Electron collisions with CFX_3 and CF_2X_2 (X=Cl, Br, I) molecules: elastic and rotational excitations cross sections

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Dissociative electron attachment of molecules containing Carbon and halogen atoms have been widely studied over many years. These molecules are used in many practical fields as in chemical etching in plasma processing, which is an important step in the semiconductor fabrication. However, more information on the cross sections for electron collisions are needed. Experimental results on the cross sections are rare, and theoretical calculations are thus necessary. In the present work we report integral, differential and momentum transfer cross sections for elastic scattering of low-energy electrons by $CFCl_3$, $CFBr_3$, CFI_3, CF_2Cl_2, CF_2Br_2 and CF_2I_2 molecules. To calculate the cross sections we employed the Schwinger multichannel [1, 2] method with pseudopotentials [3] in the fixed-nuclei static-exchange approximation for incident energies up to 30 eV. We compared the differential and integral cross section of these molecules and found similarities between them. We also found a shape resonance in the integral cross sections of $CFCl_3$, $CFBr_3$ and CFI_3, and find two shape resonance in cross sections of CF_2Cl_2, CF_2Br_2 and CF_2I_2. We also compared our results with available experimental cross sections of $CFCl_3$ and CF_2Cl_2 and found good agreement. We also included the rotation effects to calculate cross sections for $J = 0, 1, 2, 3, 4, 5, 6$ excitation levels using the Adiabatic Nuclei Rotation approximation [4]. Since all molecules studied have permanent dipole moments, we included a first Born approximation [5] of the dipole potential correction to account for the long-range potential. $CFCl_3$, $CFBr_3$ and CFI_3 belong to C_{3v} symmetry group and are symmetric tops; CF_2Cl_2, CF_2Br_2 and CF_2I_2 belong to C_{2v} and are asymmetric tops. We compare the rotationally summed and rotationally unresolved cross sections for all molecules and we verify a very good convergence.

References

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