 5320 ab initio points. The estimated depth of this potential well is quite large  $\sim 5700 \text{ cm}^{-1}$ . A two dimensional potential energy surface calculated for the equilibrium distance of  $\text{AlO}^+$  (i.e  $r = 3.04$  bohr) is represented in Figure 2.

## 2.2 $\text{AlO}^+ + \text{He}$

For the  $\text{AlO}^+ - \text{He}$  we calculated only a two dimensional potential energy surface as the well depth of this PES  $\sim 350 \text{ cm}^{-1}$  is not big enough to couple several vibrational states. A total of 646 ab initio points were computed for this system.

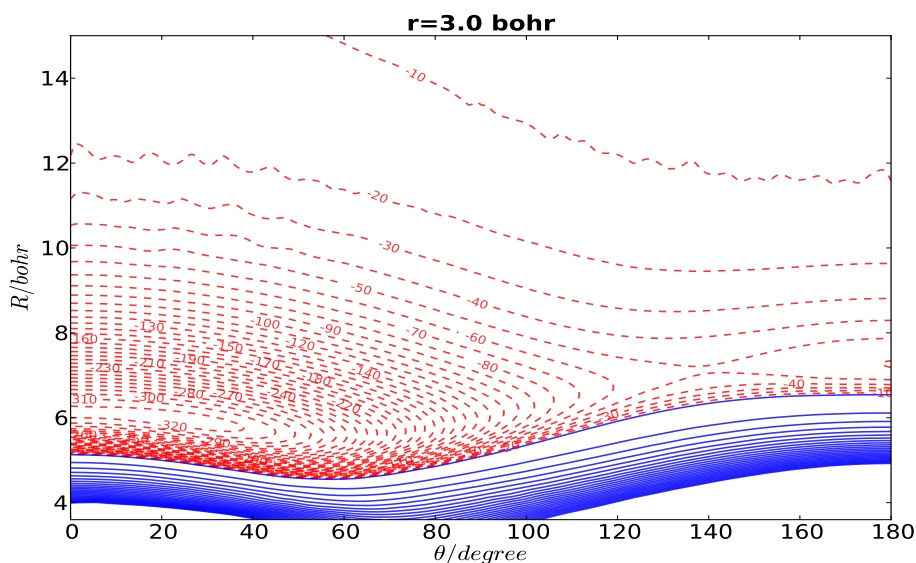


Figure 3: 2D-PES for  $\text{AlO}^+ - \text{He}$  calculated at equilibrium geometry for  $\text{AlO}^+$

We present in Figure 3 the calculated two dimensional potential energy surface for the equilibrium distance

of  $\text{AlO}^+$  (i.e  $r = 3.04$  bohr) The equilibrium geometry for this system is  $\theta = 0$  degree,  $r = 3.0$  bohr and  $R = 6.2$  bohr.

### 2.3 $\text{AlO}^+ + \text{Ne}$

For the  $\text{AlO}^+ - \text{Ne}$  we calculated the three dimensional potential energy surface from a total of 3860 ab initio points. This system is characterized by a depth of potential wells estimated  $\sim 1100 \text{ cm}^{-1}$ . We present in Figure 4 the two dimensional potential energy surface calculated at equilibrium distance for  $\text{AlO}^+$  (i.e  $r = 3.04$  bohr). The equilibrium geometry for this system is  $\theta = 0$  degree,  $r = 2.9$  bohr and  $R = 5.4$  bohr.

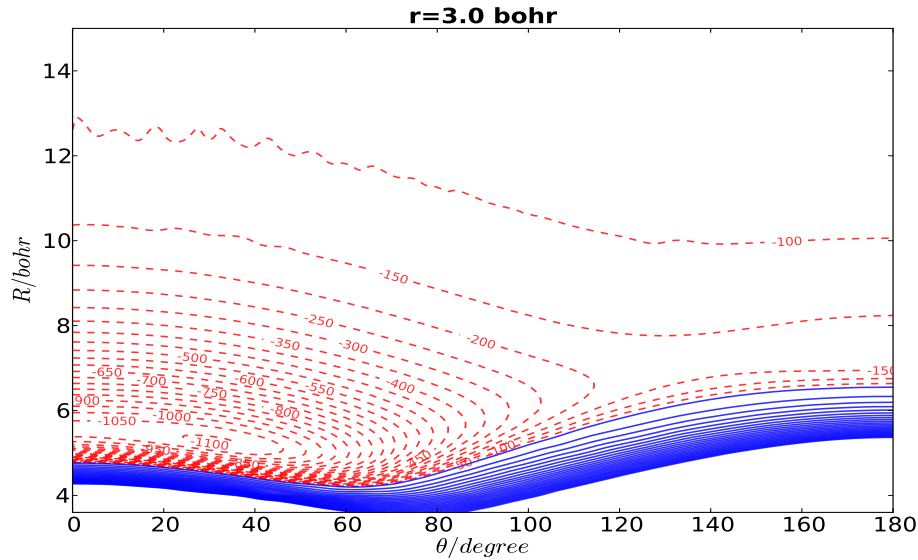


Figure 4: 2D-PES for  $\text{AlO}^+ - \text{Ne}$  calculated at equilibrium geometry for  $\text{AlO}^+$

## 3 Discussions conclusion

This internship was very fruitful to me because I had to cover many different fields. I also learnt new concept and new ways of working.

The Potential energy surface fo  $\text{AlO}^+ - \text{He}$  has an astrophysical interest, as  $\text{AlO}^+$  was detected in the interstellar midium and because Helium is the second most abundant chemical element after hydrogen. The next step of this study will then to calculate the rotational excitation of  $\text{AlO}^+$  in collisions with He. For the two other systems the two PES will be used to study the vibrational quenching of  $\text{AlO}^+$  with the Ne and Ar colliding partners.