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IAEA SPECIALISTS' MEETING ON

"REQUIRED ATOMIC DATABASE FOR NEUTRAL BEAM PENETRATION IN LARGE TOKAMAKS"

Vienna, 10-12 April 1989

SUMMARY REPORT

Prepared by R.K. Janev

July 1989

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

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Abstract

This Summary Report contains the proceedings, conclusions and recommendations of the Specialists' Meeting on the "Required Atomic Database for Neutral Beam Penetration in Large Tokamaks" convened on 10-12 April 1989, at the IAEA Headquarters in Vienna, Austria, by the IAEA Atomic and Molecular Data Unit. The existing database for collisions of energetic hydrogen atoms with electrons, protons and plasma impurity ions, as well as the new results presented at the Meeting were critically analyzed, the accuracies of the data were assessed, and recommendations were given regarding the best set of available cross section data to be used in neutral beam penetration codes.

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1. Introduction

The injection of energetic neutral beams is currently used as a standard method for heating tokamak fusion plasmas to temperatures required for ignition, and is considered as one of the major methods for power injection and current drive in the next-step, reactor level fusion devices. The development of an efficient neutral beam heating and current drive system has been identified as one of the important issues in the R&D plans for the International Thermonuclear Experimental Reactor (ITER). At the ITER Physics Group Workshop on Heating and Current Drive, held on June 13-17, 1988, in Garching (FRG), it was concluded that the uncertainties in the atomic collision database for calculation of the neutral beam penetration, beam energy deposition rates and the current drive efficiency, may have a serious impact on the neutral beam system technology. The characteristics of the neutral beam penetration and energy deposition are also important for plasma parameters control (current density and safety factor profile control) and for setting the onset of beam induced Alfven wave plasma instabilities. The same kind of problems are also met in the design of beam injection systems for other fusion test reactors, presently under consideration (NET, TIBER-II, FER, and OTR).

Recognizing the importance of establishing an accurate atomic database for the calculations of neutral hydrogen beam penetration in the next-generation fusion devices, the IAEA Atomic and Molecular Data Unit convened on April 10-12, 1989, at the IAEA Headquarters in Vienna, a relatively small Specialists' Meeting of competent experts to assess the existing database involved in the hydrogen neutral beam penetration kinetics, and to recommend the best available set of data for use in beam penetration codes. The List of Meeting Participants is given in Appendix 1, while the Meeting Agenda is given in Appendix 2.

It should be emphasized that a preparation work has been undertaken by the Meeting participants a few months prior to the Meeting, with the objective to generate new data for the most important gaps in the database, or as a cross-check for some of the existing data. Several of the participants also agreed to perform data compilation and assessment work before the Meeting for certain classes of processes, so that the efficiency of the joint work during the Meeting was very high. Some experts (Dr. V.P. Shevelko and Dr. S.C. Mukherjee), who were not able to attend the Meeting, sent the results of their cross section calculations to the Meeting, and these were included in the Meeting discussions and data analyses.

2. Meeting Proceedings

The Meeting was opened by Dr. J.J. Schmidt, the Head of the IAEA Nuclear Data Section. Then, R.K. Janev, Head of the IAEA Atomic and Molecular Data Unit and IAEA Responsible officer for the Meeting, briefly emphasized the objectives of the Meeting. At the first session of the Meeting, C.D. Boley presented beam stopping cross section results from his neutral beam penetration code. The cross section calculations were performed by inclusion of the multistep processes. An atomic database prepared by R.K. Janev was used in these calculations. Boley also presented an analysis of the sensitivity of the beam stopping cross sections on the accuracy of different classes of atomic collision cross sections. R.K. Janev provided arguments and explanations for the choice of atomic cross sections used in Boley's calculations, and stressed some inconsistencies in the existing database. M. Cox provided detailed information on the atomic data requirements for beam penetration in reactor-grade plasmas, as well as information on the structure of "standard" beam energy deposition and current drive codes. He rised the question whether the beam stopping cross section can be considered as a local quantity and stressed the necessity of checking whether the beam energy deposition codes can use a single-state beam with enhanced beam stopping cross section.

The second session of the Meeting was devoted to the particle-impact excitation data for atomic hydrogen. In the energy region considered, all electron impact processes are described well by the Born approximation. Extensive electron-impact excitation data for the $n_o\ell_o \rightarrow n_1\ell_1$ forbidden transitions in hydrogen, calculated within the 1st Born approximation, were provided by V.P. Shevelko (and presented at the Meeting by R.K. Janev). To within 5-10% accuracy the data were fitted to an analytical, two-parameter expression. For the allowed $n_o\ell_o \rightarrow n_1\ell_1$ transitions, Shevelko provided an analytical formula for the cross section (derived by a perturbational procedure and using the dipole approximation), which reproduces the 1st Born results to within 20%.

For proton induced 1s → nl excitation transitions in hydrogen, the group of S.C. Mukherjee from Jadavpur, provided extensive 1st Born cross section calculations (up to n=16). These data were distributed to the Meeting participants in the form of graphs, compared with the results calculated from the semi-empirical formula of Lodge et al.

K.-H. Schartner reviewed the experimental database for proton-impact and multicharged ion-impact excitation of hydrogen atoms, including recent data from the Giessen University group. Inconsistencies in the old Park et al. (1976) cross section data for the n=3, 4 were identified, and were attributed to an inappropriate normalization procedure. W. Fritsch reviewed the theoretical database for proton and impurity ion excitation of hydrogen and presented an extensive set of new results for the intermediate energy region (~ 30-150 keV/amu), based on the multi-state atomic-orbital close-coupling method. Fritsch presented results both for 1s → n ($2 \leq n \leq 5$) and n → m ($2 \leq n < m \leq 5$) transitions. The agreement of these calculations with the CTMC data and the results of Lodge et al formula was found satisfactory. R.E. Olson presented an extensive set of CTMC excitation cross sections for both proton and impurity ion ($q \leq 26$) impact, including also transitions between excited states. The scatter of the data, when scaled as σ/q vs E/q (q being the ionic charge), was found to be about ± 20% in the region of cross section maximum. Above 300-400 keV/amu, the CTMC data have been extrapolated by using the Bethe-Born behaviour of the excitation cross section. Dz.S. Belkic discussed the formulation of heavy particle excitation theory from the point of view of the correct boundary conditions.

In the third session of the Meeting the database for electron removal from hydrogen by proton and impurity ion impact was discussed. H.B. Gilbody presented an extensive review on the existing charge exchange and ionization database, emphasizing its experimental part, and including electron removal from excited states. D.S.F. Crothers reviewed the theoretical database for charge transfer, with emphasis on the cross section scaling relationships in different energy regions. F.J. de Heer presented the recent experimental charge exchange data, obtained within the KVI (Groningen) - FOM (Amsterdam) collaboration, including state-selective electron capture. S. Szucs reviewed the data for electron capture from excited hydrogen by He^{2+}, obtained by the group of Louvain-la-Neuve.

After these presentations and the accompanying discussions, the Meeting participants split into four Working Groups for a more detailed analysis of the data requirements and the existing database (including the new results presented at the Meeting), assessment of the accuracies of the data, and preparation of recommendations regarding the best available atomic collision data for hydrogen to be used in neutral beam penetration codes. The following Working Groups were formed:

1) Working Group on the required atomic database for neutral beam penetration;
2) Working Group for electron-impact collision data;
3) Working Group for heavy-particle impact excitation;
4) Working Group for electron removal by heavy-particle impact.

The reports of these working groups are given in the next section.

Note: A meeting follow-up

After the Meeting (May, June 1989), K.-H. Schartner performed absolute cross section measurements for the 1s → np (n=2-6) excitation transitions in the H^+ +H(1s) system for impact energies of 300 and 500 keV/amu. The new data, which have a 10-15% accuracy, agree well with the Born cross sections of Mandal et al. (reported at the Meeting), and thus resolve the controversy about the normalization of the relative Park et al. data for n=3, 4 transitions. The new Schartner's data can also be taken as justification for the use of Lodge formula in calculating the 1s → n proton-impact excitation cross sections (since his results, to within 10%, agree with the Born calculations).

3. WORKING GROUP REPORTS ON REQUIRED AND RECOMMENDED DATA

3.1. Working Group Report on the required atomic database for neutral hydrogen beam penetration in large tokamaks

M. Cox, C.D. Boley, R.K. Janev

1. Introduction. Multistep beam ionization

Injection of energetic neutral hydrogen beams is one of the major methods for plasma heating in the present-day large tokamaks (JET, TFTR, JT-60, DIII-D, ASDEX, etc.) and is envisaged to play a similar role in the next-generation fusion (such as NET, TIBER-II, FER, ITER, etc.), where this method should also provide a large contribution to the non-inductive current drive in the central part of the discharge. The efficiency of the neutral beam injection (NBI) method for heating and current drive of large tokamak plasmas relies on the deposition of beam energy and momentum in the central (near axis) plasma region, i.e. on a correct determination of the required beam energy which ensures such deposition. The attenuation of the neutral hydrogen beam penetrating a plasma depends exclusively on the atomic collision processes. These processes lead to beam-atom ionization, after which the motion of ionized beam particles is determined by the tokamak magnetic field, and their energy is dissipated in Coulomb collisions with the charged plasma particles.

The standard beam penetration and beam energy deposition codes are designed on the asumption that beam particles are all in the ground state and that beam atom ionization occurs due to ground state-continuum transitions in collisions with plasma electrons, protons and impurities, and due to the electron capture from the ground state by plasma protons and impurity ions. This approximation is valid as long as the beam velocity and plasma density are such that the collision time is much longer than the radiative lifetime of excited atomic states. However, for beam energies above 200 keV/u and plasma densities above ~ $5 \times 10^{19} m^{-3}$, the radiative and collision times of excited beam atoms become comparable, and the beam-plasma system is in a radiative-collisional regime. Inclusion of the collision processes of excited beam atoms in the beam attenuation kinetics becomes necessary, and this leads to an enhancement of the effective beam attenuation (or "stopping") cross section [1].

The effects of multistep processes on the beam attenuation (or, the multistep beam ionization) became recently an important issue in the design of beam heating and current drive systems for the next-step, reactor level fusion devices (ITER, NET, etc). The required NBI heating power in these devices is of the order of ~ 100 MW, with beam energies around ~ 1 MeV, and operating plasma densities around $10^{20} m^{-3}$. The estimated beam stopping enhancement due to multistep processes for beam-plasma parameters in this range is between 50% and 100%, [1-3] depending on the accuracy of the atomic database used in the calculations. This uncertainty is reflected in the requirements for the beam energy value and the associated beam technology, with obvious economical consequences. Therefore, an accurate determination of the required atomic database for the beam stopping calculations is necessary for resolving this important issue.

2. The required atomic database

The following processes are involved in the beam attenuation kinetics, when multistep processes are included (H stands for D or T):

2.1. Electron impact processes

1) $$e + H(n) \rightleftarrows e + H(m) \quad , \quad 1 \leq n < m \leq N \tag{1}$$

2) $$e + H(n) \rightarrow e + H^{+} + e \quad , \quad 1 \leq n \leq N \tag{2}$$

(N is defined by Eq.(8) below)

2.2. Proton impact processes

1) $$H^{+} + H(n) \rightleftarrows H^{+} + H(m) \quad , \quad 1 \leq n < m \leq N \tag{3}$$

2) $$H^{+} + H(n) \rightarrow H^{+} + H^{+} + e \quad , \quad n \geq 1 \tag{4a}$$

$$H(m) + H^{+} \qquad (m \simeq n) \tag{4b}$$

2.3. Impurity-ion impact processes

1) $A^{q+} + H(n) \rightleftarrows A^{q+} + H(m)$, $1 \leq n < m \leq N$ (5)

2) $A^{q+} + H(n) \rightarrow A^{q+} + H^{+} + e$, $n \geq 1$ (6a)

$\rightarrow A^{(q-1)+}(m) + H^{+}$, $(m \simeq n)$ (6b)

$A^{q+} = He^{2+}$, (Be^{4+}), C^{6+}, O^{8+}, Fe^{24-26+}, W^{n+} ,

2.4. Radiative processes

$H(m) \rightarrow H(n)+h\nu$, $1 \leq n < m \leq N$ (7)

2.5. Lorentz field ionization

$$H(m) + F_L \rightarrow H^{+} + e \quad , \quad m \geq N = \frac{1}{2F_L^{1/4}} \tag{8}$$

where $F_L = | \vec{V}_o \times \vec{B} |$, V_o and B are the neutral beam velocity and strength of magnetic field, respectively. For neutral beam energies E_o of about 10 keV/u and magnetic fields of $B \simeq 3$ T, $N \simeq 7$, while for $E_o \simeq 1$-2 MeV/u and $B \simeq 10$ T, $N \simeq 4$.

The computer codes for beam attenuation calculations solve the system of coupled equations

$$V_o \frac{dI_n}{dx} = \sum_{n'=1}^{N} Q_{nn'} I_{n'}(x) \quad , \quad n = 1 \ldots\ldots N \ , \tag{9}$$

$$I_n(o) = \delta_{n1} \ , \tag{10}$$

where $I_n(x)$ is the fraction of the beam in the n-th quantum state at the distance x from the point where the beam enters the plasma (x=o). The reaction matrix $Q_{nn'}$ includes the reaction rate coefficients for all the processes 2.1 - 2.4.

The stopping cross section is defined as $\sigma_s = 1/(n_e\lambda)$, where λ is the e-folding beam intensity decay distance, and n_e is the plasma density. The relative enhancement of σ_s due to multistep processes is $\delta = (\sigma_s-\sigma_s^o)/\sigma_s^o$, where σ_s^o is the stopping cross section for ground state processes only.

Previous calculations of σ_s have shown [1] that for plasma densities $n_e \lesssim 10^{21}m^{-3}$ and beam energies $E \lesssim 30$ keV/u, the effect of excitations on σ_s is only about 10-15%. The relative enhancement δ starts to increase considerably for $E \gtrsim 150$-200 keV/u, even at moderately low densities ($n_e \sim 5x10^{19}m^{-3}$). As function of E_o, n_e, and Z_{eff}, δ shows the following dependences (in the ranges 10 keV/u $\leq E_o \leq$ 10 MeV/u, $10^{19}m^{-3} \leq n_e \leq 10^{21}m^{-3}$, $1 \leq Z_e \leq 10$): logarithmic increase with E_o, almost linear increase with n_e, and linear increase with Z_{eff}.

The standard beam penetration codes calculate the beam heating rates and current-drive profiles on the base of a single-state (ground-state) beam model and local beam stopping cross sctions. With the necessity of inclusion of multistep processes, the question arises whether the codes require a full multi-state description of the beam. From heating calculations for TFTR, it appears that one can still employ a single-state model but with an appropriately enhanced beam stopping cross section. It would seem prudent, however, to check whether this remains true for the parameters of the next-step devices. As a representative example one could take the design parameters for the physics and technology phase of ITER: $n_e = (0.7 - 2) \times 10^{20}m^{-3}$, $E_o = 1 \pm 0.3$ MeV, $T_e \sim 18$-30 keV, $Z_{eff} \simeq$ 1.5-2.5 ($Z_{eff} = 2.3$ for the technology phase, with an impurity mix of He : C : O : Fe = 5 : 1.5 : 0.5 : 0.05).

Having in mind the above range of E_o, and that the relevant interaction energy parameter is E_o/q ($q \lesssim 25$ for metallic impurities), one defines the region of $E_o/q \gtrsim 20$ keV/u for which data for the heavy-particle collisions are required for the next-step fusion devices. In order to incorporate the data needs also for the presently operating tokamak devices ($E_o \gtrsim 60$ keV/u), one would have data for $E_o/q \gtrsim 1$ keV/u. As well known, the region of $E/q \sim 25$ keV/u is a critical one for the theoretical description of heavy-particle collision processes.

The required electron impact data, however, all lie in the region where the Born approximation is applicable.

3. Required data accuracies

Ideally, the total beam stopping cross section needs to be known to an accuracy of ~ 10%. It is fortunate that the cross sections for the most important, electron-removal processes involving the ground state are experimentally known to an accuracy better than 10% (as documented by the Working Group Reports of this Meeting). A rough sensitivity analysis for the beam energies and plasma densities of interest, and for penetration into a uniform plasma has shown that:

- The contribution of all electron processes to the total beam stopping cross section is of the order of 15-20%, so that the required accuracy for their cross sections would be about 50%;
- The contribution of all impurity impact excitations to σ_s is about 20% (although this fraction increases with the beam energy) and the required accuracy for the corresponding cross sections is about 50%. This is only for the most important $1 \rightarrow n$ excitations; for the less important $n \rightarrow m$ ($n \geq 2$) transition (which contribute only 5% to σ_s), the required accuracy is a factor of 2 to 3, only;
- The proton impact excitation and electron removal processes contribute about 30-40% in the beam stopping enhancement. The required accuracy of the corresponding cross sections is estimated to about 20-30% for the excitations from the ground state, and 30-50% for the electron removal.

References

1. C.D. Boley, R.K. Janev, D.E. Post, Phys. Rev. Letts. 52, 534 (1984);
2. A.S. Schlachter, J.W. Stearns, W.S. Cooper, R.E. Olson, "Penetration of an energetic D^o beam in an ETR plasma. Current Drive for ITER", Report LBL-25369; presented at the ITER Workshop on Heating and Current Drive, June 13-17, 1988, Garching, FRG;
3. V.A. Abramov, A. Yu. Pigarov, V. Pistunovich, Report presented at the ITER Workshop on Heating and Current Drive, June 13-17, 1988, Garching, FRG.

3.2. Working Group Report on Electron-Impact Processes: Recommended database for electron impact excitation and ionization

F.J. de Heer, R.K. Janev and J.J. Smith

The cross section database for the following processes was considered*:

$$e + H(n) \rightarrow e + H(m) \quad , \quad m > n \geq 1 \tag{a}$$

$$e + H(n) \rightarrow e + H^{+} + e \quad , \quad n \geq 1 \tag{b}$$

including also the specific ℓ-substates in 1 → 2; 3 excitation. The analysis concentrated on the energy range E ≥ 100 eV, which is of main interest in the context of neutral beam penetration into plasmas.

1. Excitation processes

1.1. $\underline{e + H(1s)}$ → e + H(2s)
→ e + H(2p)

→ e + H(n=2)

For σ_{ex} (2s) and σ_{ex} (2p), the cross sections of Callaway and McDowell (CAMP 13 19 (1983)) are recommended. The total n=2 excitation cross section is $\sigma_{ex}(n=2) = \sigma_{ex}(2s) + \sigma_{ex}(2p)$.
Estimated accuracy: better than 10%.

1.2. $\underline{e + H(1s)}$ → e + H(3s)
→ e + H(3p)
→ e + H(3d)

→ e + H(n=3)

* The rate of the inverse reaction of (a) can be obtained by the detailed balance principle, while the inverse reaction (b) is of no interest in the context of beam penetration.

The recommended cross sections $\sigma_{ex}(3\ell)$ are those of Callaway and McDowell (CAMP 13, 19 (1983), and the total $\sigma_{ex}(n=3)$ cross section is $\sigma_{ex}(n=3) = \sigma_{ex}(3s) + \sigma_{ex}(3p) + \sigma_{ex}(3d)$.

Estimated accuracy for $\sigma_{ex}(n=3)$: better than 10%.

1.3. $e + H(1s) \rightarrow e + H^{*}(n\geq 4)$

For individual 1s → nl transitions, recommended are (in the considered energy range) the recent calculations of Shevelko 1989, reported at this Meeting. These include: a two-parameter analytic fit of the 1st Born calculations for dipole-forbidden transitions (the fit is accurate to within 5%), and a first-order peturbation-theoretical formula (using a dipole potential) for the dipole-allowed transitions.

Estimated accuracy: 20% or better.

Alternatively, for 1s → n transitions, recommended is also the semi-empirical formula of Vriens and Smeets (Phys. Rev. A 22, 940 (1980)), which in the Born energy region agrees to within 3-5% with the $\sigma_{ex}(n)$ cross sections of Shevelko (see Fig. 1).

Estimated accuracy for $\sigma_{ex}(n)$: 20-25%, or better.

1.4. $e + H^{*}(n) \rightarrow e + H^{*}(m)$, $m > n \geq 2$

Recommended is the semi-empirical formula of Vriens and Smeets (1980), which in the high energy region agrees to within 3-5% with the Born calculations of Shevelko (see Fig. 2). For individual $n\ell_o \rightarrow m\ell_1$ transitions (when necessary), recommended are the recent calculations of Shevelko (1989, report at this Meeting).

Estimated overall accuracy for $\sigma_{ex}(n\rightarrow m)$: 20-25%, or better.

2. Ionization Processes

2.1. $e + H(1s) \rightarrow e + H^{+} + e$

For this reaction, accurate experimental data exist in a wide energy region (Shah, Elliott, Gilbody, J. Phys. B 20, 3501, 1987). An analytic fit to these data, with appropriate Bethe-Born behaviour at high energy, is also available (Lennon, Bell et al., J. Phys. Chem. Ref. Data 17, 1285, 1988). The Working Group recommends these data for $\sigma_{ion}(1s)$.

Estimated accuracy: better than 10%.

2.2a. $e + H^*(2s) \rightarrow e + H^+ + e$

Experimental data for this reaction exist in the region below the Born region ($\gtrsim 50\ E_{thr.}$) (Dixon, Harrison, Abstracts of Papers, VII ICPEAC, p.892, 1971). These data can be extended by the Born-Exchange II calculations of Kyle and Omidvar (Phys. Rev. 176, 164 1968), and further by a Bethe-Born expression (Janev et al., "Elementary Processes in Hydrogen-Helium Plasmas", Springer-Verlag, 1987).

The cross section obtained by using this procedure is recommended.

Estimated overall accuracy: better than 20%.

2.2b. $e + H^*(2p) \rightarrow e + H^+ + e$

Recommended is the Born-Exchange II cross section of Kyle and Omidvar (1968), suitably extended by a Bethe-Born type expression (Janev et al, 1987).

Estimated accuracy: better than 20%.

2.2c. $e + H^*(n=2) \rightarrow e + H^+ + e$

$$\sigma_{ion}(n=2) = \sigma_{ion}(2s) + \sigma_{ion}(2p)$$

Accuracy: $\lesssim$ 20%.

2.3. $e + H^*(n\geq3) \rightarrow e + H^+ + e$

Recommended for σ_{ion} $(n\geq3)$ is the semi-empirical formula of Vriens and Smeets (1980).

Estimated accuracy: 25-30%.

General Remark

In the Born energy region of sufficiently high energy (see Bates and Griffing, 1953), the excitation and ionization cross sections for electron and proton impact are the same on the relative collision velocity scale (see Fig. 1 in the Report of Working Group on electron removal; WG 4). This fact should be used as a cross-check for the used electron-and proton-impact cross sections, and/or to derive more accurate cross sections in cases when it is necessary and possible.

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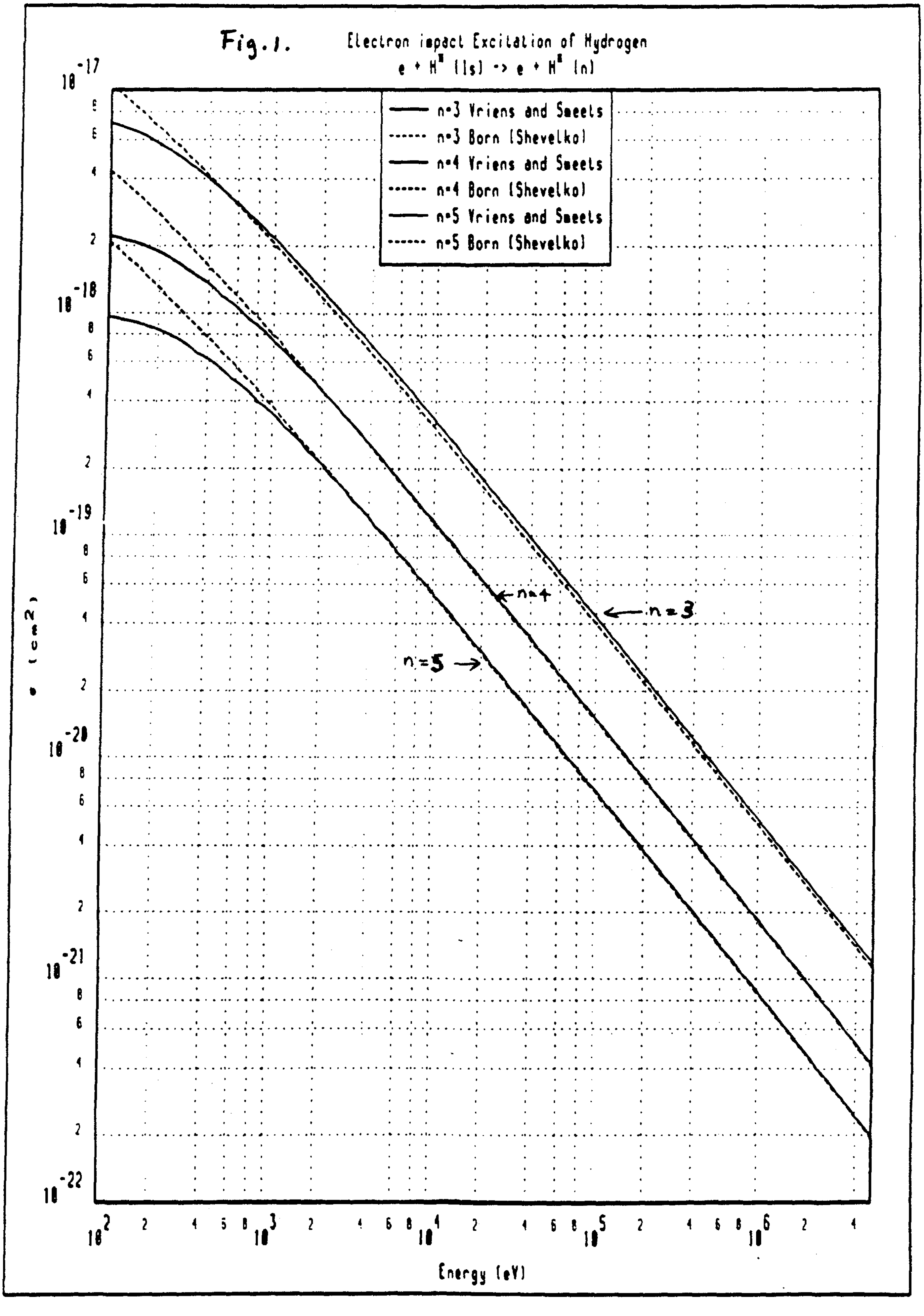
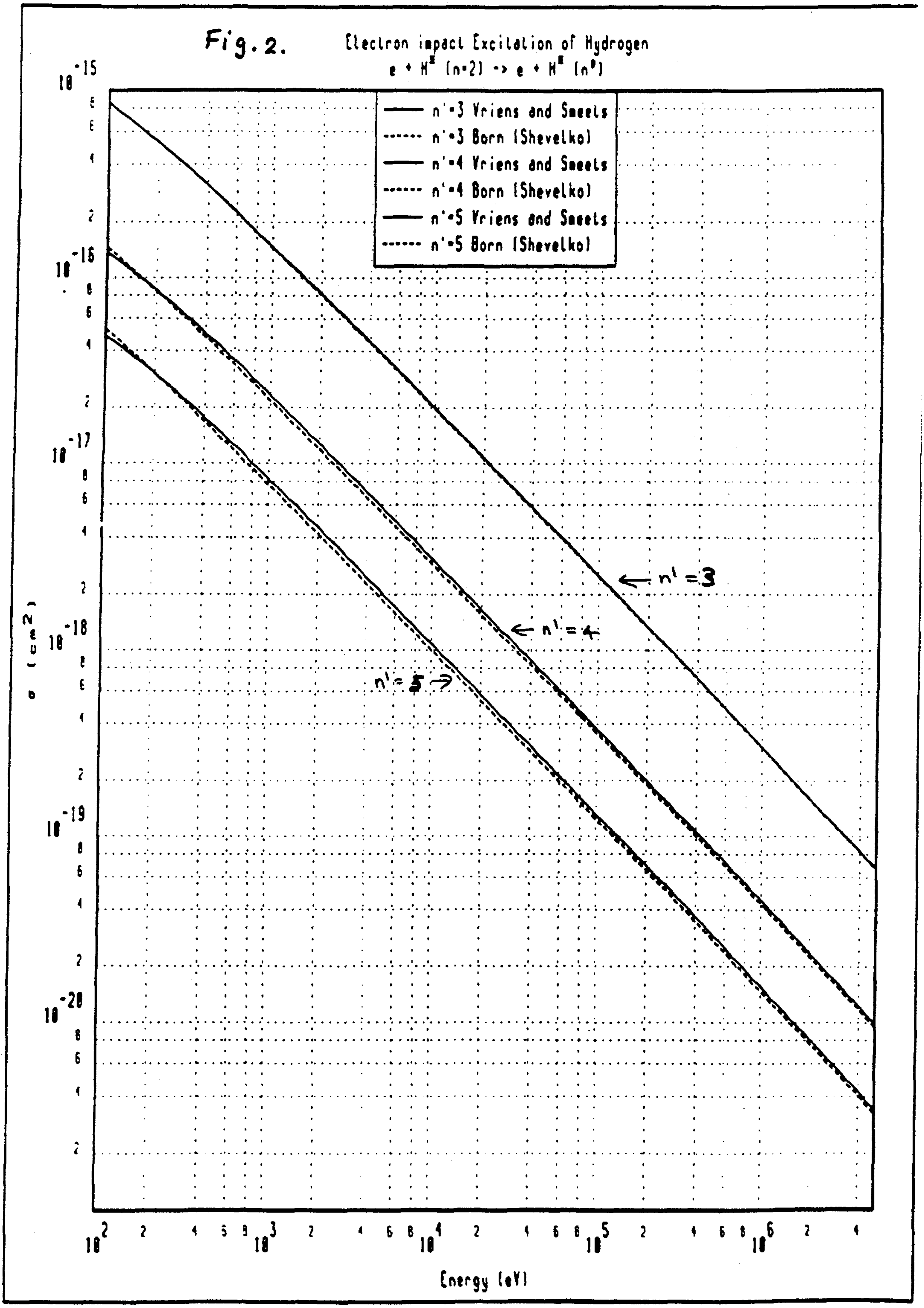


Fig. 1.
Electron impact Excitation of Hydrogen
e + H* (1s) -> e + H* (n)
n=3 Vriens and Smeets
n=3 Born (Shevelko)
n=4 Vriens and Smeets
n=4 Born (Shevelko)
n=5 Vriens and Smeets
n=5 Born (Shevelko)
n=4
n=3
n=5
σ (cm2)
Energy (eV)

Fig. 2.


Electron impact Excitation of Hydrogen
e + H* (n=2) -> e + H* (n')
n'=3 Vriens and Smeets
n'=3 Born (Shevelko)
n'=4 Vriens and Smeets
n'=4 Born (Shevelko)
n'=5 Vriens and Smeets
n'=5 Born (Shevelko)
← n' = 3
← n' = 4
n' = 5 →
σ (cm2)
Energy (eV)

3.3. Working Group Report on Ion-Impact Excitation: Recommended database for Ion-Impact Excitation of Atomic Hydrogen

W. Fritsch, R.E. Olson, K.-H. Schartner and Dz.S. Belkic

A. Proton Impact Excitation

Experimental studies of the excitation of atomic hydrogen by protons at energies above 10 keV are documented in two investigations (and in references cited therein). Park et al (1976) have measured total cross sections for ground state H(1s) excitation to n=2, 3 and 4 in an energy range between 15 keV and 200 keV. Schartner et al (1989) have obtained excitation cross sections to the 2p-level in the range between 70 keV and 700 keV. For n=2 excitation the experimental data agree within 10% with the 1st Born approximation (see Mandal et al. 1989) and also with the Lodge formula (Lodge et al. 1976). The Lodge formula is recommended because it appears to be applicable to lower energies. For higher levels of excitation, $n \geq 3$, there is a higher level of discrepancy between the theory and the experiments of Park et al. (1976). This, seemingly, is the result of a systematic error in the experimental data analysis, especially for n=4. From our evaluations, we suggest the Lodge formula will be valid to ± 20%. However, further experiments are needed, especially for $n \geq 4$, to verify this prediction.* Two recent experiments for Balmer α-emission from hydrogen, induced by H^+ or He^{++} impact, are worthwhile to be mentioned (Gilbody et al. 1989) though these may be of more relevance to plasma diagnostics.

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* After the Meeting, Dr. K.-H. Schartner has performed $H^+ + H(1s) \rightarrow H^+ + H^*(np)$ n=3-6, absolute cross section measurements for E=300 and 500 keV/amu. These data agree within 10% with the 1s → np Born calculations of Mandal et al (see Fig.1). Therefore, the use of the Lodge formula for $1 \rightarrow n$ ($n \geq 3$) excitation transitions seems fully justified.

For proton impact excitation from excited hydrogen levels, cross sections have been calculated using the Classical Trajectory Monte Carlo method (CTMC) (Olson 1989), the Atomic Orbital Close Coupling method (AO) (Fritsch 1989) and the Lodge formula. The calculated CTMC and AO results agree with each other, and within 20% with the Lodge formula. The Lodge formula is thus recommended for the atomic database.

B. Excitation in A^{q+} + H(1s) collisions (A^{q+} = He^{2+}, ..., Fe^{26+})

In the energy region of interest, E=100 - 2000 keV/amu, there is no published information on these systems except for the DACC (Dipole Approximation Close Coupling) results by Janev and Presnyakov (1980) and the one-center AO results by Fritsch and Schartner (1987). At the present Meeting, however, recently performed (specifically for the Meeting) and still unpublished results of CTMC calculation (Olson 1989), calculation within the symmetric eikonal (SE) approximation (Reinhold 1989, Reinhold and Miraglia 1987), and calculations with an enlarged one - center AO expansion (Fritsch 1989, these results should replace the earlier results by Fritsch and Schartner) were reported. The results for the 1s → n (n=2-4) excitation transitions are plotted, in figure 1, in a reduced σ/q vs. E/q form, where the q-scaled data from the Lodge formula and those of Mandal et al. are also shown (the latter only for E ≥ 100 keV/amu). They show the following features:

- CTMC : the dashed curves display approximate scaling with q, with the scatter of results for various q being approximately ± 20% (cf. the error bars of the curves). Note that for E $\gtrsim$ 400 keV/amu, the CTMC results are extended so as to satisfy the Bethe-Born cross section behaviour, but for n ≥ 3 they are consistently below the First Born data of Mandal et al.
- SE : points (circles) at 1 and 2 MeV/amu are derived for q=1; they lie on the CTMC curves and demonstrate that both the Born-extended CTMC and SE approximations agree with each other in the energy region when the 1st Born approximation is appropriate. The SE points at lower energies (triangles) are derived for q=6, and they are roughly about 20% above the CTMC results.

- AO : these results are compatible with the SE results at energies at, or above, the cross section maxima. At lower energies, there are significant deviations from the CTMC results and also from the assumed $\sigma/q = f(E/q)$ scaling.
- DACC : these results (broken lines) are above all other results for $n \geq 3$.
- q-scaled Lodge formula results : they are consistent with the q-scaled first Born, SE and the Born-extended CTMC data at higher reduced energies, and in the energy region around the cross section maximum they are about 20-30% below the AO data.
- all theories : a n^{-3} behaviour of the excitation cross section is not strictly observed but may still be adopted for $n \geq 5$.

Given this situation, it seems appropriate to recommend for the use in plasma penetration codes, the q-scaled first Born approximation for $E/q > 400$ keV/amu, extended in the region below 400 keV/u by the q-scaled Lodge formula ($\sigma \rightarrow \sigma/q$, $E \rightarrow E/q$). The estimated uncertainty is of about $\pm$ n.10% (n is the final principal quantum number) in the region $80 \lesssim E/q$ (keV/amu) $\lesssim 400$, which reduces to about $\pm$ 20% for $E/q \gtrsim 400$ keV/amu. At lower energies ($E/q \lesssim 80$ keV/amu), the uncertainties may become considerably larger (up to a factor of 2 or so, for q=6). Our analysis indicates that the "true" cross sections in the region around the reduced cross section maximum will lie above the q-scaled Lodge formula.

Further, particularly, experimental work on these systems is urgently needed to benchmark the available calculations. Also, the $H^+ + H$ system appears to be fundamental to this investigation in that it provides a test of the E/q vs. σ/q scaling in the region around the cross section maximum, $E/q \sim 80$ keV/u, even though at these low energies the H^+ results are not directly applicable to an ITER plasma.

C. Excitation in $A^{q+} + H(n)$ collisions ($n \geq 2$)

For these transitions, the CTMC results (Olson 1989) can be considered reliable (cf. Figures 2 and 3, for the $2 \rightarrow 3$, $2 \rightarrow 5$ transitions) in the energy region of cross section maximum. They agree with the available AO results (for He^{2+}, C^{6+}, Fritsch 1989). Consistent with the CTMC and AO data in this region are also the results of the q-scaled Lodge formula which in the energy region above the cross section maximum should provide an adequate description. This can be inferred also from the appropriateness of the Lodge formula for the $n \to n'$ proton induced transitions, which shows a 15-20% agreement with the AO data (Fritsch, 1989). Therefore, for the $n \to n'$ impurity ion induced transitions the Lodge formula is recommended, with an estimated accuracy of about 20% for the energy range above the cross section maximum.

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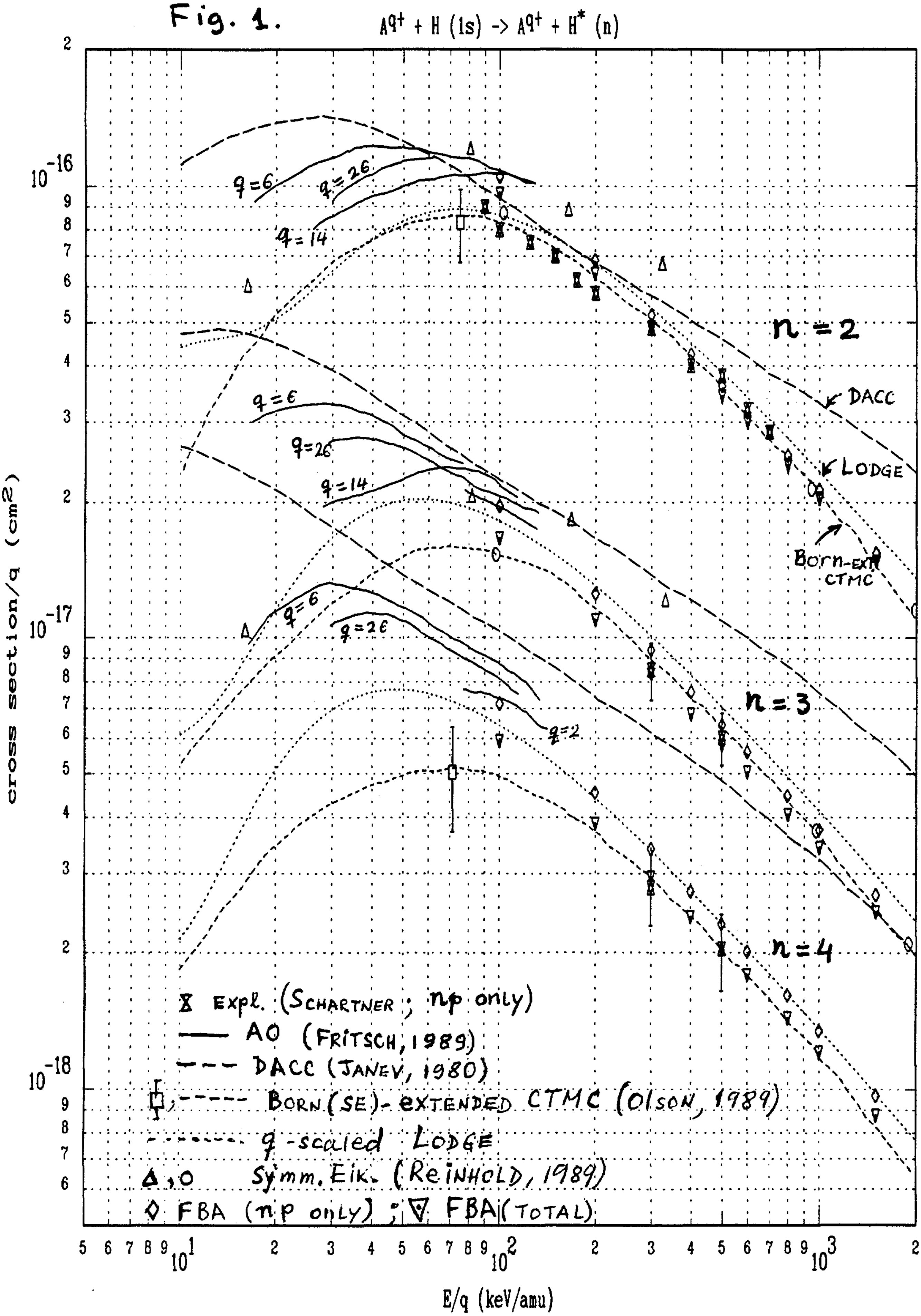
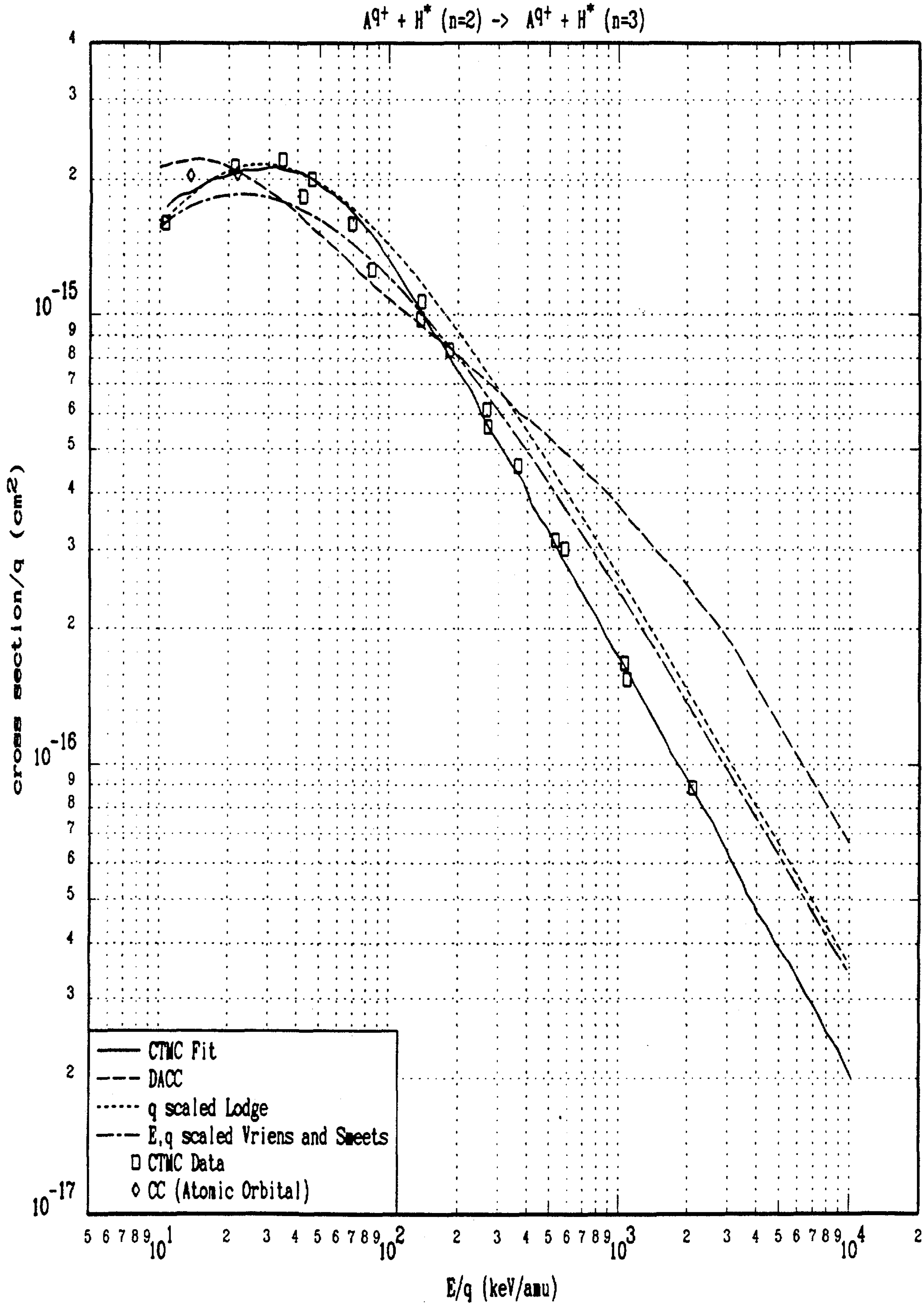


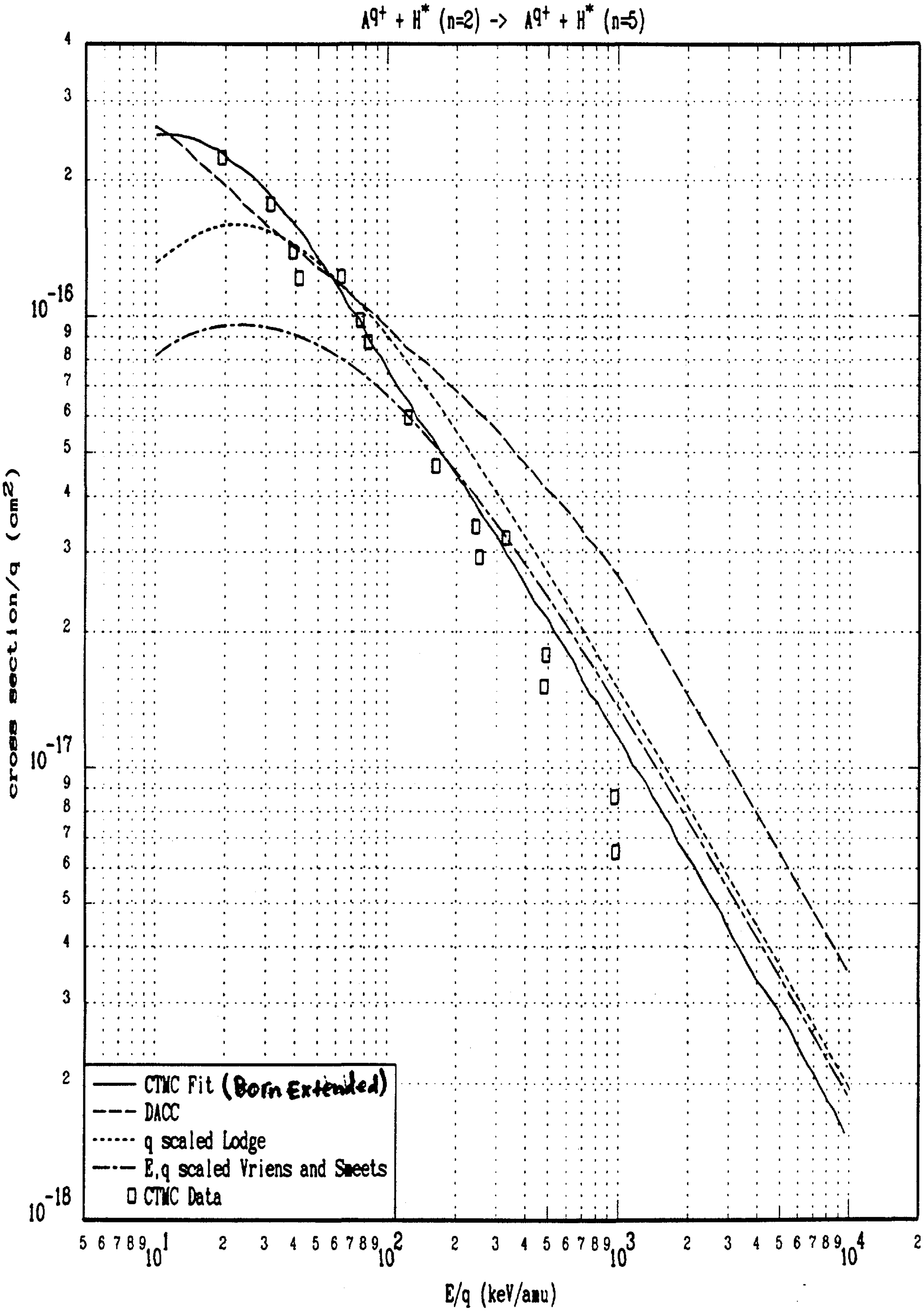
Fig. 1.
A^{q+} + H (1s) -> A^{q+} + H^* (n)
cross section/q (cm^2)
E/q (keV/amu)
n = 2
n = 3
n = 4
q=6
q=26
q=14
q=2
DACC
LODGE
Born-ext CTMC
Expl. (SCHARTNER ; np only)
AO (FRITSCH, 1989)
DACC (JANEV, 1980)
BORN(SE)-EXTENDED CTMC (OLSON, 1989)
q-scaled LODGE
Δ,O Symm. Eik. (REINHOLD, 1989)
◇ FBA (np only) ; ∇ FBA (TOTAL)

Fig 2



A^{q+} + H* (n=2) -> A^{q+} + H* (n=3)
cross section/q (cm^2)
E/q (keV/amu)
CTMC Fit
DACC
q scaled Lodge
E,q scaled Vriens and Smeets
CTMC Data
CC (Atomic Orbital)

Fig. 3



$A^{q+} + H^{*}(n=2) \rightarrow A^{q+} + H^{*}(n=5)$
cross section/q (cm²)
E/q (keV/amu)
CTMC Fit (Born Extended)
DACC
q scaled Lodge
E,q scaled Vriens and Smeets
CTMC Data

3.4. Working Group Report on Electron Removal: Recommended database for charge exchange and ionization

H.B. Gilbody, D.S.F. Crothers and S. Szucs

1. Collisions of protons with hydrogen atoms

The database for the processes:

$$H^{+} + H(1s) \rightarrow H + H^{+} \qquad \text{(charge transfer)}$$
$$\rightarrow H^{+} + H^{+} + e \qquad \text{(ionization)}$$

at energies above 10 keV u^{-1} is now quite well established, with the cross section for ionization providing an increasingly dominant contribution to electron removal from H atoms at energies above about 25 keV u^{-1} (see Fig. 1).

For ionization, the experimental cross sections of Shah and Gilbody[1] and Shah et al[2] in the range 9-1500 keV are accurate to within 10% and are well described by theoretical estimates based on CDW theory by Crothers and McCann.

For charge transfer, the absolute measurements of McClure[4] in the range 2-117 keV u^{-1} have been supplemented by other measurments which extend to 500 keV (see[5]). When considered together with the theoretical predictions of Belkic and Gayet[6] cross sections accurate to within about 10% can be derived.

For the processes

$$H^{+} + H^{*}(n) \rightarrow H(n) + H^{+}$$
$$\rightarrow H^{+} + H^{+} + e$$

when $n > 1$ there are no definitive experimental measurements. Scaling of the total cross sections for electron removal σ_e for $n = 1$ is recommended with $\tilde{\sigma}_e = \sigma_e/n^4$ and $\tilde{E} = En^2$ keV u^{-1}.

2. Collisions of fully stripped impurity ions with hydrogen atoms

The database for the processes

$$A^{Z+} + H(1s) \rightarrow A^{(Z-1)+} + H^{+}$$
$$\rightarrow A^{Z+} + H^{+} + e$$

is now quite reliable for $E/Z > 10$ keV u^{-1}.

For ionization the experimental data of Shah and Gilbody (see[4]) are satisfactorily described by the CDW calculations of Crothers and McCann[3] at progressively higher velocities as Z increases. The scaling relation due to Gillespie[7] based on the Bethe-Born approximation predicts cross sections[3]

$$\sigma_{ion} = q^2 f(q^{1/2}\alpha/\beta)\ \sigma_{Bethe}(\beta)$$

for primary ions of charge state $q > \frac{Z}{2}$, where σ_{Bethe} is the Bethe cross section for proton impact, $\beta = v/c$ and α is the fine structure constant. The term f is designed to correct for the overestimation of σ_{Bethe} at moderate velocities. Using $f\ (q^{1/2}\alpha/\beta) = \exp\ [-\lambda(q^{1/2}\alpha/\beta)^2]$ with $\lambda = 0.76$, a fit to the experimental data to within 10% is obtained for $E/q > 10$ keV u^{-1}.

For charge transfer, the experimental data are more extensive (see review[4]) and accurate to within about 10%, and at high velocities for $Z > 1$ approach the asymptotic velocity dependence predicted by the expression $\sigma = 8\ \pi\ Z^3\ a_0^2\ v^{-7}$ a.u. given by Crothers and Todd[8]. For $E/Z > 10$ keV u^{-1} and $Z > 3$ scaling based on the UDWA approximation[9] provides a universal curve of scaled cross section $\tilde{\sigma} = \sigma/Z$ plotted against

$\tilde{E} = EZ^{-0.464}$ (keV u^{-1}) which is accurate to within about 25%.

Janev[10] has also obtained an analytic fit for total cross sections σ_e for electron removal by both charge transfer and ionization. The following expression is proposed for $\tilde{E} = E/Z > 1$ keV u^{-1}.

$$\tilde{\sigma}_e = \frac{\sigma_e}{Z} = A_1\left[\frac{1}{1+A_2\tilde{E}} + \frac{A_3}{\tilde{E}+A_4}\ln(1+A_5\tilde{E})\right] \times 10^{-16}\,\mathrm{cm}^2$$

where $A_1 = 7.57$, $A_2 = 0.089$, $A_3 = 2.65$, $A_4 = 58.98$, $A_5 = 1.65$

For the processes

$$A^{Z+} + H^*(n) \rightarrow A^{(Z-1)+} + H^+$$
$$\rightarrow A^{Z+} + H^+ + e$$

there are no experimental data in the energy range of interest. The proposed Z, n-scaling of the $\sigma_e(Z{=}1,\ n{=}1)$ data[11],

$$\tilde{\sigma}_e(\tilde{E}) = \frac{\sigma_e(E)}{Zn^4},\quad \tilde{E} = \frac{En^2}{Z}\ \mathrm{keV\ u}^{-1},$$

is expected to be valid only at high velocities ($\tilde{E}$ > 25 keV/u).

For the processes

$$A^{Z+} + H^*(m) \rightarrow A^{(Z-1)+}(n) + H^+$$

an asymptotic dependence is predicted

$$\sigma = \frac{8\pi Z^3 a_0^2}{1.2v^7 m^3 n^3}$$

for $m > 1$, $n > Z$, $v > 1$ a.u.

Note that $n \leq Z$ is not strictly within the domain of the Bohr- Lindhard model. Nevertheless, the formula may well suffice for general scaling approximations.

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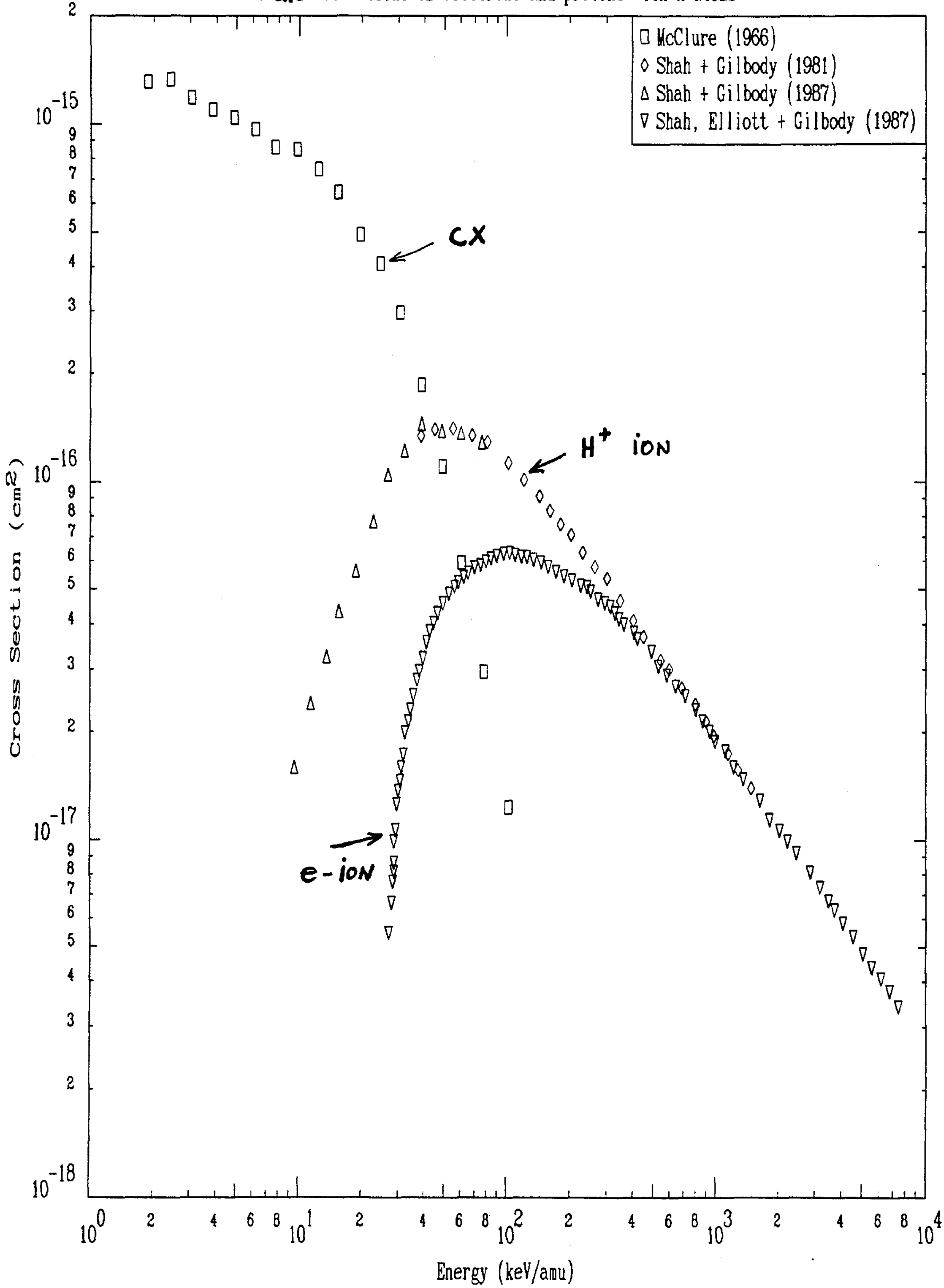
Fi G.1 Collisions of electrons and protons with H atoms



4. Meeting Conclusions and Recommendations

The results of the work of the Meeting can be summarized as follows:

1) The database on atomic hydrogen collision processes with electrons, protons and impurity ions, recommended by the Working Groups, can be considered as fully adequate for use in the neutral beam penetration codes for beam energies of interest to fusion test reactors ($E_0 \gtrsim 600$ keV/amu, reduced collision $E_0/q \gtrsim 25$ keV/amu). The assessed accuracies of existing data in this energy region are well within those required for a 10% accuracy of the calculated beam stopping cross section. The use of the q-scaling laws in the region $E_0/q \gtrsim 25$ keV/amu is justified.
2) For ion-atom interaction energies $1 \lesssim E_0/q$ (keV/amu) $\lesssim 10$, of interest to the beam penetration calculations in present large tokamak devices, or their future up-grades, the database is still not fully established. The main gaps are in the impurity ion impact excitation data, both from the ground and the excited states. While the impurity induced transitions between the excited states are not critical (required accuracy on the order of a factor of 2 to 3), excitation from the ground state are important (required accuracy about 20-30%). The q-scaling of the excitation breaks down at around $E/q \simeq 15$ keV/amu, and below this reduced energy the excitation cross sections should be known individually for each impurity ion. This is also true for the proton impact excitations from ground and excited states.
3) The database for electron removal by protons, (including removal from excited states) is well established down to very low (0.1 keV) impact energies. For impurities with $q \gtrsim 6$, the electron removal database (including excited target states) has the required accuracy down to ~ 1 keV/amu/q (q-scalings applicable), but for $q \lesssim 5$ individual charge cross sections should be used below ~ 20 keV/amu/q. The data are available for most of the important impurity species in tokamak plasmas.
4) The database for all relevant electron impact processes can be considered as firmly established in the energy region of interest.

Appendix 1

IAEA Specialists' Meeting on "Required Atomic Data Base for Neutral Beam Penetration in Large Tokamaks"

IAEA Headquarter, Vienna 10-12 April 1989

LIST OF PARTICIPANTS

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S. Szucs	Institut de Physique, Universite de Louvain, Belgium

IAEA Visiting Experts

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W. Fritsch	Hahn-Meitner-Institut für Kernforschung, Berlin, FRG
H.B. Gilbody	The Queen's University of Belfast, Northern Ireland, U.K.
R.E. Olson	Physics Department, University of Missouri-Rola, U.S.A.

IAEA Staff

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J.J. Smith	Atomic and Molecular Data Unit, Nuclear Data Section
J.J. Schmidt	Nuclear Data Section
A. Lorenz	Nuclear Data Section

OTHER CONTRIBUTORS TO THE MEETING WORK

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Appendix 2

IAEA Specialists' Meeting on "Required
Atomic Data Base for Neutral Beam Penetration in Large Tokamaks"

IAEA Headquarter, Vienna 10-12 April 1989

Meeting Agenda

Monday, 10 April 1989

9:30 : Opening of the Meeting (J.J. Schmidt) (Room: C-0453)

9:45 - 10:45 : Results of beam penetration codes. General view on required atomic data base

- Boley, Janev, Cox

10:45 - 11:00 : Coffee Break

11:00 - 12:30 : Data reviews and individual contributions

- Electron-impact processes: Shevelko (presented by Janev)
- Heavy-particle excitation: Schartner, Fritsch

Chairman: H.B. Gilbody

12:30 - 14:00 : Lunch

14:00 - 15:45 : Data reviews and individual contributions

- Heavy-particle excitation: Olson, Belkic (Data of Mukherjee et al distributed)

15:45 - 16:00 : Coffee Break

16:00 - 18:00 : Data reviews and individual contributions

- Charge exchange and ionization (electron removal): Crothers, Gilbody, de Heer, Szucs

Chairman: W. Fritsch

Tuesday, 11 April 1989 (Room: C-0453)

9:00 - 10:00 : General discussion of atomic data base

- Formation of Working Groups

Chairman: D.S.F. Crothers

10:00 - 10:15 : Coffee Break

10:15 - 12:15 : Working Group Sessions: Selection of recommended data

a) Working Group on electron-impact processes.
Room: NDS Library
b) Working Group on heavy-particle excitation processes.
Room: C-0453
c) Working Group on heavy-particle electron removal.
Room: C-0451

12:15 - 14:00 : Lunch

14:00 - 18:00 : Working Group Sessions: Selection of recommended data

Wednesday, 12 April 1989

9:00 - 12:00 : Formulation of recommended data sets and preparation of reports

a) Working group on electron-impact processes
b) Working group on heavy-particle excitation data
c) Working group on electron-removal data

12:00 - 14:00 : Lunch

14:00 - 17:00 : Plenary Session (Room: C-0453):

* Presentation and discussion of Working Group Reports and adoption of the recommended atomic data base for use in neutral beam penetration codes

* Recommendations for additional benchmark calculations/ measurements for completing the atomic data base (if necessary)

Chairman: R.K. Janev