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Effective collision strengths for allowed transitions among the $n \leq 5$ degenerate levels of Al XIII

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ABSTRACT

Aims. In this paper we report on calculations of collision strengths and effective collision strengths for allowed transitions among the $n \leq 5$ degenerate levels of Al XIII.
Methods. The Dirac atomic *R*-matrix code (DARC) has been adopted for these calculations.
Results. Collision strengths are reported over a wide energy range below 300 Ryd, and effective collision strengths are provided for electron temperatures of $4.4 \leq \log T_e \leq 6.8$ K.

Key words. atomic data – atomic processes

1. Introduction

In a recent paper (Aggarwal et al. 2005) we reported results for energy levels, radiative rates, collision strengths, and excitation rate coefficients for transitions among the $n \leq 5$ levels of Al XIII. Those calculations were a substantial improvement over our earlier results in the *LS* coupling scheme for the same ion (Aggarwal et al. 2001). However, even the more recent data for transitions among the fine-structure levels remained limited in scope, particularly for those that are allowed among the degenerate levels of a state, such as $2s\ ^2S_{1/2}$–$2p\ ^2P^o_{1/2,3/2}$. This was because collision strengths were *not* converged within the partial wave range ($J \leq 60$) considered in that paper. Extending the partial wave range in a collisional code such as DARC is impractical, because these transitions converge very *slowly* as demonstrated by Igarashi et al. (2003). Therefore, a "top-up" based on the formulations of Burgess et al. (1970) has now been fully implemented in the *Dirac atomic R-matrix code* (DARC) of Ait-Tahar et al. (1996), which enables us to calculate converged values of Ω for all allowed transitions, including the "elastic" ones, i.e. those for which $\Delta E \sim 0$. However, results for all transitions, forbidden and allowed, remain the same as already reported, *except* for those which are allowed among the degenerate levels and for which $\Delta E \sim 0$. Therefore, in this paper we present values of collision strengths (Ω) as well as effective collision strengths (Υ) for all 26 elastic transitions alone over a wide energy/temperature range, so that data for *all* transitions can be applied with confidence in plasma modelling.

2. Collision strengths

The details of our calculations have already been given in our earlier paper (Aggarwal et al. 2005) and hence are not repeated here. Additionally, results for all transitions *except* those which are allowed among the degenerate levels remain the same. Therefore in the present paper we discuss results for only the elastic transitions, i.e. those which are *allowed* within the $n \leq 5$ levels of Al XIII, and for which $\Delta E \sim 0$.

In Table 1 we list our energy levels, as reported earlier (Aggarwal et al. 2005), which will facilitate the discussion of

Table 1. Energy levels (in Ryd) for Al XIII.

Index	Configuration	Level	Energy
1.....	1s	$^2S_{1/2}$	0.000000
2.....	2s	$^2S_{1/2}$	126.988960
3.....	2p	$^2P^o_{1/2}$	126.985252
4.....	2p	$^2P^o_{3/2}$	127.081062
5.....	3p	$^2P^o_{1/2}$	150.534500
6.....	3s	$^2S_{1/2}$	150.535599
7.....	3d	$^2D_{3/2}$	150.562851
8.....	3p	$^2P^o_{3/2}$	150.562897
9.....	3d	$^2D_{5/2}$	150.572266
10.....	4p	$^2P^o_{1/2}$	158.772842
11.....	4s	$^2S_{1/2}$	158.773300
12.....	4d	$^2D_{3/2}$	158.784805
13.....	4p	$^2P^o_{3/2}$	158.784821
14.....	4d	$^2D_{5/2}$	158.788773
15.....	4f	$^2F^o_{5/2}$	158.788773
16.....	4f	$^2F^o_{7/2}$	158.790756
17.....	5s	$^2S_{1/2}$	162.584579
18.....	5p	$^2P^o_{1/2}$	162.584351
19.....	5d	$^2D_{3/2}$	162.590469
20.....	5p	$^2P^o_{3/2}$	162.590485
21.....	5f	$^2F^o_{5/2}$	162.592499
22.....	5d	$^2D_{5/2}$	162.592499
23.....	5g	$^2G_{7/2}$	162.593521
24.....	5f	$^2F^o_{7/2}$	162.593521
25.....	5g	$^2G_{9/2}$	162.594131

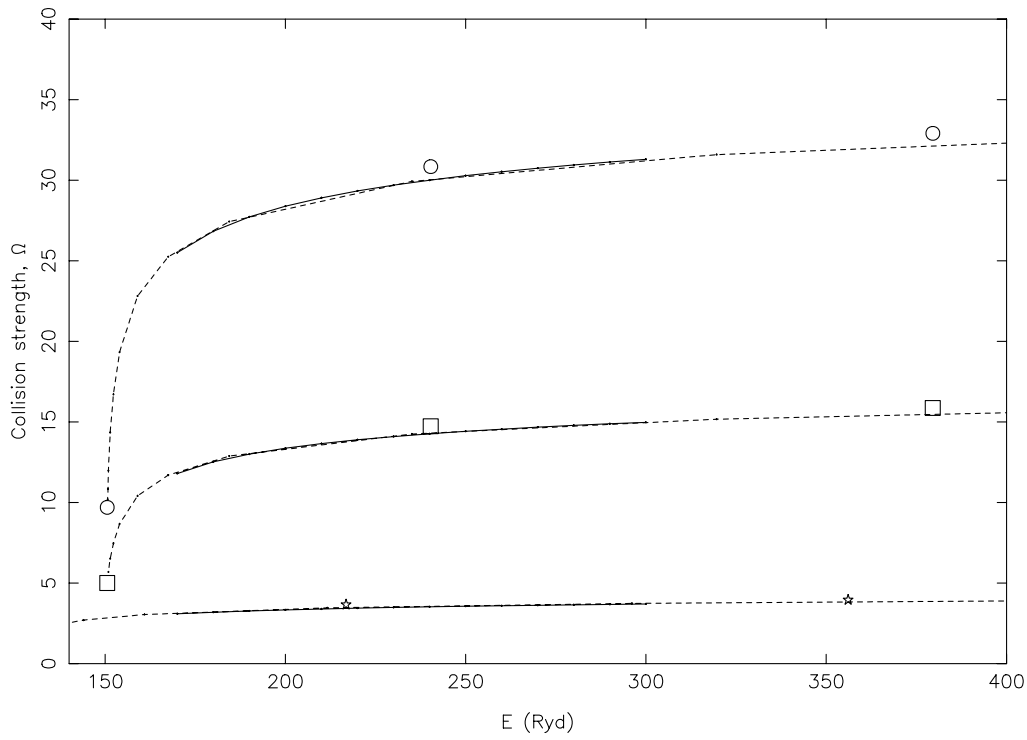

Fig. 1. Comparison of collision strengths for some "elastic" transitions of Al XIII. Continuous curves: DARC, broken curves: CC+CB, stars: 2–4 ($2s\ ^2S_{1/2}$–$2p\ ^2P^\circ_{3/2}$), squares: 5–7 ($3p\ ^2P^\circ_{1/2}$–$3d\ ^2D_{3/2}$), and circles: 8–9 ($3p\ ^2P^\circ_{3/2}$–$3d\ ^2D_{5/2}$) transitions are from FAC.

our subsequent results. It may be noted here that the energy of the $2s\ ^2S_{1/2}$ level is *higher* than that of $2p\ ^2P^\circ_{1/2}$ due to the inclusion of Lamb shift. However, we have retained this ordering (of $2s\ ^2S_{1/2}$ level before $2p\ ^2P^\circ_{1/2}$), mainly because DARC provides results in this ordering and more importantly, this is the same ordering as was adopted in our earlier paper (Aggarwal et al. 2005). Table 2 lists our results of Ω, at energies above thresholds but below 300 Ryd, for all 26 elastic transitions among the $n \le 5$ degenerate levels of Al XIII. To our knowledge, the only other results available in the literature for (qualitative) comparison purposes are those of Zygelman & Dalgarno (1987). Their values of Ω cover a wide energy range up to ∼250 Ryd, but only for transitions within the $n = 2$ levels. Similarly, they have performed calculations for several ions with $2 \le Z \le 18$, but not for $Z = 13$. Therefore, we have performed two other independent calculations to verify our results. The first uses the *Flexible Atomic Code* (FAC) of Gu (2003), available from the website `http://kipac-tree.stanford.edu/fac`. This is a fully relativistic code (as is DARC) and is based on the well known and widely used *distorted-wave* (DW) method. FAC provides background values of Ω over a wider energy range (up to ∼1400 Ryd) but only at six energies. Nevertheless, the data obtained from FAC are helpful in assessing the accuracy of our results. The other calculation is from a combination of the close-coupling (CC) and the Coulomb-Born (CB) programs of Igarashi et al. (2003, 2005), who reported collision strengths for elastic transitions, but again within the $n = 2$ levels alone. Their CC+CB programs have now been extended to calculate values of Ω up to the $n = 5$ levels for a hydrogenic ion of any nuclear charge Z.

In Fig. 1 we compare our results from DARC with those from FAC and CC+CB, but for only three transitions, namely 2–4 ($2s\ ^2S_{1/2}$–$2p\ ^2P^\circ_{3/2}$), 5–7 ($3p\ ^2P^\circ_{1/2}$–$3d\ ^2D_{3/2}$), and 8–9 ($3p\ ^2P^\circ_{3/2}$–$3d\ ^2D_{5/2}$), over a wide energy range below 400 Ryd. As is clear from this figure, there is no discrepancy among the different calculations, and the values of Ω from any calculation can be safely employed for the determination of excitation rates. Similar comparisons for other transitions have also been made but are not shown here for brevity. However, a comparison of the present results shows that the earlier reported values of Ω, with only $J \le 60$, are underestimated for all elastic transitions by over a factor of two, and by up to an order of magnitude for some transitions, such as: 17–18 ($5s\ ^2S_{1/2}$–$5p\ ^2P^\circ_{1/2}$), 19–20 ($5d\ ^2D_{3/2}$–$5p\ ^2P^\circ_{3/2}$), 21–22 ($5f\ ^2F^\circ_{5/2}$–$5d\ ^2D_{5/2}$), and 23–24 ($5g\ ^2G_{7/2}$–$5f\ ^2F^\circ_{7/2}$). Finally, based on comparisons of the different calculations for all elastic transitions, we can state with confidence that the results for Ω listed in Table 2 are accurate to better than 15%.

3. Effective collision strengths

In Table 3 we list our results of ϒ for all 26 elastic transitions among the $n \le 5$ degenerate levels of Al XIII, over a wide temperature range of $4.4 \le \log T_e \le 6.8$ K, the same as adopted in our earlier paper (Aggarwal et al. 2005). From these values of ϒ, the corresponding results for excitation and de-excitation rate coefficients can be easily determined from the simple relationships given in Eqs. (2) and (3) of Aggarwal et al. (2001). To our knowledge, there are no other results for comparison purposes, but our earlier reported values of ϒ are underestimated by over a factor of two for almost all elastic transitions, and by up to a factor of eight for some transitions, such as: 12–13 ($4d\ ^2D_{3/2}$–$4p\ ^2P^\circ_{3/2}$), 14–15 ($4d\ ^2D_{5/2}$–$4f\ ^2F^\circ_{5/2}$), 19–20 ($5d\ ^2D_{3/2}$–$5p\ ^2P^\circ_{3/2}$), and 21–22 ($5f\ ^2F^\circ_{5/2}$–$5d\ ^2D_{5/2}$). This is because our corresponding

Table 2. Collision strengths for the "elastic" transitions of Al XIII. ($a \pm b \equiv a \times 10^{\pm b}$).

Transition		Energy (Ryd)								
i	j	170.0	180.0	190.0	200.0	220.0	240.0	260.0	280.0	300.0
2	3	2.728+0	2.753+0	2.774+0	2.791+0	2.818+0	2.839+0	2.856+0	2.871+0	2.883+0
2	4	3.090+0	3.189+0	3.268+0	3.336+0	3.443+0	3.526+0	3.594+0	3.651+0	3.700+0
5	6	1.617+1	1.647+1	1.666+1	1.681+1	1.702+1	1.716+1	1.728+1	1.737+1	1.745+1
5	7	1.180+1	1.252+1	1.301+1	1.337+1	1.389+1	1.426+1	1.455+1	1.478+1	1.497+1
6	8	1.867+1	1.982+1	2.058+1	2.116+1	2.198+1	2.257+1	2.302+1	2.339+1	2.370+1
7	8	4.255+0	4.328+0	4.378+0	4.415+0	4.468+0	4.506+0	4.535+0	4.559+0	4.579+0
8	9	2.550+1	2.683+1	2.773+1	2.839+1	2.934+1	3.000+1	3.053+1	3.095+1	3.130+1
10	11	6.119+1	6.266+1	6.348+1	6.405+1	6.478+1	6.529+1	6.570+1	6.599+1	6.626+1
10	12	5.035+1	5.497+1	5.757+1	5.935+1	6.175+1	6.338+1	6.461+1	6.560+1	6.640+1
11	13	6.254+1	6.829+1	7.151+1	7.372+1	7.670+1	7.873+1	8.026+1	8.148+1	8.249+1
12	13	2.038+1	2.086+1	2.113+1	2.132+1	2.156+1	2.173+1	2.185+1	2.195+1	2.203+1
12	15	6.410+1	6.910+1	7.188+1	7.377+1	7.633+1	7.807+1	7.937+1	8.041+1	8.127+1
13	14	1.088+2	1.173+2	1.221+2	1.253+2	1.296+2	1.326+2	1.349+2	1.366+2	1.381+2
14	15	8.467+0	8.642+0	8.739+0	8.808+0	8.901+0	8.962+0	9.009+0	9.050+0	9.079+0
14	16	1.013+2	1.084+2	1.124+2	1.151+2	1.188+2	1.213+2	1.231+2	1.247+2	1.258+2
17	18	1.534+2	1.582+2	1.605+2	1.620+2	1.638+2	1.651+2	1.660+2	1.668+2	1.674+2
17	20	1.576+2	1.763+2	1.853+2	1.911+2	1.986+2	2.037+2	2.075+2	2.105+2	2.129+2
18	19	1.385+2	1.549+2	1.628+2	1.679+2	1.745+2	1.789+2	1.822+2	1.849+2	1.871+2
19	20	6.264+1	6.431+1	6.513+1	6.563+1	6.634+1	6.678+1	6.709+1	6.738+1	6.754+1
19	21	2.293+2	2.523+2	2.633+2	2.703+2	2.795+2	2.856+2	2.901+2	2.938+2	2.967+2
20	22	2.990+2	3.291+2	3.435+2	3.527+2	3.648+2	3.727+2	3.787+2	3.835+2	3.874+2
21	22	2.733+1	2.816+1	2.855+1	2.881+1	2.914+1	2.936+1	2.952+1	2.965+1	2.975+1
21	23	2.056+2	2.243+2	2.331+2	2.388+2	2.462+2	2.510+2	2.547+2	2.577+2	2.601+2
22	24	3.621+2	3.952+2	4.109+2	4.210+2	4.341+2	4.428+2	4.494+2	4.545+2	4.587+2
23	24	1.166+1	1.199+1	1.215+1	1.226+1	1.239+1	1.248+1	1.255+1	1.261+1	1.265+1
24	25	2.853+2	3.095+2	3.210+2	3.284+2	3.380+2	3.443+2	3.491+2	3.528+2	3.560+2

Table 3. Effective collision strengths for the "elastic" transitions of Al XIII. ($a \pm b \equiv a \times 10^{\pm b}$).

Transition		Temperature (log, K)												
i	j	4.400-0	4.600-0	4.800-0	5.000-0	5.200-0	5.400-0	5.600-0	5.800-0	6.000-0	6.200-0	6.400-0	6.600-0	6.800-0
2	3	8.827-1	9.764-1	1.071+0	1.190+0	1.345+0	1.488+0	1.576+0	1.650+0	1.747+0	1.866+0	1.995+0	2.126+0	2.256+0
2	4	1.332+0	1.357+0	1.392+0	1.443+0	1.514+0	1.608+0	1.727+0	1.867+0	2.026+0	2.201+0	2.392+0	2.596+0	2.809+0
5	6	6.325+0	7.014+0	7.707+0	8.554+0	9.619+0	1.056+1	1.109+1	1.149+1	1.201+1	1.265+1	1.335+1	1.406+1	1.476+1
5	7	5.355+0	5.514+0	5.742+0	6.057+0	6.469+0	6.972+0	7.555+0	8.200+0	8.885+0	9.599+0	1.034+1	1.111+1	1.189+1
6	8	8.512+0	8.769+0	9.137+0	9.645+0	1.031+1	1.112+1	1.205+1	1.308+1	1.418+1	1.532+1	1.650+1	1.772+1	1.896+1
7	8	2.665+0	2.944+0	3.197+0	3.483+0	3.831+0	4.120+0	4.248+0	4.317+0	4.430+0	4.589+0	4.768+0	4.951+0	5.132+0
8	9	1.050+1	1.099+1	1.168+1	1.260+1	1.373+1	1.501+1	1.638+1	1.781+1	1.930+1	2.081+1	2.233+1	2.387+1	2.540+1
10	11	2.377+1	2.643+1	2.901+1	3.207+1	3.583+1	3.907+1	4.074+1	4.185+1	4.338+1	4.534+1	4.747+1	4.963+1	5.176+1
10	12	2.456+1	2.544+1	2.668+1	2.838+1	3.052+1	3.302+1	3.578+1	3.871+1	4.174+1	4.483+1	4.795+1	5.112+1	5.429+1
11	13	2.930+1	3.053+1	3.227+1	3.460+1	3.751+1	4.082+1	4.437+1	4.810+1	5.196+1	5.588+1	5.984+1	6.385+1	6.785+1
12	13	1.213+1	1.334+1	1.441+1	1.562+1	1.708+1	1.828+1	1.876+1	1.898+1	1.939+1	1.999+1	2.067+1	2.138+1	2.208+1
12	15	2.746+1	3.084+1	3.406+1	3.789+1	4.272+1	4.704+1	4.958+1	5.159+1	5.422+1	5.744+1	6.090+1	6.443+1	6.794+1
13	14	4.662+1	5.238+1	5.787+1	6.441+1	7.263+1	8.000+1	8.433+1	8.774+1	9.220+1	9.767+1	1.036+2	1.096+2	1.155+2
14	15	5.304+0	5.794+0	6.214+0	6.685+0	7.259+0	7.722+0	7.888+0	7.945+0	8.080+0	8.300+0	8.557+0	8.823+0	9.087+0
14	16	4.662+1	5.124+1	5.594+1	6.180+1	6.931+1	7.602+1	7.981+1	8.267+1	8.645+1	9.114+1	9.620+1	1.013+2	1.064+2
17	18	6.551+1	7.284+1	7.975+1	8.771+1	9.736+1	1.055+2	1.094+2	1.117+2	1.151+2	1.196+2	1.245+2	1.295+2	1.345+2
17	20	7.673+1	8.112+1	8.714+1	9.485+1	1.036+2	1.124+2	1.208+2	1.292+2	1.383+2	1.480+2	1.579+2	1.679+2	1.778+2
18	19	6.706+1	7.086+1	7.607+1	8.273+1	9.035+1	9.799+1	1.053+2	1.127+2	1.207+2	1.291+2	1.378+2	1.465+2	1.552+2
19	20	3.806+1	4.157+1	4.456+1	4.788+1	5.192+1	5.516+1	5.626+1	5.657+1	5.742+1	5.886+1	6.057+1	6.235+1	6.412+1
19	21	1.129+2	1.240+2	1.352+2	1.492+2	1.670+2	1.828+2	1.916+2	1.980+2	2.066+2	2.174+2	2.290+2	2.408+2	2.526+2
20	22	1.475+2	1.621+2	1.767+2	1.950+2	2.183+2	2.389+2	2.504+2	2.588+2	2.700+2	2.841+2	2.992+2	3.147+2	3.300+2
21	22	2.497+1	2.691+1	2.846+1	3.018+1	3.232+1	3.399+1	3.438+1	3.432+1	3.459+1	3.524+1	3.606+1	3.694+1	3.780+1
21	23	1.018+2	1.126+2	1.233+2	1.361+2	1.522+2	1.663+2	1.737+2	1.789+2	1.859+2	1.947+2	2.042+2	2.139+2	2.236+2
22	24	1.794+2	1.984+2	2.173+2	2.401+2	2.685+2	2.933+2	3.065+2	3.156+2	3.279+2	3.434+2	3.602+2	3.773+2	3.943+2
23	24	1.047+1	1.127+1	1.192+1	1.264+1	1.354+1	1.423+1	1.440+1	1.437+1	1.448+1	1.476+1	1.511+1	1.547+1	1.584+1
24	25	1.434+2	1.588+2	1.739+2	1.919+2	2.141+2	2.333+2	2.431+2	2.496+2	2.585+2	2.699+2	2.824+2	2.951+2	3.076+2

values of Ω were also underestimated, as stated earlier. However, based on the comparisons made in our earlier paper for the forbidden (and other allowed) transitions, and the comparisons of Ω values discussed above in Sect. 2, we expect our present results for Υ to be accurate to better than 15% at all temperatures. Furthermore, the results presented here, along with those already

reported for radiative rates and effective collision strengths in our earlier work (Aggarwal et al. 2005), form a complete set of atomic data for all transitions in Al XIII, and will hopefully be useful for plasma modelling.

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