Queen's University Belfast

Atomic Data for Fe-peak Ions using RMATRX II

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Introduction

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One of the major outstanding problems in atomic collision physics .....

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The accurate treatment of scattering from open d-shell systems

Open 3d-shell Systems

1 H																	2 He
3 Li	4 Be										5 B	6 C	7 N	8 O	9 F	10 Ne
11 Na	12 Mg										13 Al	14 Si	15 P	16 S	17 Cl	18 Ar
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
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
55 Cs	56 Ba	71 Lu	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
87 Fr	88 Ra	103 Lr	104 Rf	105 Db	106 Sg	107 Bh	108 Hs	109 Mt	110 Ds	111 Rg	112 Uub	113 Uut	114 Uuq	115 Uup	116 Uuh	117 Uus	118 Uuo

Ions of the astrophysically important Fe-peak elements have an open 3d-shell

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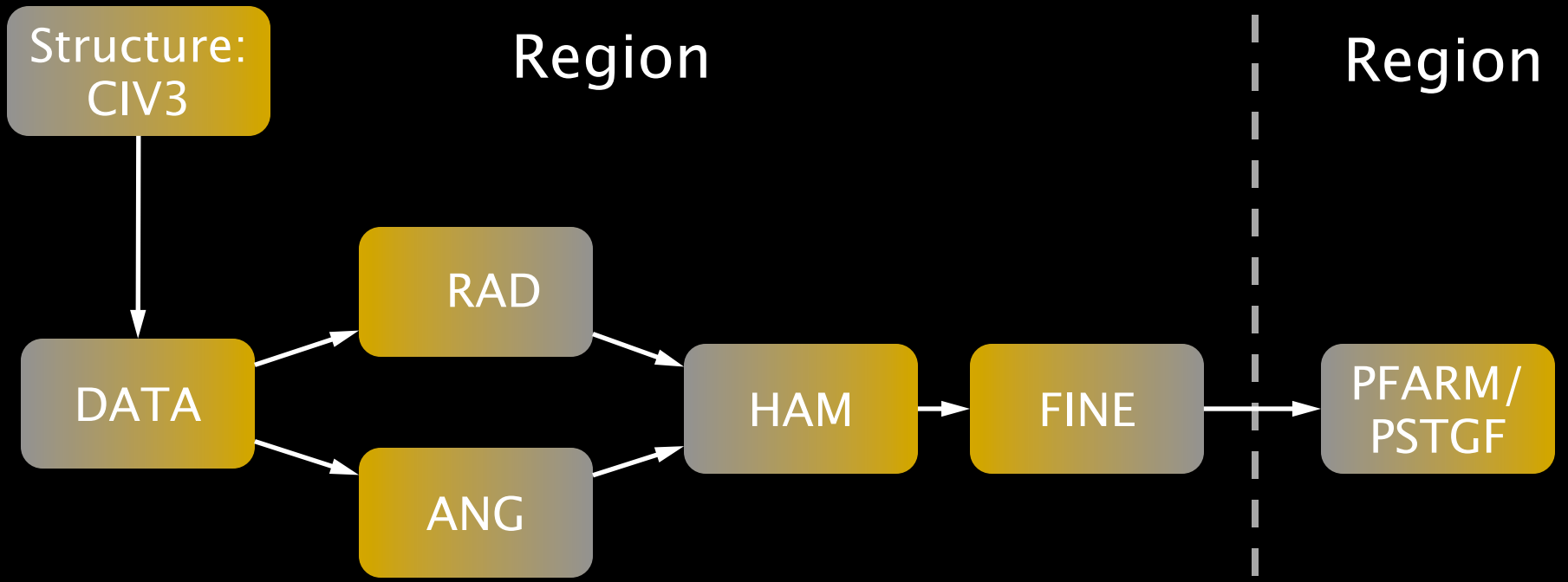
RMATRX II Codes



Target Model – Fe II

Fe II Target Configurations	No. of Target States (LS)	No. of Channels (LS)	No. of Target States (jj)	No. of Channels (jj)
$3d^6 4s$	24	73	63	420
$3d^7$	32	98	82	540
$3d^6 4p$	100	315	262	1800
$3d^5 4s^2$	116	366	299	2052
$3d^5 4s4p$	261	818	716	5076

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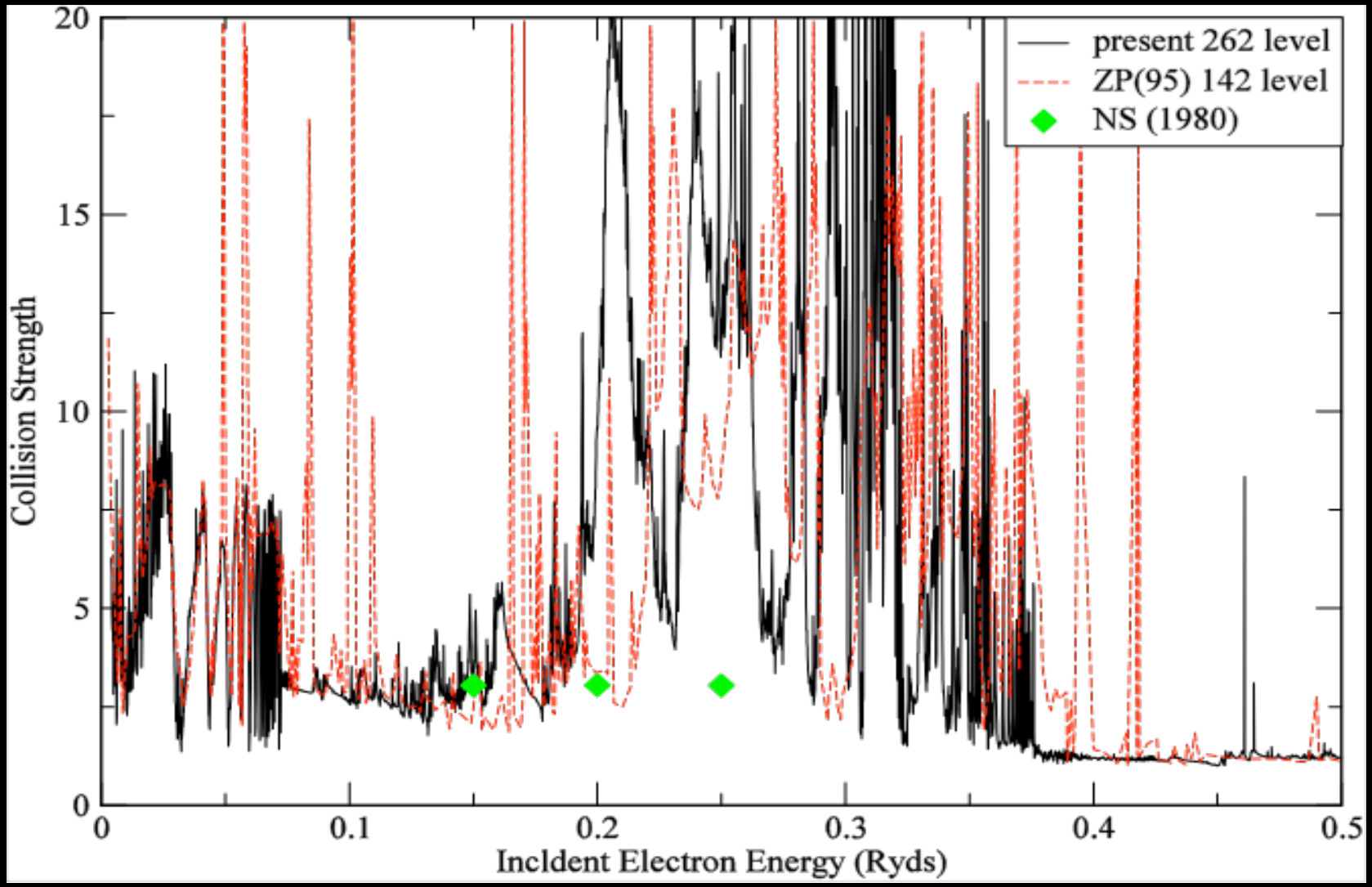
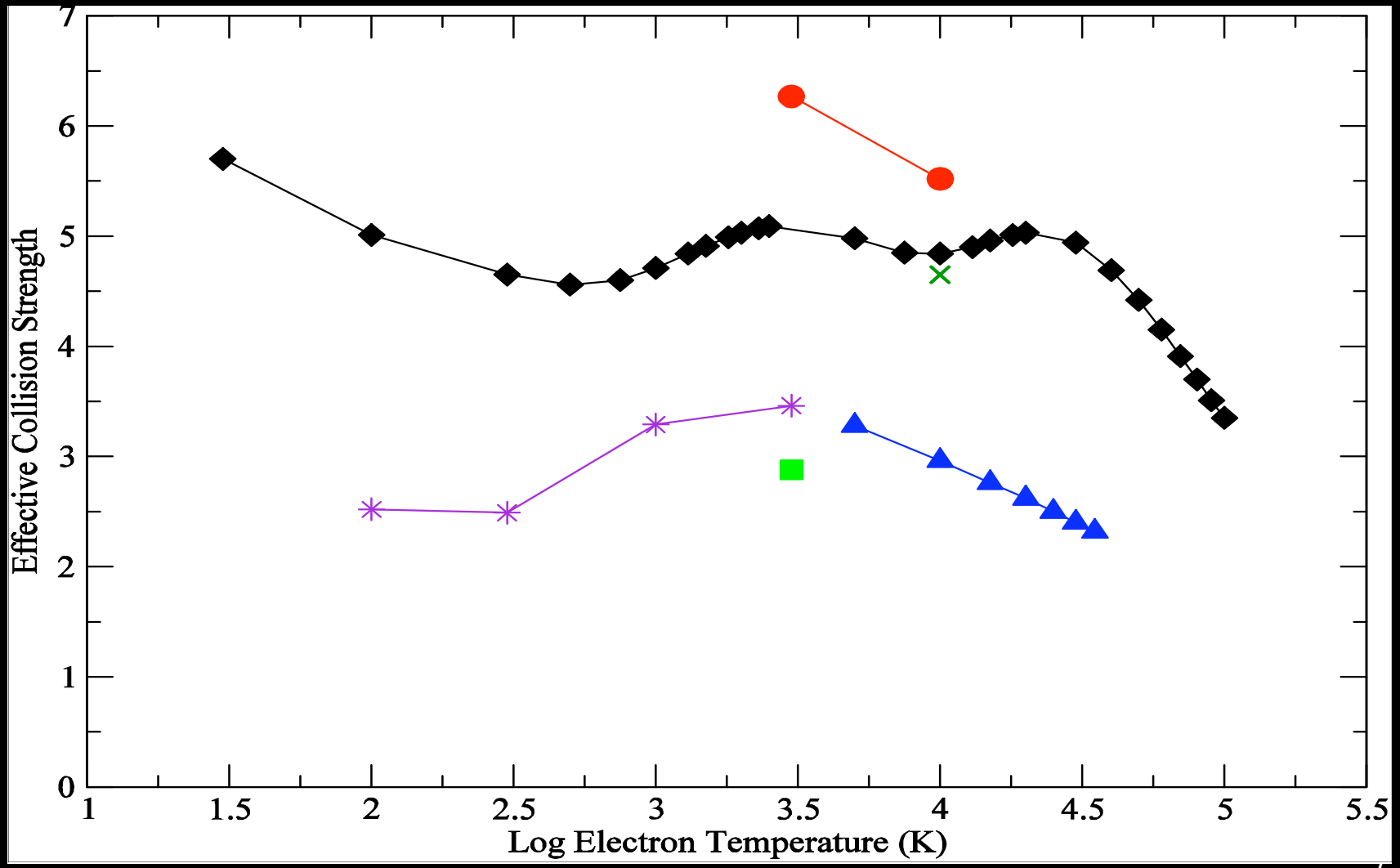
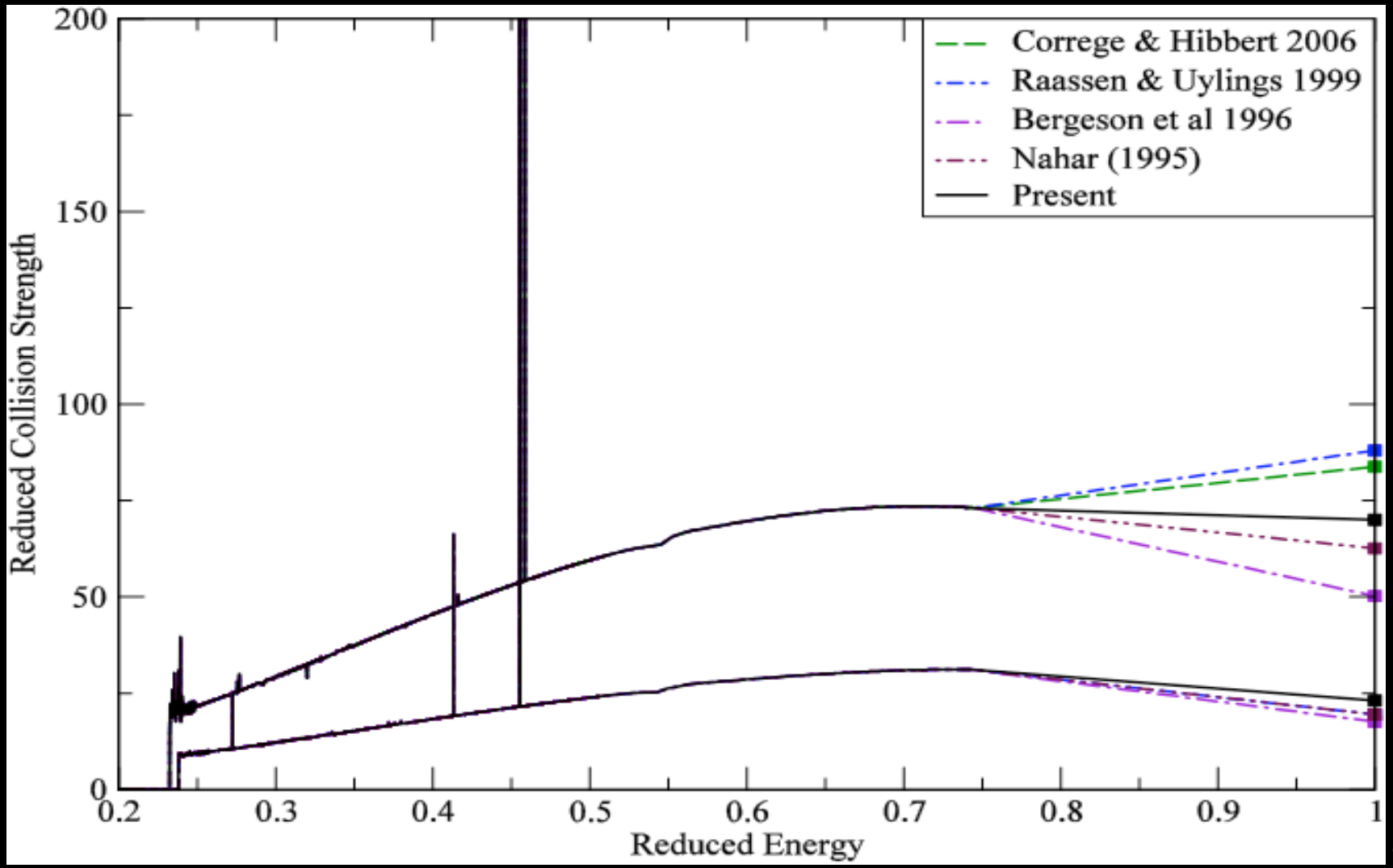
$3d^64s\ {}^6D^e_{9/2} - 3d^64s$



ZP(95), Berr (88), Keenan(88), BP(96)



$3d^6 4s\ {}^6D^e_{9/2}$ – $3d^6 4p\ {}^6F^o_{11/2}, {}^6P^o_{7/2}$



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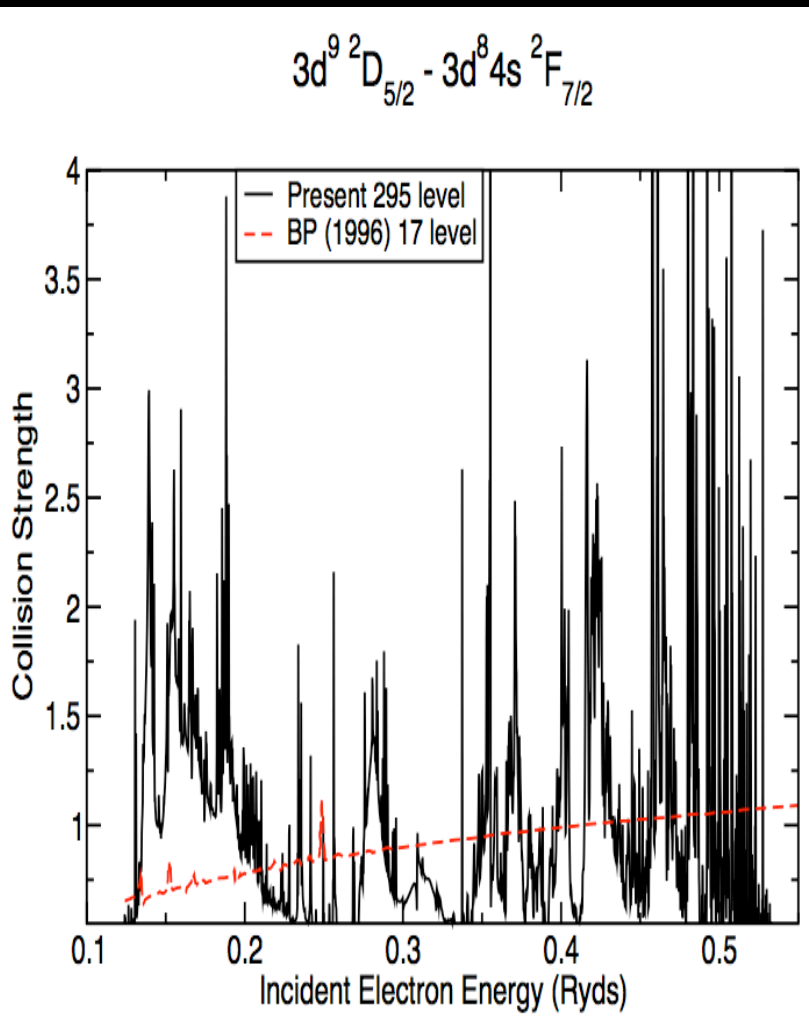
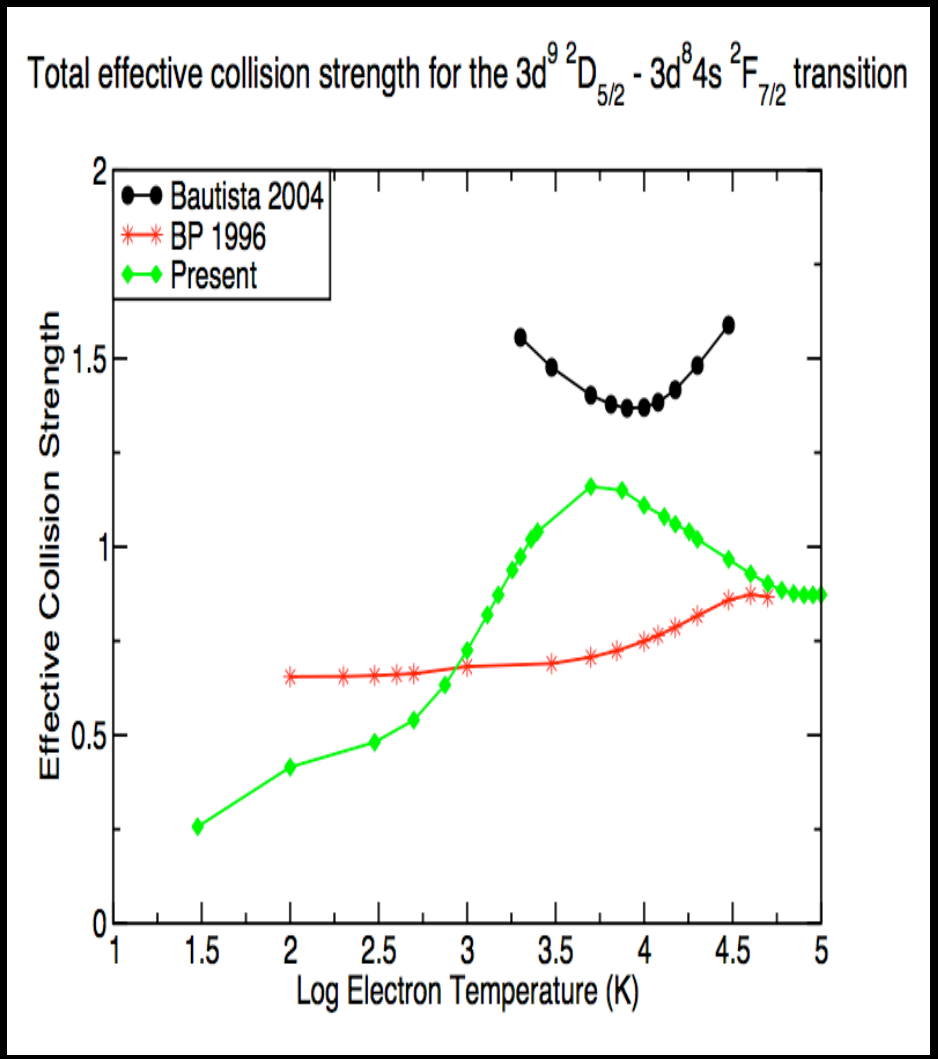
No. Jπ target states	Max no. Channels	Max size of (N+1) electron H matrix	Total no. transitions
262	1800	36,055	34,453
716	5076	>100,000	256,686

Target Model – Ni II

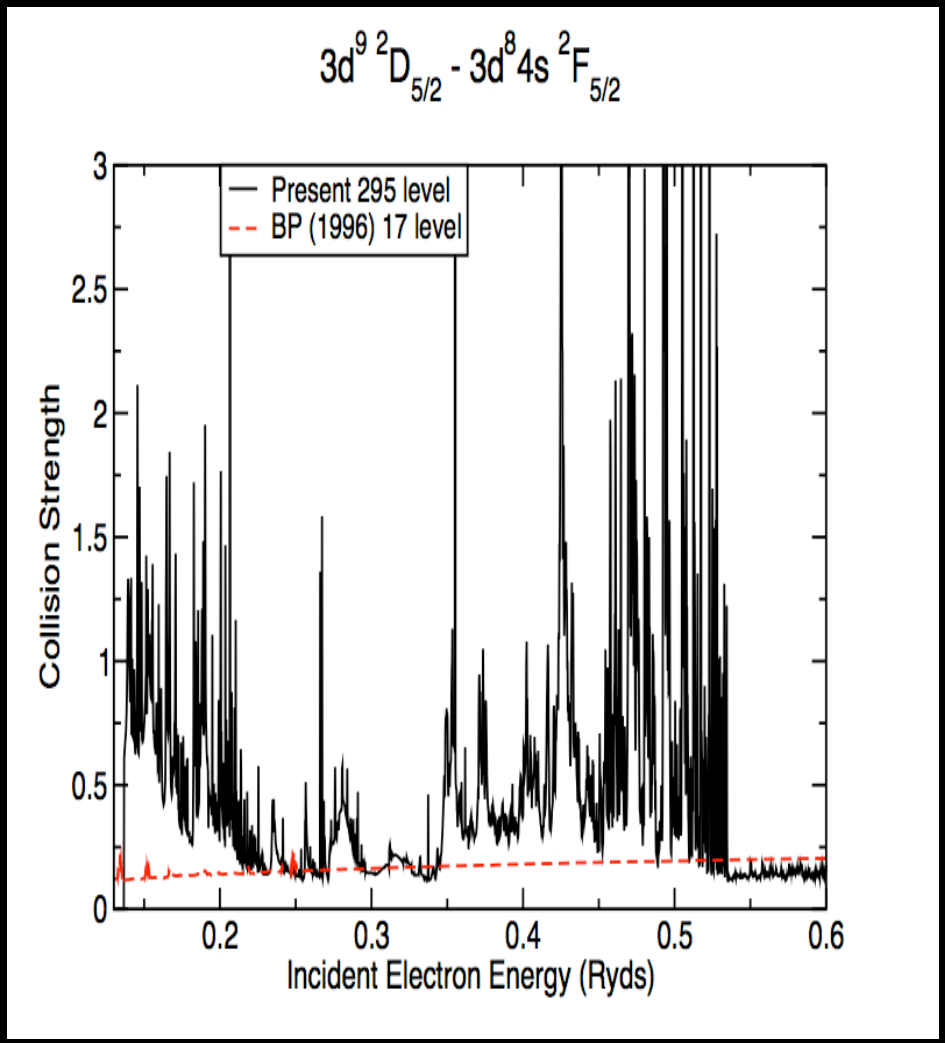
Ni II Target Configurations	No. of Target States (LS)	No. of Channels (LS)	No. of Target States (jj)	No. of Channels (jj)
$3d^9$	1	3	2	10
$3d^8 4s$	8	20	18	100
$3d^7 4s^2$	16	46	37	220
$3d^8 4p$	35	99	82	490
$3d^7 4s 4p$	113	327	295	1930

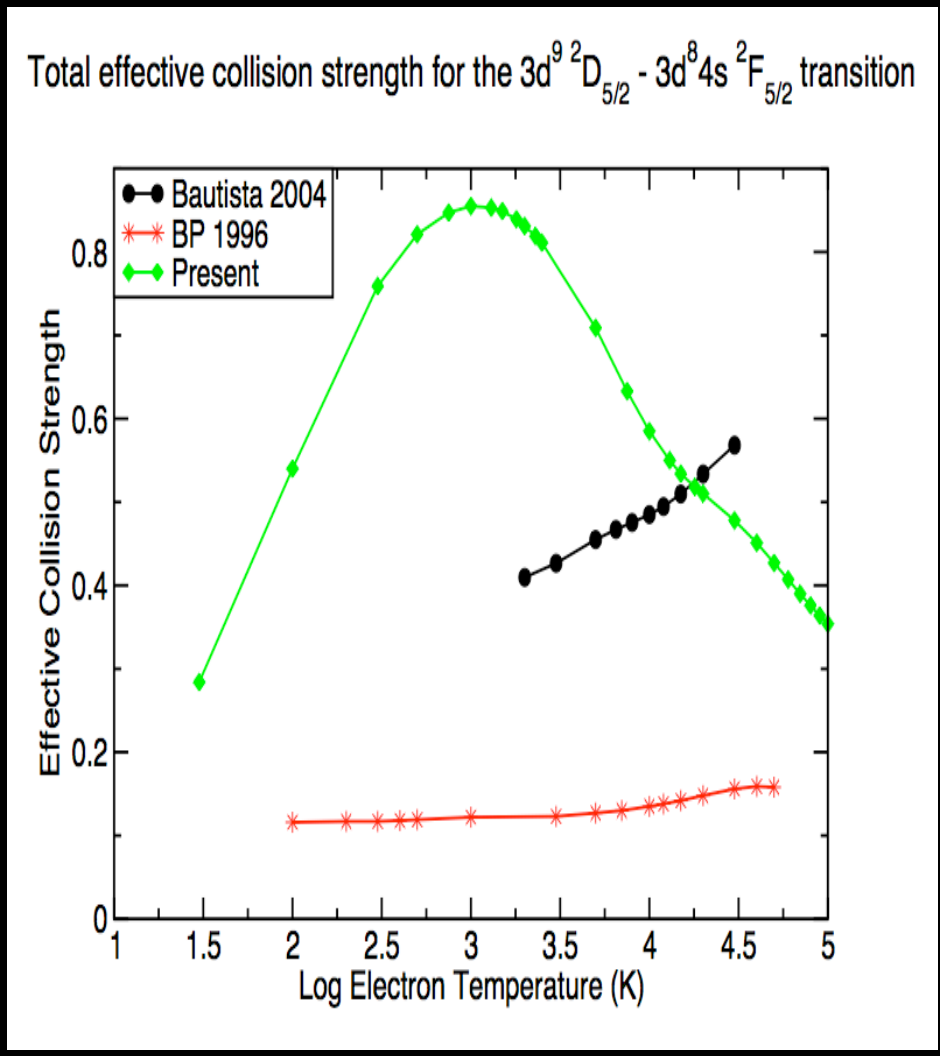
Collisions with Ni II





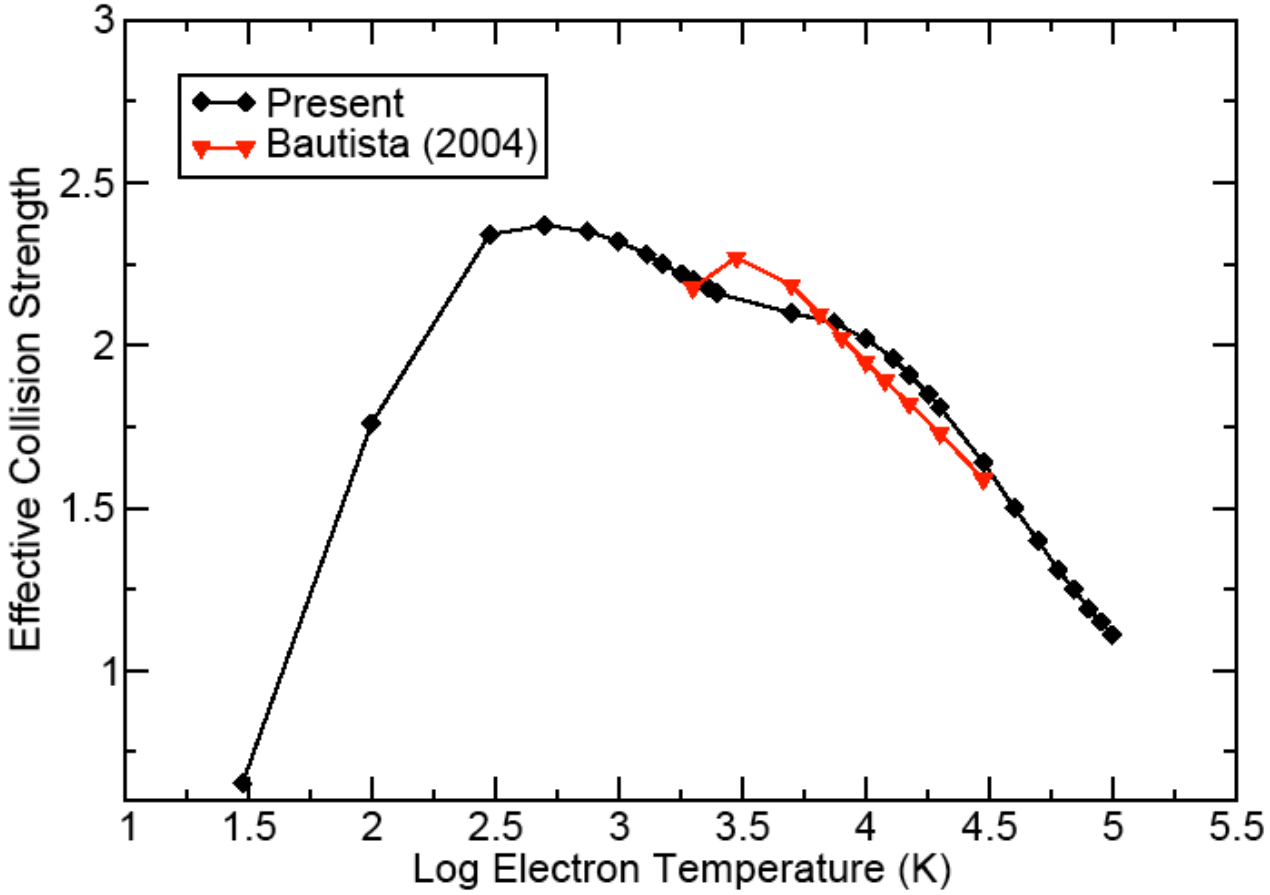
Collisions with Ni II





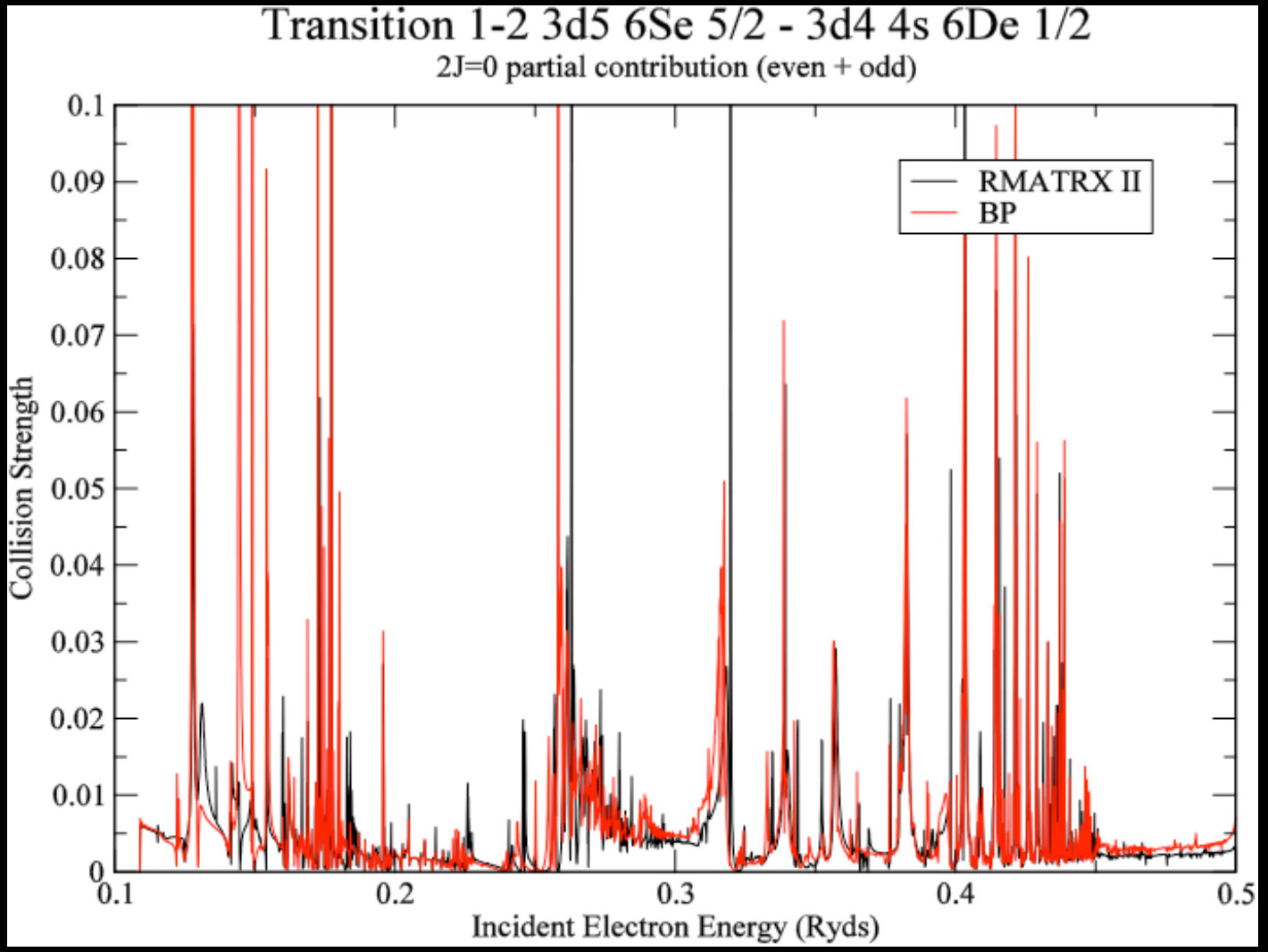
Effective Collision Strengths

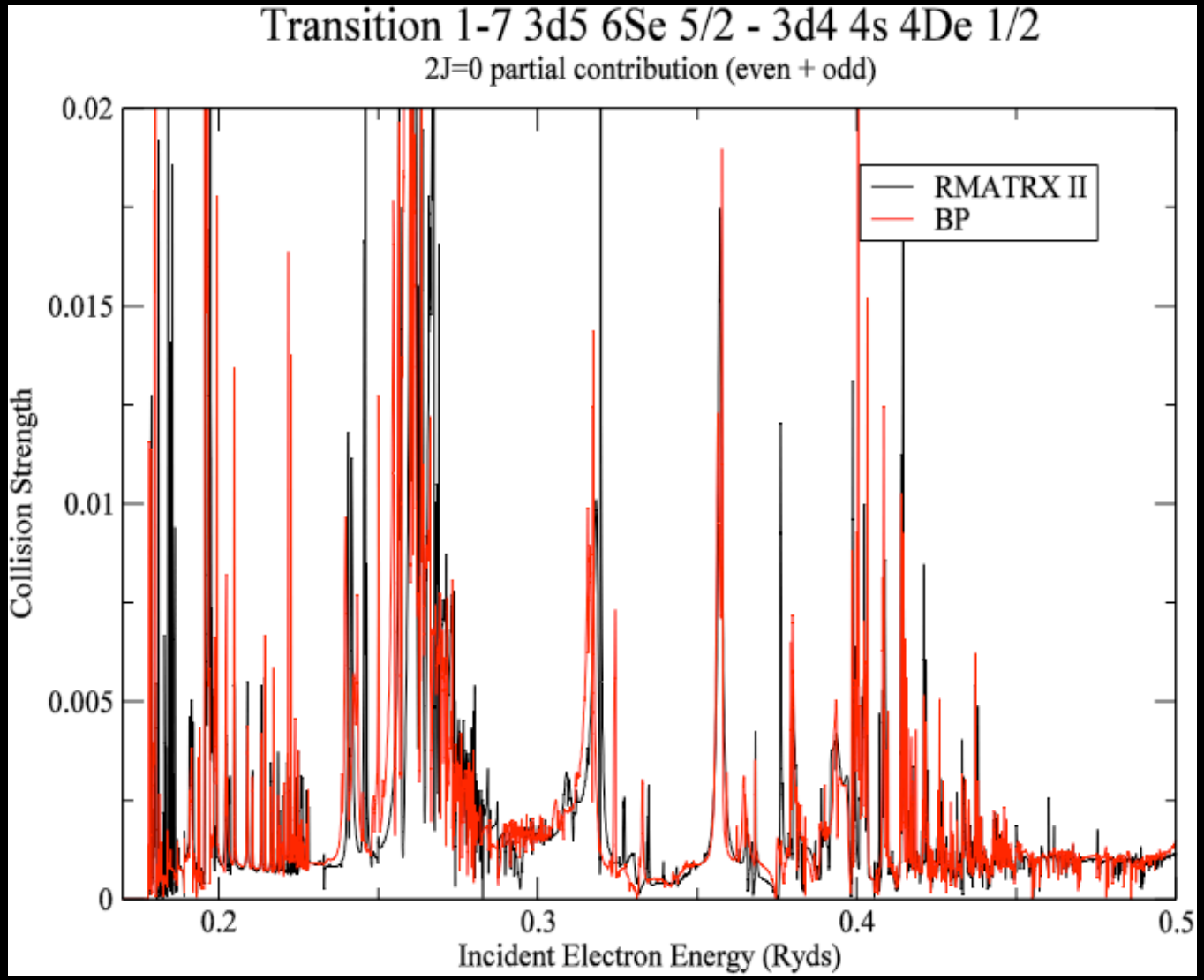
Total effective collision strength for the $3d^9\ ^2D_{5/2}$ - $3d^9\ ^2D_{3/2}$ transition



Target Model – Cr II

Ni II Target Configurations	No. of Target States (LS)	No. of Channels (LS)	No. of Target States (jj)	No. of Channels (jj)
$3d^5$	16	51	37	252
$3d^4 4s$	40	124	100	672
$3d^4 4p$	108	342	280	1932
$3d^3 4s^2$	116	366	299	2052
$3d^3 4s4p$	194	591	512	3492


Transition 1-2 3d5 6Se 5/2 - 3d4 4s 6De 1/2
2J=0 partial contribution (even + odd)
RMATRX II
BP
Collision Strength
Incident Electron Energy (Ryds)
0.1
0.09
0.08
0.07
0.06
0.05
0.04
0.03
0.02
0.01
0
0.1
0.2
0.3
0.4
0.5


Transition 1-7 3d5 6Se 5/2 - 3d4 4s 4De 1/2
2J=0 partial contribution (even + odd)
RMATRX II
BP
Collision Strength
0.02
0.015
0.01
0.005
0
0.2
0.3
0.4
0.5
Incident Electron Energy (Ryds)

Looking to the future…

- We need to continue to push the boundaries on the scale of these calculations.
- Calculations completed for Fe II and Fe III.
- Calculations ongoing for Ni II, Ni V and Cr II with exciting results to follow!

Complete Sets of Data

- Electron-impact collision strengths and effective collision strengths.
- Radiative data – oscillator strengths and transition probabilities.
- Photoionization cross sections

Thank you!

http://web.am.qub.ac.uk/apa/