Calculation of Isotropic, Partial Cross Sections and rate coefficients for Electron Ionization of CF_4

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Ionization processes play an important role in many applications such as discharges and plasmas, gas lasers, mass spectrometry, and chemical analysis. Even though cross sections for the single step multiple ionization of a molecule are significantly smaller than cross sections for single ionization, multiple ionization processes are important in fusion plasmas and other high-temperature environments.

In the present work we calculate the isotropic/ angular cross sections for the production of singly charged ions (CF_3^+, CF_2^+, CF^+, F^+, and C^+) produced through the dissociative channels and doubly charged ions (CF_3^{++} and CF_2^{++}) produced through dissociative- double ionization of the CF_4 molecule by electron impact using a semi-empirical formulation based on the Jain-Khare approach [1,2]. The calculations are made at fixed incident electron energy of 100 eV. As no previous data seem for these cross sections, we have derived the partial and total ionization cross sections from the corresponding angular cross sections in the energy range of ionization threshold to 500 eV. Where possible we compare the present results with the recent experimental data [3] and theoretical data including those of BEB- calculations [4] and DM- calculations [5]. A satisfactory agreement with the available theoretical and experimental data has been noticed.

From the perspective of applications, in particular applications to fusion plasmas, it s often more desirable to have ionization rate coefficients available rather than electron impact ionization cross sections. We have computed ionization rate coefficients for CF_4 as a function of incident electron energy using the calculated ionization cross sections.

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References

1. S.Pal; Chem. Phys. **302**(2004) 119.
2. S.Pal, J.Kumar, T.D.Märk; J. Chem. Phys. **120** (2004) 4658.
3. B. G. Lindsay, K. F. McDonald, W. S. Yu, R. F. Stebbings, and F. B. Yousif. J. Chem. Phys. **121**, 1350-1356 (2004).
4. BED calculations, see www.physics.nist.gov/ionXsections/
5. H.Deutsch, K.Becker, S.Matt and T.D.Märk, Int. J.Mass Spectrom **197** (2000) 37.