New atomic data for plasma diagnostics: Be and Mg-like isoelectronic sequences

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Be- and Mg-like ion lines in space

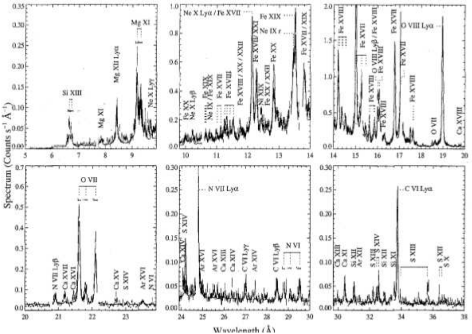
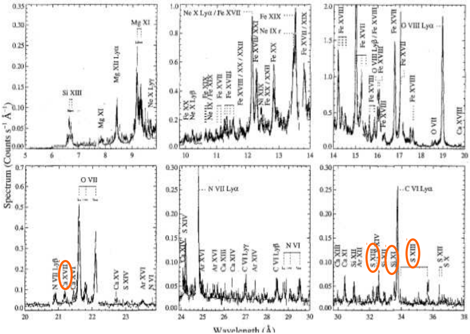


Figure: XMM-Newton RGSI spectrum of Capella together with a best-fit model

Be- and Mg-like ion lines in space



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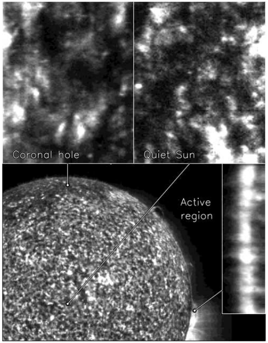

Figure: Observed solar regions by the Extreme Ultraviolet Imaging Telescope (EIT). The full Sun image is in $\mathrm{He\,II}$. The expanded regions are the observed $\mathrm{Si\,III}$ data, summed over the $1113.0 - 1113.7\,\mathrm{\AA}$ spectral region

New adf04 files

- From B^{+} to Kr^{32+}
  `~adas/adas/adf04/copaw#be/belike_lfm14#*.dat`
  L. Fernández-Menchero, G. Del Zanna and N. R. Badnell 2014
  Astron. Astrophys. **566**, A104.
- From Al^{+} to Kr^{24+}
  `~adas/adas/adf04/copaw#mg/mglike_lfm14#*.dat`
  L. Fernández-Menchero, G. Del Zanna and N. R. Badnell 2014
  Astron. Astrophys. **572**, A115.

Previous calculations: Be-like sequence

- D. H. Sampson, S. J. Goett and R. E. H. Clark 1984, Atomic Data and Nuclear Data Tables, 30, 125
  Coulomb-Born, intermediate coupling up to $n = 3$ from Ne^{6+} to W^{70+}
- K. A. Berrington, P. G. Burke, P. L. Dufton and A. E. Kingston 1985, Atomic Data and Nuclear Data Tables, 33, 195
  R-Matrix, 10 IC levels, C^{2+}, O^{4+}, Ne^{6+}, Si^{10+}.
- M. C. Chidichimo, G. Del Zanna, H. E. Mason, N. R. Badnell, J. A. Tully, and K. A. Berrington 2005, Astronomy and Astrophysics, 430, 331
  Fe^{22+}, *R*-matrix, up to $n = 4$.
- M. C. Chidichimo, N. R. Badnell, and J. A. Tully 2003, Astronomy and Astrophysics, 401, 1177
  Ni^{24+}, *R*-matrix, up to $n = 4$.
- F. P. Keenan 1988, Physica Scripta, 37, 57 and F. P. Keenan, K. A. Berrington, P. G. Burke, P. L. Dufton and A. E. Kingston 1986, Physica Scripta, 34, 216
  Interpolated values for N^{3+}, F^{5+}, Na^{7+}, Mg^{8+}, Al^{9+}, P^{11+}, S^{12+}, Cl^{13+}, K^{15+}.

Previous calculations: Mg-like sequence

- R. B. Christensen, D. W. Norcross and A. K. Pradhan 1986, Physical Review A, 34, 4704
  Distorted Wave, 16 levels, S^{4+}, Ar^{6+}, Ca^{8+}, Cr^{12+}, Ni^{16+}.
- D. C. Griffin, N. R. Badnell and M. S. Pindzola 1998 J. Phys. B: At. Mol. Opt. Phys. 31, 3713
  R-matrix, 45 levels, Ar^{6+} and Ti^{10+}.
- E. Landi 2011, At. Data Nucl. Data Tables. 97, 587
  Distorted Wave, up to $n = 5$, Fe^{14+}.
- K. A. Berrington, P. G. Burke, P. L. Dufton and A. E. Kingston 1985, Atomic Data and Nuclear Data Tables, 33, 195
  R-Matrix, 10 IC levels, C^{2+}, O^{4+}, Ne^{6+}, Si^{10+}.
- M. C. Chidichimo, G. Del Zanna, H. E. Mason, N. R. Badnell, J. A. Tully, and K. A. Berrington 2005, Astronomy and Astrophysics, 430, 331
  Fe^{22+}, *R*-matrix, up to $n = 4$.
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University of Strathclyde Science

Contents

Atomic structure

Atomic structure calculated with AUTOSTRUCTURE program N. R. Badnell 2011, Comput. Phys. Commun., 182, 1528
Breit-Pauli Hamiltonian including fine structure terms: mass-velocity, spin-orbit and Darwin.
Multielectronic potential introduced through a Thomas-Fermi-Dirac-Amaldi model. Scaling parameters λ determined variationally, minimising the sum of the energy of the terms.

Basis set: Be-like sequence

Orbitals:
1s,
2s, 2p,
3s, 3p, 3d,
4s, 4p, 4d, 4f,
5s, 5p, 5d, 5f, 5g,
6s, 6p, 6d,
7s, 7p, 7d
Total 21 orbitals
Configurations $1\mathrm{s}^2\,\{2\mathrm{s}^2,\ 2\mathrm{s}\,2\mathrm{p},\ 2\mathrm{p}^2,\ 2\mathrm{s}\,nl,\ 2\mathrm{p}\,nl\}$. With $n = 3 - 7$, $l = \mathrm{s}, \mathrm{p}, \mathrm{d}, \mathrm{f}, \mathrm{g}$
Total 39 configurations, 130 *LS* tems, 238 fine structure levels.
Values of λ can be found in L. Fernández-Menchero, G. Del Zanna and N. R. Badnell 2014 *Astron. Astrophys.* **566**, A104, or the adf04 files.

Basis set: Mg-like sequence

Orbitals:
1s,
2s, 2p,
3s, 3p, 3d,
4s, 4p, 4d, 4f,
5s, 5p, 5d, 5f, 5g
Total 15 orbitals
Configurations
$1\mathrm{s}^2\,2\mathrm{s}^2\,2\mathrm{p}^6\,\{3\mathrm{s}^2,\ 3\mathrm{s}\,3\mathrm{p},\ 3\mathrm{s}\,3\mathrm{d},\ 3\mathrm{p}^2,\ 3\mathrm{p}\,3\mathrm{d},\ 3\mathrm{d}^2,\ 3\mathrm{s}\,nl,\ 3\mathrm{p}\,nl,\ 3\mathrm{d}\,nl\}$. With $n = 4, 5,\ l = \mathrm{s, p, d, f, g}$
Total 33 configurations, 149 *LS* tems, 283 fine structure levels.
Values of λ can be found in L. Fernández-Menchero, G. Del Zanna and N. R. Badnell 2014 *Astron. Astrophys.* **572**, A115, or the adf04 files.

Atomic energies

Level energies (cm^{-1}) for Fe^{14+}.
NIST: J. Sugar and C. Corliss, 1985, *J. Phys. Chem. Ref. Data*, **14, Suppl. 2**, 1–664
CHIANTI: Landi, 2011, *At. Data Nucl. Data Tables*, **97**, 587

i	Conf.	Level	E_{th} (%)	E_{NIST}	E_{CHIANTI} (%)
1	$3s^2$	$^1S_0^+$	0. (0.0)	0.	0. (0.0)
2	$3s\,3p$	$^3P_0^-$	233066. (0.3)	233842.	233068. (0.3)
3	$3s\,3p$	$^3P_1^-$	238974. (0.3)	239660.	238900. (0.3)
4	$3s\,3p$	$^3P_2^-$	253015. (0.3)	253820.	252918. (0.4)
5	$3s\,3p$	$^1P_1^-$	356807. (1.4)	351911.	356127. (1.2)
6	$3p^2$	$^3P_0^+$	557614. (0.6)	554524.	556995. (0.4)
7	$3p^2$	$^1D_2^+$	561312. (0.3)	559600.	560266. (0.1)
8	$3p^2$	$^3P_1^+$	567380. (0.5)	564602.	566833. (0.4)
9	$3p^2$	$^3P_2^+$	584191. (0.4)	581803.	583564. (0.3)
10	$3p^2$	$^1S_0^+$	666738. (1.1)	659627.	665768. (0.9)
11	$3s\,3d$	$^3D_1^+$	682739. (0.6)	678772.	680146. (0.2)
12	$3s\,3d$	$^3D_2^+$	684031. (0.6)	679785.	681129. (0.2)
13	$3s\,3d$	$^3D_3^+$	686015. (0.7)	681416.	682667. (0.2)
14	$3s\,3d$	$^1D_2^+$	772235. (1.3)	762093.	769370. (1.0)
15	$3p\,3d$	$^3F_2^-$	932223. (0.4)	928241.	928787. (0.1)
16	$3p\,3d$	$^3F_3^-$	942210. (0.4)	938126.	938555. (0.0)
17	$3p\,3d$	$^1D_2^-$	952970. (0.5)	948513.	949447. (0.1)
18	$3p\,3d$	$^3F_4^-$	953701. (0.4)	949658.	949928. (0.0)
19	$3p\,3d$	$^3D_1^-$	989033. (0.6)	982868.	986083. (0.3)
20	$3p\,3d$	$^3P_2^-$	989882. (0.6)	983514.	986408. (0.3)

Contents

Scattering

R-matrix formalism combied with and Intermediate Coupling Frame Transformation.
Electron exchange: $2J = 0 - 30$
Non exchange: $2J = 31 - 80$
Burgess sum rules: $2J > 80$.

Distribution function

$$\Upsilon(i-j) = \frac{\sqrt{\pi}}{2}\int_0^\infty \mathrm{d}E \left(\frac{E}{kT_{\mathrm{eff}}}\right)^{-1/2} f(E)\,\Omega(i-j)$$

- Maxwell distribution:

$$f(E,T) = \frac{2}{\sqrt{\pi}}\frac{1}{kT}\left(\frac{E}{kT}\right)^{1/2} e^{-\frac{E}{kT}}$$

$T = T_{\mathrm{eff}}$: electron temperature; k: Boltzmann constant.

- κ distribution:

$$f(E;\kappa,T_{\mathrm{eff}}) = \frac{\Gamma(\kappa+1)}{\Gamma(\kappa-\frac{1}{2})}\frac{2}{\sqrt{\pi}}\frac{1}{\kappa E_\kappa}\left(\frac{E}{\kappa E_\kappa}\right)^{1/2}\left(1+\frac{E}{\kappa E_\kappa}\right)^{-(\kappa+1)}$$

$kT_{\mathrm{eff}} = \kappa E_\kappa/(\kappa-\frac{3}{2})$; T_{eff}: effective temperature, $kT_{\mathrm{eff}} = \frac{2}{3}\overline{E}$; $\overline{E}$: mean electron energy.

Paul Bryans 2005. PhD Thesis. University of Strathclyde.

Contents

Collision strengths

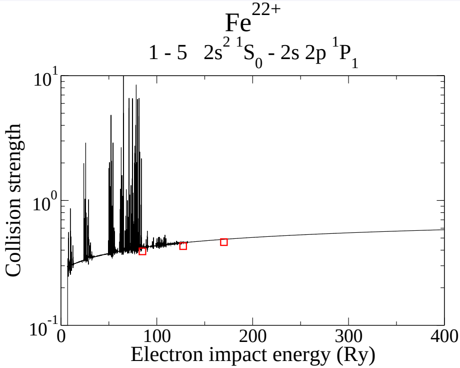


Figure: Electron impact excitation collision strength for the transition of Fe^{22+} $2s^2\,{}^1S_0 - 2s2p\,{}^1P_1$. Full line: present calculation; □: distorted wave results of A. K. Bhatia and H. E. Mason 1981, *Astron. Astrophys.*, **103**, 324

Collision strengths

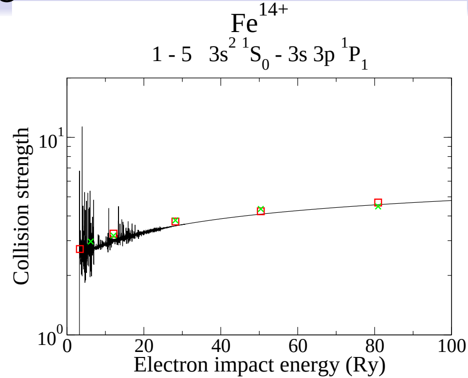


Figure: Electron impact excitation collision strength for the transition of Fe^{14+} $3\mathrm{s}^2\,{}^1\mathrm{S}_0 - 3\mathrm{s}3\mathrm{p}\,{}^1\mathrm{P}_1$. Full line: present calculation; □: distorted wave results of E. Landi 2011, *At. Data Nucl. Data Tables*, **97**, 587; × distorted wave results with same atomic structure.

Effective collision strengths

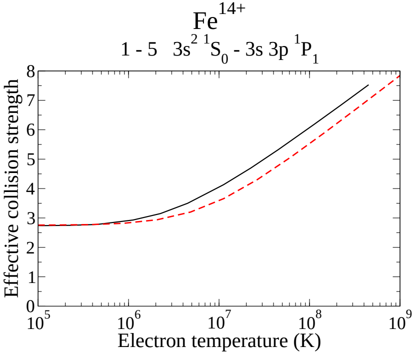


Figure: Effective collision strength for the transition of Fe^{14+} $3s^2\,{}^1S_0 - 3s3p\,{}^1P_1$. Full line: present calculation; Dashed line: K. A. Berrington, C. P. Ballance, D. C. Griffin and N. R. Badnell 2005, *J. Phys. B: At., Mol. Opt. Phys.*, **38**, 1667
$\lambda = 284.16$ Å

Effective collision strengths

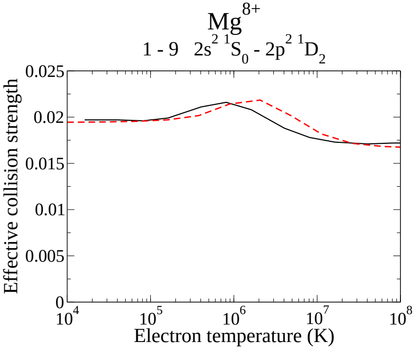


Figure: Effective collision strength for the transition of $\mathrm{Mg}^{8+}\ 2\mathrm{s}^2\ ^1\mathrm{S}_0 - 2\mathrm{p}^2\ ^1\mathrm{D}_2$. Full line: present calculation; Dashed line: G. Del Zanna, I. Rozum and N. R. Badnell 2008, *Astron. Astrophys.*, **487**, 1203
$\lambda = 749.55, 383.13, 379.55$ Å

Non Maxwellian

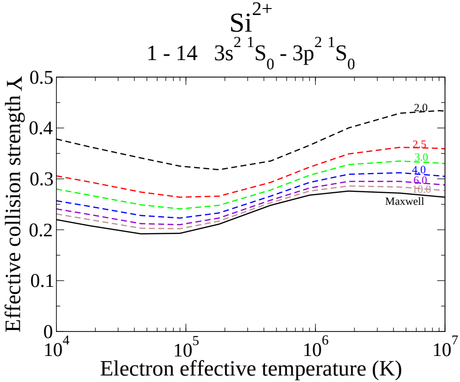


Figure: Effective collision strength for the transition of Si^{2+} $3\mathrm{s}^2\ {}^1\mathrm{S}_0 - 3\mathrm{p}^2\ {}^1\mathrm{S}_0$. Dashed line: κ distribution; full line: Maxwell distribution.
$\lambda = 1417.2\,\mathrm{\AA}$

Non Maxwellian

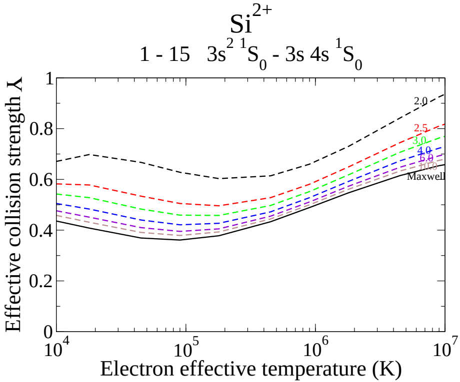


Figure: Effective collision strength for the transition of Si^{2+} $3\mathrm{s}^2\,{}^1\mathrm{S}_0 - 3\mathrm{s}4\mathrm{s}\,{}^1\mathrm{S}_0$.
Dashed line: κ distribution; full line: Maxwell distribution.
$\lambda = 1412.6\,\text{Å}$

Contents

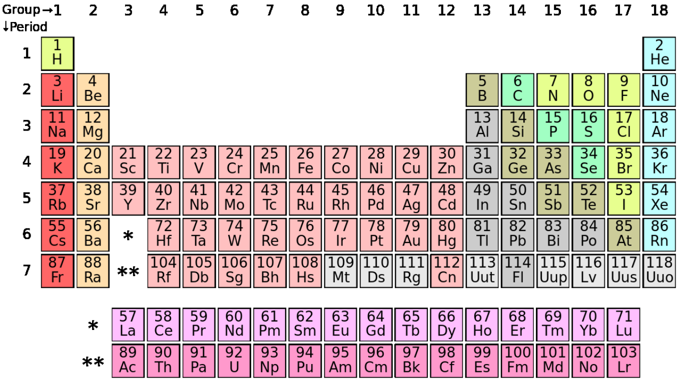
Conclusions

- High quality data have been calculated for all the ions in the Berylium- and Magnesium like isoelectronic sequences, up to Zn^{q+}.
- Excited states have been included in basis set up to $n = 7$ for Be-like, and up to $n = 5$ for Mg-like. Cascading effects can be included in Collision Radiative modelling up to such levels.
- Present work compliments previous ones in sequences:

F-like: M. C. Witthoeft, A. D. Whiteford, and N. R. Badnell 2007, *J. Phys. B: At. Mol. Opt. Phys.*, **40**, 2969
Ne-like: G. Y. Liang and N. R. Badnell 2010, *Astron. Astrophys.*, **518**, A64
Li-like: G. Y. Liang and N. R. Badnell 2011, *Astron. Astrophys.*, **528**, A69
Na-like: G. Y. Liang, A. D. Whiteford and N. R. Badnell 2009, *Astron. Astrophys.*, **500** 1263
B-like: G. Y. Liang, A. D. Whiteford and N. R. Badnell 2009, *Astron. Astrophys.*, **499**, 943

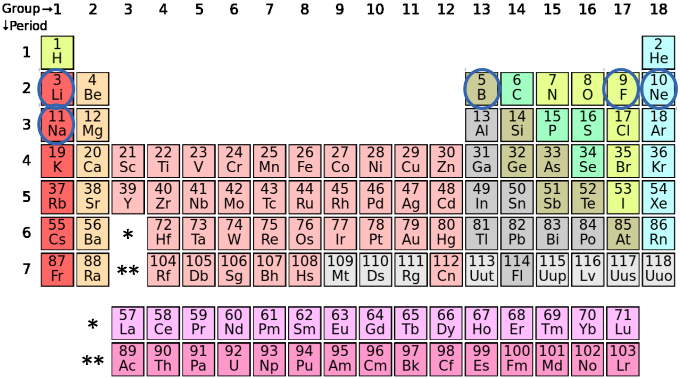
- Work is in progress in the C-, N- and O-like sequences. Then the L shell will be completed.

Sequences studied



Group→ ↓Period	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
1	1 H																	2 He
2	3 Li	4 Be											5 B	6 C	7 N	8 O	9 F	10 Ne
3	11 Na	12 Mg											13 Al	14 Si	15 P	16 S	17 Cl	18 Ar
4	19 K	20 Ca	21 Sc	22 Ti	23 V	24 Cr	25 Mn	26 Fe	27 Co	28 Ni	29 Cu	30 Zn	31 Ga	32 Ge	33 As	34 Se	35 Br	36 Kr
5	37 Rb	38 Sr	39 Y	40 Zr	41 Nb	42 Mo	43 Tc	44 Ru	45 Rh	46 Pd	47 Ag	48 Cd	49 In	50 Sn	51 Sb	52 Te	53 I	54 Xe
6	55 Cs	56 Ba	*	72 Hf	73 Ta	74 W	75 Re	76 Os	77 Ir	78 Pt	79 Au	80 Hg	81 Tl	82 Pb	83 Bi	84 Po	85 At	86 Rn
7	87 Fr	88 Ra	**	104 Rf	105 Db	106 Sg	107 Bh	108 Hs	109 Mt	110 Ds	111 Rg	112 Cn	113 Uut	114 Fl	115 Uup	116 Lv	117 Uus	118 Uuo
		*	57 La	58 Ce	59 Pr	60 Nd	61 Pm	62 Sm	63 Eu	64 Gd	65 Tb	66 Dy	67 Ho	68 Er	69 Tm	70 Yb	71 Lu	
		**	89 Ac	90 Th	91 Pa	92 U	93 Np	94 Pu	95 Am	96 Cm	97 Bk	98 Cf	99 Es	100 Fm	101 Md	102 No	103 Lr	

Sequences studied



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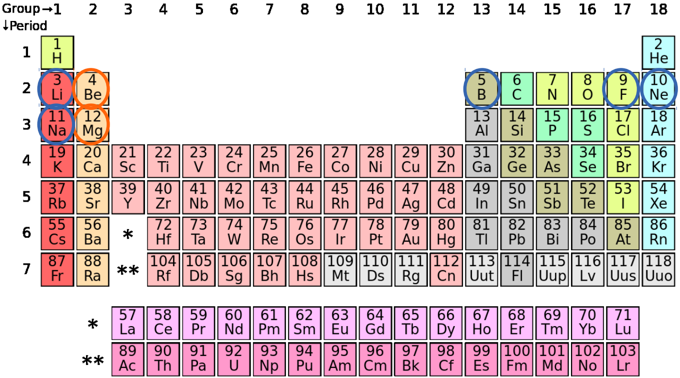

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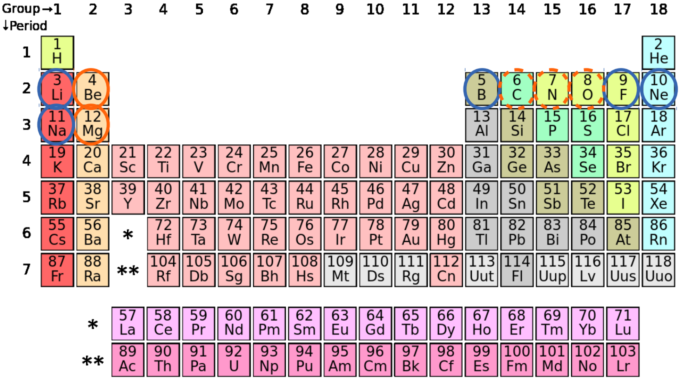

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Acknowledgement

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L. Fernández-Menchero, G. Del Zanna and N. R. Badnell 2014 *Astron. Astrophys.* **566**, A104.

L. Fernández-Menchero, G. Del Zanna and N. R. Badnell 2014 *Astron. Astrophys.* **572**, A115. *R*-matrix electron-impact excitation data for the Mg-like iso-electronic sequence

G. Del Zanna, L. Fernández-Menchero and N. R. Badnell 2015 *Astron. Astrophys.* **574**, A99. Benchmarking atomic Data for Astrophysics: Si III