Electron scattering by CF$_3$I and CF$_3$Br

Matheus B. Kiataki, Márcio H. F. Bettega

UFPR - PR - Brasil

Electron scattering from CF$_3$I and CF$_3$Br and other halofluorocarbons molecules have been studied by many scientists due to their use as feedstocks gases in industrial plasmas and relation with its global warming potentials. Among them, CF$_3$I is the most environment-friendly gas since its lifetime in Earth’s atmosphere is just a few days, and therefore, a good alternative gas to replace traditional pollutant gases used in the plasmas industry, such as SF$_6$ and fully fluorinated hydrocarbons. CF$_3$Br, on the other hand, is known to be an ozone-layer depleting agent. Furthermore, CF$_3$I and CF$_3$Br are also utilized as fire suppressants. We present in this work calculated elastic differential and integral cross sections for low energy electron collisions with these halofluorocarbons (CF$_3$I, CF$_3$Br). To calculate the cross sections we employed the Schwinger Multi-channel Method with pseudopotentials in the static-exchange and static-exchange plus polarization approximations. The halofluorocarbons belong to C3v point group and differ from each other by the different heavy central atom and both have permanent dipole moments. In order to account for the long-range interaction of the dipole moment we included the Born Closure procedure. We found two shape resonances for the CF$_3$I, belonging to A1 and E symmetries and three shape resonances for the CF$_3$Br, where two of them belong to A1 symmetry and one to the E symmetry. For the CF$_3$Br we found a bound state in A1 symmetry in the static-exchange plus polarization approximation. The present results are compared with the results available in the literature and in general find a good agreement. Finally, we discuss the similarity and differences between the cross sections of these molecules.