

# Atomic Data Generation at QUB

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# Atomic Data:

- **Energy Levels**
- **Oscillator Strengths/Transition probabilities**
- **Electron-impact excitation collision strengths**
- **Maxwellian averaged effective collision strengths**
- **Photoionisation Cross Sections**
- **Radiative Recombination Rates**
- **Proton Rates**

# Atomic Properties of the Elements

**Frequently used fundamental physical constants**  
 For the most accurate values of these and other constants, visit [physics.nist.gov/constants](http://physics.nist.gov/constants)  
 1 second = 9 192 631 770 periods of radiation corresponding to the transition between the two hyperfine levels of the ground state of <sup>133</sup>Cs

speed of light in vacuum	<i>c</i>	299 792 458 m s <sup>-1</sup>	(exact)
Planck constant	<i>h</i>	6.6261 × 10 <sup>-34</sup> J s	( <i>h</i> = <i>h</i> /2π)
elementary charge	<i>e</i>	1.6022 × 10 <sup>-19</sup> C	
electron mass	<i>m<sub>e</sub></i>	9.1094 × 10 <sup>-31</sup> kg	
	<i>m<sub>e</sub>c<sup>2</sup></i>	0.5110 MeV	
proton mass	<i>m<sub>p</sub></i>	1.6726 × 10 <sup>-27</sup> kg	
fine-structure constant	<i>α</i>	1/137.036	
Rydberg constant	<i>R<sub>∞</sub></i>	10 973 732 m <sup>-1</sup>	
	<i>R<sub>∞</sub>c</i>	3.289 842 × 10 <sup>15</sup> Hz	
	<i>R<sub>∞</sub>hc</i>	13.6057 eV	
Boltzmann constant	<i>k</i>	1.3807 × 10 <sup>-23</sup> J K <sup>-1</sup>	

- Solids
- Liquids
- Gases
- Artificially Prepared

Physics Laboratory <a href="http://physics.nist.gov">physics.nist.gov</a>		Standard Reference Data Group <a href="http://www.nist.gov/srd">www.nist.gov/srd</a>					VIIIA										
13 IIIA	14 IVA	15 VA	16 VIA	17 VIIA	18	2											
5 B Boron 10.811 1s <sup>2</sup> 2s <sup>2</sup> 2p 8.2980	6 C Carbon 12.0107 1s <sup>2</sup> 2s <sup>2</sup> 2p <sup>2</sup> 11.2603	7 N Nitrogen 14.0067 1s <sup>2</sup> 2s <sup>2</sup> 2p <sup>3</sup> 14.5341	8 O Oxygen 15.9994 1s <sup>2</sup> 2s <sup>2</sup> 2p <sup>4</sup> 13.8181	9 F Fluorine 18.9984032 1s <sup>2</sup> 2s <sup>2</sup> 2p <sup>5</sup> 17.4226	10 Ne Neon 20.1797 1s <sup>2</sup> 2s <sup>2</sup> 2p <sup>6</sup> 21.5645	2 He Helium 4.002602 1s <sup>1</sup> 24.5874											
11 Na Sodium 22.989770 [Ne]3s 5.1391	12 Mg Magnesium 24.3050 [Ne]3s <sup>2</sup> 7.6482	13 Al Aluminum 26.981538 [Ne]3s <sup>2</sup> 3p 5.9858	14 Si Silicon 28.0855 [Ne]3s <sup>2</sup> 3p <sup>2</sup> 8.1517	15 P Phosphorus 30.973761 [Ne]3s <sup>2</sup> 3p <sup>3</sup> 10.4887	16 S Sulfur 32.065 [Ne]3s <sup>2</sup> 3p <sup>4</sup> 10.3800	17 Cl Chlorine 35.453 [Ne]3s <sup>2</sup> 3p <sup>5</sup> 12.9676	18 Ar Argon 39.948 [Ne]3s <sup>2</sup> 3p <sup>6</sup> 15.7596										
19 K Potassium 39.0983 [Ar]4s 4.3407	20 Ca Calcium 40.078 [Ar]4s <sup>2</sup> 6.1132	21 Sc Scandium 44.955910 [Ar]3d <sup>1</sup> 4s 6.5615	22 Ti Titanium 47.887 [Ar]3d <sup>2</sup> 4s 6.8281	23 V Vanadium 50.9415 [Ar]3d <sup>3</sup> 4s 6.7462	24 Cr Chromium 51.9961 [Ar]3d <sup>5</sup> 4s 6.7665	25 Mn Manganese 54.938049 [Ar]3d <sup>5</sup> 4s 7.4340	26 Fe Iron 55.845 [Ar]3d <sup>6</sup> 4s 7.9024	27 Co Cobalt 58.933200 [Ar]3d <sup>7</sup> 4s 7.6910	28 Ni Nickel 58.6934 [Ar]3d <sup>8</sup> 4s 7.6398	29 Cu Copper 63.546 [Ar]3d <sup>10</sup> 4s 7.7264	30 Zn Zinc 65.409 [Ar]3d <sup>10</sup> 4s 9.3942	31 Ga Gallium 69.723 [Ar]3d <sup>10</sup> 4s <sup>2</sup> 4p 5.9993	32 Ge Germanium 72.64 [Ar]3d <sup>10</sup> 4s <sup>2</sup> 4p <sup>2</sup> 7.6994	33 As Arsenic 74.92160 [Ar]3d <sup>10</sup> 4s <sup>2</sup> 4p <sup>3</sup> 9.7886	34 Se Selenium 78.96 [Ar]3d <sup>10</sup> 4s <sup>2</sup> 4p <sup>4</sup> 9.7524	35 Br Bromine 79.904 [Ar]3d <sup>10</sup> 4s <sup>2</sup> 4p <sup>5</sup> 11.8138	36 Kr Krypton 83.798 [Ar]3d <sup>10</sup> 4s <sup>2</sup> 4p <sup>6</sup> 13.9996
37 Rb Rubidium 85.4678 [Kr]5s 4.1771	38 Sr Strontium 87.62 [Kr]5s <sup>2</sup> 5.6949	39 Y Yttrium 88.90585 [Kr]4d <sup>1</sup> 5s 6.2173	40 Zr Zirconium 91.224 [Kr]4d <sup>2</sup> 5s 6.6330	41 Nb Niobium 92.90638 [Kr]4d <sup>4</sup> 5s 6.7589	42 Mo Molybdenum 95.94 [Kr]4d <sup>5</sup> 5s 7.0924	43 Tc Technetium (98) [Kr]4d <sup>5</sup> 5s 7.28	44 Ru Ruthenium 101.07 [Kr]4d <sup>7</sup> 5s 7.3855	45 Rh Rhodium 102.90550 [Kr]4d <sup>8</sup> 5s 7.4589	46 Pd Palladium 106.42 [Kr]4d <sup>10</sup> 5s 8.3389	47 Ag Silver 107.8682 [Kr]4d <sup>10</sup> 5s 7.5782	48 Cd Cadmium 112.411 [Kr]4d <sup>10</sup> 5s <sup>2</sup> 8.0938	49 In Indium 114.818 [Kr]4d <sup>10</sup> 5s <sup>2</sup> 5p 5.7884	50 Sn Tin 118.710 [Kr]4d <sup>10</sup> 5s <sup>2</sup> 5p <sup>2</sup> 7.3430	51 Sb Antimony 121.760 [Kr]4d <sup>10</sup> 5s <sup>2</sup> 5p <sup>3</sup> 8.6084	52 Te Tellurium 127.60 [Kr]4d <sup>10</sup> 5s <sup>2</sup> 5p <sup>4</sup> 9.0096	53 I Iodine 126.90447 [Kr]4d <sup>10</sup> 5s <sup>2</sup> 5p <sup>5</sup> 10.4513	54 Xe Xenon 131.293 [Kr]4d <sup>10</sup> 5s <sup>2</sup> 5p <sup>6</sup> 12.1298
55 Cs Cesium 132.90545 [Xe]6s 3.8939	56 Ba Barium 137.327 [Xe]6s <sup>2</sup> 5.2117	57 La Lanthanum 138.90549 [Xe]5d <sup>1</sup> 6s 6.8251	58 Ce Cerium 140.116 [Xe]4f <sup>1</sup> 5d <sup>1</sup> 6s 5.5387	59 Pr Praseodymium 140.90765 [Xe]4f <sup>3</sup> 6s 5.473	60 Nd Neodymium 144.24 [Xe]4f <sup>4</sup> 6s 5.5250	61 Pm Promethium (145) [Xe]4f <sup>5</sup> 6s 5.582	62 Sm Samarium 150.36 [Xe]4f <sup>6</sup> 6s 5.6437	63 Eu Europium 151.964 [Xe]4f <sup>7</sup> 6s 5.6704	64 Gd Gadolinium 157.25 [Xe]4f <sup>7</sup> 5d <sup>1</sup> 6s 6.1406	65 Tb Terbium 158.92534 [Xe]4f <sup>9</sup> 6s 5.8938	66 Dy Dysprosium 162.500 [Xe]4f <sup>10</sup> 6s 5.9389	67 Ho Holmium 164.93032 [Xe]4f <sup>11</sup> 6s 6.0215	68 Er Erbium 167.259 [Xe]4f <sup>12</sup> 6s 6.1077	69 Tm Thulium 168.93421 [Xe]4f <sup>13</sup> 6s 6.1843	70 Yb Ytterbium 173.04 [Xe]4f <sup>14</sup> 6s 6.2542	71 Lu Lutetium 174.967 [Xe]4f <sup>14</sup> 5d <sup>1</sup> 6s 5.4250	
87 Fr Francium (223) [Rn]7s 4.0727	88 Ra Radium (226) [Rn]7s <sup>2</sup> 5.2784	89 Ac Actinium (227) [Rn]6d <sup>1</sup> 7s 5.17	90 Th Thorium 232.0381 [Rn]6d <sup>2</sup> 7s 6.3087	91 Pa Protactinium 231.03688 [Rn]5f <sup>2</sup> 6d <sup>1</sup> 7s 5.89	92 U Uranium 238.02891 [Rn]5f <sup>3</sup> 6d <sup>1</sup> 7s 6.1941	93 Np Neptunium (237) [Rn]5f <sup>4</sup> 6d <sup>1</sup> 7s 6.2637	94 Pu Plutonium (244) [Rn]5f <sup>6</sup> 7s 6.0280	95 Am Americium (243) [Rn]5f <sup>7</sup> 7s 5.9738	96 Cm Curium (247) [Rn]5f <sup>8</sup> 7s 5.9914	97 Bk Berkelium (247) [Rn]5f <sup>9</sup> 7s 6.1979	98 Cf Californium (251) [Rn]5f <sup>10</sup> 7s 6.2917	99 Es Einsteinium (252) [Rn]5f <sup>11</sup> 7s 6.42	100 Fm Fermium (257) [Rn]5f <sup>12</sup> 7s 6.50	101 Md Mendelevium (258) [Rn]5f <sup>13</sup> 7s 6.58	102 No Nobelium (259) [Rn]5f <sup>14</sup> 7s 6.65	103 Lr Lawrencium (262) [Rn]5f <sup>14</sup> 7s <sup>2</sup> 7p 4.97	

IA	IIA	IIIB	IVB	VB	VIB	VII B	VIII	IB	IIB				
1 H Hydrogen 1.00794 1s 13.5984	2 He Helium 4.002602 1s <sup>1</sup> 24.5874	3 Li Lithium 6.941 1s <sup>2</sup> 2s 5.3917	4 Be Beryllium 9.012182 1s <sup>2</sup> 2s <sup>2</sup> 9.3227	11 Na Sodium 22.989770 [Ne]3s 5.1391	12 Mg Magnesium 24.3050 [Ne]3s <sup>2</sup> 7.6482	19 K Potassium 39.0983 [Ar]4s 4.3407	20 Ca Calcium 40.078 [Ar]4s <sup>2</sup> 6.1132	37 Rb Rubidium 85.4678 [Kr]5s 4.1771	38 Sr Strontium 87.62 [Kr]5s <sup>2</sup> 5.6949	55 Cs Cesium 132.90545 [Xe]6s 3.8939	56 Ba Barium 137.327 [Xe]6s <sup>2</sup> 5.2117	87 Fr Francium (223) [Rn]7s 4.0727	88 Ra Radium (226) [Rn]7s <sup>2</sup> 5.2784

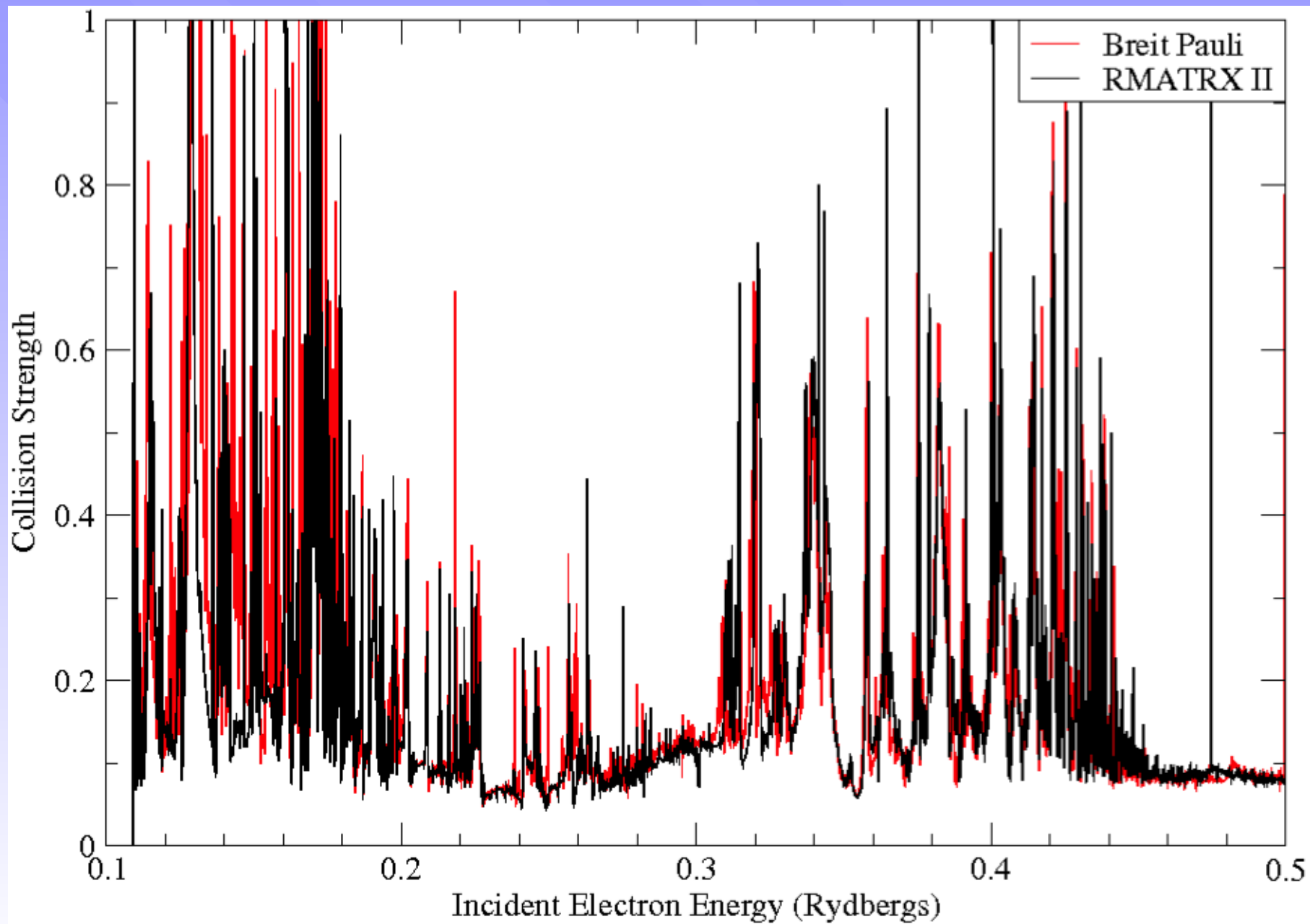
Atomic Number: 58  
 Ground-state Level: 1G<sub>4</sub>  
 Symbol: Ce  
 Name: Cerium  
 Atomic Weight: 140.116  
 Ground-state Configuration: [Xe]4f<sup>1</sup>5d<sup>1</sup>6s<sup>2</sup>  
 Ionization Energy (eV): 5.5387

Lanthanides  
 Actinides



# R-matrix Methodologies:

- **RMATRX I (LS coupling)**
- **BP (1 body terms included in Hamiltonian)**
- **DARC (all 1+2 body terms included)**
- **RMATRX II (LS + transformation)**
- **ICFT (LS + transformation)**
- **B-spline R-matrix**



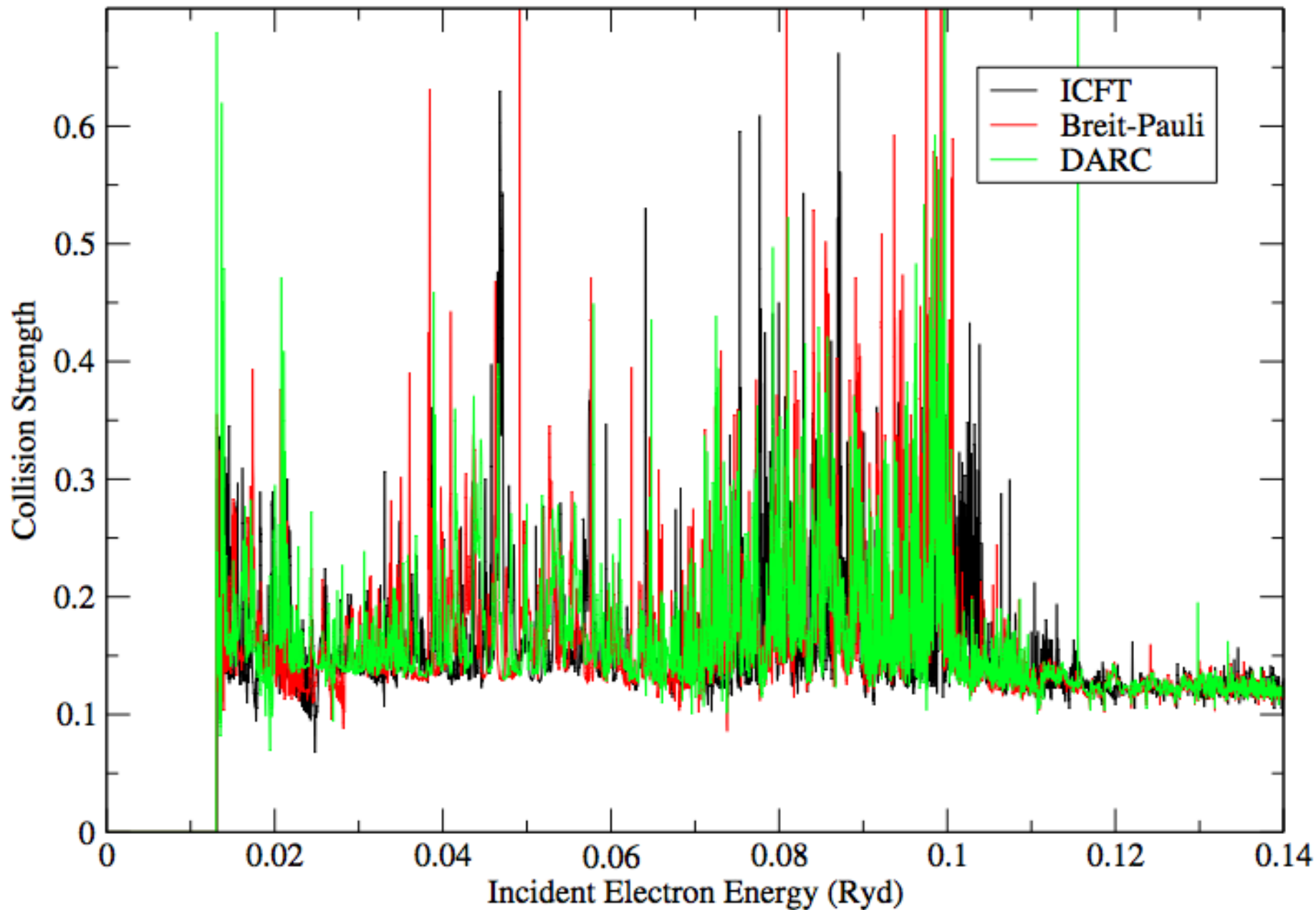


Figure 9.7: Collision strengths for the  $3d^3\ ^4F_{3/2} - 3d^3\ ^2P_{3/2}$  transition.

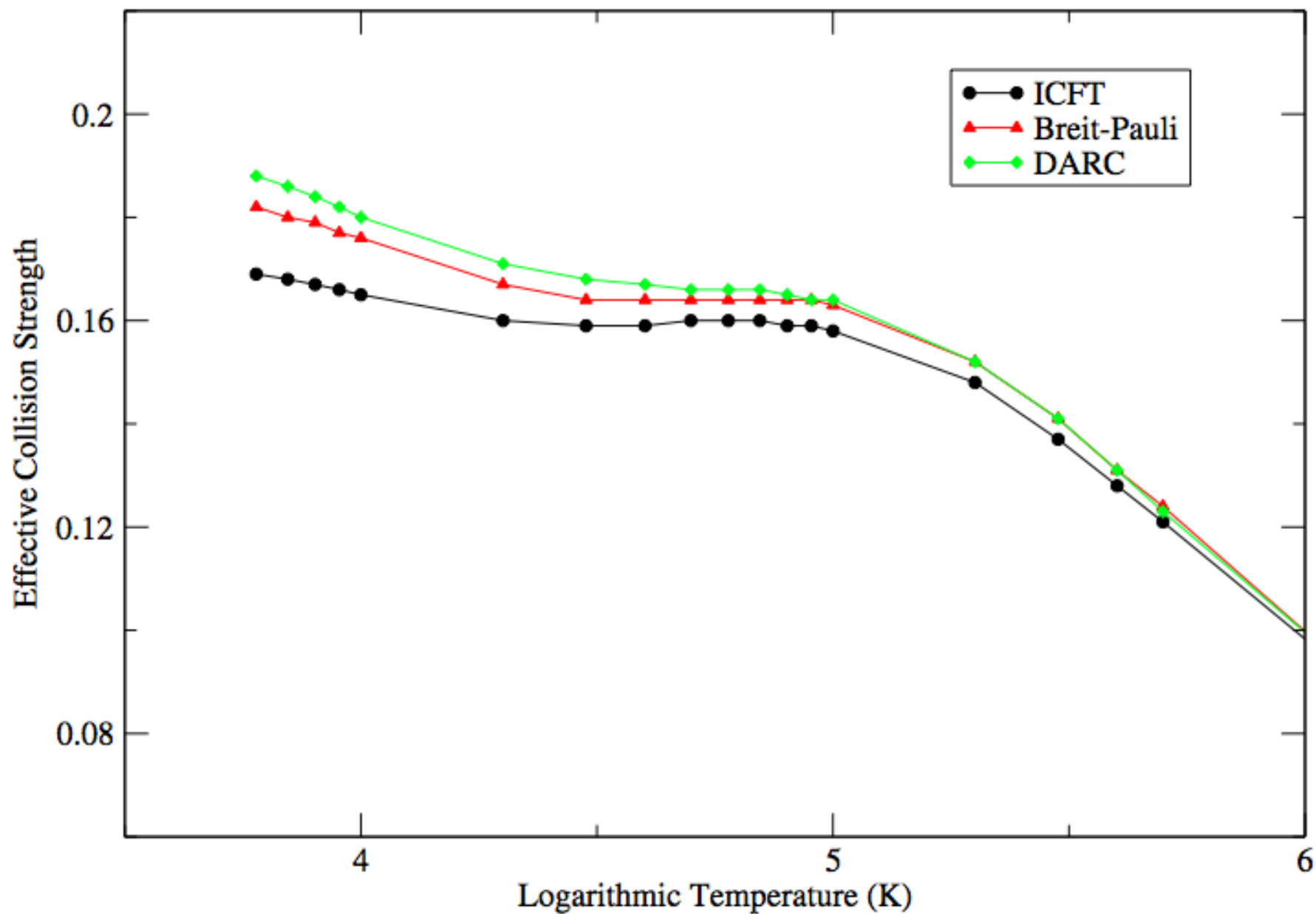


Figure 9.8: Effective collision strengths for the  $3d^3\ ^4F_{3/2} - 3d^3\ ^2P_{3/2}$  transition.



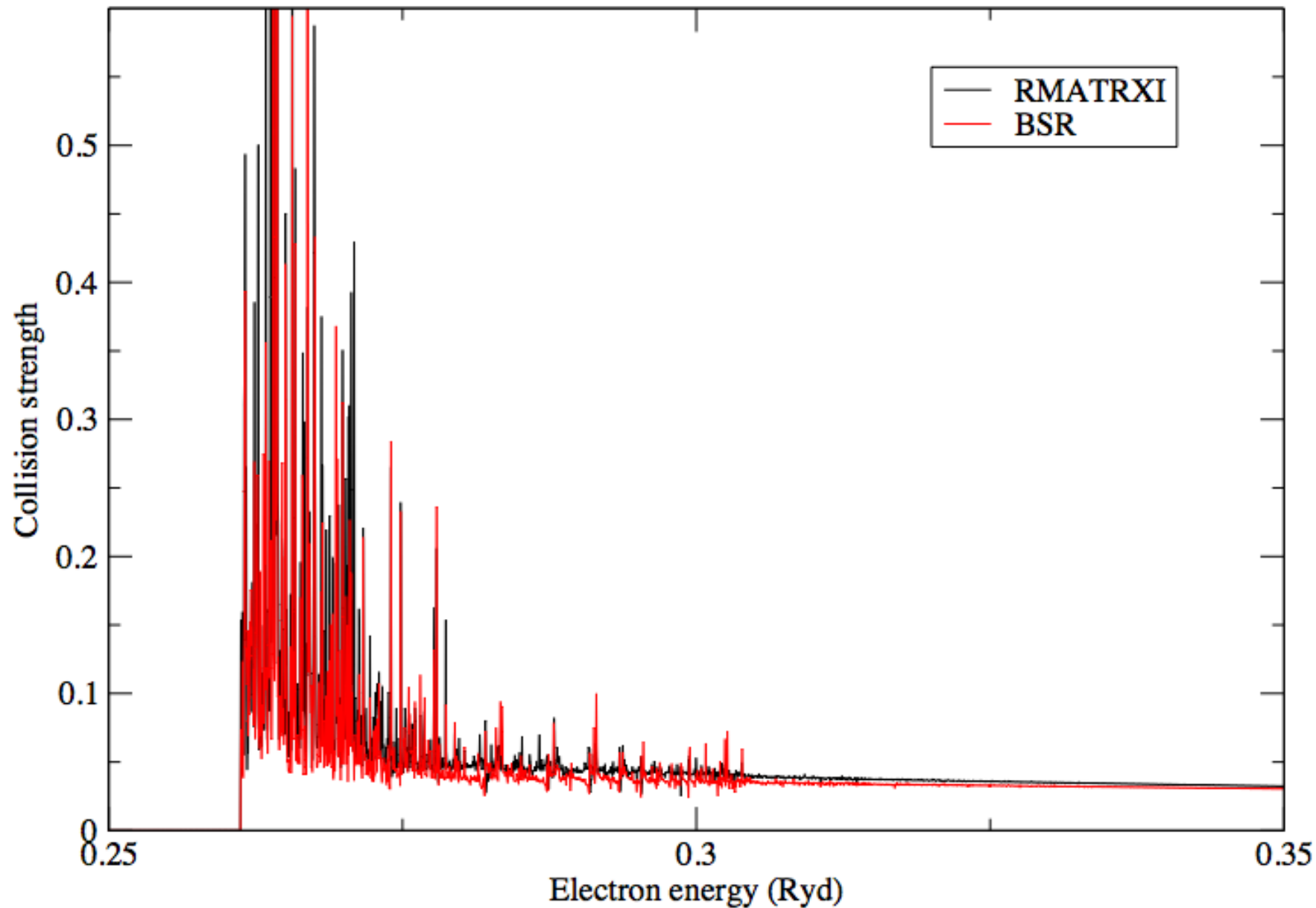


Figure D.1: Collision strength as a function of incident electron energy for the  $2s^22p\ ^2P_{1/2}^o - 2p^3\ ^2P_{3/2}^o$  transition.

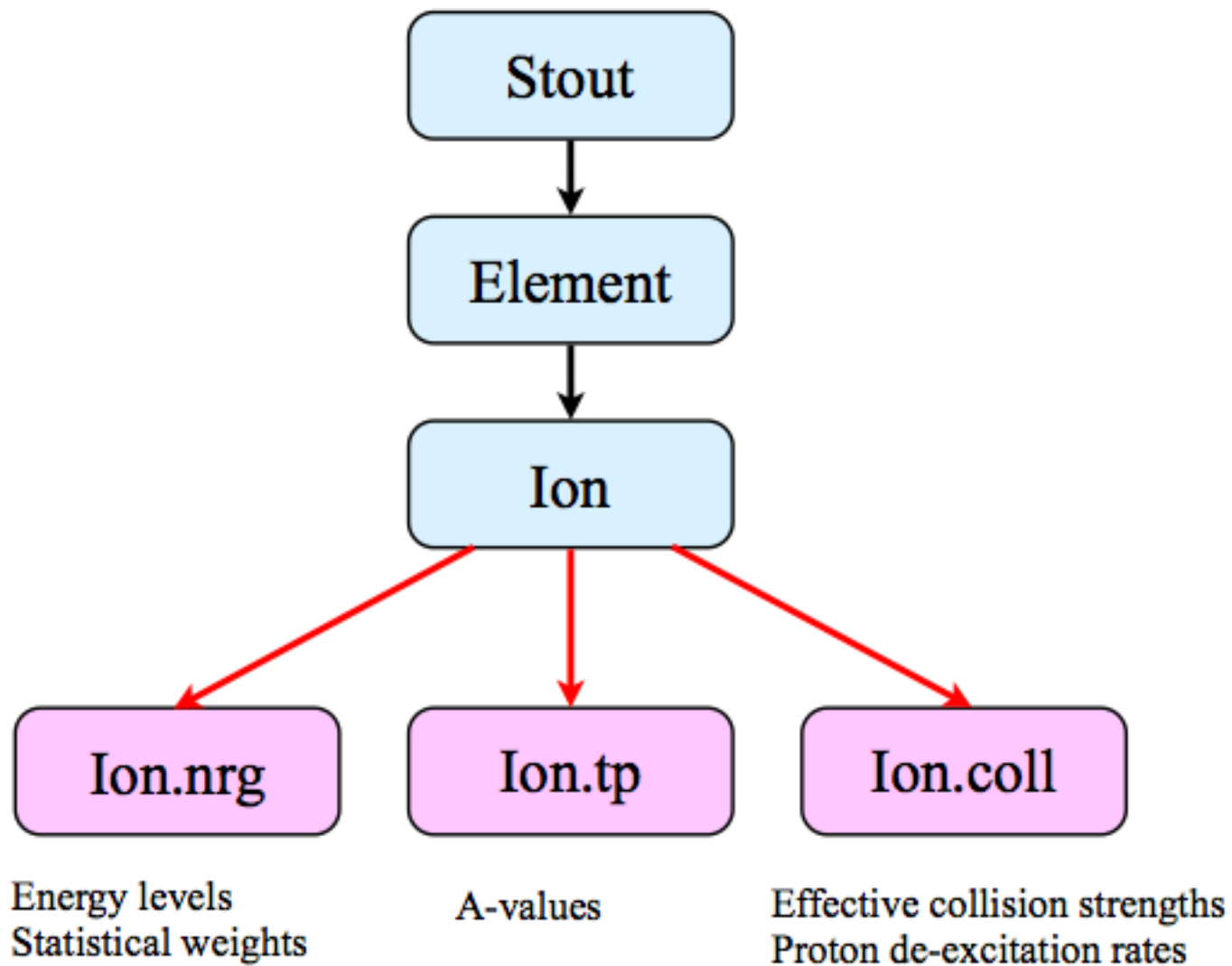
# Main Applications:

## **CLOUDY**

- Energy Levels
- A values
- Effective Collision Strengths
- Proton Rates

## **Supernovae**

- Energy Levels
- A values
- Photoionization Cross Sections
- Recombination Rates



# Main Applications:

## **CLOUDY**

- Energy Levels
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# Fusion Applications:

- **Iter**
- **All ionization Levels of W ions**
- **Energy Levels**
- **Radiative Atomic Data**
- **Collisional Atomic Data**

Fe II

(NZ=26 :NELC=25)

Ground state:  $1s^2 2s^2 2p^6 3s^2 3p^6 3d^6 4s$

$1s^2 2s^2 2p^6 3s^2 3p^6 3d^7$

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

