EIPAM REPORT

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Reference number

1290

Dates of visit

Starting date: 06.12.2006
Ending date: 05.02.2007

The title of your project

Electron-attachment resonances of the molecular models of DNA constituents. Quantum scattering calculations.

1. Purpose of the visit

Study the electron-attachment resonances of the molecular models of DNA constituents. Very recent experimental findings obtained in the group of David Field (University of Aarhus, Denmark)[1] have suggested the change of the target from DNA to OCS. Several theoretical and experimental studies of electron collisions with OCS have been also published previously. For example, Bettega et al.[2] have calculated elastic integral, differential and momentum transfer cross section for electron-OCS collisions. One should also cite the calculations of Lynch et al.[3] employing the continuum multiple-scattering model and a joint theoretical-experimental study on electron-OCS collisions carried out by Michelin et al.[4] Most recently, the group in Rome has also carried out calculations on the integral and differential cross sections at low energies.[5] The aim of our calculations is to be able to obtain elastic and rotationally inelastic cross sections at low energies nearing the various threshold openings and closer to the experimental data obtained in the Aarhus group.

2. Description of the work carried out during the visit

The carbon oxysulfide (OCS) molecule is well known to be of importance for the role it plays in the carbon chemistry and sulphur chemistry chains of reactions in astrophysics. It is also of interest in the realm of cold molecular plasmas because of its reaction quenching properties.

Collisional processes induced by low-energy electrons in molecular gas have triggered the interest of both experimentalists and theoreticians, intrigued by the possible role that the permanent dipole of the OCS molecule might play in the scattering phenomena.

During all visit in Rome I completed the following tasks:

Calculations of the rotational excitation of OCS molecule have been performed with using several programs, both commercial and developed in the MQSQD (Rome Group on Molecular Quantum Structures and Quantum Dynamics) led by Prof. Gianturco. The first step was to calculate electronic eigen functions (at the HF level) for different interatomic distances and polarizability tensor of OCS molecule (at the HF level), both were done using the Gaussian 98 package. In case of the calculations of the polarization tensor I have used an extended basis set, cc-pVQZ, augmented with six d-type and ten f-type diffusion functions. The calculations of interaction potential (static exchange + polarization) between the scattering partners (i.e. impinging electron and OCS in its ground state) were carried out with Volloc – a package developed in the MQSQD group, which uses a Single Centre Expansion technique to calculate multicentral potentials. The radial grid of points, at which the interaction potential is calculated, was generated in such a way that it is dense at the vicinity of the nuclei, and much sparser at long distances, where the main interaction is dominated by polarization member. The CC package allows calculations the elastic and rotationally inelastic cross sections for linear molecules. The first step consisted of the choosing adequate parameters (e.g. numbers of rotational levels, magnitude of the integration step). All of the calculations were performed on work station JAMAICA, at the CASPUR (Inter-University Consortium for the Application of Super-Computing for Universities and Research) in Rome.

3. Description of the main results obtained

I A Convergence tests

First step consisted of finding the calculation parameters which yield a converged cross section. On the following figures I show the results of tests for: the number of included rotational levels of the target (Fig. 1 for 0.01eV and 0.1eV, respectively), number of terms in multipolar potential expansion (λ) (Fig. 2) and number of values of the total angular momentum of the system (i.e. electron + OCS molecule) (Fig. 3, Fig. 4).

I B Cross sections

At the moment, due to a rather long computational time, I have obtained the cross section values at 0.01eV, 0.1eV and 1.0eV, which are shown in Fig. 5

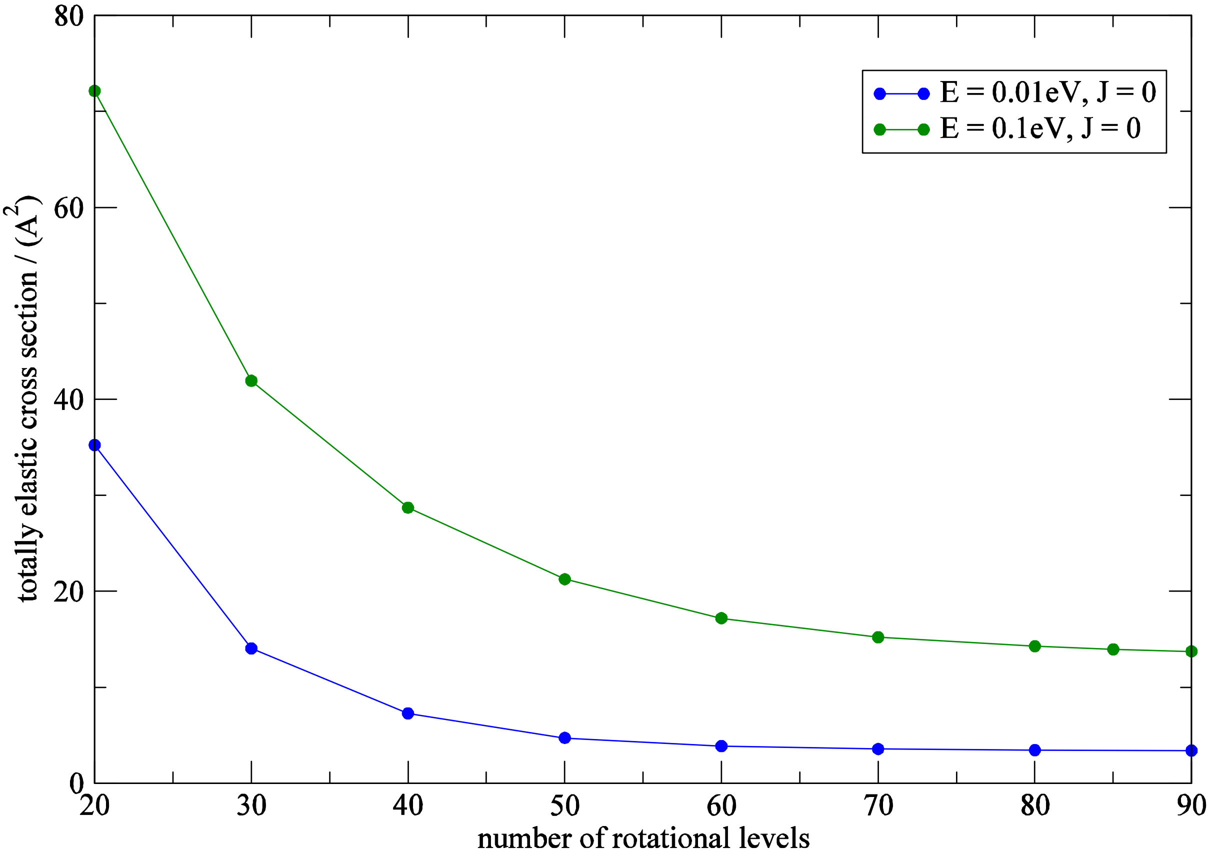

Fig. 1 Total elastic integral cross section in the function of the number of included rotational channels

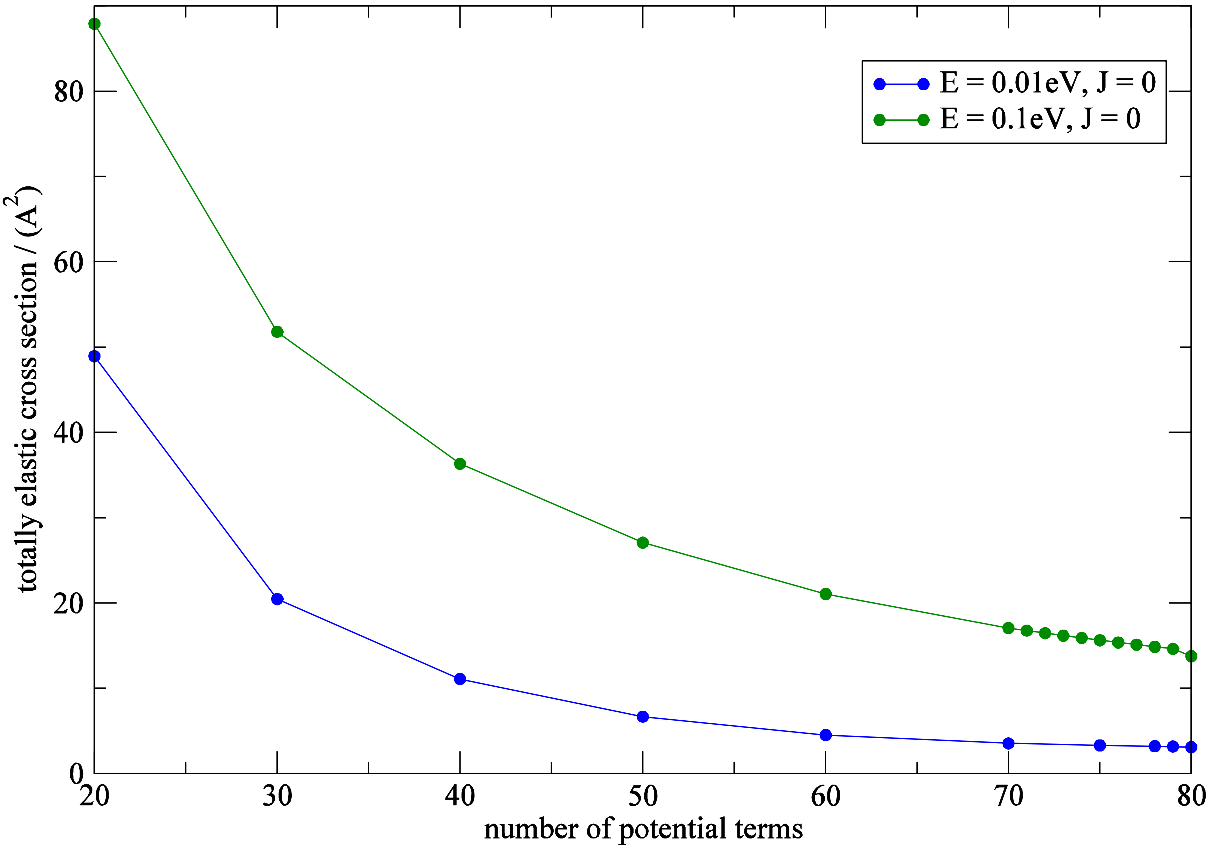

Fig. 2 Total elastic integral cross section in the function of the number of included potential terms

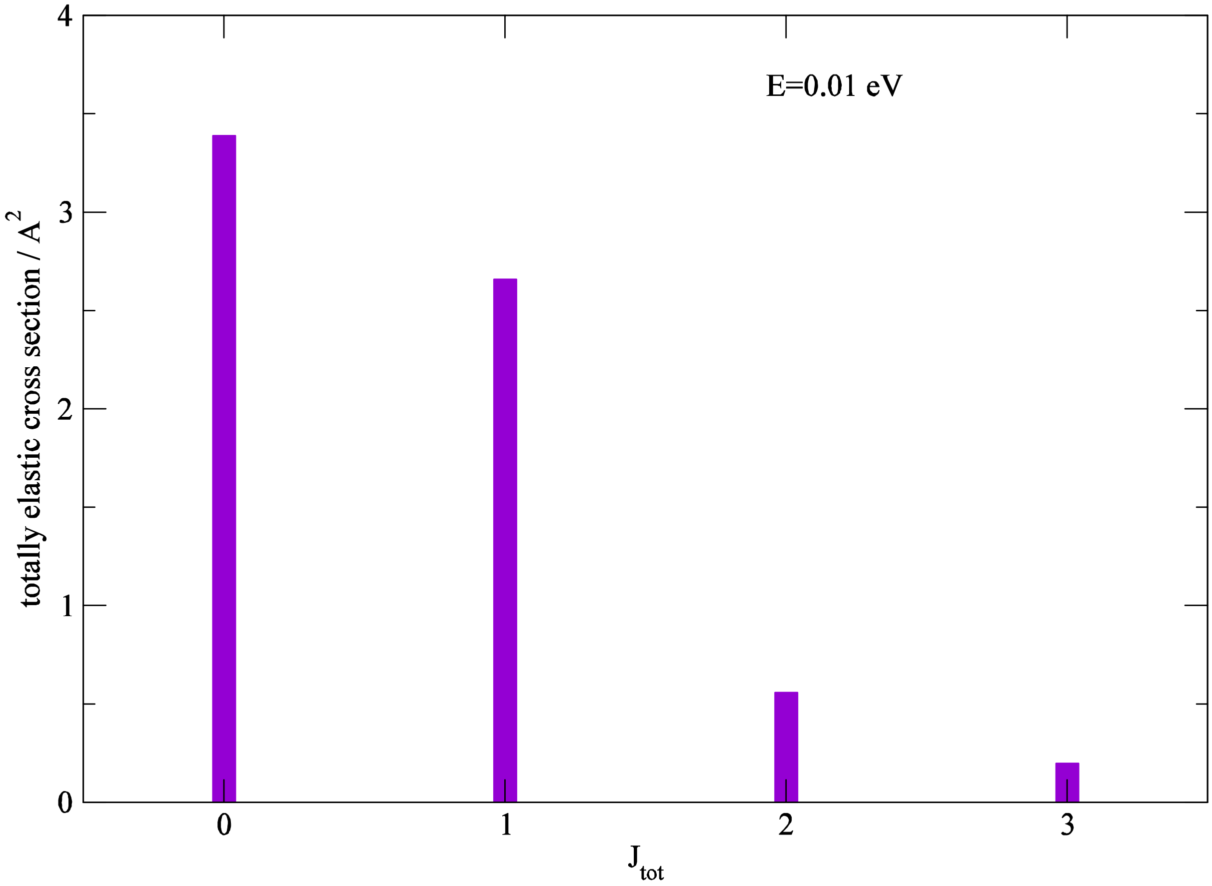

Fig. 3 Total elastic integral cross section in the function of the number of included total angular momentum values for 0.01eV energy

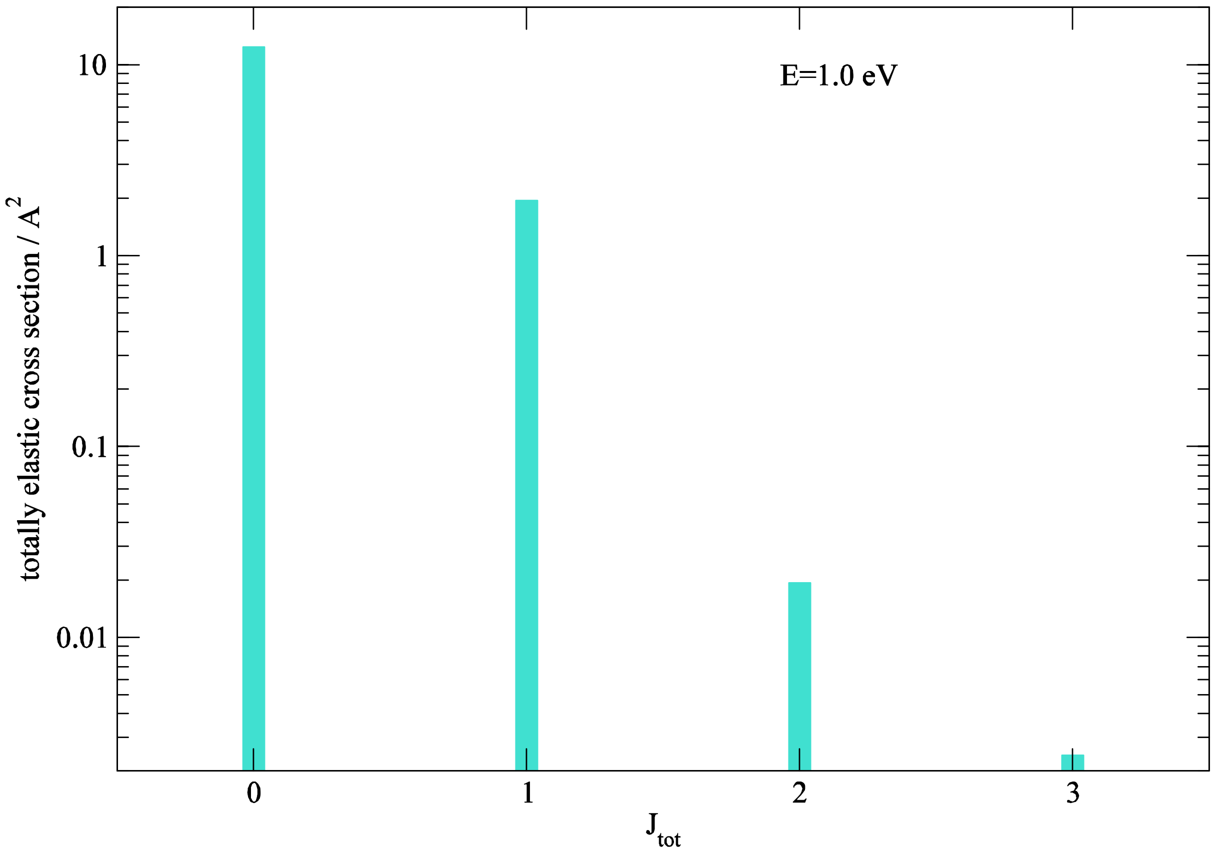

Fig. 4 Total elastic integral cross section in the function of the number of included total angular momentum values for 1.0eV

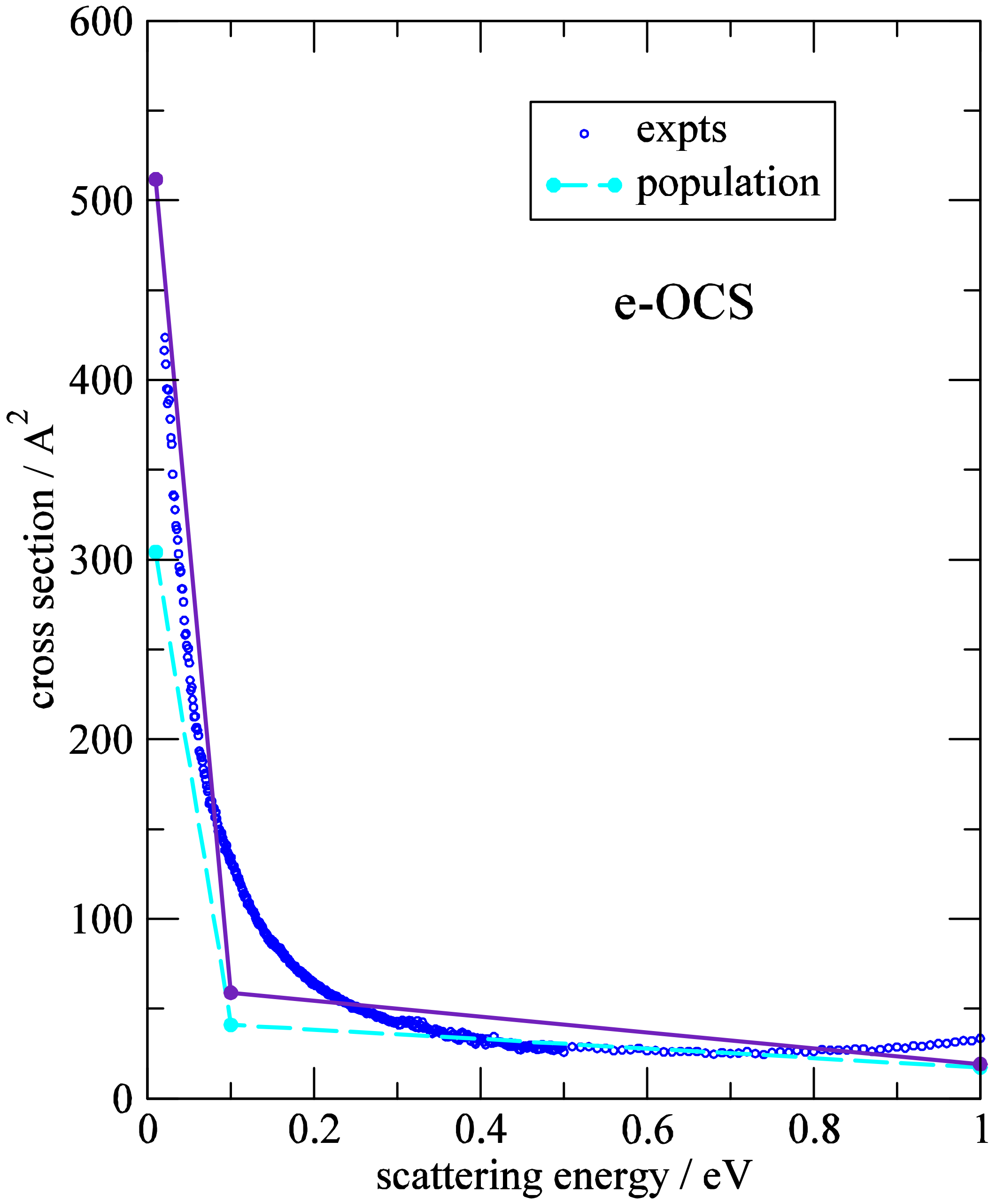

Fig. 5 Cross section for the electron scattering from OCS molecule in the j=0 level in the low energy region. Comparison between experimental findings obtained in the Aarhus group and two sets of theoretical calculations. Solid line: calculations performed assuming that all target molecules where in their ground state; broken line: calculations taking into account rotational state population at 300 K and summing over all populated states.

Conclusion

As it has been shown in the previous figures I have managed to obtain the convergence of cross sections to less than 1%, to analyze the rotational cross sections for their overall energy dependence over the broad range of energies which is experimentally available. One can see (Fig. 5) that present calculations follow closely the experimental findings from 0.3 eV to 0.7 eV. Our initial theoretical results (only 3 points) seem to be shifted towards the lower energies with respect to measurements. It may be caused by the chosen exchange model SCE though the effect requires further investigation.

4. Future collaboration with host institution (if applicable)

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5. Projected publications/articles resulting or to result from your grant

The obtained results, after completion, are to be published in one of the leading journals of the field.

6. Other comments (if any)

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References

[1] D. Field, N. Jones, private communications (unpublished results)
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[3] M.G. Lynch, D. Dill, J. Siegel, J.L. Dehmer, *J. Chem. Phys.*, 71, 4249, 1979
[4] S.E. Michelin, T. Kroin, I. Iga, M.G.P. Homen, H.S. Moglio, M.T. Lee, *J. Phys. B*, 33, 3293, **2000**
[5] T. Stoecklin, F.A. Gianturco, *Chem. Phys.*, **2007** (in press)