Rerseach Notes

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Research Note

Semi-Empirical Electron-Impact Ionization Cross-Sections of Some Hydrocarbons

ARJUN TAN and S. T. WU
The Research Institute The University of Alabama in Huntsville Huntsville, AL 35807 U. S. A.

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Semi-empirical expressions for the electron impact ionization cross-sections of CH, CH_2, CH_3, and CH_4 are given with the appropriate values of the parameters. They constitute convenient interpolation formulas in the study of the Jovian ionosphere.

CROSS-SECTIONS for electron and proton collisions with various gases are important in plasma physics, atmospheric and ionospheric physics, planetary physics and other areas. Green and Barth[1] initiated the study of electron energy deposition in various atomic and molecular excitations and ionizations of a gaseous medium. Semiempirical analytic expressions have been sought for the cross-sections by adjusting various parameters and matching with experimental data. Cross-sections in parametric form have been worked out for He[2], N_2[3], O_2[4], N[5] and other constituents of the earth's atmosphere. This way of fitting provides direct applications where values over a broad energy are needed. It also provides convenient interpolation formulas between the fragmentary experimental data, which are restricted in energy range and also subject to experimental errors. The analytical formulas tend to smooth out the errors.

In this study, the ionization cross-sections of CH, CH_2, CH_3, and CH_4 for electron impact are matched with parametric expressions and the various parameters determined. CH, is a major constituent of the atmospheres of the Jovian planets and CH, CH_2, and CH_3 are the important products of photolysis of CH_4[6]. The ionization of these constituents due to energetic electrons from the solar wind and Jupiter's radiation belt could be an important source of ion production under Jovian conditions, particularly in high latitude regions.

Ionization cross-sections are usually treated in a series form, based on Born approximation. The differential cross-section for an ionization continuum state i may be written as

$$S_i(E, T) = \frac{q_0 A_0}{W^2} \left(\frac{I}{W}\right)^{\beta} \left(\frac{W}{E}\right)^{\alpha} \left[1 - \left(\frac{W}{E}\right)^{\beta}\right]^{\nu}, \qquad (1)$$

(1) A. E. S. Green and C. A. Barth: J. Geophys. Res. 70, 1083 (1965).
(2) A. E. S. Green and S. K. Dutta: J. Geophys. Res. 72, 3933 (1967).
(3) A. T. Jusick, C. E. Watson, L. R. Peterson and A. E. S. Green: J. Geophys. Res. 72, 3943 (1967).
(4) C. E. Watson, V. A. Dulock, Jr., R. S. Stolarski and A. E. S. Green: J. Geophys. Res. 72, 3961 (1967).
(5) S. S. Prasad and A. E. S. Green: J. Geophys. Res. 76, 2419 (1971).
(6) S. S. Prasad, L. A. Capone and L. J. Schneck: Geophys. Res. Letters 2, 161 (1975).

where E = primary electron energy
I = ionization potential
T = secondary electron energy
$W = T + I$
$q_0 = 4\pi a_0^2 R_y^2 = 6.514 \times 10^{-14}$ cm² eV²
a_0 = the Bohr radius
R_y = the Rydberg energy = 13.6 eV

and A_0, P, Ω, β, and ν are the parameters to be adjusted to experimental data.

In the present study, the values $\beta = 1, \nu = 2, p = 1$ have been chosen. Experimental ionization cross-sections of CH, CH_2, CH, and CH, for electrons of energy between 20 and 500eV have been taken from Adamczyk et *al.*[7]. The method used consisted essentially of obtaining a good fit with the exprimental data by properly adjusting the parameters I, Ω, and A_0. Initial values of the parameters are supplied bearing in mind that I determines the threshold of the curve, Ω gives a measure of the slope, while A_0 is directly proportional to the height. A rapid convergence is obtained by a good guess. The lower portion of the curve is first fitted and then the higher energy portion. In case of non-convergence with say 30 iterations, two or more curves are needed. In that case the lower energy portion is fitted first and the residual part is next fitted with another curve using a higher ionization potential I. This is exemplified by the cases of CH and CH_3.

The results of our study are given in Table I and Fig. 1-4. Cross-sections for CH_2 could be fitted with a single curve, whereas those of CH and CH, required two curves. The case of CH_4 presents an interesting example, requiring three curves for a proper fit.

Table 1. Parameters for Electron Impact Ionization Cross-Sections of Some Hydrocarbons

		I		A_0
CH	Component 1	21.0	4.0	0.75
	Component 2	45.0	1.35	0.09
CH_2	Component 1	13.0	0.86	0.058
CH_3	Component 1	15.0	1.8	1.1
	Component 2	45.0	1.02	0.1
CH_4	Component 1	9.0	0.8	0.243
	Component 2	50.0	1.6	0.6
	Component 3	230.0	1.0	0.1

(7) B. Adamczyk, A. J.H. Boerboom, B. L. Schram and J. Kistemaker: J. Chem. Phys. **44** 4640 (1966).

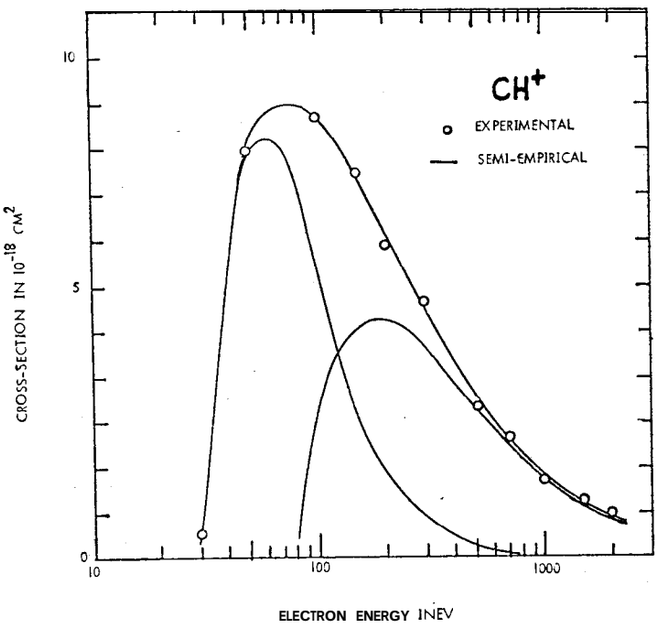

Fig. 1. Electron-impact Ionization Cross-Sections of CH.

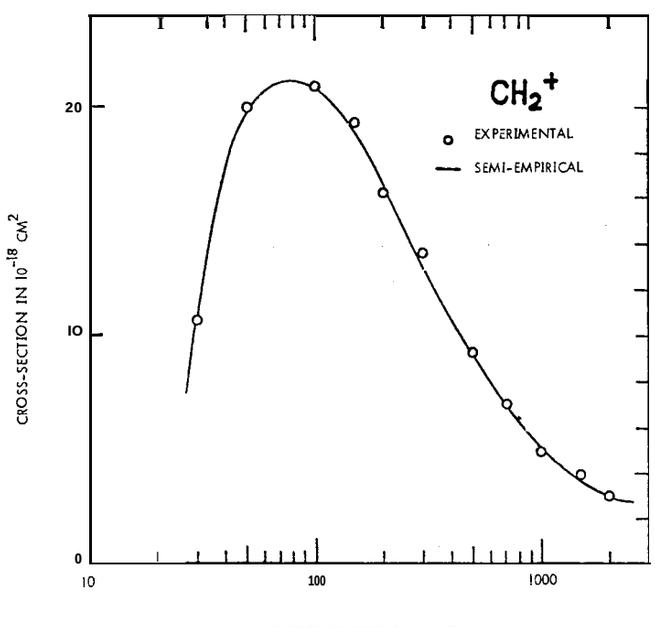

Fig. 2. Electron-impact Ionization Cross-Sections of CH_2.

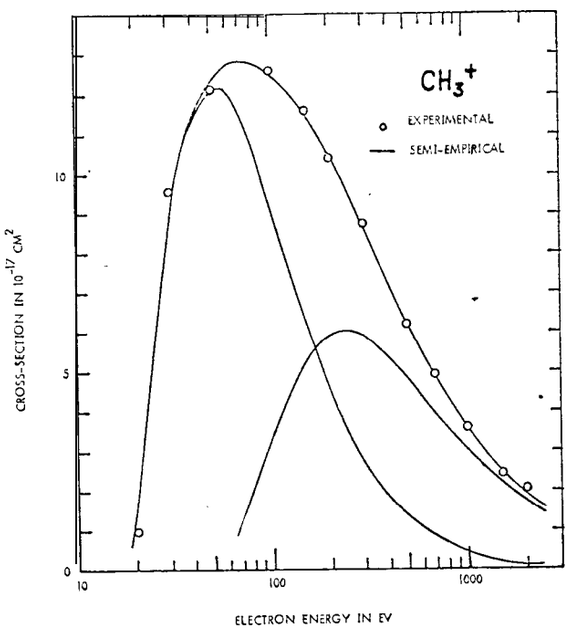

Fig. 3. Electron-Impact Ionization Cross-Sections of CH_3.

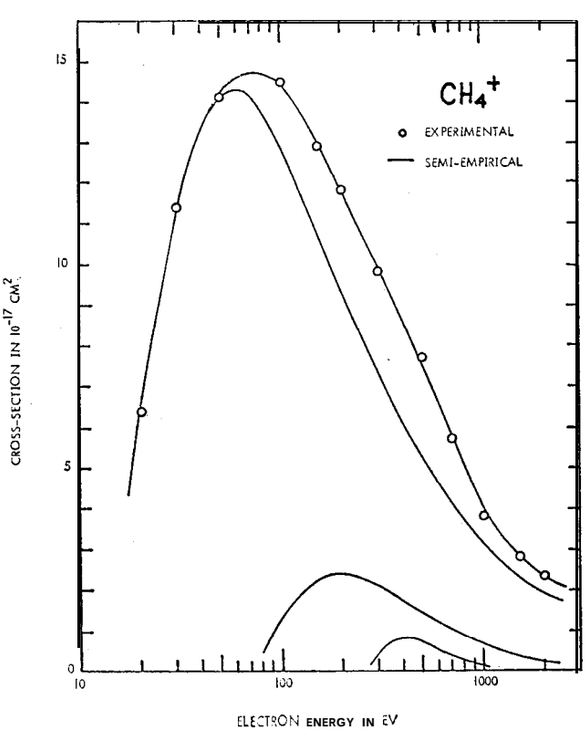

Fig. 4. Electron-Impact Ionization Cross-Sections of CH_4.