

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)

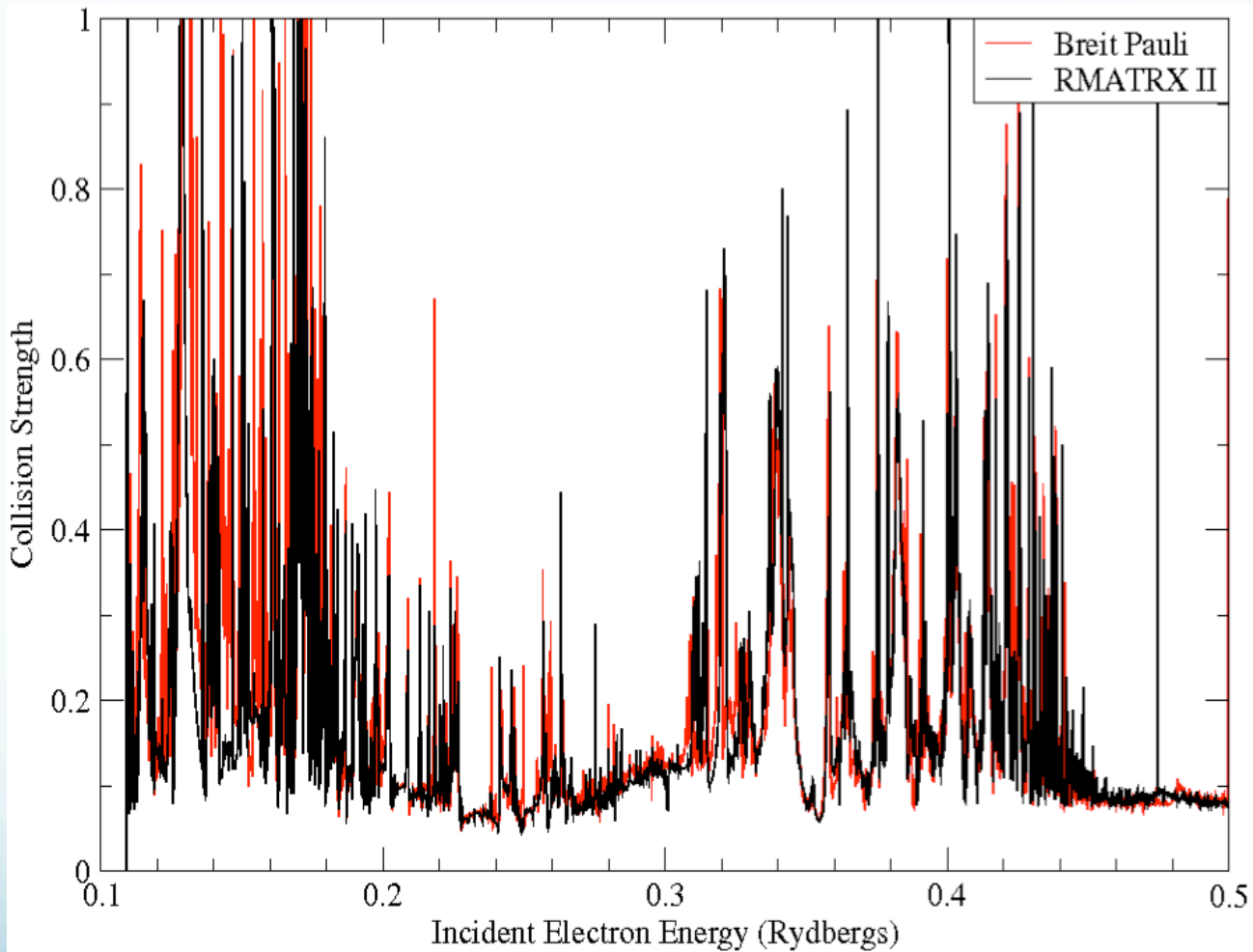
**CLOUDY
CHIANTI
XSTAR**

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graph TD; A["Radiative Data (f- and A-values, energy levels, wavelengths)"] --> B((CLOUDY CHIANTI XSTAR)); C["Collision data (cross sections, excitation rates, recombination rates, proton rates)"] --> B;
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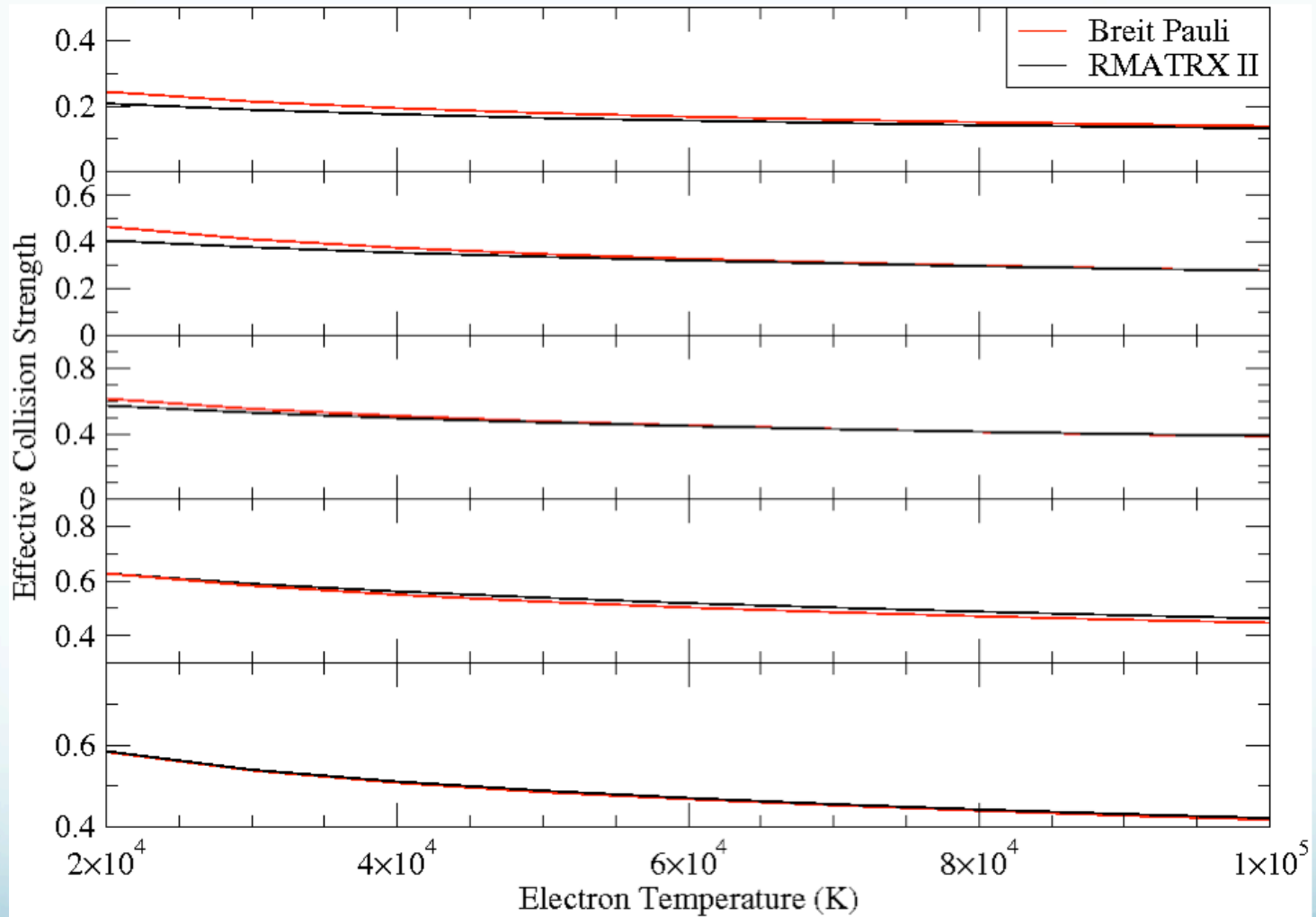
R-matrix Methodologies:

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

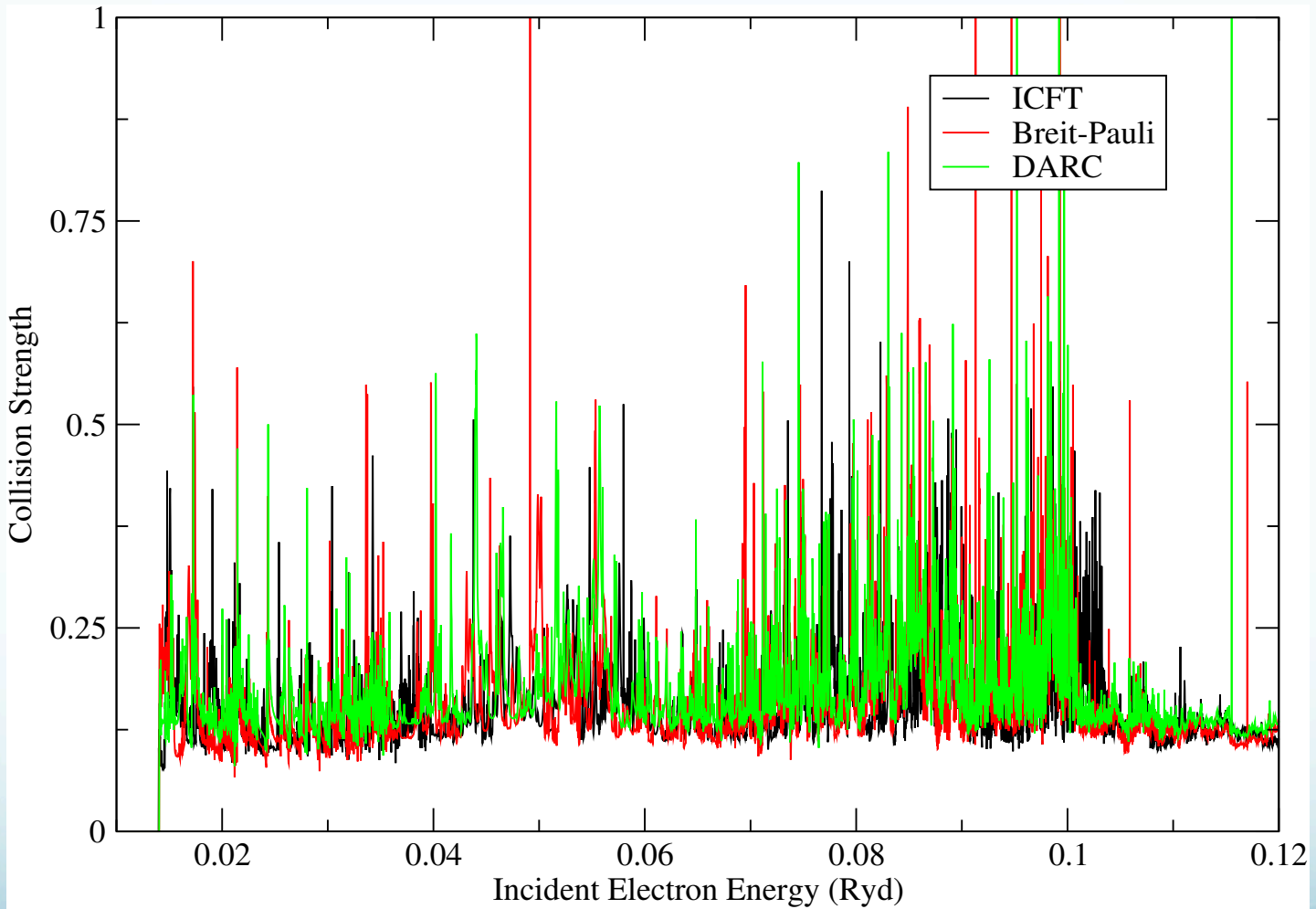
Cr II $3d^5\ ^6S_{5/2} - 3d^44s\ ^6D_{1/2}$



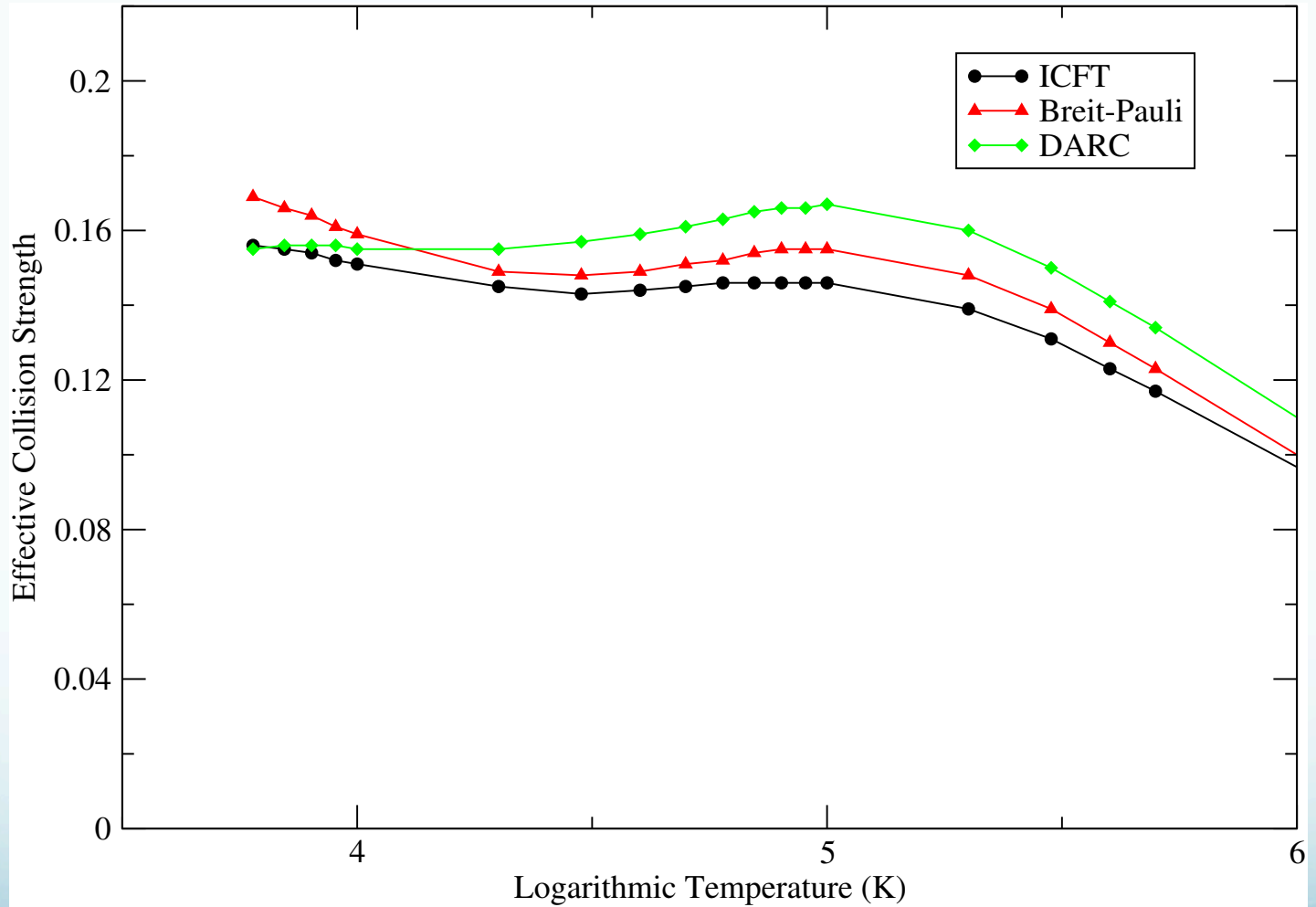
Cr II $3d^5\ ^6S_{5/2} - 3d^44s\ ^6D_{1/2,3/2,5/2,7/2,9/2}$



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

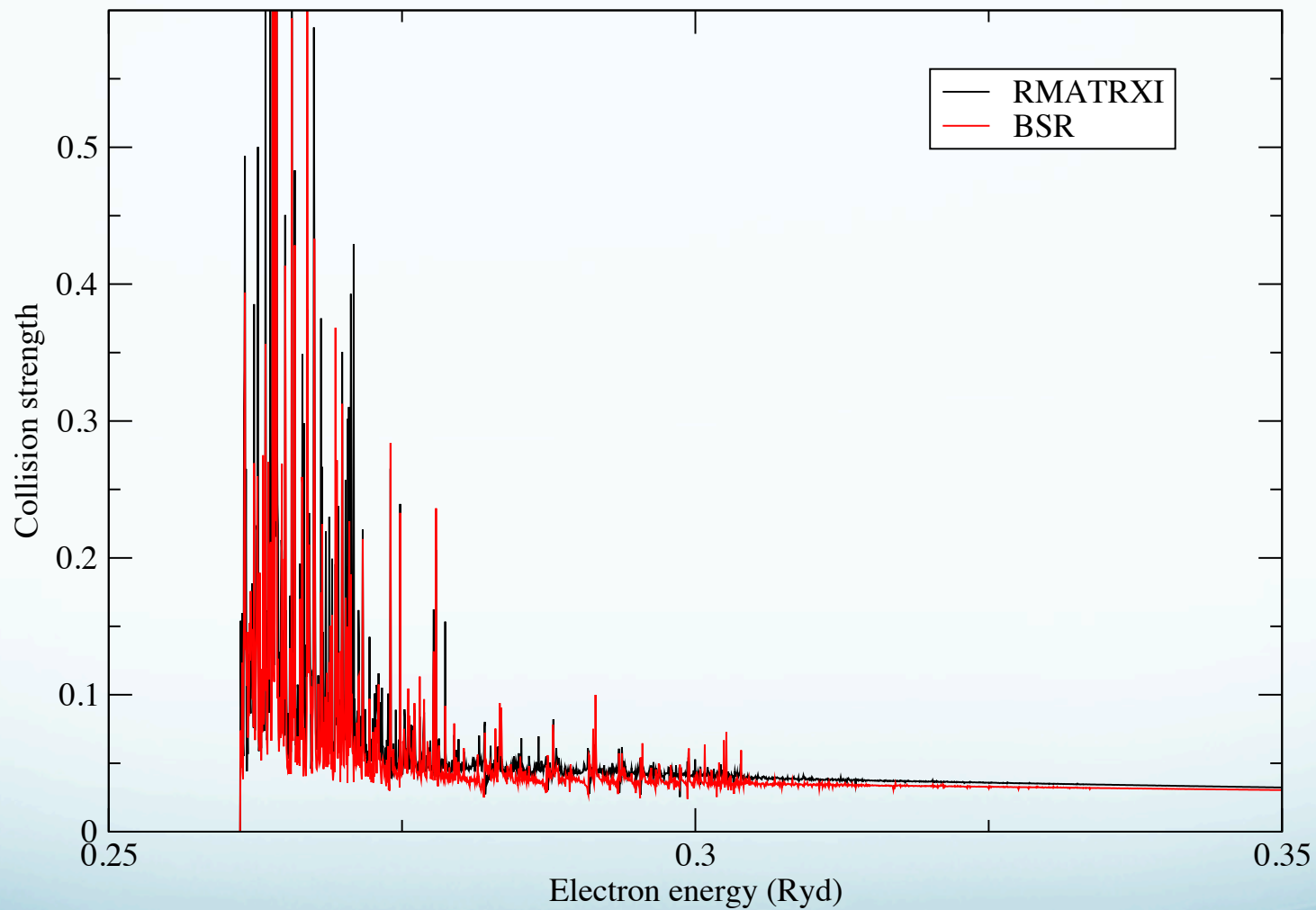


Mn V $3d^3\ ^4F_{3/2} - 3d^3\ ^2D_{5/2}$



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

Mg VIII $2s^22p\ ^2P^o_{1/2} - 2p^3\ ^2P^o_{3/2}$



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

1 1A 11A																	18 VIII 8A
1 H Hydrogen 1.008																	2 He Helium 4.003
3 Li Lithium 6.941	4 Be Beryllium 9.012											5 B Boron 10.811	6 C Carbon 12.011	7 N Nitrogen 14.007	8 O Oxygen 15.999	9 F Fluorine 18.998	10 Ne Neon 20.180
11 Na Sodium 22.990	12 Mg Magnesium 24.305	3 IIIB 3B	4 IVB 4B	5 VB 5B	6 VIB 6B	7 VIIB 7B	8 VIII 8	9 VIII 8	10 VIII 8	11 IB 1B	12 IIB 2B	13 Al Aluminum 26.982	14 Si Silicon 28.086	15 P Phosphorus 30.974	16 S Sulfur 32.066	17 Cl Chlorine 35.453	18 Ar Argon 39.948
19 K Potassium 39.098	20 Ca Calcium 40.078	21 Sc Scandium 44.956	22 Ti Titanium 47.88	23 V Vanadium 50.942	24 Cr Chromium 51.996	25 Mn Manganese 54.938	26 Fe Iron 55.933	27 Co Cobalt 58.933	28 Ni Nickel 58.693	29 Cu Copper 63.546	30 Zn Zinc 65.39	31 Ga Gallium 69.732	32 Ge Germanium 72.61	33 As Arsenic 74.922	34 Se Selenium 78.09	35 Br Bromine 79.904	36 Kr Krypton 84.80
37 Rb Rubidium 84.468	38 Sr Strontium 87.62	39 Y Yttrium 88.906	40 Zr Zirconium 91.224	41 Nb Niobium 92.906	42 Mo Molybdenum 95.94	43 Tc Technetium 98.907	44 Ru Ruthenium 101.07	45 Rh Rhodium 102.906	46 Pd Palladium 106.42	47 Ag Silver 107.868	48 Cd Cadmium 112.411	49 In Indium 114.818	50 Sn Tin 118.71	51 Sb Antimony 121.760	52 Te Tellurium 127.6	53 I Iodine 126.904	54 Xe Xenon 131.29
55 Cs Cesium 132.905	56 Ba Barium 137.327	57-71	72 Hf Hafnium 178.49	73 Ta Tantalum 180.948	74 W Tungsten 183.85	75 Re Rhenium 186.207	76 Os Osmium 190.23	77 Ir Iridium 192.22	78 Pt Platinum 195.08	79 Au Gold 196.967	80 Hg Mercury 200.59	81 Tl Thallium 204.383	82 Pb Lead 207.2	83 Bi Bismuth 208.980	84 Po Polonium [208.982]	85 At Astatine 209.987	86 Rn Radon 222.018
87 Fr Francium 223.020	88 Ra Radium 226.025	89-103	104 Rf Rutherfordium [261]	105 Db Dubnium [262]	106 Sg Seaborgium [266]	107 Bh Bohrium [264]	108 Hs Hassium [269]	109 Mt Meitnerium [268]	110 Ds Darmstadtium [269]	111 Rg Roentgenium [272]	112 Cn Copernicium [277]	113 Uut Ununtrium unknown	114 Fl Flerovium [289]	115 Uup Ununpentium unknown	116 Lv Livermorium [298]	117 Uus Ununseptium unknown	118 Uuo Ununoctium unknown

Lanthanide Series	57 La Lanthanum 138.906	58 Ce Cerium 140.115	59 Pr Praseodymium 140.908	60 Nd Neodymium 144.24	61 Pm Promethium 144.913	62 Sm Samarium 150.36	63 Eu Europium 151.966	64 Gd Gadolinium 157.25	65 Tb Terbium 158.925	66 Dy Dysprosium 162.50	67 Ho Holmium 164.930	68 Er Erbium 167.26	69 Tm Thulium 168.934	70 Yb Ytterbium 173.04	71 Lu Lutetium 174.967
Actinide Series	89 Ac Actinium 227.028	90 Th Thorium 232.038	91 Pa Protactinium 231.036	92 U Uranium 238.029	93 Np Neptunium 237.048	94 Pu Plutonium 244.064	95 Am Americium 243.061	96 Cm Curium 247.070	97 Bk Berkelium 247.070	98 Cf Californium 251.080	99 Es Einsteinium [254]	100 Fm Fermium 257.095	101 Md Mendelevium 258.1	102 No Nobelium 259.101	103 Lr Lawrencium [262]

Alkali Metal	Alkaline Earth	Transition Metal	Semimetal	Nonmetal	Basic Metal	Halogen	Noble Gas	Lanthanide	Actinide
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W XLV (Z=74: NELC=30)

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

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

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

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

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

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

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

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

$1s^2 2s^2 2p^6 3s^2 3p^6 3d^{10} 4d 4f \rightarrow 35au$

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 $J\pi$ 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 $J\pi$ 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 $3d^9 4s 4p 4d$, neglect $3d^9 4s 4p^2$
and $3d^9 4s 4d^2$**

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

313 $J\pi$ levels: inclusive

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

Radiation Damping Included (Type I)

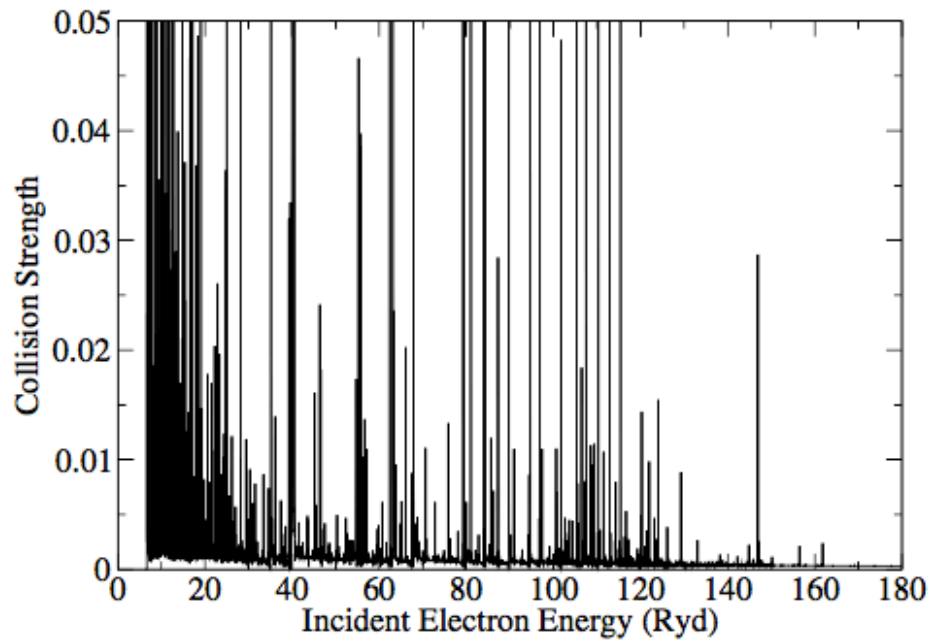
Top-up of high partial waves included

W XLV Energy Levels in au

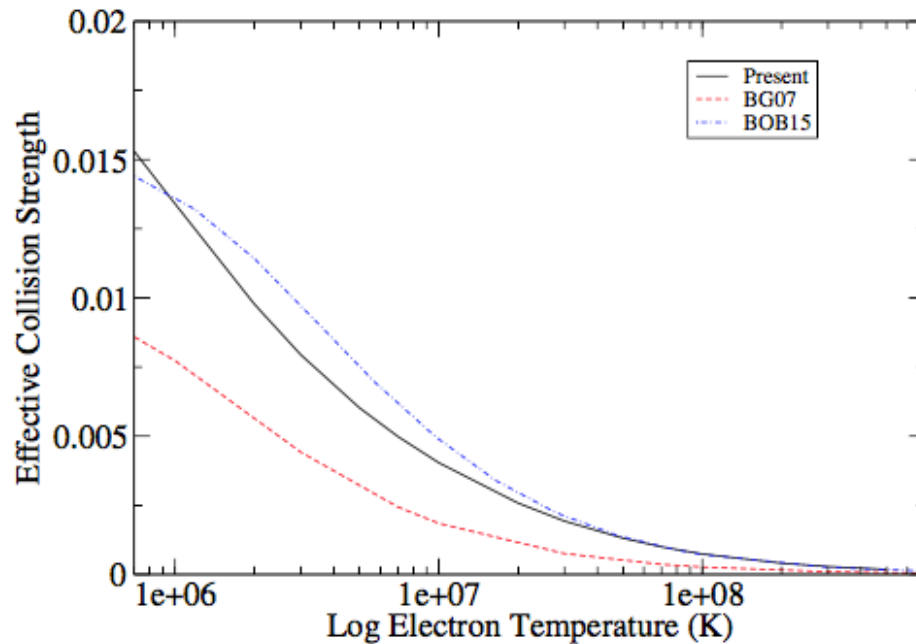
Index	Level	Present	NIST ^a	BG ^b	Q ^c	SS ^d	F ^e	VI ^f
1	4s ² 1S ₀	0.000	0.000	0.000	0.000	0.000	0.000	0.000
2	4s4p 3P ₀ ^o	3.165	3.167	3.175	3.170	3.175	3.187	3.173
3	4s4p 3P ₁ ^o	3.423	3.429	3.445	3.436	3.428	3.450	3.425
4	4s4p 3P ₂ ^o	6.833	6.809	6.887	6.844	6.859	6.860	6.853
5	4p ² 3P ₀	7.246	7.236	7.306	7.290	7.242		7.236
6	4s4p 1P ₁ ^o	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 ₂ ^o	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



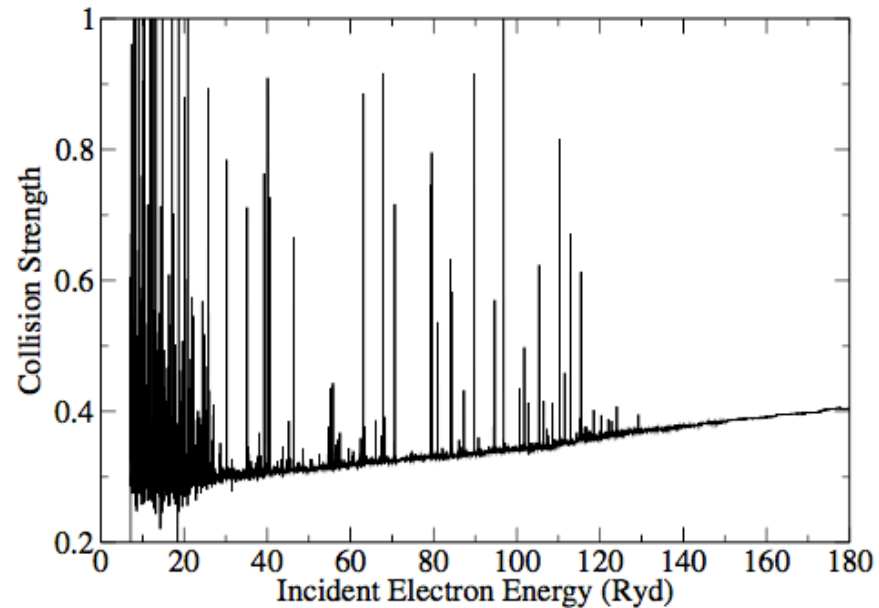
(a) 1-2 Collision Strength



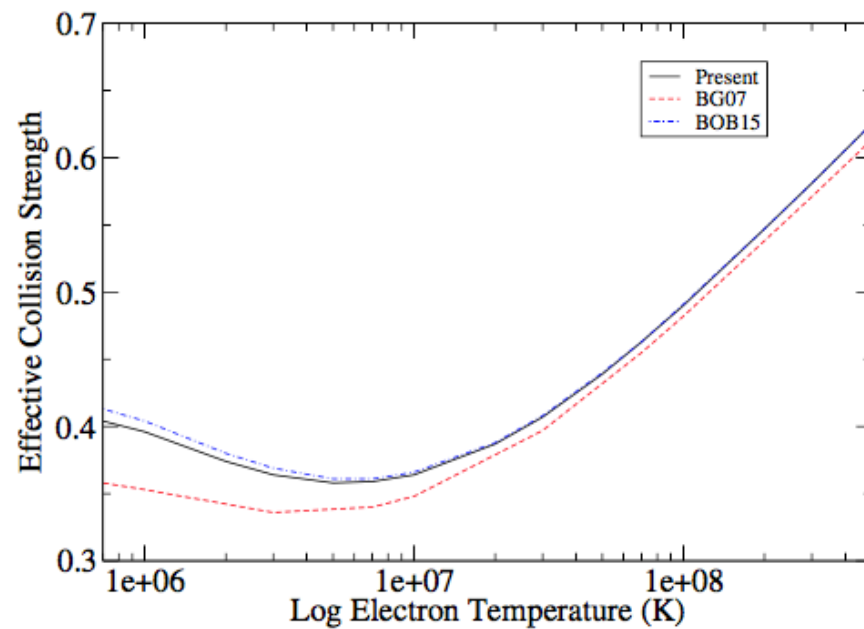
(b) 1-2 Effective Collision Strength

BP Present
BG07
BOB15

W XLV 1-3



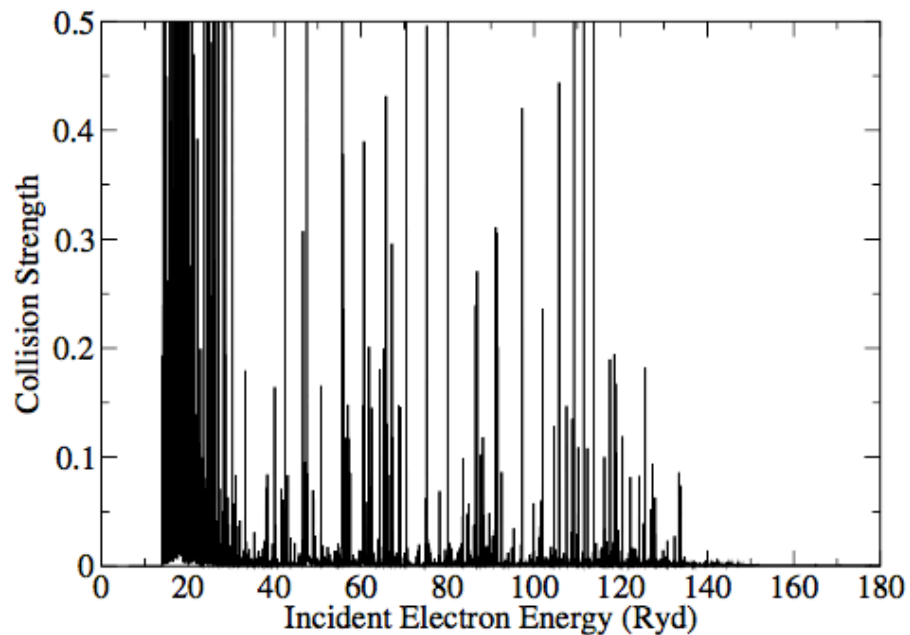
(c) 1-3 Collision Strength



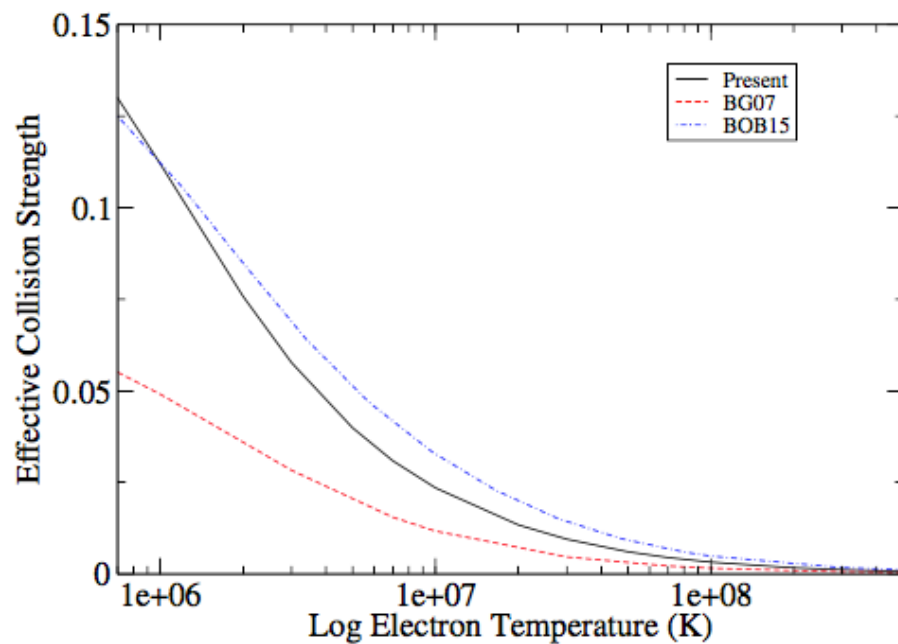
(d) 1-3 Effective Collision Strength

BP Present
BG07
BOMB15

W XLV 1-4



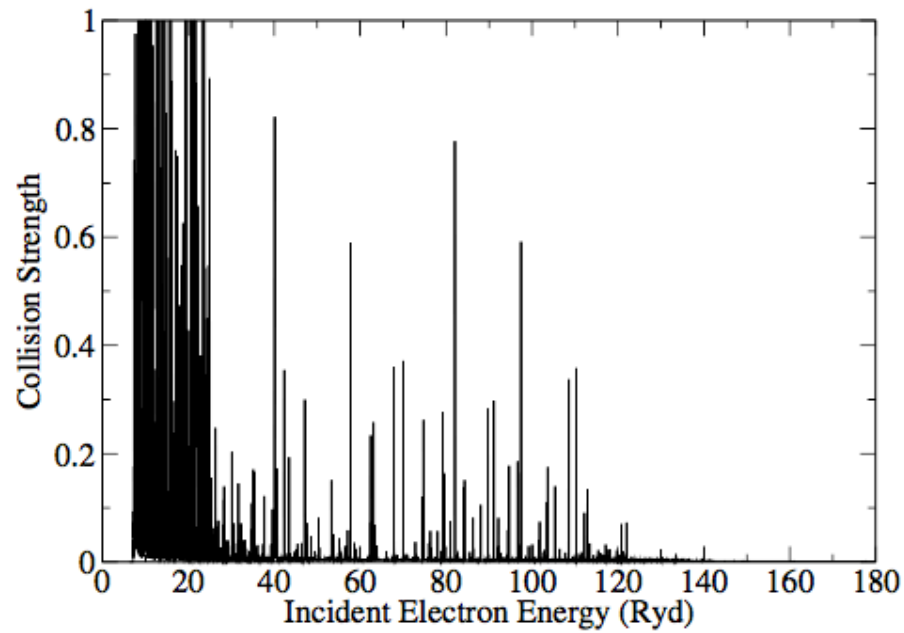
(e) 1-4 Collision Strength



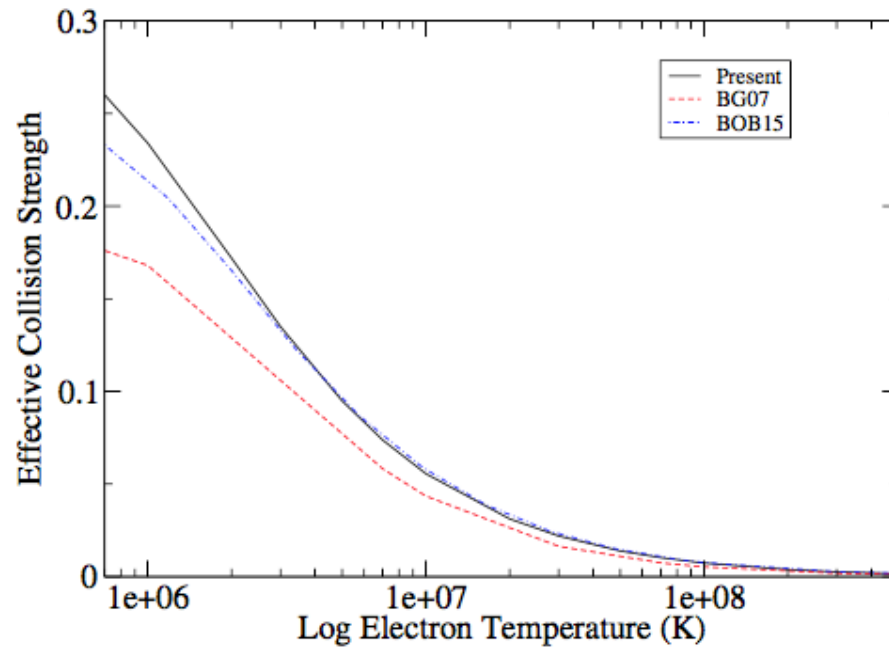
(f) 1-4 Effective Collision Strength

BP Present
BG07
BOB15

W XLV 2-3



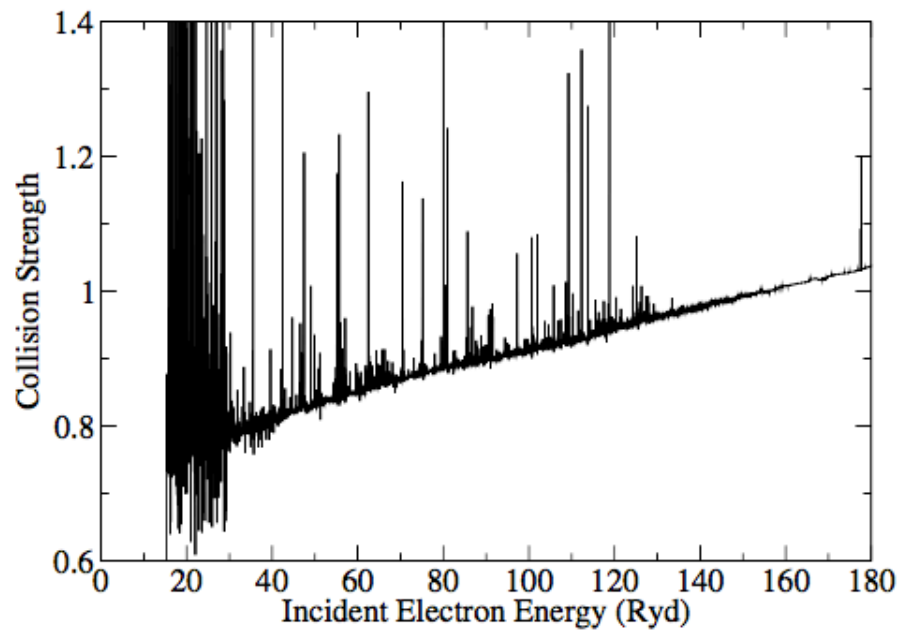
(g) 2-3 Collision Strength



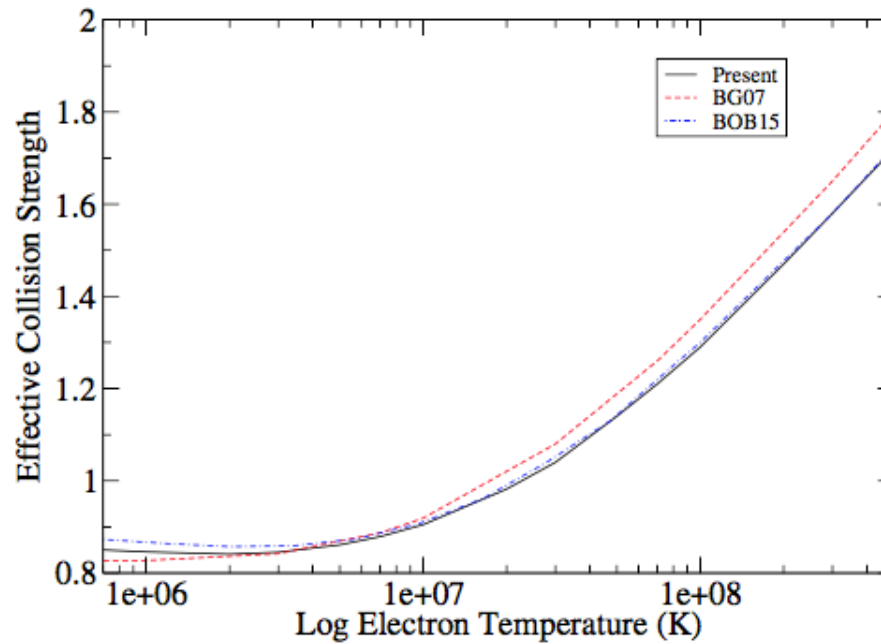
(h) 2-3 Effective Collision Strength

BP Present
BG07
BOMB15

W XLV 1-6



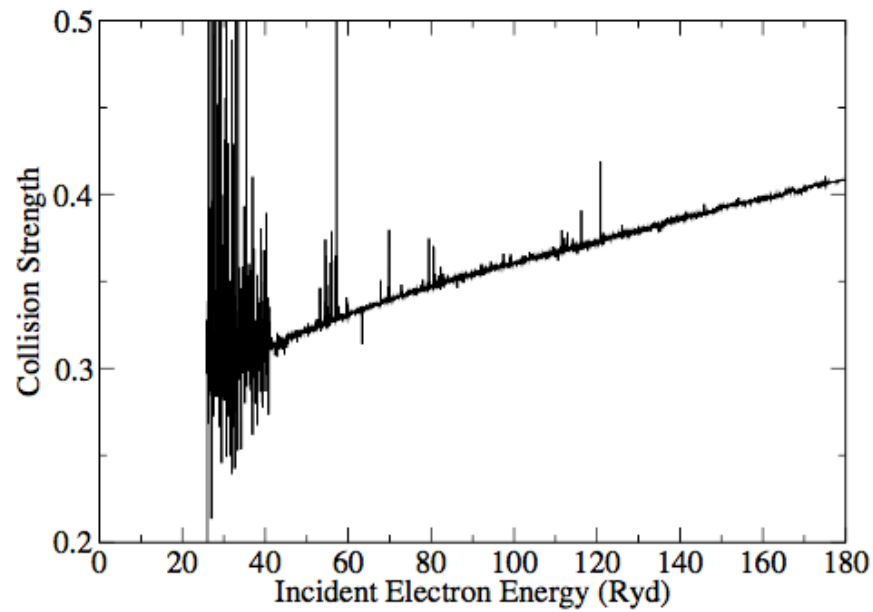
(i) 1-6 Collision Strength



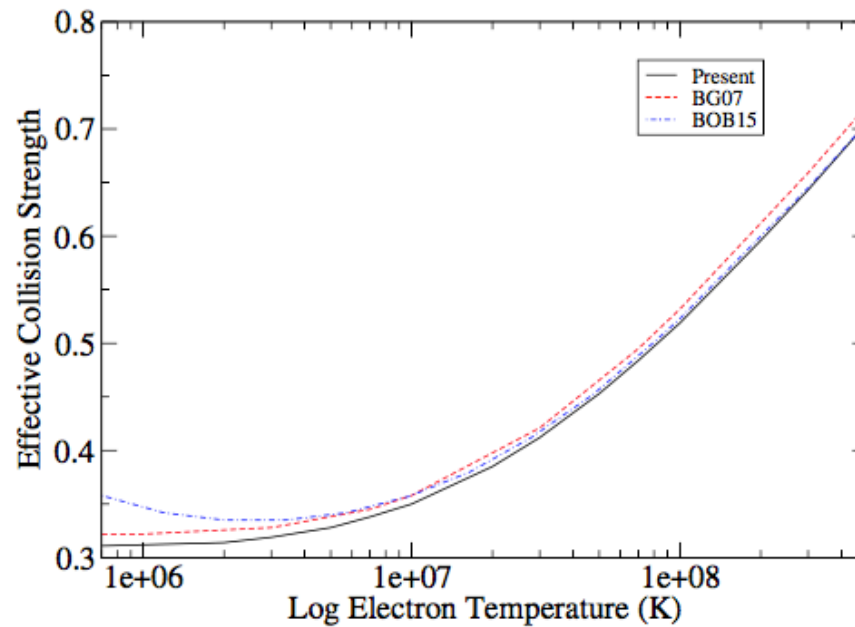
(j) 1-6 Effective Collision Strength

BP –present
BG07
BOB15

W XLV 2-9



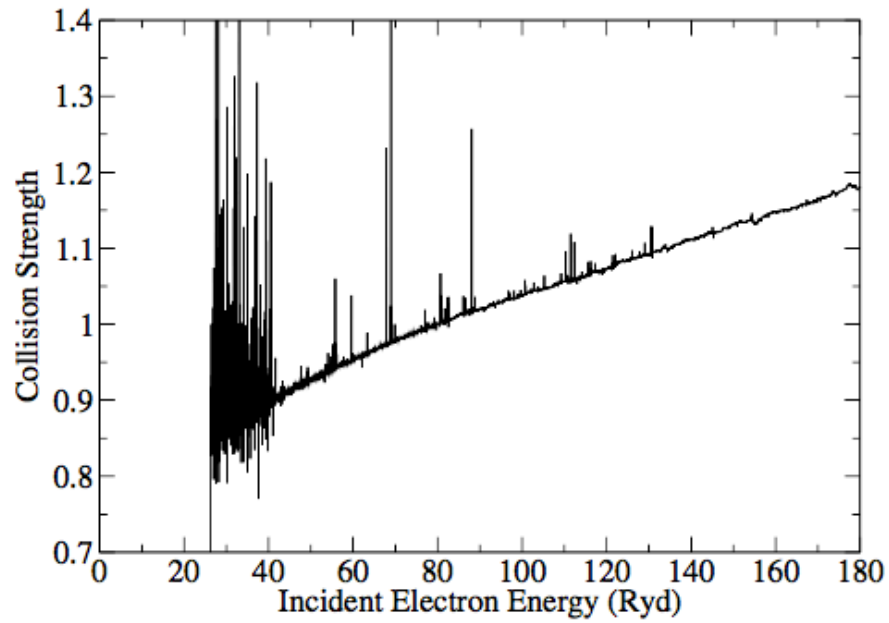
(k) 2-9 Collision Strength



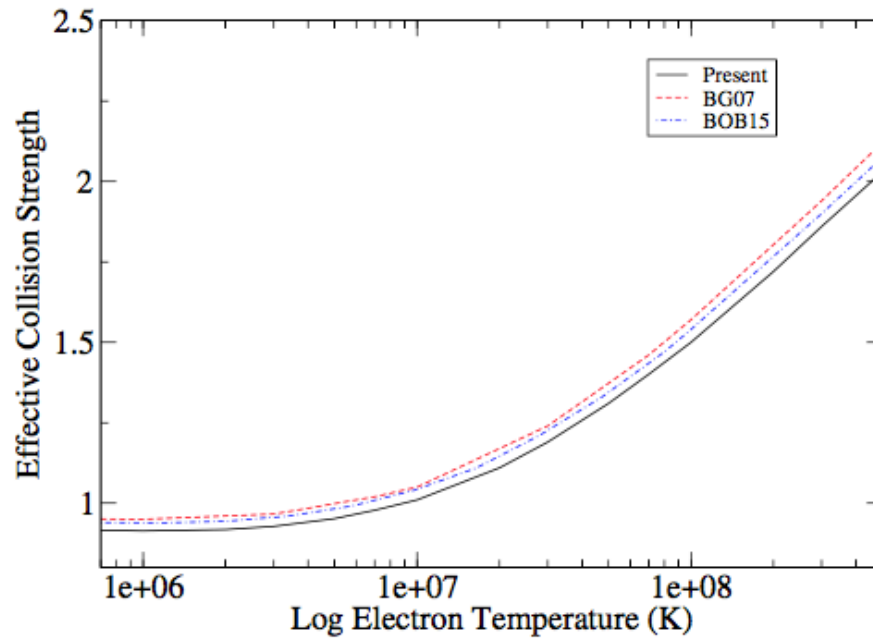
(l) 2-9 Effective Collision Strength

BP –present
BG07
BOB15

W XLV 3-10



(m) 3-10 Collision Strength



(n) 3-10 Effective Collision Strength

BP –present
BG07
BOMB15

Strong Dipole Transition

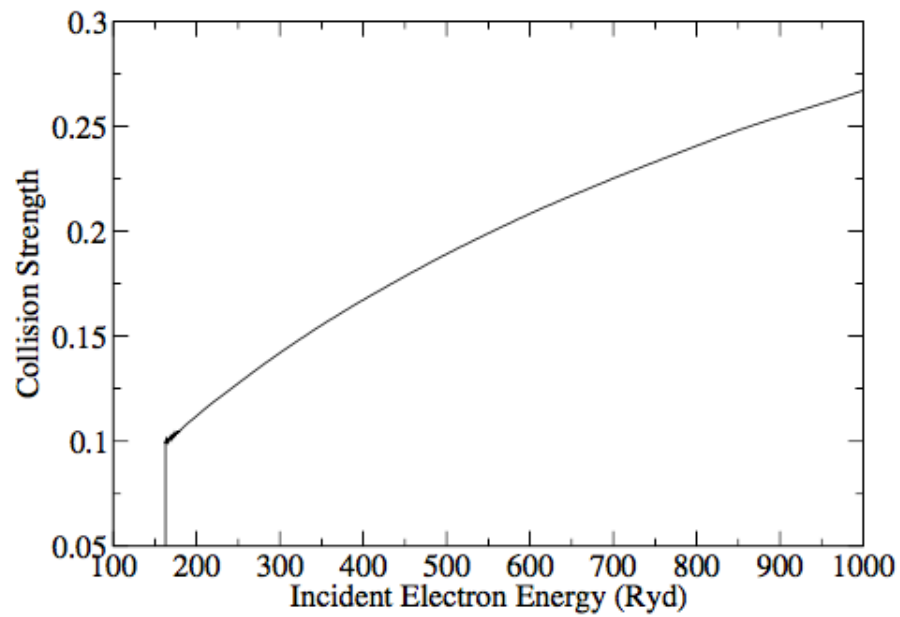


1-177 ($f_1=3.109$, $A_{ij}=2.205 \times 10^{14}$)

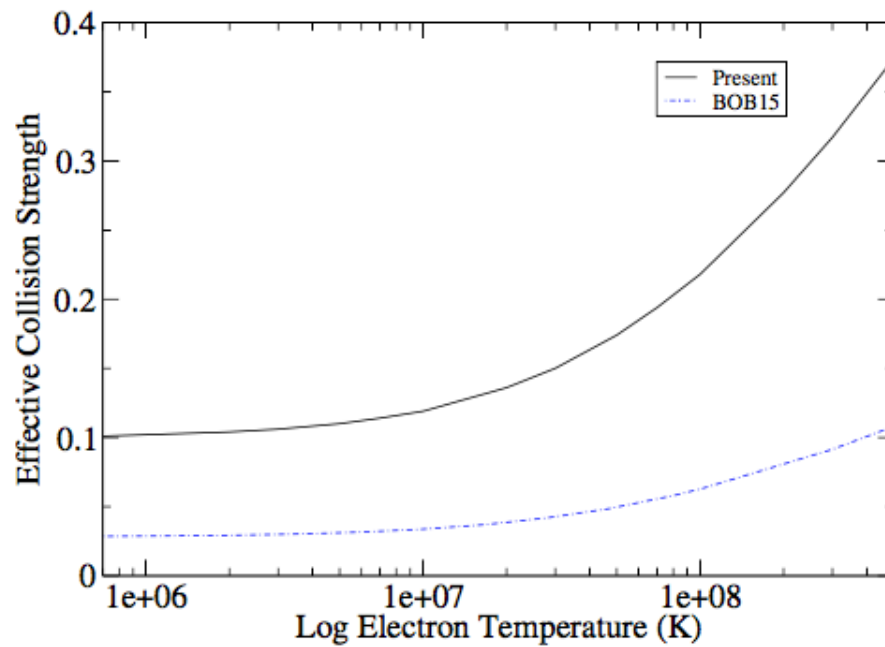
Index	Level	Contr. %	Energy (a.u.)	Index	Level	Contr. %	Energy (a.u.)
158	4s ² 4f 3P ^o ₀	100	77.6166	175	4s ² 4f 3D ^o ₃	37	80.6121
159	4s ² 4f 3P ^o ₁	75	77.7227		4s ² 4f 1F ^o ₃	24	
	4s ² 4f 3D ^o ₁	25		176	4s ² 4f 3G ^o ₄	46	80.6649
160	4s ² 4f 3H ^o ₅	53	77.8745		4s ² 4f 1G ^o ₄	30	
	4s ² 4f 1H ^o ₅	44			4s ² 4f 3F ^o ₄	23	
161	4s ² 4f 3D ^o ₂	56	77.9015	177	4s ² 4f 1P ^o ₁	78	81.3494
	4s ² 4f 3P ^o ₂	29			4s ² 4f 3D ^o ₁	15	
	4s ² 4f 3F ^o ₂	15		178	4s4d ² 5D ₂	35	83.5747
162	4s ² 4f 3F ^o ₃	56	78.0210		4s4d ² 5F ₂	21	
	4s ² 4f 3D ^o ₃	26			4s4d ² 5P ₂	13	
	4s ² 4f 3G ^o ₃	13		179	4s4d ² 5P ₁	45	83.5820
163	4s ² 4f 3H ^o ₅	100	78.0413		4s4d ² 5D ₁	34	
164	4s ² 4f 3G ^o ₄	51	78.0612	180	4s4d ² 5F ₃	26	83.6167
	4s ² 4f 1G ^o ₄	22			4s4d ² 5D ₃	18	
	4s ² 4f 3F ^o ₄	15			4s4d ² 5G ₃	14	

W XLV 1-177

BP –present
BOMB15



(o) 1-177 Collision Strength



(p) 1-177 Effective Collision Strength

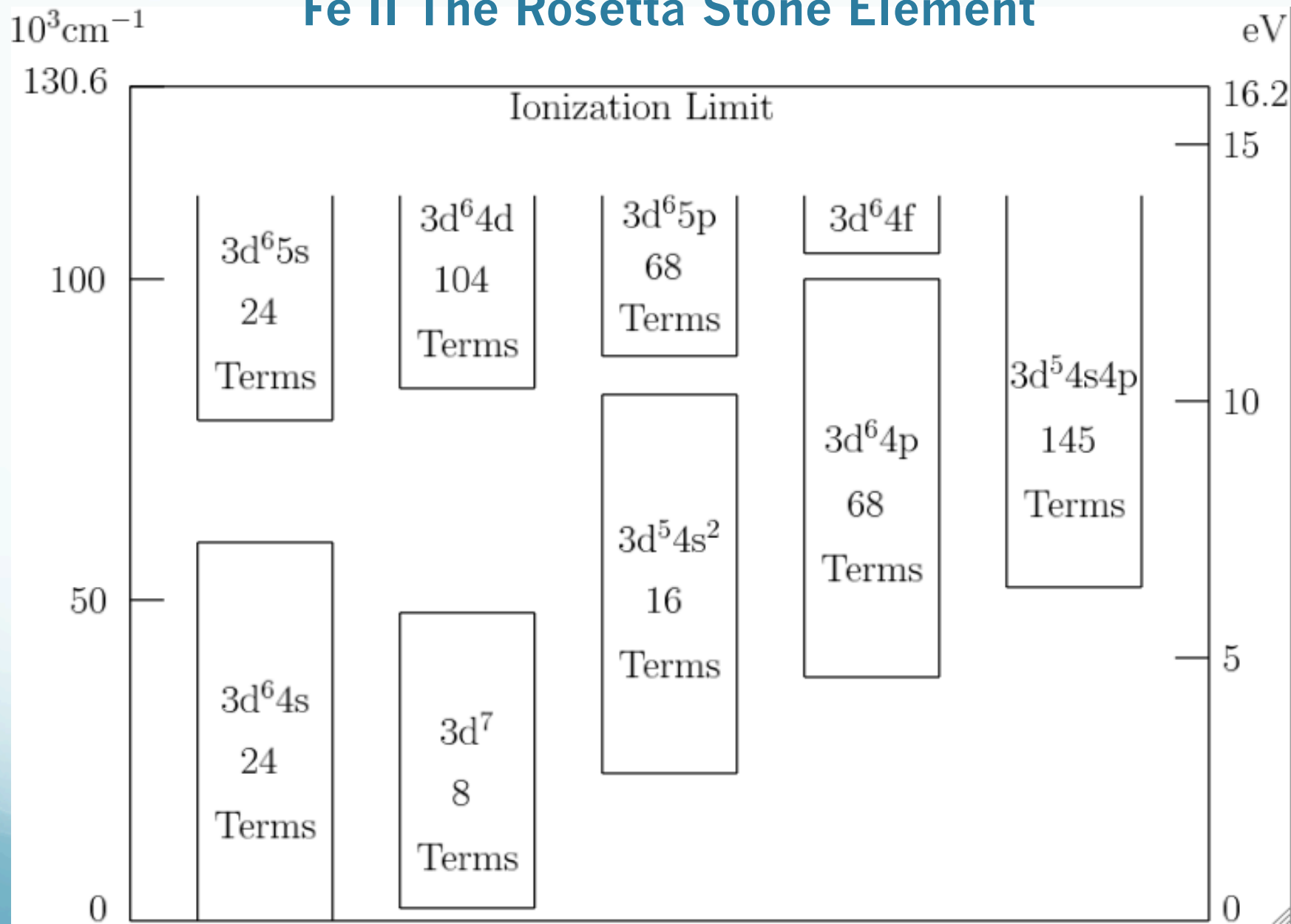
Periodic Table of the Elements

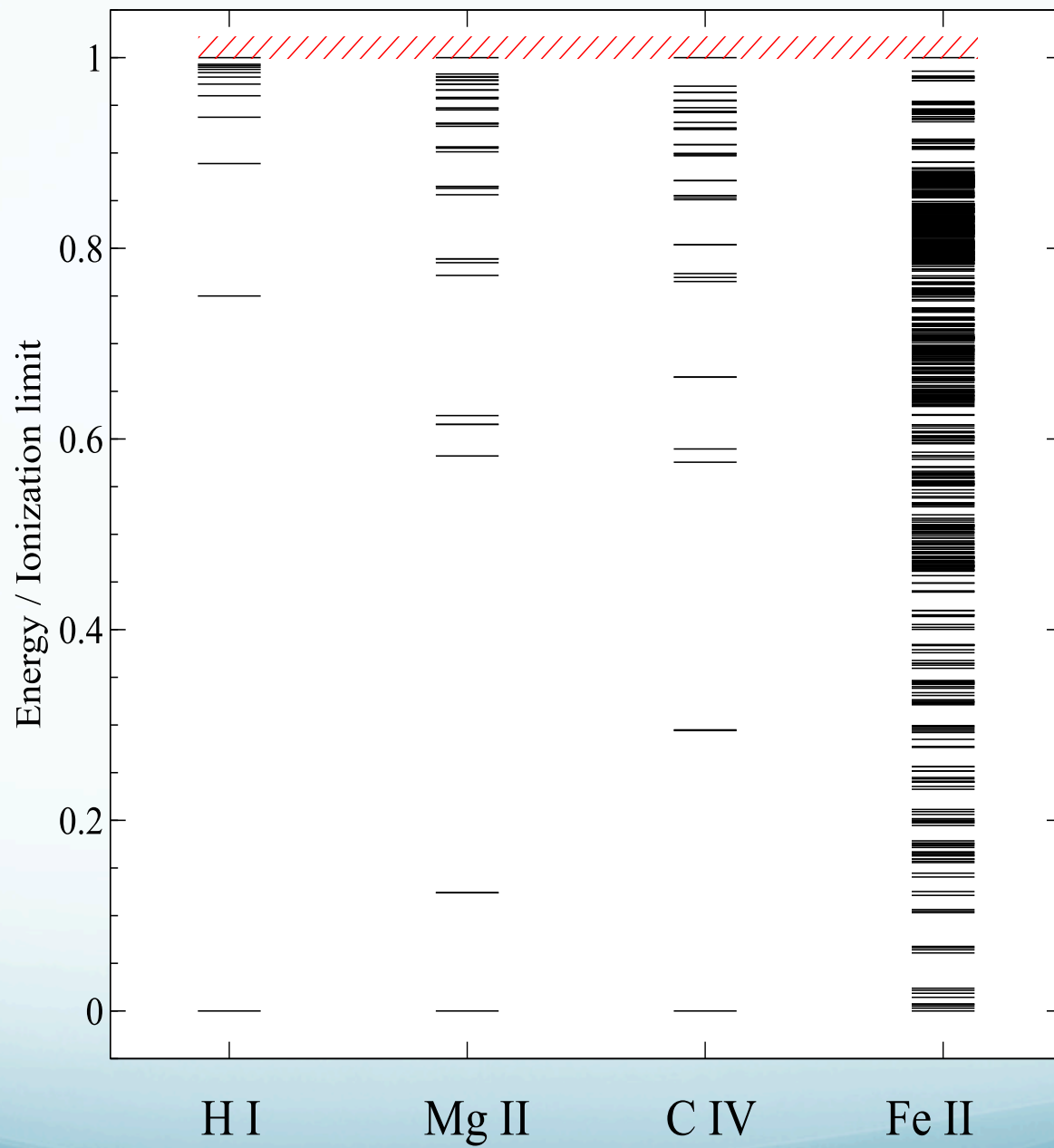
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37 Rb Rubidium 84.468	38 Sr Strontium 87.62	39 Y Yttrium 88.906	40 Zr Zirconium 91.224	41 Nb Niobium 92.906	42 Mo Molybdenum 95.94	43 Tc Technetium 98.907	44 Ru Ruthenium 101.07	45 Rh Rhodium 102.906	46 Pd Palladium 106.42	47 Ag Silver 107.868	48 Cd Cadmium 112.411	49 In Indium 114.818	50 Sn Tin 118.71	51 Sb Antimony 121.760	52 Te Tellurium 127.6	53 I Iodine 126.904	54 Xe Xenon 131.29
55 Cs Cesium 132.905	56 Ba Barium 137.327	57-71 Lanthanide Series	72 Hf Hafnium 178.49	73 Ta Tantalum 180.948	74 W Tungsten 183.85	75 Re Rhenium 186.207	76 Os Osmium 190.23	77 Ir Iridium 192.22	78 Pt Platinum 195.08	79 Au Gold 196.967	80 Hg Mercury 200.59	81 Tl Thallium 204.383	82 Pb Lead 207.2	83 Bi Bismuth 208.980	84 Po Polonium [208.982]	85 At Astatine 209.987	86 Rn Radon 222.018
87 Fr Francium 223.020	88 Ra Radium 226.025	89-103 Actinide Series	104 Rf Rutherfordium [261]	105 Db Dubnium [262]	106 Sg Seaborgium [266]	107 Bh Bohrium [264]	108 Hs Hassium [269]	109 Mt Meitnerium [268]	110 Ds Darmstadtium [269]	111 Rg Roentgenium [272]	112 Cn Copernicium [277]	113 Uut Ununtrium unknown	114 Fl Flerovium [289]	115 Uup Ununpentium unknown	116 Lv Livermorium [293]	117 Uus Ununseptium unknown	118 Uuo Ununoctium unknown

Lanthanide Series	57 La Lanthanum 138.906	58 Ce Cerium 140.115	59 Pr Praseodymium 140.908	60 Nd Neodymium 144.24	61 Pm Promethium 144.913	62 Sm Samarium 150.36	63 Eu Europium 151.966	64 Gd Gadolinium 157.25	65 Tb Terbium 158.925	66 Dy Dysprosium 162.50	67 Ho Holmium 164.930	68 Er Erbium 167.26	69 Tm Thulium 168.934	70 Yb Ytterbium 173.04	71 Lu Lutetium 174.967
Actinide Series	89 Ac Actinium 227.028	90 Th Thorium 232.038	91 Pa Protactinium 231.036	92 U Uranium 238.029	93 Np Neptunium 237.048	94 Pu Plutonium 244.064	95 Am Americium 243.061	96 Cm Curium 247.070	97 Bk Berkelium 247.070	98 Cf Californium 251.080	99 Es Einsteinium [254]	100 Fm Fermium 257.095	101 Md Mendelevium 258.1	102 No Nobelium 259.101	103 Lr Lawrencium [262]

Alkali Metal	Alkaline Earth	Transition Metal	Semimetal	Nonmetal	Basic Metal	Halogen	Noble Gas	Lanthanide	Actinide
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Fe II The Rosetta Stone Element





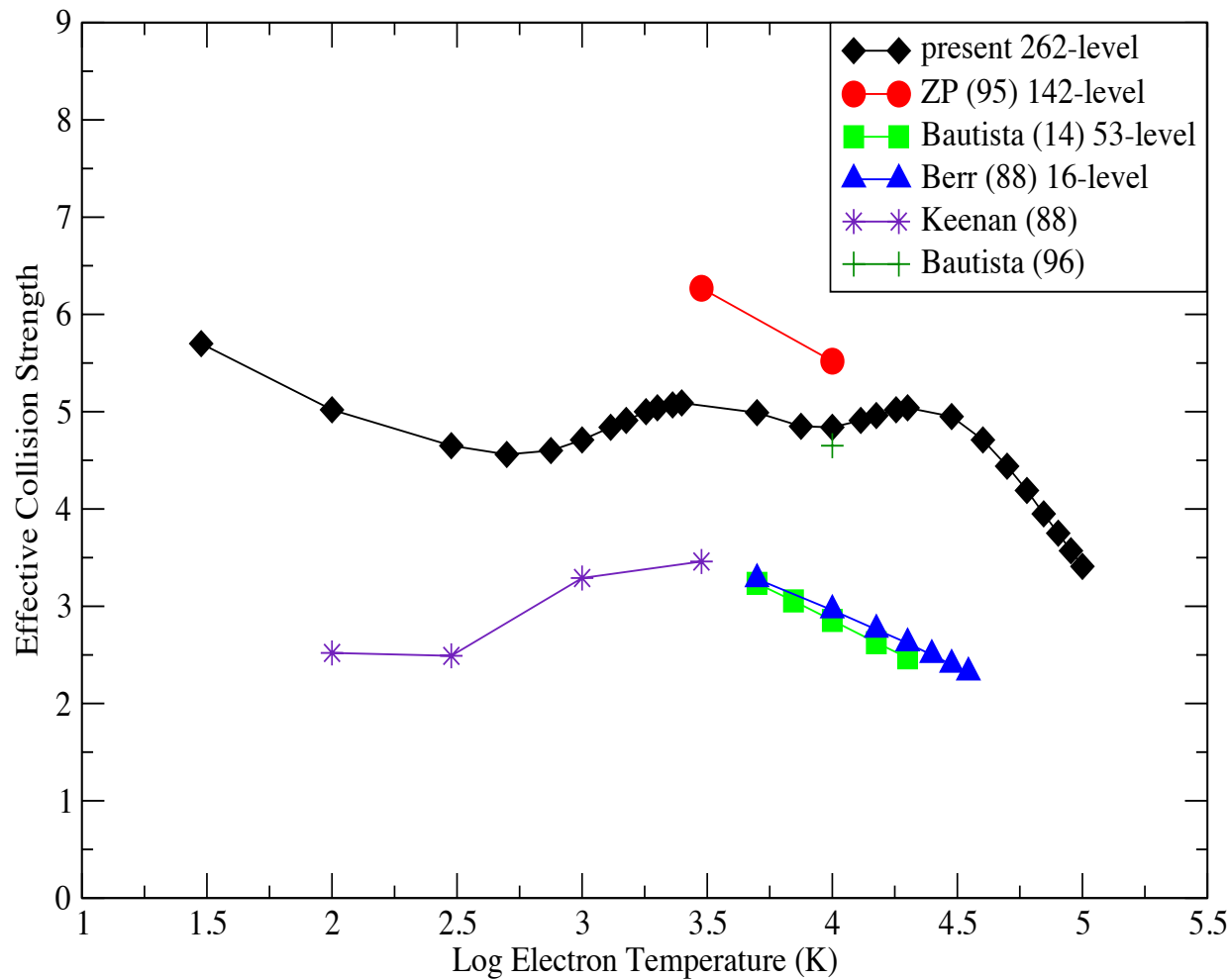
Model	LSπ		Jπ	
No. Configs	States	Channels	States	Channels
1	24	72	63	420
2	32	98	82	540
3	100	315	262	1800
4	116	363	299	2052
5	261	805	716	5076
6	285	877	779	5496
7	389	1239	1055	7596

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

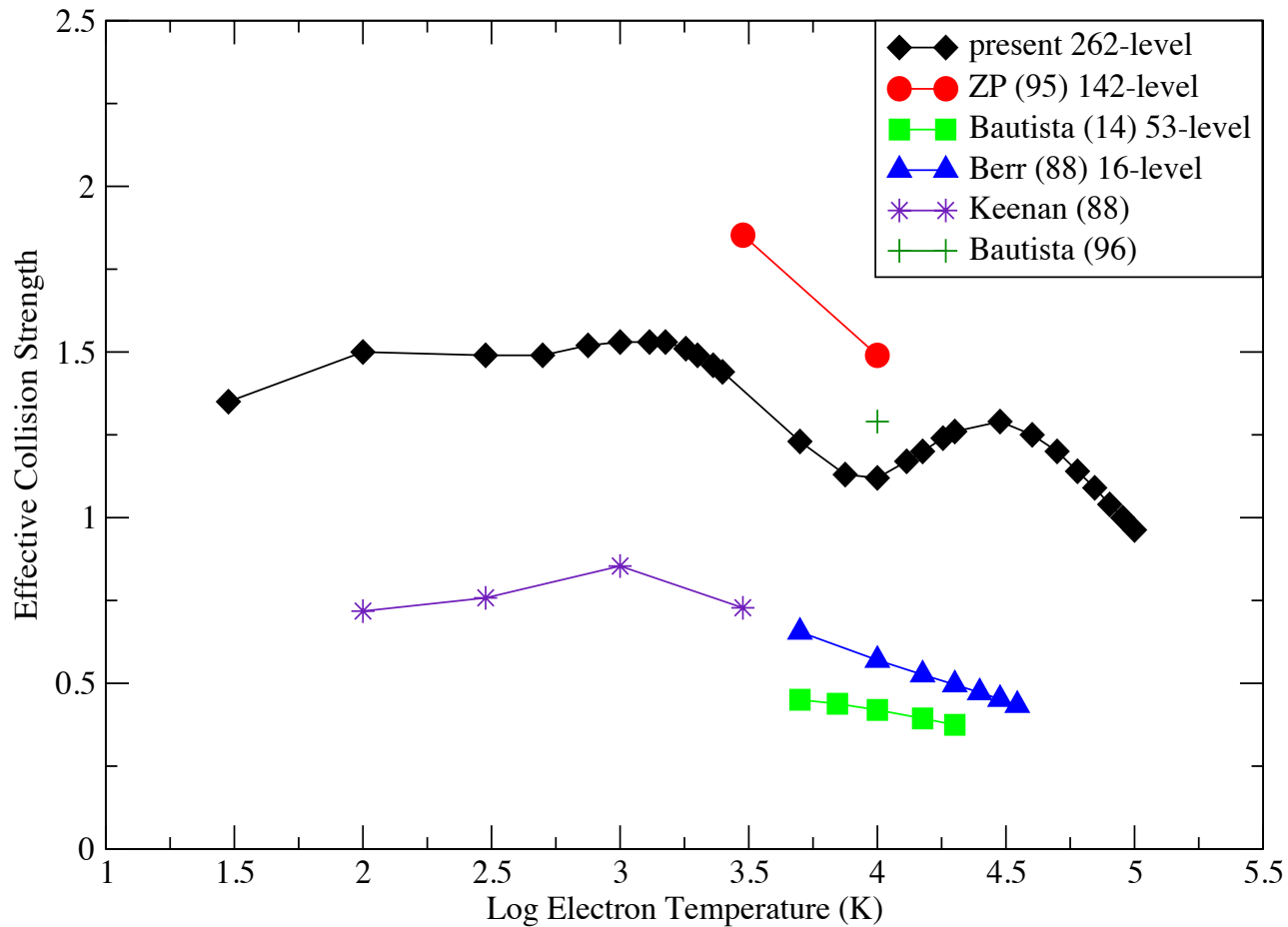
Model	LS π		J π	
No. Configs	States	Channels	States	Channels
1	24	72	63	420
2	32	98	82	540
3	100	315	262	1800
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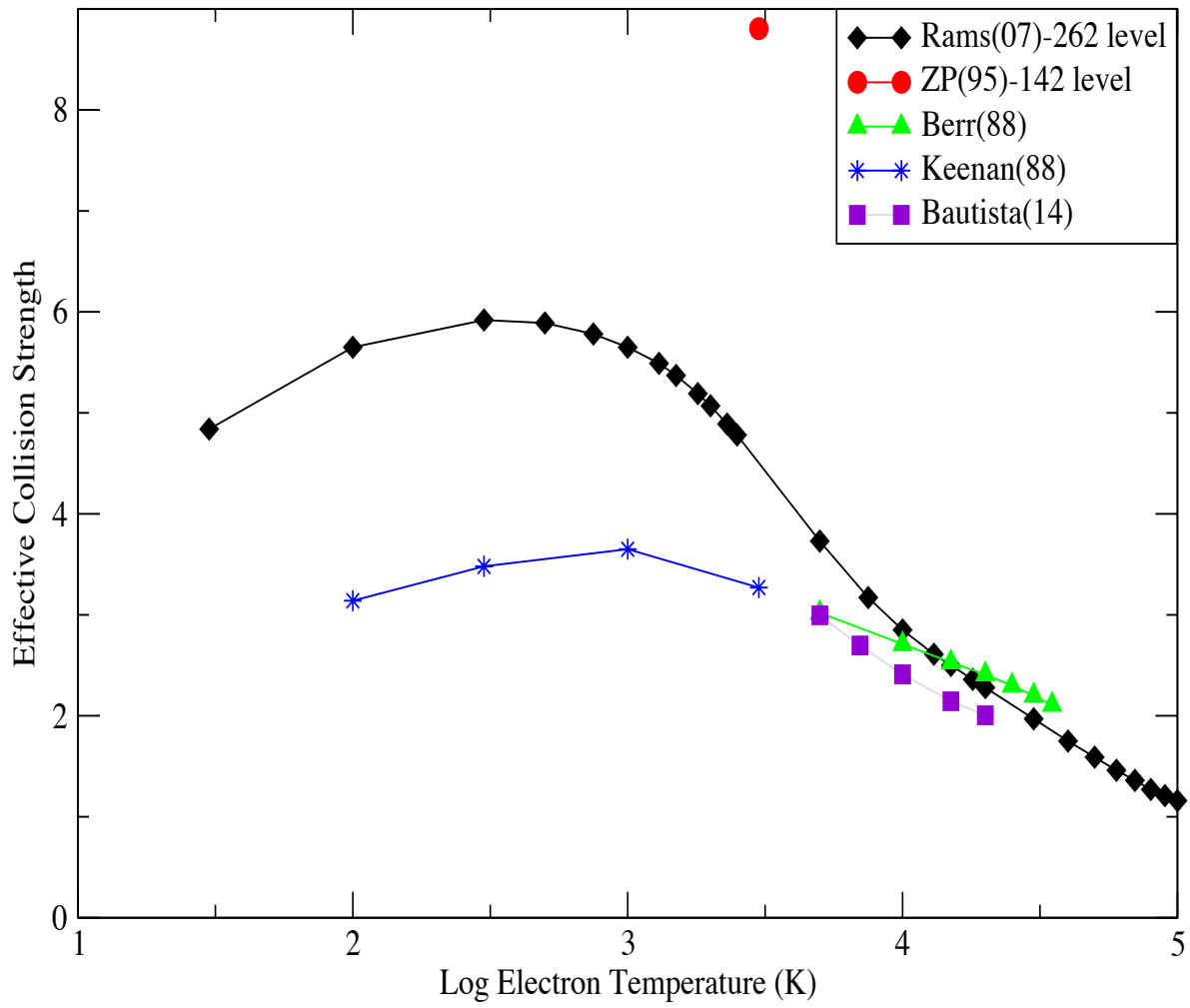
Fe II $3d^64s\ ^6D_{9/2} - 3d^64s\ ^6D_{7/2}$



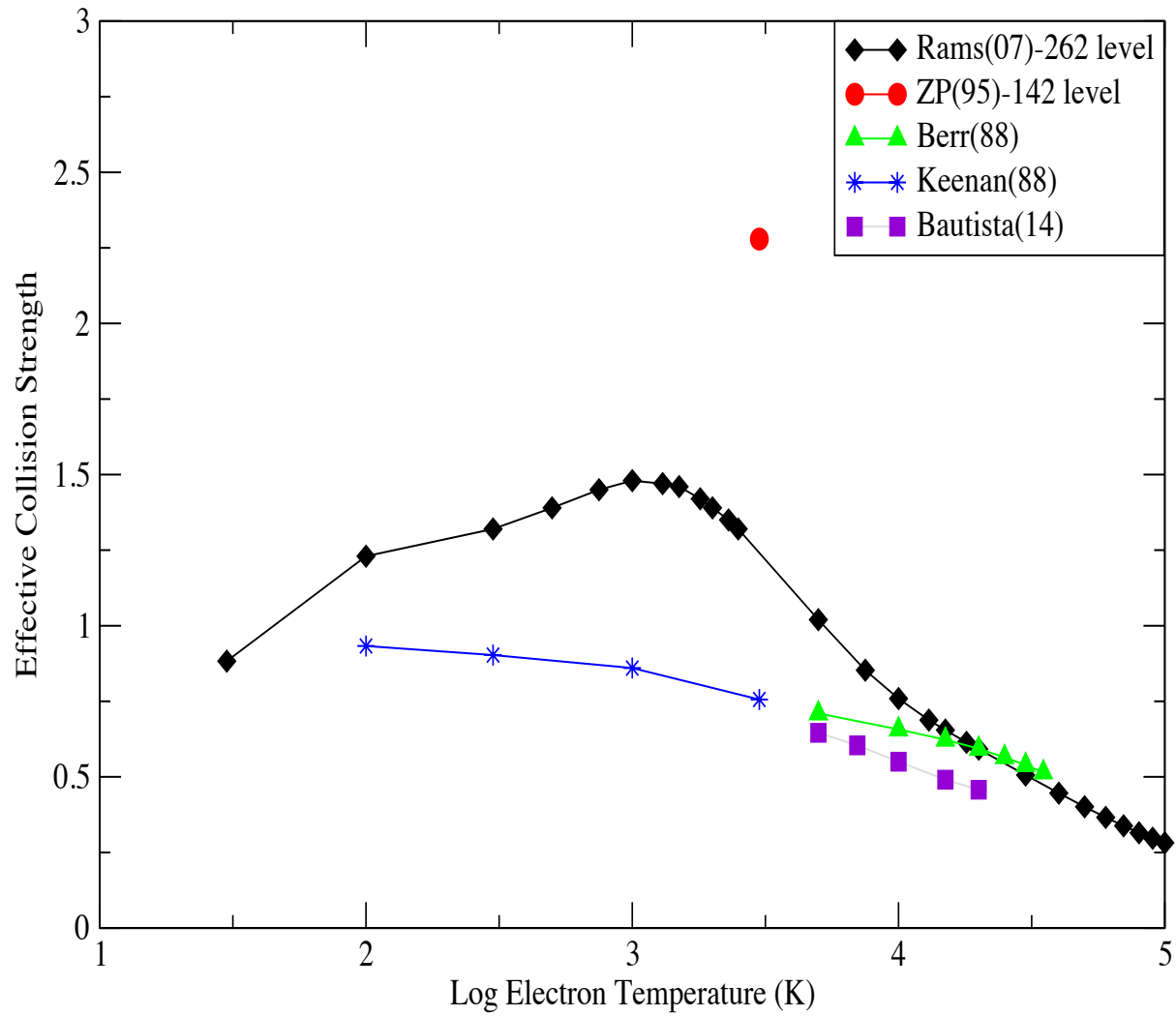
Fe II $3d^6 4s \ ^6D_{9/2} - 3d^6 4s \ ^6D_{5/2}$



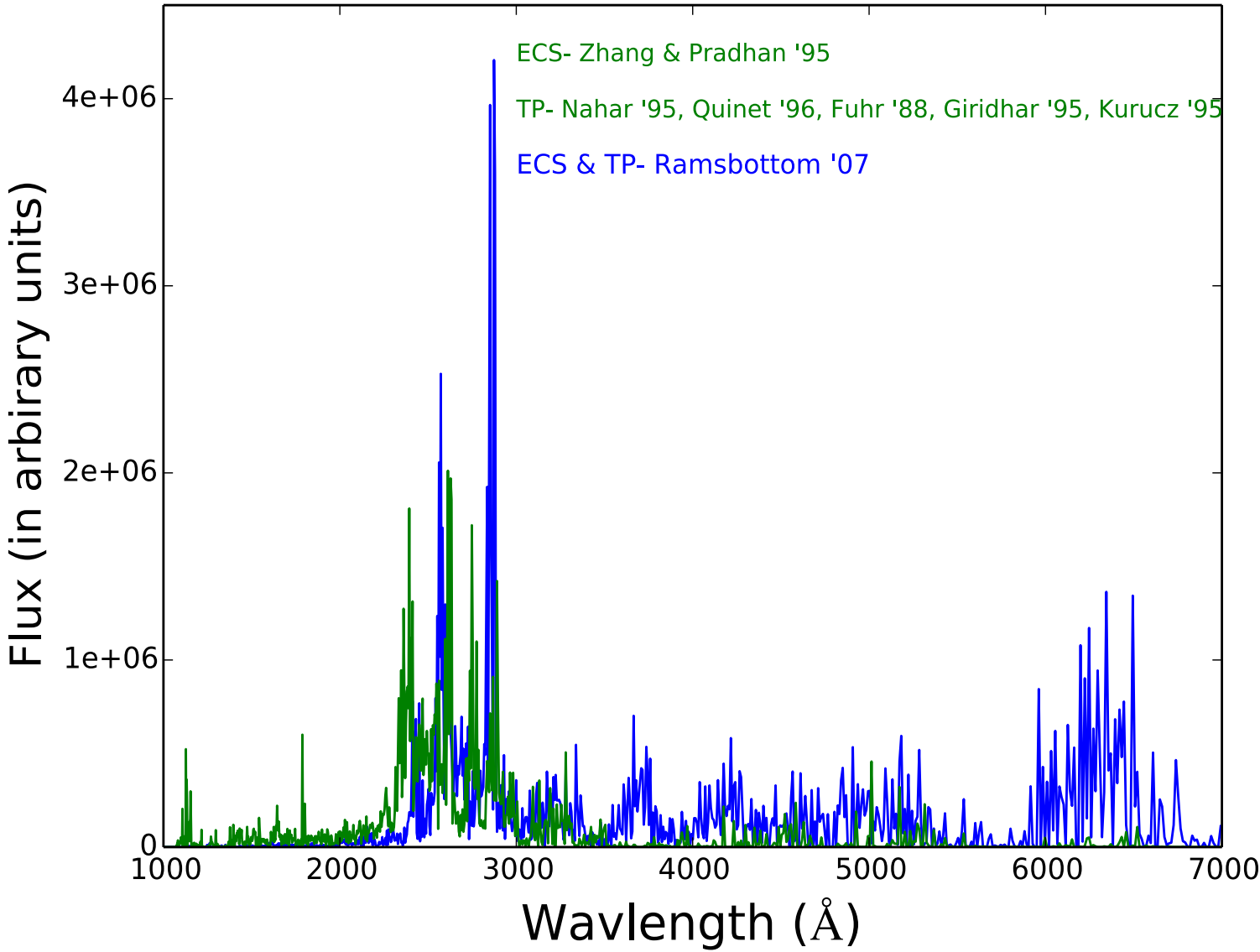
Fe II Transition 6-7



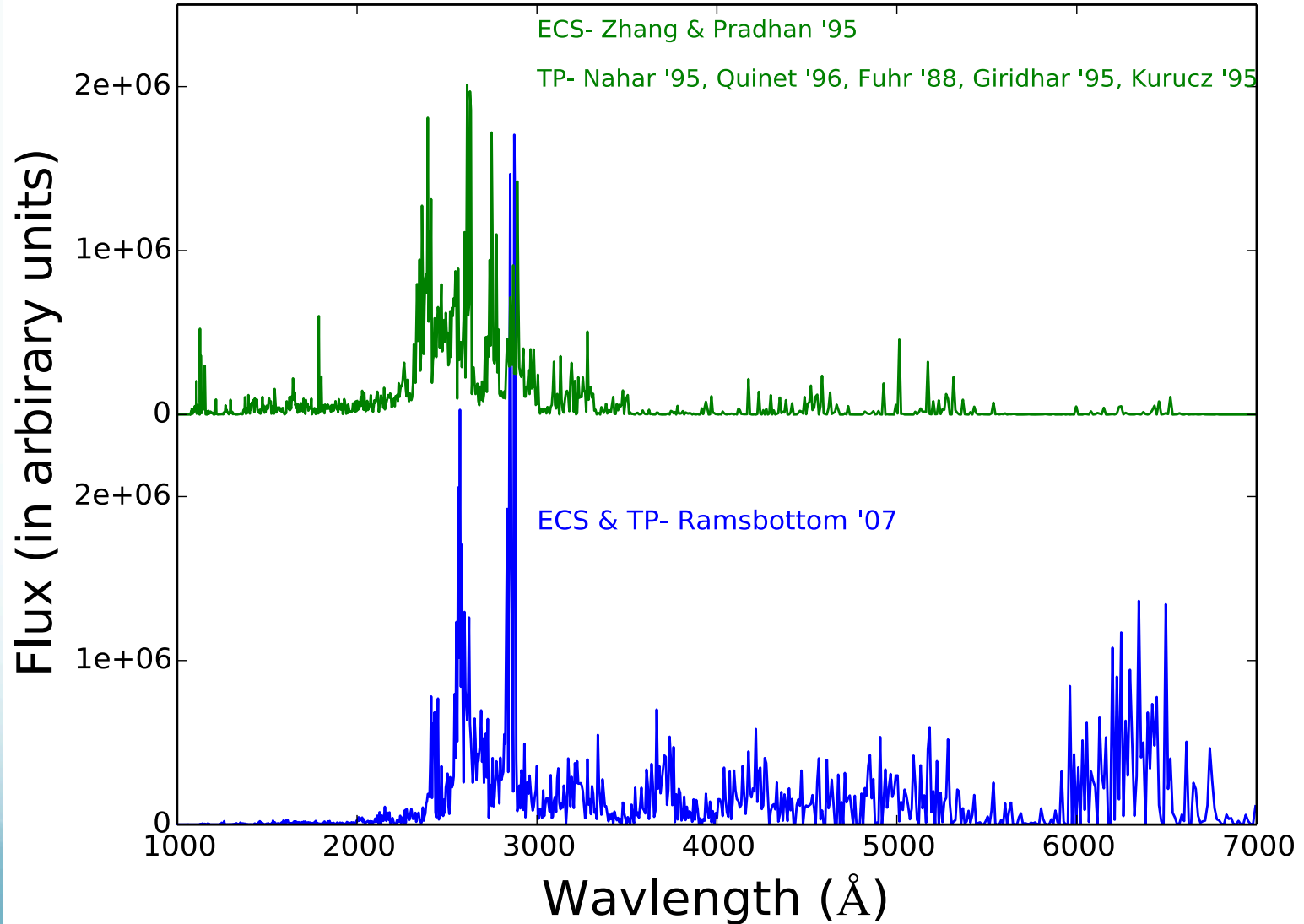
Fe II Transition 7-9



Cloudy Models



Cloudy Models



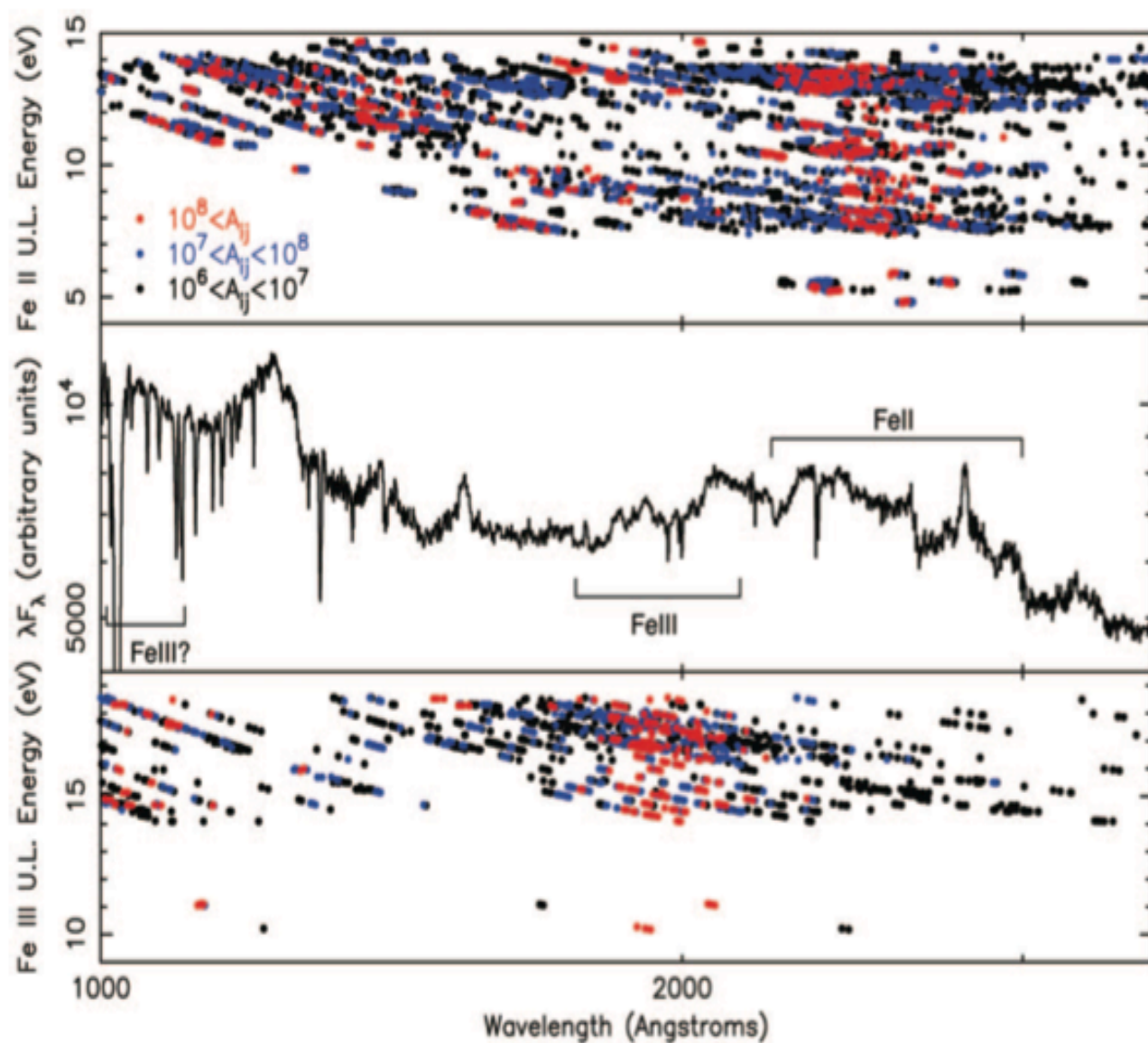
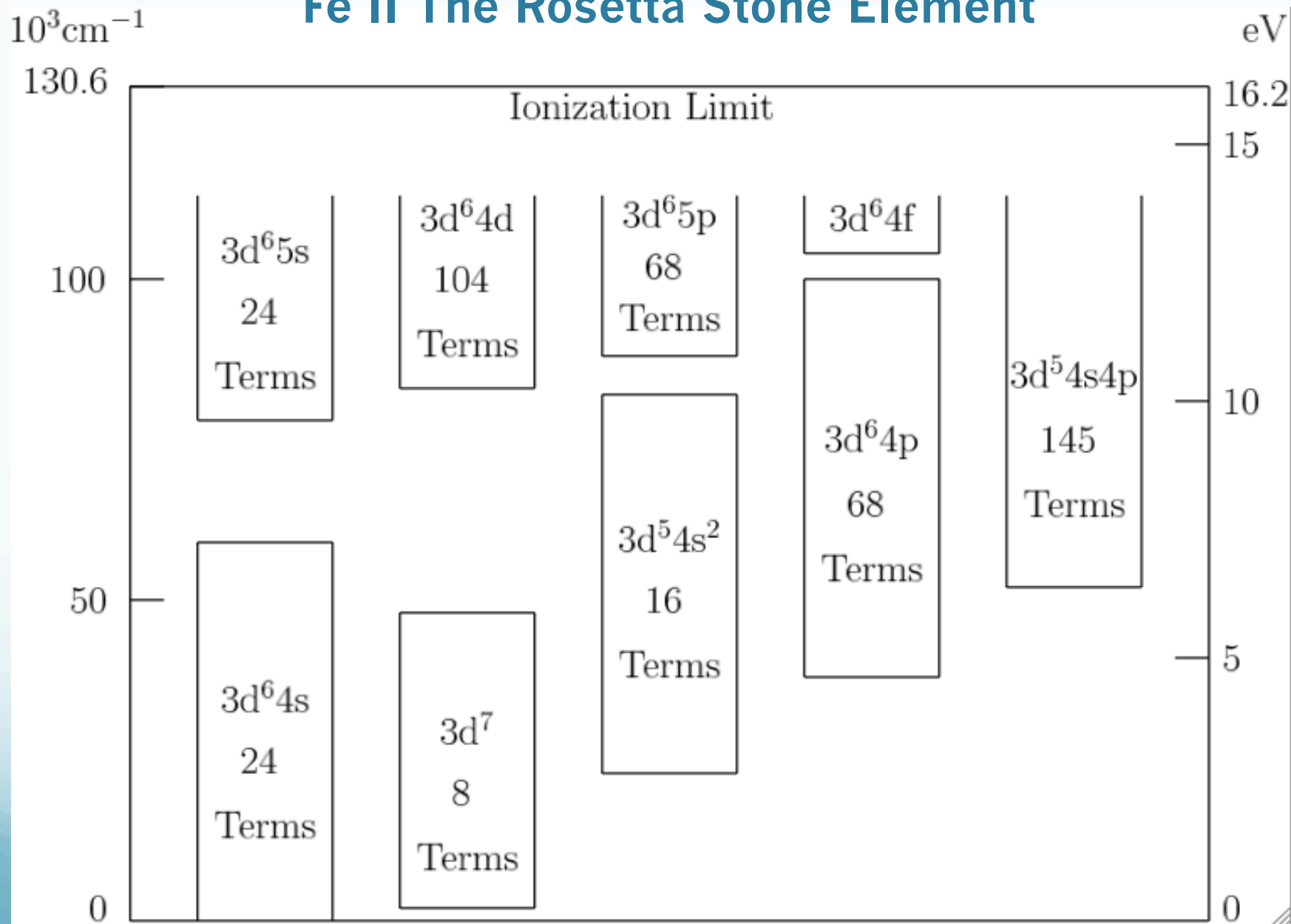


FIG. 6.—*Top:* Upper level energies for Fe II emission lines, color coded according to their A_{ij} value. *Middle:* λF_{λ} spectrum of PHL 1811. *Bottom:* Same as the top panel, for Fe III.

Fe II The Rosetta Stone Element



Latest Calculation from QUB

- 262 LS or 716 $J\pi$ target states with configs $3d^64s$, $3d^7$, $3d^64p$, $3d^54s^2$, $3d^54s4p$
- Last target threshold approximately 23eV
- Breit-Pauli + DARC treatments
- Target energies shifted to NIST where possible
- Highly applicable to recent quasar studies

Thank You