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

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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 ≥ 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 ≥ 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 → n (n ≥ 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 $E \geq 100$ 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 $n \geq 3$ 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 ± n.10% (n is the final principal quantum number) in the region $80 \lesssim E/q$ (keV/amu) $\lesssim 400$, which reduces to about ± 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 → 3, 2 → 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 → n' proton induced transitions, which shows a 15-20% agreement with the AO data (Fritsch, 1989). Therefore, for the n → 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.

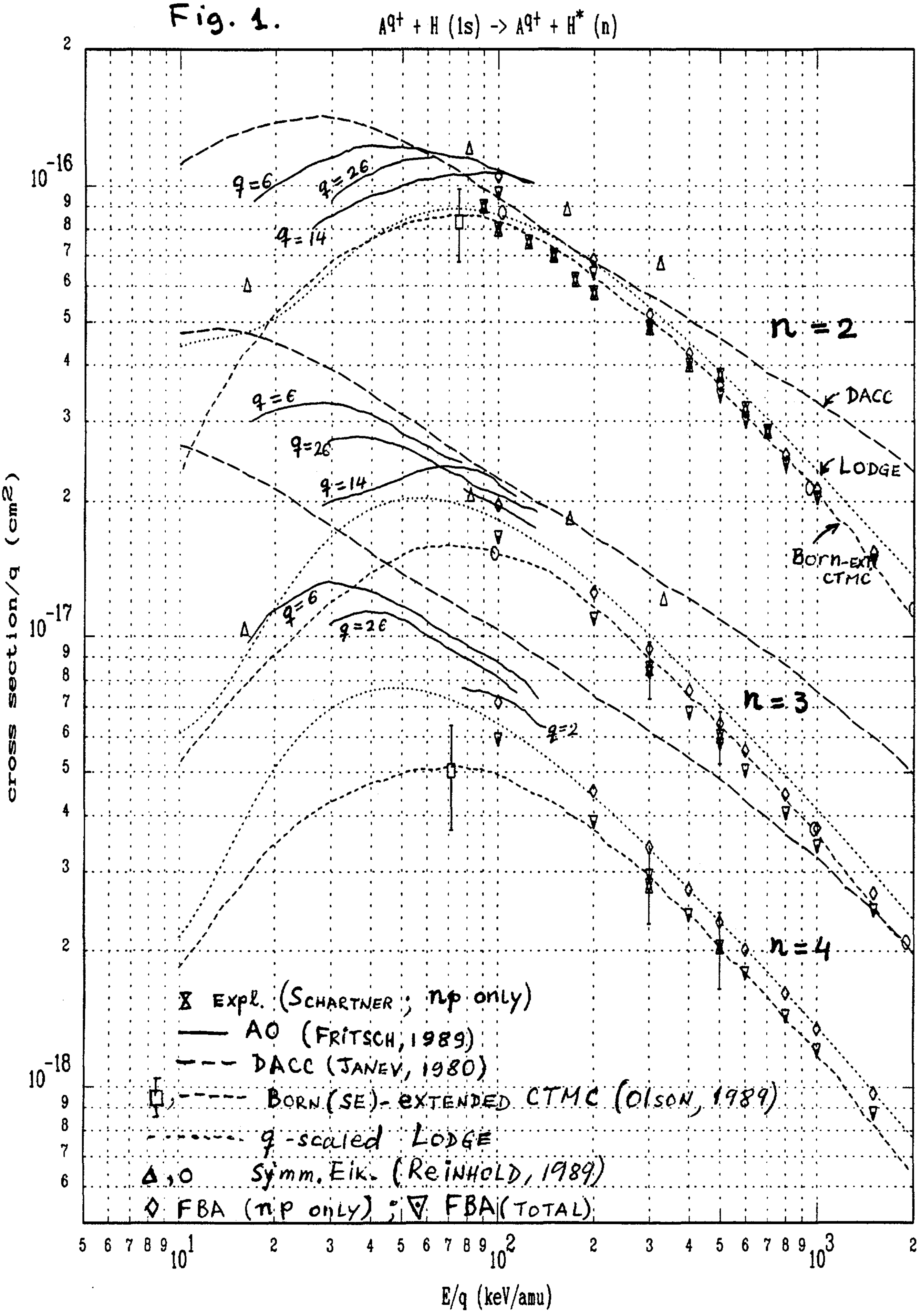

$A^{q+} + H(1s) \rightarrow A^{q+} + H^*(n)$
cross section/q (cm^2)
E/q (keV/amu)
10^{-16}
10^{-17}
10^{-18}
2
9
8
7
6
5
4
3
5 6 7 8 9
10^1
10^2
10^3
q=6
q=26
q=14
q=2
n=2
n=3
n=4
DACC
LODGE
Born-ext CTMC
Expl. (Schartner; np only)
AO (Fritsch, 1989)
DACC (Janev, 1980)
Born (SE) - extended CTMC (Olson, 1989)
q-scaled Lodge
Δ, O Symm. Eik. (Reinhold, 1989)
◇ FBA (np only) ; ∇ FBA (total)

Fig 2

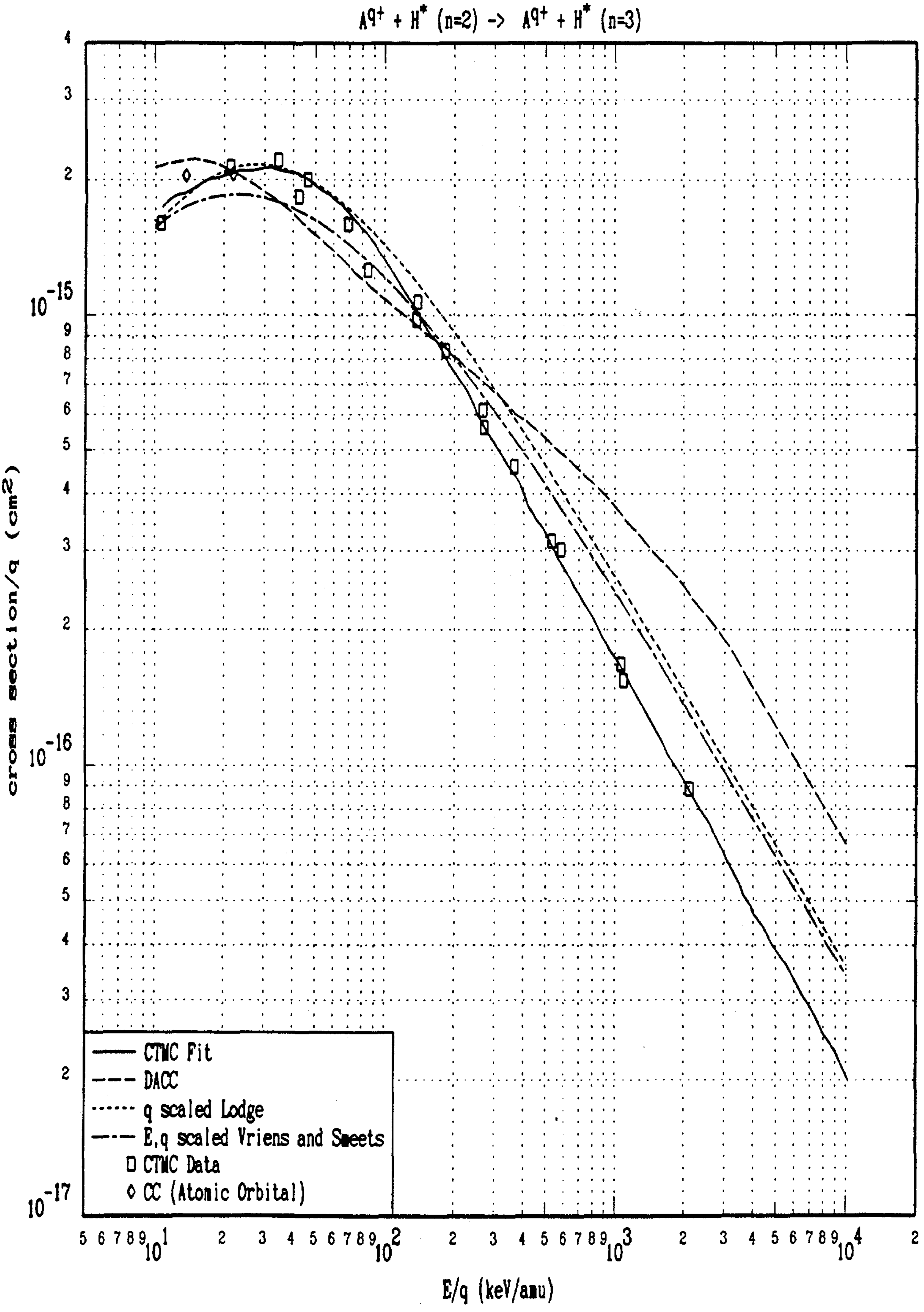
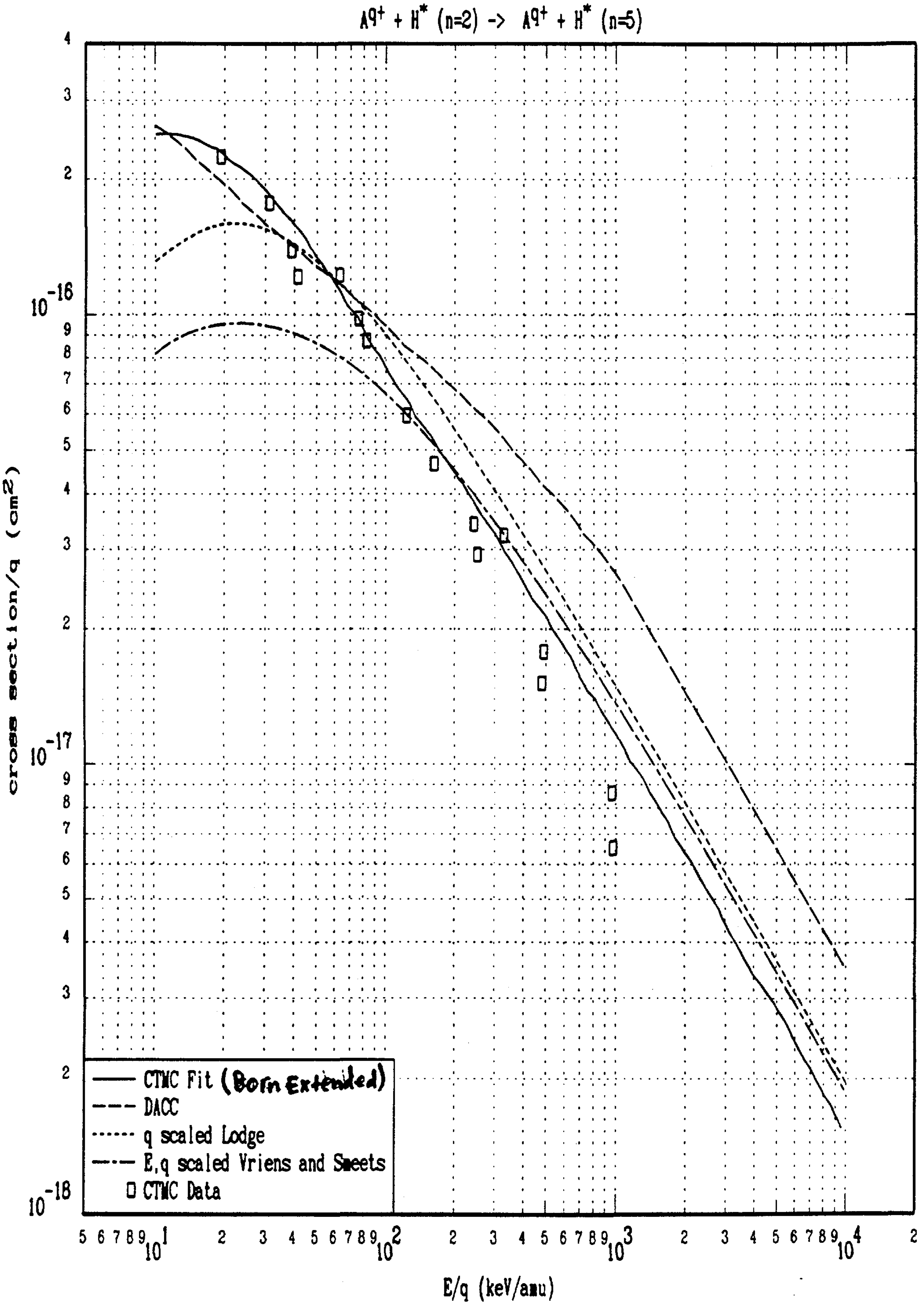

A^{q+} + H* (n=2) -> A^{q+} + H* (n=3)
cross section/q (cm²)
10^{-15}
10^{-16}
10^{-17}
4
3
2
9
8
7
6
5
E/q (keV/amu)
10^1
10^2
10^3
10^4
CTMC Fit
DACC
q scaled Lodge
E,q scaled Vriens and Smeets
□ CTMC Data
◇ CC (Atomic Orbital)

Fig. 3


A^{q+} + H* (n=2) -> A^{q+} + H* (n=5)
cross section/q (cm²)
E/q (keV/amu)
10^-16
10^-17
10^-18
10^1
10^2
10^3
10^4
4
3
2
9
8
7
6
5
CTMC Fit (Born Extended)
DACC
q scaled Lodge
E,q scaled Vriens and Smeets
CTMC Data