Validity of the ICFT *R*-matrix method: Be-like Al^{9+} a case of study

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- Work on Be-like isoelectronic sequence. 238-level CI/CC expansion, ICFT.
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  K. M. Aggarwal, F. P. Keenan 2015, *Mon. Not. R. Astr. Soc.*, **447**, 3849.
- Reply: L. Fernández-Menchero, G. Del Zanna and N. R. Badnell 2015, *Mon. Not. R. Astr. Soc.*, **450**, 4174.

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Motivation

- 238-level ICFT of MZB-2014 gives in general larger results for the effective collision strengths Υ than 98-level DARC of AK-2014.
- Electron exchange included by AK-2014 for more angular momenta than MZB-2015: $2J = 81$ vs $2J = 23$.
- Energy step length of AK-2014 slight finer than MZB-2014, depends on ion.
- AK-2014 goes further in scattering energy than MZB-2014: 12 times versus 3 times the ionization potential plus interpolation up to $E = \infty$ in Burgess–Tully domain.
- DARC vs ICFT.

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- AK-2014 goes further in scattering energy than MZB-2014: 12 times versus 3 times the ionization potential plus interpolation up to $E = \infty$ in Burgess–Tully domain.
- DARC vs ICFT.
- MZB-2014 has a much larger configuration interaction and close coupling expansion than AK-2014: 238 levels vs 98 levels.

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Atomic energies

238-level CI structure[1] configurations $1s^2\,\{2s^2, 2s2p, 2p^2\}$, $1s^2\,2\{s, p\}\,nl$, with $n = 3 - 7$ and $l = s, p, d, f, g$ for $n = 3 - 5$ and $l = s, p, d$ for $n = 6 - 7$.
Total 130 terms, 238 levels.

98-level CI structure[2] configurations $1s^2\,\{2s^2, 2s2p, 2p^2\}$, $1s^2\,2\{s, p\}\,nl$, with $n = 3 - 4$ and $l = s, p, d, f$.
Total 54 terms, 98 levels.

[1] L. Fernández-Menchero, G. Del Zanna and N. R. Badnell 2014, *Astron. Astrophys.*, **566**, A104.
[2] Present work (for test comparison).

Atomic energies

Table: Al^{9+} target levels. All energies are in cm^{-1}.

i	Conf.	Level	E_{NIST}	E_{98} (%)	E_{238} (%)
1	$2s^2$	$^1S_0$	0.	0. (0)	0. (0)
2	2s 2p	$^3P^o_0$	155148.	155722. (0.4)	155539. (0.3)
3	2s 2p	$^3P^o_1$	156798.	157487. (0.4)	157404. (0.4)
4	2s 2p	$^3P^o_2$	160429.	161146. (0.4)	161278. (0.5)
5	2s 2p	$^1P^o_1$	300490.	309273. (2.9)	307209. (2.2)
6	$2p^2$	$^3P_0$	404574.	408026. (0.9)	407826. (0.8)
7	$2p^2$	$^3P_1$	406517.	409969. (0.8)	409888. (0.8)
8	$2p^2$	$^3P_2$	409690.	413420. (0.9)	413526. (0.9)
9	$2p^2$	$^1D_2$	449732.	458157. (1.9)	457831. (1.8)
10	$2p^2$	$^1S_0$	553783.	567794. (2.5)	567267. (2.4)

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Atomic energies

Table: Al^{9+} target levels. All energies are in cm^{-1}.

i	Conf.	Level	E_{NIST}	E_{98} (%)	E_{238} (%)
88	$2p\,4f$	$^3P_3$	–	2712961. (–)	2706897. (–)
89	$2p\,4f$	$^3P_4$	–	2713531. (–)	2707350. (–)
90	$2p\,4f$	$^3P_5$	–	2715225. (–)	2708632. (–)
91	$2p\,4f$	$^3D_3$	–	2716473. (–)	2710743. (–)
92	$2p\,4f$	$^1D_4$	–	2717105. (–)	2710218. (–)
93	$2p\,4f$	$^3D_2$	–	2717141. (–)	2711361. (–)
94	$2p\,4p$	$^1S_0$	–	2717922. (–)	2706869. (–)
95	$2p\,4f$	$^3D_1$	–	2718397. (–)	2712736. (–)
96	$2p\,4f$	$^1D_2$	–	2719895. (–)	2713991. (–)
97	$2p\,4d$	$^1F^o_3$	–	2722212. (–)	2715080. (–)
98	$2p\,4d$	$^1P^o_1$	–	2723448. (–)	2716711. (–)

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Infinite energy point

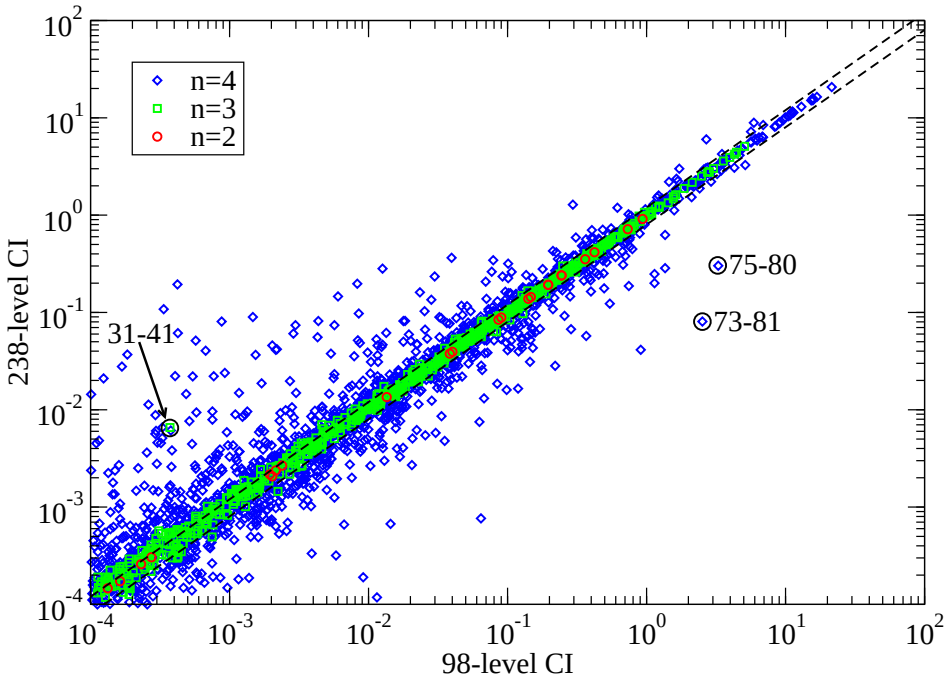

Figure: Transition infinite energy points $y_\infty = \Omega^{\mathrm{PWB}}_\infty$ or $\frac{4}{3}S$ for two different atomic structures: 98-level CI versus 238-level CI.

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Result comparison

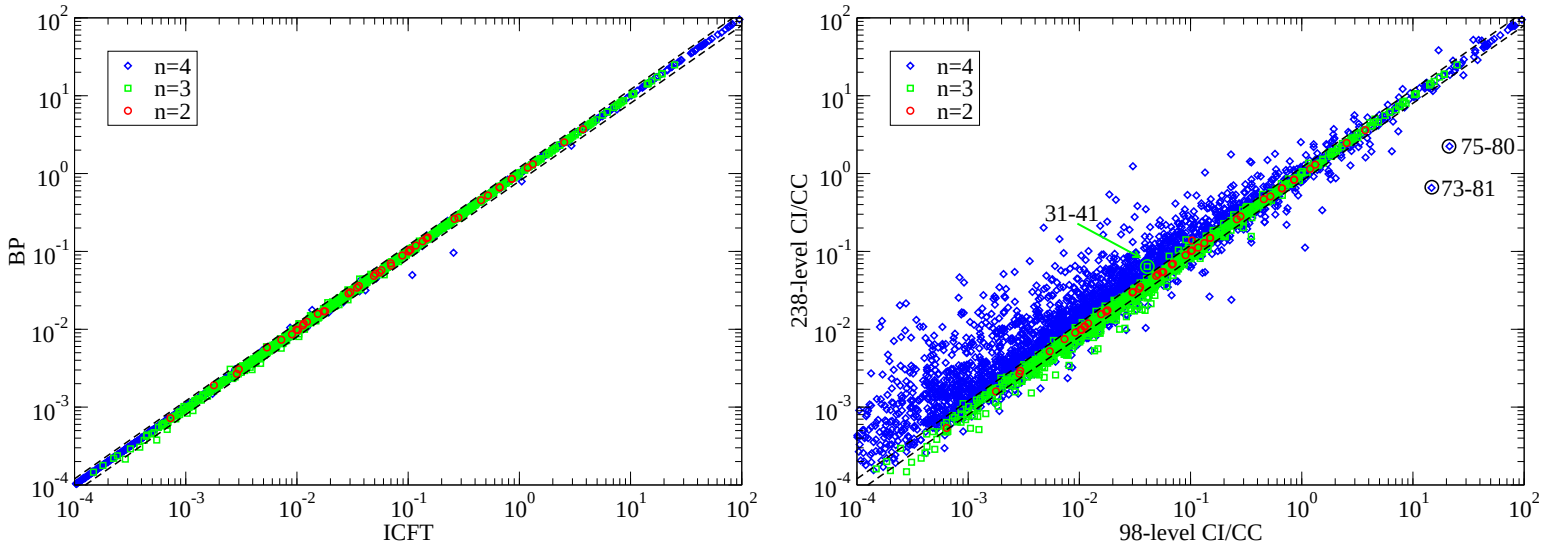

Figure: Effective collision strengths for electron-impact excitation of the ion Al^{9+} at $T = 10^6\,\mathrm{K}$. Left: Breit–Pauli versus ICFT, 98 level CI/CC; right: 98-level CI/CC versus 238-level CI/CC, ICFT.

Result comparison

Table: Number of transitions in figures which differ by more than a certain relative error $\delta = |\Upsilon_A - \Upsilon_B|/\Upsilon_B$ (or $\Upsilon \rightarrow y_\infty$), as a percentage.

Rel. error (%)	y_∞ 98 vs 238 CI	98 CI/CC Υ BP vs ICFT	ICFT Υ 98 vs 238 CI/CC
1	3778	1336	4579
2	3600	803	4400
3	3416	500	4243
4	3266	350	4077
5	3141	260	3928
6	3022	206	3798
7	2914	158	3676
8	2804	127	3569
9	2722	106	3460
10	2644	82	3357
20	2068	22	2582
30	1643	9	2090
40	1356	4	1725
50	1163	2	1449
75	846	2	1113
100	707	2	901
150	538	1	647
200	443	0	505
300	336	0	320
1000	187	0	88
Total	4035	4753	4753

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Result comparison

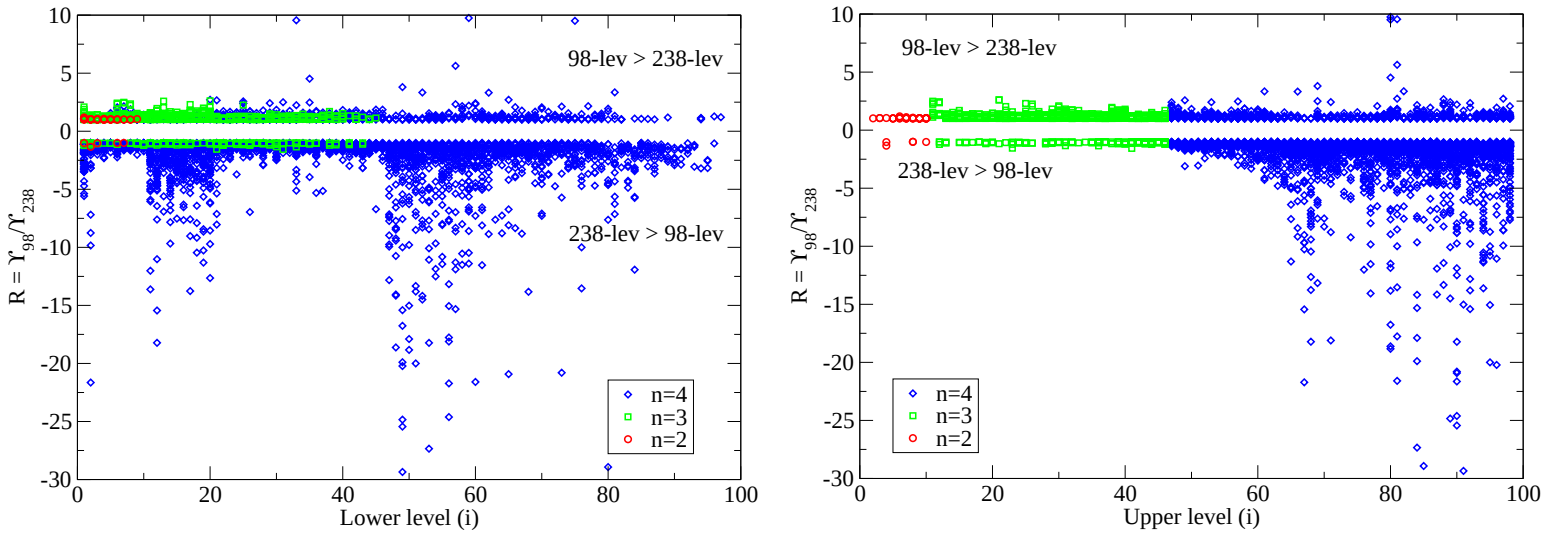

Figure: The ratio of effective collision strengths from 98- vs 238-level CI/CC ICFT R-matrix calculations vs left: lower level and right: upper level index for all inelastic transitions amongst the 98 lowest common levels of Al^{9+} at $T = 10^6\,\mathrm{K}$. Positive values indicate $\Upsilon_{98} > \Upsilon_{238}$ and negative values $\Upsilon_{238} > \Upsilon_{98}$.

Result comparison

- Comparing different relativistic formalism the differences are minimal. Only a few spin-change transitions present differences, and they are much smaller compared with CI/CC differences.
- Comparing different atomic structures, differences in the results Υ are same order as differences in the atomic structure $\Omega_{\infty}^{\mathrm{PWB}}$, $\frac{4}{3}S$.
- Υ for 238-level CI/CC expansion are in general larger than the ones for 98-level CI/CC expansion, while $\Omega_{\infty}^{\mathrm{PWB}}$, $\frac{4}{3}S$ was symmetrical.
- Differences are considerable larger for transitions to the $n = 4$ shell than for the $n = 2, 3$ ones.
- 98-level CC expansion is not converged for the $n = 4$ atomic shell.
- 238-level CI expansion gives a much more accurate atomic structure than 98-level.

Result comparison

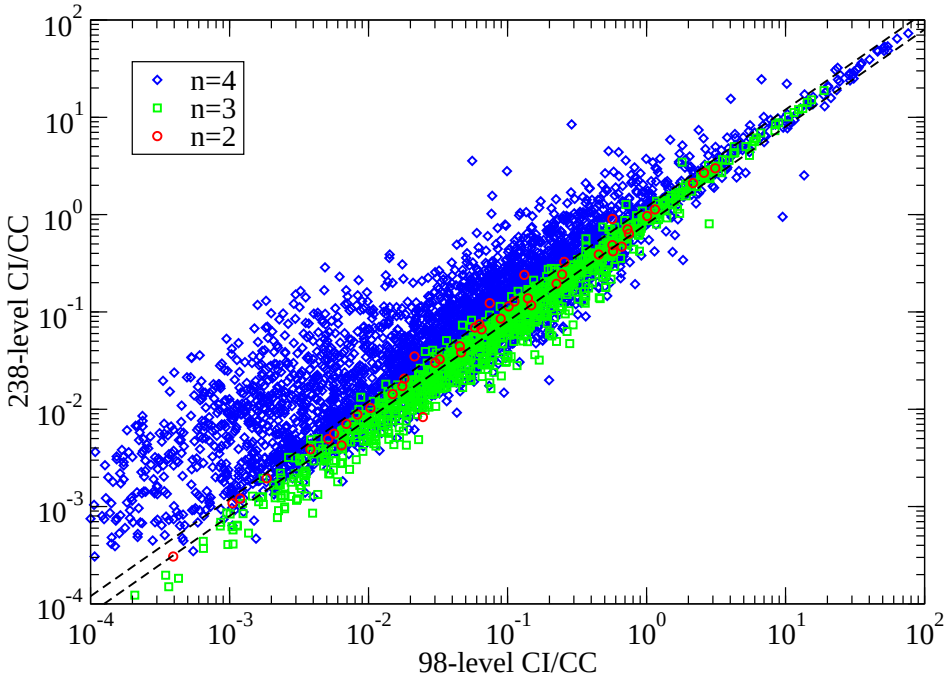

Figure: Effective collision strengths for electron-impact excitation of the ion Al^{9+} at $T = 2 \times 10^4\,\mathrm{K}$. 98-level CI/CC versus 238-level CI/CC, ICFT.

Result comparison

- Differences between atomic structures much larger than at the peak abundance temperature.
- Position or resolution of resonances.
- Both same step lengths and checked convergence. Resolution of the resonances discarded.
- Differences in position of the resonances due to atomic structure.
- 238-level CI expansion much more reliable than 98-level one, mainly for levels in the $n = 4$ atomic shell.

Result comparison

Table: Comparison of effective collision strengths, Υ, at $T = 2 \times 10^7$ K and the reduced quantity y_∞ at infinite temperature. $A\,(B)$ denotes $A \times 10^B$.

	DARC	ICFT			
i–j	98-level CI/CC	98-level CI/CC		238-level CI/CC	
$T\,(K)$	2×10^7	2×10^7	∞	2×10^7	∞
1–52	3.01 (−2)	3.20 (−2)	2.40 (−2)	3.22 (−2)	2.64 (−2)
1–64	1.70 (−4)	1.96 (−4)	1.01 (−4)	9.40 (−5)	1.63 (−5)
1–70	5.29 (−6)	4.23 (−6)	2.68 (−6)	2.18 (−5)	2.18 (−5)
1–80	8.45 (−6)	7.05 (−6)	–	1.09 (−5)	–

DARC: K. M. Aggarwal and F. P. Keenan 2014, *Mon. Not. R. Astr. Soc.*, **438**, 1223
98-level ICFT: present work
238-level ICFT: L. Fernández-Menchero, G. Del Zanna, N. R. Badnell 2014, *Astron. Astrophys.*, **566**, A104.

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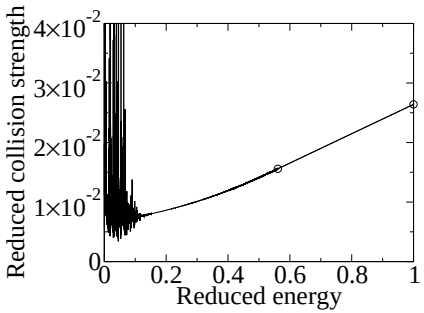
Differences at high temperature

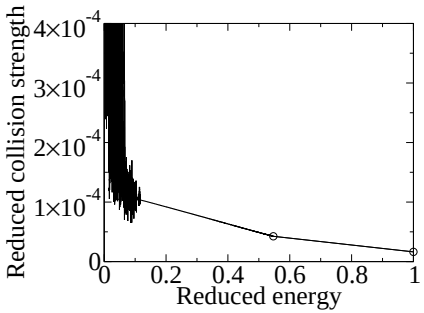
MZB-2014 calculated Ω up to three times the ionization potential and interpolated in Burgess–Tully domain.
A. Burgess and J. A. Tully 1992. *Astron. Astrophys.*, **254**, 436–453.
AK-2014 calculated Ω up to twelve times the ionization potential and did not perform any interpolation up to infinity.

Burgess–Tully diagram



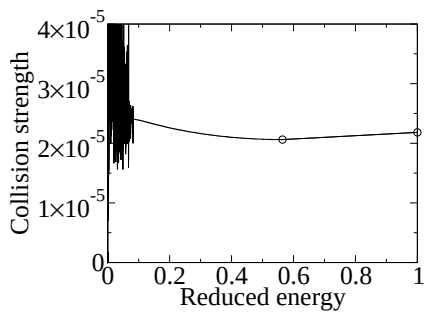
$1 - 52$

$2s^2\ ^1S_0 - 2s4p\ ^1P^o_1$



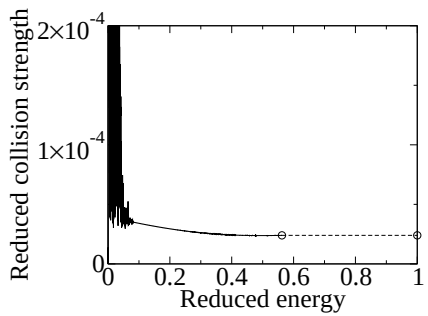
$1 - 64$

$2s^2\ ^1S_0 - 2p4s\ ^1P^o_1$



$1 - 70$

$2s^2\ ^1S_0 - 2p4p\ ^3P_0$



$1 - 80$

$2s^2\ ^1S_0 - 2p4f\ ^1F_3$

Figure: Reduced collision strengths versus energy from 238-level CI/CC ICFT R-matrix calculations for selected transitions of Al^{9+}.

Result comparison

- Calculated Ω reached asymptotic form. Interpolation in Burgess–Tully domain properly done.
- Differences in the infinite energy point lead to differences in the Υ for high temperature.
- Infinite energy points more reliable for 238-level CI expansion than for 98-level CI expansion.

Contents

Conclusions

- Three main error sources: atomic structure, close coupling expansion and inclusion of relativistic effects.
- Different atomic structures / CI expansions lead to large differences, mainly at high temperature / energy.
- A larger CC expansion improves strongly the results, mainly for the higher excited terms / levels.
- Method to consider the relativistic effects (ICFT, BP, DARC) does not change meaningfully the results.
- No calculation can guarantee the quality of the results for the last terms / levels included in the close-coupling expansion.
- Nothing special about Be-like Al^{9+}. Same conclusions can be applied to other ions and sequences.
  For example: Fe^{13+}: G. Del Zanna, N. R. Badnell, L. Fernández-Menchero, G. Y. Liang, H. E. Mason and P. J. Storey 2015. *Mon. Not. R. Astron. Soc. In press.*

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Thank you for your attention

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