CHARGE EXCHANGE PROCESSES INVOLVING IRON IONS*

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CONF-8509180--1

DE86 001353

ABSTRACT

A review and evaluation is given of the experimental data which are available for charge exchange processes involving iron ions and neutral H, H₂ and He. Appropriate scaling laws are presented, and their accuracy estimated for these systems. A bibliography is given of available data sources, as well as of useful data compilations and review articles. A procedure is recommended for providing single approximate formulae to the fusion community to describe total cross sections for electron capture by partially-stripped Fe^{q+} ions in collisions with H, H₂ and He, based on the scaling relationships suggested by Janev and Hvelplund.

Report prepared for the IAEA Advisory Group Meeting on
Atomic Data for Fusion Plasma Modelling, Vienna, Austria
September 18-20, 1985

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*Research sponsored by the Office of Fusion Energy, U.S. Department of Energy, under Contract No. DE-AC05-84OR21400 with Martin Marietta Energy Systems, Inc.

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1. INTRODUCTION

Charge exchange (electron capture) collisions involving multiply charged ions and neutral species have been studied extensively during the last decade. Much of the experimental and theoretical work has been motivated by data requirements of controlled-thermonuclear fusion research, and as a result, much of the available data is for species which are of particular importance in fusion plasmas. Iron is an example of a specific ion which has received attention because of its importance as an impurity in nearly all magnetically-confined plasmas.

The subject of charge exchange collisions of multiply charged ions with neutrals (especially hydrogen atoms and molecules) has been reviewed from the perspective of fusion research by a number of researchers. Gilbody (1982) and de Heer (1983) have analyzed this subject from an experimental perspective, and the theory has been covered in a number of review articles, including those of Bransden (1983) and Janev and Presnyakov (1985). Experiments and theory for state-selective electron capture have also been analyzed recently by Janev and Winter (1985). The present report will concentrate on the data base for Fe ions in collision with H, H₂ and He. These are considered to be the most important reactant combinations for present-day plasmas and future reactors. The process we shall consider is the following:

A = H, H₂ or He

n = 1 for H; n = 1,2 for H₂ or He

2. GENERAL FEATURES

Charge exchange cross sections are characterized by a number of general features. Discussion of the process is usually divided into two energy regions, depending on whether the relative collision velocity is fast or slow compared to the mean velocity of the bound electron which is to be captured. For capture from hydrogen, this velocity is 1 a.u., or 2.2×10^8 cm/s, which corresponds to a collision energy of 25 keV/amu. In the low-velocity (adiabatic) region, the electronic structure of the interacting species can adjust to the changing internuclear field as the particles approach and separate, and a quasi-molecular description of the collision process is required. In the high velocity (diabatic) region, the collision is relatively fast, and a perturbation-type treatment becomes applicable.

Some general features of cross sections for electron capture by multiply charged ions from neutrals are summarized below.

For a given neutral species at low velocities:

1. For multiply-charged, partially stripped ions, the cross sections tend to be large, velocity and ion-species independent, and to scale approximately linearly with q .
2. For nearly-fully-stripped ions at the lowest energies, the capture is highly state-selective, the cross sections do not scale with q in a simple way, and are velocity-dependent.

For a given neutral species at high velocities:

1. The cross sections fall rapidly with increasing velocity.
2. The cross sections for partially-stripped ions depend only on q and are almost ion-species-independent.

3. Cross sections scale as q^n , where n varies between 2 and 3, increasing with velocity.
4. The distribution of final states of principal quantum number n becomes broader with increasing collision velocity.

3. DATA BASE FOR IRON

Total electron-capture cross section measurements have been reported for a number of charge states of iron ions in collisions with hydrogen atoms and molecules, but iron data is available for helium only at an energy of 7.1 MeV/amu for $q=26$. The available experimental data for multiply-charged ions colliding with atomic hydrogen have been compiled by Tawara et al. (1983a). The corresponding data for H_2 have been compiled by Tawara et al. (1983b) and by Huber and Kahlert (1982). A search of the current bibliographic files of the ORNL Controlled-Fusion Atomic Data Center indicated these compilations to be complete, and failed to identify any subsequent data in the energy range judged relevant to fusion-energy research (0.001 - 1000 keV/amu).

All of the data have been obtained by the fast ion beam - gas target method, in which a mass-per-charge and velocity selected ion beam is directed through a differentially-pumped gas target cell. The total electron-capture cross section is determined from the variation with gas density of the fraction of ions which capture an electron, which is linear under single-collision conditions. The target-thickness (product of gas density and effective cell length) is determined either by gas pressure measurement, or by normalization to a well-established cross section for some projectile ion such as H^+ . All the data for hydrogen atoms were obtained by use of a thermal-dissociation gas target, in which H_2 is

admitted into a tungsten tube heated to about 2300 K. The dissociation fraction is determined by measuring a double-electron-capture signal for some incident ion as a function of oven-tube temperature under single-collision conditions. Since double electron capture is not possible from hydrogen atoms, this signal decreases as the H_2 becomes dissociated.

In principle, the methods discussed above are capable of producing total cross sections with accuracies of 10-15% for H_2 and He targets, and 15-20% for H. The actual absolute accuracy of a particular experiment depends on the care which was exercised to ensure that the gas target was well-characterized, and that all product ions were detected and counted with unit or known efficiency. These considerations are relatively more important at the lower collision energies. In general, the projectile ion beam will contain some unknown fraction of ions in metastable states, regardless of whether the ion beam was produced directly in an ion source, or by stripping a lesser-charged fast ion beam in a thin foil or gas cell. In any case, the state distribution of the incident ions will probably be representative of those which will exist in the plasmas for which these data are intended to be applied. The presence of metastable states does, however, complicate many comparisons of experiment and theory, the latter of which is almost always for the ionic ground state. Nevertheless, the electron-capture process for multiply charged ions tends to be dominated by the strong ionic Coulomb field, and is not expected to be influenced significantly by the quantum state of the projectile ion.

The available sources of experimental data for charge exchange collisions of Fe ions with H, H_2 and He are listed in Table 1. An estimated accuracy is also given for each source. A few double electron capture cross

sections have also been measured for H_2 and He targets at the higher collision energies, and are typically 10% or less of the single capture cross sections. Thus double electron capture can probably be safely ignored for most fusion plasma applications.

The availability and consistency of experimental data for charge exchange in $Fe^{5+} + H$ and $Fe^{6+} + H$ collisions are shown in Figure 1, reproduced from the compilation by Tawara et al. (1983a). In this case, data are available both at low and at high energies. However, there are no low-energy experimental data for ionic charges q greater than 14. Thus theoretical predictions and scaling laws must be considered for these cases, as will be discussed later.

4. EXPERIMENTAL RESULTS AND SCALING LAWS

A. Low Energies

The relative energy-independence of the total capture cross sections for partially-stripped ions at low energies is clearly shown by the data in Figure 1 for Fe^{5+} and Fe^{6+} colliding with H-atoms. The data for H_2 show a similar energy-independence. In these many-electron collision systems, the energy-level structure of the final ionic state is complex, and thus a number of curve-crossings occur which are favorable for capture. For fully or nearly fully stripped ions, the levels in the final ionic state become highly degenerate, fewer curve crossings occur which are favorable for capture, and the resonant selectivity of the capture process at low velocities can produce large or small cross sections, which are velocity-dependent (see for example Meyer et al., 1985).

The scaling of low-energy electron capture cross sections for Fe^{q+} ions colliding with H atoms is shown in Figure 3, from Phaneuf (1983),

where these data are compared with similar data for $\text{Xe}^{q+} + \text{H}$ collisions, and also with predictions of the absorbing-sphere, the tunneling and the classical over-barrier models. The dashed line represents the simple empirical relationship:

$$\sigma_{q,q-1}(\text{H}) = q \times 10^{-15} \text{ cm}^2 \quad (1)$$

and describes the data with an rms deviation of 26%. This relationship was found to give a comparable average representation of similar data for Al^{q+} ions. In the case of molecular hydrogen, the following scaling relationship was found:

$$\sigma_{q,q-1}(\text{H}_2) = 0.85 \times q \times 10^{-15} \text{ cm}^2 \quad (2)$$

The above relationships are expected to be valid in the low-velocity region to within 30% on the average for any partially stripped projectile ion.

No experimental data are available at low velocities for fully-stripped or nearly-stripped Fe ions. The only theoretical data available for Fe^{26+} at these velocities are the multichannel-Landau-Zener-with-rotational-coupling (MLZRC) calculations of Janev et al. (1983), and the perturbed-stationary-state calculations of Salop and Olson (1979). The MLZRC calculations agree within 30% or better with the measurements of Meyer et al. (1985) for bare ions of charges $Z = 6-10$ colliding with H-atoms. Their theory also predicts quite well the observed velocity dependences for these systems. However, it is dangerous to extrapolate the reliability of such calculations from $Z=10$ to $Z=26$.

B. High Energies

The situation at higher energies is much better in hand, in part because fast projectile beams can be produced more easily by foil or gas stripping, and in part because the cross sections behave in a more orderly and predictable manner. Figure 3, taken from a paper by Meyer et al. (1979), shows the scaling of total electron-capture cross sections with ionic charge at fixed collision energies for Fe and Si projectiles in H and H₂. The cross sections scale with charge as q^p , where the power p varies from 1.7 at 60 keV/amu to 2.8 at 161 keV/amu. Berkner et al. (1981) found a similar scaling for $\text{Fe}^{q+} + \text{H}_2$ collisions. At energies above 275 keV/amu, they found that their data can be described by the formula:

$$\sigma_{q,q-1}(\text{H}_2) = (1.2 \times 10^{-8}) \times q^{3.15} \times E^{-4.48} \text{ cm}^2, \quad E(\text{keV/amu}) > 275 \quad (3)$$

It has been shown by Crothers and Todd (1980) that semiclassical OBK, eikonal, continuum intermediate-state and continuum distorted-wave theories all predict a q^3 scaling at asymptotically-high velocities for collisions of fully-stripped ions with hydrogen atoms.

The fact that electron-capture cross sections in this high-velocity range depend strongly on the ionic charge q , but weakly on ionic species is illustrated in Figure 4, from Meyer et al. (1979) for seven- and fourteen-times charged O, Si, Fe, Mo, Ta, W and Au ions colliding with H-atoms and molecules. The rapid fall-off with increasing velocity is also apparent. On the basis of the Bohr-Lindhard (1954) model, Crothers and Todd (1980) have shown that the cross section for a bare ion colliding with a hydrogen atom at high energies is given by the expression

$$\sigma_{q,q-1}(\text{H}) = 7.03 \times 10^{-16} q^3 (v/v_0)^{-7} \text{ cm}^2, \quad v_0 = 2.188 \times 10^8 \text{ cm/s.} \quad (4)$$

This prediction is compared to the available measurements for collisions with bare ions in Figure 5, adapted from a paper by Goffe et al. (1979). The agreement at energies above about 50 keV/amu is seen to be quite reasonable.

This uniform behavior in the high velocity region has led to a number of attempts to establish scaling laws for electron capture for partially-stripped ions in various gas targets. Janev and Hvelplund (1981) discussed the status of such scaling laws for electron capture, target ionization and total electron loss by the neutral target, which is the sum of capture plus ionization. For electron capture, they found that the available cross section data for multiply charged ions colliding with H and He could each be described quite well by a single curve, if σ/q were plotted versus $E/q^{1/2}$. This representation follows from adiabatic considerations in the low-velocity region, and at high energies from the Bohr-Lindhard (1954) classical theory and also the Born approximation. The maximum deviations of individual data points from these curves are about a factor of two, but the rms deviation is much smaller.

Knudsen et al. (1981a) have examined such scalings for H and H₂ targets within the context of the Bohr-Lindhard model. In Figure 7, taken from their paper, they plot the ratio $\sigma(\text{H}_2)/\sigma(\text{H})$ versus a reduced energy $E/q^{4/7}$ for the available data on multiply charged ions. The ratio is 0.76 over a wide range in the low-energy region, and increases to 3.84 at high energies. Since the empirical curve in Figure 6 for H suggests that the cross section at low energies is energy-independent and proportional to the

charge q , it is interesting to compare the predictions from Figures 6 and 7 with the empirical relationships of Eqs. 1 and 2. For H, Janev and Hvelplund's value is about 90% of that from Eq. 1, and for H_2 , about 80% of that from Eq. 2. It should be noted that the low-energy data of Phaneuf (1983) were not available at the time these scalings were examined.

Knudsen et al. (1981b) have performed a comparative analysis of available data for electron-capture collisions of multiply-charged ions with atomic hydrogen and noble gas atoms. On the basis of the Bohr-Lindhard model, they analytically derive a set of formulae to describe capture from an arbitrary target atom of nuclear charge Z . The agreement of this relatively simple classical theory with the data for H, He, Ar and Kr is surprisingly good.

A number of other theoretical methods have been applied to electron capture by multiply charged ions from atomic hydrogen. The most successful have been the classical-trajectory Monte-Carlo (CTMC) method introduced by Olson and Salop (1977), and the unitarized-distorted-wave (UDWA) method introduced by Ryufuku and Watanabe (1979). Both methods produce cross sections which are in good agreement with experimental data for partially-stripped ions at energies above roughly 100 keV/amu. Figure 8 is taken from a recent paper by McDowell and Janev (1985), and shows a comparison of their CTMC calculations with available data for $Fe^{13+} + H$. The agreement is seen to be very good. In this case, allowance was made for the fact that the incident ion is not fully stripped via a variable charge potential.

There are no experimental data available in the energy range of interest to fusion on partial cross sections for electron-capture into specific final states for Fe^{q+} ions incident on neutrals. The subject of

state-selective electron capture by multiply charged ions has been recently reviewed in depth by Janev and Winter (1985). CTMC calculations of (n, l) final-state distributions for capture by bare projectiles from H atoms are shown in Figure 9, from Olson (1981). The distributions broaden with increasing collision velocity, and the predicted peaks in the n -distributions occur at $n \sim q^{3/4}$. The UDWA calculations are generally consistent with the CTMC results. Since there are no experimental data available at present for state-selective capture by bare or partially-stripped Fe projectile ions, a recommendation at this time is probably premature. Such data are of principle importance at present for diagnostics of bare ions using injected neutral hydrogen beams (Isler et al., 1981). In such applications, the CTMC or UDWA results for bare ions are the best estimates available.

5. RECOMMENDATION

In terms of recommending data to the fusion community for total electron capture in collisions of Fe^{9+} ions with H, H_2 and He, it is suggested that advantage be taken of the low and high energy scaling properties exhibited by the data and predicted by theory.

For H and H_2 , the available experimental cross-section data, for Fe^{9+} ions only, should be plotted in terms of the scaled variables suggested by Janev and Hvelplund (1981), as discussed in Part 4 of this report. A least-squares fit of an appropriate functional form should be then be made to these data, and an analysis performed of the deviations from this functional fit. The uncertainties in the recommended cross sections should then be estimated from this analysis, and from an analysis of the individual experiments.

For collisions with He atoms, a similar procedure should be followed, except that all the available data for multiply-charged ions in the range of atomic numbers $10 < Z < 80$ should be included, since none exist specifically for Fe ions. The uncertainty in the data recommended using this procedure should be determined from an analysis of the variation of the experimental cross sections with Z for fixed ionic charge.

Should the Advisory Group determine that this procedure is appropriate for recommending electron-capture data to the international fusion-research community, the ORNL Controlled-Fusion Atomic Data Center would be willing to perform this analysis. One advantage of such a procedure is that it could easily be updated, should new data become available.

ACKNOWLEDGMENTS

The author is indebted to R. K. Janev for many useful discussions on the electron capture process, and on the applicability of scaling laws.

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Table 1. Experimental charge exchange data for iron ions

Neutrals	Charge States	Energy Range keV/amu	Accuracy	Reference	Comments
H, H ₂	3 < q < 14	0.01 - 0.095	25%	Phaneuf (83)	laser-plasma source time-of-flight analysis
H, H ₂	5,6	0.3 - 2.2	20% H 15% H ₂	Crandall et al. (1980)	PIG ion source electrostatic analysis
H ₂	3,5	0.02 - 0.05	?	Huber and Kahlert (1982)	not published
H	4 < q < 13	27 - 290	35%	Gardner et al.	foil stripped fast beam magnetic analysis
H, H ₂	4 < q < 15	60 - 161	20% H 15% H ₂	Meyer et al. (1979)	foil, gas-stripped fast beam, magnetic analysis
H ₂	11 < q < 22 9 12	1,100 277 14,262	15%	Berkner et al. (1978)	foil-stripped fast beam, magnetic analysis
H ₂	3 < q < 13 9 < q < 16 16 < q < 22 20 < q < 25	103 294 1,160 3,400	20%	Berkner et al. (1981)	foil-stripped fast beam magnetic analysis
H ₂	20 < q < 25	3,400	20%	Berkner et al. (1977)	foil-stripped fast beam, magnetic analysis
He	26	7,143	45%	Jolly et al. (1984)	foil-stripped fast beam, X-ray measurements

FIGURE CAPTIONS

Fig. 1. Compiled experimental cross section data for $\text{Fe}^{5+} + \text{H}$ and $\text{Fe}^{6+} + \text{H}$ collisions, from the compilation by Tawara et al. (1983).

Fig. 2. Ionic charge scaling of experimental total electron capture cross sections for $\text{Fe}^{q+} + \text{H}$ (solid circles) and $\text{Xe}^{q+} + \text{H}$ (open circles) at collision velocities near 1×10^7 cm/s, from Phaneuf (1983). The data are compared to the predictions of various generalized theoretical models. The short-dashed line represents the empirical scaling of Eq. 1.

Fig. 3. Scaling of experimental total electron-capture cross sections for Fe^{q+} and Si^{q+} ions colliding with H and H_2 at a number of fixed collision energies, from Meyer et al. (1979). The lines represent power-law least-squares fits to the data.

Fig. 4. Comparison of experimental cross sections plotted as functions of collision velocity for a number of different projectile ions of charge $q=7$ and $q=14$ incident on H and H_2 , from Meyer et al. (1979).

Fig. 5. Comparison of experimental cross sections plotted versus energy for a number of bare ions colliding with H and H_2 , adapted from Goffe et al. (1979). The dashed and chain-dashed curves represent experimental data, and the solid curve is the q^3 scaling law of Crothers and Todd (1980), represented by Eq. 4.

Fig. 6. Reduced experimental cross sections plotted versus reduced collision energy for electron capture by multiply-charged ions from H and He , from Janev and Hvelplund (1981). All experimental data which were

available at the time are included. The solid line represents the slope of a q^3 scaling in this reduced representation of the cross sections.

Fig. 7. Ratio of experimental cross sections for electron capture by multiply charged ions from H to those for capture from H_2 , as a function of reduced collision energy, from Knudsen et al. (1981a).

Fig. 8. Comparison of classical-trajectory Monte-Carlo calculations (points denoted by x) with experimental data for electron capture by Fe^{13+} from H-atoms, from McDowell and Janev (1985).

Fig. 9. Classical-trajectory Monte-Carlo calculations of partial cross sections for electron capture by bare projectiles of various charges Z , as functions of principal quantum number n in (a), and orbital angular momentum quantum number, l in (b). Graphs are taken from a paper by Olson (1981).

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