ASTRONOMY & ASTROPHYSICS
SUPPLEMENT SERIES

Astron. Astrophys. Suppl. Ser. **133**, 245–248 (1998)

Atomic data from the IRON Project

XXXII. On the accuracy of the effective collision strength for the electron impact excitation of the quadrupole transition in Ar III

M.E. Galavís[1,3], C. Mendoza[2,3], and C.J. Zeippen[3]

[1] Departamento de Física, Universidad Metropolitana, PO Box 76819, Caracas 1070A, Venezuela
[2] Centro de Física, Instituto Venezolano de Investigaciones Científicas (IVIC), PO Box 21827, Caracas 1020A, Venezuela
[3] URA 173 (associée au CNRS et à l'Université Paris 7) et DAEC, Observatoire de Paris, 92195 Meudon, France

Received April 7; accepted June 5, 1998

Abstract. Since Burgess et al. (1997) have recently questioned the accuracy of the effective collision strength calculated in the IRON Project for the electron impact excitation of the $3s^2 3p^4\ ^1D - ^1S$ quadrupole transition in Ar III, an extended R-matrix calculation has been performed for this transition. The original 24-state target model was maintained, but the energy regime was increased to 100 Ryd. It is shown that in order to ensure convergence of the partial wave expansion at such energies, it is necessary to take into account partial collision strengths up to $L = 30$ and to "top-up" with a geometric series procedure. By comparing effective collision strengths, it is found that the differences from the original calculation are not greater than 25% around the upper end of the common temperature range and that they are much smaller than 20% over most of it. This is consistent with the accuracy rating (20%) previously assigned to transitions in this low ionisation system. Also the present high-temperature limit agrees fairly well (15%) with the Coulomb–Born limit estimated by Burgess et al., thus confirming our previous accuracy rating. It appears that Burgess et al., in their data assessment, have overextended the low-energy behaviour of our reduced effective collision strength to obtain an extrapolated high-temperature limit that appeared to be in error by a factor of 2.

Key words: atomic and molecular data

1. Introduction

This communication is a reply to Burgess et al. (BCT, 1997) who question the accuracy of the effective collision strength computed within the IRON Project (IP) by Galavís et al. (IP-X, 1995) for the electron impact excitation of the $3s^2 3p^4\ ^1D - ^1S$ transition in Ar III. The IP (Hummer et al. 1993; Butler 1996) is an international on-going collaboration whose goal is to compute collisional and radiative data for ions of astrophysical interest. Since the initial stages of the IP targeted isoelectronic sequences rather than single ionic systems, general practical approximations had to be adopted. The issue of accuracy consequently became a main concern because tricky individual features perhaps did not get the attention that was required. In their assessment of the IP data for the quadrupole transition in Ar III, BCT made use of a helpful technique developed by Burgess & Tully (BT, 1992) whereby the effective collision strength is scaled and mapped onto the finite reduced electron-temperature interval (0,1). In this particular case, they computed the limiting point at infinite temperature (i.e. reduced temperature $T_r = 1$), and they adjusted the scaling parameter in such a way that an electron temperature interval of 10^5 K occupied 90% of the unitary scale. In their analysis, BCT suggested that the IP data could be in error by a factor of 2 due to the neglect of the contribution of high partial waves. Since the accuracy rating quoted in IP-X for the slightly ionised species is 20%, the magnitude of the alleged discrepancy indeed deserves some consideration.

We have rerun the IP-X calculation examining in detail possible sources of error. Also, the original energy range has been extended so as to study the high-temperature behaviour of the effective collision strength with respect to the limit estimated by BCT. The present report is organised as follows. We provide short summaries of the original IP calculation and the BT formalism in Sects. 2 and 3, respectively, followed in Sect. 4 by a presentation and analysis of the recalculated collisional data. Some conclusions are drawn in Sect. 5.

Send offprint requests to: C.J. Zeippen

2. The IP-X calculation

Following the general policy of the IP, collision strengths for Ar III were computed in IP-X with a suite of programs based on the R-matrix method (Burke et al. 1971) and asymptotic techniques developed by Seaton (1985). Target wavefunctions were obtained with the atomic structure code SUPERSTRUCTURE (Eissner et al. 1974; Nussbaumer & Storey 1978; Eissner 1991). The target representation adopted included the 24 terms arising from the configurations: $3s^23p^4$, $3s3p^5$, $3s^23p^33d$ and $3p^6$. Configuration interaction was limited to single and double excitations within the $n = 3$ complex. The λ_{nl} scaling parameters in the Thomas–Fermi statistical model potential used to generate the $P_{nl}(r)$ radial orbitals were adjusted by minimising the weighted sum of the energies of the 24-term target model. Following the earlier five-state R-matrix calculation by Johnson & Kingston (1990) on this system, partial collision strengths were computed for $L \leq 9$. The energy range was taken to be $E < 3.7$ Ryd, and effective collision strengths were determined for the electron temperature range $10^3 \leq T \leq 10^5$ K.

3. The BT method

In order to analyse collisional data and to present them in compact form, BT introduce a scaling procedure where the collision strength $\Omega(E)$ is mapped onto the reduced form $\Omega_r(E_r)$, where the infinite energy E range is scaled to the finite E_r interval $(0, 1)$. For a quadrupole transition, such as $^1D - ^1S$ in Ar III, the BT scaling prescription is given by

$$E_r = \frac{E}{\Delta E}\left(\frac{E}{\Delta E} + C\right)^{-1} \quad (1)$$

$$\Omega_r(E_r) = \Omega(E) \quad (2)$$

with ΔE being the transition energy, E the electron energy with respect to the reaction threshold and C an adjustable scaling parameter. A key aspect of the BT approach lies in the fact that the limiting points $\Omega_r(0)$ and $\Omega_r(1)$ are both finite and can be computed. BT have discussed that for a quadrupole transition these points are

$$\Omega_r(0) = \Omega(0) \quad (3)$$

$$\Omega_r(1) = \Omega_{CB} \quad (4)$$

where Ω_{CB} is the Coulomb–Born high-energy limit. This formalism can also be extended to treat the effective collision strength

$$\Upsilon(T) = \int_0^\infty \Omega(E)\exp(-E/\kappa T)\mathrm{d}(E/\kappa T)\ , \quad (5)$$

through the analogous relations

$$T_r = \frac{\kappa T}{\Delta E}\left(\frac{\kappa T}{\Delta E} + C\right)^{-1} \quad (6)$$

$$\Upsilon_r(T_r) = \Upsilon(T) \quad (7)$$

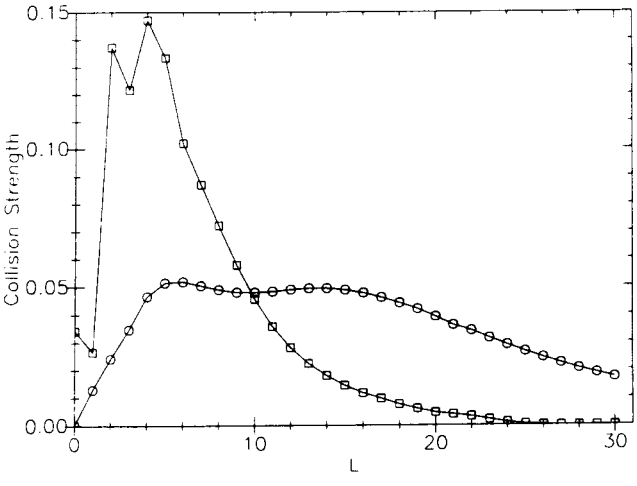

Fig. 1. Partial collision strength for the $3s^23p^4\ ^1D - ^1S$ transition in Ar III as a function of the total orbital angular momentum L. Squares: 10 Ryd. Circles: 100 Ryd

where T is the electron temperature and κ the Boltzmann constant; the limiting points now become

$$\Upsilon_r(0) = \Omega(0) \quad (8)$$

$$\Upsilon_r(1) = \Omega_{CB}\ . \quad (9)$$

A second important point in the BT approach is that the reduced effective collision strength can be neatly fitted in its entire range. A 5-point spline is usually sufficient, and thus leads to a notably compact way of presenting collisional data.

With specific reference to the questioned transition in Ar III, BCT have computed a Coulomb–Born high-energy limit of ~ 1.64. This computation includes configuration interaction effects that are found only to cause changes of a few per cent. Then, in a plot of the IP-X effective collision strengths, they scale the fairly low temperature range of $0 - 10^5$ K to occupy 90% of the reduced temperature interval and they find an extrapolated high-energy limit of ~ 0.8, a factor of 2 lower than the Coulomb–Born limit, which led them to question the accuracy of the calculation.

4. Revised collision strength

Since there is good agreement between the 24-state results by IP-X and those from the 5-state calculation by Johnson & Kingston (1990) for electron temperatures below 24000 K, we have rerun the calculation with the original IP-X target representation. Since we are interested in the high-temperature behaviour of the effective collision strength in order to check the match with the Coulomb–Born limit quoted by BCT, we now extend the calculation of collision strengths to 100 Ryd. Convergence of the partial-wave expansion is ensured by examining the partial collision strength L profile at the highest energy point (100 Ryd) and by topping up with a simple geometric series procedure at every energy point. In Fig. 1 we plot

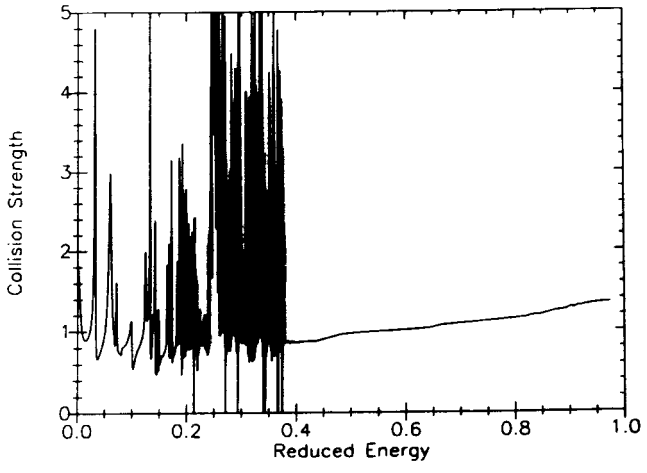

Fig. 2. Total collision strength for the $3s^2 3p^4\ ^1D - ^1S$ transition in Ar III plotted as a function of the reduced energy with $C = 9.0$. It is seen that the non-resonant region increases slowly and approaches the point $\Omega_r(1) \approx 1.4$

the partial collision strength as a function of L at both 10 Ryd and 100 Ryd. This plot illustrates the computational difficulty in obtaining a converged collision strength for this transition particularly as the energy is increased. While at 10 Ryd there is a well defined peak at around $L = 4$, at 100 Ryd the expansion becomes a flat and broad plateau for $5 \leq L \leq 20$. Using a geometric series top-up in this L range would certainly lead to a significant overestimate of the total collision strength at the high energies. At 100 Ryd, say, it is only for $L > 30$ that the top-up procedure can be safely implemented, and the latter amounts to a barely acceptable 20% of the total collision strength. In Fig. 2 the total collision strength for this transition is plotted using the reduced energy method of BT. A further difficulty with this transition becomes apparent: for the non-resonant region the collision strength, rather than flattening out as in most quadrupole transitions, displays a slow increase. As discussed before, this effect makes the management of the convergence of the partial wave expansion particularly difficult at the high energies. It also causes difficulties in determining the high-temperature trend of the effective collision strength as will be shown below. The present reduced collision strength seems to converge to the point $\Omega_r(1) \approx 1.4$ which is in reasonable agreement ($\sim 15\%$) with the high-energy Coulomb–Born limit of 1.64 estimated by BCT.

In Fig. 3 the present reduced effective collision strength is compared with earlier work, and in Table 1 we list the present effective collision strength in the extended range of $3 \leq \log(T) \leq 7$ and compare them with the data by IP-X. It may be seen that the low-temperature regime is dominated by the contribution from resonances (see Fig. 2), particularly a resonance sitting at threshold that is responsible for the high value of $\Upsilon_r(0) = 1.82$. The good overall agreement (10%) at low temperatures with

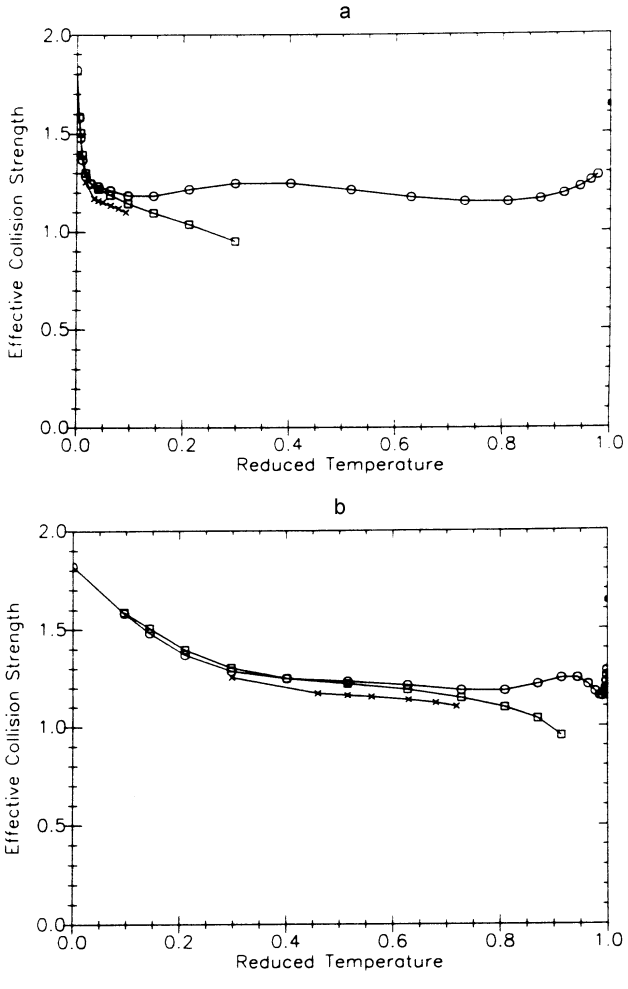

Fig. 3. Effective collision strength for the $3s^2 3p^4\ ^1D - ^1S$ transition in Ar III as a function of the reduced temperature with **a)** $C = 0.2$ and **b)** $C = 5.0$. Circles: present calculation. Squares: IP-X. Crosses: Johnson & Kingston (1990). Filled square: High-energy Coulomb–Born limit by BCT

the work by Johnson & Kingston (1990) is reinforced. It is shown that the differences with IP-X, mainly due to the neglect of partial collision strengths for $L > 9$ at the higher energies, are less than 10% up to $\log(T) = 4.6$, they are well below 20% up to $\log(T) = 4.8$ and they reach $\sim 25\%$ only towards the upper limit of the temperature range considered in IP-X. In our opinion, such differences are consistent with the level of accuracy ($\sim 20\%$) claimed in IP-X for the lower members of the Si and S isoelectronic sequences. Furthermore, it is found that the fairly steep climb of the reduced effective collision strength to its high-temperature limiting value of $\Upsilon_r(1) \approx 1.4$ only starts at relatively high temperatures, and certainly stands out from the gently oscillating patterns at intermediate temperatures. As shown in Fig. 3, the characteristic features in each temperature regime can be enhanced by a suitable choice of the scaling parameter C. For instance, in Fig. 3b we have used a C parameter similar to that used by BCT

Table 1. Comparison of present effective collision strengths for the $3s^2 3p^4\ ^1D - ^1S$ transition in Ar III with those in IP-X. Electron temperatures are given in K. It may be seen that discrepancies are not larger than 25%

log(T)	Present	IP-X
3.0	1.582	1.587
3.2	1.481	1.506
3.4	1.369	1.395
3.6	1.286	1.302
3.8	1.247	1.248
4.0	1.232	1.219
4.2	1.211	1.188
4.4	1.185	1.145
4.6	1.183	1.096
4.8	1.216	1.038
5.0	1.247	0.951
5.2	1.247	
5.4	1.214	
5.6	1.175	
5.8	1.153	
6.0	1.151	
6.2	1.166	
6.4	1.193	
6.6	1.226	
6.8	1.258	
7.0	1.284	

which stretches the low-temperature regime suggesting a value of $\Upsilon_r(1) = 0.8$ for IP-X; with this choice of scaling parameter the high-temperature behaviour of the present data appears almost as a vertical climb. It is worth mentioning that an estimate of the effective collision strengths for $T > 10^{6.5}$ K requires an energy range greater than 100 Ryd. Therefore a top-up procedure was introduced where the collision strength for $E > 100$ Ryd was assumed constant at $\Omega = 1.40$.

5. Discussion

We have revisited the $^1D - ^1S$ quadrupole transition of Ar III, looking in detail at the different factors that affect the accuracy of the effective collision strength. It is found that differences with the data computed in IP-X are not greater than 25% at the upper limit of the common temperature range. This is consistent with their original accuracy rating and with the general level of reliability that is usually attained in the type of massive computations where several ionic systems are treated simultaneously. Furthermore, a high-temperature limit of the present reduced effective collision strength has been estimated and is in good agreement (15%) with the high-energy Coulomb–Born limit of BCT. We are therefore confident about the accuracy ranking for this transition (20%). It appears that the suspicion of BCT arose because they overstretched the behaviour of the IP-X reduced effective collision strength at low temperatures to obtain an extrapolated high-temperature limit that appeared to be grossly discrepant with the Coulomb–Born limit. It has been shown here that for this transition the high-temperature trend is only reached at relatively high temperatures and differs significantly from those at the low- and intermediate-temperature regimes. Finally, it is hoped that we conveyed the computational difficulties that must be addressed in order to ensure reliable data throughout a chosen integration region.

Acknowledgements. Calculations were carried out on the IBM SP2 computer at CeCalCULA, Universidad de Los Andes, Mérida, Venezuela. The present collaboration also benefited from funding by the CNRS, IVIC, the Observatoire de Paris and the Ministère des Affaires Etrangères. This research has been supported by CONICIT under contract No. S1-95000521.

References

Burgess A., Chidichimo M.C., Tully J.A., 1997, J. Phys. B 30, 33
Burgess A., Tully J.A., 1992, A&A 254, 436
Burke P.G., Hibbert A., Robb W.D., 1971, J. Phys. B 4, 153
Butler K, 1996, Phys. Scr. T65, 63
Eissner W., 1991, J. Phys. IV C1, 3
Eissner W., Jones M., Nussbaumer H., 1974, Comput. Phys. Commun. 8, 270
Galavís M.E., Mendoza C., Zeippen C.J., 1995, A&AS 111, 347
Hummer D.G., Berrington K.A., Eissner W., et al., 1993, A&A 279, 298
Johnson C.T., Kingston A.E., 1990, J. Phys. B 23, 3393
Nussbaumer H., Storey P.J., 1978, A&A 64, 139
Seaton M.J., 1985, J. Phys. B 18, 2111