

ELECTRON INTERACTIONS WITH CCl_2F_2

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We have completed a critically evaluated synthesis of the available information on cross sections and rate coefficients for collisional interactions of low energy electrons with dichlorodifluoromethane (CCl_2F_2) [1]. This gas has many industrial uses and is of significant atmospheric and environmental interest. While the available data are limited, particularly for electron collision cross sections, a reasonably complete set of cross sections and transport data are assembled.

The work presented here includes a review, an assessment, and a discussion of the following processes related to electron interactions with CCl_2F_2 : (1) *electron scattering*, including cross sections for total electron scattering, momentum transfer, differential elastic electron scattering, integral elastic electron scattering, and inelastic electron scattering for rotational and vibrational (direct and indirect) excitation; (2) *electron impact ionization*, including cross sections for total, partial, and double ionization, and coefficients for electron impact ionization; (3) *electron attachment*, including cross sections, rate

constants, and coefficients, and their energy and temperature dependencies, dissociative attachment fragment anions, and negative ion states; (4) *optical emission under electron impact*; and (5) *electron transport*, including electron drift velocity and ratio of transverse electron diffusion coefficient to electron mobility.

Figure 1 shows the cross sections (as a function of electron energy, ϵ) for total electron scattering, total direct vibrational excitation, integral elastic electron scattering, total ionization, and total electron attachment. These data are based primarily upon available experimental data. Stated uncertainties of the data from which these cross sections were derived vary from $\pm 5\%$ to $\pm 25\%$. Other cross sections, not presented here, due to space limitations or uncertain reliability, are discussed in Ref. [1].

The structure in the total electron scattering and total electron attachment cross sections is due to negative ion resonances. The average positions of these resonances

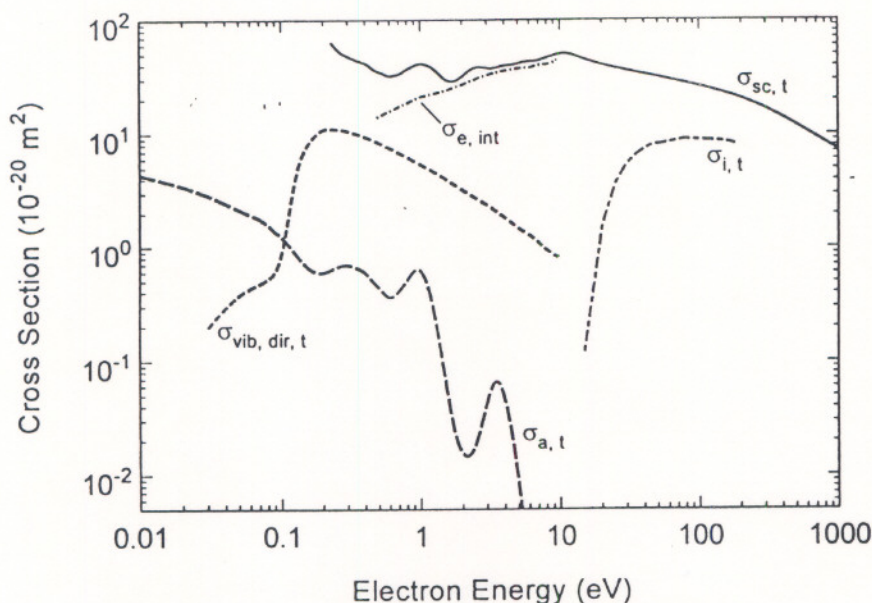


Fig. 1 Recommended cross sections for: total electron scattering, $\sigma_{sc,t}(\epsilon)$; integral elastic electron scattering, $\sigma_{e,int}(\epsilon)$; Bohr dipole approximation of total direct vibrational excitation, $\sigma_{vib,dir,t}(\epsilon)$; total ionization, $\sigma_{i,t}(\epsilon)$; and total electron attachment, $\sigma_{a,t}(\epsilon)$. Values for $\sigma_{e,int}(\epsilon)$ and $\sigma_{vib,dir,t}(\epsilon)$ are from Ref. [3], and the values for $\sigma_{i,t}(\epsilon)$ are from Ref. [4]. Values for $\sigma_{sc,t}$ and $\sigma_{a,t}$ are synthesized from several independent measurements.

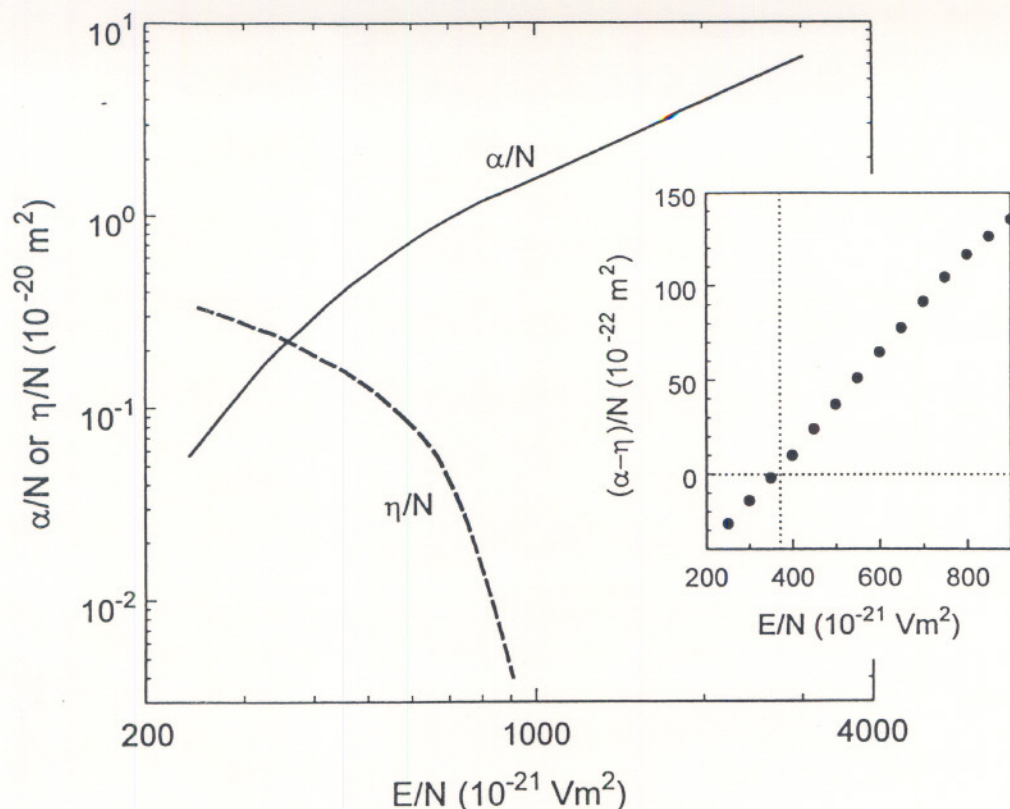


Fig. 2 Recommended density-reduced coefficients, based upon several experimental measurements, for electron impact ionization, α/N ; attachment, η/N ; and effective ionization $(\alpha-\eta)/N$.

(below 10 eV), determined from the results of a number of experimental methods, are: 0.9 eV, 2.5 eV, 3.5 eV, 6.2 eV, and 8.9 eV. The 8.9 eV resonance lies in the region of electronic excitation and most likely is associated with excited electronic states. The 0.9 eV resonance is likely to be due to the lowest negative ion state which has a shallow minimum about 0.4 eV below the zero-level, as is indicated by the positive value of the adiabatic electron affinity of CCl_2F_2 reported by Dispert and Lacmann [2].

The CCl_2F_2 molecule fragments rather extensively under electron impact, principally via dissociative ionization and dissociative attachment; the latter process is temperature dependent. No measurements have been made to investigate dissociation into neutral fragments.

Figure 2 shows a plot of our recommended values for the coefficients of electron attachment, ionization, and effective ionization. Stated uncertainties for the coefficient data from which these values are derived range from $\pm 3\%$ to $\pm 15\%$. Analysis of experimental measurements indicates that the effective ionization is zero when $E/N = (371 \pm 5) \times 10^{-21} \text{ Vm}^2$ (one standard deviation).

The data in Figs. 1 and 2 can form the basis of Boltzmann and/or Monte Carlo calculations to determine model-dependent collision cross section sets for this molecule.

Such information is required along with additional experimental measurements on a wide range of electron collision processes for this molecule, foremost electron-impact cross sections for momentum transfer and dissociation of CCl_2F_2 into neutral species.

The recommended data for this molecule, and for CF_4 (Ref. [5]) and CHF_3 (Ref. [6]), can be found on the WWW at <http://www.eeel.nist.gov/811/refdata>.

- [1] L. G. Christophorou, J. K. Olthoff, and Y. Wang, *J. Phys. Chem. Ref. Data* (submitted).
- [2] H. Dispert and K. Lacmann, *Intern. J. Mass Spectrom. Ion Phys.* **28**, 49 (1978).
- [3] A. Mann and F. Linder, *J. Phys. B* **25**, 1633 (1992).
- [4] K. Leiter, P. Scheier, G. Walder, and T. D. Märk, *Intern. J. Mass Spectrom. Ion Processes* **87**, 209 (1989).
- [5] L. G. Christophorou, J. K. Olthoff, and M. V. V. S. Rao, *J. Phys. Chem. Ref. Data* **25**, 1341 (1996).
- [6] L. G. Christophorou, J. K. Olthoff, and M. V. V. S. Rao, *J. Phys. Chem. Ref. Data* **26**(1), in press (1997).

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