

## Electron Collisions with $\text{CF}_x$ Radicals

Iryna Rozum and Jonathan Tennyson

Department of Physics and Astronomy  
University College London  
Gower St., London WC1E 6BT, UK

The plasma processing technology used in the fabrication of materials for micro-electronics has become one of the most vibrant and commercially successful industries. Despite its high cost and technical importance, plasma equipment is still largely designed empirically, with little help from computer simulations. Models of technological plasmas require quantitative data on the reactions of all the constituent neutral species and ions, especially data on collisional, reactive processes occurring within the plasma.

The molecular reactants currently used ( $\text{CF}_4$  and  $\text{C}_2\text{F}_6$ ) in plasma processing procedure have been found to be detrimental to the terrestrial environment and global climate as both are strong greenhouse gases.

$\text{CF}_3\text{I}$  and  $\text{C}_2\text{F}_4$  have been proposed as the next generation of plasma reactant since both have a low global warming potential. When bombarded with electrons these systems fragment into various  $\text{CF}_x$  radicals, about which little is known. In particular, there appears to be essentially no information available on how these radicals interact with low-energy electrons.

The purpose of this work is to develop a full description of electron  $\text{CF}_x$  radical collisions at energies up to 10 eV with particular emphasis placed on the energy range 2–5 eV as this is the typical energies of etching plasmas. We have performed calculations to obtain resonance parameters as well as elastic cross-sections and excitation cross-sections for the  $\text{CF}_2$  and  $\text{CF}_x$  molecular radicals in the incident electron energy range below 10 eV. Several low lying resonances were detected and fitted using our program RESON. We also performed several test target calculations for  $\text{CF}_3$  for several target models using different basis sets (6-31G\*, 6-311G\* and Sadlej-pVTZ). Surprisingly, there are no data on vertical excitation energies of  $\text{CF}_3$  available in the literature, so this is a necessary precursor to scattering calculations.