# Atomic Structure and Collisional Calculations in W LXIV

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# Introduction

- Na-like Tungsten
- Ground State $1s^2 2s^2 2p^6 3s\ {}^2S$
- Can we use non-relativistic orbitals?

# Structure Calculation - Energy Levels

| Configuration | J | CIV3 (Ry) | NIST (Ry) | GRASP0 (Ry) |
|---|---|---|---|---|
| $2p^6 3s\ ^2S$ | 0.5 | 0.00 | 0.00 | 0.00 |
| $2p^6 3p\ ^2P^o$ | 0.5 | 11.53 | 11.73 | 11.87 |
| | 1.5 | 37.03 | 39.19 | 39.63 |
| $2p^6 3d\ ^2D$ | 1.5 | 52.28 | 52.97 | 53.53 |
| | 2.5 | 58.25 | 59.21 | 59.93 |
| $2p^6 4s\ ^2S$ | 0.5 | 237.98 | 239.12 | 239.56 |
| $2p^6 4p\ ^2P^o$ | 0.5 | 241.58 | 243.92 | 244.46 |
| | 1.5 | 254.17 | 255.18 | 255.82 |
| $2p^6 4d\ ^2D$ | 1.5 | 258.97 | 260.37 | 261.11 |
| | 2.5 | 262.08 | 263.09 | 263.87 |
| $2p^6 4f\ ^2F^o$ | 2.5 | 265.32 | 265.94 | 266.50 |
| | 3.5 | 266.51 | 267.09 | 267.84 |

# Structure Calculation - Energy Levels

| Configuration | J | CIV3 (Ry) | NIST (Ry) | GRASP0 (Ry) |
|---|---|---|---|---|
| $2p^6 5s\ ^2S$ | 0.5 | 348.56 | - | 346.74 |
| $2p^6 5p\ ^2P^o$ | 0.5 | 350.58 | - | 348.53 |
| | 1.5 | 353.22 | - | 354.23 |
| $2p^6 5d\ ^2D$ | 1.5 | 358.30 | - | 356.83 |
| | 2.5 | 358.30 | 357.54 | 358.25 |
| $2p^6 5f\ ^2F^o$ | 2.5 | 360.87 | 358.84 | 359.63 |
| | 3.5 | 358.93 | 359.46 | 360.24 |
| $2p^6 5g\ ^2G$ | 3.5 | 359.19 | 359.77 | 360.43 |
| | 4.5 | 359.54 | 360.11 | 360.80 |

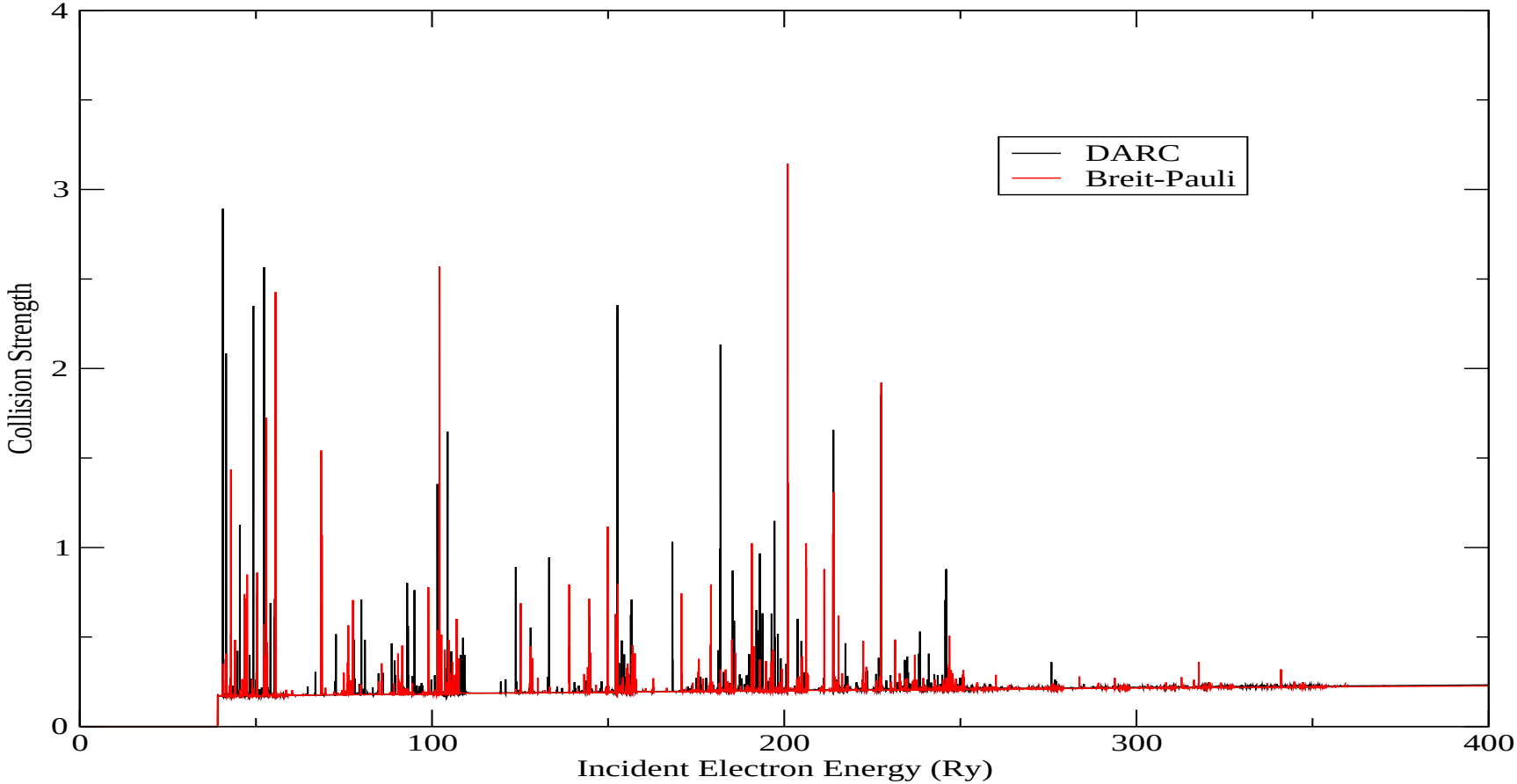
# Structure Calculation - A-values

| Transition | CIV3 | GRASP0 | $\Delta$ (%) |
|---|---|---|---|
| $3s\ ^2S_{1/2} \rightarrow 3p\ ^2P^o_{3/2}$ | 1.49E+12 | 1.82E+12 | +22.15 |
| $3s\ ^2S_{1/2} \rightarrow 4p\ ^2P^o_{3/2}$ | 5.13E+13 | 3.80E+13 | -25.93 |
| $4p\ ^2P^o_{3/2} \rightarrow 4d\ ^2D_{5/2}$ | 5.22E+10 | 5.66E+10 | +8.43 |
| $4p\ ^2P^o_{3/2} \rightarrow 5d\ ^2D_{5/2}$ | 2.41E+13 | 2.29E+13 | -4.98 |
| $3p\ ^2S_{1/2} \rightarrow 3p\ ^2P^o_{3/2}$ | 4.78E+06 | 7.52E+06 | +57.32 |
| $4d\ ^2D_{3/2} \rightarrow 5d\ ^2D_{3/2}$ | 1.51E+10 | 1.37E+10 | -9.27 |

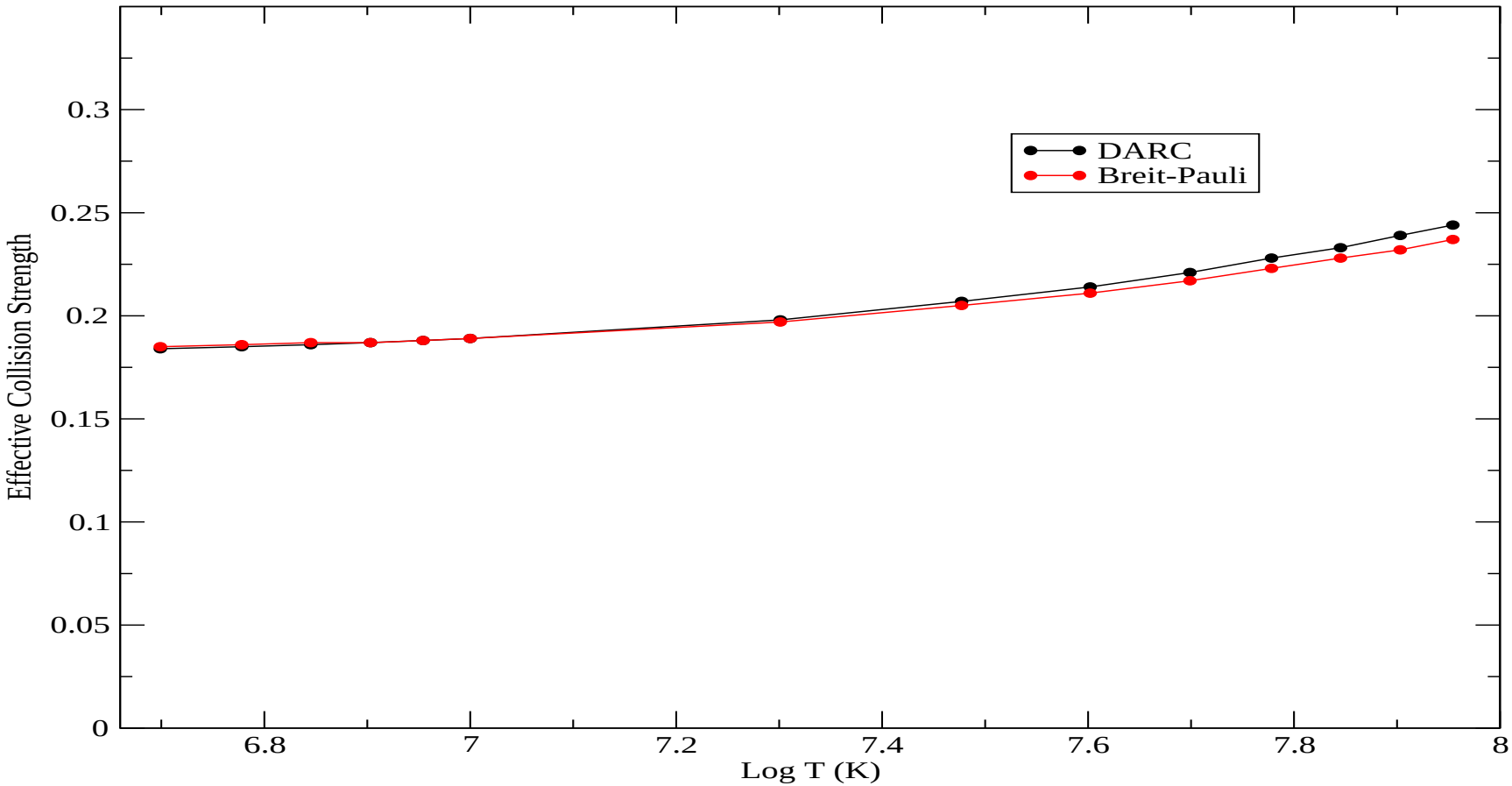
# R-Matrix Calculations

- Used Breit-Pauli and DARC suites of R-matrix codes
- Calculations made as similar as possible
- Energies shifted to NIST values in both calculations

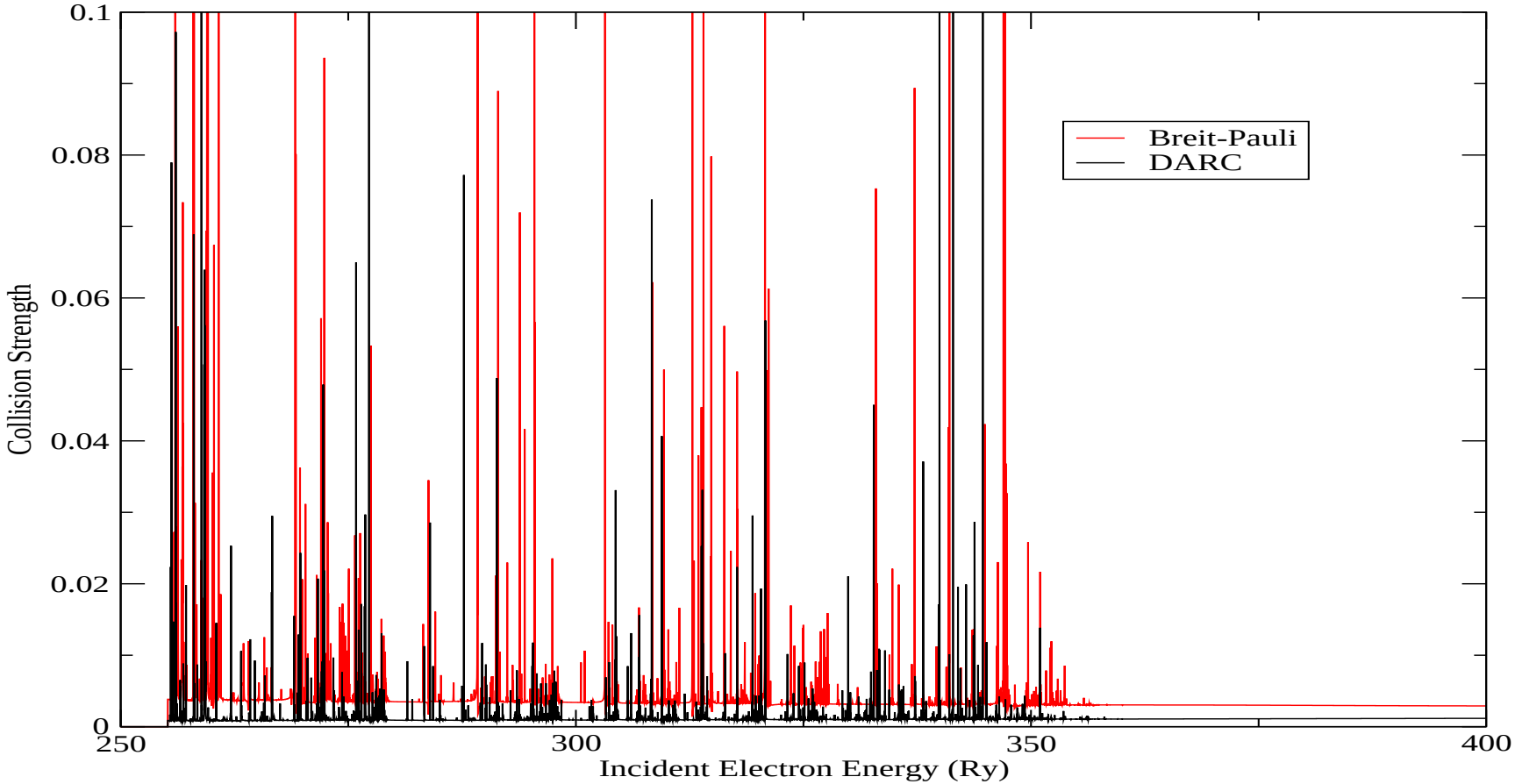
# $3s\ ^2S_{1/2} \rightarrow 3p\ ^2P^o_{3/2}$ transition



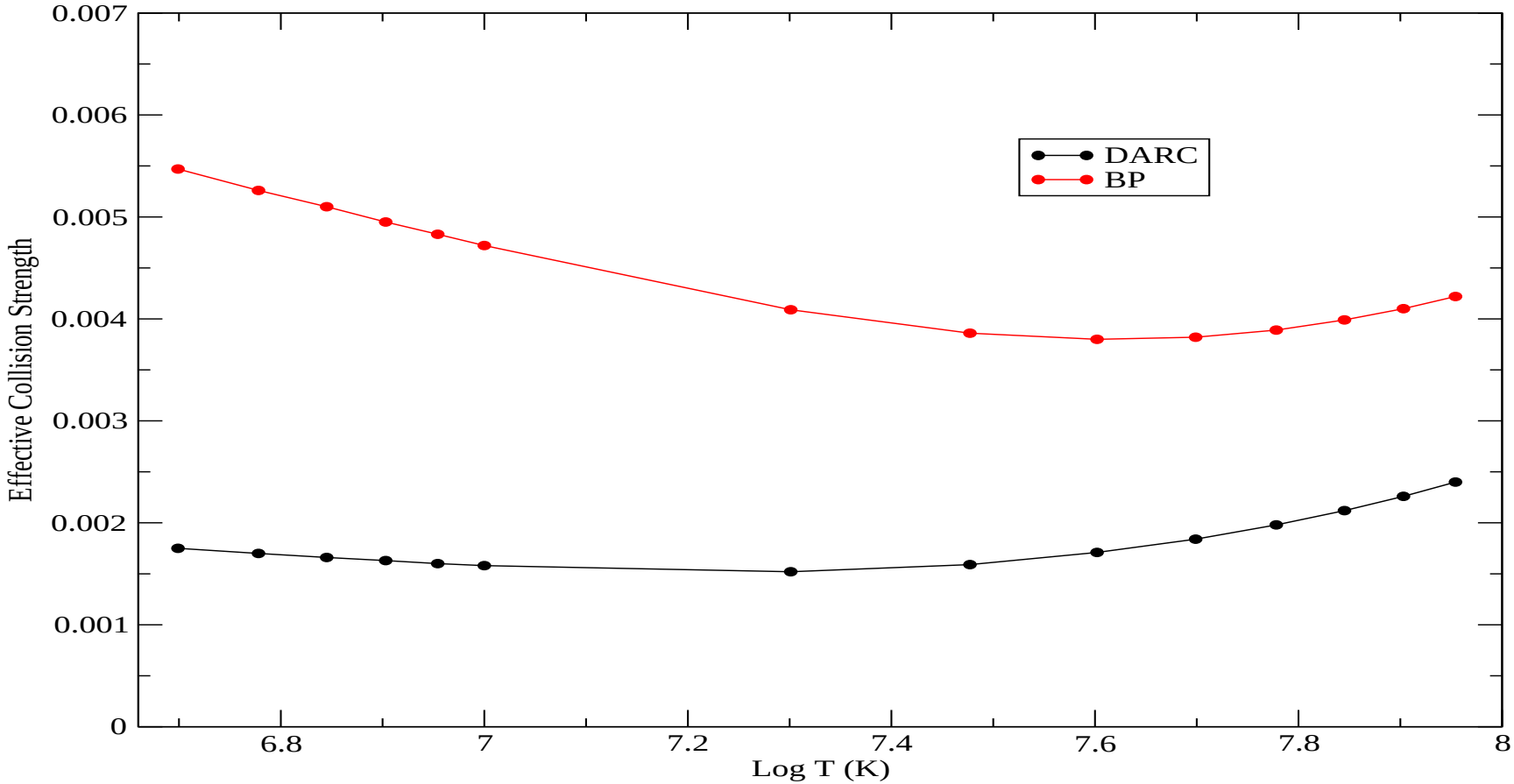
# $3s\ ^2S_{1/2} \rightarrow 3p\ ^2P^o_{3/2}$ transition



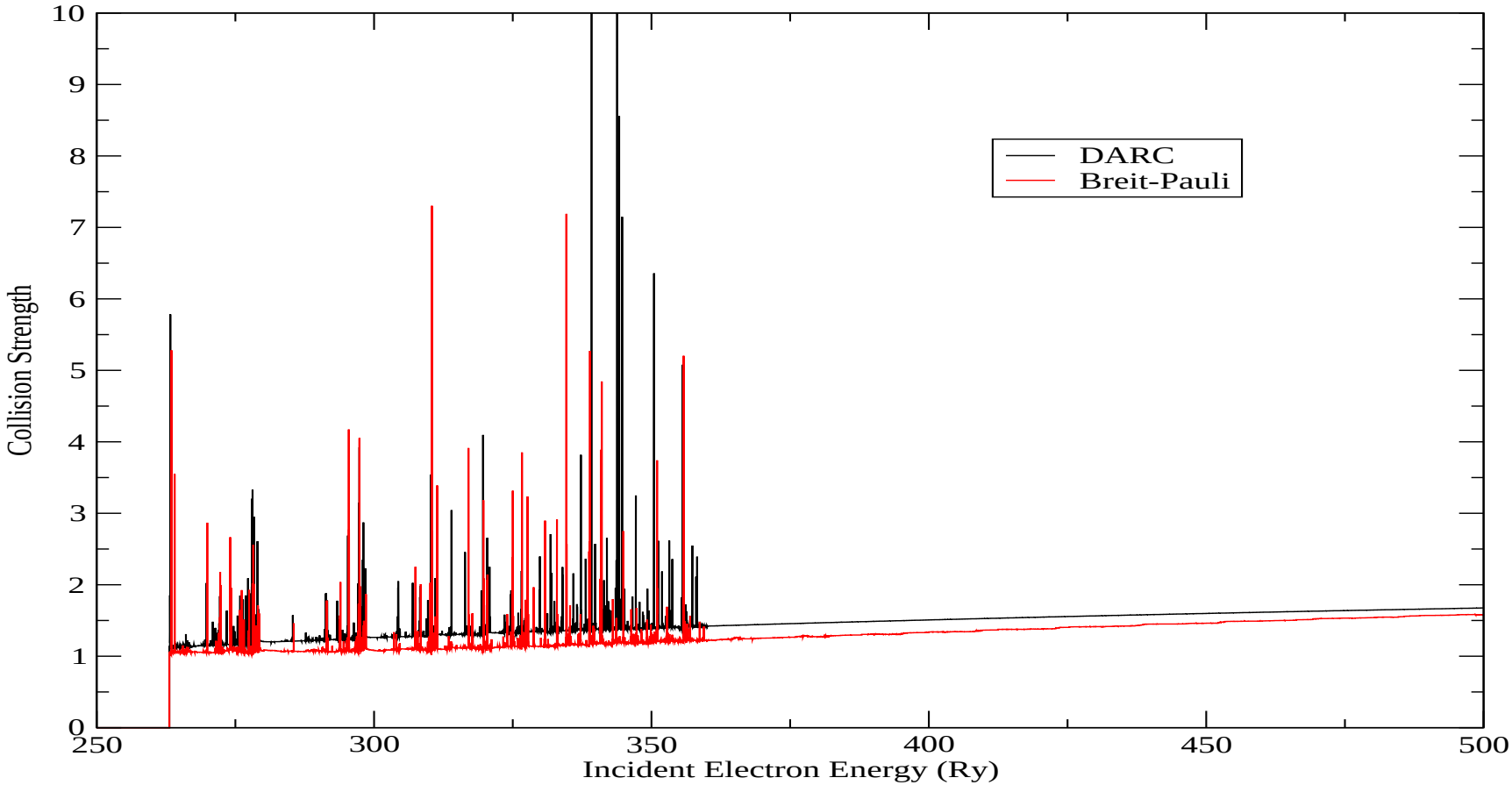
# $3s\ ^2S_{1/2} \rightarrow 4p\ ^2P^o_{3/2}$ transition



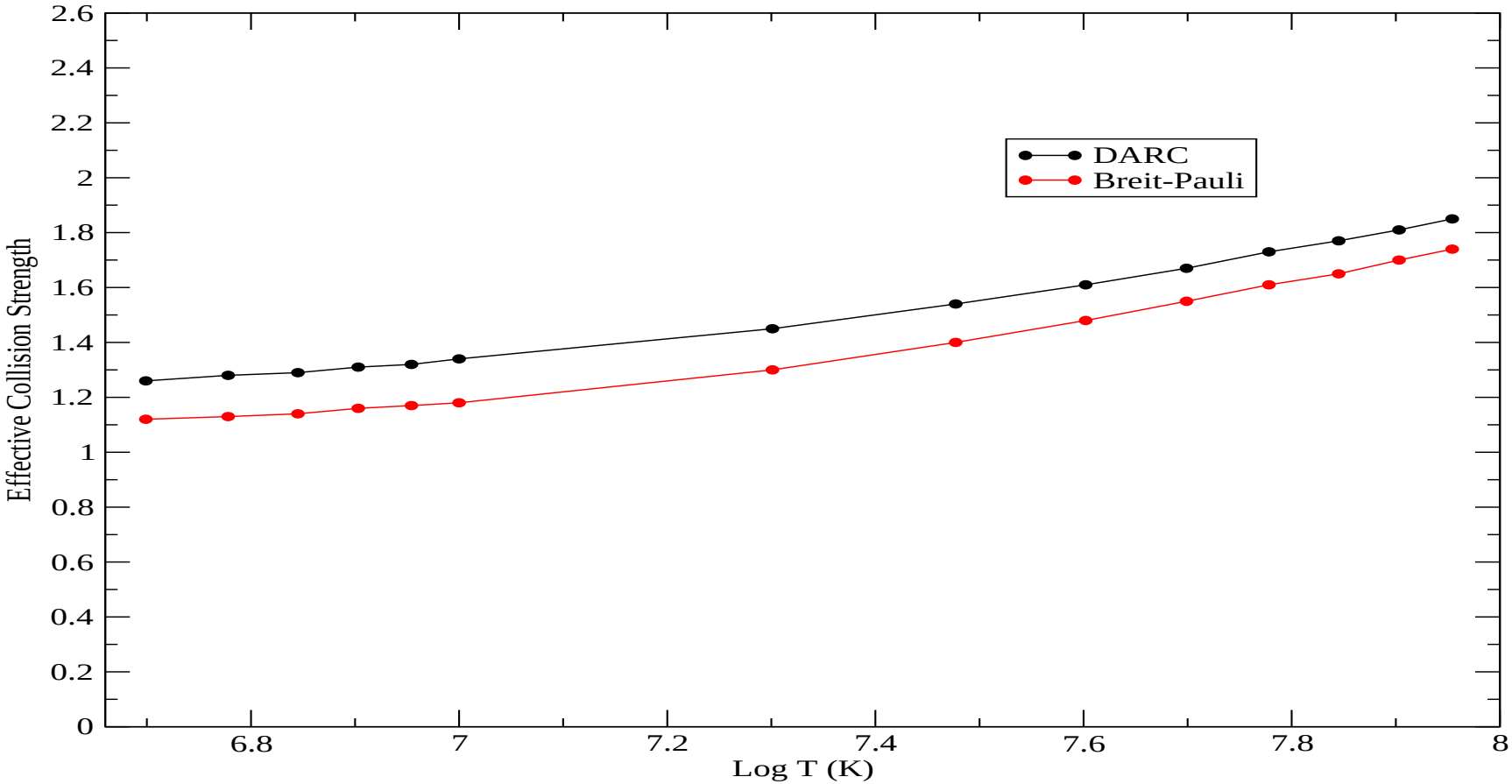
# $3s\ ^2S_{1/2} \rightarrow 4p\ ^2P^o_{3/2}$ transition



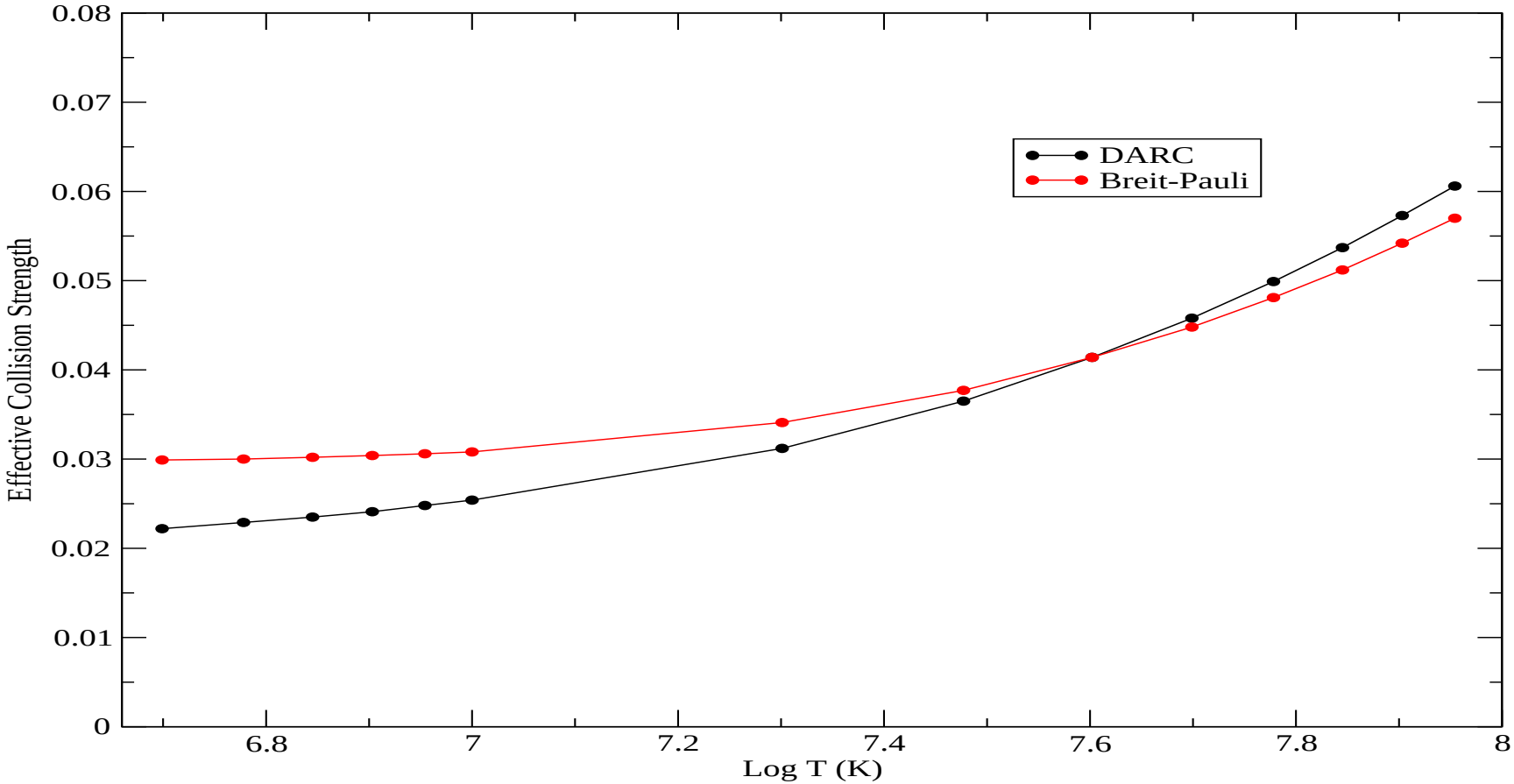
# $4p\ ^2P^o_{3/2} \rightarrow 4d\ ^2D_{5/2}$ transition



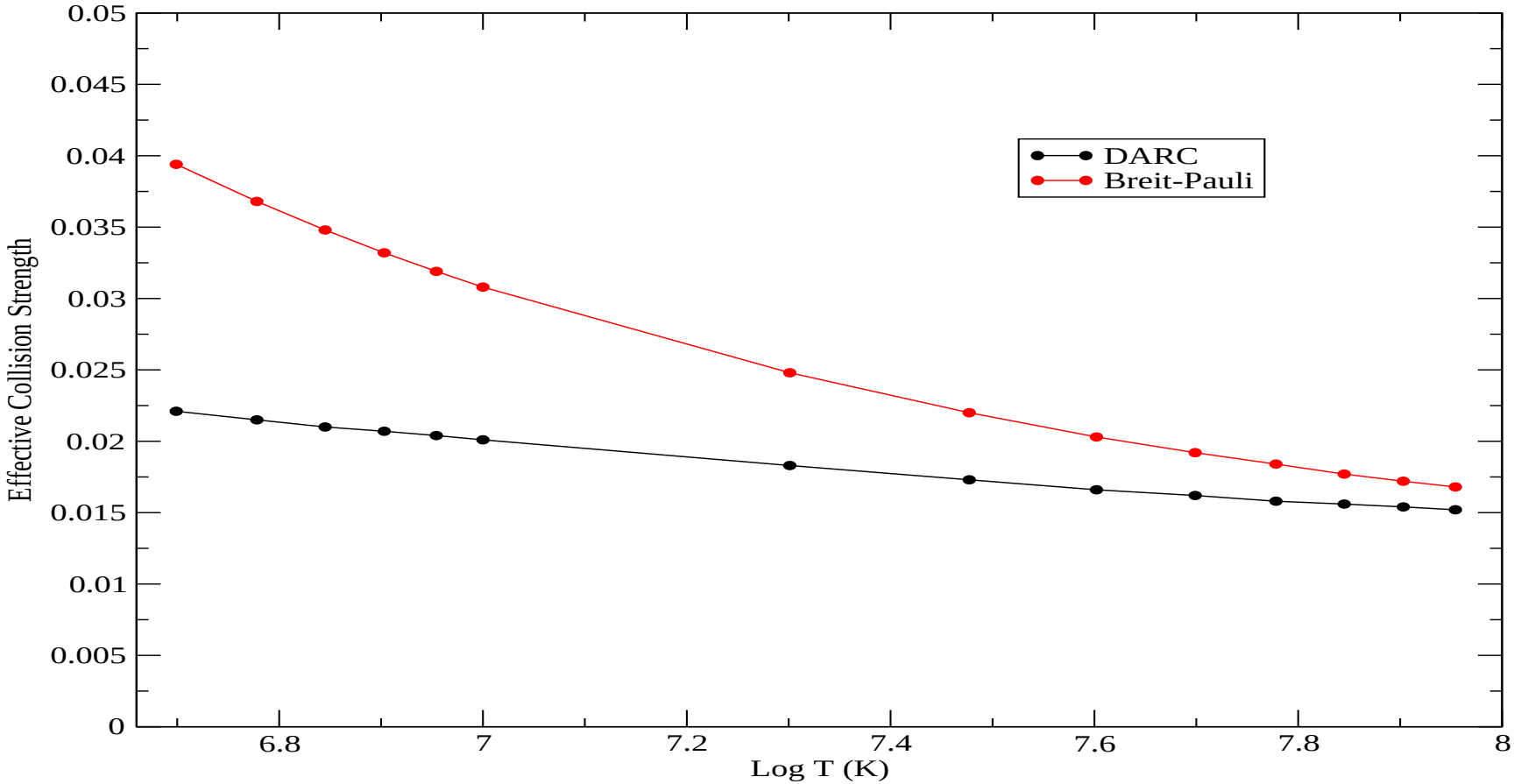
# $4p\ ^2P^o_{3/2} \rightarrow 4d\ ^2D_{5/2}$ transition



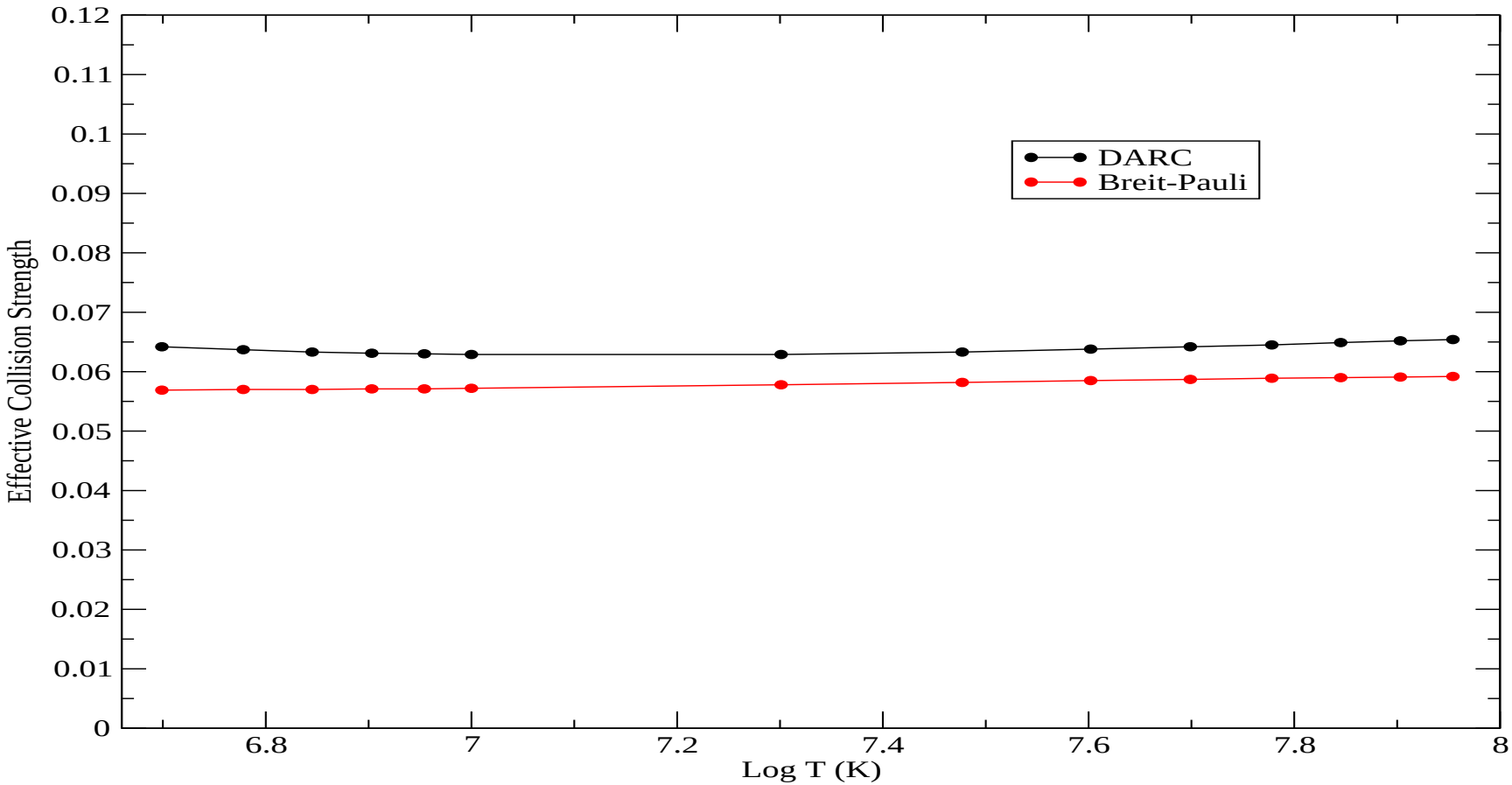
# $4p\ ^2P^o_{3/2} \rightarrow 5d\ ^2D_{5/2}$ transition



# $3p\ ^2S_{1/2} \rightarrow 3p\ ^2P^o_{3/2}$ transition



# 4d $^2D_{3/2} \rightarrow$ 5d $^2D_{3/2}$ transition



# Summary

A comparison between effective collision strengths using both methods for all transitions showed

- an average difference of 16.6%
- maximum difference of 150%