

# Bromine iso-electronic sequence: Lifetimes of the $4p^4 4d^4 D_{7/2}$ metastable level

J.P. Desclaux\*

15 Chemin du Billery, Sassenage F-38360, France

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## Abstract

The relativistic multiconfiguration Dirac–Fock method is applied to the calculation of the radiative decay rates from the lowest  $J = 7/2$  level of the  $4s^2 4p^4 d$  configuration along the Bromine iso-electronic sequence. It is shown that only a limited number of configurations is needed to include the most relevant contributions to the variation in correlation effects between this excited level and the ground  $4s^2 4p^5 P_{3/2}$  state. The transition from LS to  $jj$  recoupling schemes along the sequence is studied and its impact on decay rates is discussed.

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## 1. Introduction

Metastable levels are important in dilute plasmas because they are not depopulated by collisions but accurate values of their lifetimes are difficult to obtain both from experiment and from theory. For *ab initio* methods, how much of correlation effects have to be included is a critical issue since, excepted for few electron systems, a full correlated approach becomes intractable. On the other side, *semi empirical* methods rely on fitting some parameters to experimental results, these methods are not relevant to study trends along iso-electronic sequences. Indeed experimental results may be available near the neutral end of the sequence but the fitted values cannot be used for the high  $Z$  end of the sequence because of strong relativistic effects. To include in a consistent way both relativistic corrections, intermediate coupling and correlation contributions, we use here the multiconfiguration Dirac–Fock method with the purpose to include only the contributions significant for energies and probabilities of radiative decays. Our motivation to select the Bromine iso-electronic sequence was because of the importance of the  $M2$  decay channel for the single excited KrII

ion and, to our knowledge, no estimate of how this importance evolves along the sequence is known.

This paper is organized as follows: in Section 2, the method used to compute wave functions and transition probabilities is outlined. The next section contains a detailed discussion of the excited  $4s^2 4p^4 4d^4 D_{7/2}$  level of KrII, for which an accurate experimental result and previous theoretical calculations are available [1], in order to assess the accuracy of the present calculations. Section 4 gives the trends along the iso-electronic sequence before we draw our conclusions.

## 2. Outline of the calculation method

### 2.1. The MCDF method

In this work, the 2007 version of the Dirac–Fock program of the author and P. Indelicato, named *mdfgme* [2] is used. Details on the Hamiltonian, angular momentum recoupling and numerical methods can be found elsewhere [3–6] below is just a brief summary for the sake of self-contained. The total energies associated with the various levels of the atomic system are given by the eigenvalues of the equation:

$$\mathcal{H}\Psi_{\Pi,J,M}(\dots, \mathbf{r}_i, \dots) = E_{\Pi,J,M}\Psi_{\Pi,J,M}(\dots, \mathbf{r}_i, \dots), \quad (1)$$

\* Corresponding author.

E-mail address: [jean-paul.desclaux@wanadoo.fr](mailto:jean-paul.desclaux@wanadoo.fr).

where  $\Pi$  is the parity,  $J$  the total angular momentum eigenvalue, and  $M$  is the eigenvalue of its projection  $J_z$  on the  $z$  axis. The Hamiltonian  $\mathcal{H}$  is given by

$$\mathcal{H} = \sum_i h_D(r_i) + \sum_{i<j} V_{ij}(|\mathbf{r}_i - \mathbf{r}_j|) \quad (2)$$

with  $h_D$  the one electron Dirac operator and  $V_{ij}$  an operator representing the electron–electron interaction of order one in the fine structure constant  $\alpha$ . The expression of  $V_{ij}$  in Coulomb gauge, and in atomic units, is

$$V_{ij} = \frac{1}{r_{ij}} \quad (3)$$

$$-\frac{\boldsymbol{\alpha}_i \cdot \boldsymbol{\alpha}_j}{r_{ij}} \quad (4)$$

$$-\frac{\boldsymbol{\alpha}_i \cdot \boldsymbol{\alpha}_j}{r_{ij}} \left[ \cos\left(\frac{\omega_{ij} r_{ij}}{c}\right) - 1 \right] + c^2 (\boldsymbol{\alpha}_i \cdot \nabla_i)(\boldsymbol{\alpha}_j \cdot \nabla_j) \frac{\cos(\omega_{ij} r_{ij}/c) - 1}{\omega_{ij}^2 r_{ij}}, \quad (5)$$

where  $r_{ij} = |\mathbf{r}_i - \mathbf{r}_j|$  is the inter-electronic distance,  $\omega_{ij}$  the energy of the exchanged photon between the two electrons,  $\alpha_i$  are the Dirac matrices and  $c$  is the speed of light. It has been demonstrated that the Coulomb gauge provides energies free from spurious contributions at the ladder approximation level and must be used in many-body atomic structure calculations [7,8].

In the equations above, the term (3) is the Coulomb interaction, (4) is the Gaunt (magnetic) interaction, and the last two terms (5) stand for the retardation in the electron–electron interaction. In this expression the  $\nabla$  operators act only on  $r_{ij}$  and not on the following wave functions.

Expanding the operators of Eq. (5) in powers of  $\omega_{ij} r_{ij}/c$  one obtains, at the limit  $\omega_{ij} \rightarrow 0$ :

$$B_{ij}^R = \frac{\boldsymbol{\alpha}_i \cdot \boldsymbol{\alpha}_j}{2r_{ij}} - \frac{(\boldsymbol{\alpha}_i \cdot \mathbf{r}_{ij})(\boldsymbol{\alpha}_j \cdot \mathbf{r}_{ij})}{2r_{ij}^3}, \quad (6)$$

i.e., the retardation part of the Breit interaction which includes the leading retardation contribution of order  $1/c^2$ . The total Breit interaction is the sum of the Gaunt interaction (4) and the Breit retardation (6).

In the calculations reported here, the electron–electron interaction for the self-consistent determination of the wave functions is taken as the sum of the Coulomb and the Breit interactions. Higher orders in  $1/c$ , arising from the difference between operators (5) and (6) are treated here only as a first order perturbation. Radiative corrections are also added by perturbation, a detailed description of what is included in the most recent version of the *mdfgme* code can be found in [9]. All calculations are done for finite nuclei using a Fermi distribution with a thickness parameter of 2.3 fm. The nuclear radii are taken or evaluated using formulas from Ref. [10].

The MCDF method is defined by the particular choice of the total wave function to solve Eq. (1) taken as a linear combination

of configuration state functions (CSF):

$$|\Psi_{\Pi,J,M}\rangle = \sum_{\nu=1}^{N_\nu} c_\nu |v, \Pi, J, M\rangle. \quad (7)$$

The label  $\nu$  stands for all other quantities (principal quantum number, degeneracy, ...) necessary to define unambiguously the CSF besides the parity  $\Pi$ , the total angular momentum  $J$  and its projection  $J_z$ . Each CSF is an antisymmetric products of one-electron wave functions taken as a linear combination of Slater determinants of Dirac 4-spinors:

$$|v, \Pi, J, M\rangle = \sum_{i=1}^{N_D^v} d_i^v \begin{vmatrix} \phi_1^i(\mathbf{r}_1) & \cdots & \phi_n^i(\mathbf{r}_1) \\ \vdots & \ddots & \vdots \\ \phi_1^i(\mathbf{r}_n) & \cdots & \phi_n^i(\mathbf{r}_n) \end{vmatrix}, \quad (8)$$

where the coefficients  $d_i^v$  are determined by requiring the CSF to be an eigenstate of  $J^2$  and  $J_z$  and the  $\phi$ -s are the one-electron Dirac 4-spinors:

$$\phi(r) = \begin{pmatrix} \chi_k^\mu(\Omega) P(r) \\ i \chi_{-k}^\mu(\Omega) Q(r) \end{pmatrix} \quad (9)$$

with  $\chi_k^\mu$  a two-component spinor, and  $P$  and  $Q$  respectively the large and small component of the radial wave function. The convergence process is based on the self-consistent field process (SCF). For a given set of configurations, initial one-electron radial functions are used to build the Hamiltonian matrix and get a first set of mixing coefficients  $c_\nu$ . Direct and exchange potential are constructed for all orbitals, and the integro-differential equations obtained from the variational principle are solved. Then a new set of potentials is constructed and the whole process is repeated. Each time the largest variation for all radial functions has been reduced by an order of magnitude, the Hamiltonian matrix is re-diagonalized, and a new cycle is started until convergence is reached.

## 2.2. Transition probabilities

To perform the calculations reported in the next sections, some of the specific options of *mdfgme* code are used:

- First with the option *radiative* it is enough to define the CSF for the initial and final states and, after the SCF optimization of both states, all allowed transitions probabilities for all multipoles of the electric and magnetic decay channels are computed, so that there is no need to perform separated calculations of each of the decay channels in order to find the dominant one. Transition probabilities are computed with the full operator, i.e., without low frequency approximation.
- To introduce correlation, two main options are available: either give explicitly the list of CSF to include or let the program build all single and double excitations from a reference state. In this latter case, orbitals to be excited and non-closed shells in which excitations will occur have to be specified. The second option is indeed split in more than one possibility but it is not our purpose to reproduce here part of the code's

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