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INDC INTERNATIONAL NUCLEAR DATA COMMITTEE

INDC International Nuclear Data Committee

IAEA SPECIALISTS' MEETING ON

"CARBON AND OXYGEN COLLISION DATA FOR FUSION PLASMA RESARCH"

Vienna, 12-13 May 1988

Prepared by R.K. Janev

<u>SUMMARY REPORT</u>

September 1988

IAEA NUCLEAR DATA SECTION, WAGRAMERSTRASSE 5, A-1400 VIENNA

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Abstract

Summary report of an IAEA Specialists' Meeting on the "Carbon and Oxygen Collision Data for Fusion Plasma Research", convened on 12, 13 May 1988 by the IAEA Atomic and Molecular Data Unit is provided. The review of the data status and requirements for these ions is presented through the Reports of the Working Groups. The conclusions and recommendations of the meeting are also summarized.

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1. SUMMARY OF THE MEETING

1.1. Introduction

In the broad spectrum of impurity species present in present-day fusion experiment devices, carbon and oxygen have a special place. Due to its high reactivity, oxygen is an omnipresent impurity species, with concentrations on the level of several percents of the plasma density even after the most carefull cleaning of the vessel walls. Carbon enters as a constituent in most plasma facing system components, and, due to many good properties, it is today in fact one of the preferred plasma facing materials (limiters, RF antenas, carbonized walls, etc). Its concentration in present fusion devices may be as high as 5-10% of plasma density. In controlled quantities, the presence of carbon and oxygen impurities may have positive effects on the overall plasma performance, providing an efficient mechanism for the near-wall plasma radiation cooling.

The knowledge of collisional and spectroscopic properties of carbon and oxygen ions is, therefore, of primary interest to fusion research (energy balance calculations, scrape-off plasma modelling, diagnostics, etc). The purpose of the IAEA Specialists' Meeting on the "Carbon and Oxygen Collision Data for Fusion Plasma Research" was to review the data status for these ions, to identify the gaps in the data base, and through specific original contributions, to contribute to the enlargement of the data base for these ions.

The response of the atomic physics community to the invitation by the IAEA Atomic and Molecular Data Unit to contribute to the evaluation and completion of the carbon and oxygen collision data base for fusion was very enthusiastic. More than twenty experts participated in the Meeting (see Appendix 1), and several have submitted written contributions to the meeting. Below, we summarize the proceeding and the main results of the meeting.

1.2. Meeting proceedings and results

The Meeting worked in five sessions: (see Appendix 2: Meeting Agenda)

1) Electron-atom/ion collisions: excitation and ionization,
2) Electron-ion recombination,
3) Collisions of C^{q+} and O^{q+} with H, H_2 and He,
4) Electron capture reactions,
5) Preparation and adoption of conclusion and recommendations.

At the first session, a comprehensive review of the data status for electron impact excitation and ionization of C^{q+} and O^{q+} ions was presented by Dr. R.A. Phaneuf, with an appropriate discussion of the data accuracies, uncertainties, gaps in the data base and requirements. Recommended data for excitation rate coefficients of He-like ions were presented by Dr. H. Tawara (on behalf of Dr. T. Kato). Original contributions to the ionization and excitation data base for these ions were given by Dr. P. Defrance and Drs. V.P. Shevelko, L.A. Vainshtein and E.A. Yukov (the results presented by R.K. Janev).

At the session devoted to electron-ion recombination, very detailed reviews of the data base and recent calculations for these processes were presented by Dr. D.C. Griffin and Dr. Y. Hahn. The problem of enviormental effects on the dielectronic recombination rates (electric fields, density effects) were thorougly discussed. Dr. L. Roszman presented results on dielectronic recombination of some oxygen ions with density effects included.

At the sessions devoted to the C^{q+}, O^{q+} - H, H_2, He collision processes, comprehensive reviews of the data status were presented by Prof. H.B. Gilbody (total electron capture and ionization), Dr. A. Salin (theoretical methods and results for state selective electron capture) and Dr. H. Tawara (the status of charge transfer data for C^{q+} and O^{q+}). Dr. Y. Nakai presented a semi-emprical fitting formula for the total charge transfer cross sections in C^{q+}, O^{q+} - H, H_2, He collisions, while Dr. T. Watanabe discussed in detail the theoretical methods for these processes. Original cross section data for these collision systems were presented by Dr. Dz.S. Belkic (high energy charge exchange, theory), Dr. R.D. Rivarola (high energy charge transfer and ionization, theory), Dr. R. Hoekstra (state-selective electron capture, experiment), and Dr. A. Bárány (state-selective electron capture, experimental). Dr. F. Aumayr presented some comments on the electron capture measurements in the presence of metastable ion fractions in the beam.

The main results of the meeting can be summarized as follows:

- A detailed analysis of the existing data base for carbon and oxygen ions colliding with electrons, H, H_2 and He was performed both through the reviews prepared by some of the participants and during the discussions of Working Groups. This analysis has identified the status of the data (availability, quality) and the gaps in the data base. Such data analysis was particularly needed for the radiative and dielectronic recombination, and for the state-selective electron capture processes.
- A significant amount of new data for the processes considered at the meeting was reported for the first time. The meeting, thus, contributed to the enlargement of the collisional data base for the carbon and oxygen ions. This particularly holds for the data on dielectronic recombination, state-selective electron capture, heavy-particle ionization, and electron impact excitation and ionization.

A more detailed account of the performed data analyses is given in the Working Group Reports (see section 2).

2. Meeting Follow-ups

(i) The participants agreed to continue cross section (or reaction rate coefficient) calculations and measurements of the processes involving carbon and oxygen ions in the period after the meeting, and to submit new sets of such data to the Organizer by September 1988. The contributions to the meeting, together with the new sets of calculated/measured data will be published as a Topical Issue of "Physica Scripta". Theoretical groups, not represented at the Meeting, also agreed to provide new data for this "Physica Scripta" volume.

(ii) As a follow-up of the Meeting, a two-day Workshop was organized by Dr. D. Griffin on August 8-9, 1988, at the Oak Ridge National Laboratory on finalizing the recommendations regarding the dielectronic recombination data for carbon and oxygen ions. Participants of this workshop were: N. Badnel, Ch. Bottcher, P. Dittner, D. Griffin, Y. Hahn, M. Pindzola and L. Roszman. The results of this Workshop are also incorporated in the Working Group Report on electron-ion collisions (see next section).

2. REVIEW OF THE DATA STATUS AND DATA REQUIREMENTS

2.1. Report of the Working Group on the Spectroscopic and Electron-Impact Collision Data Base for C^{q+} and O^{q+} Ions

R.A. Phaneuf (Chairman), P. Defrance, D.C. Griffin, Y. Hahn, M.S. Pindzola, L. Roszman, and W. Wiese

Abstract

A brief overview is given of the status of the carbon and oxygen atomic data base for electron-impact excitation, ionization and recombination, and for spectroscopic data. Deficiencies for fusion plasma research applications are identified. Additional data are most critically needed for dielectronic and radiative recombination.

1. Introduction

In this report, spectroscopic data and data for electron collisions with C^{q+} and O^{q+} ions (q = 0, 1, ..., Z), are assessed with respect to availability and accuracy. The designations which have been adopted to represent the estimated reliability of the data are given in Table 1.

Table 1. Criteria for data-base evaluation

Level of accuracy	Designation
3% or better	A+
Between 3% and 10%	A
Between 10% and 25%	B
Between 25% and 50%	C
Between 50% and 100%	D
Worse than a factor of 2	E

References are given to the most recent data compilations, and to available sourses of evaluated or recommended data.

2. Spectroscopic Data

Spectroscopic information is fundamental to studies of all collision processes. The spectroscopic data base for C^{q+} and O^{q+} (q = 0, 1, ..., Z-1) is extensive, and may be divided for convenience into energy levels [1, 2], wavelengths [1, 2], and transition probabilities [2]. The energy levels and outer-shell transition wavelengths are well-established, and all have accuracies of A+. The outer-shell transition probabilities range in accuracy from A+ for H-, He- and Li-like ions, to B for some of the more complex electronic configurations.

3. Electron-Impact Ionization Data

Electron-impact ionization is an important process in determining the ionization balance, impurity transport, and power loss in fusion plasmas, particularly in the edge region. The data base for electron-impact

Table 2. Data base for electron-impact ionization of C^{q+} and O^{q+}

Species	Beams	Experimental Data Trapped-Ion	Plasma	Theoretical Data Direct	Indirect	Accuracy
C	X					A
C^{+}	X	X		X		A
C^{2+}	X	X		X		A
C^{3+}	X	X		X	X	B
C^{4+}	X,*	X	X	X		B
C^{5+}		X	X	X		B
O	X					A
O^{+}	X	X		X		A
O^{2+}	X	X		X		A
O^{3+}	X	X		X		A
O^{4+}	X	X		X		A
O^{5+}	X	X	X	X	X	A
O^{6+}	*	X				B
O^{7+}		X				B

*: new data presented at this meeting.

ionization of C^{q+} and O^{q+} (q = 0, 1, ..., Z-1) consists predominantly of experimental cross-section data. Crossed-beams measurements provide good energy resolution (a few eV or better), and thus are capable of providing information about indirect ionization mechanisms having well-defined threshold energies. Crossed-beams measurments from different laboratories have absolute accuracies in the 10% range, and usually agree within 5%. A trapped-ion technique using an electron-beam ion source (EBIS) has provided data for the higher charge states at higher energies. These data are somewhat model-dependent and lower in absolute accuracy, but provide the only experimental results for H-like C^{5+} and O^{7+}. Consistency with crossed-beams data for other charge states is within 20% or better. Ionization rate-coefficient measurements from plasmas have lower absolute accuracy and energy resolution because of integration over a Maxwellian (or other) energy distribution, but are useful for comparative purposes.

The widely applied Lotz semiempirical formula gives a reasonable estimate for the cross section when indirect ionization mechanisms are relatively unimportant. Indirect excitation-autoionization contributions have been included in some theoretical calculations, which agree well with experiment. The available data have recently been evaluated and cross sections and rate coefficients have been recommended for applications in fusion research [3, 4]. A comprehensive compilation of cross-section data for electron-impact ionization of ions has also been published more recently [5]. New crossed-beams data for He-like C^{4+} and O^{6+} were presented by P. Defrance at this meeting. In this experiment, careful analysis was made of the contribution due to a 1s2s metastable component in the reactant beams, and the ground-state ionization cross section were also made in the Coulomb-Born approximation. The new results for He-like C^{4+} and O^{6+} are consistent with earlier recommendations [3].

The data base for electron-impact ionization of C^{q+} and O^{q+} is summarized in Table. 2.

Double-ionization cross-section data are available only for neutral oxygen. Double-ionization cross sections for the Li-like and higher ionization stages will be negligibly small. The crossed-beams measurments for single ionization of Li-like C^{3+} deviate from isoelectronic trends and have considerable scatter. This may be due to a small O^{4+} contaminant in the reactant beam, which has the same m/q as C^{3+}. Although systematic checks were made of beam purity, crossed-beams measurements with a reactant beam of $^{13}C^{3+}$ will probably be necessary to more accurately establish the cross section.

4. Electron-Impact Excitation Data

Electron-impact excitation is important for plasma radiative power loss and diagnostics, particularly of the edge region. The data base for electron-impact excitation of C^{q+} and O^{q+} (q = 0, 1, ..., Z-1) is extensive, covering some 140 different transitions, and consisting almost entirely of theoretical calculations based on the close-coupling (R-matrix), distorted-wave and Coulomb-Born approximations. The close-coupling methods are in principle more reliable in the near-threshold region where the effects of resonance may be large, provided that all of the important interacting levels have been accounted for in the calculation. The distorted-wave and Coulomb-Born approximations are particularly useful at energies above a few times the excitation threshold, and may be accurate near threshold if effects such as exchange are accounted for. This extensive theoretical data base is self-consistent, with estimated accuracies ranging from A to D, depending on the ion and transition. Cross-beams experimental data for outer-shell excitation are available only for 2s-2p excitation of C^{+} and C^{3+}, and substantiate theory in these two cases. Some plasma rate-coefficient measurements are available with reduced accuracy, and are generally consistent with theoretical results. Experimental data are also available for 1s-nl inner-shell excitation of Li-like C^{3+} and O^{5+} from crossed-beams measurements of electron-impact ionization; these also compare favorably with theory.

The data for electron-impact excitation of C^{q+} and O^{q+} have been recently reviewed [3, 6-10], and recommended data are available for more than 140 transitions, with accuracies ranging from B to D. A need exists for experimental checks on the accuracy of the theoretical data base, particularly for the lower ionization stages (e.g., C^{2+}, O^{+}, O^{2+}, O^{3+}, and O^{4+}), where resonance effects are predicted to be large. New merged-beams experiments are being developed at several laboratories to determine electron-impact excitation cross sections in the critical near-threshold region. Cross-checks between theory and experiment should also be accompained by internal tests of the sensitivity and completeness of the theoretical calculations for transitions which cannot be readily addressed experimentally (i.e., between excited levels).

5. Radiative Recombination Data

Radiative recombination, the inverse of photoionization, is the dominant electron-ion recombination process in plasmas at low temperatures, and is therefore most important in the edge region. The available data base consists primarily of theoretical calculations. The cross section for radiative recombination into the ground state is obtained from the calculated ground-state photoionization cross section by detailed balance. Hydrogenic models have been used to determine cross sections for recombination into higher subshells of partially stripped ions. The total radiative recombination cross section is then obtained by summing over all subshells. An analytic formula for the radiative recombination rate coefficient has been derived by Seaton based on a modified version of the hydrogenic photoionization formula of Kramers. Specific calculations are available for radiative recombination into the ground state, with the Seaton formula applied for recombination into excited levels to determine the total radiative recombination rate coefficient. Such calculations for partially stripped ions have an accuracy rating of "C". There are a number of spectroscopic measurements of free-bound continuum radiation due to the capture of electrons by singly charged ions. The associated determinations of absorption coefficients (or cross sections) are estimated to have accuracies of the order of "C" on an absolute scale.

Direct experimental measurements of radiative recombination cross sections are needed to adequately test the theory for the higher ionization stages. A number of heavy-ion storage rings will be placed into operation during the next several years. The electron-beam ion coolers on such machines may be useful in providing data on electron-ion recombination processes. There is also a need for distorted-wave (or better) calculations for the lower-lying states, where the hydrogenic approximation is known to be unreliable.

6. Dielectronic Recombination Data

Dielectronic recombination is the dominant electron-ion recombination process in plasmas at higher temperatures, and is therefore important in determing the ionization balance. Some theoretical and experimental data are available for C^{q+} and O^{q+} ions. Most of the theoretical work has been based on the isolated resonance approximation, in which dielectronic recombination is treated as a two-step process: resonant excitation with recombination into a doubly excited state (the inverse of autoionization), followed by radiative stabilization into a bound state. The branching ratio for radiative stabilization versus autoionization must be calculated for each doubly excited state. The total dielectronic recombination cross section or rate coefficient is determined by summing over all resonant excitations and doubly excited levels. Merged-beams experimental data are available for $\Delta n=0$ transitions of some charge states of C and O, and provide tests of theory. Comparison of experiment and theory is complicated by the presence of external electric fields in the experiments, which produce large effects on the measured cross section for $\Delta n=0$ transitions. This results both from Stark mixing of levels with different angular momentum quantum number ℓ, and from field ionization of recombined ion states with large n. Some rate-coefficient measurements from plasmas are also available from satellite-line intensity measurements, providing consistency checks for theory. The available data for C^{q+} and O^{q+} are summarized in Table 3. Included are only those theoretical calculations which are sufficiently complete to be applicable at the higher electron temperatures relevant to fusion plasmas, and which are specific to a particular ionization stage of C or O.

On the basis of the data currently available, the widely-applied Burgess-Merts formula is known to be inaccurate by as much as a factor of 5 in some cases. The effect of the fusion plasma environment on the dielectronic recombination rate is also known to be very important, especially for $\Delta n=0$ transitions. The majority of theoretical calcualtions performed thus far for C^{q+} and O^{q+} ions refer to the limit of no external-field or plasma-density effects. These effects are strongly interrelated, and accurate calculations for specific plasma conditions are extremely tedious. However, the establishment of limits

Table 3. Fusion-relevant data base for dielectronic recombination of C^{q+} and O^{q+}

Species	Experimental Data $\Delta n=0$	Experimental Data $\Delta n>0$	Theoretical Data $\Delta n=0$	Theoretical Data $\Delta n>0$	Accuracy $\Delta n=0$	Accuracy $\Delta n>0$
C^{+}	b		2		B	
C^{2+}	b		2		C	
C^{3+}	b		1		B	?
C^{4+}	n/a	r	n/a	3	n/a	B
C^{5+}	n/a	r	n/a	2	n/a	B
O^{+}			1		?	
O^{2+}			2	1	D	
O^{3+}	b		2	1	B	
O^{4+}	b		2	2	C	?
O^{5+}	b		3	2	B	D
O^{6+}	n/a		n/a	2	n/a	B
O^{7+}	n/a		n/a	2	n/a	A

b: beams experiment
r: plasma rate measurement
numbers: number of independent calculations

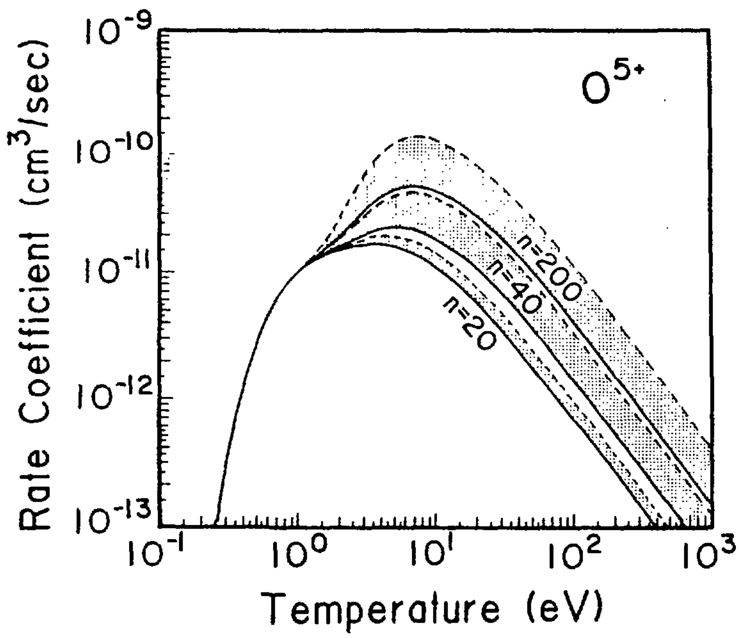

Fig. 1. Calculated dielectronic recombination rate coefficient for O^{5+} incorporating plasma field and density effects. The shaded bands are labeled by the highest final-state principal quantum number, n, included in the calculation. For strong fields or high densities, high-n product states are ionized and thus do not contribute to the recombination rate. For each band, the solid lower curve is a spherical basis calculation (no Stark effect), while the dashed upper curve is a parabolic basis calculation which estimates maximum state mixing due to either fields or collisions. (Caculation by M.S. Pindzola, 1988).

for such effects can be much more readily accomplished. The effects of plasma density and electric fields are summarized in Fig. 1, which presents the calculated $\Delta n=0$ dielectronic recombination rate coefficient for O^{5+} as a function of n_{max}, which represents the lowest final-state principal quantum number which is not ionized due to the plasma environment.

Data needs include further experimental and theoretical studies of the effects of external fields, primarily for $\Delta n=0$ transitions. Experimental data are also required for $\Delta n>0$ transitions, where external field effects are predicted to be negligibly small, and comparisons with theory would be more definitive. Such measurements are planned for a number of heavy-ion storage rings which will be placed into operation during the next several years. More than one experimental measurement and one theoretical calculation for each case would be helpful in establishing the consistency and accuracy of data. Theoretical tests of the validity of the isolated-resonance approximation should be made, and limits should be established for effects due to the plasma environment.

7. References to Data Compilations

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10. "Electron Excitation Collision Strengths for Positive Atomic Ions: A Collection of Theoretical Data", A.L. Merts, J.B. Mann, W.D. Robb, and N.H. Magee, LA-8267-MS, Los Alamos Scientific Laboratory (1980).

2.2. Report of Working Group on the Data Base for Collisions of C^{q+} and O^{q+} Ions with H, H_2 and He

J.B. Gilbody and A. Salin (Co-Chairmen), R. Aumayr, A. Barany, Dz.S. Belkic, R. Hoekstra, R.K. Janev, Y. Nakai, R.D. Rivarola, H. Tawara and T. Watanabe

1. Introduction

The processes of main interest are:

charge transfer or one-electron capture,

$$X^{q+} + Y \rightarrow X^{(q-1)+} + Y^{+} \qquad (1)$$

(where X refers to C or O and Y to H, H_2 or He)

and single ionization

$$X^{q+} + Y \rightarrow X^{q+} + Y^{+} + e\ . \qquad (2)$$

In the case of charge transfer there is also a need for cross sections for capture into specified excited states (n,ℓ) of the product ion as in

$$X^{q+} + Y \rightarrow X^{(q-1)}\ (n,\ell) + Y^{+}\ . \qquad (3)$$

Accurate data on the major as well as on the minor collision product channels are important. For H_2 targets there are a number of dissociative collision channels available involving charge transfer and ionization as well as the transfer-ionization process

$$X^{q+} + H_2 \rightarrow X^{q-1)+} + H^{+} + H^{+} + e\ . \qquad (4)$$

Two-electron processes involving capture or ionization must also be considered in the case of helium.

The energies of interest range from a few eV to several MeV.

A recent compilation of all the available data for carbon and oxygen ions [1] shows that, while some data are available for the majority of collision combinations with different charge states q, the data base is still incomplete and the accuracy of some cross sections is limited.

2. Current Work

Over the past decade experimental data on (1) has been obtained by the use of beam-static gas target methods and, in the case of atomic hydrogen, with a tungsten tube furnace target. Measurements originally mainly confined to comparatively high impact energies, are currently being extended through the availability of special ion sources down to energies ~ 0.1 keV amu^{-1} for all charge states. Measurements based on translational energy spectroscopy (TES) and photon emission spectroscopy (PES) are now providing detailed information on (3). For measurements with some partially ionized ions, it is necessary to consider the often strong influence of any metastable ions present in the primary beam.

Measurements on ionization are being carried out by variants of the condenser plate method and crossed beam techniques. Coincidence counting techniques allow data on transfer ionization in He and H_2 or dissociative processes in H_2 to be separately obtained.

A number of theoretical techniques based on both quantal and classical models have been developed and are being applied to predict total cross sections for charge transfer and ionization as well as the detailed n,ℓ distributions in electron capture processes. Cross-checks of predictions based on different approximations and comparisons with experimental data are establishing the range of validity of each type of calculation. In some cases, it is necessary to rely on theory to provide the state-to-state electron capture cross sections.

3. The Present Data Base and Recommendations for Future Work

Measurements of cross sections for (1) in H, H_2 and He at high energies (greater than about 25 keV amu^{-1}) are now of acceptable accuracy. At velocities above the cross section peaks, cross sections can be described by simple q scaling relations. A number of more general scaling predictions provide an approximate description of the data over a wide energy range. Classical trajectory Monte-Carlo (CTMC) calculations provide a satisfactory description of (1) at moderate velocities while, at high velocities, it has been shown recently that a correct formulation of the first Born approximation yields reliable data.

At energies below about 25 keV/amu where a molecular description of (1) is required, cross sections for electron capture are determined mainly by curve crossings leading to a limited number of excited product channels. With the exception of fully stripped ions, where the electron capture process is now well understood, the accuracy of the experimental data is often poor and the energy range inadequate. Many more studies of state selective capture are also required to identify and quantify the role of particular collision product channels. Theoretical studies based on close coupling calculations in characterising the n,ℓ distributions which are not always accessible to experiments. The unknown effect of the presence of metastable primary ions in beams on measured cross sections for some partially ionized species is another factor which at present limits the accuracy of the low energy data base. At the very low energies, both experimental and theoretical data are still very fragmentary.

For helium, measurements and calculations indicate that two-electron capture is much less likely than single capture, except in the case of C^{4+} and O^{8+} impact.

The availability of total (T) and state-selective (SS) electron capture is presented in Table 1. The accuracies and energy ranges for these data can be found in Refs. [2, 3]. (Other data compilations are contained in Refs. [4-6]. The state-selective data are of relatively high accuracy (~ 20-50%) only for the dominantly populated electron shells ($n_{max} \simeq q^{0.768}$, for hydrogen atom target) and sub-shells.

Accurate measurements of ionization by C^{q+} and O^{q+} for $q \geq 2$ in H and H_2 at energies greater than about 10 keV amu^{-1} and a number of theoretical treatments provide a satisfactory description of the high energy behaviour. At velocities above the cross section peak, cross sections are q rather than species dependent and scale in a manner similar to cross sections for (1). More general scaling relations provide an approximate fit to the ionization data at high velocities. Data for helium are less extensive. For H, H_2 and He there are no

Table 1. Total and State-selective Electron Capture Cross Section Data for C^{q+}, O^{q+} – H, H_2, He Collisions

Ion/ Target	H		H_2		He	
	T	SS	T	SS	T	SS
C^{+}	X		X			
C^{2+}	X	X	X		X,#	(X)
C^{3+}	X,*	X,*	X,#	X	X,#	X
C^{4+}	X	X	X	X,#	#	X,#
C^{5+}	X	*	X		X	
C^{6+}	X	X	X	X,#	X	X,#
O^{+}	X	(X)	X		X	
O^{2+}	X	X	X		X,#	X
O^{3+}	X	X	X		X	
O^{4+}	X	*	X		X	
O^{5+}	X	*	X		X	
O^{6+}	X	X	X	X,#	X	X,(#)
O^{7+}	X		X		X	
O^{8+}	X	X	X	X	X	X,#

T = total cross section data
SS = state-selective cross section data
* = new data reported at the meeting
# = also data for two-electron capture

Table 2. One-electron ionization cross section data for C^{q+}, O^{q+} – H, H_2, He Collisions

Ion/T	H	H_2	He
C^{+}	X, *, ϕ	X, ϕ	X, *, ϕ
C^{2+}	X, *	X, *	X, *, ϕ
C^{3+}	X, *	X, *	X, *, ϕ
C^{4+}	X, *, #	X, *	X, *
C^{5+}	X, *, #	X, *, (ϕ+1)	X, *
C^{6+}	X, *, #, ϕ	X, *, (ϕ+1)	X, *, #
O^{+}	X, *, ϕ	X, ϕ	X, *, ϕ
O^{2+}	X, *	X, *	X, *, ϕ
O^{3+}	X, *	X, *	X, *, ϕ
O^{4+}	X, *	X, *	X, *
O^{5+}	X, *	X, *	X, *
O^{6+}	X, *	*, ϕ	X, *, #
O^{7+}	X, ϕ	*, ϕ	X, *
O^{8+}	X, *, ϕ	*, ϕ	X, #

X = theoretical or experimental data available in certain energy range
* = semi-empirical scaling relationships is used for constructing σ_{ion} in the energy regions where no data are available
ϕ = no experimental data available
(ϕ+1) = one experimental point available
= new data reported at the meeting

measurments below about 10 keV amu^{-1} and there are no reliable theoretical predictions. In H_2 dissociative ionization is important at low energies and the process of transfer ionization needs to be fully investigated for both H_2 and He.

The availability of ionization data in C^{q+}, O^{q+} - H, H_2, He collisions is presented in Table 2 ([1, 2]). It should be noted that for generating ionization cross sections in a broad energy range (E $\gtrsim$ 10q keV/amu), appropriate scaling relations have been used in Refs. [1, 2] for many collision partners.

Studies of electron capture involving excited hydrogen atoms are desirable for calculation of the hydrogen neutral beam penetration into plasmas. At present there are no experimental data and the theoretical studies are limited. For the same purpose, excitation of H to $2 \leq n \leq 7$ states by C^{q+} and O^{q+} ions, as well as cross sections for the $n \rightarrow n'$ and $n \rightarrow$ continuum transitions are required. Charge transfer collisions between He^{2+} and C^{q+} or O^{q+} ions need to be investigated both experimentally and theoretically over a wide energy range (E $\leq$ 3.5 MeV) in relation to the alpha particle confinement in fusion reactors.

References to Data Compilations

[1] R.A. Phaneuf, R.K. Janev and, M.S. Pindzola, "Collisions of Carbon and Oxygen Ions with Electrons, H, H_2 and He", Atomic Data for Fusion, Vol. 5, Report ORNL-6090 (Oak Ridge Natl. Lab., Oak Ridge, 1987)

[2] R.K. Janev, R.A. Phaneuf and H. Hunter, "Recommended Cross Sections for Electron Capture and Ionization in Collisions of C^{q+} and O^{q+} Ions with H, H_2 and He", At. Data Nucl. Data Tables, xxx (1988) (in press)

[3] H. Tawara, "Total and Partial Cross Sections for Electron Capture for C^{q+}(q=6-2) and O^{q+}(q=8-2) ions in collisions with H, H_2 and He". Report IPPJ-AM-56 (Inst. Plasma Phys. Nagoya Univ., Nagoya, 1987)

[4] H. Tawara, T. Kato and Y. Nakai, At. Data Nucl. Data Tables 32, 235 (1985). Also: "Cross Sections for Charge Transfer of Highly Ionized Ions on hydrogen atoms", Report IPPJ-AM-30 (Inst. Plasma Phys., Nagoya Univ., Nagoya, 1983)

[5] H. Tawara, T. Kato and Y. Nakai, "Electron Capture and Loss Cross Sections for Collisions between Heavy Ions and Hydrogen Molecules", Report IPPJ-AM-28. (Inst. Plasma Phys. Nagoya Univ., Nagoya, 1983)

[6] B.A. Huber and H.J. Kahlert, "Total Cross Sections for Electron Capture by Multiply Charged Ions in H, H_2 and He". Report No. 82-05-104 (Ruhr-Univ., Bochum, 1982)

3. CONCLUSIONS AND RECOMMENDATIONS OF THE MEETING

The participants of the Specialists' Meeting on the "Carbon and Oxygen Collision Data for Fusion Plasma Research" during two-day discussions have thoroughly reviewed the status of the collisional and spectroscopic data base for these plasma impurities in all stages of ionization, and through original contributions presented at the meeting and additional, post-meeting research work have significantly enlarged the data base for certain processes.

The conclusions and recommendations of the Meeting can be summarized as follows:

(1) The spectroscopic data base (energy levels, wavalengths, transition probabilities) for carbon and oxygen ions is very extensive particularly for the outer shells. Data on inner-shell are, however, still limited, especially for the doubly excited configurations.

(2) The data base for electron-impact single-ionization of carbon and oxygen ions can be considered to be in a satisfactory shape, with cross section accuracies better than 25%. The data for double- and multiple-ionization of these ions are still very fragmentary, and more systematic data on these processes are required (particularly for the low-charged ions) for the ionization-balance calculations of fusion edge plasmas.

(3) The electron-impact excitation data for the lower states of carbon and oxygen ions are available and are based almost entirely on theoretical calculations (accuracy between 20-100%). Experimental checks of these data is required.

(4) The data on radiative electron-ion recombination are based on hydrogenic formulae (for capture into high excited states) and their modifications (through the Gaunt factor), or on specific, more elaborate calculations (for capture in the ground or lower excited states). The theoretical data (accuracy 25-50%) are consistent with the plasma spectroscopy observations, but improvements in their quality are possible and have to be made.

(5) The data base on dielectronic recombination for C^{q+} and O^{q+} ions is virtually complete for both $\Delta n=0$ and $\Delta n > 0$ transitions, but is based on a very limited number of theoretical or experimental (for $\Delta n=o$ only) investigations. The assessment of accuracy is, therefore, in many cases uncertain. More theoretical calculations are required for cross-checking, as well as experimental data for $\Delta n > 0$ transitions. Environmental effects (external electric fields and finite electron density) have to be assessed in each case, and appropriate limits on the rates due to these effect should be established.

(6) The total one-electron capture cross section data for C^{q+}, O^{q+} - H, H_2, He collisions form an almost complete set at least for energies above 10/q (keV/amu). The only exception is the C^+ -He system for which no data exist (but the cross section is expected to be small). In the low energy region the data are rather scarce.

(7) The data base for electron capture into specific ion states is still incomplete, and the existing data in many cases disagree with each other, except for the dominantly populated levels. In view of the

importance of this process for plasma diagnostics and detailed radiation loss calculations, completion of the data base for state-selective electron capture on these ions is strongly recommended.

(8) Ionization of H, H_2, and He by C^{q+}, O^{q+} impact has not been studied systematically and data are limited to only a number of collision systems. Particularly critical in this respect is the energy region below the cross section maximum. Although the semi-empirical scaling relationships proved to be fairly successful in describing the existing data, their check in the cases of lowest and highest charge states is strongly recommended, as well as their validity in the low energy region.

(9) Excitation data for H, H_2 and He by C^{q+} and O^{q+} impact do not exist, except for few cases [C^{6+}, O^{8+} + H → H (2p)]. Such data are urgently required for the H target in the energy region around and above the cross section maximum in relation to the calculation of neutral hydrogen beam stopping into fusion plasmas.

(10) The data base for two-electron transition processes, such as dissociative capture in H_2, transfer ionization in H_2 and He, are also very poorly docummented and require more attention.

Specialists' Meeting on the "Carbon and Oxygen Collision Data for Fusion Plasma Research"

12, 13 May 1988

at

IAEA Headquarters in Vienna, Austria

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IAEA Specialists' Meeting on

"Carbon and Oxygen Collision Data for Fusion Plasma Research"

Vienna, 12 and 13 May 1988

IAEA Headquarters, Meeting room: C7-IV

Meeting Agenda

Thursday, 12 May 1988

9:15 -	Opening: Prof. V.A. Konshin, Director of the IAEA Division of Physical and Chemical Sciences Adoption of meeting agenda
	Session I: Electron-atom/ion collisions: excitation and ionization
	Chairman: Y. Hahn
10:00 - 10:45	R.A. Phaneuf (ORNL, Oak Ridge) Electron-impact excitation and ionization: status of the data base for C^{q+} and O^{q+}
10:45 - 11:00	Coffee Break
11:00 - 11:25	P. Defrance (Univ. Catholique de Louvain-la-Neuve) Electron-impact ionization of C^{4+} and O^{6+}
11:25 - 11:50	T. Kato / H. Tawara (IPP, Nagoya) Recommended data for excitation rate coefficients of He-like ions
11:50 - 12:00	V.P. Shevelko, L.A. Vainshtein, E.A. Yukov (Lebedev Inst. Moscow) cross sections and rate coefficients for inelastic electron collisions with carbon and oxygen ions
12:00 - 12:15	A. Bárány / P. Hvelplund (Inst. At. Physics, Stockholm, Inst. of Physics, Aarhus) State selective capture in C^{q+}, O^{q+} - He collisions with translational spectroscopy
12:15 - 14:00	Lunch Break
	Session II: Electron-ion recombination
	Chairman: W.L. Wiese
14:00 - 14:40	D.C. Griffin (Rollins College, Florida) A review of recombination data for collisions of electrons with carbon and oxygen ions
14:40 - 15:15	Y. Hahn (Univ. of Connecticut, Storrs) Radiative and DR rates for C and O ions
15:15 - 15:45	L.S. Roszman (NBS, Gaithersburg) Some density effects and atomic structure problems in the DR of some oxygen ions
15:45 - 16:00	Coffee Break

Session III: Collisions of C^{q+} and O^{q+} with H, H_2 and He

Chairman: R.A. Phaneuf

16:00 - 16:40	H.B. Gilbody (Queen's University, Belfast) Total cross sections for charge exchange and ionisation in C^{q+}, O^{q+} - H, H_2, He collisions
16:40 - 17:10	Y. Nakai (JAERI) Semi-empirical formula for the cross sections for A^{q+} + H, H_2, He → $A^{(q-1)+}$
17:10 - 17:40	R.D. Rivarola (Inst. de Fisica, Rosario) Electron ionization by impact of carbon and oxygen ions on hydrogen and helium atoms
17:40 - 18:10	Dz.S. Belkic (Inst. of Physics, Belgrade) Cross sections for C^{q+} -H collisions at intermediate energies in the first Born approximation with correct boundary conditions

Friday, 13 May 1988

Session IV: Electron capture reactions

Chairman: H.B. Gilbody

9:00 - 9:40	A. Salin (Univ. of Bordeaux) Theoretical methods and results for state selective electron capture
9:40 - 10:10	T. Watanabe (RIKEN, Saitama) Theoretical aspects on electron capture by C^{q+} and O^{q+} from H, H_2 and He
10:10 - 10:30	Coffee Break
10:30 - 11:00	H. Tawara (IPP, Nagoya) The present status of charge transfer data for C^{q+}, O^{q+} ions
11:00 - 11:20	R. Hoekstra (KVI, Groningen) Absolute line emission cross sections for electron capture in collisions of C^{q+} and O^{q+} on H and H_2
11:20 - 12:00	F. Aumayr (TUW, Vienna) Comments on electron capture in presence metastable ions in the beam
12:00 - 14:00	Lunch Break

Session V: Preparation and adoption of Meeting conclusions and recommendations

Chairman: R.K. Janev

14:00 - 14:30	General discussion on the C^{q+}, O^{q+} data base, formation of working groups to determine the data status, propose recommended data sets and formulate immediate actions for completing the data base for: 1) electron-ion collision processes 2) C^{q+}, O^{q+} - H, H_2, He collision processes
14:30 - 17:00	Discussions in working groups and preparation of working reports (Meeting Rooms: C07-IV and C07-37)
17:00 - 18:00	Discussion of working group reports, adoption of recommendations and further actions