Electron Scattering by HOOC1 Molecules.

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Introduction

In 1974, Rowland and Molina found that chlorine atoms produced by the UV irradiation of chlorofluorocarbons (CFCs) are involved in the ozone depletion [1]. Since then, species with chlorine and oxygen has been studied for better understanding of this process, therefore several models of reactions were proposed for ozone depletion, where this kind of species plays an important role as intermediate agents. Theoretical calculation indicates that HClO₂ molecule has three stable isomers: HOOC1, HOC1O and HClOO [2]. Because of the thermal stability and the prospect of formation in the stratosphere the HOOC1 molecule could be the most important reservoir for chlorine [3]. However, there is no experimental data about this molecule because it has never been observed experimentally. The objective of this work is to perform a study of the interaction of low-energy electrons (1-10eV) with HOOC1 in the gas-phase.

Methodology

In this work, the interactions between free electrons and HOOC1 molecules were studied and cross sections were calculated using the UK R-Matrix-R codes. In the R-Matrix formulation, the space is split into an inner and an outer region limited by a sphere of radius $r = a$, which should contain all the electronic density of the target molecule, centered on its center of mass. The system in the inner region is formed by $N + 1$ electrons, N electrons from the molecule plus one continuum electron, where the short-range effects such as polarization, exchange and correlation effects are important. In the outer region, the solutions are obtained by solving a set of one-electron, coupled, second-order differential equation. In this region of long-range effects, the interaction of the continuum electron with the molecular dipole is relevant [4]. The target description is performed by Hartree-Fock method with three different atomic bases: TZV, 6311G* and ccpVTZ.

Results and Discussion

A systematic study was performed to obtain reliable cross sections, various parameters in the R-matrix method was tested such as, the radius a , basis set, polarization and long-range effects. For all basis sets the best radius was $10a_0$. In figure 1, the dependence of eigenphase-sums for all set basis are shown. The resonance structure is ranging from 1.4-2 eV. A study of convergence of polarization effects was performed. In the figure 2 and 3, we present our ICS including or not (with or without Born corrections) long-range interactions, due to permanent molecular dipole moment. In the figure 2, the peaks in the ICS represent the resonance position.

Figure 1: Atomic basis dependence in the Eigenphase sums.

Figure 2: Integral Cross Section in SE level with Born corrections (CB).

Figure 3: Integral Cross Section in SE level and no Born correction (WB).

Conclusions

The eigenphase-sums results show the existence of a resonance around 2 eV, the correct value depends of atomic set basis. The ICS with and without Born corrections show that the long-range effects are dominant over short-range polarization effects.

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References

- [1] T. Yoshinobu, N. Akai, A. Kawai, and K. Shibuya, Chem. Phys. Lett., vol. 477, 70, 2009.
- [2] K. Johnsson, A. Engdahl, and B. Nelander, J. Phys. Chem., vol. 100, 3923, 1996.
- [3] T. J. Lee and A. P. Rendell, J. Phys. Chem., vol. 97, 6999, 1993.
- [4] J. Tennyson, Phys. Rep., vol. 491, 29, 2010.