Atomic data and collisional-radiative model for Beryllium and its ions

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Introduction

Be is foreseen as a plasma-facing material in the main chamber of ITER. For interplay at high-Z experiments, measurements and modelling of the Be impurity transport in the edge and divertor plasma, collisional atomic data (cross sections of elementary processes) are required. The "effective" rate coefficients given in existing atomic databases (e.g. ADAS) are sometimes insufficient for applications. Due to high toxicity of Be the experimental cross sections are practically unavailable in the literature. As a rule the most accurate theoretical methods, such as convergent close-coupling (CCC) or the K-matrix with pseudostates (RPMs) demand very large computation time (especially at intermediate energies when continuum coupling effects are important). For the relatively fast calculation simpler but accurate enough methods such as K-matrix can be used.

Convergent close-coupling calculations for Be I

- All transitions with \( \alpha \leq 4 \) for collision energies \( E \leq 400 \text{ eV} \) included.
- For energies below 10 eV (relative to the ground state) - 10 partial waves, and 16 above. Extrapolation to infinity done using the Born approximation.

Code ATOM

Computes atomic characteristics:
- Radiative: \( f, \Delta \) (photodissociation/recombination), autoreionization
- Collisional: \( \kappa \) (\( \nu \)) of excitation, ionization by electrons and protons

Included in ATOM:
- For wave functions: exchange, scaled potential, core polarization
- For collisions: Coulomb field, exchange, normalization, configuration interaction (with optional matrix of eigenvectors)
- One-electron radial equation:

\[
\frac{d^2 \psi}{d \rho^2} + \frac{1}{\rho} \frac{d \psi}{d \rho} + \left( \frac{\mu}{\rho^2} - \frac{1}{\rho^2} \right) \psi = \frac{1}{\rho^2} \sum_n \psi_n \left( \frac{\mu}{\rho^2} - \frac{1}{\rho^2} \right) \psi_n
\]

- For \( \alpha = 0 \), the experimental energy bound is used
- The scale parameter is such an eigenvalue such that \( P(\rho) = 0 \) and \( P(\rho) \exp(-\alpha \rho) \rightarrow \sigma \). In this case \( a \) gives the correct asymptotic behavior of \( P(\rho) \).

K-matrix method (transitions between terms)

- A chosen list of atomic states (basis) is used as an input information.
- For all pairs of states \( |a_i, \epsilon_i, k_i \rangle < |a_f, \epsilon_f, k_f \rangle \) from the basis, for a set of partial waves \( \langle n, l, \lambda \rangle \) of the outer electron and for total angular momenta \( n, l, \lambda \), the transition amplitudes \( \delta^{gf} \) are calculated in Born approximation by the exchange between the incident and target electrons.
- From transition amplitudes the full matrix \( \delta^{gf} \) is constructed. The final unitary scattering matrix \( \delta \) is obtained according to the matrix equation

\[
K \delta = \delta - 1
\]

- The cross section is expressed in terms of S-matrix:

\[
\sigma_{gg'} = \frac{1}{4} \sum_k \left| \delta_{kk'} \right|^2
\]

The method takes into account:
- Normalization (electron flux conservation)
- Step transitions (e.g., 2s \( \rightarrow \) 2p)
- Other less straightforward consequences of the channel interaction

K-matrix method (basic formule)

The full set of quantum numbers \( P = \alpha \lambda \Delta \langle \nu \rangle \). Usually \( \alpha = 0, \Delta = 1, \lambda = 0 \).

The elements of \( \delta_{kk'} \) are equal to the matrix elements of interaction:

\[
K_{\alpha_1 \lambda_1 \Delta_1 \langle \nu_1 \rangle}^{\gamma_1 \lambda_1 \Delta_1 \langle \nu_1 \rangle} = \sum_n \sum_n^{\alpha_2 \lambda_2 \Delta_2 \langle \nu_2 \rangle} \left( \sum_n \psi_n \right) \sum_n^{\alpha_1 \lambda_1 \Delta_1 \langle \nu_1 \rangle} \left( \sum_n \psi_n \right) \frac{1}{\rho^2} \sum_n \psi_n \left( \frac{\mu}{\rho^2} - \frac{1}{\rho^2} \right) \psi_n
\]

The direct \( \kappa \) and exchange \( \kappa' \) radial integrals are expressed through radial functions \( P_\lambda \) and \( P_\lambda \) of the optical and outer electron, respectively:

\[
\kappa = \left( \frac{\mu}{\rho^2} - \frac{1}{\rho^2} \right) \frac{1}{2} \left( \sum \psi_n \right) \sum \psi_n \frac{1}{\rho^2} \sum \psi_n \left( \frac{\mu}{\rho^2} - \frac{1}{\rho^2} \right) \psi_n
\]

\[
\kappa' = \left( \frac{\mu}{\rho^2} - \frac{1}{\rho^2} \right) \frac{1}{2} \left( \sum \psi_n \right) \sum \psi_n \frac{1}{\rho^2} \sum \psi_n \left( \frac{\mu}{\rho^2} - \frac{1}{\rho^2} \right) \psi_n
\]

Comparison between CCC and K-matrix for Be I

- Good agreement was found for dipole transitions, if oscillator strength \( g \) is not very small. We note also the significant influence of the configuration mixing. For intercombination transitions the difference is somewhat larger because the exchange is normally more important compared to the used approximations.
- Poor agreement was found in cases of very strong configuration interaction when the description of atomic structure used in ATOM can be inadequate and for transitions with extremely small values for which the cancellation effects are important.
- Some questionable cases, e.g. the transition 2s1/2 \( \rightarrow \) 2p1/2 1D

Steady-state dependencies on Ne and Te for Be I

- The excitation rates:\( \kappa _{g} \) are given in Table 10.

Effective ionization and recombination rate coefficients

- Quasi-steady-state approximation, \( \alpha_{nl}/\alpha_{nl} - 0 \) for the excitation and ionization rates for ground and metastable states.
- The excited states make essential contribution to the effective rates.
- Nonmonotonic recombination rate due to competition between the recombination to and the collisional ionization from excited states.

Radiative power losses and cooling rates

- The radiative power losses include the following contributions:
  - Line radiation (continuum):
    - Be I: \( \sum \sigma_{\alpha \lambda} L_{\alpha \lambda} \)
  - Radiative and dielectronic recombination:
    - Be II: \( \sum \sigma_{\alpha \lambda} L_{\alpha \lambda} \)
  - Acceleration of electrons by the ions (bremsstrahlung):
    - Be I: \( \sum \sigma_{\alpha \lambda} L_{\alpha \lambda} \)
  - Be II: \( \sum \sigma_{\alpha \lambda} L_{\alpha \lambda} \)

Conclusion

- Electron impact excitation and ionization cross sections were calculated using two independent methods: the sophisticated Convergent Close-Coupling (for Be I) and Coulomb-Born-Exchange (for all Be ions). The comparison of cross sections for Be I ion demonstrates reasonable agreement.
- The EBE results for \( \text{He}^+ \), \( \text{Be}^+ \) and \( \text{Be}^2+ \) are presented on IAEE website: http://www-nds.iaea.org/Atom/AKM.
- Similar calculations (possibly including fine structure transitions) can be done for other light (small-electron) elements (e.g., for alkali or alkaline earth atoms and their isoelectronic ions).
- Collisions with negative ions for Be I ion and all Be ions include the new improved version of CCC and excitation and ionization cross sections was constructed. Fractional ion abundances, electron cooling rates, radiative power losses and effective emission coefficients were calculated as functions of electron temperature in a wide range of plasma densities by the NOMAD code.