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Research Report

quantum dynamical study of low-energy electron scattering off mono-fluorinated methane

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visiting time: **16 April - 31 May 2009**

Purpose of the visit

Fluoro-methane (CH_3F) is of fundamental importance in plasma processing (see e.g. [1]). However in the literature only total elastic cross-sections are available [2].

The purpose of the visit in the group of Prof. Gianturco at the University of Rome *La Sapienza* is to calculate vibrational-inelastic electron-cross sections for this molecule in order to provide more data for plasma modelling.

We have decided to extend these studies and to also investigate positron scattering. CH_3F shows enhanced positron annihilation near the vibrational thresholds [3, 4]. Therefore we consider studies on the molecule vibrational dynamics of this molecule an important step towards the understanding of the underlying mechanism of enhanced positron annihilation in small molecules.

Work carried out

The vibrational-inelastic cross sections are calculated with the vibrational close-coupling Volterra-integration method (for more details see e.g. [5]).

Fluoromethane has point group symmetry C_{3v}. We have started our study by investigating one component of the anti-symmetric CH-stretching mode. The mode belongs to the irreducible representation E and is doubly degenerated. By perturbing the molecule along the vibrational normal coordinates of this mode, the symmetry is lowered to C_S symmetry. The lowering of the symmetry results in a huge increase of the number of coupled channels. In order to tackle this problem, it was necessary to rewrite several parts of the vibrational-close-coupling program code and to implement more efficient computer routines.

Main results

We have performed Hartree-Fock geometry optimization and frequency calculation to obtain the vibrational normal modes using the TURBOMOLE program suite [6].

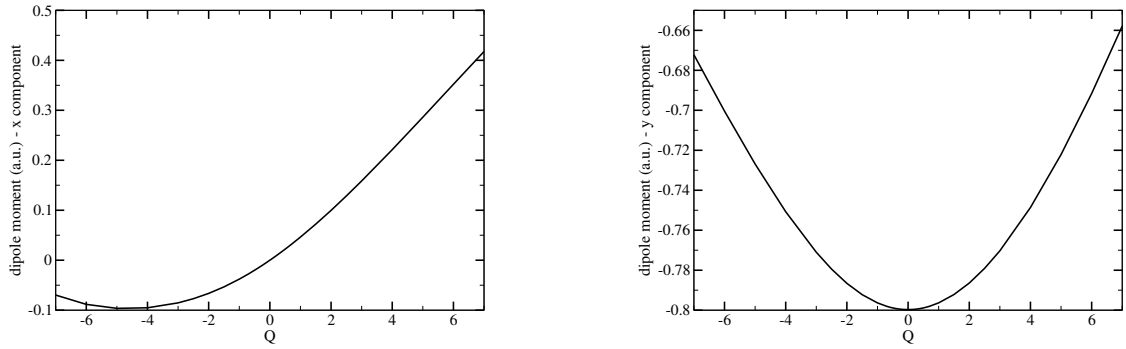

Figure 1: x and y components of the dipole moment as a function the elongation along the vibrational normal coordinate of the antisymmetric CH-stretching mode.

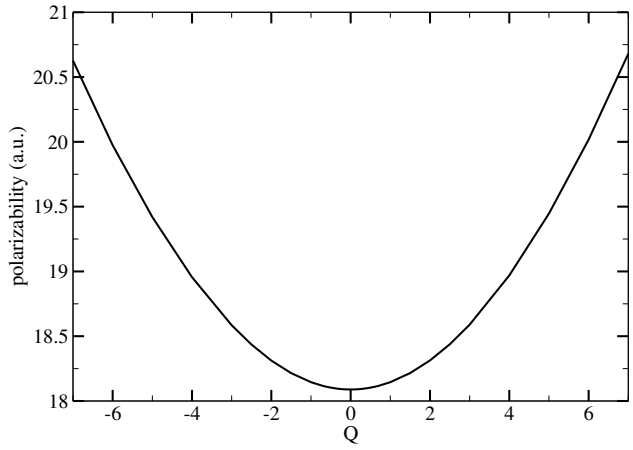

Figure 2: the dipole polarizability as a function the elongation along the vibrational normal coordinate of the antisymmetric CH-stretching mode.

Figure 1 is showing the x- and y component of the dipole moment as a function of the vibrational normal coordinate along the antisymmetric CH-stretching mode.

Figure 2 shows the polarizability along the same mode. The polarizability was shifted by 6.042 a.u. in order to match the more reliable value obtained from density functional calculations using the PBE-functional and the aug-cc-pVTZ basis set at equilibrium geometry.

Figure 3 shows some preliminary results for the computed positron cross sec-

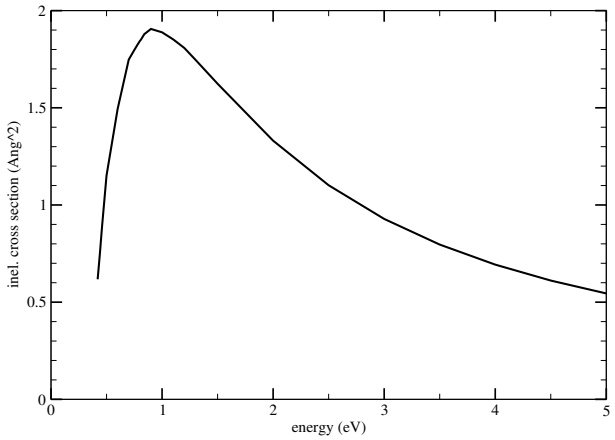

Figure 3: cross sections for the excitation out of the vibrational ground state into the first excited state the antisymmetric CH-stretching mode by positron impact.

tions for the excitation from the vibrational ground state into the first excited state. Analogous calcualtions for electron scattering are underway.

References

[1] L. G. Christophorou, and J. K. Olthoff. Fundamental Electron Interactions with Plasma Processing Gases, Springer-Verlag, Berlin, 2003

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[3] J. A. Young, and C. M. Surko. *Phys. Rev. A* **78** (2008), 032702.

[4] G. F. Gribakin, and C. M. R. Lee. *Phys. Rev. Lett.* **97** (2006), 193201.

[5] J. Franz, and F. A. Gianturco. *Eur. Phys. J. D* **39** (2006) 407-413

[6] R. Ahlrichs *el al.*, TURBOMOLE, Version 5 (University of Karlsruhe, 2002).

Future collaboration with host insitution

We will continue collaboration on vibrational-inelastic electron and positron scattering off polyatomic molecules.

Projected publications resulting from the grant

It is envisaged to publish the results on vibrational inelastic electron and positron scattering off CH_3F later this year.

Other comments

We acknowledge computer time, which has been made available by the CASPUR computer consortium (Rome, Italy). Furthermore we thank Prof. Sigrid D. Peyerimhoff for valuable computer time at the University of Bonn (Germany).