Queen's University Belfast

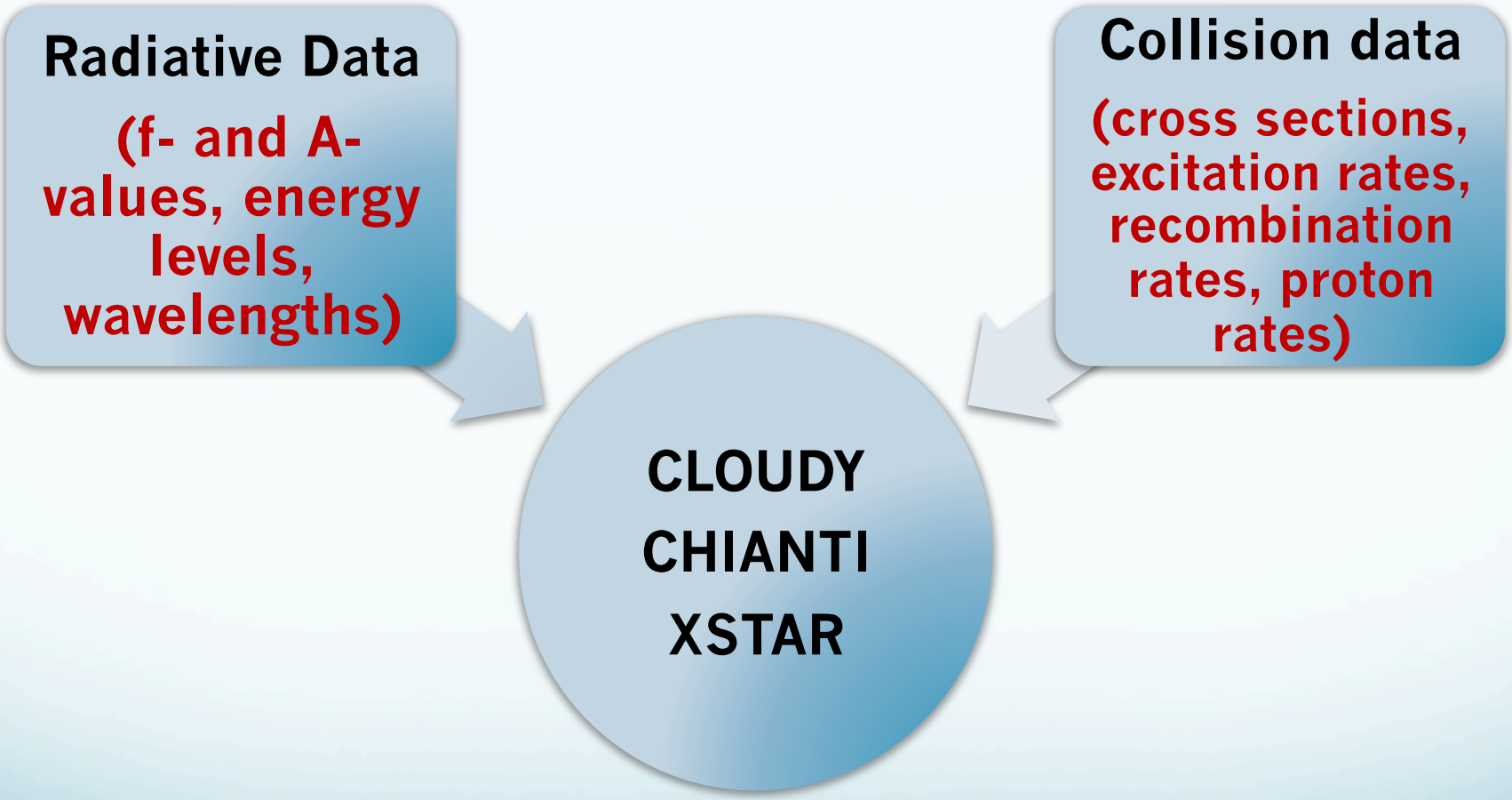
A Selection of Atomic Collision Calculations from QUB

Dr Cathy Ramsbottom

The Group

- Cathy Ramsbottom (QUB)
- Connor Ballance (QUB)
- Alan Hibbert (QUB)
- Phil Burke (Daresbury)
- Val Burke (Daresbury)
- Sibasish Laha
- Niall Tyndall
- Stefan Spencer
- Michael Turkington

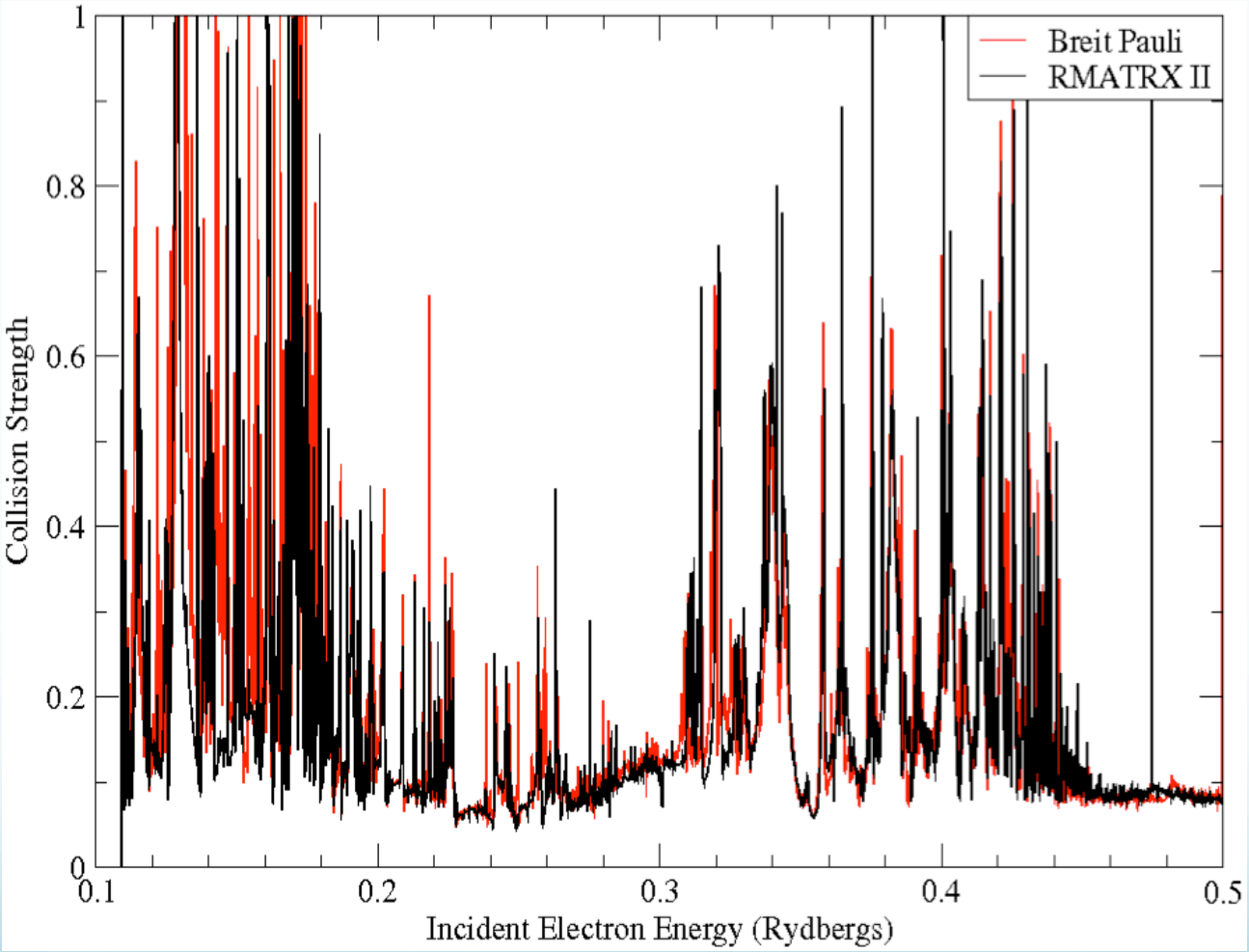
Modelling


Radiative Data
(f- and A-values, energy levels, wavelengths)
Collision data
(cross sections, excitation rates, recombination rates, proton rates)
CLOUDY
CHIANTI
XSTAR

R-matrix Methodologies:

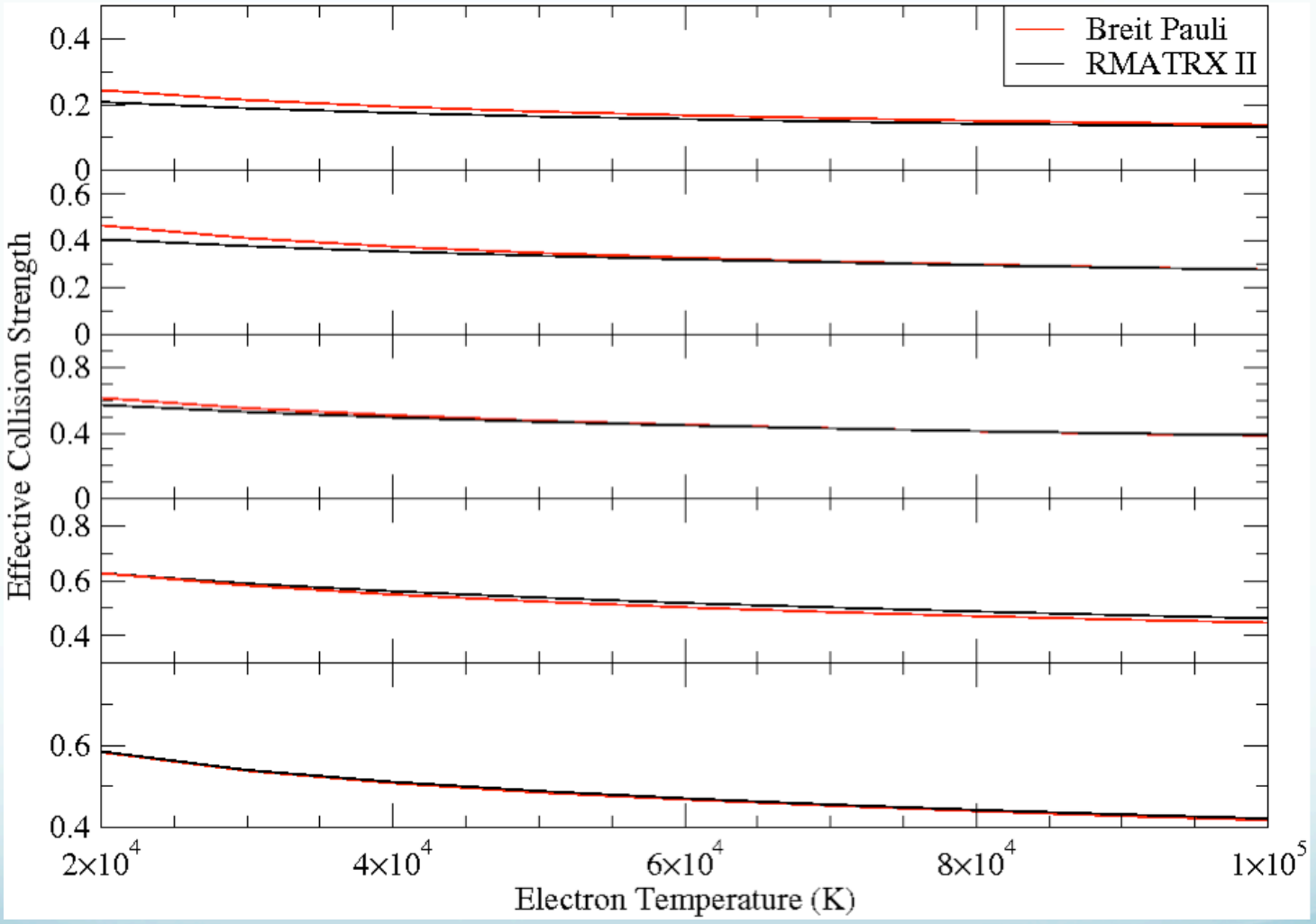
- RMATRX I (LS coupling)
- BP RMATRX I
- DARC
- RMATRX II (LS + transformation)
- ICFT (LS + transformation)
- B-spline R-Matrix BSR

Cr II $3d^5\ ^6S_{5/2} - 3d^4 4s\ ^6D_{1/2}$



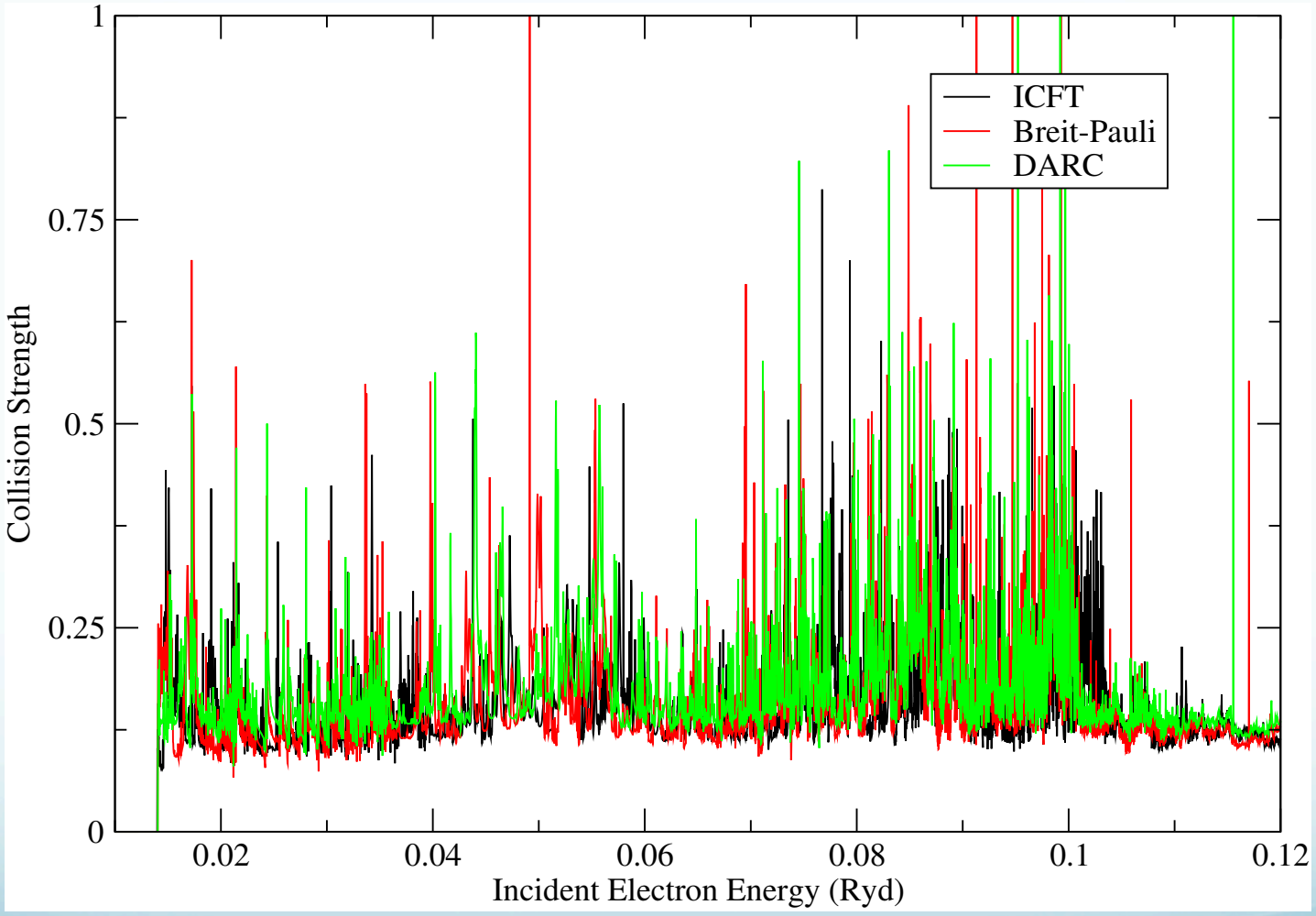
Wasson IR, Ramsbottom CA & Scott MP, 2010, a&A, 524,A35

Cr II $3d^5\ ^6S_{5/2}$ – $3d^4 4s\ ^6D_{1/2,3/2,5/2,7/2,9/2}$



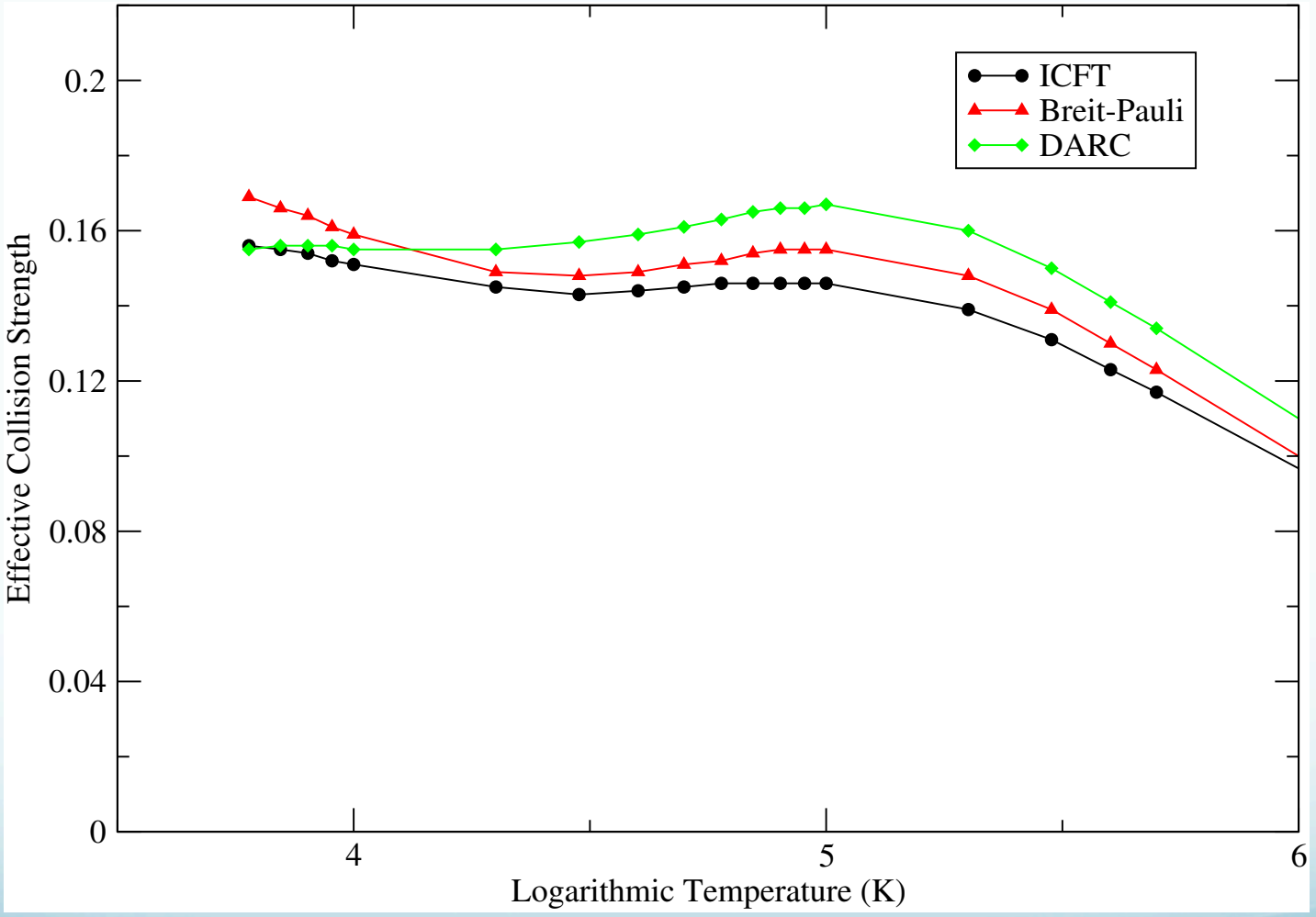
Wasson IR, Ramsbottom CA & Scott MP, 2010, a&A, 524,A35

Mn V $3d^3\ ^4F_{3/2} - 3d^3\ ^2D2_{5/2}$



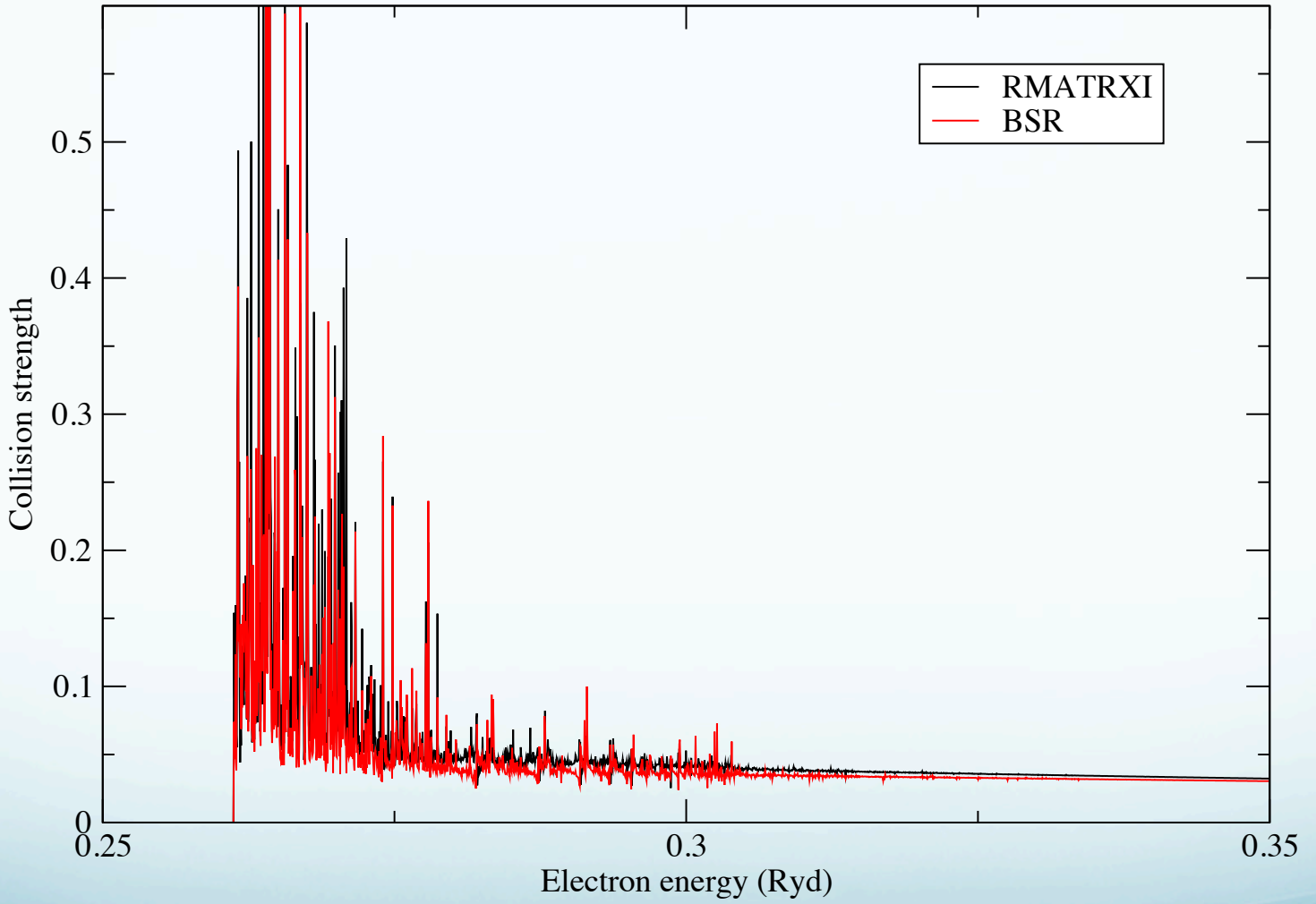
Grieve MFR, Ramsbottom CA, Hibbert A, Ferland G & Keenan FP, in preparation

Mn V $3d^3\ {}^4F_{3/2} - 3d^3\ {}^2D2_{5/2}$



Grieve MFR, Ramsbottom CA, Hibbert A, Ferland G & Keenan FP, in preparation

Mg VIII $2s^2 2p\ ^2P^o_{1/2} - 2p^3\ ^2P^o_{3/2}$



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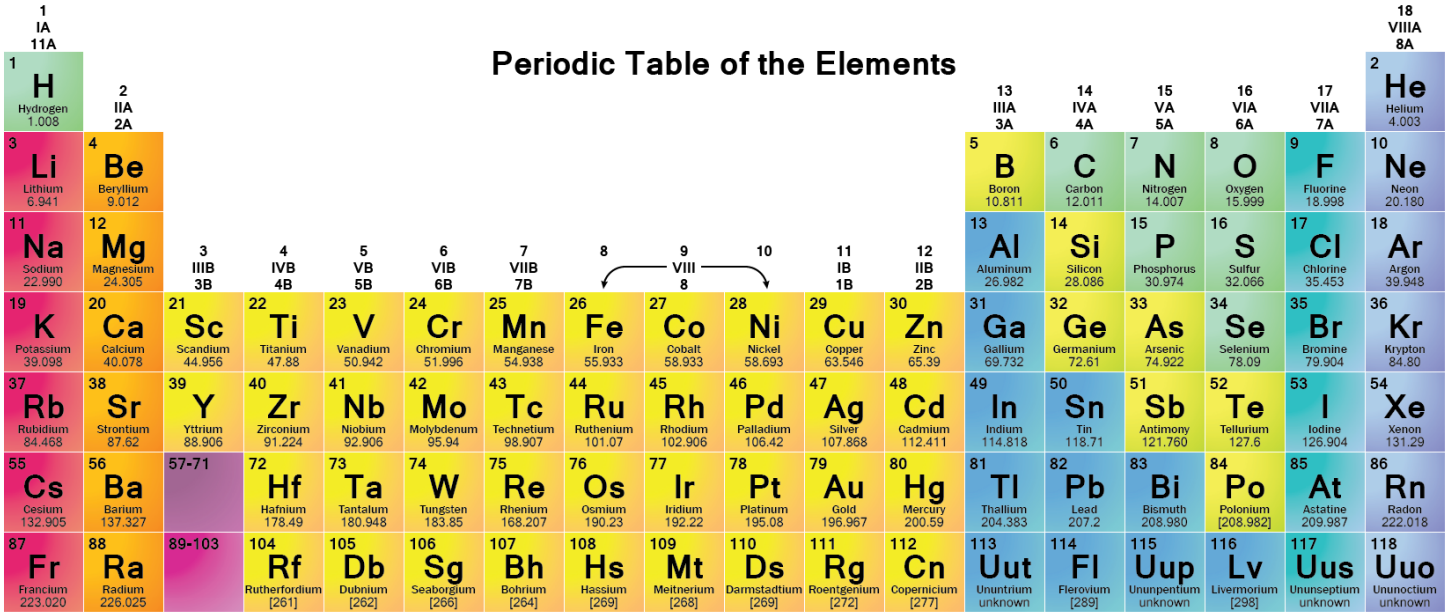
Electron-impact excitation of W XLV

Atomic Data

- Energy Levels
- Electron impact excitation collision strengths
- Maxwellian averaged effective collision strengths

Periodic Table of the Elements



W XLV (Z=74: NELC=30)

$1s^2 2s^2 2p^6 3s^2 3p^6 3d^{10} 4s^2$

$1s^2 2s^2 2p^6 3s^2 3p^6 3d^{10} 4s4p$

$1s^2 2s^2 2p^6 3s^2 3p^6 3d^{10} 4p^2$

$1s^2 2s^2 2p^6 3s^2 3p^6 3d^{10} 4s4d$

$1s^2 2s^2 2p^6 3s^2 3p^6 3d^{10} 4p4d$

$1s^2 2s^2 2p^6 3s^2 3p^6 3d^{10} 4s4f$

$1s^2 2s^2 2p^6 3s^2 3p^6 3d^{10} 4p4f$

$1s^2 2s^2 2p^6 3s^2 3p^6 3d^{10} 4d^2$

$1s^2 2s^2 2p^6 3s^2 3p^6 3d^{10} 4d4f$ → 35au

W XLV
(Z=74: NELC=30)

$1s^2 2s^2 2p^6 3s^2 3p^6 3d^9 4s^2 4p$

$1s^2 2s^2 2p^6 3s^2 3p^6 3d^9 4s^2 4d$

$1s^2 2s^2 2p^6 3s^2 3p^6 3d^9 4s 4p^2$

$1s^2 2s^2 2p^6 3s^2 3p^6 3d^9 4s 4d^2$

$1s^2 2s^2 2p^6 3s^2 3p^6 3d^9 4s^2 4f$

➔ **89 au**

W XLV Models

Present Breit-Pauli:

14 configs: listed including $3d^9$ open core terms

10 orbitals: up to n=4 including 4f. All non-relativistic and orthogonal produced with CIV3

311 Jπ levels: fully inclusive

Fine mesh of incident electron energies 10^{-6} scaled Ryds (12 000 points)

Radiation Damping Included (Type I)

Top-up of high partial waves included

W XLV Models

Ballance & Griffin 2007 (BG07):

Fully relativistic DARC calculation

22 configs: not including $3d^9$ open core terms

15 orbitals: up to n=5. Relativistic and produced with GRASP0

168 Jπ levels: not inclusive

Fine mesh of incident electron energies 10^{-6} scaled Ryds (40 000 points)

Radiation Damping Included (Type I + II)

Top-up of high partial waves included

W XLV Models

Bluteau, O Mullane & Badnell 2015 (BOMB15):

Fully relativistic DARC calculation

13 configs: listed already including $3d^9$ open core terms. Exactly same $3d^{10}$ configs, add $3d^9 4s4p4d$, neglect $3d^9 4s4p^2$ and $3d^9 4s4d^2$

10 orbitals: up to n=4 including 4f. Relativistic and produced with GRASP0

313 Jπ levels: inclusive

Fine mesh of incident electron energies 10^{-6} scaled Ryds (48 000 points)

Radiation Damping Included (Type I)

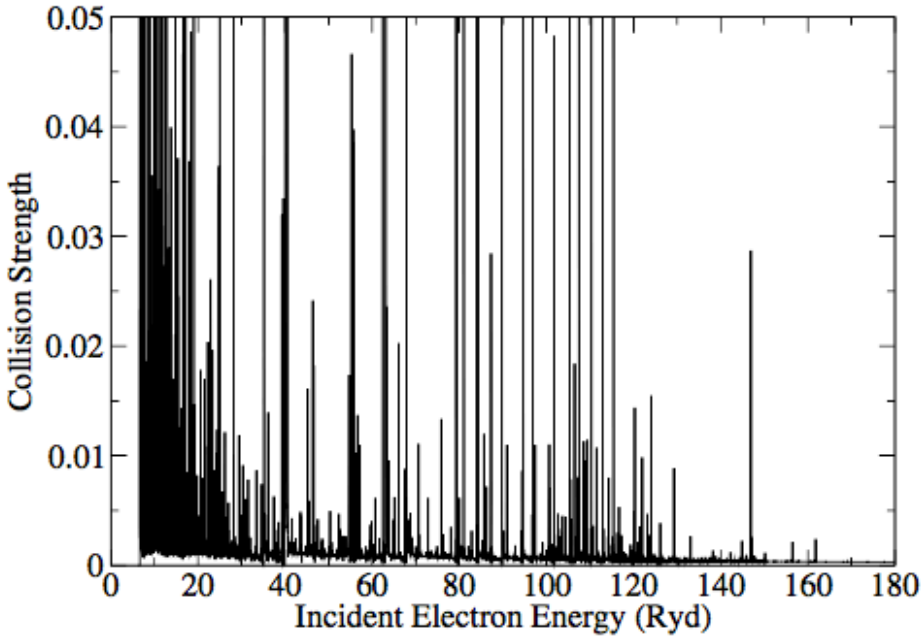
Top-up of high partial waves included

W XLV Energy Levels in au

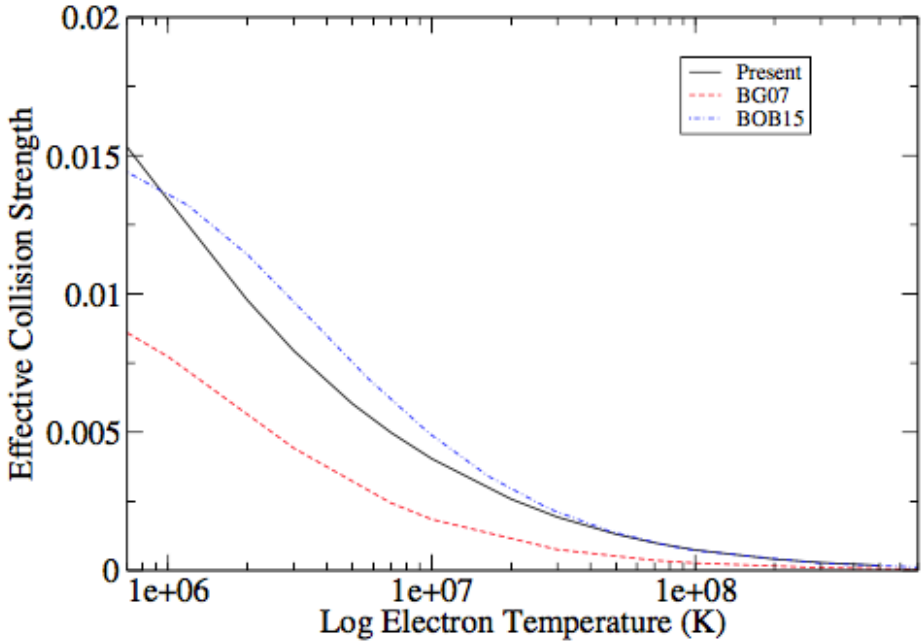
Index	Level		Present	NIST[a]	BG[b]	Q[c]	SS[d]	F[e]	VI[f]
1	$4s^2$	$^1S_0$	0.000	0.000	0.000	0.000	0.000	0.000	0.000
2	4s4p	$^3P^o_0$	3.165	3.167	3.175	3.170	3.175	3.187	3.173
3	4s4p	$^3P^o_1$	3.423	3.429	3.445	3.436	3.428	3.450	3.425
4	4s4p	$^3P^o_2$	6.833	6.809	6.887	6.844	6.859	6.860	6.853
5	$4p^2$	$^3P_0$	7.246	7.236	7.306	7.290	7.242		7.236
6	4s4p	$^1P^o_1$	7.486	7.478	7.552	7.509	7.481	7.511	7.474
7	$4p^2$	$^3P_1$	10.687	10.688	10.777	10.726	12.674		10.688
8	$4p^2$	$^1D_2$	10.752	10.765	10.825	10.771	13.659		10.743
9	4s4d	$^3D_1$	12.976	12.679	12.764	12.699	10.697		12.670
10	4s4d	$^3D_2$	13.086	12.801	12.895	12.827	10.752	12.861	12.794
11	4s4d	$^3D_3$	13.709	13.413	13.554	13.470	13.452	13.499	13.446
12	4s4d	$^1D_2$	13.840	13.617	13.761	13.678	12.799	13.716	13.652
13	$4p^2$	$^3P_2$	14.690	14.630	14.761	14.676	14.631	14.725	14.619
14	$4p^2$	$^1S_0$	14.813	14.804	14.933	14.848	14.815		14.802
15	4p4d	$^3F^o_2$	16.314		16.116		19.980		16.015

Index	Level	Pres BP	NIST	BG07	BOMB15
1	$4s^2\ ^1S_0$	0.000	0.000	0.000	0.000
2	$4s4p\ 3P^o_0$	3.165	3.167	3.175	3.174
3	$4s4p\ 3P^o_1$	3.423	3.429	3.445	3.440
4	$4s4p\ 3P^o_2$	6.833	6.809	6.887	6.882
5	$4p^2\ ^3P_0$	7.246	7.236	7.306	7.337
6	$4s4p\ 1P^o_1$	7.486	7.478	7.552	7.539
7	$4p^2\ ^3P_1$	10.687	10.688	10.777	10.800
8	$4p^2\ ^1D_2$	10.752	10.765	10.825	10.848
9	$4s4d\ ^3D_1$	12.976	12.679	12.764	12.790
10	$4s4d\ ^3D_2$	13.086	12.801	12.895	12.921
11	$4s4d\ ^3D_3$	13.709	13.413	13.554	13.579
12	$4s4d\ ^1D_2$	13.840	13.617	13.761	13.786
13	$4p^2\ ^3P_2$	14.690	14.630	14.761	14.785
14	$4p^2\ ^1S_0$	14.813	14.804	14.933	14.960
15	$4p4d\ 3F^o_2$	16.314	-	16.116	16.142
16	$4p4d\ 3D^o_1$	16.927	-	16.767	16.797
17	$4p4d\ 3F^o_3$	17.383	-	17.256	17.283

W XLV 1-2



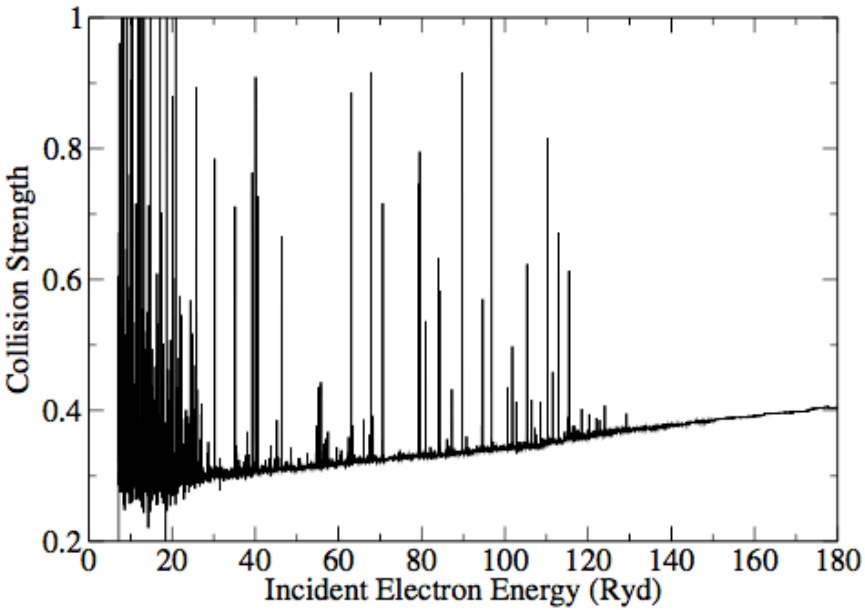
(a) 1-2 Collision Strength



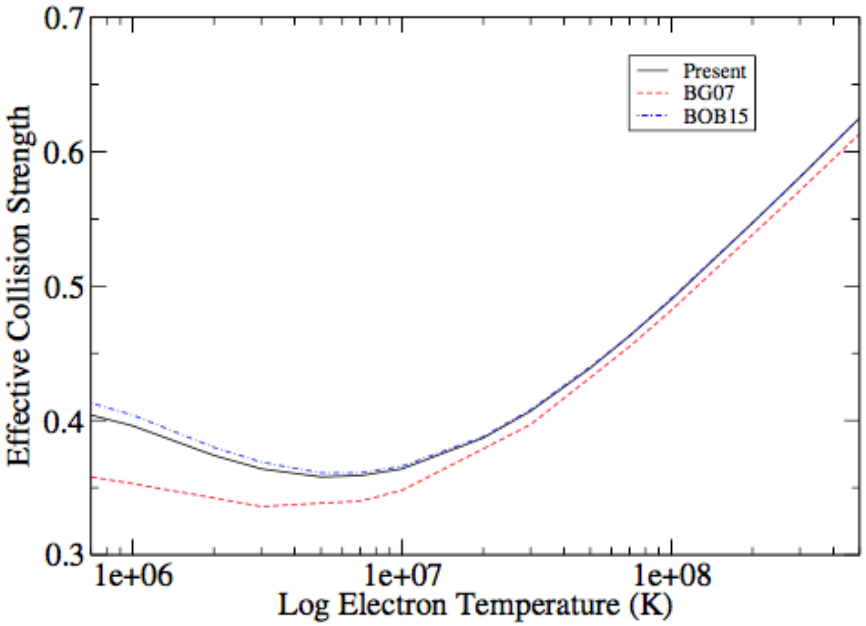
(b) 1-2 Effective Collision Strength

BP Present
BG07
BOMB15

W XLV 1-3



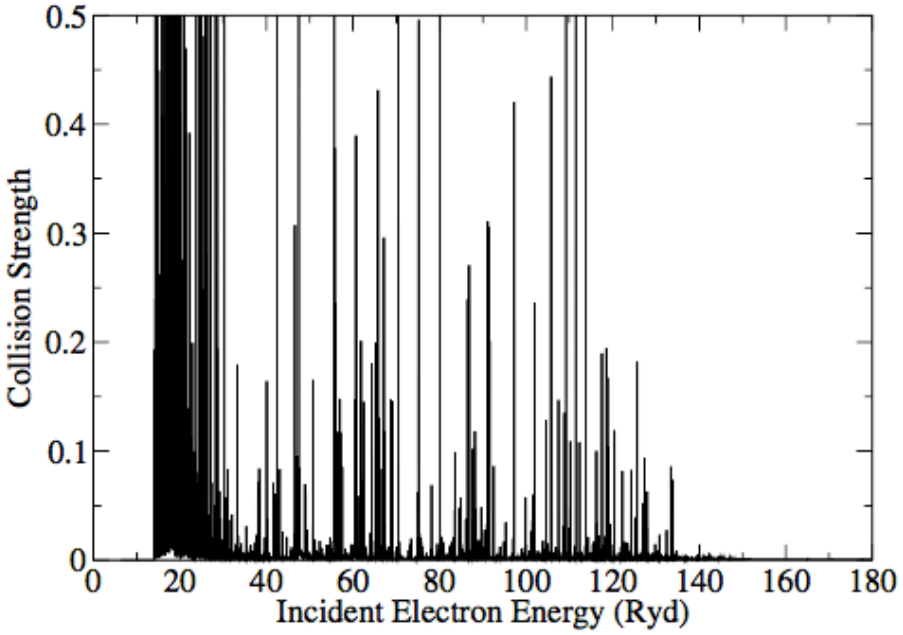
(c) 1-3 Collision Strength



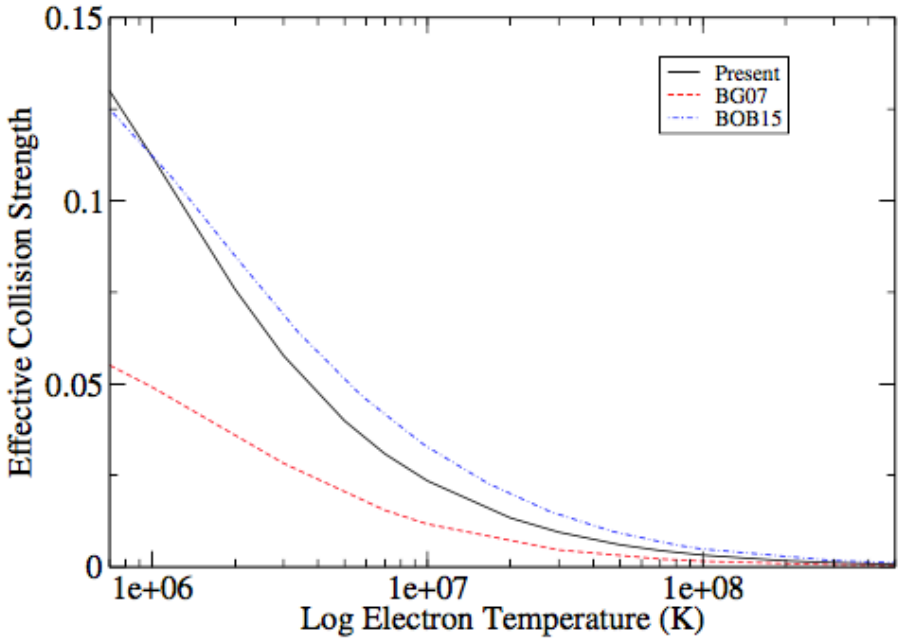
(d) 1-3 Effective Collision Strength

BP Present
BG07
BOMB15

W XLV 1-4



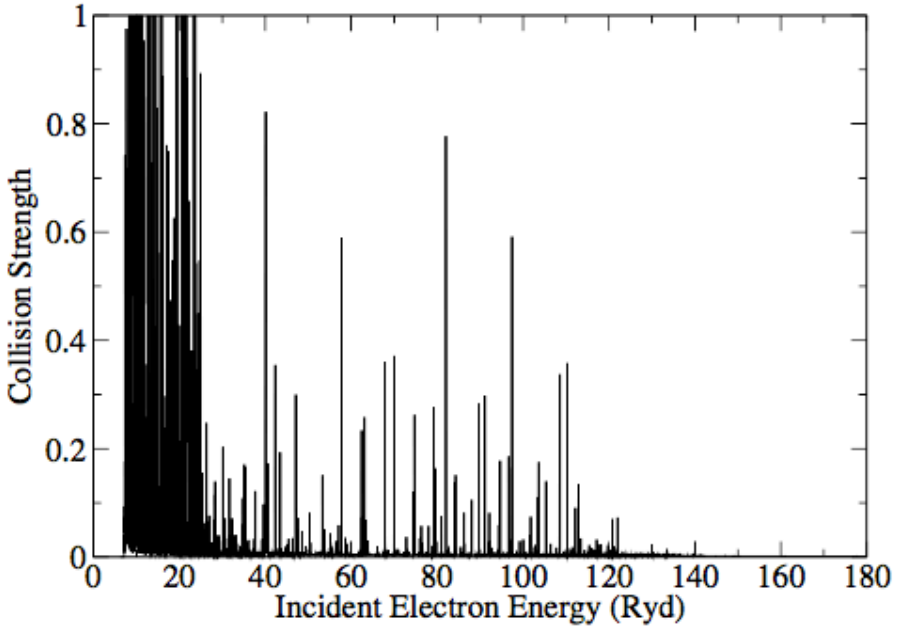
(e) 1-4 Collision Strength



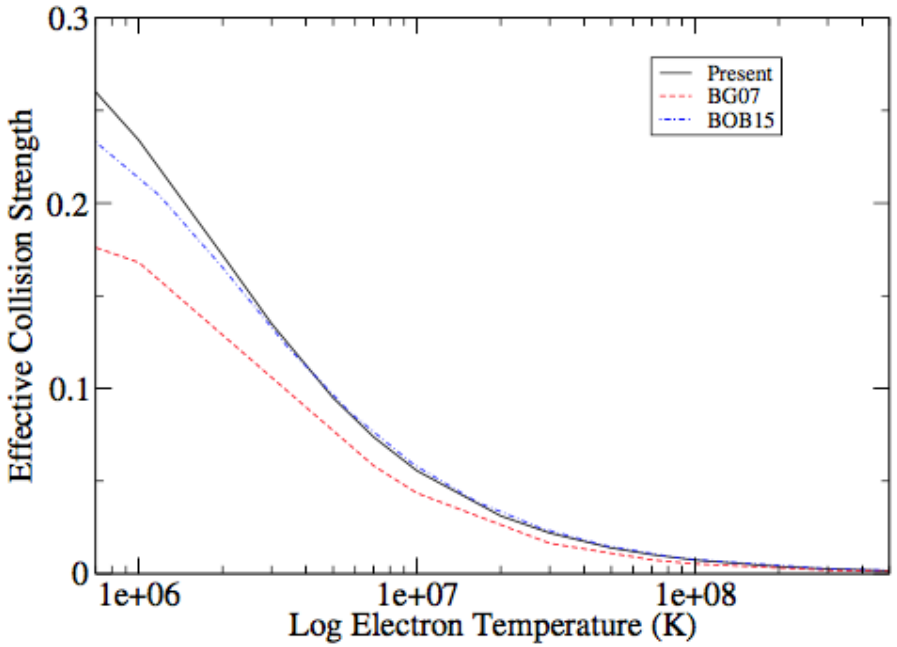
(f) 1-4 Effective Collision Strength

BP Present
BG07
BOMB15

W XLV 2-3



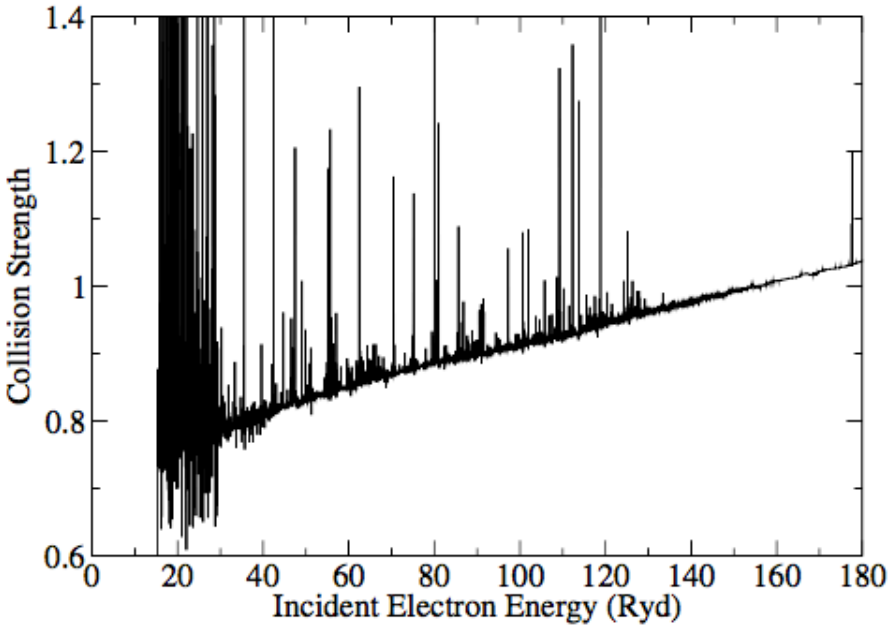
(g) 2-3 Collision Strength



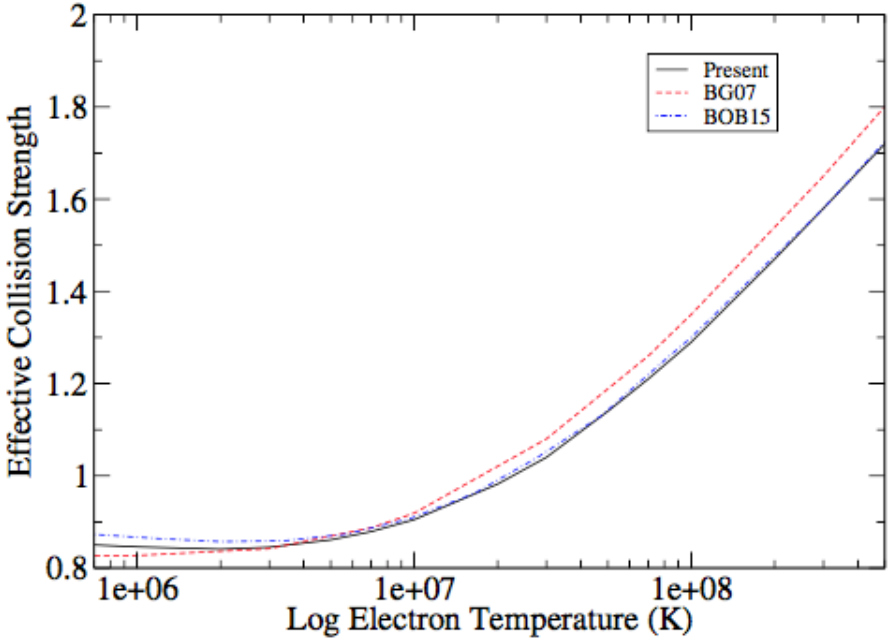
(h) 2-3 Effective Collision Strength

BP Present
BG07
BOMB15

W XLV
1-6



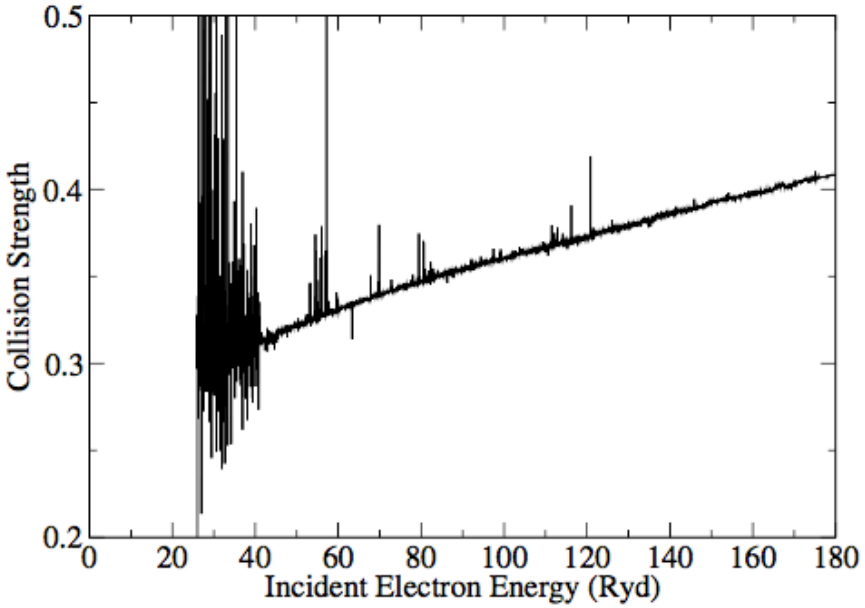
(i) 1-6 Collision Strength



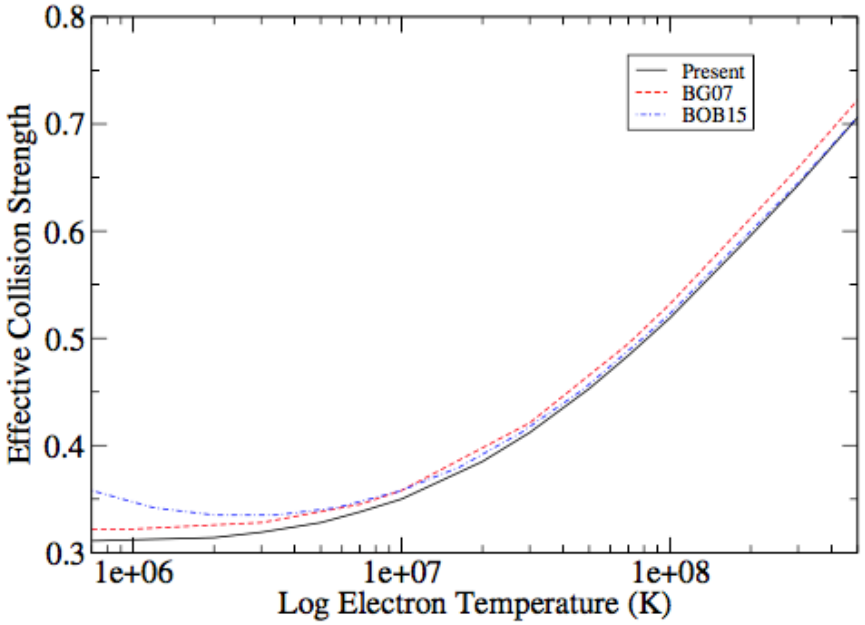
(j) 1-6 Effective Collision Strength

BP –present
BG07
BOMB15

W XLV
2-9



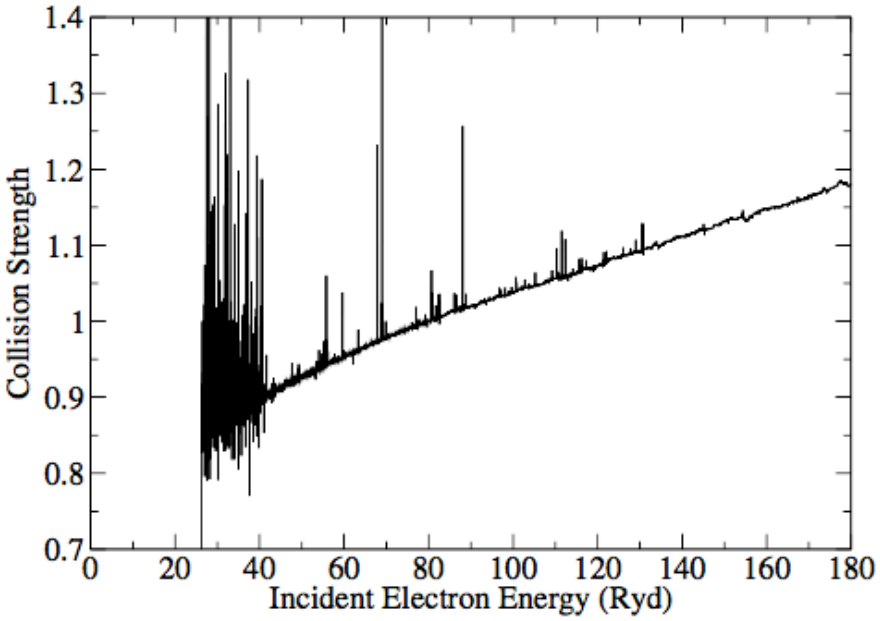
(k) 2-9 Collision Strength



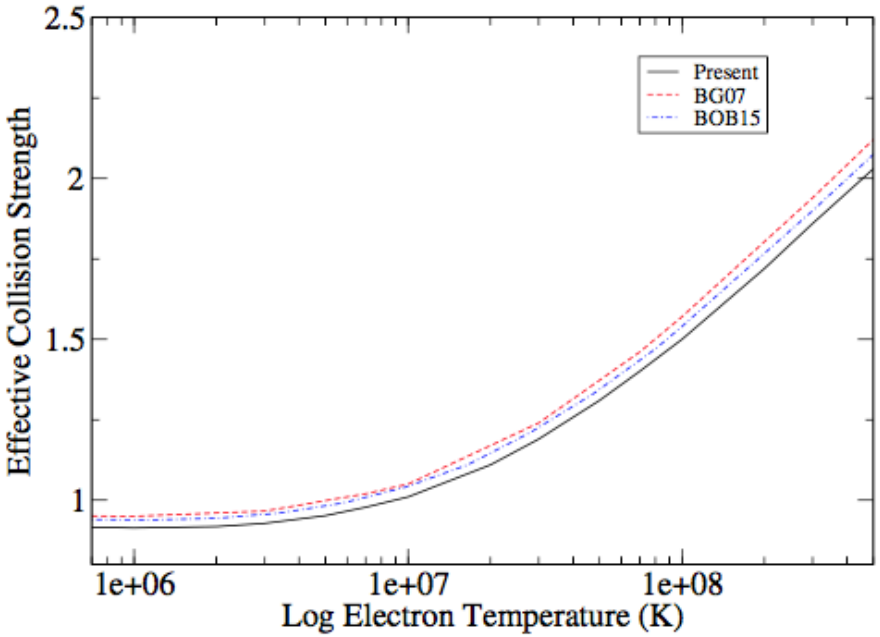
(l) 2-9 Effective Collision Strength

BP –present
BG07
BOMB15

W XLV 3-10



(m) 3-10 Collision Strength



(n) 3-10 Effective Collision Strength

BP –present
BG07
BOMB15

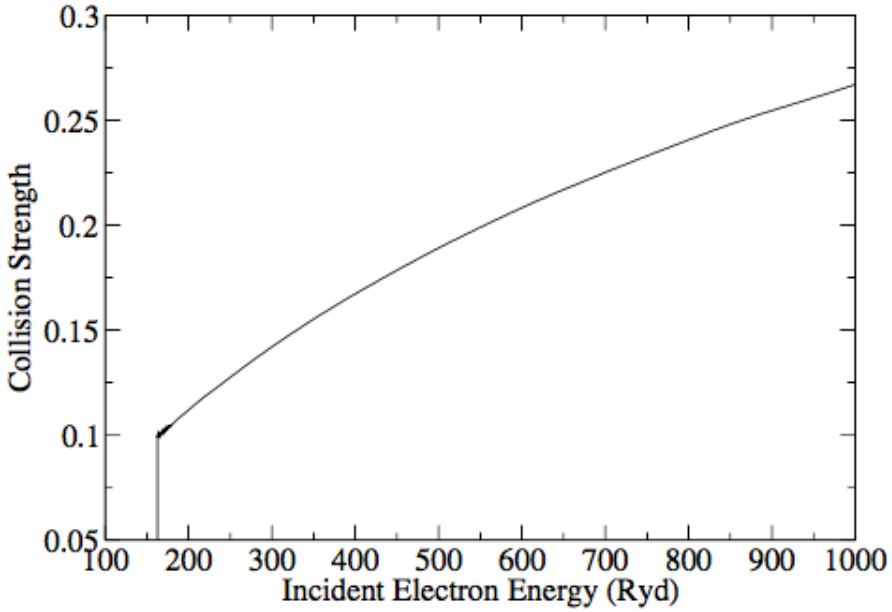
Strong Dipole Transition

$3d^{10}4s^2\ {}^1S_0 - 3d^9 4s^2 4f\ {}^1P^o_1$

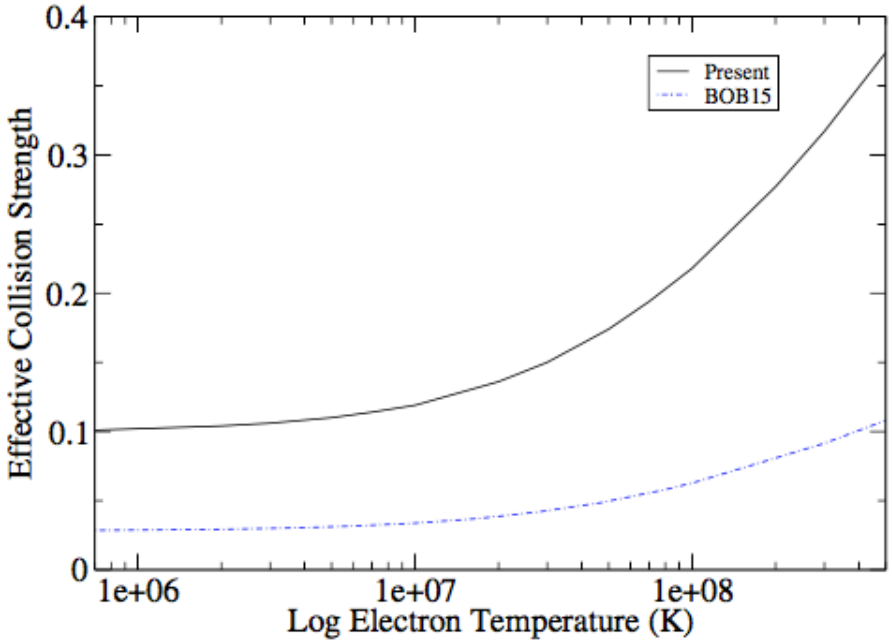
1-177 (f_i=3.109, A_{ij}=2.205x10^{14})

Index	Level		Contr. %	Energy (a.u.)	Index	Level		Contr. %	Energy (a.u.)
158	$4s^24f$	$^3P^o_0$	100	77.6166	175	$4s^24f$	$^3D^o_3$	37	80.6121
159	$4s^24f$	$^3P^o_1$	75	77.7227		$4s^24f$	$^1F^o_3$	24	
	$4s^24f$	$^3D^o_1$	25		176	$4s^24f$	$^3G^o_4$	46	80.6649
160	$4s^24f$	$^3H^o_5$	53	77.8745		$4s^24f$	$^1G^o_4$	30	
	$4s^24f$	$^1H^o_5$	44			$4s^24f$	$^3F^o_4$	23	
161	$4s^24f$	$^3D^o_2$	56	77.9015	177	$4s^24f$	$^1P^o_1$	78	81.3494
	$4s^24f$	$^3P^o_2$	29			$4s^24f$	$^3D^o_1$	15	
	$4s^24f$	$^3F^o_2$	15		178	$4s4d^2$	$^5D_2$	35	83.5747
162	$4s^24f$	$^3F^o_3$	56	78.0210		$4s4d^2$	$^5F_2$	21	
	$4s^24f$	$^3D^o_3$	26			$4s4d^2$	$^5P_2$	13	
	$4s^24f$	$^3G^o_3$	13		179	$4s4d^2$	$^5P_1$	45	83.5820
163	$4s^24f$	$^3H^o_5$	100	78.0413		$4s4d^2$	$^5D_1$	34	
164	$4s^24f$	$^3G^o_4$	51	78.0612	180	$4s4d^2$	$^5F_3$	26	83.6167
	$4s^24f$	$^1G^o_4$	22			$4s4d^2$	$^5D_3$	18	
	$4s^24f$	$^3F^o_4$	15			$4s4d^2$	$^5G_3$	14	

W XLV
1-177



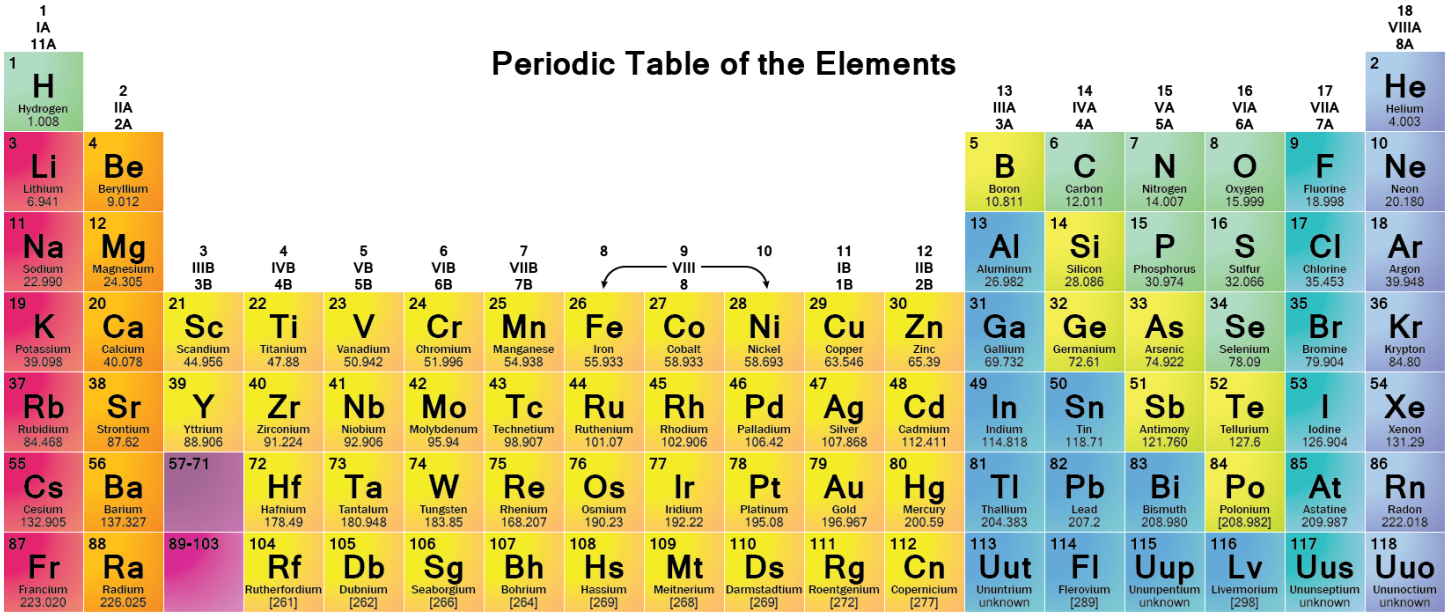
(o) 1-177 Collision Strength



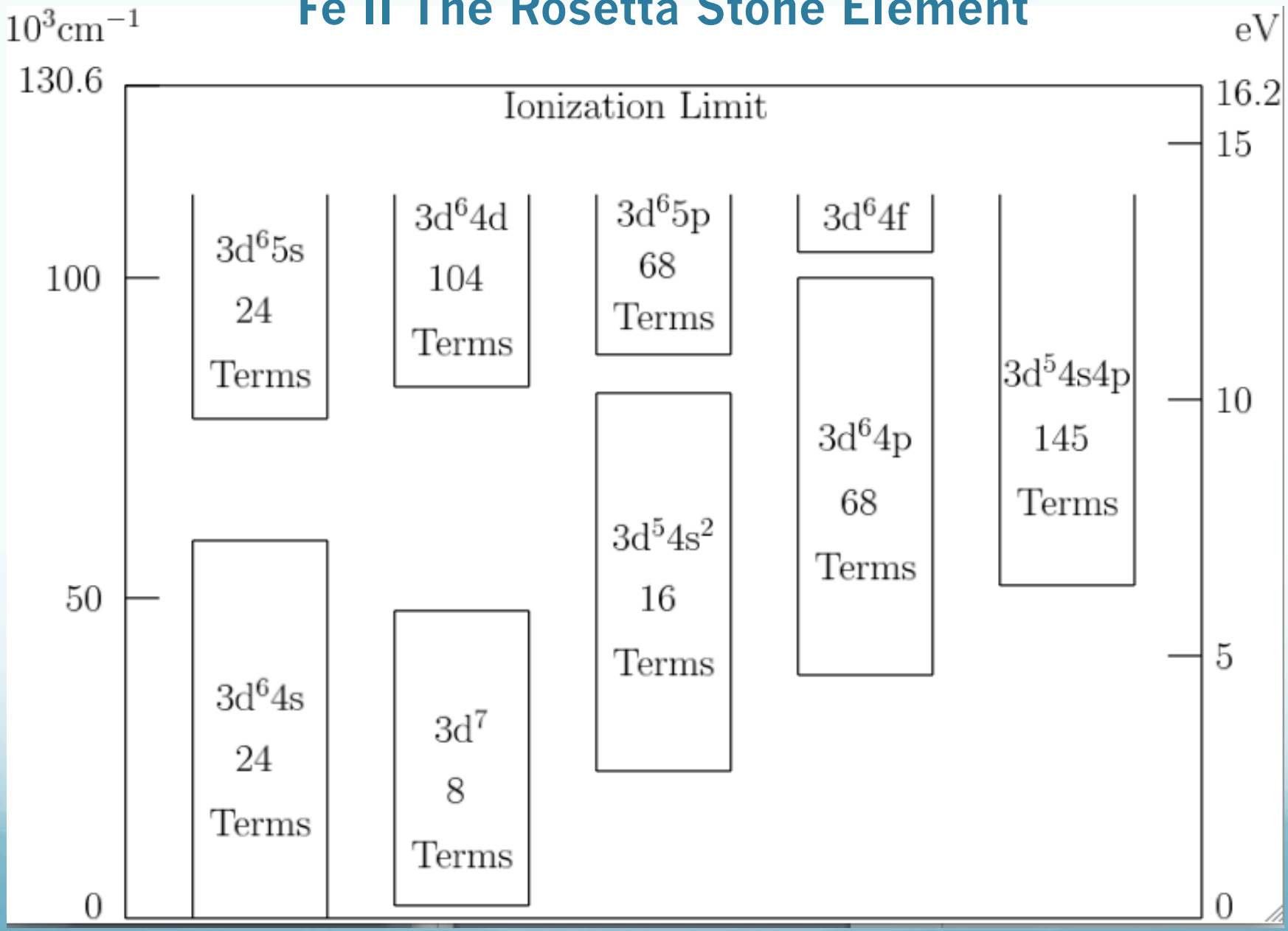
(p) 1-177 Effective Collision Strength

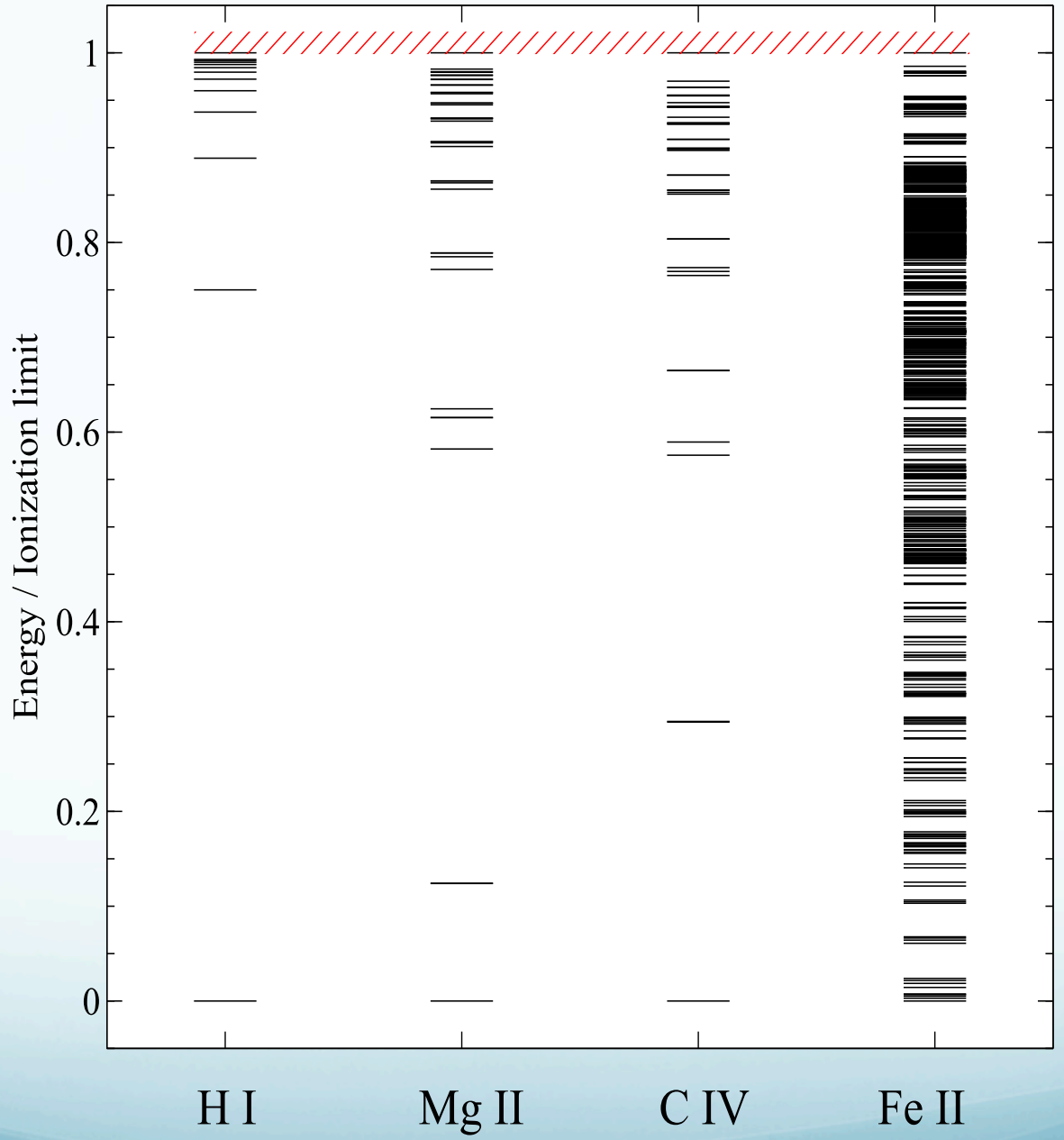
BP –present
BOMB15

Periodic Table of the Elements



Fe II The Rosetta Stone Element




Energy / Ionization limit
1
0.8
0.6
0.4
0.2
0
H I
Mg II
C IV
Fe II

Model	LSπ		Jπ	
No. Configs	States	Channels	States	Channels
1	24	72	63	420
2	32	98	82	540
3	100	315	262	1800
4	116	363	299	2052
5	261	805	716	5076
6	285	877	779	5496
7	389	1239	1055	7596

No. Target States	Max No. Channels	Max size (N+1) H matrix	Total No. Transitions
100 (LSπ)	315	12 660	5050
262 (Jπ)	1800	36 055	34 453
716 (Jπ)	5076	> 100 000	256 686

Model	LSπ		Jπ	
No. Configs	States	Channels	States	Channels
1	24	72	63	420
2	32	98	82	540
3	100	315	262	1800
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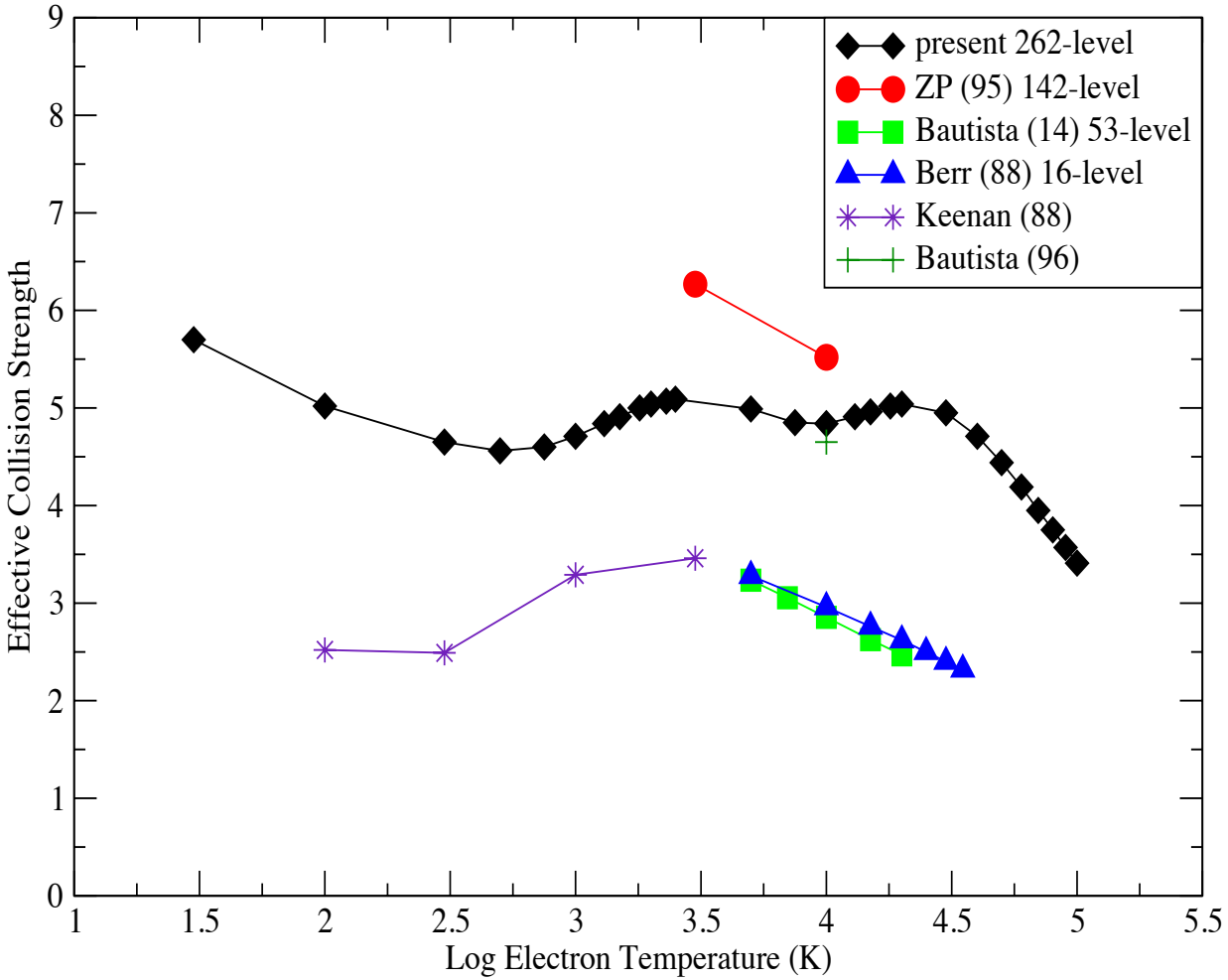
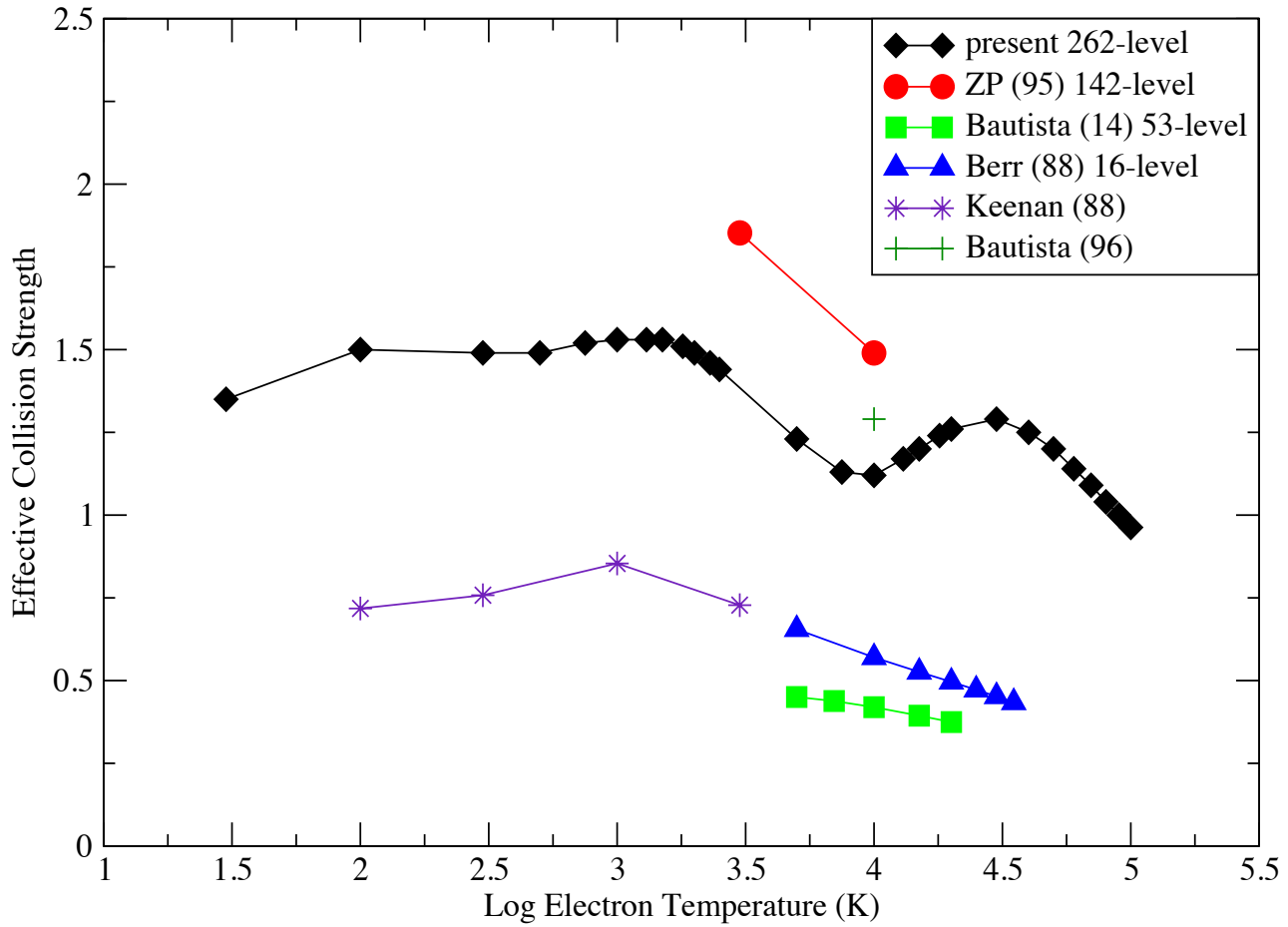
100 (LSπ)	315	12 660	5050
262 (Jπ)	1800	36 055	34 453
716 (Jπ)	5076	> 100 000	256 686

Fe II $3d^6 4s\ {}^6D_{9/2} - 3d^6 4s\ {}^6D_{7/2}$



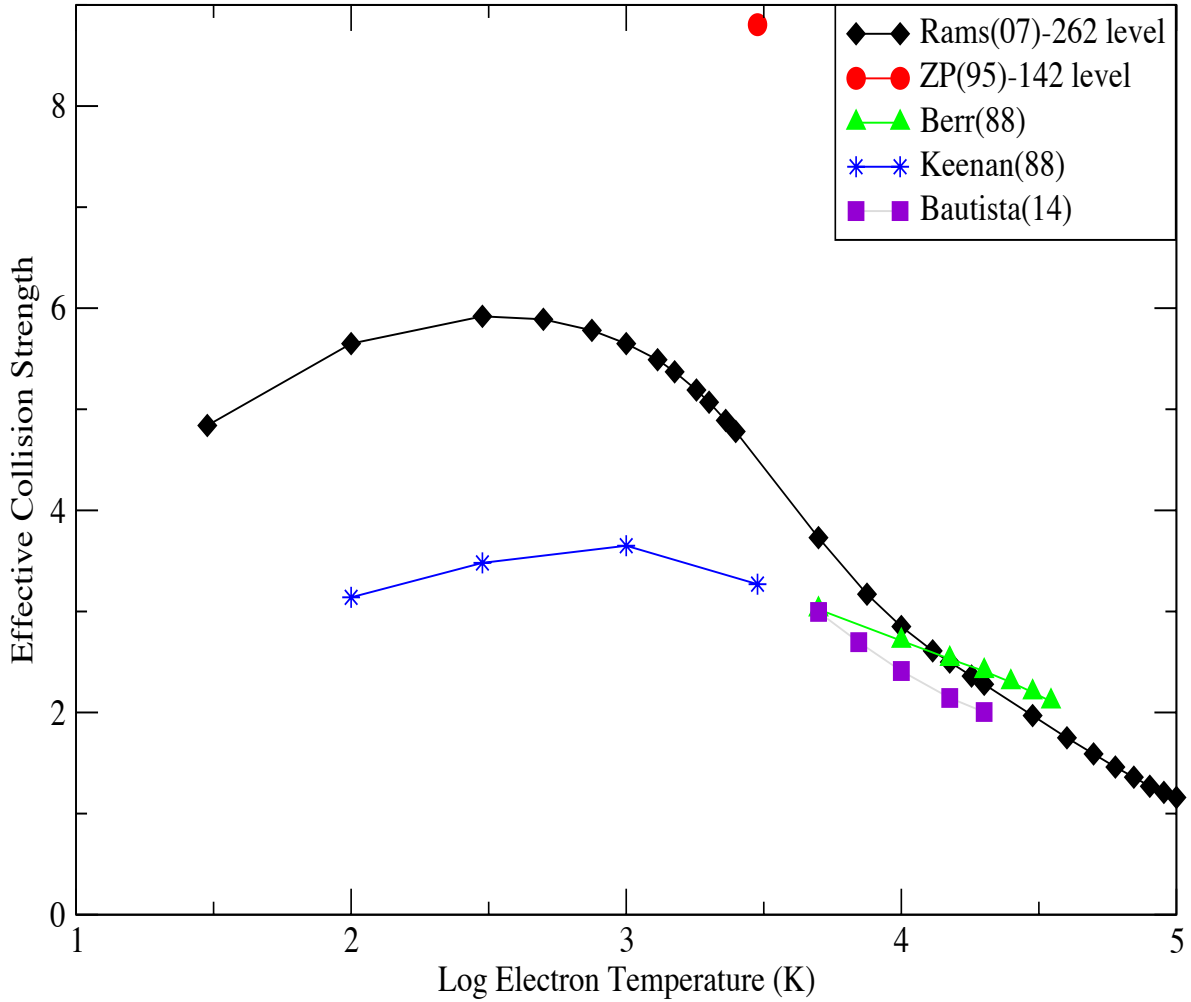
Ramsbottom CA, Hudson CE, Norrington PH & Scott MP, 2007, A&A, 475, 765

Fe II $3d^6 4s\ {}^6D_{9/2} - 3d^6 4s\ {}^6D_{5/2}$

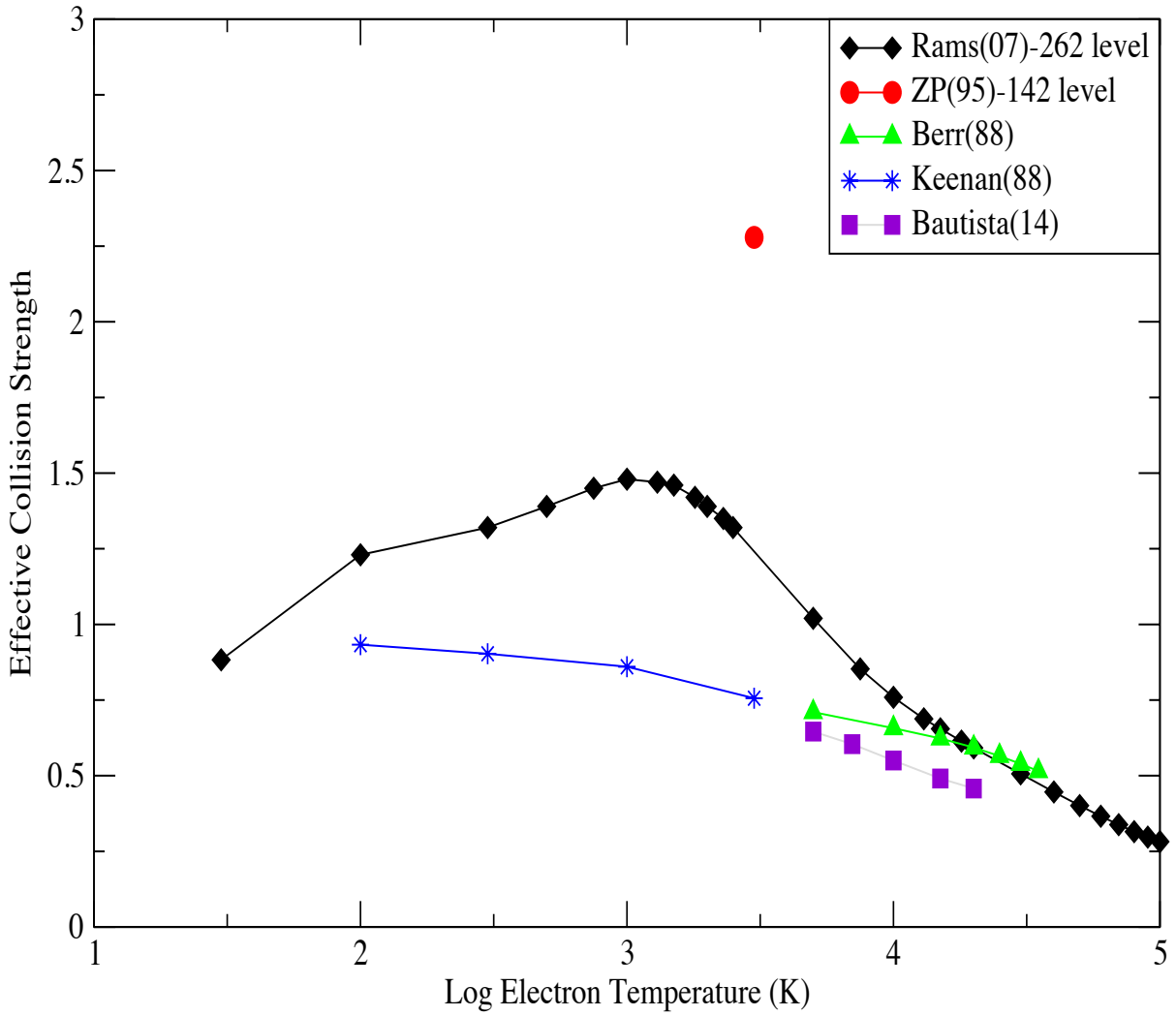


Ramsbottom CA, Hudson CE, Norrington PH & Scott MP, 2007, A&A, 475, 765

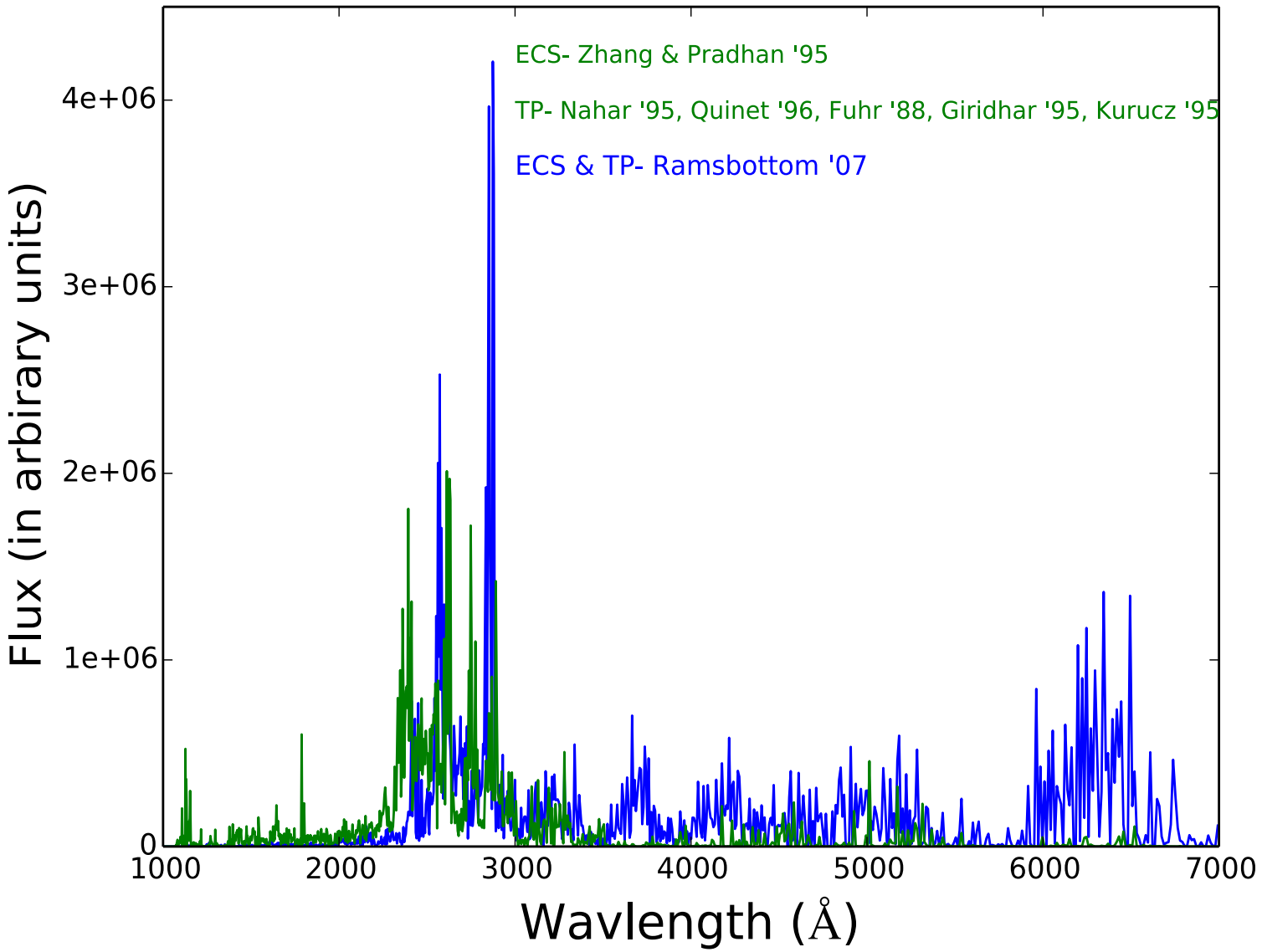
Fe II Transition 6-7



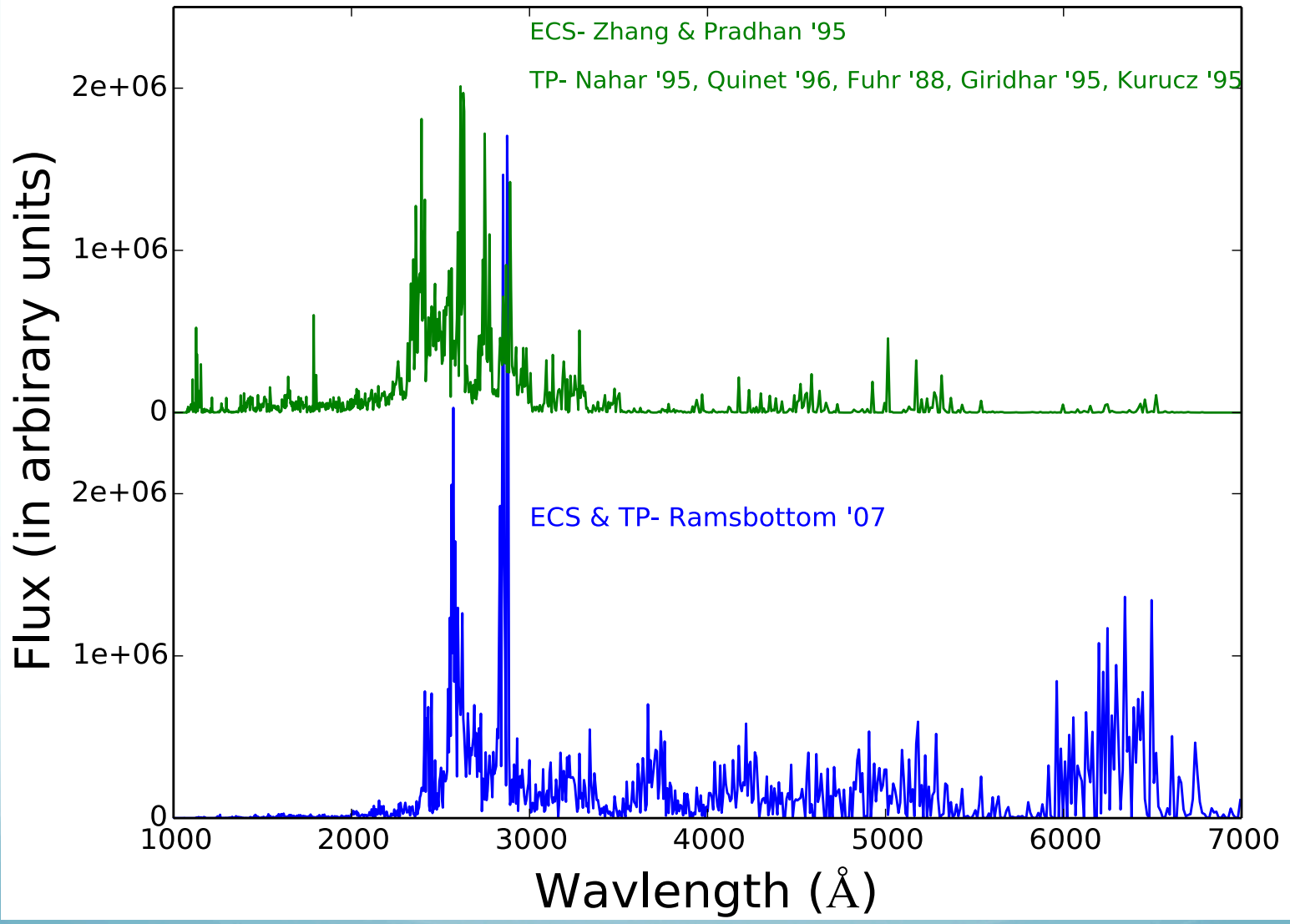
Fe II Transition 7-9



Cloudy Models



Cloudy Models



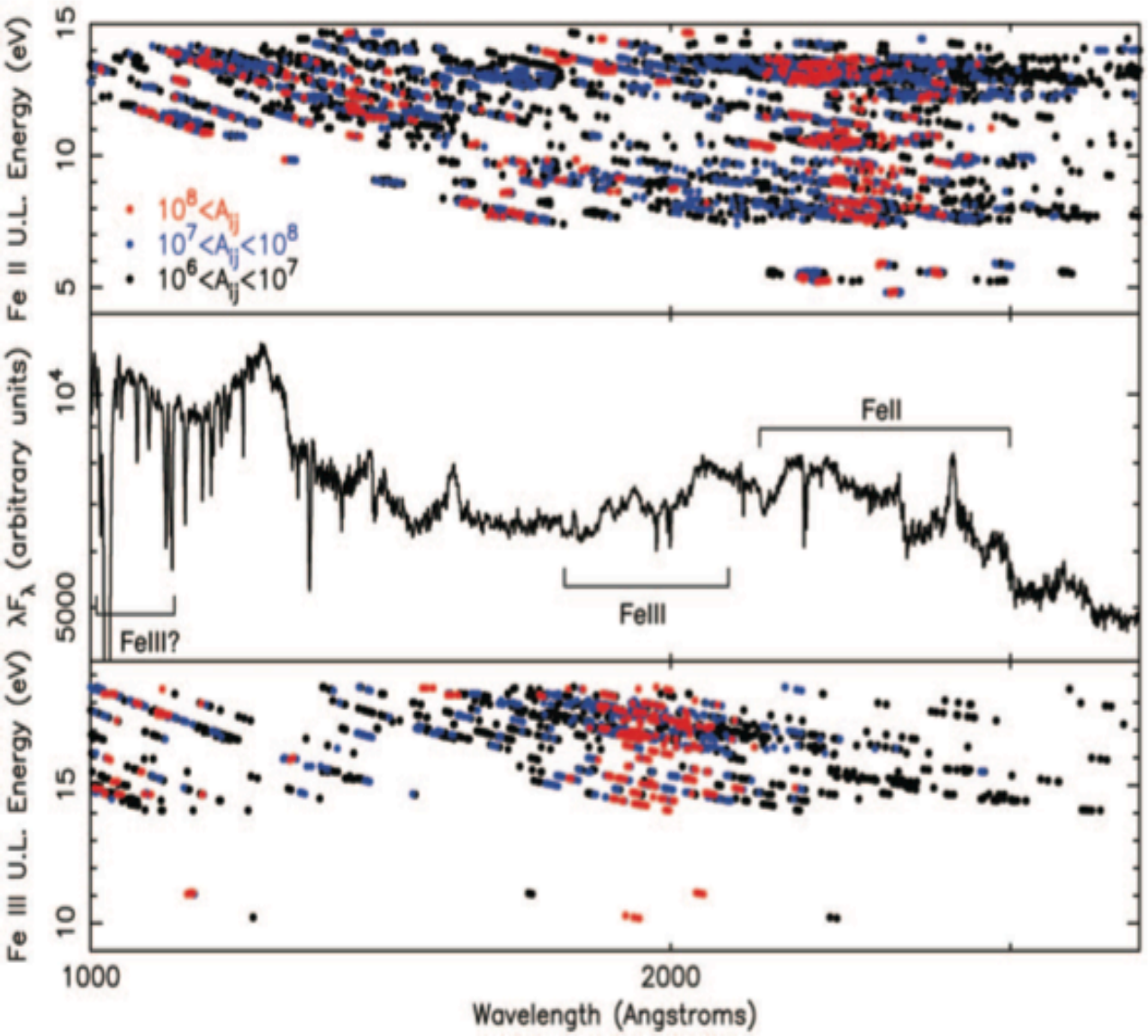
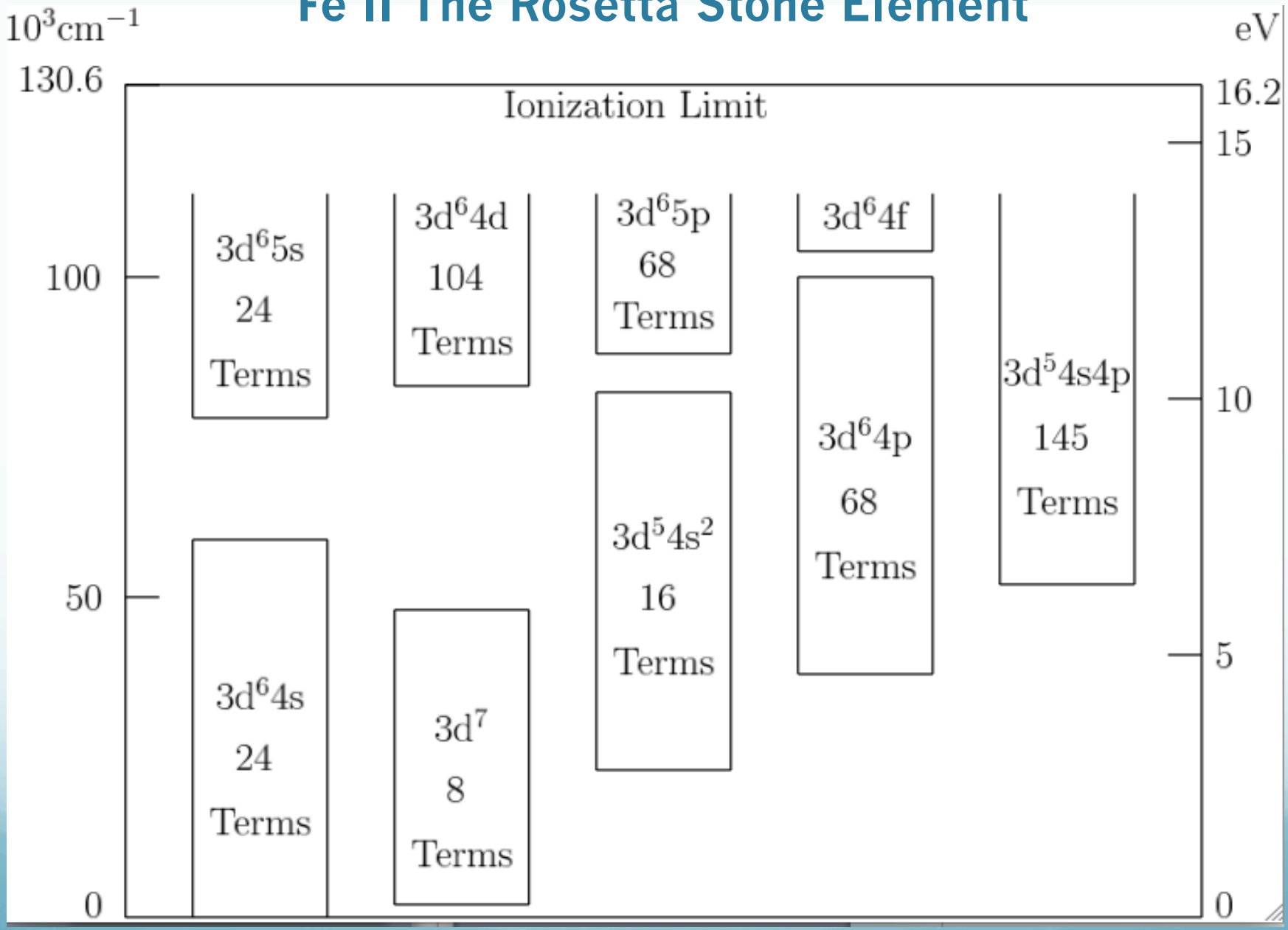


FIG. 6.—*Top*: Upper level energies for Fe II emission lines, color coded according to their A_{ij} value. *Middle*: λF_λ spectrum of PHL 1811. *Bottom*: Same as the top panel, for Fe III.

Leighly KM, Halpern JP, Jenkins EB & Casebeer D, 2007, ApJSS, 173, 1

Fe II The Rosetta Stone Element



Latest Calculation from QUB

- 262 LS or 716 Jπ target states with configs $3d^6 4s$, $3d^7$, $3d^6 4p$, $3d^5 4s^2$, $3d^5 4s4p$
- Last target threshold approximately 23eV
- Breit-Pauli + DARC treatments
- Target energies shifted to NIST where possible
- Highly applicable to recent quasar studies

Thank You