3. WORKING GROUP REPORTS

3.1. SPECTROSCOPIC AND ELECTRON-ION COLLISION DATA FOR PLASMA IMPURITIES

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A. Introduction

In this report we critically review and summarize the available spectroscopic and electron-ion collision data which are of primary importance to fusion research. We address plasma impurities on present and future fusion research machines and include also some elements, such as Li, Ne and Ar, which are not impurities per se, but are introduced for diagnostic purposes.

In a series of recent advisory meetings at the IAEA, various electron-ion collision data have been already reviewed for specific groups of plasma impurities, such as Helium[1], beryllium and boron[2], carbon and oxygen[3], and intermediate Z metallic elements[4] in the range 22<Z<29. We therefore refer to these reports for details and shall not repeat the same information here. Instead, we turn our attention primarily to the heavy metal impurities Ga, Mo, Ta and W plus three light elements utilized (or considered) for diagnostics: Li, Ne and Ar.

B. Current Data Situation

1. Spectroscopy Data:

The spectroscopic data situation has not been discussed in the earlier cited IAEA advisory meetings, except for the C and O impurities.[3] We therefore review the status of spectroscopic data in toto. Extensive data are available for most of the chemical elements of fusion interest, including many pertinent ions. However, there is a noticeable degradation in quality and completeness from the lighter to the heavier elements, and for numerous ions of heavy elements almost no data are available as yet. The data are summarized in Table 1, where the the elements of interest are divided into three groups.

TABLE 1. STATUS OF SPECTROSCOPIC DATA

Elements, Including Ions	Completeness	Quality
1. H, He, Li, C, N, O, Be, Ne:		
Energy Levels	High	Excellent
Wavelengths	High	Excellent
Transition Probabilities	High	Often very good (<5%), but some only fair
2. Ar, Ti, Cr, Fe, Ni, Cu:		
Energy Levels	Moderate	Excellent
Wavelengths	Moderate	Excellent
Transition Probabilities	Some Large Gaps in Data	Fair (±10 to ±50%)
3. Mo, Ta, W		
Energy Levels	Poor (few data)	Very good
Wavelengths	" " "	" "
Transition Probabilities	" " "	Most data of poor quality (factors of 2), but Mo I in good shape

Completeness and quality of data are listed for (a) wavelengths and energy levels (these quantities are closely related) and (b) for transition probabilities. Energy level and wavelength data--especially the experimental data--are typically of very high accuracy, usually better than 1 part in 10^5 and often 1 part in 10^6. Transition probability data, which are by orders of magnitude less accurate than energy levels and wavelengths, are typically available with accuracies ranging from 5 to 20% for the light elements, in the range from 10 to 50% for medium heavy elements and are often much less accurate for complex heavy elements. A complete listing of all spectroscopic data tables compiled at the U. S. National Institute of Standards and Technology (NIST) is given in the IAEA Techn. Report INDC (NDS)-243/M7(1990).[5]

A comprehensive bibliographic database is being built up at NIST and contains at present about 25,000 literature references. Also, two comprehensive numerical databases of critically evaluated spectroscopy data are in operation at NIST and at VNIIFTRI, and are being updated and enlarged.

2. Ionization Data:

In a series of IAEA advisory meetings, a great deal of understanding of the important physical processes involved in ionization of ions by electrons and their data situation has been obtained. Instead of repeating the description of these processes, in Table 2 we show a summary of the present status of ionization data for typical impurities expected in plasmas. In the following comments, the pertinent literature sources for these data are summarized:

(a) He: In a June 1991 IAEA advisory meeting, the data situation has been discussed in detail[1]. The recommended data seem to be of good accuracy.

(b) Li: The recommended data have been given by Bell et al.[6].

(c) Be, B: In another June 1991 advisory meeting, detailed discussions have been presented and recommended data have been proposed by Berrington et al.[2], based largely on the scaling properties because experimental data are still scarce.

(d) C, O: Detailed discussions and recommendations have been reported in Phys. Scripta T28 (1989)[4].

(e) Ne, Ar: These gases are intended to be used for diagnostics purposes. Recommended data have been reported by Bell et al.[6] and Lennon et al.[7]

(f) Intermediate-z metallic species: The data situation has been discussed in detail for Ti, Cr, Fe, Ni and Cu in a previous 1990 advisory meeting.[4] Since then, some new data have been added.[8] However, the over-all situation seems to be largely unchanged.

TABLE 2. DATA

	ELEMENT																
	He	Li	Be	B	C	O	Ne	Ar	Ti	Cr	Fe	Ni	Cu	Ga	Mo	Ta	W
Charge:																	
0	A	A	B	A	A	A	A	A							B		
1	A	A	C	B	A	A	A	A	B	B	B	B	B	A	B	B	B
2		A	A	C	A	A	A	A	B	D	B	C	B				
3			A	A	B	A	A	A	B	F	C	B	B			B	
4				A	B	A	A	A	D	F	C	C					
5					B	A	A	A	B	F	B	B					
6						B	B	B	D	B	B	B					
7						B	B	B	D	B	B	B					
8							B	B	D	B	B	B					
9							B	B	D	D	B	B					
10								B	D	B	B	B					
11								B	B		B	B					
12								B	C		B	B					
13								C	C	B	B	B					
14								C	C		B	B					
15								C	C		B	B					
16								C	C		C	B					
17								C	C		C	B					
18									C		C	C					
19									B		C	C					
20									B		C	C					
21									B		C	C					
22											C	C					
23											B	C					
24											B	C					
25											B	B					
26												B					
27												B					

Accuracy ratings: A=0-10%, B=10-25%, C=25-50%, D=50-100%, F = >100%

(g) Ga: This element is a candidate for a proposed liquid metal divertor system--an idea which is still in the conceptual stage. Very limited data are available so far.

(h) Heavy metallic elements: Recommended data for Mo, Ta and W have been reported only for a small number of ions of different charge states[9].

3. Excitation and Recombination Data:

The data situation is similar to that for ionization data. For the elements He, Be, B, C, O and the intermediate-Z metals, the data have been reviewed in recent IAEA advisory meetings.[1-4] Some additional excitation data for O I and O V are contained in three new papers, Refs. 10-12.

Radiative (RR) and dielectronic (DR) recombination data on various ions of the other elements of fusion interest--such as Li, Ne, Ar, Ga, Mo--may be found in a number of recent papers.[13-27]

It should be noted that recent developments of powerful ion sources and progress in accelerator technologies as well as measuring techniques have made it possible to directly determine excitation and recombination cross sections of higher ions. For example, direct measurements of excitation cross sections, using electron-ion crossed beam techniques, have been reported for Ar^{7+} and Si^{3+} ions.[28,29] Also, some recombination cross sections have been determined[30,31] based on new storage and cooling techniques in ion sources or accelerators. These techniques should soon provide systematic data for such processes involving multiply charged ions.

C. Data Requirements:

1. Spectroscopy Data:

Data are especially needed for ions of low and intermediate charge states of heavier elements. Also, the quality of transition probability data needs substantial improvements for many atomic species.

2. Ionization Data:

As seen in Table 2, more systematic studies should be devoted to very heavy elements with high melting points because there are plans for big machines such as ITER to use these materials for high heat load areas. For these heavy elements, multiple electron ionization processes should become more important than for light elements.

Also in multi-electron ions, significant fractions of the ions are often present in metastable states in the parent ion beams and show significant contributions to ionization. The recommended data should carefully take into account the effects of metastable ions in the measured data.

One should distinguish between the following, and thus provide individual cross sections for:

- direct ionization from the valence shell
- direct ionization from inner shells when it is important and provide branching ratios for resulting autoionizing states
- excitation to autoionizing states plus branching ratios[32]

3. Excitation Data:

Cross sections are needed for $\Delta n > \sim 1$ transitions from metastables.

Cross sections are needed for transitions to autoionizing states with branching ratios.[32]

4. Radiative Recombination Data:

Cross sections for recombination to specific states are needed (ground state of recombined ion plus excited states which result from $\Delta n = 0$ or 1 excitations).

Approximate cross sections to higher excited states of recombined states are needed (the recombining ions may be initially in the ground or metastable states).

5. Dielectronic Recombination Data:

Cross sections or rates for specific core transitions are needed A's are the first priority. One should distinguish between the various possible $\Delta n = 0$ transitions and a single effective rate for all $\Delta n > 0$ transitions. If possible, cross sections or rates for specific $\Delta n > 0$ transitions should be determined (recombining ions may be initially in the ground or metastable states).

Finite density effects, particularly for $\Delta n = 0$ core transitions, should be evaluated.

D. Other Recommendations

1. Presentation of Data:

Analytic fits are useful, but they should always be accompanied by the tables used to generate them.

When analytic fits are provided they should, if possible, be asymptotically correct, or sensible, or a prescription should be provided to extend them outside the interval over which the fit was made. This is necessary considering the wide range of temperatures of interest to fusion.

2. Evaluation of Empirical Expressions:

The group recognizes the utility of simple empirical expressions for cross sections and rates to complement existing recommended data. Evaluations of empirical expressions should be made for the various processes of interest, and recommendations should be made.

3. Data from the Opacity Project (OP):

The working group recommends that contacts with members of the Opacity Project should be intensified, and they should be encouraged to make the results of their calculations of excitation cross sections widely available to the fusion research community.

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32. Footnote: When the branching ratio for autoionization is nearly one, the cross section can be added to the cross section for direct ionization from the valence shell.