1 Ba atom

Ground configuration $1s^22s^22p^63s^23p^63d^{10}4s^24p^64d^{10}5s25p^66s^2$.

Excited configurations $1s^22s^22p^63s^23p^63d^{10}4s^24p^64d^{10}5s25p^66snl$.

5p-core-excited configurations $1s^22s^22p^63s^23p^63d^{10}4s^24p^64d^{10}5s^25p^5nln'l'n''l''$.

2 Method of calculations

The calculations of energies, radiative and autoionization probabilities, electron impact excitation and ionization cross sections were performed in the basis of mixed relativistic configurations by using FAC computer code (M. F. Gu, The flexible atomic code, Can. J. Phys. **86**, 675 (2008)). The radial orbitals for the construction of basis state wave functions were derived from a modified self-consisted Dirac-Fock-Slater iteration on the fictitious mean configuration with fractional occupation numbers representing the average electron cloud of the configurations included in the calculation.

In order to optimize the local central potential including the approximated exchange part, the configurations $5p^66s^2$. The following singly excited $5p^66snl$ $n = 6, ..., 12$, $l = 0, 1, 2$, $nl =$4f,5f and 5p-core excited $5p^5nln'l'n'l'$ $nl =$6s,5d, $n'l' =$6s,7s,6p,5d,6d, $n''l'' =$7s,...,10s; 7p,...,10p; 5d,...,10d; 5f configurations were used to take into account the correlation effects. Since the local potential was optimized only for singly excited states, to reduce the errors on total energies the following correction procedure was applied. Before the potential for the mean configuration with fractional occupation numbers was calculated, the optimized potential for each configuration was obtained, and the average energy for the configuration was calculated by using this potential. Then, the average energy for each configuration was calculated with the potential optimized for the mean configuration with fractional occupation numbers. The difference of the two average energies was then applied as a correction to the state energies within each configuration after the Hamiltonian was diagonalized. The total number of both odd and even states included in the calculation was 10199. The same basis set was used to calculate cross sections and autoionization probabilities. The final states $5p^6nlLSJ$ of Ba$^+$ were obtained by using $5p^6nl$, $nl =$6s,7s,6p,7p,5d,6d configurations.

The excitation cross sections were calculated in a relativistic distorted wave approximation. The contributions from large angular momentum partial waves for the allowed transition were taken into account by the Coulomb-Bethe approximation. To include the long-range contributions to the continuum-continuum radial integrals, the phase-amplitude method for continuum

wave functions was used. The autoionization probabilities were calculated in relativistic distorted wave and isolated resonance approximations.

3 Energy levels

The energy levels are presented in eV from the lowest energy level marked by 0.

The non-relativistic configuration is denoted by the standard spectroscopic notation, e.g. 5p2 for 2 electrons in 5p shell. Only open and nonempty shell are given. No coupling information is available in this name.

Each state is denoted with relativistic configuration and jjJ quantum numbers. For example, the label 4p+3(3)3 5s+1(1) 4 5p-1(1) 3 means $4p_{3/2}^5(3/2)3/2\ 5s_{1/2}(1/2)\ 2\ 5p_{1/2}(1/2)\ 3/2$ or, for any state, $nl^N[2(l+1/2)](2j)(2j)n'l'[2(l'+1)](2j')2J_0n''l''[2(l''-1/2)](2j'')2J$. The number in the parenthesis is 2 times the total angular momentum of the occupied shell. Immediately after the parenthesis, there is a number indicate the $2J$ value when all preceding shells are coupled. Therefore, 4p+2(2)2 4p2(2)0 represents a state $[4p_{3/2}^2(J=1)4p_{1/2}^2(J=1)]J=0$. Each shell is denoted such that 5p+2(2) represents 2 electrons in $5p_{3/2}(J=1)$ and 5p-2(2) represents 2 electrons in $5p_{1/2}(J=1)$.

4 Radiative transition probabilities

The weighted oscillator strength gf of the transition between states N_i and N_f is presented. It is related to the multipole matrix element M as

$$gf = (2L+1)^{-1}2E(2\alpha E)^{2L-2}|M|^2,$$

where L is the multipole rank, E is transition energy in atomic units. α is fine structure constant, g is the statistical weight of the level.

The weighted radiative transition probability is related to gf as

$$gA = 2\alpha^3 E^2 gf.$$

5 Autoionization probabilities

The autoionization probabilities were calculated in relativistic distorted-wave and isolated resonance approximations. In the case of the core-excited alkaline atoms, there is only one autoion-

ization channel up to the first excited state of alkaline ion, therefore the presented autoionization probabilities A^a are a total autoionization rates of the states.

6 Electron-impact excitation

Electron-impact excitation cross sections and collision strengths are calculated in relativistic distorted wave approximation. The energy grid is presented for the scattered electrons. Then, the energy E_i of the impacting electron is $E_i = E_{ex} + E_{ejected}$, where E_{ex} is the excitation threshold energy of the state.

The Born limit of the collision strength at high energies is

$$\Omega = b_0 \ln(x) + b_1,$$

where

$$x = \frac{E_0}{E_{th}}.$$

Here E_{th} is the energy of the excitation threshold, B_0 is given by Bethe, if it is an allowed transition in dipole approximation. It is equal to zero for forbidden transitions. The parameter b_1 is calculated at an energy which is chosen to be very high, about $100\ E_{th}$. These numbers are useful to extrapolate the collision strength to high energies with correct asymptotic behavior.

The collision strength is related to the excitation cross section as (atomic units):

$$\sigma = \frac{\pi}{k_0^2 g_0}\Omega,$$

where g_0 is the statistical weight of the initial state, k_0 is the kinetic momentum of the incident electron.

7 Electron-impact excitation rates

Electron-impact excitation rates were obtained by integration of the excitation cross sections over the Maxwellian electron energy distribution.

8 Electron-impact ionization

The ionization cross sections and strengths are calculated in Binary-Encounter-Dipole approximation. The energy grid is for the impacting electrons. The collision strength for ionizationΩ

is related to the ionization cross section as (atomic units):

$$\sigma = \frac{1}{k_0^2 g_0}\Omega,$$

where k_0 is the kinetic momentum of the incident electron, and g_0 is the statistical weight of the initial state. The missing factor π as compared to the formula for the collisional excitation is due to the different normalization for bound and free states.

The parameters b_0, b_1, b_2 and b_3 could be used in the fitting formula for the ionization strength

$$\Omega = b_0 \ln x + b_1 y^2 + b_2 \frac{1}{x} y^2 + b_3 \frac{1}{x^2} y,$$

where $x = E_0/E_{th}$, $y = 1 - 1/x$. E_0 is the energy of the incident electron, E_{th} is the ionization threshold. The parameter b_0 is obtained from the bound-free oscillator strength, which is more reliable than one would get by fitting the calculated collision strengths.

9   Electron-impact ionization rates

Electron-impact ionization rates were obtained by integration of the ionization cross sections over the Maxwellian electron energy distribution.