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# INTERNATIONAL NUCLEAR DATA COMMITTEE

### IAEA Consultants' Meeting on

# ELECTRON-IMPACT EXCITATION CROSS SECTION DATA FOR HELIUM

20 - 21 November 1995 Vienna, Austria

### SUMMARY REPORT

K. Bartschat, I. Bray, F.J. de Heer, W.C. Fon, R.K. Janev

December 1995

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### Abstract

Brief proceedings and a summary of the conclusions of the IAEA Consultants' Meeting on "Electron-Impact Excitation Cross Section Data for Helium", held on 20-21 November 1995, in the IAEA Headquarters in Vienna, Austria, are provided. The main emphasis in the database analysis is given to the transitions between the states with principal quantum numbers n=2-4. The most important gaps in the existing database for these transitions have been identified, as well as the recently developed theoretical methods which can generate highly accurate cross sections. A course of action has been suggested for completing the electron-impact excitation database for helium in a timeframe conformal with the needs of present fusion energy research.

December 1995



# Table of Contents

1.	Introduction	7
2.	Meeting proceedings	8
3.	Status of e-He excitation database	9
4.	Recent developments in cross section calculation capabilities	11
5.	Conclusions and recommendations	.19

# Appendices

Appendix 1: List of Meeting Participants	 .21
Appendix 2: Meeting Agenda	 .23

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### 1. Introduction

The IAEA Consultants' Meeting on "Electron-Impact Excitation Cross Section Data for Helium" was convened on 20-21 November 1995, at the IAEA Headquarters in Vienna, Austria, with the objectives to review and critically assess the existing database on the e-He excitation processes, identify its most important deficiencies and gaps, and analyze the possible ways and means of its improvement and completion. The meeting was attended by four prominent experts in the field (see Appendix 1), three theoreticians and one experimentalist, and by part of the IAEA Atomic and Molecular Data Unit staff.

The organization of this IAEA consultancy meeting was in line with the Agency's effort to establish a complete and highly accurate cross section database for all processes involving helium (ground state and excited) atoms and the major fusion plasma constituents (electrons, protons and dominant impurity ions). The main applications of such a database in fusion energy research are the modeling of neutral helium beam attenuation in fusion plasmas and the transport of helium in fusion reactor divertors. Energetic (30-200 keV) neutral helium beams are introduced in fusion plasmas for diagnostic purposes and the attenuation of their intensity in the plasma is strongly affected by the plasma density and atomic processes of beam atoms with plasma particles. The beam intensity attenuation results from the loss of beam particles due to their ionization or charge exchange in collisions with plasma electrons and ions. When the neutral beam velocity is such that the collision times of excited beam atoms become comparable with (or longer than) their radiative lifetimes, multistep collision processes (such as excitation followed by ionization or charge exchange) begin to play an important role in the beam attenuation kinetics, resulting in a significant The enhancement of beam increase of the effective "beam stopping" cross section. attenuation at high beam energies is related with the increase of the population of excited states in the beam and the increase of electron removal cross section with increasing the excited state principal quantum number. At the considered collision energies, the excitation of the first few excited singlet states takes place much more effectively by heavy particle impact (protons, impurity ions) than by electrons. However, the excitation of higher excited states from the lower ones is more efficient by electron than by heavy-particle impact. Transitions between the states of different spin multiplicity (singlet-triplet and triplet-singlet transitions) are possible only by electron collisions. Therefore, the electron-impact transitions between the excited states of helium play a very important role in the beam attenuation kinetics.

The energy levels of the excited states of He with principal quantum numbers  $n \ge 5$  can be considered degenerate and, consequently, the corresponding states can be regarded as hydrogen-like. For the transitions between the states with  $n \ge 5$  one can use the hydrogenic approximations (e.g. for the electron wave function) or suitable cross section scaling relationships. The transitions between the states in the group with n=2-4, however, require to be treated individually.

The need of a radiative-collisional treatment of the kinetics of helium atoms in fusion reactor divertors stems not from the helium particle velocity but from the high electron plasma density in these regions. In this case, however, helium excitation from the ground state is also an important electron-impact process.

## 2. Meeting proceedings

At the beginning of the meeting, the Head of the IAEA Atomic and Molecular Data Unit reiterated the objectives of the meeting and then the Meeting Agenda (see Appendix 2) was discussed and adopted. The Agenda for the first working day included an analysis and critical assessment of the existing cross section data for electron-impact excitation of ground state and excited helium atoms. The discussions on the most critical gaps in the database and the existing computational capabilities for generation of the required data were left for discussion during the second day of the meeting.

Since the transitions from the ground state have been subject of a detailed analysis at a previous IAEA experts' meeting related to the "Helium Beam Fusion Alpha Particle Diagnostics" (June 1991) and its findings reported in Nuclear Fusion A+M Supplement vol. 3 (1992), the present consultancy meeting focused its work on the assessment of available cross sections for transitions from excited states, mainly within the group of states with principal quantum numbers n=2-4. A comprehensive compilation of all the existing theoretical and experimental (for a few transitions) data has been prepared and reported at the meeting by <u>Dr. F.J. de Heer</u>. This collection served as a basis for the data intercomparison and assessment analyses performed at the meeting. <u>Prof. K. Bartschat</u> reviewed the recent developments of the R-matrix method with inclusion of pseudo-states (RMPS-method) at the Queen's University of Belfast and reported on its first results. <u>Prof. I. Bray</u> described the basic features of the convergent close-coupling (CCC) method recently developed at the Flinders University of South Australia and reported the cross section results obtained by this method for many transitions from the 2<sup>1,3</sup>S states of helium. <u>Prof. W.C. Fon</u> provided extensive comments on the standard R-matrix method, its various features and limits of applicability.

The analysis of database completeness for the transitions with the n=2-4 group of states revealed that for the transitions from  $2^{1,3}$ S the available cross section information is, generally speaking, adequate (with the exception of a few cases), but for the transitions from  $2^{1,3}$ P and  $n^{1,3}$ L (n=3,4; L=S,P,D) the cross section information is either absent or of, generally, very low accuracy. The recently developed CCC and RMPS codes have been identified as currently the most powerful available theoretical tools for generation of the missing (or of inadequate accuracy) excitation cross section data. Details of the findings of the meeting regarding the data status and the ways of its possible improvements are given in the following sections of this Report.

### 3. Status of e-He excitation database

### 3.1 Excitation from the ground state of He

The experimental data for electron impact excitation of  $He(1^{1}S)$  to  $He(n^{1.3}L)$ , n=2-6, have been recently critically reviewed (F.J. de Heer et. al., Supplement to the Journal Nuclear Fusion 3 (1992) 7). A preferred data set is now being established and combined with theoretical close-coupling approximation data below the ionization threshold and Born approximation data at high energy. The experimental data are between 30 and 2000eV electron impact energy for singlet excitation merging well with the theoretical Born data, and up to less high impact energy for triplet excitation (because the cross section becomes very small with increasing energy, as it follows from the Ochkur approximation). Below 30eV an extrapolation is made towards the close-coupling (29-states R-matrix) calculations from threshold up to the ionization energy (Berrington et. al., personal communication). Except for the metastable 2<sup>1</sup>S and 2<sup>3</sup>S states, most experimental data are from photon emission cross section measurements. For metastables the (integrated) cross sections have been obtained by using angular differential inelastic (energy loss selected) scattering cross sections.

The errors are, generally, smallest for singlet states (optical measurements) above about 40eV, i.e.  $\leq 10\%$  and the recommended R-matrix and Born data are accurate to better than 10% and 5%, respectively. At low energies (< 40eV) errors in experiment may increase up to about 30%.

Errors in experimental triplet cross sections (optical data) are relatively large, in particular at high energies, because secondary effects, such as collision transfer, are difficult

to eliminate. Some experimental data are missing (e.g. for  $3^3$ S) or showed severe scatter (e.g. for  $3^3$ D) and were estimated via cross section ratios in a term series. Generally, below 100 eV the error is ~ 30% for all triplet level cross sections, and above 100 eV there is an increasing uncertainty. Below the ionization threshold, the R-matrix (29-states) data for triplet levels may be accurate to about 10%.

Some improvement of the assessment of the above data (de Heer et. al, in preparation) will be done by considering new experiments (inelastic differential scattering experiments, see for instance Trajmar et. al., J. Phys. B 25 (1992) 4889). These will not change the general status of experimental data. However, new theoretical 75-state CCC data, discussed further on, which can be used over the entire energy range and demonstrate consistency with our singlet excitation data, show that the assessment of the triplet cross sections can be improved, in many cases to better than 20-10%. The R-matrix (29-states) data of Saway and Berrington (Atomic Data and Nuclear Data Tables 55 (1993) 81) up to 33 eV overlap partly the RM-29 data mentioned in de Heer et al.

At higher energies for triplet excitation it would be useful to compare different theoretical calculations such as CCC, CBE (Shevelko) and Ochkur. Ochkur calculations done so far only go up to 100 eV.

### 3.2 Excitation from the $2^{1,3}$ S states of He

Theoretical data for electron impact excitation of neutral helium in the He( $2^{1,3}$ S) states have been reviewed and a preferred data set has been established for excitation to the He( $n^{1,3}$ L) states with n=2-4 (F.J. de Heer et. al., Nucl. Fusion A+M Suppl. <u>6</u> (1995) 7). This work is an improvement of a previous report (F.J. de Heer et al, FOM-report 95 0653, April 1995) made possible by new theoretical data, in particular the 75-state convergent close coupling (CCC) data of Bray and Fursa, valid for the entire impact energy range of interest. Except for the smallest cross sections, i.e. for some spin changing collisions at higher energies, the CCC cross sections are expected to have an accuracy of about 10%. They are consistent with the most reliable low energy R-matrix data of the Belfast group<sup>1</sup> summarized by F.J. de Heer et. al. and with high energy Born data. For <u>spin allowed transitions</u> new CBE

<sup>&</sup>lt;sup>1</sup> Note: Unpublished RM-29 data of the Belfast group, used in the quoted papers of F.J. de Heer et. al. have been improved and should be incorporated in the final data assessment (see Sawey and Berrington, Atomic Data and Nuclear Data Tables 55 (1993) 81).

data (see Shevelko and Tawara, in Supplement to the Journal of Nuclear Fusion, <u>6</u>, (1995) 27) also coincide with Born at high energies, but generally overestimate the cross sections at lower energies. The new FOMBT (DWA) data (see Cartwright and Csanak, Phys. Rev. A <u>51</u> (1995) 454) are also relatively large at intermediate energies, as are many other considered distorted wave calculations. Only the (D)MET data of Flannery, McCann and Mansky with coupling of 10 states (Phys. Rev. A <u>12</u> (1975) 846 and J. Phys. B <u>23</u> (1990) 4573) show reasonable agreement with the CCC data in the intermediate energy region for most transitions considered by them.

For <u>spin changing transitions</u> the various new calculations (CCC, FOMBT (DWA), CBE) and the older ones of Ochkur and Bratsev (Soviet Astronomy - A.J. 2 (1966) 797) give different results, for instance at intermediate energies, and only CCC and CBE approach each other at higher energies, except for spin changing S-S transitions. In particular for the latter case more study is necessary, as for instance about the influence of the choice of the wave functions used for the relevant He states.

The few experiments of Rall et al. (optical, emission of radiation, Phys. Rev. Lett. 62 (1989) 2253) and Müller-Fiedler at al. (differential angular scattering, J. Phys. B <u>17</u> (1964) 259) are not giving sufficiently accurate data for the assessment of the cross sections.

# 3.3 Cross sections for transitions between other excited states of He, $n^{1.3}L - n'^{1.3}L'$ (n,n' = 2-4)

So far these other transitions have not yet received an extended attention as have the transitions considered before (see sub-sections 3.1 and 3.2). The most extensive cross section calculations on these transitions are contained in the following references:

- Cross Sections for Electron-Impact Induced Transitions Between Excited States in He; n,n'=2,3 and 4 (CBE approximation), V.P. Shevelko and H. Tawara (in Supplement to the Journal Nuclear Fusion, <u>6</u> (1995) 27).
- Collision Strengths from a 29-state R-matrix calculation on Electron Excitation in Helium, P.M.J. Sawey and K.A. Berrington, Atomic Data and Nuclear Data Tables <u>55</u> (1993) 81.

# 4. Recent developments in cross section calculation capabilities

4.1 General remarks

The often used perturbative techniques yield good results for the direct transition at high energies, so long as good wave functions are used. For exchange transitions these calculations often give a good estimation of the cross section (see Fig. 1) though on occasion the discrepancy with the more sophisticated theories may be substantial (see Fig. 2). (Both figures are from de Heer et al.: Nucl. Fusion A+M Suppl. vol. 6, in press).

At low energies there are RM-5 (Fon et al., J. Phys. B <u>14</u>, 2921 (1981)), RM-11 (Berrington et al. J. Phys. B <u>18</u>, 4135 (1985)), RM-19 (Berrington and Kingston, J. Phys. B <u>20</u> 6631 (1987)), and RM-29 (Sawey et al., J. Phys. B. <u>23</u>, 4321 (1990), At. Data Nucl. Data Tables <u>55</u>, 81 (1993)) R-matrix calculations in which only the lowest discrete states (from n=1 to n=2,3,4 and 5 respectively) were included in the close-coupling wave functions. As no continuum states were included, one would not expect these calculation to be highly accurate at energies above the ionization threshold (where loss of flux into such channels should be taken into account). However, at energies below ionization, where resonances dominate and the ionization continuum effects are less significant, it was shown by Berrignton and Kingston (J. Phys. B <u>20</u>, 6631 (1987)) that R-matrix calculations for e-He scattering at low energies in which physical discrete states with increasing principal quantum number n are used yield qualitatively accurate excitation cross sections in the energy range up to the highest threshold explicitly included while quantitatively they could be wrong by 10% in magnitude. This also implies that the 2<sup>3</sup>S-3<sup>3</sup>S cross section will not have the correct qualitative shape at energies  $\ge n=3$  thresholds.

The R-matrix method, as described above, is by nature a low-energy method to treat collision processes, but can be accurate at intermediate energies for ionic targets where the Coulomb force dominates. For the helium target, a calculation including physical target states with principal quantum number n can be expected to provide a qualitative description for transitions involving levels up to n-1. In general, predicted cross sections from the ground state to levels with principal quantum number n can be expected to be somewhat too large (by about 10%). However, in the case of transitions between very strongly coupled states, even a calculation with very few states can be accurate. An example is given in Fig. 2 for the transition 2s  ${}^{3}S \rightarrow 2s {}^{1}S$  where the 5-state calculation of Fon et al. (1981, see above) is in good agreement with the recent "convergent close-coupling" (CCC) results of Bray and Fursa (J. Phys. B 28, L 197 (1995)).





	Recommended cross section
•	Bray and Fursa (1995), CCC, this work
Ο	Burke et al. (1969), R(5), [10]
¥	Fon et al. (1981), R(5), [9]
0	Berrington et al. (1981), R(11), [11]
Δ	Kingston et al. (1992), R(29), [4]
0	Kim and Inokuti (1969), FBA, [12]
۲	Ton-That et al. (1977), FBA, [13]
۵	Vanderpoorten (1970), FBA, [15]
۵	Ochkur and Brattsev (1966), Ochkur, [17]
	Shevelko and Tawara (1995), CBE, [6]
٠	Flannery and McCan (1975), MET, [18]
•	Mansky et al. (1990,1992), DMET, [19,20]
Ο	Mathur et al. (1987), DWA, [21]
٠	Badnell (1984), DWA, EDW, [22]
▽	Khurana et al. (1987), DWA, [23]
	Cartwright and Csanak (1995), DWA, FOMBT, [7]
o	Khayrallah et al. (1978), GLAUBER, [25]
ಶ	Willis et al. (1981), 3-state C_C, (27)
ø	Katiyar and Srivastava (1988), DWA, [28]
0	Rall et al. (1989), Exp., [26]



Fig. 2



	Recommended cross section
٠	Bray and Fursa (1995), CCC, this work
o	Burke et al. (1969), R(5), [10]
▼	Fon et al. (1981), R(5), [9]
0	Berrington et al. (1981), R(11), [11]
۵	Kingston et al. (1992), R(29), [4]
0	Kim and Inokuti (1969), FBA, [12]
۵	Ton-That et al. (1977), FBA, [13]
۵	Vanderpoorten (1970), FBA, [15]
۵	Ochkur and Brattsev (1966), Ochkur, [17]
m	Shevelko and Tawara (1995), CBE, [6]
٠	Flannery and McCan (1975), MET, [18]
0	Mansky et al. (1990, 1992), DMET. [19,20]
Ø	Mathur et al. (1987), DWA, [21]
٠	Badnell (1984), DWA, EDW, [22]
⊽	Khurana et al. (1987), DWA, [23]
۸	Cartwright and Csanak (1995), DWA, FOMBT, [7]
0	Khayrallah et al. (1978), GLAUBER, [25]
Ø	Willis et al. (1981), 3-state C_C, [27]
۲	Katiyar and Srivastava (1988), DWA, [28]
0	Rali et al. (1989), Exp., [26]



### 4.2 Recent (1995) Developments

### A. Convergent Close-Coupling (CCC) Method

A major advance in the ability to calculate e-He cross sections has occurred due to the extension of the CCC method for e-H scattering to the helium target (Fursa and Bray, Phys. Rev. A <u>52</u> (1995) 1279). The method involves the expansion of the total wave function in a set of target states. These states are obtained by diagonalizing the target Hamiltonian in an antisymmetric two-electron basis constructed from an orthogonal Laguerre basis. The use of such a basis ensures that the obtained target states are all square integrable, but allow for a systematic treatment of both the target true discrete and continuum subspaces. The reliability of the results is tested by progressively increasing the basis size until convergence to a desired accuracy in the cross section of interest is observed. Since both the discrete and continuum subspaces are treated the method is equally valid over the entire energy range of interest and for all scattering processes, including ionization.

### B. R-matrix method with pseudo-states (RMPS)

Along the same lines of accounting for the target continuum states, the recently developed "R-matrix with Pseudo States" (RMPS) method (K. Bartschat, E.T. Hudson, M.P. Scott, P.G. Burke and V.M. Burke 1995, J. Phys. B, in press) extends the range of applicability of the standard low-energy R-matrix method described above to "intermediate energies" above the ionization threshold. The method allows for a systematic treatment of N-electron target correlation effects and (N+1) electron continuum effects. An important feature of this method is its applicability to general complex multi-electron atomic and ionic targets. It was recently applied to e-He collisions involving levels with  $n \leq 2$  (K. Bartschat, E.T. Hudson, M.P. Scott, P.G. Burke and V.M. Burke 1995, submitted to Phys. Rev. Lett..) and is currently being extended to levels with  $n \leq 3$ . As an example, Table 1 (taken from the second of the above cited articles) shows the good agreement between the CCC and RMPS predictions (and with experiment) for some S-S transitions. Furthermore, the importance of accounting for the target continuum states is demonstrated by comparison with a standard 5-state close-coupling calculation which predicts results of up to a factor of three too large.

**Table 1.** Total cross sections (in  $10^{-18}$ cm<sup>2</sup>) for electron impact excitation of helium. "CCC" refers to the 75-state (frozen core) calculation of Fursa and Bray (Phys. Rev. A <u>52</u>, 1279 (1995)) and "5-state" to a (frozen core) model with physical states alone. The experimental data for the elastic cross section are taken from Register et al. (Phys. Rev. A <u>21</u>, 1134 (1980)) and for excitation from de Heer et al. (Nucl. Fusion A+M Suppl. <u>3</u>, 19 (1992)).

Transition	Energy	5-state	ccc	this work	experiment
$1^{1}S \rightarrow 1^{1}S$	30 eV	201	225	219	211
	40 eV	154	169	166	158
	50 eV	124	134	133	126
	80 eV	73.2	75.9	78.4	71.2
$1^{1}S \rightarrow 2^{3}S$	30 eV	4.95	1.91	1.76	1.90
	40 eV	1.63	1.14	1.10	1.18
	50 eV	0.709	0.732	0.694	0.740
	80 eV	0.151	0.256	0.225	0.260
$1^{1}S \rightarrow 2^{1}S$	30 eV	5.84	2.19	2.29	2.40
	40 eV	3.97	1.87	2.02	2.11
	50 eV	3.12	1.67	1.84	1.94
	80 eV	1.66	1.37	1.40	1.50

### 4.3 What can be done with CCC and RMPS

a) <u>e-He collisions</u>: Data are required for transitions between ALL levels up to n=4. These can be obtained by the CCC method at all energies of interest. For transitions involving levels with n ≤ 3, RMPS results are expected to be available for collision energies below 100 eV. This would allow for a much needed consistency check of the two approaches.

We also note that both of these methods allow for the prediction of total ionization cross sections from both ground and excited states.

b) <u>Other collision systems</u>: Electron impact cross section data is also required for other targets, including neutral Li, Be, B, C, O, Ne, Ar, Ti, Cr, Fe, Ni, Cu, Mo, W and the multitude of their positive ions. For quasi-one and quasi-two electron systems, the CCC method is likely to be able to provide accurate results for all required transitions and collision energies. RMPS is expected to yield similar results at low and intermediate energies. In addition, the RMPS can be applied to even more complex systems in a straightforward way.

### **Conclusions and Recommendations**

Based on the analysis performed at the meeting, the current status of electron-impact excitation database for helium and of the existing possibilities for generation of excitation cross section data for this collision system can be summarized as follows:

- 1) The cross section database for the transitions from the ground to n<sup>1,3</sup>L (n=2-4, L=S,P,D) states is, generally, in a good shape, having an accuracy of 5-10% for the singlet states. For the transitions to triplet states the uncertainties are on the level of about 30%, but this can be improved (down to about 10%) by performing new CCC, RMPS and CBE calculations. Systematic CCC and RMPS calculations for all 1<sup>1</sup>S → n<sup>3</sup>L (n=2-4) transitions would be desirable up to 1000 eV to compare with the CBE results and reduce the cross section uncertainties to about 10% in the high energy region as well. The recent critical assessment of the data for these transitions (F.J. de Heer et al., Nucl. Fusion A+M Suppl. 3, 7 (1992)) remains still valid in its major part.
- 2) The cross sections for  $2^{1,3}S \rightarrow n^{1,3}L$  (n=2-4) transitions have also been recently critically assessed (F.J. de Heer et al., Nucl. Fusion A+M Suppl. <u>6</u> (1995) 7) and supplemented with new results from extensive CCC calculations (Bray and Fursa, Sept.-Oct. 1995). The database for these transitions can now be considered as reasonably well established.
- 3) For the transitions  $2^{1,3}P \rightarrow n^{1,3}L$  (n=2-4) and  $n^{1,3}L \rightarrow n_1^{1,3}L_1$  (n,n<sub>1</sub>=3,4) a complete set of CBE cross sections is now available (Shevelko and Tawara, Nucl. Fusion A+M Suppl. <u>6</u> (1995) 27) and could be useful in a consistency check of the planned CCC calculations at high energies. Systematic CCC and RMPS calculations are necessary in the low and intermediate energy range to improve the present status of the database for these transitions and to check the consistency of earlier RM-19 and RM-29 results in the threshold region.

- 4) The recently developed CCC and RMPS methods (and the corresponding computational codes) open the possibility for generation of all required excitation cross section in e-He (n=1-4) collisions in the entire energy range of interest to fusion (and other) applications in a time-frame of one-to-two years. These two methods are capable to achieve cross section accuracy of about 10% (or better, in some energy regions), and to provide cross section information also for ionization (from the same run of the code). The CCC and RMPS methods can be applied with the same success to excitation and ionization of more complex many-electron atoms and ions of fusion interest (subject to construction of adequately good electron wave functions).
- 5) The co-ordinating role of the International Atomic Energy Agency in establishing a recommended collisional database for helium has been instrumental in the past. The Agency should continue to play this role also in the future and provide the technical assistance in both formatting the data (e.g. in a parametrized form suitable for fusion application) and their dissemination to the fusion research community.

# Appendix 1

### IAEA Consultants' Meeting on 'Electron-Impact Excitation Cross Section Data for Helium'

## 20-21 November, 1995, IAEA Headquarters, Vienna, Austria

### List of Meeting Participants

Prof. I. Bray	Electronic Structure of Material Centre, Department of Physics, Flinders University, GPO 2100, Adelaide 5001, AUSTRALIA
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IAEA	
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### Appendix 2

### IAEA Consultants' Meeting on 'Electron-Impact Excitation Cross Section Data for Helium''

20-21 November, 1995, IAEA Headquarters, Vienna, Austria

### Meeting Agenda

Monday, November 20

Meeting Room: A-2312

- 10:00 10:30: Opening - Adoption of Agenda
- 10:30 12:00: Analysis of available database: critical assessment
- 12:00 14:00: Lunch
- 14:00 18:00: Analysis of available database: critical assessment

### Tuesday, November 21

- 10:00 12:00: Identification of most critical gaps in the He database
- 12:00 14:00: Lunch
- 14:00 16:00: Discussion of ways for He-database improvements Formulation of meeting conclusions

Note: Within each working session a 30 min. coffee break is envisaged