

Collisions electrons of low-energy by SiF_4 and GeF_4

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Synopsis In this work we calculated integral and differential elastic cross sections for silicon and germanium tetrahalides. We found a Ramsauer-Townsend minimum for the SiF_4 molecule and we observed a presence of a virtual state for GeF_4 molecule, and both molecules presented form resonances.

The knowledge of the scattering cross section for electron-molecule collisions is of great importance in technological applications. For example, the scattering of low-energy electrons by molecules plays an important role in plasma processing materials, the simulation of the environment where the discharge depends on various input data, such as the scattering cross sections [1]. In particular the SiF_4 and GeF_4 molecules (the geometric structures are shown in the figure 1) are employed in industry, as feed gases in cold plasmas.

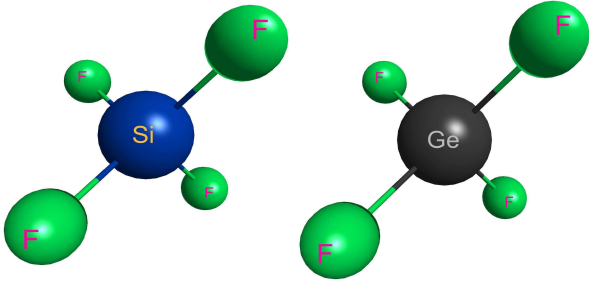


Figure 1. Geometrial structure of SiF_4 and GeF_4 .

The scattering problem it is treated by the Schwinger multichannel method (SMC) [2] implemented with pseudopotentials (SMCPP) [3] of Bachelet, Hamann and Schlüter [4]. The SMC method is a variational approximation to the scattering amplitude. To take polarizations effects into account, we considered single excitations of the target, from the occupied (hole) orbitals to the unoccupied (particle) orbitals. To represent the particle and scattering orbitals in polarizations calculations we used the improved virtual orbitals (IVOs) [6].

We present integral and differential cross sections for silicon tetrafluoride and germanium tetrafluoride in the static-exchange (SE) and

static-exchange plus polarization (SEP) approximations for collision energy up to 12 eV.

The ground-state geometry (the bond lengths between Si/Ge atom and the fluorines) were optimized using the package GAMESS [7] employing Møller-Plesset perturbation theory of second order with the 6-31G(*d*) basis.

In SiF_4 molecule we found a shape resonance located at about 8.5 eV which is associated in the T_2 symmetry. This system has also a Ramsauer-Townsend minimum at around 0.45 eV. The GeF_4 molecule showed an anomaly in low energy (below at 2 eV), this behavior was associated as a virtual state. Also found a form resonance at about 6 eV in the T_2 symmetry. In general we results are in good agreement with the previously shown in the literature for both the cases.

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