# Production and Compilation of Charge Changing Cross Sections of Ion-Atom and Ion-Molecule Collisions

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## Abstract

Single electron capture cross sections  $\sigma_{10}$ ,  $\sigma_{21}$  for singly and doubly ionized ions and double electron capture cross sections  $\sigma_{20}$  for doubly ionized ions of Be, B, Fe and Ni with atomic and molecular gas targets are derived experimentally in the energy range of 0.5 - 32 keV. The current status of our compilation of experimental cross sections for charge changing collisions is also presented.

## Keywords:

electron capture, charge exchange, cross section, beryllium, boron, iron, nickel, collisional database

## 1. Introduction

Charge changing processes of ions for high-Z materials including stainless consisting elements as well as low-Z materials such as Be and B are of practical importance for controlled thermonuclear fusion research. Upon this point of view, we have been cooperating in production and compilation of experimental charge changing cross sections for ion-atom and ion-molecule collisions since 1983, as a part of data center activities of JAERI [1].

We have measured single and double electron capture cross sections for  $C^{q+}$  (q = 1 - 4) ions with H<sub>2</sub>, CH<sub>4</sub>, C<sub>2</sub>H<sub>6</sub>, C<sub>3</sub>H<sub>8</sub> and CO<sub>2</sub> molecules in the collision energy range of (1 - 20)q keV [2], and now devoted to the single and double electron capture cross sections,  $\sigma_{10}$ ,  $\sigma_{21}$  and  $\sigma_{20}$ , and even the electron loss cross sections  $\sigma_{12}$  for Be, B, Cr, Fe and Ni ions colliding with He, Ne, Ar, Kr, H<sub>2</sub>, CO, CO<sub>2</sub>, CH<sub>4</sub>, C<sub>2</sub>H<sub>6</sub>, C<sub>3</sub>H<sub>8</sub>, CO, CO<sub>2</sub> and N<sub>2</sub> atoms and molecules at collision energies of 0.5–32 keV. In this paper, results for electron capture cross sections for Be, B, Fe and Ni ions are presented with the current status of the data compilation.

#### 2. Experiment

The experiment has been performed using the Van de Graaff Accelerator Facility of the Quantum Science and Engineering Center, Kyoto University. As is illustrated in Fig.1, incident ions were obtained by Ion-

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Fig. 1 The experimental setup.

Impact-Ion-Source [3], in which a pump beam of 0.8 MeV  $CO_2^+$  impacts a metal wire. For production of Be, Fe and Ni ions, pure metallic wires of  $\geq 99.9\%$  purity were set in the ion-source, while a wire of Fe, B and Si alloy was used for B ion. A combination of a Wien-filter and an electric field for removing neutrals (Neutral Particle Rejecter; NPR) selects the incident ion by its charge state. Another role of the NPR is to remove the backscattered fragments of the pump beam, because the charged fragments at equal velocity can pass the Wien Filter. The selected ion beam collides with the target gas, filled in a gas cell, whose pressure was monitored with a high-sensitivity-Pirani gauge calibrated with a capacitance manometer (MKS Baratron). Outgoing ions were electrostatically separated and de-

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tected with position sensitive detector utilizing a micro channel plate (MCP-PSD). All the charge-separated ions and neutrals were detected with a single MCP so that the detection efficiencies cancel each other on deriving the charge fractions. Signals from MCP-PSD were recorded event by event to confirm that the detection efficiencies for each charge fraction do not differ under different counting rates by reproducing the pulse height distributions for each detector position. Cross sections were derived by a growth method under single collision condition with gas target pressures of  $10^{-2} - 10^{-1}$  Pa, while the base pressure of the vacuum chamber was kept below  $8 \times 10^{-8}$  Torr. To guarantee the blow out of the target gas from both ends of the gas cell, we included the half diameter of the entrance and exit apertures (0.5 and 4.0 mm, respectively) to the gas cell length (45.0 mm). The validity of this calibration had been confirmed by measuring  $H^+ + H_2 \rightarrow H$  single capture cross section with the present apparatus at 7.5 keV. The total uncertainties are estimated to be 9-20 %, which mainly come from the effect of residual gases and the uncertainty of Pirani gauge reading.

## 3. Experimental results

The measured cross sections are presented in Figs. 2 and 3 for low-Z (Be, B) and high-Z (Fe, Ni) projectile ions, respectively, with theoretical results for  $Be^{q+}$  (q = 1, 2) + He collision systems by Shimakura  $(\sigma_{10})$  [4], Fritsch  $(\sigma_{21,20})$  [5] and Suzuki *et al.*  $(\sigma_{21})$ [6],  $\sigma_{21}$  for Be<sup>2+</sup> + H<sub>2</sub> collision system by Kimura and Lane [7] and Schultz *et al.* [8], and  $\sigma_{10}$  for B<sup>+</sup> + He collision system by Shimakura et al. [9] and Hansen and Dubois [10]. As for high-Z ions, no data has been published for the present collision systems in this energy range except for the experimental measurement of  $\sigma_{10}$ for  $Fe^+$  + Ar, N<sub>2</sub> collisions by Layton *et al.* [11], which covers the higher continuous energy region. In the Fig. 2(a), the calculations of Shimakura [4] and Fritsch [5] for the single electron capture cross sections  $\sigma_{10}$  and  $\sigma_{21}$ , respectively, for He target are found to have an excellent agreement with the present experiment. Also the calculation of Kimura and Lane [7] for H<sub>2</sub> target shows an excellent agreement with the present experiment in the Fig. 2(a'). The calculation of Schultz et al. [8] was derived by classical trajectory Monte Carlo (CTMC) method and has no calculation point in the present energy range, but its interpolation coincides very well with our measurement. The present cross sections for  $Fe^+$  + Ar, N<sub>2</sub> collisions fairly well connect the experimental results by Layton et al. [11], although the present values are found to be a little higher, which may come from the metastable fractions of Fe<sup>+</sup> ion produced in the impact-ion-source. Our preliminary result for single electron capture cross section of  $Cr^+$  indicates that the metastable fractions may give rise to the electron capture by a factor of 10 or so. It is also demonstrated in the Fig. 3 that the cross sections for double electron capture  $\sigma_{20}$  to form the neutral atom are larger than or comparable to those for single electron capture  $\sigma_{10}$  for Ni ions in the energy range investigated. For better understanding the electron capture collisions of transition metal ions, further studies are required both in experimentally and theoretically.

## 4. Data compilation

We have been compiling experimental total cross section data for electron capture or loss since 1983, and partial cross section data since 1992, published in journals of our selection. Experimental cross sections for some related interactions, like inner-shell ionization of target, ion-ion collisions, cluster collisions and so on, are also under the compilation since 1995. This compilation has been done not specifying the projectile ion or target of the collision system, taking its aim at a larger area of applications as well as fusion research. All the compiled data after 1989 are stored numerically, including the case that only a figure is published. An electrical version of this compilation is under the development now, utilizing Oracle database management system. We have defined the database structure, which consisted of 8 tables. The collected papers are indexed by document number key "docno" and the data are indexed by a combination of document and system number keys "docno, sysno", for cases that single paper includes multiple collision systems. The most important tables are the ones called COL, DATA and DOC, which store collision system information, numeric data and bibliographic indexes, respectively. In case that cross section data for some collision system are required, "docno, sysno" keys for the desired system are looked up in the table COL and the numeric data are derived from the table DATA using those "docno, sysno" keys. If the bibliographic information is additionally required, it can be looked up in the DOC table with "docno" key. Reference with specifying the known paper's information is also possible by looking the "docno" key up in the table DOC and look into COL and DATA tables. We intend to open this electrical version to the public through web browsers, and to make it possible for other database systems to make an SQL query through provided account and password by opening the database specifications.

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Fig. 2 Single and double electron capture cross sections  $\sigma_{10}$ ,  $\sigma_{21}$  and  $\sigma_{20}$  for (a), (a') Be ions and (b), (b') B ions. In the (a) and (b) quadrants, circles, down triangles, squares and diamonds denote He, Ne, Ar and Kr targets, respectively, while circles, down triangles, squares, diamonds, up triangles and hexes denote H<sub>2</sub>, CH<sub>4</sub>, C<sub>2</sub>H<sub>6</sub>, C<sub>3</sub>H<sub>8</sub>, CO and CO<sub>2</sub> targets, respectively, in the (a') and (b') quadrants. Present value: symbols connected with full and dashed lines,  $\sigma_{10}$  and  $\sigma_{21}$ , respectively; small symbols connected with dotted lines,  $\sigma_{20}$ . Theories: (a) full line,  $\sigma_{10}$  for He by Shimakura [4]; long and short dashed line,  $\sigma_{21}$  for He by Fritsch [5] and Suzuki *et al.* [6], respectively; dotted line,  $\sigma_{20}$  for He by Fritsch [5]; (a') full and dashed line,  $\sigma_{21}$  for H<sub>2</sub> by Kimura and Lane [7] and Schultz *et al.* [8], respectively; (b) full and dashed line,  $\sigma_{10}$  for He by Shimakura *et al.* [9] and Hansen and Dubois [10], respectively.



Fig. 3 Single and double electron capture cross sections  $\sigma_{10}$ ,  $\sigma_{21}$  and  $\sigma_{20}$  for (a), (a') Fe<sup>+</sup> ion, (b1), (b1') Ni<sup>+</sup> ion and (b2), (b2') Ni<sup>2+</sup> ion. In the (a), (b1) and (b2) sections, circles, squares and diamonds denote He, Ar and Kr targets, respectively, while dark circles, down triangles, squares, diamonds, up triangles, hexes and pale circles denote H<sub>2</sub>, CH<sub>4</sub>, C<sub>2</sub>H<sub>6</sub>, C<sub>3</sub>H<sub>8</sub>, CO, CO<sub>2</sub> and N<sub>2</sub> targets, respectively, in the (a'), (b1') and (b2') sections. Present value: symbols connected with full and dashed lines,  $\sigma_{10}$  and  $\sigma_{21}$ , respectively; small symbols connected with dotted lines,  $\sigma_{20}$ . Smaller square and circle with full line in the (a) and (a') sections denote experimental values  $\sigma_{10}$  for Ar and N<sub>2</sub> targets, respectively, by Layton *et al.* [11]

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