Benchmark calculations for electron collisions with complex atoms

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Benchmark calculations for electron collisions with general B-spline R-matrix package (BSR)

Benchmark results:
- maximum accuracy
- possible source of uncertainties
- convergence
- uncertainty estimations

OVERVIEW:
1. General features of BSR:
   - R−matrix method (close−coupling expansion)
   - B−spline as universal basis
   - non−orthogonal orbitals technique
   - Examples: e + Ne, Ar, Kr, Xe
2. New DBSR code – extension to the Dirac Hamiltonian
   - Example: e + Xe
3. MPI versions
   - Continuum pseudo−state approach (RMPS)
   - Ionization (complete set of data)
   - Example: e + He, Ne, Ar, C, N, F, Fe−ions
4. Final remarks
Benchmark calculations for electron collisions with general B-spline R-matrix package (BSR)

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4. Summary
The B-Spline R-Matrix (BSR) Method

- The method is based on the non-perturbative close-coupling expansion.

- Standard method of treating low-energy scattering

- Based upon an “exact” expansion of the total scattering wavefunction over target states

\[ \Psi_{E}^{LS \pi}(r_1, \ldots, r_{N+1}) = A \sum_{i} \Phi_{i}^{LS \pi}(r_1, \ldots, r_{N}, \hat{r}) \frac{1}{r} F_{E,i}(r) + \sum_{j} \Phi_{j}^{LS \pi}(r_1, \ldots, r_{N+1}) \]

- Simultaneous results for transitions between all states in the expansion

- Problems:
  - close-coupling expansion must be cut off
  - accuracy (expansions) of target states are limited

Main source of uncertainties
The B-Spline R-Matrix (BSR) Method


• The method is based on the non-perturbative close-coupling expansion.
• The close-coupling equations are solved using the R-matrix method.

**Basic Idea:** indirect calculations – inner \( r < a \) and outer regions \( r > a \).

**Complete set** of inner-region solutions is found from diagonalization of total Hamiltonian modified with Bloch operator.

**Scattering parameters** can then obtained from matching with solutions in external region – allows us obtain cross sections at many energy points rather cheaply.
The B-Spline R-Matrix (BSR) Method

• The method is based on the non-perturbative **close-coupling** expansion.
• The close-coupling equations are solved using the **R-matrix method**.

**Computer Codes:**

- PRMAT - parallelized version of RMARX-I
- Badnell's Rmax complex - http://amdpp.phys.strath.ac.uk/, with possibility for radiative damping
- DARC – relativistic version, http://web.am.qub.ac.uk/DARC/
- Enormous number of calculations

**Principal ingredient:** a single set of orthogonal one-electron orbitals

- \(< P_{n\ell} | P_{n'\ell} > = 0 \) → difficulties to achieve accurate target representation for different states
- \(< P_{n\ell} | u_{k\ell} > = 0 \) → large \((N+1)\)-electron expansions needed for completeness (may lead to appearance of pseudo-resonances)
The B-Spline R-Matrix (BSR) Method

• The method is based on the non-perturbative close-coupling expansion.
• The close-coupling equations are solved using the R-matrix method.
• Atomic-structure calculations − frozen-core approximation

Distinctive feature:

Allows for non-orthogonal orbital sets to represent both bound and continuum radial functions

• independent generation of target states − much more accurate target representation (term-dependence, relaxation effects, correlation)

• no artificial orthogonality constraints for continuum orbitals − more consistent treatment of N-electron target and (N+1)-electron collision system → no pseudo–resonances
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\begin{itemize}
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    \item \textit{no artificial orthogonality constraints for continuum orbitals} – more consistent treatment of N-electron target and (N+1)-electron collision system \rightarrow \textit{no pseudo-resonances}
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Distinctive feature:

Allows for non-orthogonal orbital sets to represent both bound and continuum radial functions

• independent generation of target states – much more accurate target representation (term-dependence, relaxation effects, correlation)

It allows us considerably (almost completely) reduce the uncertainties due to accuracy of target states

more consistent treatment of N-electron target and (N+1)-electron collision system → no pseudo-resonances
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• independent generation of target states — much more accurate target representation (term-dependence, relaxation effects, correlation)
• no artificial orthogonality constraints for continuum orbitals — more consistent treatment of N-electron target and (N+1)-electron collision system → (no pseudo-resonances, improved convergence)

Additional source of uncertainties
\( e + K^+ (3p^6) \rightarrow e + K^+ (3p^5n l \ 1,3L) \)

**BSR versus Belfast RMATRX**

- BSR –43, Tayal and Zatsarinny (2008)

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**Graphs**

- **4p \(^3S_1\)**: Cross section for \(4p\) states with different calculations.
- **4p \(^1S_0\)**: Cross section for \(4p\) states with different calculations.
- **4p \(^3P_0\)**: Cross section for \(4p\) states with different calculations.
- **4p \(^1P_1\)**: Cross section for \(4p\) states with different calculations.

**Axes**

- **Electron energy (eV)**
- **Cross section (10^{-16} cm^2)**

**Notations**

- **CC-expansion**: Cross section calculation method.
Example of spurious resonances
\( e + O \text{ III (} ^2P_j \) 

\[ \Psi_{E}^{LS\pi}(r_1, ..., r_{N+1}) = A \sum \int \Phi_{i}^{LS\pi}(r_1, ..., r_N, \hat{r}) \frac{1}{r} F_{E,i}(r) + \sum_{j} \Phi_{j}^{LS\pi}(r_1, ..., r_{N+1}) \]

overloaded

RM −19, Palay et al. (2012)

not used at all

BSR −202, Tayal et al. (2014)

CC−edge

Collision Strength

Electron Energy (Ry)
On the convergence of close-coupling results for low-energy electron scattering from magnesium

K Bartschat, O Zatsarinny, I Bray, D V Fursa and A T Stelbovics

There are still many questions to resolve due to code limitations.
Why B-splines?

- **excellent numerical properties** – machine accuracy with Gaussian quadratures.
- **flexibility** in the choice of radial grid.
- effective **completeness** of B-spline basis – no Buttle correction required; finite representation of whole Rydberg series or continuum spectra.
- avoid finite-difference algorithms – established **Linear Algebra packages** can be used.

\[
\psi(r) = \sum_i c_i B_i(r) \quad \quad H\Psi = E\Psi \quad \rightarrow \quad Hc = ES_c
\]

• first R-matrix calculation with B-splines: e-H scattering (van der Hart 1997)

However – scattering calculations require relatively big basis: \( n \sim 50-100 \)
BSR – general B-spline R-matrix package

1. First implementation: Li photoionization (2000)
2. First presentation: ICPEAC XXX, Rosario, Argentina (2005)
5. RMPS extension and e-He,Ne scattering (2011-2012)

Calculations:

1. Electron scattering from neutrals (including inner-core excitations)
   He, C, N, O, S, Cl, Ne, Na, Mg, Si, Ar, K, Ca, Cu, Zn, I, Kr, Rb, Xe, Cs, Kr, Xe, Cs, Au, Hg, Pb
2. Electron-ion collisions (rate coefficients)
   S II, K II, Fe II, Fe VII, Fe VIII, Fe IX
3. Photodetachment and photoionization
   He-, Li-, B-, O-, Ca-, Li, K, Zn
4. Atomic structure: energies, oscillator strengths, polarizabilities
   C, Ne, S, SII, F, CL, Ar, Kr, Xe
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* Lanthanides
+ Actinides
Metastable production in electron collisions with noble gases (status on 2002)


Experiment: metastable count rate (Buckman et al, 1983)

at best – qualitative agreement between theory and experiment
Metastable production in Electron Collisions with noble gases

BSR calculations

Cross Section ($a_0^2$) vs. Electron Energy (eV)

- Ne
- Ar
- Kr
- Xe

BSR calculations for different noble gases, showing the cross section as a function of electron energy.
Metastable production in Electron Collisions with noble gases

Uncertainty question:
BSR – general B-spline R-matrix package  
Present design and perspectives

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   - R-matrix method (close-coupling expansion)
   - Examples: e + Ne, Ar, Kr, Xe

2. New DBSR code – extension to the Dirac Hamiltonian
   - Example: e + Xe

3. MPI versions
   - Continuum pseudo-state approach (RMPS)
   - Ionization (complete set of data)
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4. Conclusions and Outlook
Dirac–Coulomb–Breit Hamiltonian

\[ H_{DCB} = \sum_i h_i(r_i) + \sum_{i<j} \left( \frac{1}{r_{ij}} + b_{ij} \right) \]

\[ h_D = c \mathbf{\alpha} \cdot \mathbf{p} + \beta c^2 + V_{\text{nuc}}(r) \]

\[ b_{ij}^0 = -\frac{1}{2r_{ij}} \left[ \mathbf{\alpha}_i \cdot \mathbf{\alpha}_j + \frac{(\mathbf{\alpha}_i \cdot \mathbf{r}_{ij})(\mathbf{\alpha}_j \cdot \mathbf{r}_{ij})}{r_{ij}^2} \right] \]

R-matrix basis functions:

\[ \Psi^{\alpha JM}(x_1, \ldots, x_{N+1}) = A \sum_{ij} \left[ \Phi_i^{\alpha_i J M_i}(x_1, \ldots, x_N) \cdot \phi_j(x_{N+1}) \right]^{JM} + \sum_i \chi_i^{JM}(x_1, \ldots, x_{N+1}) b_i^{JM} \]

\[ \phi_{nkm}(r) = \frac{1}{r} \left( \frac{P_{nk}(r)\chi_{km}(\hat{r})}{iQ_{nk}(r)\chi_{-km}(\hat{r})} \right) \]

\[ P(r) = \sum_i p_i B_{i}^{k_p}(r); \quad Q(r) = \sum_i q_i B_{i}^{k_q}(r) \quad k_p \neq k_q \quad \text{!!!} \]

Spurious–states problem – Froese Fischer & Zatsarinny, CPC, 2009

- Retain key feature: both bound and continuum radial functions can be represented by non-orthogonal term-dependent radial orbitals.
- Target wave-functions – GRASP2K (Jönsson, He and Froese Fischer, CPC, 2007)
e-Xe: \(6s^{3/2}_2 + 6s^{1/2}_0\)

- Buckman et al (1983)

**BSR-31**

**DBSR-31**
Buckman et al (1983)
BSR-31
DBSR-31
DBSR-75

Cross Section ($a_0^2$)
Electron Energy (eV)
e-Xe: $6s[3/2]_2 + 6s[1/2]_0$

- Buckman et al (1983)
- BSR-31
- DBSR-31
- DBSR-75
TOPICAL REVIEW

The $B$-spline $R$-matrix method for atomic processes: application to atomic structure, electron collisions and photoionization

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Many more examples can be found here!
BSR – general B-spline R-matrix package
Present design and perspectives

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   - R−matrix method (close−coupling expansion)
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2. New DBSR code – extension to the Dirac Hamiltonian
   - Example:  e + Xe

3. MPI versions
   - Continuum pseudo−state approach (RMPS)
   - Ionization  (complete set of data)
   - Example:  e + He, Ne, Ar

4. Conclusions and Outlook
We use the box-base approach:

Both physical and pseudo-states are found by directly solving the close-coupling (frozen-cores) equations for N-electron atomic wavefunctions with zero boundary conditions.
Electron-impact excitation of neon at intermediate energies


Target states:

\[ \Phi(2s^2 2p^5 nl, J) = A \sum_{ij,LS} a_{ij} \varphi(2s^2 2p^5; \mathbf{P}) \cdot B_i(r) |l_j s >, LS \} \]
\[ + A \sum_{ij,LS} a_{ij} \varphi(2s^2 p^6; \mathbf{S}) \cdot B_i(r) |l_j s >, LS \} \]

Total number of states: - 457
Bound states: - 87
Continuum pseudostates: - 370
(l = 0 - 3)
Continuum energy cover: - 40eV
Number of channels: - 2260
R-matrix radius: - 30 \text{a}\_o
Number of B-splines: - 70
Hamiltonian matrix: - 150000

Number of processors used: - up to 1000
Resources used: - 200000 \text{PU} (1 hour x 1 processor)
(for 50 partial waves)
Total Cross Section for Electron Impact Excitation of Neon

Effect of Channel Coupling to Discrete and Continuum Spectrum

Electron Energy (eV)

Cross Section (10^{-18} cm^2)

3s[3/2]_2

BSR-457

BSR-31

BSR-5

3s'[1/2]_0

3s[3/2]_1

Cross Section (10^{-18} cm^2)

3s'[1/2]_1


Phillips et al (1985)


Electron Energy (eV)
Differential Cross Section for Electron Impact Excitation of Neon at 30 eV

- **30 eV**
  - **3s[3/2]_2**
  - **3s'[1/2]_0**

Khakoo et al. x 0.55 !!!

DCS (10^{-19} cm^2/sr)

- **3s[3/2]_1**
- **3s'[1/2]_1**

Scattering Angle (deg)
Effect of Channel Coupling to Discrete and Continuum Spectrum for $2p^{5}3d$ excitation in Ne

The $2p^{5}3d$ states are really affected – factors of 5–10 !!!
Effect of Channel Coupling to Discrete and Continuum spectrum in Ar

How to estimate uncertainties here?
Total Cross Section for Electron Impact Excitation of Argon

Convergence study

Final uncertainty within 5–10 percent, just based on the convergence study.
Electron Impact Excitation of Fluorine ($2p^5 \, ^2P$)

Total number of states $-$ 690
Bound states $-$ 53
Continuum pseudostates $-$ 637
(\(l=0-3, \, L=0-5\))

Continuum energy cover $-$ 20eV
Number of channels $-$ 1727
R–matrix radius $-$ 30\(a_o\)
Number of B–splines $-$ 68
Hamiltonian matrix $-$ 100000

Dipole transitions:
- Crucial dependence on continuum pseudostates
- In less extent – on target description
- Most problematic – $2p^5$ excitation
Electron Impact Excitation of **Fluorine** \((2p^5 \, ^2P)\)

None – dipole transitions:

- Crucial dependence on continuum pseudostates for all transitions
- Target description is more important
- Uncertainties are different!
Electron Impact Excitation of Nitrogen ($2p^3 \, ^4S$)

- $2p-2p$ – converged
- Target continuum – important
- Experiment – ?
- Uncertainties – 10 %
Electron Impact Excitation of Carbon (2p$^2$ 3P)

Total number of states = 696
Bound states = 51
Continuum pseudostates = 645
(1 = 0 − 3)
Continuum energy cover = 30eV
Number of channels = 1543
R−matrix radius = 30a$_o$
Number of B−splines = 83
Hamiltonian matrix = 120000

Crucial dependence on both target description and continuum pseudostates

First check target − then convergence!
Elastic Scattering on Nitrogen

Cross Section $(10^{-16} \text{ cm}^2)$

Electron Energy (eV)

- BSR-690 (tuned)
- BSR-690
- BSR-61
- momentum-transfer

Neynaber et al. (1963)
Miller et al. (1970)

$(2p^3)^4S^o$

Tuned to position of the $2p^4^3P$ resonance at 62 meV (Mazeau et al. 1978)
You never get this position from ab-initio calculations! – Experiment is crucial!
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4. Conclusions and Outlook
Ionization in the Close−Coupling Formalism 
(non−perturbation approach) 

- We are interested in the ionization process 

\[ e_0 (k_0 \mu_0) + A(L_0 S_0 M_{L_0} M_{S_0}) \rightarrow e_1 (k_1 \mu_1) + e_2 (k_2 \mu_2) + A^+ (L_f S_f M_{L_f} M_{S_f}) \]

- Pseudo−state approach for ionization amplitude:

\[ f(L_0 M_0 S_0 M_{S_0} \rightarrow L_f M_f S_f M_{S_f}) = \sum_p <\Psi_f^{k_2(-)}(\mu_2) | \Phi(L_p S_p) > f_p (L_0 M_0 S_0 \rightarrow L_p M_p S_p) \]

This direct projection to the true continuum is the essential idea: allows to consider ionization plus excitation as well

\[ \Psi_f^{k_2 \mu_2(-)}(X) = \frac{1}{\sqrt{k_2}} \sum_{l_2 m_2} i^{l_2} \exp(-i \sigma_{l_2}) Y_{l_2 m_2}^*(\hat{k}_2) \]

\[ \sum_{L,M,S,M_S} (L_f M_f, l_2 m_2 | LM)(S_f M_{S_f}, \frac{1}{2} \mu_2 | SM_S) \Psi_{LMMS_S}^{L_f M_f S_f M_{S_f}, k_2(-)}(X) \]

\[ \frac{d \sigma^f}{d \Omega_1 d \Omega_2 dE} = \frac{k_1 k_2}{k_0} \frac{1}{2(2L_0 + 1)(2S_0 + 1)} \sum_{M_0, M_f, M_{S_f}, \mu_0, \mu_1, \mu_2} |f(L_0 M_0 S_0 M_{S_0}, \mu_0 \rightarrow L_f M_f S_f M_{S_f}, \mu_1 \mu_2)|^2 \]
Ionization in the Close-Coupling Formalism (non-perturbation approach)

$$e_0(k_0\mu_0) + A(L_0S_0M_{L_0}M_{S_0}) \rightarrow e_1(k_1\mu_1) + e_2(k_2\mu_2) + A^+(L_fS_fM_{L_f}M_{S_f})$$

**Total (ionization) cross-section** are much easier to get – just add up the results for all the (positive-energy) pseudo-states.

$$\sigma^{tot} = \sum_p \sigma^p$$

**Ionization-excitation** can be estimated from channel decomposition of continuum pseudostates:

$$\sigma^f = \sum_{p,kl} \langle \Phi^p | f, kl \rangle^2 \sigma^p$$

**OR** from direct integration of TDCS over ejected energies and angles.
Example of He pseudo–state expansion (to model the $1s^1l$ and $2s^1l$ continuum):

$$
\Phi^p (LS) = A \sum_j \{ \varphi(1s) P(n_j l_j) \}^{LS} + A \sum_j \{ \varphi(2s) P(n_j l_j) \}^{LS} + A \sum_j \{ \varphi(2p) P(n_j l_j) \}^{LS} + \Phi(1s^2)
$$

$$
P_{nl}(r) = \sum_k a_k B_k (r)
$$

The $B$-splines $B_k(r)$ represent the radial part of the outer orbitals.

Expansion coefficient are found by direct diagonalization of $N$–electron Hamiltonian with zero boundary conditions.

Number and density of pseudo–states depend on box radius $a$ and number of $B$–splines.

The same expansion is used for real continuum spectrum (needed for ionization amplitude) with ingoing-wave boundary conditions.

Extensive usage of nonorthogonal orbital technique:

$$
< \Psi_{LS}^{f,k_2(-)} | \Phi^p (LS) > = a^{cont.} | O | a^p >
$$

He: 525 states with $L=0$–3 to cover ejected–electron spectrum up to 300 eV

$a = 15 \ a_o$; $ns=64$; $ks = 8$; number of $kl$ channels $= 1300$;

matrix to diagonalize – 80000 for $L^T=0$–25
First test calculation: total ionization of helium
(Paint Physical Review A 85, 062709, 2012)

- Including correlation in the ground state reduces the theoretical result.
$e + \text{He}(1s^2) - \text{He}^+(2p) + 2e$

How we can estimate the uncertainty in this case? Only order of magnitude.
We estimate uncertainty around 10% for this correlated process.
Triple-Differential Cross Section Ratio $n=1/n=2$

Comparison BSR−527 ($n=2$) and BSR−1255 ($n=3$) models

$\theta_1 = 24^\circ$

$\theta_1 = 36^\circ$

$\theta_1 = 48^\circ$

$E_1=44$ eV

$E_2=44$ eV

$\theta_1 = 28^\circ$

$\theta_1 = 40^\circ$

$\theta_1 = 52^\circ$

$\theta_1 = 32^\circ$

$\theta_1 = 44^\circ$

$\theta_1 = 56^\circ$

$n=1/n=2$ Cross Section Ratio

$\theta_1 = 40^\circ$

$\theta_1 = 52^\circ$
Ionization of complex targets

- Ionization Cross Section (10\(^{-17}\) cm\(^2\))
- Electron energy (eV)

**e + C - C\(^+\) + 2e**

\((2p^2)^3P\)

**e + N - N\(^+\) + 2e**

\((2p^3)^4S^0\)

**e + F - F\(^+\) + 2e**

**e^- + Ne - 2e^- + Ne\(^+\)**

Correlation in the initial state is important – up to 20 to 50%

- **expt.**, Brook et al. (1978)
- **BEB + 2s2p^3 3S**, Kim & Desclaux (2002)
- **BSR-696, Wang et al. (2013)**

- **expt.**, Brook et al. (1978)
- **BEB (3P:1D:1S - 9:5:1)**
- **N\(^+\)(2s^22p^2)^3P-ionization**
- **2s-ionization**

- **expt.**, BSR-690
- **BEB**
- **2s-ionization**
- **(2p^3)4S**

- **expt.**, BSR-690
- **Krishnakumar & Strivastava (1988)**
- **Pindzola et al. (2000), TDCC**
- **Ballance et al. (2009), RMPS-347**
- **BSR-679**
Comparison with BEB calculations

Very big overestimation of the autoionization–excitation contribution
Total Cross Sections
(BSR can do this as a single theory for energies between 0.01 eV and 300 eV!)

Ne

Ar

Kr

Xe
Total Cross Sections
(BSR can do this as a **single** theory for energies between 0.01 eV and 300 eV!)

- **Ne**
  - Total Cross Section (10^{-16} cm^2)
  - BSR-679, elastic
  - elastic + excitation
  - total

- **Ar**
  - Total Cross Section (10^{-16} cm^2)
  - BSR-500, elastic
  - elastic + excitation
  - total

- **Kr**
  - Total Cross Section (10^{-16} cm^2)

- **Xe**
  - Total Cross Section (10^{-16} cm^2)

- **These results (and more) are now in the LXCAT database:**

- **Excellent results in modeling of low-temperature Ne and Ar plasmas**
Electron−impact excitations of Fe ions
(large−scale BSR calculations for astrophysical applications)

FeVII \[3p^63d^2, 3p^53d^3, 3p^63d4l, 3p^53d5s, 3p^63d5p\]
182 fine−structure levels

FeVIII \[3p^63d, 3p^53d^2, 3p^64l, 3p^53d4s, 3s3p^63d^2, 3p^65l\]
102 fine−structure levels

FeIX \[3p^6, 3p^53d, 3s3p^63d, 3p^43d^2, 3p^54l, 3s3p^53d^2, 3s3p^64l, 3p^55s\]
344 fine−structure levels
(in progress)

• Direct Breit−Pauli (intermediate coupling) calculations
• More accurate target description
• Complete set of scattering and radiative parameters
  (rate coefficient and oscillator strengths between all levels)
• Extensive calculation of resonance structure (~20000 energy points)
• Do we get convergence?
Electron-impact excitation of Fe VII

![Graphs and data points](image)

- DW Zeng et al. (2005)
- RM-80 Berrington et al. (2000)
- BSR-189 Tayal & Zatsarinny (2013)

Convergence still a question
Electron-impact excitation of Fe VIII

--- RM-77(LS−33), Griffin et al. (2000)
--- BSR-102, Tayal & Zatsarinny (2011)

- 3d − relaxation
- Direct Breit–Pauli approx.
- Difference:
  < 30% for 90% of transitions
  < 10% for 50% of transitions
Electron-impact excitation of Fe XI

- $3s^23p^6$
- $3s^23p^53d$
- $3s^23p^63s$
- $3s^23p^64p$
- $3s^23p^64d$
- $3s^23p^65s$
- $3s^23p^64f$
- $3s^23p^53d$
- $3s^23p^54d$
- $3s^23p^55s$
- $3s^23p^54s$
- $3s^33p^6$
- $3s3p^53d$
- $3s3p^54p$
- $3s3p^54d$
- $3s3p^55s$
- $3s3p^54s$
- $3s3p^53d$
- $3s3p^54p$
- $3s3p^56$

- Collision strength
- Scattered energy (Ry)

- Effective collision strength
- log T (K)

- $3p^6 \ ^1S_0 - 3p^54s \ ^1P_1$
- $3p^6 \ ^1S_0 - 3p^54p \ ^1S_0$

- $\times$ DW O’Dwyer et al. (2012)
- ○ RM-64LS Storey et al. (2002)
- — BSR-370 Tayal & Zatsarinny (2014)
Summary

- For complex targets, the **BSR method with non-orthogonal orbitals** has advantages:
  - highly **accurate** target description
  - more **consistent** description of (N+1)-electron scattering system
  - considerable improvement for **low-energy region** and **near-threshold resonance** phenomena
  - provide benchmark results for uncertainty estimations

- **DBSR** — new **Dirac-based** version of the B-spline R-matrix method
  - it is a general **all-electron code**
  - higher accuracy for heavy atoms

- Recent development: **MPI versions** and **continuum pseudostate implementation**
  - accurate results for intermediate energy scattering (drastic difference with previous results)
  - **ionization** through pseudo-state approach
  - detailed treatment ionization processes in complex targets: ionization plus excitation, TDCS

- **Complete set of data**
  Application for low–energy modeling of the Ne and Ar plasma shows excellent results
Uncertainty's questions

- Benchmark results:
  - considerable reduction (elimination) of \textit{target description} uncertainty
  - systematic check of \textit{convergence} (including target continuum)
- Many existing databases for neutrals should be re-evaluated
- \textbf{ABSOLUTE} experimental data are difficult to obtain!
- Comparison with \textit{simplified} calculations is questionable (not productive).
- Comparison different \textit{codes} and \textit{models}.
  - Repeating calculations are encouraged.
  - Non-critical using the existing codes – expert proof is still important.
- Each atom – unique!
  (the automatic calculations for whole iso-electronic or iso-nuclear series can be deceptive)
- Using other (more detailed) \textit{variables} to support the accuracy.
- How to present uncertainties for big set of cross sections or rates?
  (each energy or temperature?)
- Comparison of published results or different databases is very time consuming:
  (It is desirable to encourage development of \textit{new software} for extracting and comparison of data in different databases and sharing the results)
THANK YOU
For Your Attention!