Database for Electron-Impact Total Ionization Cross Sections of Atoms and Molecules*

Y.-K. Kim and D. S. Zucker
National Institute of Standards and Technology,
Gaithersburg, MD 20899-0001

M. A. Ali
Chemistry Department, Howard University,
Washington, DC 20059

M. E. Rudd
Department of Physics and Astronomy,
University of Nebraska-Lincoln, Lincoln, NE 68588-0111

1 Introduction

A database for electron-impact total ionization cross sections of 43 atoms and molecules is available as part of the NIST Physics Laboratory web presentation:

http://physics.nist.gov/PhysRefData/Ionization/Xsection.html

This database presents theoretical cross sections based on the Binary-Encounter-Bethe (BEB) model for a large number of atoms, molecules, and radicals of interest in modeling low-temperature plasmas in magnetic fusion devices, plasma processing of semiconductors, radiation damages to materials, and cleaning of air pollutants by corona discharge. The database includes molecules such as H_2, H_2O, NO_2, O_3, SiH_4, and SF_6. For each target, the database compares the BEB cross section to available theoretical and experimental data.

2 Theory

The BEB model [1]-[4] combines a modified form of the Mott cross section with the Bethe cross section for high incident energy, T. The BEB model requires three constants per orbital, viz., the binding energy B, the average kinetic energy U, and the electron occupation number N. Then, the ionization cross section per orbital is given by:

$$\sigma_{BEB} = \frac{S}{t+u+1}\left[\frac{Q\ln t}{2}\left(1-\frac{1}{t^2}\right)+(2-Q)\left(1-\frac{1}{t}-\frac{\ln t}{t+1}\right)\right], \quad (1)$$

where t=T/B, u=U/B, $S=4\pi a_0^2 N(R/B)^2$, a_0=0.529 Å, R=13.61 eV and Q is a weighted integral of the target=s continuum oscillator strength [1]. For most targets, Q=1 is an excellent approximation. The total ionization cross section, σ_i, is obtained by summing σ_{BEB} over occupied orbitals.

* Work at NIST was supported in part by the Office of Fusion Sciences, USDOE.

The first logarithmic term in eq (1) is associated with the dipole interaction term from the Bethe theory, 1 – 1/t comes from the direct and exchange Coulomb interaction in the Mott cross section, and the last logarithmic term results from the interference between the direct and exchange terms of the Coulomb interaction.

Equation (1) is not a fitting formula, nor does it contain any adjustable or empirical parameters. Instead, the model uses ab initio constants obtained from the ground-state wave function of the target (with Q = 1). To match the experimental threshold, however, we recommend using the experimental vertical ionization potential for the outermost valence orbital, if available. Experimental ionization potentials (mostly adiabatic) of many molecules and radicals are available from another NIST database [5].

3 Results

The BEB model was found to be very effective in reproducing known ionization cross sections from threshold to several keV (within ±10% of *reliable* experimental data at the peak) for most of more than 50 atoms, molecules, and radicals we have tested so far. As an example, the BEB cross sections for CH and CF_4 are compared to available experimental data in Figures 1 and 2.

Using this database, a user can (a) calculate the BEB cross section on-line by typing in the desired incident energy; (b) look at graphical comparison of the BEB cross section to other theory and experiment with full references; and (c) download orbital constants and BEB cross sections in ASCII form. We found so far that the BEB model works extremely well for hydrocarbons, both stable molecules and radicals. The BEB model works better for closed-shell molecules than open shell molecules, and better for molecules than atoms.

4 Outlook

Ionization cross sections for more atoms and molecules will be added to the database as they become available. For instance, preliminary studies indicate that the BEB model produces reliable cross sections for closed-shell compounds of fluorine, such as CF_4, CHF_3, and C_4F_8, while substantial disagreement with experiments (sometimes a factor of 2) is found for radicals of fluorine compounds, such as CF and NF.

References

[1] Y.-K. Kim and M. E. Rudd, *Phys. Rev. A* **50**, 3954 (1994)

[2] W. Hwang, Y.-K. Kim, and M. E. Rudd, *J. Chem. Phys.* **104**, 2956 (1996)

[3] Y.-K. Kim, W. Hwang, N. M. Weinberger, M. A. Ali, and M. E. Rudd, *J. Chem. Phys.* **106**, 1026 (1997)

[4] M. A. Ali, Y.-K. Kim, W. Hwang, N. M. Weinberger, and M. E. Rudd, *J. Chem. Phys.* **106**, 9602 (1997)

[5] S. G. Lias, J. F. Liebman, R. D. Levin, and S. A. Kafafi, *"NIST Positive Ion Energetics Database"*

[6] V. Tarnovsky, A. Levin, H. Deutsch, and K. Becker, *J. Phys. B* **29**, 139 (1996)

[7] H. U. Poll, C. Winkler, D. Margreiter, V. Grill and T. D. Märk, *Int. J. Mass Spectrom. Ion Processes* **112**, 1 (1992)

[8] R. A. Bonham, *private communication* (1997)

[9] M. V. V. S. Rao and S. K. Srivastava, *Abstracts of the XXth International Conference on the Physics of Electronic and Atomic Collisions*, 23-24 July 1997, Vienna, Austria, p. MO150

[10] J. A. Beran and L. Kevan, *J. Phys. Chem.* **73**, 3866 (1969)

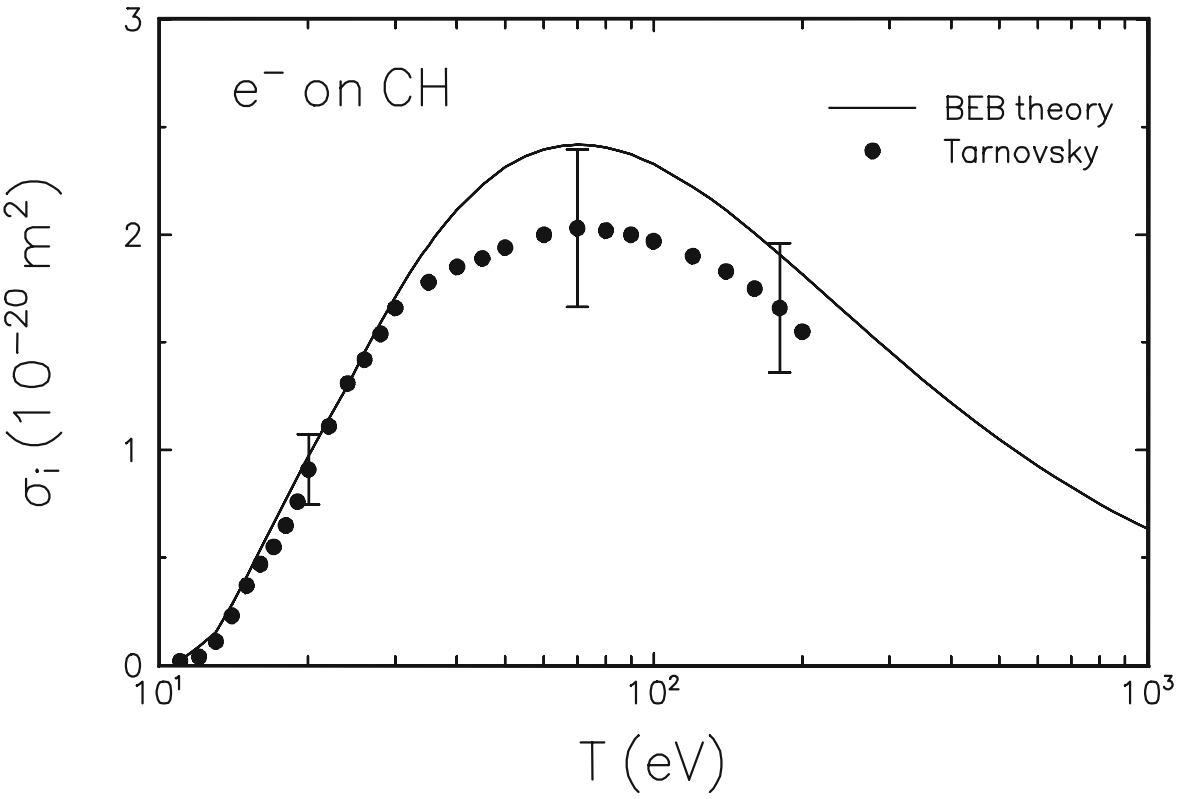

Figure 1: Comparison of ionization cross sections for CH. σ_i, total ionization cross section; T, incident energy; solid curve, BEB cross section; circles, experimental data by Tarnovsky et al. [6].

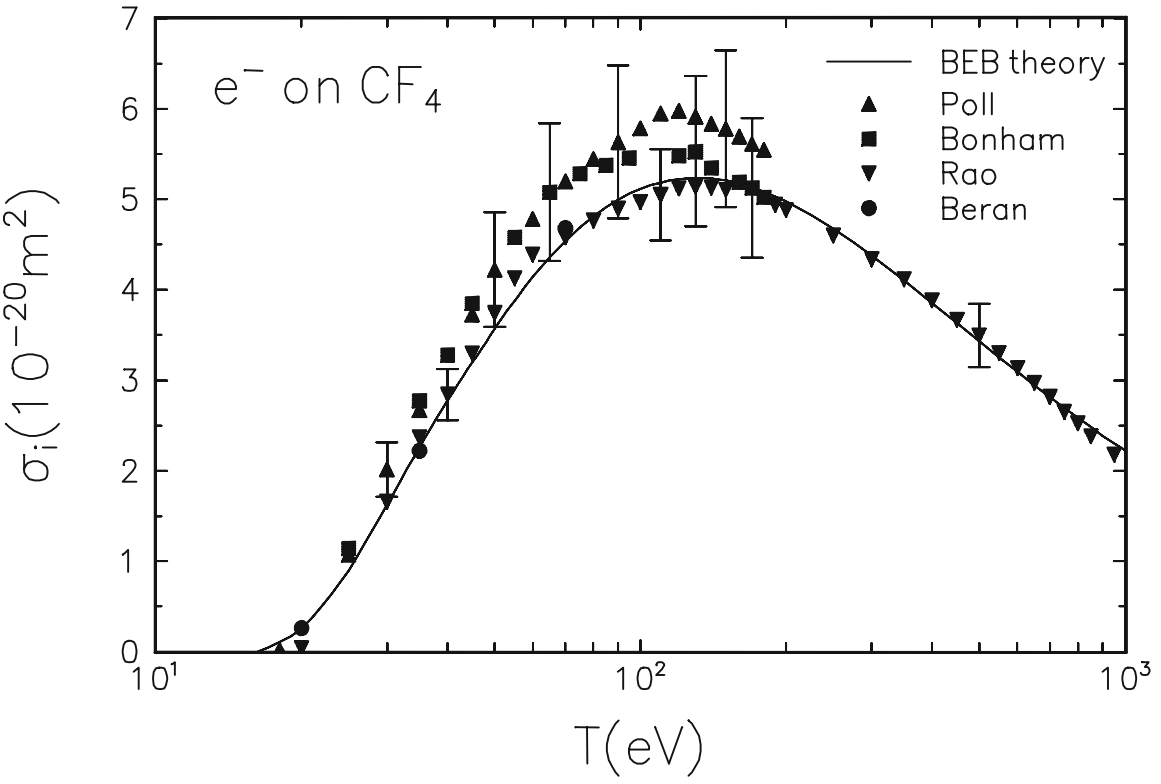

Figure 2: Comparison of ionizations cross sections for CF_4. σ_i, total ionization cross section; T, incident energy; solid curve, BEB cross section; upright triangle, experimental data by Poll et al. [7]; squares, data by Bonham [8]; inverted triangles, data by Rao and Srivastava [9]; circles, data by Beran and Kevan [10].