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Construction of the energy matrix for complex atoms

Part V: Electrostatically correlated spin-orbit and electrostatically correlated hyperfine interactions

Magdalena Elantkowska[1,a], Jarosław Ruczkowski[2], and Jerzy Dembczyński[2]

[1] Institute of Materials Research and Quantum Engineering, Faculty of Technical Physics, Poznan University of Technology Piotrowo 3, 60-965 Poznań, Poland
[2] Institute of Control and Information Engineering, Faculty of Electrical Engineering, Poznan University of Technology Piotrowo 3A, 60-965 Poznań, Poland

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Abstract. The continuation of the previous series of papers related to the construction of the energy matrix for complex atoms is presented. The contributions from the second-order perturbation theory concerning electrostatically correlated spin-orbit interactions (CSO), as well as electrostatically correlated hyperfine interactions (CHFS) to the atomic structure of nl^N, $nl^N n_1 l_1^{N_1}$ and $nl^N n_1 l_1^{N_1} n_2 l_2^{N_2}$ configurations, are considered. This theory assumes that the electron excitation $n_0 l_0 \rightarrow nl$ affects spin-orbit splitting and magnetic dipole and electric quadrupole hyperfine structure in the same way which will be discussed below. Part I of the series presented, in general terms, a method allowing the analysis of complex electronic systems. Parts II, III and IV provided a description of an electrostatic interaction up to second-order perturbation theory; they constitute the basis for the design of an efficient computer program package for large-scale calculations of accurate wave functions. Analyses presented in the entire series of our papers clearly demonstrate that obtaining the precise wave functions is impossible without considering the contribution from the second-order effects into fine and hyperfine atomic structure.

1 Introduction

This paper is the fifth in the series on *Construction of the energy matrix for complex atoms*. In the first work [1] we introduced in general terms a method allowing the analysis of a complex electronic system composed of a configuration of up to four open shells, taking into account all electromagnetic interactions expected in an atom. The wave functions corresponding to the atomic energy states are expanded in the system of interacting configurations. On this basis, the energy matrix of the Hamiltonian [2–5] describing the fine structure of an atom is constructed, accounting for the interactions up to the first order of the perturbation theory. The calculation details of the matrix elements of the particular Hamiltonian constituents were discussed, and the formulae were presented in our earlier works [6, 7]. These works focused on $(nd + n's)^{N+2} + nd^N n_1 l_1 n_2 l_2$ configurations. In the analysis of the spectra of complex atoms, electrostatic interactions appear between many types of configurations involving up to four open electronic shells. Therefore, in our second paper in the series [8], we presented 36 new formulae for the first-order electrostatic interactions between configurations up to four open shells.

However, even though many interacting configurations were included, the perturbations produced by all weakly interacting configurations remained. In spite of the fact that a correction from a single distant perturbing configuration is rather small, its cumulative influence may be considerable, due to the increasing density of states as the continuum is approached. The second-order effects, the so-called configuration interaction (CI) effects, are observed both in the fine and hyperfine structure study. Therefore, our energy matrix is extended by the elements comprising electrostatic coupling and electrostatically correlated spin-orbit coupling between the configurations of the system analysed and the distant configurations. Generally, for the configurations containing up to three open electronic shells, these matrix

[a] e-mail: magdalena.elantkowska@put.poznan.pl

elements originate from the second-order perturbation theory and can be schematically expressed as follows:

$$\mathrm{C} = -\sum_{\psi'' \neq \psi, \psi'} \left[\langle \psi | \mathbf{G} | \psi'' \rangle \times \langle \psi'' | \mathbf{G} | \psi' \rangle \right] / \Delta E = -(\text{angular part}) \times (\text{radial part}), \tag{1}$$

where ψ, ψ' represent particular states of the considered system of configurations:

$$\begin{aligned} \psi &= (n_0 l_0)^{4l_0+2}\ {}^1S, (n_1 l_1)^{N_1} S_1 L_1, (n_2 l_2)^{N_2} S_2 L_2, (n_3 l_3)^{N_3} S_3 L_3; SL, \\ \psi' &= (n_0 l_0)^{4l_0+2}\ {}^1S, (n_1 l_1)^{N_1'} S_1' L_1', (n_2 l_2)^{N_2'} S_2' L_2', (n_3 l_3)^{N_3'} S_3' L_3'; SL, \end{aligned} \tag{2}$$

and ψ'' denotes all perturbing virtual states included in our system, defined directly in sections containing formulae (see sect. 3 in [9] and sect. 5 in [10]), $\mathbf{G}$ denotes the two-body operator of an electrostatic interaction, and ΔE denotes the energy difference between the centre of gravity of the considered configuration and the particular perturbing configuration. The angular coefficients are the result of the coupling of angular momenta of the operator $\mathbf{G}$. They are determined by means of our computer codes. The radial integrals are treated adjustable parameters, which can be determined by fitting the calculated levels to the experimental ones with the least squares method. The radial parameters have denotations which code the interacting configurations and specify the interactions. Denotations of particular radial parameters take the form

$$R^t \left(n_a l_a n_b l_b, n_c l_c n_d l_d \right) R^{t'} \left(n_a' l_a' n_b' l_b', n_c' l_c' n_d' l_d' \right), \tag{3}$$

where R^t and $R^{t'}$ represent the Slater radial integrals which arise from the radial parts of one-electron eigenfunctions.

The Slater radial integrals R^t are defined by [11]

$$R^t \left(n_a l_a n_b l_b, n_c l_c n_d l_d \right) = e^2 \int_0^\infty \int_0^\infty \frac{r_<^t}{r_>^{t+1}} R_{n_a l_a}(r_1) R_{n_b l_b}(r_2) R_{n_c l_c}(r_1) R_{n_d l_d}(r_2)\, \mathrm{d}r_1 \mathrm{d}r_2, \tag{4}$$

where e is the electron charge, r_1 and r_2 are the coordinates of electrons, $r_<$ and $r_>$ indicate the distances from the nucleus to the closer and more distant electrons, respectively. In order to specify particular interactions more precisely, the symbol R^t (where t stands for the order) is replaced, respectively, by D^t in the case of direct interactions, E^t for exchange interactions, or R^t for interactions involving two equivalent electrons. In our procedure, excitations of one or two electrons from a closed shell to all open shells are studied under the following conditions:

$$|l_i - l_0| = 0, 2 \quad \text{and} \quad N_1 + N_2 + N_3 = N_1' + N_2' + N_3'. \tag{5}$$

The matrix elements determined from relation (1) under condition (5) were included in the fine-structure energy matrix and were clearly defined in the papers [9,10].

In the third part [9] of our series, we started discussing the second-order electrostatic effects, concentrating on the excitation of two equivalent electrons from a closed shell into an open shell or into an empty shell. As a result, we presented 22 new formulae for the second-order electrostatic intra- and interconfigurations matrix elements up to third open shells. In the fourth part [10] we introduced 138 new formulae for the second-order electrostatic intra- and interconfiguration matrix elements up to third open shells, describing the effects of one electron excitation from a closed shell into an open shell or into an empty shell.

The next section of the current paper contains the detailed description of electrostatically correlated spin-orbit interactions and electrostatically correlated hyperfine interactions. The current state of the art is also presented. The method of the reduced matrix elements calculation is described in sect. 3. Section 4 contains the explanation of the symbols used in this work. In sect. 5, explicit formulae for electrostatically correlated spin-orbit interactions as well as for electrostatically correlated hyperfine interactions are presented. This section is the most extensive part of the paper. The results of semi-empirical calculations for the $(5d + 6s)^3$ configurations system of lanthanum atom, as an example of the method described above, are presented in sect. 6.

2 Electrostatically correlated spin-orbit interactions and electrostatically correlated hyperfine interactions: the current state of the art

Contributions from the second-order perturbation theory for electrostatically correlated spin-orbit interactions (CSO) as well as for electrostatically correlated hyperfine interactions (CHFS), are defined as follows:

$$-\sum_{\psi'' \neq \psi, \psi'} \left[\langle \psi | \mathbf{G} | \psi'' \rangle \times \langle \psi'' | \mathbf{T}^{(\kappa k) K} | \psi' \rangle + \langle \psi | \mathbf{T}^{(\kappa k) K} | \psi'' \rangle \times \langle \psi'' | \mathbf{G} | \psi' \rangle \right] / \Delta E = -\left(\text{angular part} \right) \times \left(\text{radial part} \right), \tag{6}$$

where ψ, ψ' represent particular states of the considered system configurations:

$$\psi = (n_0 l_0)^{4l_0+2}\ {}^1S, (n_1 l_1)^{N_1} S_1 L_1, (n_2 l_2)^{N_2} S_2 L_2, (n_3 l_3)^{N_3} S_3 L_3; SLJ,$$
$$\psi' = (n_0 l_0)^{4l_0+2}\ {}^1S, (n_1 l_1)^{N_1'} S_1' L_1', (n_2 l_2)^{N_2'} S_2' L_2', (n_3 l_3)^{N_3'} S_3' L_3'; S'L'J \tag{7}$$

and ψ'' denotes all perturbing virtual states included in our system, defined below in sect. 5. The symbol $\mathbf{G}$ denotes the two-body operator of an electrostatic interaction, a double tensor $\mathbf{T}^{(\kappa k)K}$ of rank κ in the spin space and of rank k in the orbit space denotes the one-body operator of either spin-orbit ($H_{\rm so}$ for $K = 0$) interaction or a hyperfine ($H_{\rm hfs}$ for $K > 0$) interaction, and ΔE denotes the energy difference between the centre of gravity of the considered configuration and the particular perturbing configuration.

The radial parameters $P^t(n_i l_i n_0 l_0, n_i l_i n_i' l_i') P^{\kappa k}(n_0 l_0, n_i l_i)$ specify the coupling between configurations. The radial integral $P^t(n_i l_i n_0 l_0, n_i l_i n_i' l_i')$ describes electrostatic coupling of the configurations, *i.e.* it specifies the electrons involved and the type of their interaction. In the actual description the symbol P^t is replaced, as above, with D^t or E^t, respectively. $P^{\kappa k}$ is the radial part of a one-body operator $\mathbf{T}^{\kappa k}$ which couples the electrons $n_0 l_0$ and $n_i l_i$. In our procedure, the excitations of one electron from the closed shell $(n_0 l_0)^{4l_0+2}$ to each of three open shells $(n_1 l_1)^{N_1}$, $(n_2 l_2)^{N_2}$ and $(n_3 l_3)^{N_3}$ are considered. In the case of the spin-orbit interaction, the symbol $P^{\kappa k}$ is replaced by the spin-orbit parameter $\zeta(n_0 l, nl)$.

The off-diagonal radial integrals $\zeta(n_0 l, nl)$ of the spin-orbit interaction are defined by [12]

$$\zeta(n_0 l, nl) = \langle nl|\xi(r)|n_0 l\rangle, \tag{8}$$

where $\xi(r)$ is the radial part of the spin-orbit operator defined by [11]

$$\xi(r) = \frac{\alpha^2}{2}\frac{1}{r}\left(\frac{\mathrm{d}V(r)}{\mathrm{d}r}\right), \tag{9}$$

where $V(r)$ is the central-field potential-energy function, α is the fine-structure constant, and $\zeta(n_0 l, nl)$ has the same units as $V(r)$ if r is in Bohr units.

The above description of the parameters is a simplified notation. The parameters are precisely defined as sums over all closed (or open) shells. For example, in the case of the lanthanum atom:

$$E^2(n_0 d6s, 6s5d)\,\zeta_{n_0 d,5d} = \sum_{n_0=3}^{4} E^2(n_0 d6s, 6s5d)\,\zeta(n_0 d, 5d)/\Delta E, \tag{10}$$

where ΔE is the energy difference between the relevant closed- and open-shell orbitals.

In the case of CSO, the following condition has to be fulfilled:

$$|l_0 - l_1| = 0 \quad \text{and} \quad \kappa k = 11,\ K = 0. \tag{11}$$

The matrix elements determined from relation (6) under condition (11) were included in the fine-structure energy matrix.

In the case of CHFS, the following relations hold: for magnetic dipole interactions $K = 1$:

$$|l_0 - l_1| = 0 \quad \text{if } \kappa k = 01, 10 \quad \text{and} \quad |l_0 - l_1| = 0, 2 \quad \text{if } \kappa k = 12 \tag{12}$$

and for electric quadrupole interactions $K = 2$:

$$|l_0 - l_1| = 0, 2 \quad \text{if } \kappa k = 02 \quad \text{and} \quad |l_0 - l_1| = 0 \quad \text{if } \kappa k = 11, 13. \tag{13}$$

The radial part $P^{\kappa k}$ of a one-body operator $\mathbf{T}^{\kappa k}$ in the two-body hyperfine-structure (hfs) radial parameter $P^t(n_i l_i n_0 l_0, n_i l_i n_i' l_i') P^{\kappa k}(n_0 l_0, n_i l_i)$ is an integral $\langle n_0 l_0|r^{-3}|n_i l_i\rangle^{\kappa k}$.

The parameters are precisely defined as sums over all closed (or open) shells. For example, in the case of the lanthanum atom:

$$E^2(n_0 d6s, 6s5d)\,P^{02} n_0 d, 5d = \sum_{n_0=3}^{4} E^2(n_0 d6s, 6s5d)\,\left\langle n_0 l_0 \left| r^{-3} \right| 5d \right\rangle^{02} / \Delta E \tag{14}$$

or for "core polarization"

$$E^2(n_0 s5d, 5d6s)\,P^{10}(n_0 s, 6s) = 4\pi \sum_{n_0=1}^{5} \Psi_{6s}(0)\Psi_{n_0 s}(0)\,E^2(n_0 s5d, 5d6s)/\Delta E, \tag{15}$$

where ΔE is the energy difference between the relevant closed- and open-shell orbitals.

The matrix elements resulting from relation (6) and conditions (12) and (13) were calculated by our computer code and included in the hyperfine structure energy matrix.

The spin-orbit interaction (where $\kappa k = 11$) and hfs interactions, for $\kappa k = 01$, are diagonal in the one-electron orbital quantum number $l > 0$, but not in the principal quantum number n. The spin-orbit interaction vanish for s electrons, therefore the hyperfine interaction related to the excitations from $n_0 s$ closed shell to ns open shell or from $n_0 s$ closed shell to $n'''s$ empty shell will be discussed separately.

2.1 Electrostatically correlated spin-orbit interactions (CSO)

The first detailed investigation of the electrostatically correlated spin-orbit interaction (CSO) was carried out by Rajnak and Wybourne [13]. It was done for the l^N configuration. This study resulted in the formulae on the matrix elements of the relevant effective operator; the radial parameters of CSO were defined as well. The CSO for the l^N configuration was examined also by Pasternak and Goldshmidt [14]. They gave the effective operator for the electrostatically correlated spin-orbit interaction explicitly. The expressions for matrix elements of this operator are the same as those calculated by Rajnak and Wybourne [13] if the terms proportional to the spin-orbit interaction are subtracted. This suggests that a mistake from [13] is repeated in [14]. Probably it arose from the wrong definition of the CSO (eq. (6)) correction in [13], where the identity $\langle\psi|\mathbf{G}|\psi''\rangle \times \langle\psi''|\mathbf{H}_{\rm so}|\psi'\rangle = \langle\psi|\mathbf{H}_{\rm so}|\psi''\rangle \times \langle\psi''|\mathbf{G}|\psi'\rangle$ seems to be assumed, which is generally not true.

Further progress in the theoretical CSO formalism was achieved for the $l^N l'$ configuration. For this configuration, a number of formulae to calculate the matrix elements of CSO was given by Goldschmidt and Mallow [15].

The method of parametrization of the electrostatically correlated spin-orbit interaction for complex atoms in extended model space of $(nd + n's)^{N+2} + \sum_{i,j} nd^{N+2-w_i-w_j} n_i l_i^{w_i} n_j l_j^{w_j}$ configurations was presented in our paper from 1996 [6],which also included corrections of errors from earlier papers of other authors [13,14]. Although the interconfiguration CSO interactions were included for the first time in the work [6], the contributions with the integrals involving the l' orbital (or l''), as well as excitations from these orbitals were neglected.

2.2 Electrostatically correlated hyperfine interactions (CHFS)

The development of the hyperfine structure theory was initiated in the classic paper of Sandars and Beck [16]. They developed a theory which simplifies the calculation and interpretation of relativistic hfs effects in many-electron atoms. This theory leads to three effective radial integrals for each open shell and for each multipole interaction. As shown by Judd [17,18] and Sandars [19], the configuration interaction (CI) effects caused by excitations from closed shells to empty shells can be included in an effective Hamiltonian of the same form. This theory was applied by Lindgren and Rosen [20] to analyse a large number of experimental hfs data mainly in atomic ground configurations, and by Büttgenbach [21] to analyse hfs in $4d$- and $5d$-shell atoms. In these analyses of hfs data, the effective radial integrals were treated as free parameters which were fitted to the experimental results in order to examine some relativistic CI effects. The experimental hfs radial parameters obtained in this way show a rather poor agreement with theoretical results of relativistic Hartree-Fock calculations [20–22] It demonstrates that more contributions exist to the hfs splittings which should be taken into account. Bauche-Arnoult [23,24], Armstrong [2] as well as Lindgren and Morrison [3] showed that configuration effects for the second order perturbation theory can be split into two parts: the first (one-body) part, which is common to all terms of a given configuration, and the other (two-body) part depending on the SL-terms studied. Bauche-Arnould [23,24] defined the effective operators, which described the crossed second-order effects of electrostatic and hyperfine interactions for all types of excitations appearing in the configurations l^N or $l^N l'$. Assuming pure SL-coupling, Bauche-Arnoult found regularities in the contributions from electrostatically correlated second-order hfs to the different effective radial parameters. Later, in 1985, Dembczyński [25] elaborated a new parametrization method which took into account simultaneously one- and two-body interactions in atomic hfs structure of the configurations $(3d+4s)^{N+2}$. This method was applied to the interpretation of iron, vanadium, titanium and cobalt atoms [26–29]. In the following years, the above mentioned method of parametrization of interactions in the hfs was extended up to three open electronic shells [6,30]. Remarks on the interpretation of very high-precision measurements of hyperfine structure splittings in neutral and singly ionised complex atoms were presented in our papers [31,32].

2.3 Parametrization of the configuration interaction effects

Computer procedures of experimental data analysis concerning the fine and hyperfine structure (fs and hfs) of complex atoms have been developed in our group for many years. For the configurations containing up to three open electronic shells we considered all contributions to fs and hfs, within the framework of the second order perturbation theory,

which originate from the excitations "open shell-empty shell" or "closed shell-open shell" and "closed shell-empty shell". In the work of 2010 [33] we presented our new method. We analysed the configuration system $(5d+6s)^N$ of the lanthanum atom, which is well isolated from any disturbing configurations, and the conditions for the application of the perturbation theory are fulfilled. It yields an excellent possibility of an alternative analysis of the contributions mentioned within the second-order perturbation theory according to the excitation model, either "open shell-empty shell" or "closed shell-open shell". A simultaneous application of both models is not possible due to the fact that in both models an implicit linear dependence between angular coefficients corresponding to certain radial parameters has to occur, which makes the solution of a redundant set of linear equations impossible, thus hindering the determination of the respective radial parameters. It provides an excellent test to confirm the correctness of the complex formulae derived, *e.g.* for the configurations with three open shells, which require recoupling of five or more angular momenta and strict observance of the electron permutation rules, in particular for interconfiguration matrix elements. When both the fine and the hyperfine structure are considered independently within the framework of both excitation models, two independent sets of radial parameters describing the atomic structure are obtained. On the basis of the theoretically predicted relations between the radial parameters originating from both models, we proved the correctness of the obtained description of the atomic structure, as well as precisely defined the information provided by the radial parameters determined from the experimental data. In sect. 5 of paper [33] we provided the relations which allow to recalculate the parameters obtained for the model space $(5d+6s)^3$ within both excitation models: "closed shell-open shell" (c-o) and "open shell-empty shell" (o-e) into the radial parameters characteristic of the individual configurations $5d^3$, $5d^2 6s$ and $5d6s^2$.

In summary, on the basis of our considerations included in [33], we suggest considering the broadest possible basis of configurations in the first-order of the perturbation theory, while the second-order effects of the perturbation theory should be described by both the excitation of two electrons from a closed shell to an open shell or an empty shell and the excitation of one electron from a closed shell to an open shell or an empty shell. In our method, each orbital appearing in closed n_0l_0 shells or open nl, n_1l_1, n_2l_2 shells, and also $n'l'$ empty shells, is common for all configurations in the system under study. The existence of the factor containing the number of electrons in the core (N) removes the linear dependence between parameters for the configurations with different N number. Therefore, we obtain different values of the angular coefficients of the parameters for the configurations with the same parameter describing the excitations either to empty, or to open shells. For example, in the case of even configurations of lanthanum atom, the excitation to the $6s$ shell represents, for $5d^3$ configuration, the excitation to an empty shell, while the same parameter describes the excitation to an open shell in $5d^2 6s$ configuration.

Recently, we have presented the appropriate formulae describing the excitation of one or two electrons from a closed shell to an open shell for the following configurations: nl^N, $nl^N n_1 l_1^{N_1}$, $nl^N n_1 l_1^{N_1} n_2 l_2$ and $nl^N n_1 l_1 n_2 l_2^{N_2}$, as well as between the configurations [9,10].

3 Removal of the J-dependence and the method of the reduced matrix elements calculation

In this paper we concentrate on the excitation of one electron from a closed shell into an open shell or into an empty shell for the extended model configuration space. The formulae describing the intra- and interconfiguration electrostatically correlated spin-orbit interaction and electrostatically correlated hyperfine interaction are presented in the form of the reduced matrix elements. Each two-body contribution to the spin-orbit parameter and to the hfs magnetic-dipole and electric-quadrupole constants can be written as reduced matrix elements using the Wigner-Eckart theorem.

3.1 Electrostatically correlated spin-orbit interaction

By substituting $\kappa k = 11$ and $K = 0$ into the eq. (6), the general formula for the matrix elements of CSO reads

$$\langle \Psi(\Gamma\alpha SLJM)|\mathbf{CSO}|\Psi'(\Gamma'\alpha'S'L'J'M')\rangle = -\sum_{\Psi''\neq\Psi,\Psi'} \left[\langle\Psi|\mathbf{G}|\Psi''\rangle \times \langle\Psi''|\mathbf{H}_{\rm so}|\Psi'\rangle + \langle\Psi|\mathbf{H}_{\rm so}|\Psi''\rangle \times \langle\Psi''|\mathbf{G}|\Psi'\rangle\right]/\Delta E =$$

$$\delta(M,M')\delta(J,J')(-1)^{J+S'+L} \begin{Bmatrix} S & S' & 1 \\ L & L' & J \end{Bmatrix} \langle \Psi(\Gamma\alpha SL)\|\mathbf{CSO}\|\Psi'(\Gamma'\alpha'S'L')\rangle =$$

$$\delta(M,M')\delta(J,J')(-1)^{J+S'+L} \begin{Bmatrix} S & S' & 1 \\ L & L' & J \end{Bmatrix}$$

$$\times \left[-\sum_{\psi''} \left\langle n_0 l_0^{4l_0+2}\ {}^1S\ , \Gamma\alpha SL; SL\,|\mathbf{G}|\,n_0 l_0^{4l_0+1}\ {}^2l_0, \Gamma''\alpha''S''L''; SL \right\rangle \right.$$

$$\times \left\langle n_0 l_0^{4l_0+1}\ {}^2l_0, \Gamma''\alpha''S''L''; SL \,\|\mathbf{H}_{\rm so}\|\, n_0 l_0^{4l_0+2}\ {}^1S\ , \Gamma'\alpha'S'L'; S'L' \right\rangle$$
$$- \sum_{\psi''} \left\langle n_0 l_0^{4l_0+1}\ {}^2l_0, \Gamma''\alpha''S''L''; SL \,\|\mathbf{H}_{\rm so}\|\, n_0 l_0^{4l_0+2}\ {}^1S\ , \Gamma'\alpha'S'L'; S'L' \right\rangle$$
$$\times \left\langle n_0 l_0^{4l_0+2}\ {}^1S\ , \Gamma'\alpha'S'L'; S'L' \,|\mathbf{G}|\, n_0 l_0^{4l_0+2}\ {}^1S, \Gamma'\alpha'S'L' \right\rangle \Bigg] =$$
$$\delta(M,M')\ \delta(J,J')(-1)^{J+S'+L} \begin{Bmatrix} S & S' & 1 \\ L & L' & J \end{Bmatrix} \delta(l_i,l_0)\ t^{11}_{coeff}(n_0l_0,n_il_i)$$
$$\times \text{(angular part)} \sum_{n_0l_0} R^t\,(n_il_in_0l_0, n_il_in_i'l_i')\,\zeta_{n_0l_i,n_il_i}/\Delta E, \tag{16}$$

where Γ, Γ' designate the configurations being considered, ΔE is the (positive) energy difference between the relevant closed- and open or empty-shell orbitals, $\kappa k = 11$ and $t^{11}_{coeff}(n_0l_0, n_il_i)$ is the angular part of the spin-orbit operator $\widehat{s}_i\widehat{l}_i$:

$$\left\langle n_0l_0 \left\| \widehat{s}_i\widehat{l}_i \right\| n_il_i \right\rangle = t^{\kappa k}_{coeff}(n_0l_0,n_il_i)\ \zeta_{n_0l_i,n_il_i} = \frac{3}{2}\sqrt{l(l+1)(2l+1)}\ \zeta_{n_0l_i,n_il_i}. \tag{17}$$

3.2 Electrostatically correlated hyperfine interaction

In the case of CHFS, the following relations hold:

a) for magnetic dipole interactions $K = 1$:

$$\langle \Psi(\Gamma\alpha SLJM)|\mathbf{CHFS}|\Psi'(\Gamma'\alpha'S'L'J'M')\rangle = -\sum_{\Psi''\neq\Psi,\Psi'} \left[\langle\Psi|\mathbf{G}|\Psi''\rangle \times \langle\Psi''|\mathbf{t}^{\kappa k}|\Psi'\rangle + \langle\Psi|\mathbf{t}^{\kappa k}|\Psi''\rangle \times \langle\Psi''|\mathbf{G}|\Psi'\rangle\right]/\Delta E =$$
$$\delta(M,M')\delta(J,J')\sqrt{\frac{3(2J+1)}{J(J+1)}} \begin{Bmatrix} S & S' & \kappa \\ L & L' & k \\ J & J & 1 \end{Bmatrix} \langle\Psi(\Gamma\alpha SL)\|\mathbf{CHFS}\|\Psi'(\Gamma'\alpha'S'L')\rangle =$$
$$\delta(M,M')\delta(J,J')\sqrt{\frac{3(2J+1)}{J(J+1)}} \begin{Bmatrix} S & S' & \kappa \\ L & L' & k \\ J & J & 1 \end{Bmatrix}$$
$$\times \Bigg[-\sum_{\psi''} \left\langle n_0 l_0^{4l_0+2}\ {}^1S\ , \Gamma\alpha SL; SL \,|\mathbf{G}|\, n_0 l_0^{4l_0+1}\ {}^2l_0, \Gamma''\alpha''S''L''; SL \right\rangle$$
$$\left\langle n_0 l_0^{4l_0+1}\ {}^2l_0, \Gamma''\alpha''S''L''; SL \left\|\mathbf{t}^{\kappa k}\right\| n_0 l_0^{4l_0+2}\ {}^1S\ , \Gamma'\alpha'S'L'; S'L' \right\rangle$$
$$- \sum_{\psi''} \left\langle n_0 l_0^{4l_0+1}\ {}^2l_0, \Gamma''\alpha''S''L''; SL \left\|\mathbf{t}^{\kappa k}\right\| n_0 l_0^{4l_0+2}\ {}^1S\ , \Gamma'\alpha'S'L'; S'L' \right\rangle$$
$$\times \left\langle n_0 l_0^{4l_0+2}\ {}^1S\ , \Gamma'\alpha'S'L'; S'L' \,|\mathbf{G}|\, n_0 l_0^{4l_0+2}\ {}^1S, \Gamma'\alpha'S'L' \right\rangle \Bigg] =$$
$$\delta(M,M')\ \delta(J,J')\sqrt{\frac{3(2J+1)}{J(J+1)}} \begin{Bmatrix} S & S' & \kappa \\ L & L' & k \\ J & J & 1 \end{Bmatrix} t^{\kappa k}_{coeff}(n_0l_0,n_il_i)$$
$$\times \text{(angular part)} \sum_{n_0l_0} R^t\,(n_il_in_0l_0, n_il_in_i'l_i')\,\langle n_0l_0|r^{-3}|n_il_i\rangle/\Delta E, \tag{18}$$

b) for electric quadrupole interactions $K = 2$:

$$\langle \Psi(\Gamma\alpha SLJM)|\mathbf{CHFS}|\Psi'(\Gamma'\alpha'S'L'J'M')\rangle = -\sum_{\Psi''\neq\Psi,\Psi'} \left[\langle\Psi|\mathbf{G}|\Psi''\rangle \times \langle\Psi''|\mathbf{t}^{\kappa k}|\Psi'\rangle + \langle\Psi|\mathbf{t}^{\kappa k}|\Psi''\rangle \times \langle\Psi''|\mathbf{G}|\Psi'\rangle\right]/\Delta E =$$
$$\delta(M,M')\delta(J,J')\sqrt{\frac{20J(2J+1)(2J-1)}{(J+1)(2J+3)}} \begin{Bmatrix} S & S' & \kappa \\ L & L' & k \\ J & J & 2 \end{Bmatrix} \langle\Psi(\Gamma\alpha SL)\|\mathbf{CHFS}\|\Psi'(\Gamma'\alpha'S'L')\rangle =$$

$$\delta(M,M')\ \delta(J,J')\sqrt{\frac{20J(2J+1)(2J-1)}{(J+1)(2J+3)}}\begin{Bmatrix} S & S' & \kappa \\ L & L' & k \\ J & J & 2 \end{Bmatrix} t^{\kappa k}_{coeff}(n_0l_0,n_il_i)$$
$$\times\ (\text{angular part})\sum_{n_0l_0} R^t\,(n_il_in_0l_0,n_il_in_i'l_i')\,\langle n_0l_0|r^{-3}|n_il_i\rangle^{\kappa k}/\Delta E, \tag{19}$$

where Γ, Γ' designate configurations being studied, ΔE is the (positive) energy difference between the relevant closed- and open- or empty-shell orbitals, $\kappa k = 01, 12, 10$ or 02 and $t^{\kappa k}_{coeff}(n_0l_0,n_il_i)$ is the angular part of the hfs operator $\mathbf{t}^{\kappa k}$:

$$\left\langle n_0l_0\left\|t^{\kappa k}\right\|n_il_i\right\rangle = t^{\kappa k}_{coeff}(n_0l_0,n_il_i)\ \langle n_0l_0|r^{-3}|n_il_i\rangle^{\kappa k}. \tag{20}$$

The radial integrals of the hfs operator $\mathbf{t}^{\kappa k}$ corresponding there to $\kappa k = 01, 12, 10$ or 02 are defined as

$$\left\langle n_0l_0\left\|t^{01}\right\|n_il_i\right\rangle = \left\langle n_0l_0\left\|\widehat{l}_ir^{-3}\right\|n_il_i\right\rangle = \delta(l_0,l_i)\sqrt{2l_0(l_0+1)(2l_0+1)}\langle n_0l_0|r^{-3}|n_il_0\rangle^{01},$$
$$\left\langle n_0l_0\left\|t^{12}\right\|n_il_i\right\rangle = \left\langle n_0l_0\left\|-\sqrt{10}(\widehat{s}_i\widehat{C}^2_i)^{(1)}r^{-3}\right\|n_il_i\right\rangle = -\sqrt{15}(l_0\|\mathbf{C}^2\|l_i)\langle n_0l_0|r^{-3}|n_il_i\rangle^{12},$$
$$\left\langle n_0l_0\left\|t^{10}\right\|n_il_i\right\rangle = \left\langle n_0l_0\left\|\widehat{s}_ir^{-3}\right\|n_il_i\right\rangle = \delta(l_0,l_i)\sqrt{3/2}\sqrt{2l_0+1}\langle n_0l_0|r^{-3}|n_il_0\rangle^{10},$$
$$\left\langle n_0l_0\left\|t^{02}\right\|n_il_i\right\rangle = \left\langle n_0l_0\left\|-\widehat{C}^2_ir^{-3}\right\|n_il_i\right\rangle = \sqrt{2}(l_0\|\mathbf{C}^2\|l_i)\langle n_0l_0|r^{-3}|n_il_i\rangle^{02}. \tag{21}$$

Reduced matrix elements for particular configurations are presented in sect. 5.

4 Explanation of used symbols

In all the formulae given below, symbol $\mathbf{G}^t$ denotes a particular term of Coulomb repulsion represented by irreducible tensors of rank t: $\sum_{i>j} r^t_</r^{t+1}_>(\mathbf{C}^t_i\cdot\mathbf{C}^t_j)$, where $r_<$ and $r_>$ indicate the distances from the nucleus to the closer and more distant electron, respectively. The summation over t is omitted. The expressions describing $\mathbf{G}^t$ element contain coupling schemes used for the derivation of the formula.

For nj-coefficients the generally accepted notations were used.

The antisymmetric states for N equivalent electrons, allowed by the Pauli principle, were constructed from a linear combination of products of parent states with $(N-1)$ electrons using Racah's coefficients of fractional parentage [34,35]. In the one-electron fractional parentage coefficient $(nl^N\alpha_0S_0L_0\{|nl^{N-1}\bar{\alpha}\bar{S}\bar{L})$, $\alpha_0S_0L_0$ denote the states of a group nl^N of equivalent electrons and α_0 is an additional quantum number introduced to distinguish terms with identical values of S_0L_0. In an analogous manner, $\bar{\alpha}\bar{S}\bar{L}$ denote the states of nl^{N-1} equivalent electrons. For two-electron coefficients, introduced for the first time by Donlan [36], $(nl^N\alpha_0S_0L_0\{|nl^{N-2}\bar{\alpha}\bar{S}\bar{L},nl^2\hat{\alpha}\hat{S}\hat{L})$, $\alpha_0S_0L_0$, $\bar{\alpha}\bar{S}\bar{L}$ and $\hat{\alpha}\hat{S}\hat{L}$ denote the states of a group nl^N, nl^{N-2} and nl^2 of equivalent electrons, respectively.

The expression $[x,y]$ represents $(2x+1)(2y+1)$. The reduced matrix elements $\mathbf{C}^t$ and $\mathbf{U}^t$ represent

$$(l_1\|\mathbf{C}^t\|l_2) = (-1)^{l_1}\,[(2l_1+1)(2l_2+1)]^{1/2}\begin{pmatrix} l_1 & t & l_2 \\ 0 & 0 & 0 \end{pmatrix}, \tag{22}$$
$$\left\langle nl^N\alpha_0S_0L_0\left\|\mathbf{U}^t\right\|nl^N\alpha_0'S_0'L_0'\right\rangle = \delta(S_0,S_0')\ N\ (-1)^{L_0+l+t}\ [L_0,L_0']^{1/2}$$
$$\times\sum_{\bar{\alpha}\bar{S}\bar{L}}(-1)^{\bar{L}}\left(nl^N\alpha_0S_0L_0\{|nl^{N-1}\bar{\alpha}\bar{S}\bar{L}\right)\left(nl^N\alpha_0'S_0'L_0'\{|nl^{N-1}\bar{\alpha}\bar{S}\bar{L}\right)\begin{Bmatrix} l & l & t \\ L_0 & L_0' & \bar{L} \end{Bmatrix}. \tag{23}$$

The consideration of the configuration with three open shells, where the second and third shell contain up to three electrons, requires the coupling of four angular momenta. Therefore, it is necessary to use $12j$-coefficients, introduced by Jahn and Hope [37] and studied by Ord-Smith [38], who found 16 symmetry relations including a convenient new notation. In the comprehensive work of Yutsis *et al.* [39], the $12j$-coefficients of this form were referred to as symbols of the first kind. Additionally, Yutsis introduced more convenient symbols of the second kind with 24 symmetry properties and presented a number of useful sum rules on nj-coefficients, which we primarily use in this paper. The most important sum rules, which we used, are described by the formulae (A 6.13), (A 6.14), (A 6.25), (A 6.26), (A 6.35–6.40) and (A 6.45–6.49) presented in the paper of Yutsis *et al.* [39]. Without these sum rules, it would be impossible to write the formulae, presented below in sect. 5 in such a compressed form. Therefore, the formulae in

Yutsis's work contain the nj-coefficients of the first kind and of the second kind, so it is convenient to use the following relation between the different types of $12j$-coefficients:

$$\begin{Bmatrix} j_1 & j_2 & j_3 & j_4 \\ l_1 & l_2 & l_3 & l_4 \\ k_1 & k_2 & k_3 & k_4 \end{Bmatrix} = \begin{Bmatrix} l_1 & k_1 & k_2 & k_3 \\ j_1 & l_4 & k_4 & j_3 \\ j_2 & j_4 & l_2 & l_3 \end{Bmatrix}, \tag{24}$$

$$\begin{bmatrix} j_1 & j_2 & j_3 & j_4 \\ l_1 & l_2 & l_3 & l_4 \\ k_1 & k_2 & k_3 & k_4 \end{bmatrix} (-1)^{-j_1+j_2+j_3-j_4+k_1-k_2-k_3+k_4} = \begin{bmatrix} k_3 & j_1 & k_1 & j_2 \\ l_2 & l_1 & l_3 & l_4 \\ k_4 & j_3 & k_2 & j_4 \end{bmatrix}. \tag{25}$$

In this work we use $15j$-coefficients defined by Yutsis *et al.* [39] as 3 nj-coefficients. The sum of a product of $6j$-coefficients which represents $15j$-coefficients of the first kind is of the form

$$\begin{Bmatrix} j_1 & j_2 & j_3 & j_4 & j_5 \\ l_1 & l_2 & l_3 & l_4 & l_5 \\ k_1 & k_2 & k_3 & k_4 & k_5 \end{Bmatrix} = \sum_x [x]\ (-1)^{R_5+4x} \begin{Bmatrix} j_1 & k_1 & x \\ k_2 & j_2 & l_1 \end{Bmatrix} \begin{Bmatrix} j_2 & k_2 & x \\ k_3 & j_3 & l_2 \end{Bmatrix} \begin{Bmatrix} j_3 & k_3 & x \\ k_4 & j_4 & l_3 \end{Bmatrix} \begin{Bmatrix} j_4 & k_4 & x \\ k_5 & j_5 & l_4 \end{Bmatrix} \begin{Bmatrix} j_5 & k_5 & x \\ j_1 & k_1 & l_5 \end{Bmatrix} \tag{26}$$

and the sum which gives $15j$-coefficients of the second kind is

$$\begin{bmatrix} j_1 & j_2 & j_3 & j_4 & j_5 \\ l_1 & l_2 & l_3 & l_4 & l_5 \\ k_1 & k_2 & k_3 & k_4 & k_5 \end{bmatrix} = \sum_x [x]\ (-1)^{R_5+5x} \begin{Bmatrix} j_1 & k_1 & x \\ k_2 & j_2 & l_1 \end{Bmatrix} \begin{Bmatrix} j_2 & k_2 & x \\ k_3 & j_3 & l_2 \end{Bmatrix} \begin{Bmatrix} j_3 & k_3 & x \\ k_4 & j_4 & l_3 \end{Bmatrix} \begin{Bmatrix} j_4 & k_4 & x \\ k_5 & j_5 & l_4 \end{Bmatrix} \begin{Bmatrix} j_5 & k_5 & x \\ k_1 & j_1 & l_5 \end{Bmatrix}, \tag{27}$$

where $R_n = j_1 + j_2 + j_3 + j_4 + j_5 + l_1 + l_2 + l_3 + l_4 + l_5 + k_1 + k_2 + k_3 + k_4 + k_5$.

5 Explicit formulae for electrostatically correlated spin-orbit interactions as well as for electrostatically correlated hyperfine interactions. Excitation of one electron from a closed shell into an open shell

The formulae for electrostatically correlated spin-orbit interactions (or electrostatically correlated hyperfine interactions) are presented below.

5.1 nl^N configuration

The states ψ and ψ' for nl^N configuration are defined as follows:

$\psi = n_0 l_0^{4l_0+2}\ {}^1S, nl^N \alpha SL; \alpha SL,$
$\psi' = n_0 l_0^{4l_0+2}\ {}^1S, nl^N \alpha' S'L'; \alpha' S'L'.$

5.1.1 Excitation of one electron from a closed $n_0 l_0^{4l_0+2}$ shell to an open nl^N shell

In this case the perturbing virtual states are defined as $\psi'' = n_0 l_0^{4l_0+1}\ {}^2l_0, nl^{N+1}\alpha'' S''L''; S'''L'''$, where $S'''L'''$ has a value SL or $S'L'$, depending on the operators occurring in eq. (6),

$$-\sum_{\psi'' \neq \psi, \psi'} \left[\langle \psi | \mathbf{G} | \psi'' \rangle \times \langle \psi'' \| \mathbf{T}^{(\kappa \mathbf{k})\mathbf{K}} \| \psi' \rangle + \langle \psi \| \mathbf{T}^{(\kappa \mathbf{k})\mathbf{K}} \| \psi'' \rangle \times \langle \psi'' | \mathbf{G} | \psi' \rangle \right] / \Delta E =$$

$$-\sum_{\Psi''} \left\langle n_0 l_0^{4l_0+2}\ {}^1S\ , nl^N \alpha SL; SL\, |\mathbf{G}|\, n_0 l_0^{4l_0+1}\ {}^2l_0, nl^{N+1}\alpha'' S''L''; SL \right\rangle$$

$$\times \left\langle n_0 l_0^{4l_0+1}\ {}^2l_0, nl^{N+1}\alpha'' S''L''; SL \| \mathbf{T}^{(\kappa \mathbf{k})\mathbf{K}} \| n_0 l_0^{4l_0+2}\ {}^1S\ , nl^N \alpha' S'L'; S'L' \right\rangle$$

$$-\sum_{\Psi''} \left\langle n_0 l_0^{4l_0+1}\ {}^2l_0, nl^{N+1}\alpha'' S''L''; SL \| \mathbf{T}^{(\kappa \mathbf{k})\mathbf{K}} \| n_0 l_0^{4l_0+2}\ {}^1S\ , nl^N \alpha' S'L'; S'L' \right\rangle$$

$$\times \left\langle n_0 l_0^{4l_0+2}\ {}^1S\ , nl^N \alpha' S'L'; S'L'\, |\mathbf{G}|\, n_0 l_0^{4l_0+2}\ {}^1S, nl^N \alpha' S'L' \right\rangle =$$

$$(N+1)\sum_{\alpha''S''L''}(-1)^{S''+S'+L'+3/2}\,[S''L'']\begin{Bmatrix}S & S' & \kappa\\ 1/2 & 1/2 & S''\end{Bmatrix}\begin{Bmatrix}L & L' & k\\ l & l_0 & L''\end{Bmatrix}$$
$$\times\Bigg[\sum_{\bar\alpha\bar S\bar L}\delta(\bar S,S)\,(-1)^{L}\,(nl^{N+1}\alpha''S''L''\{|nl^N\bar\alpha\bar S\bar L)(nl^{N+1}\alpha''S''L''\{|nl^N\alpha'S'L')\,\langle nl^N\bar\alpha\bar S\bar L\,\|\mathbf{U}^t\|\,nl^N\alpha SL\rangle\begin{Bmatrix}\bar L & t & L\\ l_0 & L'' & l\end{Bmatrix}$$
$$+\sum_{\bar\alpha'\bar S'\bar L'}\delta(\bar S',S')\,(-1)^{L'}\,(nl^{N+1}\alpha''S''L''\{|nl^N\bar\alpha'\bar S'\bar L')(nl^{N+1}\alpha''S''L''\{|nl^N\alpha SL)\,\langle nl^N\bar\alpha'\bar S'\bar L'\,\|\mathbf{U}^t\|\,nl^N\alpha'S'L'\rangle$$
$$\times\begin{Bmatrix}\bar L' & t & L'\\ l_0 & L'' & l\end{Bmatrix}\Bigg](l_0\|\mathbf{C}^t\|l)(l\|\mathbf{C}^t\|l)\sum_{n_0l_0}R^t\,(n_0l_0nl,nlnl)\,\langle n_0l_0|r^{-3}|nl\rangle^{\kappa k}/\Delta E. \tag{28}$$

This parameter occurs for all types of configurations with nl^N core.

5.1.2 Excitation of one electron from a closed $n_0l_0^{4l_0+2}$ shell into an empty n_1l_1 shell

In this case the perturbing virtual states are defined as $\psi''=n_0l_0^{4l_0+1}\ ^2l_0,(nl^N\alpha_1''S_1''L_1'',n_1l_1)S''L'';S'''L'''$,

$$-\sum_{\psi''\neq\psi,\psi'}\Big[\langle\psi|\mathbf{G}|\psi''\rangle\times\langle\psi''\|\mathbf{T}^{(\kappa\mathbf{k})\mathbf{K}}\|\psi'\rangle+\langle\psi\|\mathbf{T}^{(\kappa\mathbf{k})\mathbf{K}}\|\psi''\rangle\times\langle\psi''|\mathbf{G}|\psi'\rangle\Big]/\Delta E=$$
$$\sum_{\alpha''S''L''}(-1)^{2S+S'+3S''+1/2}\,[S'',L'']\begin{Bmatrix}S & S' & \kappa\\ 1/2 & 1/2 & S''\end{Bmatrix}\begin{Bmatrix}L & L' & k\\ l_1 & l_0 & L''\end{Bmatrix}$$
$$\times\Bigg[\delta(S,S_1'')\,\delta(\alpha_1''S_1''L_1'',\alpha'S'L')\,(-1)^{l_0+l_1}\,\langle nl^N\alpha SL\,\|\mathbf{U}^t\|\,nl^N\alpha_1''S_1''L_1''\rangle\begin{Bmatrix}l_1 & t & l_0\\ L & L'' & L_1''\end{Bmatrix}$$
$$+\delta(S',S_1'')\,\delta(\alpha_1''S_1''L_1'',\alpha SL)\,(-1)^{L'+L}\,\langle nl^N\alpha'S'L'\,\|\mathbf{U}^t\|\,nl^N\alpha_1''S_1''L_1''\rangle\begin{Bmatrix}l_1 & t & l_0\\ L' & L'' & L_1''\end{Bmatrix}\Bigg]$$
$$\times(l\|\mathbf{C}^t\|l)(l_0\|\mathbf{C}^t\|l_1)\sum_{n_0l_0}R^t\,(n_0l_0nl,n_1l_1nl)\,\langle n_0l_0|r^{-3}|n_1l_1\rangle^{\kappa k}/\Delta E$$
$$+N\sum_{\alpha''S''L''}(-1)^{2S+S'+L'+3S''+L''+l+1/2}\,[S'',L'']\begin{Bmatrix}S & S' & \kappa\\ 1/2 & 1/2 & S''\end{Bmatrix}\begin{Bmatrix}L & L' & k\\ l_1 & l_0 & L''\end{Bmatrix}$$
$$\times\Bigg[\delta(\alpha_1''S_1''L_1'',\alpha'S'L')\,(-1)^{S+S_1''+l_0+l_1}\,[S_1'',L_1'',S,L]^{1/2}$$
$$\times\sum_{\bar\alpha\bar S\bar L}\left(nl^N\alpha SL\{|nl^{N-1}\bar\alpha\bar S\bar L\right)\left(nl^N\alpha_1''S_1''L_1''\{|nl^{N-1}\bar\alpha\bar S\bar L\right)\begin{Bmatrix}1/2 & \bar S & S_1''\\ 1/2 & S'' & S\end{Bmatrix}\begin{Bmatrix}\bar L & l & L_1''\\ l & t & l_1\\ L & l_0 & L''\end{Bmatrix}$$
$$+\delta(\alpha_1''S_1''L_1'',\alpha SL)\,(-1)^{S'+S_1''}\,[S_1'',L_1'',S',L']^{1/2}$$
$$\times\sum_{\bar\alpha'\bar S'\bar L'}\left(nl^N\alpha'S'L'\{|nl^{N-1}\bar\alpha'\bar S'\bar L'\right)\left(nl^N\alpha_1''S_1''L_1''\{|nl^{N-1}\bar\alpha'\bar S'\bar L'\right)\begin{Bmatrix}1/2 & \bar S' & S_1''\\ 1/2 & S'' & S'\end{Bmatrix}\begin{Bmatrix}\bar L' & l & L_1''\\ l & t & l_1\\ L' & l_0 & L''\end{Bmatrix}\Bigg]$$
$$\times(l\|\mathbf{C}^t\|l_1)(l_0\|\mathbf{C}^t\|l)\sum_{n_0l_0}R^t\,(n_0l_0nl,nln_1l_1)\,\langle n_0l_0|r^{-3}|n_1l_1\rangle^{\kappa k}/\Delta E. \tag{29}$$

5.2 $nl^Nn_1l_1^{N_1}$ configuration

The states ψ and ψ' for $nl^Nn_1l_1^{N_1}$ configuration are defined as follows:

$\psi=n_0l_0^{4l_0+2}\ ^1S,(nl^N\alpha_1S_1L_1,n_1l_1^{N_1}\alpha_2S_2L_2)SL;SL,$
$\psi'=n_0l_0^{4l_0+2}\ ^1S,(nl^N\alpha_1'S_1'L_1',n_1l_1^{N_1}\alpha_2'S_2'L_2')S'L';S'L'.$

5.2.1 Excitation of one electron from a closed $n_0 l_0^{4l_0+2}$ shell into an open nl^N shell

In this case the perturbing virtual states are defined as $\psi'' = n_0 l_0^{4l_0+1}\ ^2l_0, (nl^{N+1}\alpha_1'' S_1'' L_1'', n_1 l_1^{N_1}\alpha_2'' S_2'' L_2'')S'' L''; S''' L'''$,

$$
\begin{aligned}
&- \sum_{\psi'' \neq \psi, \psi'} \Big[\langle \psi | \mathbf{G} | \psi'' \rangle \times \langle \psi'' \| \mathbf{T}^{(\kappa \mathbf{k}) \mathbf{K}} \| \psi' \rangle + \langle \psi \| \mathbf{T}^{(\kappa \mathbf{k}) \mathbf{K}} \| \psi'' \rangle \times \langle \psi'' | \mathbf{G} | \psi' \rangle \Big] / \Delta E = \\
&(N+1)\ N_1\ (-1)^{2S_2+L+L_2+L_2'+l_1}\ [S, L, S', L', L_2, L_2']^{1/2} \\
&\times \sum_{\psi''} \left(nl^{N+1}\alpha_1'' S_1'' L_1'' \{ | nl^N \alpha_1 S_1 L_1 \right) \left(nl^{N+1}\alpha_1'' S_1'' L_1'' \{ | nl^N \alpha_1' S_1' L_1' \right) [S'', L'', S_1'', L_1''] \begin{Bmatrix} S' & S & \kappa \\ 1/2 & 1/2 & S'' \end{Bmatrix} \\
&\times \Bigg[\delta(\alpha_2' S_2' L_2', \alpha_2'' S_2'' L_2'')\ \delta(S_2, S_2'')\ (-1)^{2S_1'+L_1} \begin{Bmatrix} L' & L & k \\ l_0 & l & L'' \end{Bmatrix} \begin{Bmatrix} 1/2 & S_1' & S_1'' \\ S_2' & S'' & S' \end{Bmatrix} \begin{Bmatrix} l & L_1' & L_1'' \\ L_2' & L'' & L' \end{Bmatrix} \begin{Bmatrix} S_2 & S'' & S_1'' \\ 1/2 & S_1 & S \end{Bmatrix} \begin{Bmatrix} L_2 & t & L_2' \\ L_1 & l & L_1'' \\ L & l_0 & L'' \end{Bmatrix} \\
&\times \sum_{\bar\alpha_2 \bar S_2 \bar L_2} (-1)^{S+3S''+\bar L_2+1/2}\ (n_1 l_1^{N_1}\alpha_2 S_2 L_2 \{ | n_1 l_1^{N_1-1} \bar\alpha_2 \bar S_2 \bar L_2)(n_1 l_1^{N_1}\alpha_2' S_2' L_2' \{ | n_1 l_1^{N_1-1} \bar\alpha_2 \bar S_2 \bar L_2) \begin{Bmatrix} L_2' & L_2 & t \\ l_1 & l_1 & \bar L_2 \end{Bmatrix} \\
&+ \delta(\alpha_2 S_2 L_2, \alpha_2'' S_2'' L_2'')\ \delta(S_2', S_2'')\ (-1)^{2S_1+L_1'} \begin{Bmatrix} L' & L & k \\ l & l_0 & L'' \end{Bmatrix} \begin{Bmatrix} 1/2 & S_1 & S_1'' \\ S_2 & S'' & S \end{Bmatrix} \begin{Bmatrix} l & L_1 & L_1'' \\ L_2 & L'' & L \end{Bmatrix} \begin{Bmatrix} S_2' & S'' & S_1'' \\ 1/2 & S_1' & S' \end{Bmatrix} \begin{Bmatrix} L_2' & t & L_2 \\ L_1' & l & L_1'' \\ L' & l_0 & L'' \end{Bmatrix} \\
&\times \sum_{\bar\alpha_2' \bar S_2' \bar L_2'} (-1)^{S+3S''+\bar L_2'+1/2}\ (n_1 l_1^{N_1}\alpha_2 S_2 L_2 \{ | n_1 l_1^{N_1-1} \bar\alpha_2' \bar S_2' \bar L_2')(n_1 l_1^{N_1}\alpha_2' S_2' L_2' \{ | n_1 l_1^{N_1-1} \bar\alpha_2' \bar S_2' \bar L_2') \begin{Bmatrix} L_2 & L_2' & t \\ l_1 & l_1 & \bar L_2' \end{Bmatrix} \Bigg] \\
&\times (l_0 \| \mathbf{C}^t \| l)(l_1 \| \mathbf{C}^t \| l_1) \sum_{n_0 l_0} R^t\ (n_0 l_0 n_1 l_1, n l n_1 l_1)\ \langle n_0 l_0 | r^{-3} | n l \rangle^{\kappa k} / \Delta E \\
&+ (N+1)\ N_1\ [S, L, S', L', S_2, L_2, S_2', L_2']^{1/2} \\
&\times \sum_{\psi''} \left(nl^{N+1}\alpha_1'' S_1'' L_1'' \{ | nl^N \alpha_1 S_1 L_1 \right) \left(nl^{N+1}\alpha_1'' S_1'' L_1'' \{ | nl^N \alpha_1' S_1' L_1' \right)\ [S'', L'', S_1'', L_1''] \\
&\times \Bigg[\delta(\alpha_2' S_2' L_2', \alpha_2'' S_2'' L_2'') \sum_{\bar\alpha_2 \bar S_2 \bar L_2} (-1)^{3S+3S_1+2S_1'+3S_2'+S_2+\bar S_2+L_2+L_2'+L_1''+L''+\bar L_2+l+t+3/2} \\
&\times (n_1 l_1^{N_1}\alpha_2 S_2 L_2 \{ | n_1 l_1^{N_1-1} \bar\alpha_2 \bar S_2 \bar L_2)(n_1 l_1^{N_1}\alpha_2' S_2' L_2' \{ | n_1 l_1^{N_1-1} \bar\alpha_2 \bar S_2 \bar L_2) \\
&\times \begin{Bmatrix} 1/2 & S_1' & S_1'' \\ S_2' & S'' & S' \end{Bmatrix} \begin{Bmatrix} 1/2 & S_1'' & S_1 \\ S & S_2 & \bar S_2 \end{Bmatrix} \begin{Bmatrix} \bar S_2 & S_2' & 1/2 \\ S'' & S & S_1'' \end{Bmatrix} \begin{Bmatrix} S' & S & \kappa \\ 1/2 & 1/2 & S'' \end{Bmatrix} \begin{Bmatrix} L' & L & k \\ l_0 & l & L'' \end{Bmatrix} \begin{Bmatrix} l & L_1' & L_1'' \\ L_2' & L'' & L' \end{Bmatrix} \begin{Bmatrix} L'' & L & l_0 & t \\ L_1'' & L_1 & l & \bar L_2 \\ L_2' & L_2 & l_1 & l_1 \end{Bmatrix} \\
&+ \delta(\alpha_2 S_2 L_2, \alpha_2'' S_2'' L_2'')\ \delta(S_2', S_2'') \sum_{\bar\alpha_2' \bar S_2' \bar L_2'} (-1)^{2S'+S+2S_1+3S_1'+3S_2+S_2'+\bar S_2'+L+L'+L_2+L_2'+L_1''+L''+\bar L_2'+l+t+3/2} \\
&\times (n_1 l_1^{N_1}\alpha_2 S_2 L_2 \{ | n_1 l_1^{N_1-1} \bar\alpha_2' \bar S_2' \bar L_2')(n_1 l_1^{N_1}\alpha_2' S_2' L_2' \{ | n_1 l_1^{N_1-1} \bar\alpha_2' \bar S_2' \bar L_2') \\
&\times \begin{Bmatrix} 1/2 & S_1 & S_1'' \\ S_2 & S'' & S \end{Bmatrix} \begin{Bmatrix} 1/2 & S_1'' & S_1' \\ S' & S_2' & \bar S_2' \end{Bmatrix} \begin{Bmatrix} \bar S_2' & S_2 & 1/2 \\ S'' & S' & S_1'' \end{Bmatrix} \begin{Bmatrix} S' & S & \kappa \\ 1/2 & 1/2 & S'' \end{Bmatrix} \begin{Bmatrix} L' & L & k \\ l & l_0 & L'' \end{Bmatrix} \begin{Bmatrix} l & L_1 & L_1'' \\ L_2 & L'' & L \end{Bmatrix} \begin{Bmatrix} L'' & L' & l_0 & t \\ L_1'' & L_1' & l & \bar L_2' \\ L_2 & L_2' & l_1 & l_1 \end{Bmatrix} \Bigg] \\
&\times (l_0 \| \mathbf{C}^t \| l_1)(l_1 \| \mathbf{C}^t \| l) \sum_{n_0 l_0} R^t\ (n_0 l_0 n_1 l_1, n_1 l_1 n l)\ \langle n_0 l_0 | r^{-3} | n l \rangle^{\kappa k} / \Delta E. \qquad (30)
\end{aligned}
$$

5.2.2 Excitation of one electron from a closed $n_0 l_0^{4l_0+2}$ shell to an open $n_1 l_1^{N_1}$ shell

In this case the perturbing virtual states are defined as $\psi'' = (n_0 l_0^{4l_0+1}\ ^2l_0, nl^N \alpha_1'' S_1'' L_1'')S'' L'', n_1 l_1^{N_1+1}\alpha_2'' S_2'' L_2''; S''' L'''$.

The first type of electrostatic integrals:

$$
- \sum_{\psi'' \neq \psi, \psi'} \Big[\langle \psi | \mathbf{G} | \psi'' \rangle \times \langle \psi'' \| \mathbf{T}^{(\kappa \mathbf{k}) \mathbf{K}} \| \psi' \rangle + \langle \psi \| \mathbf{T}^{(\kappa \mathbf{k}) \mathbf{K}} \| \psi'' \rangle \times \langle \psi'' | \mathbf{G} | \psi' \rangle \Big] / \Delta E =
$$

$$
\begin{aligned}
&(N_1+1)\ N_1\ [S,L,S',L']^{1/2}\sum_{\psi''}\delta(\alpha_1 S_1 L_1,\alpha_1'' S_1'' L_1'')\ \delta(\alpha_1' S_1' L_1',\alpha_1'' S_1'' L_1'')[S'',L'',S_2'',L_2'']\\
&\times\Bigg[\Big(n_1 l_1^{N_1+1}\alpha_2'' S_2'' L_2''\{|n_1 l_1^{N_1}\alpha_2' S_2' L_2'\Big)\ [S_2,L_2]^{1/2}\begin{Bmatrix}S'' & 1/2 & S_1\\ S_2 & S & S_2''\end{Bmatrix}\begin{Bmatrix}L'' & l_0 & L_1\\ L_2 & L & L_2''\end{Bmatrix}\begin{Bmatrix}S & S'' & S_2''\\ S' & S_1' & S_2'\\ \kappa & 1/2 & 1/2\end{Bmatrix}\begin{Bmatrix}L & L'' & L_2''\\ L' & L_1' & L_2'\\ k & l_0 & l_1\end{Bmatrix}\\
&\times\sum_{\bar\alpha\bar S\bar L,\hat\alpha\hat S\hat L}(-1)^{3S+L+2S''+2S_2+2S_2'+S_1'+L_1'+\bar S+\bar L+\hat L+l_0+\kappa+k+1/2}\ [\hat S,\hat L]^{1/2}\begin{Bmatrix}\bar S & 1/2 & S_2\\ 1/2 & S_2'' & \hat S\end{Bmatrix}\begin{Bmatrix}\bar L & l_1 & L_2\\ l_0 & L_2'' & \hat L\end{Bmatrix}\\
&\times\Big(n_1 l_1^{N_1+1}\alpha_2'' S_2'' L_2''\{|n_1 l_1^{N_1-1}\bar\alpha\bar S\bar L, n_1 l_1^2\hat\alpha\hat S\hat L\Big)\Big(n_1 l_1^{N_1}\alpha_2 S_2 L_2\{|n_1 l_1^{N_1-1}\bar\alpha\bar S\bar L\Big)\begin{Bmatrix}l_1 & l_0 & t\\ l_1 & l_1 & \hat L\end{Bmatrix}\\
&+\Big(n_1 l_1^{N_1+1}\alpha_2'' S_2'' L_2''\{|n_1 l_1^{N_1}\alpha_2 S_2 L_2\Big)\ [S_2',L_2']^{1/2}\begin{Bmatrix}S'' & 1/2 & S_1'\\ S_2' & S' & S_2''\end{Bmatrix}\begin{Bmatrix}L'' & l_0 & L_1'\\ L_2' & L' & L_2''\end{Bmatrix}\begin{Bmatrix}S & S_2 & S_1\\ S' & S_2'' & S''\\ \kappa & 1/2 & 1/2\end{Bmatrix}\begin{Bmatrix}L & L_2 & L_1\\ L' & L_2'' & L''\\ k & l_1 & l_0\end{Bmatrix}\\
&\times\sum_{\bar\alpha'\bar S'\bar L',\hat\alpha'\hat S'\hat L'}(-1)^{S+L+2S'+2S''+2S_2+S_1+L_1+2S_2'+\bar S'+\bar L'+\hat L'+l_1+\kappa+k+1/2}\ [\hat S',\hat L']^{1/2}\begin{Bmatrix}\bar S' & 1/2 & S_2'\\ 1/2 & S_2'' & \hat S'\end{Bmatrix}\begin{Bmatrix}\bar L' & l_1 & L_2'\\ l_0 & L_2'' & \hat L'\end{Bmatrix}\\
&\times\ \Big(n_1 l_1^{N_1+1}\alpha_2'' S_2'' L_2''\{|n_1 l_1^{N_1-1}\bar\alpha'\bar S'\bar L', n_1 l_1^2\hat\alpha'\hat S'\hat L'\Big)\Big(n_1 l_1^{N_1}\alpha_2' S_2' L_2'\{|n_1 l_1^{N_1-1}\bar\alpha'\bar S'\bar L'\Big)\begin{Bmatrix}l_1 & l_0 & t\\ l_1 & l_1 & \hat L'\end{Bmatrix}\Bigg]\\
&\times(l_0\|\mathbf{C}^t\|l_1)(l_1\|\mathbf{C}^t\|l_1)\sum_{n_0 l_0}R^t\,(n_0 l_0 n_1 l_1, n_1 l_1 n_1 l_1)\,\langle n_0 l_0|r^{-3}|n_1 l_1\rangle^{\kappa k}/\Delta E. \qquad (31)
\end{aligned}
$$

The second type of electrostatic integrals:

$$
\begin{aligned}
&-\sum_{\psi''\neq\psi,\psi'}\Big[\langle\psi|\mathbf{G}|\psi''\rangle\times\langle\psi''\|\mathbf{T}^{(\kappa\mathbf{k})\mathbf{K}}\|\psi'\rangle+\langle\psi\|\mathbf{T}^{(\kappa\mathbf{k})\mathbf{K}}\|\psi''\rangle\times\langle\psi''|\mathbf{G}|\psi'\rangle\Big]/\Delta E=\\
&(N_1+1)\ [S,L,S',L']^{1/2}\sum_{\psi''}[S'',L'',S_2'',L_2'']\Big(n_1 l_1^{N_1+1}\alpha_2'' S_2'' L_2''\{|n_1 l_1^{N_1}\alpha_2 S_2 L_2\Big)\Big(n_1 l_1^{N_1+1}\alpha_2'' S_2'' L_2''\{|n_1 l_1^{N_1}\alpha_2' S_2' L_2'\Big)\\
&\times\Bigg[\delta(\alpha_1' S_1' L_1',\alpha_1'' S_1'' L_1'')\ \delta(S_1,S_1'')\ (-1)^{3S+L+S_2''+L_2''+2S''+L''+2S_2'+S_1'+L_1'+L_1+t+\kappa+k+1/2}\\
&\times\langle nl^N\alpha_1 S_1 L_1\,\|\mathbf{U}^t\|\,nl^N\alpha_1'' S_1'' L_1''\rangle\begin{Bmatrix}S_2 & S & S_1\\ S'' & 1/2 & S_2''\end{Bmatrix}\begin{Bmatrix}L_2 & L & L_1\\ L'' & l_1 & L_2''\end{Bmatrix}\begin{Bmatrix}L'' & L_1 & l_1\\ t & l_0 & L_1''\end{Bmatrix}\begin{Bmatrix}S & S'' & S_2''\\ S' & S_1' & S_2'\\ \kappa & 1/2 & 1/2\end{Bmatrix}\begin{Bmatrix}L & L'' & L_2''\\ L' & L_1' & L_2'\\ k & l_0 & l_1\end{Bmatrix}\\
&+\delta(\alpha_1 S_1 L_1,\alpha_1'' S_1'' L_1'')\ \delta(S_1',S_1'')\ (-1)^{S+L+2S'+S_2''+L_2''+2S''+L''+2S_2+S_1+L_1+L_1'+\kappa+k+1/2}\\
&\times\langle nl^N\alpha_1' S_1' L_1'\,\|\mathbf{U}^t\|\,nl^N\alpha_1'' S_1'' L_1''\rangle\begin{Bmatrix}S_2' & S' & S_1'\\ S'' & 1/2 & S_2''\end{Bmatrix}\begin{Bmatrix}L_2' & L' & L_1'\\ L'' & l_1 & L_2''\end{Bmatrix}\begin{Bmatrix}L'' & L_1' & l_1\\ t & l_0 & L_1''\end{Bmatrix}\begin{Bmatrix}S & S_2 & S_1\\ S' & S_2'' & S''\\ \kappa & 1/2 & 1/2\end{Bmatrix}\begin{Bmatrix}L & L_2 & L_1\\ L' & L_2'' & L''\\ k & l_1 & l_0\end{Bmatrix}\Bigg]\\
&\times(l_0\|\mathbf{C}^t\|l_1)(l\|\mathbf{C}^t\|l)\sum_{n_0 l_0}R^t\,(n_0 l_0 nl, n_1 l_1 nl)\,\langle n_0 l_0|r^{-3}|n_1 l_1\rangle^{\kappa k}/\Delta E\\
&+\ (N_1+1)\ N\ [S,L,S',L']^{1/2}\sum_{\psi''}[S_2'',L_2'',L'']\Big(n_1 l_1^{N_1+1}\alpha_2'' S_2'' L_2''\{|n_1 l_1^{N_1}\alpha_2 S_2 L_2\Big)\Big(n_1 l_1^{N_1+1}\alpha_2'' S_2'' L_2''\{|n_1 l_1^{N_1}\alpha_2' S_2' L_2'\Big)\\
&\times\Bigg[\delta(\alpha_1' S_1' L_1',\alpha_1'' S_1'' L_1'')\ \delta(S'',\bar S)(-1)^{3S+L+2S_1+L_1+S_1'+L_1'+2S_2'+L_1''+S_2''+L_2''+l_1+l+l_0+\kappa+k+1/2}\\
&\times[S_1'',L_1'',S_1,L_1]^{1/2}\begin{Bmatrix}S_2 & S & S_1\\ S'' & 1/2 & S_2''\end{Bmatrix}\begin{Bmatrix}L_2 & L & L_1\\ L'' & l_1 & L_2''\end{Bmatrix}\begin{Bmatrix}S & S'' & S_2''\\ S' & S_1' & S_2'\\ \kappa & 1/2 & 1/2\end{Bmatrix}\begin{Bmatrix}L & L'' & L_2''\\ L' & L_1' & L_2'\\ k & l_0 & l_1\end{Bmatrix}
\end{aligned}
$$

$$\times \sum_{\bar{\alpha}\bar{S}\bar{L}} \left(nl^N \alpha_1 S_1 L_1 \{|nl^{N-1} \bar{\alpha}\bar{S}\bar{L}\right) \left(nl^N \alpha_1'' S_1'' L_1'' \{|nl^{N-1} \bar{\alpha}\bar{S}\bar{L}\right) \begin{Bmatrix} \bar{L} & L_1'' & l \\ l_0 & t & L'' \end{Bmatrix} \begin{Bmatrix} L_1 & L'' & l_1 \\ t & l & \bar{L} \end{Bmatrix}$$

$$+ \delta(\alpha_1 S_1 L_1, \alpha_1'' S_1'' L_1'') \delta(S'', \bar{S}) \ (-1)^{S+L+2S'+S_1+L_1+2S_1'+L_1'+2S_2+L_1''+S_2''+L_2''+l+\kappa+k+1/2}$$

$$\times [S_1'', L_1'', S_1', L_1']^{1/2} \begin{Bmatrix} S_2' & S' & S_1' \\ S'' & 1/2 & S_2'' \end{Bmatrix} \begin{Bmatrix} L_2' & L' & L_1' \\ L'' & l_1 & L_2'' \end{Bmatrix} \begin{Bmatrix} S & S_2 & S_1 \\ S' & S_2'' & S'' \\ \kappa & 1/2 & 1/2 \end{Bmatrix} \begin{Bmatrix} L & L_2 & L_1 \\ L' & L_2'' & L'' \\ k & l_1 & l_0 \end{Bmatrix}$$

$$\times \sum_{\bar{\alpha}'\bar{S}'\bar{L}'} \left(nl^N \alpha_1' S_1' L_1' \{|nl^{N-1} \bar{\alpha}'\bar{S}'\bar{L}'\right) \left(nl^N \alpha_1'' S_1'' L_1'' \{|nl^{N-1} \bar{\alpha}'\bar{S}'\bar{L}'\right) \begin{Bmatrix} \bar{L}' & L_1'' & l \\ l_0 & t & L'' \end{Bmatrix} \begin{Bmatrix} L_1' & L'' & l_1 \\ t & l & \bar{L}' \end{Bmatrix} \Bigg]$$

$$\times (l_0 \| \mathbf{C}^t \| l)(l \| \mathbf{C}^t \| l_1) \sum_{n_0 l_0} R^t \left(n_0 l_0 nl, nln_1 l_1\right) \langle n_0 l_0 | r^{-3} | n_1 l_1 \rangle^{\kappa k} / \Delta E. \tag{32}$$

5.2.3 Excitation of one electron from a closed $n_0 l_0^{4l_0+2}$ shell into an empty $n_2 l_2$ shell calculated only for $N_1 = 1$

The states ψ and ψ' for $nl^N n_1 l_1$ configuration are defined as follows:

$$\psi = (n_0 l_0^{4l_0+2}\ {}^1S, nl^N \alpha_1 S_1 L_1) \alpha_1 S_1 L_1, n_1 l_1; SL,$$
$$\psi' = (n_0 l_0^{4l_0+2}\ {}^1S, nl^N \alpha_1' S_1' L_1') \alpha_1' S_1' L_1', n_1 l_1; S' L'.$$

In this case the perturbing virtual states are defined as $\psi'' = (n_0 l_0^{4l_0+1}\ {}^2l_0, nl^N \alpha_1'' S_1'' L_1'') S'' L'', (n_1 l_1, n_2 l_2) S_2'' L_2''; S''' L'''$.

The first type of electrostatic integrals:

$$- \sum_{\psi'' \neq \psi, \psi'} \Big[\langle \psi | \mathbf{G} | \psi'' \rangle \times \langle \psi'' \| \mathbf{T}^{(\kappa \mathbf{k}) \mathbf{K}} \| \psi' \rangle + \langle \psi \| \mathbf{T}^{(\kappa \mathbf{k}) \mathbf{K}} \| \psi'' \rangle \times \langle \psi'' | \mathbf{G} | \psi' \rangle \Big] / \Delta E =$$

$$= N \ [S, L, S', L']^{1/2} \sum_{\psi''} [L'', S_2'', L_2'']$$

$$\times \Bigg[\delta(\alpha_1' S_1' L_1', \alpha_1'' S_1'' L_1'') \ (-1)^{2S+S'+L'+2S_1'+S''+L''+2S_2''+L_1+L_1''+l_0+l+l_1+l_2}$$

$$\times [S_1, L_1, S_1'', L_1'']^{1/2} \ \begin{Bmatrix} 1/2 & S & S_1 \\ S'' & 1/2 & S_2'' \end{Bmatrix} \begin{Bmatrix} l_1 & L & L_1 \\ L'' & l_2 & L_2'' \end{Bmatrix} \begin{Bmatrix} 1/2 & \kappa & 1/2 \\ 1/2 & S' & S_1' \\ S_2'' & S & S'' \end{Bmatrix} \begin{Bmatrix} l_2 & k & l_0 \\ l_1 & L' & L_1' \\ L_2'' & L & L'' \end{Bmatrix}$$

$$\times \sum_{\bar{\alpha}\bar{S}\bar{L}} \delta(S'', \bar{S}) \left(nl^N \alpha_1 S_1 L_1 \{|nl^{N-1} \bar{\alpha}\bar{S}\bar{L}\right) \left(nl^N \alpha_1'' S_1'' L_1'' \{|nl^{N-1} \bar{\alpha}\bar{S}\bar{L}\right) \begin{Bmatrix} \bar{L} & l & L_1 \\ l_2 & L'' & t \end{Bmatrix} \begin{Bmatrix} l & t & l_0 \\ L'' & L_1'' & \bar{L} \end{Bmatrix}$$

$$+ \delta(\alpha_1 S_1 L_1, \alpha_1'' S_1'' L_1'') \ (-1)^{2S_1+3S'+L'+S''+L''+2S_2''+L_1'+L_1''+l+l_1} \ [S_1', L_1', S_1'', L_1'']^{1/2}$$

$$\times \begin{Bmatrix} 1/2 & S' & S_1' \\ S'' & 1/2 & S_2'' \end{Bmatrix} \begin{Bmatrix} l_1 & L' & L_1' \\ L'' & l_2 & L_2'' \end{Bmatrix} \begin{Bmatrix} 1/2 & \kappa & 1/2 \\ 1/2 & S & S_1 \\ S_2'' & S' & S'' \end{Bmatrix} \begin{Bmatrix} l_2 & k & l_0 \\ l_1 & L & L_1 \\ L_2'' & L' & L'' \end{Bmatrix}$$

$$\times \sum_{\bar{\alpha}'\bar{S}'\bar{L}'} \delta(S'', \bar{S}') \left(nl^N \alpha_1' S_1' L_1' \{|nl^{N-1} \bar{\alpha}'\bar{S}'\bar{L}'\right) \left(nl^N \alpha_1'' S_1'' L_1'' \{|nl^{N-1} \bar{\alpha}'\bar{S}'\bar{L}'\right) \begin{Bmatrix} \bar{L}' & l & L_1' \\ l_2 & L'' & t \end{Bmatrix} \begin{Bmatrix} l & t & l_0 \\ L'' & L_1'' & \bar{L}' \end{Bmatrix} \Bigg]$$

$$\times (l_0 \| \mathbf{C}^t \| l)(l \| \mathbf{C}^t \| l_2) \sum_{n_0 l_0} R^t \left(n_0 l_0 nl, nln_2 l_2\right) \langle n_0 l_0 | r^{-3} | n_2 l_2 \rangle^{\kappa k} / \Delta E$$

$$+ N \ [S, L, S', L']^{1/2} \sum_{\psi''} [S'', L'', S_2'', L_2'']$$

$$\times \Bigg[\delta(\alpha_1' S_1' L_1', \alpha_1'' S_1'' L_1'') \ \delta(S_1'', S_1) \ (-1)^{2S+S'+L'+2S_1+2S_1'+2S_2''+3S''+l_0+l} \ [L_1, L_1'']^{1/2}$$

$$\times \begin{Bmatrix} l_0 & L_1'' & L'' \\ L_1 & l_2 & t \end{Bmatrix} \begin{Bmatrix} 1/2 & S & S_1 \\ S'' & 1/2 & S_2'' \end{Bmatrix} \begin{Bmatrix} l_1 & L & L_1 \\ L'' & l_2 & L_2'' \end{Bmatrix} \begin{Bmatrix} 1/2 & \kappa & 1/2 \\ 1/2 & S' & S_1' \\ S_2'' & S & S'' \end{Bmatrix} \begin{Bmatrix} l_2 & k & l_0 \\ l_1 & L' & L_1' \\ L_2'' & L & L'' \end{Bmatrix}$$

$$\times \sum_{\bar{\alpha}\bar{S}\bar{L}} (-1)^{\bar{L}} \left(nl^N \alpha_1 S_1 L_1 \{|nl^{N-1}\bar{\alpha}\bar{S}\bar{L}\right) \left(nl^N \alpha_1'' S_1'' L_1'' \{|nl^{N-1}\bar{\alpha}\bar{S}\bar{L}\right) \begin{Bmatrix} t & l & l \\ \bar{L} & L_1 & L_1'' \end{Bmatrix}$$

$$+ \delta(S_1'', S_1') \ (-1)^{2S_1+3S'+L'+2S_1'+2S_2''+3S''+l_0+l+l_1+l_2} \ [L_1', L_1'']^{1/2} \begin{Bmatrix} l_0 & L_1'' & L'' \\ L_1' & l_2 & t \end{Bmatrix} \begin{Bmatrix} 1/2 & S' & S_1' \\ S'' & 1/2 & S_2'' \end{Bmatrix} \begin{Bmatrix} l_1 & L' & L_1' \\ L'' & l_2 & L_2'' \end{Bmatrix}$$

$$\times \begin{Bmatrix} 1/2 & \kappa & 1/2 \\ 1/2 & S & S_1 \\ S_2'' & S' & S'' \end{Bmatrix} \begin{Bmatrix} l_2 & k & l_0 \\ l_1 & L & L_1 \\ L_2'' & L' & L'' \end{Bmatrix} \sum_{\bar{\alpha}'\bar{S}'\bar{L}'} (-1)^{\bar{L}'} \left(nl^N \alpha_1' S_1' L_1' \{|nl^{N-1}\bar{\alpha}'\bar{S}'\bar{L}'\right) \left(nl^N \alpha_1'' S_1'' L_1'' \{|nl^{N-1}\bar{\alpha}'\bar{S}'\bar{L}'\right) \begin{Bmatrix} t & l & l \\ \bar{L}' & L_1' & L_1'' \end{Bmatrix} \Bigg]$$

$$\times (l_0 \| \mathbf{C}^t \| l_2)(l \| \mathbf{C}^t \| l) \sum_{n_0 l_0} R^t \left(n_0 l_0 nl, n_2 l_2 nl\right) \langle n_0 l_0 | r^{-3} | n_2 l_2 \rangle^{\kappa k} / \Delta E. \tag{33}$$

The second type of electrostatic integrals:

$$- \sum_{\psi'' \neq \psi, \psi'} \Big[\langle \psi | \mathbf{G} | \psi'' \rangle \times \langle \psi'' \| \mathbf{T}^{(\kappa \mathbf{k}) \mathbf{K}} \| \psi' \rangle + \langle \psi \| \mathbf{T}^{(\kappa \mathbf{k}) \mathbf{K}} \| \psi'' \rangle \times \langle \psi'' | \mathbf{G} | \psi' \rangle \Big] / \Delta E =$$

$$[S, L, S', L']^{1/2} \sum_{\psi''} \delta(\alpha_1 S_1 L_1, \alpha_1'' S_1'' L_1'') \ \delta(\alpha_1' S_1' L_1', \alpha_1'' S_1'' L_1'') \ [S'', L'', S_2'', L_2'']$$

$$\times \Bigg[(-1)^{2S+S'+L'+2S_1'+S''+L''+S_2''+1} \begin{Bmatrix} S'' & 1/2 & S_1 \\ 1/2 & S & S_2'' \end{Bmatrix} \begin{Bmatrix} L'' & l_0 & L_1 \\ l_1 & L & L_2'' \end{Bmatrix} \begin{Bmatrix} l_0 & l_1 & t \\ l_2 & l_1 & L_2'' \end{Bmatrix} \begin{Bmatrix} 1/2 & \kappa & 1/2 \\ 1/2 & S' & S_1' \\ S_2'' & S & S'' \end{Bmatrix} \begin{Bmatrix} l_2 & k & l_0 \\ l_1 & L' & L_1' \\ L_2'' & L & L'' \end{Bmatrix}$$

$$+ (-1)^{2S_1+3S'+L'+S''+L''+S_2''+l_0+l_2+1} \begin{Bmatrix} S'' & 1/2 & S_1' \\ 1/2 & S' & S_2'' \end{Bmatrix} \begin{Bmatrix} L'' & l_0 & L_1' \\ l_1 & L' & L_2'' \end{Bmatrix} \begin{Bmatrix} l_0 & l_1 & t \\ l_2 & l_1 & L_2'' \end{Bmatrix} \begin{Bmatrix} 1/2 & \kappa & 1/2 \\ 1/2 & S & S_1 \\ S_2'' & S' & S'' \end{Bmatrix} \begin{Bmatrix} l_2 & k & l_0 \\ l_1 & L & L_1 \\ L_2'' & L' & L'' \end{Bmatrix} \Bigg]$$

$$\times (l_0 \| \mathbf{C}^t \| l_1)(l_1 \| \mathbf{C}^t \| l_2) \sum_{n_0 l_0} R^t \left(n_0 l_0 n_1 l_1, n_1 l_1 n_2 l_2\right) \langle n_0 l_0 | r^{-3} | n_2 l_2 \rangle^{\kappa k} / \Delta E$$

$$+ [S, L, S', L']^{1/2} \sum_{\psi''} \delta(\alpha_1 S_1 L_1, \alpha_1'' S_1'' L_1'') \ \delta(\alpha_1' S_1' L_1', \alpha_1'' S_1'' L_1'') \ [S'', L'', S_2'', L_2'']$$

$$\times \Bigg[(-1)^{2S+S'+L'+2S_1'+S''+L''+S_2''+1} \begin{Bmatrix} S'' & 1/2 & S_1 \\ 1/2 & S & S_2'' \end{Bmatrix} \begin{Bmatrix} L'' & l_0 & L_1 \\ l_1 & L & L_2'' \end{Bmatrix} \begin{Bmatrix} l_0 & l_2 & t \\ l_1 & l_1 & L_2'' \end{Bmatrix} \begin{Bmatrix} 1/2 & \kappa & 1/2 \\ 1/2 & S' & S_1' \\ S_2'' & S & S'' \end{Bmatrix} \begin{Bmatrix} l_2 & k & l_0 \\ l_1 & L' & L_1' \\ L_2'' & L & L'' \end{Bmatrix}$$

$$+ (-1)^{2S_1+3S'+L'+S''+L''+2S_2''+L_2''+l_0+l_2+1} \begin{Bmatrix} S'' & 1/2 & S_1' \\ 1/2 & S' & S_2'' \end{Bmatrix} \begin{Bmatrix} L'' & l_0 & L_1' \\ l_1 & L' & L_2'' \end{Bmatrix} \begin{Bmatrix} l_0 & l_2 & t \\ l_1 & l_1 & L_2'' \end{Bmatrix} \begin{Bmatrix} 1/2 & \kappa & 1/2 \\ 1/2 & S & S_1 \\ S_2'' & S' & S'' \end{Bmatrix} \begin{Bmatrix} l_2 & k & l_0 \\ l_1 & L & L_1 \\ L_2'' & L' & L'' \end{Bmatrix} \Bigg]$$

$$\times (l_0 \| \mathbf{C}^t \| l_2)(l_1 \| \mathbf{C}^t \| l_1) \sum_{n_0 l_0} R^t \left(n_0 l_0 n_1 l_1, n_2 l_2 n_1 l_1\right) \langle n_0 l_0 | r^{-3} | n_2 l_2 \rangle / {}^{\kappa k} / \Delta E. \tag{34}$$

5.3 $nl^N n_1 l_1^{N_1} n_2 l_2$ configuration

The states ψ and ψ' for $nl^N n_1 l_1^{N_1} n_2 l_2$ configuration are defined as follows:

$$\psi = (n_0 l_0^{4l_0+2} \ {}^1S, nl^N \alpha_1 S_1 L_1) S_1 L_1, (n_1 l_1^{N_1} \alpha_2 S_2 L_2, n_2 l_2) S_3 L_3; SL,$$
$$\psi' = (n_0 l_0^{4l_0+2} \ {}^1S, nl^N \alpha_1' S_1' L_1') S_1' L_1', (n_1 l_1^{N_1} \alpha_2' S_2' L_2', n_2 l_2) S_3' L_3'; S' L'.$$

5.3.1 Excitation of one electron from a closed $n_0 l_0^{4l_0+2}$ shell into an open nl^N shell

In this case the perturbing virtual states are defined as

$$\psi'' = (n_0 l_0^{4l_0+1}\ ^2l_0, nl^{N+1}\alpha_1'' S_1'' L_1'') S'' L'', (n_1 l_1^{N_1}\alpha_2'' S_2'' L_2'', n_2 l_2) S_3'' L_3''; S''' L'''.$$

The first type of electrostatic integrals:

$$
\begin{aligned}
&-\sum_{\psi''\neq\psi,\psi'}\Big[\langle\psi|\mathbf{G}|\psi''\rangle\times\langle\psi''\|\mathbf{T}^{(\kappa\mathbf{k})\mathbf{K}}\|\psi'\rangle+\langle\psi\|\mathbf{T}^{(\kappa\mathbf{k})\mathbf{K}}\|\psi''\rangle\times\langle\psi''|\mathbf{G}|\psi'\rangle\Big]/\Delta E=\\
&(N+1)\ [S,L,S',L']^{1/2}\sum_{\psi''}\left(nl^{N+1}\alpha_1'' S_1'' L_1''\{|nl^N\alpha_1 S_1 L_1\right)\left(nl^{N+1}\alpha_1'' S_1'' L_1''\{|nl^N\alpha_1' S_1' L_1'\right)[L'',S_1'',L_1'']\\
&\times\Bigg[\delta(S_1,S'')\ \delta(S_2,S_2'')\ \delta(S_3,S_3'')\ \delta(\alpha_2' S_2' L_2',\alpha_2'' S_2'' L_2'')\ \delta(S_3' L_3',S_3'' L_3'')\ \left\langle n_1 l_1^{N_1}\alpha_2 S_2 L_2\left\|\mathbf{U}^t\right\|n_1 l_1^{N_1}\alpha_2'' S_2'' L_2''\right\rangle\\
&\times(-1)^{2S+L+S'+L'+L_2+3S_1'+L_1'+S_1''+2S_3+L_3+S_3'+L_3'+S''+L''+L_3''+l_2+\kappa+k+3/2}\ [L_3,L_3'']^{1/2}\\
&\times\begin{Bmatrix}L_1 & t & L''\\ L_3'' & L & L_3\end{Bmatrix}\begin{Bmatrix}t & L_2 & L_2''\\ l_2 & L_3'' & L_3\end{Bmatrix}\begin{Bmatrix}l & L_1 & L_1''\\ L'' & l_0 & t\end{Bmatrix}\begin{Bmatrix}S_1' & S'' & \kappa\\ 1/2 & 1/2 & S_1''\end{Bmatrix}\begin{Bmatrix}L_1' & L'' & k\\ l_0 & l & L_1''\end{Bmatrix}\begin{Bmatrix}S & S' & \kappa\\ S_1' & S'' & S_3'\end{Bmatrix}\begin{Bmatrix}L & L' & k\\ L_1' & L'' & L_3'\end{Bmatrix}\\
&+\delta(S_1',S'')\ \delta(S_2',S_2'')\ \delta(S_3',S_3'')\ \delta(\alpha_2 S_2 L_2,\alpha_2'' S_2'' L_2'')\ \delta(S_3 L_3,S_3'' L_3'')\ \left\langle n_1 l_1^{N_1}\alpha_2' S_2' L_2'\left\|\mathbf{U}^t\right\|n_1 l_1^{N_1}\alpha_2'' S_2'' L_2''\right\rangle\\
&\times(-1)^{3S'+L_2'+3S_1+L_1+3S_1''+S_3+L_3+2S_3'+L_3'+3S''+L''+L_3''+l_2+\kappa+k+1/2}\ [L_3',L_3'']^{1/2}\\
&\times\begin{Bmatrix}L_1' & t & L''\\ L_3'' & L' & L_3'\end{Bmatrix}\begin{Bmatrix}t & L_2' & L_2''\\ l_2 & L_3'' & L_3'\end{Bmatrix}\begin{Bmatrix}l & L_1' & L_1''\\ L'' & l_0 & t\end{Bmatrix}\begin{Bmatrix}S_1 & S'' & \kappa\\ 1/2 & 1/2 & S_1''\end{Bmatrix}\begin{Bmatrix}L_1 & L'' & k\\ l_0 & l & L_1''\end{Bmatrix}\begin{Bmatrix}S & S' & \kappa\\ S'' & S_1 & S_3\end{Bmatrix}\begin{Bmatrix}L & L' & k\\ L'' & L_1 & L_3\end{Bmatrix}\Bigg]\\
&\times(l_1\|\mathbf{C}^t\|l_1)(l_0\|\mathbf{C}^t\|l)\sum_{n_0 l_0}R^t\left(n_0 l_0 n_1 l_1, nln_1 l_1\right)\langle n_0 l_0|r^{-3}|nl\rangle^{\kappa k}/\Delta E\\
&+(N+1)\ N_1\ [S,L,S',L']^{1/2}\sum_{\psi''}\left(nl^{N+1}\alpha_1'' S_1'' L_1''\{|nl^N\alpha_1 S_1 L_1\right)\left(nl^{N+1}\alpha_1'' S_1'' L_1''\{|nl^N\alpha_1' S_1' L_1'\right)[S_1'',L_1'',S'',L'']\\
&\times\Bigg[\delta(\alpha_2' S_2' L_2',\alpha_2'' S_2'' L_2'')\ \delta(S_3' L_3',S_3'' L_3'')\ (-1)^{3S''+S'+L'+S_3'+L_3'+3S_1''+L_1''+2S_1+3S_3+S_3''+L_1+L_2+L_2''+3S_1'+L_1'+l_1+\kappa+k+3/2}\\
&\times[S_2,L_2,S_2'',L_2'',S_3,L_3,S_3'',L_3'']^{1/2}\begin{Bmatrix}S_1' & S'' & \kappa\\ 1/2 & 1/2 & S_1''\end{Bmatrix}\begin{Bmatrix}L_1' & L'' & k\\ l_0 & l & L_1''\end{Bmatrix}\begin{Bmatrix}S & S' & \kappa\\ S_1' & S'' & S_3'\end{Bmatrix}\begin{Bmatrix}L & L' & k\\ L_1' & L'' & L_3'\end{Bmatrix}\\
&\times\sum_{\bar\alpha\bar S\bar L}\left(n_1 l_1^{N_1}\alpha_2 S_2 L_2\{|n_1 l_1^{N_1-1}\bar\alpha\bar S\bar L\right)\left(n_1 l_1^{N_1}\alpha_2'' S_2'' L_2''\{|n_1 l_1^{N_1-1}\bar\alpha\bar S\bar L\right)\begin{bmatrix}S_3 & 1/2 & S_3'' & 1/2\\ 1/2 & S & \bar S & S_1''\\ S_2 & S_2'' & S_1 & S''\end{bmatrix}\begin{bmatrix}L_1 & L_3 & L_2 & l_1 & l\\ & L & l_2 & \bar L & t & L_1''\\ L'' & L_3'' & L_2'' & l_1 & l_0\end{bmatrix}\\
&+\delta(\alpha_2 S_2 L_2,\alpha_2'' S_2'' L_2'')\ \delta(S_3 L_3,S_3'' L_3'')\ (-1)^{S''+2S_1'+L_1'+3S_3'+S_3''+L_2'+L_2''+S_1''+L_1''+3S_1+L_1+S_3+L_3+S'+L'+l+l_1+l_0+\kappa+k+1/2}\\
&\times[S_2',L_2',S_2'',L_2'',S_3',L_3',S_3'',L_3'']^{1/2}\begin{Bmatrix}S_1 & S'' & \kappa\\ 1/2 & 1/2 & S_1''\end{Bmatrix}\begin{Bmatrix}L_1 & L'' & k\\ l_0 & l & L_1''\end{Bmatrix}\begin{Bmatrix}S & S' & \kappa\\ S'' & S_1 & S_3\end{Bmatrix}\begin{Bmatrix}L & L' & k\\ L'' & L_1 & L_3\end{Bmatrix}\\
&\times\sum_{\bar\alpha'\bar S'\bar L'}\left(n_1 l_1^{N_1}\alpha_2' S_2' L_2'\{|n_1 l_1^{N_1-1}\bar\alpha' \bar S' \bar L'\right)\left(n_1 l_1^{N_1}\alpha_2'' S_2'' L_2''\{|n_1 l_1^{N_1-1}\bar\alpha' \bar S' \bar L'\right)\begin{bmatrix}S_3' & 1/2 & S_3'' & 1/2\\ 1/2 & S' & \bar S' & S_1''\\ S_2' & S_2'' & S_1' & S''\end{bmatrix}\\
&\times\begin{bmatrix}L_1' & L_3' & L_2' & l_1 & l\\ & L' & l_2 & \bar L' & t & L_1''\\ L'' & L_3'' & L_2'' & l_1 & l_0\end{bmatrix}\Bigg](l_1\|\mathbf{C}^t\|l)(l_0\|\mathbf{C}^t\|l_1)\sum_{n_0 l_0}R^t\left(n_0 l_0 n_1 l_1, n_1 l_1 nl\right)\langle n_0 l_0|r^{-3}|nl\rangle^{\kappa k}/\Delta E. \qquad (35)
\end{aligned}
$$

The second type of electrostatic integrals:

$$
\begin{aligned}
&-\sum_{\psi''\neq\psi,\psi'}\Big[\langle\psi|\mathbf{G}|\psi''\rangle\times\langle\psi''\|\mathbf{T}^{(\kappa\mathbf{k})\mathbf{K}}\|\psi'\rangle+\langle\psi\|\mathbf{T}^{(\kappa\mathbf{k})\mathbf{K}}\|\psi''\rangle\times\langle\psi''|\mathbf{G}|\psi'\rangle\Big]/\Delta E=\\
&(N+1)\ [S,L,S',L']^{1/2}\sum_{\psi''}\left(nl^{N+1}\alpha_1'' S_1'' L_1''\{|nl^N\alpha_1 S_1 L_1\right)\left(nl^{N+1}\alpha_1'' S_1'' L_1''\{|nl^N\alpha_1' S_1' L_1'\right)[L'',S_1'',L_1'']\\
&\times\delta(\alpha_2 S_2 L_2,\alpha_2'' S_2'' L_2'')\ \delta(\alpha_2' S_2' L_2',\alpha_2'' S_2'' L_2'')
\end{aligned}
$$

$$\times \Bigg[\delta(S_1,S'')\;\delta(S_3,S_3'')\;\delta(S_3'L_3',S_3''L_3'')\;(-1)^{S''+L''+S_3'+L_3'+S'+L'+3S_1'+L_1'+3S_1''+L+L_2+l_2+\kappa+k+1/2}\;[L_3,L_3'']^{1/2}$$
$$\times \begin{Bmatrix} L_1 & t & L'' \\ L_3'' & L & L_3 \end{Bmatrix} \begin{Bmatrix} L_3 & L_3'' & t \\ l_2 & l_2 & L_2 \end{Bmatrix} \begin{Bmatrix} l_0 & l & t \\ L_1 & L'' & L_1'' \end{Bmatrix} \begin{Bmatrix} S_1' & S'' & \kappa \\ 1/2 & 1/2 & S_1'' \end{Bmatrix} \begin{Bmatrix} L_1' & L'' & k \\ l_0 & l & L_1'' \end{Bmatrix} \begin{Bmatrix} S & S' & \kappa \\ S_1' & S'' & S_3' \end{Bmatrix} \begin{Bmatrix} L & L' & k \\ L_1' & L'' & L_3' \end{Bmatrix}$$
$$+\,\delta(S_1',S'')\;\delta(S_3',S_3'')\;\delta(S_3L_3,S_3''L_3'')\;(-1)^{3S_1+L_1+3S''+L''+S_3+L_3+S'+S_1''+L_2'+l_0+l+l_2+\kappa+k+3/2}\;[L_3',L_3'']^{1/2}$$
$$\times \begin{Bmatrix} L_1' & t & L'' \\ L_3'' & L' & L_3' \end{Bmatrix} \begin{Bmatrix} L_3' & L_3'' & t \\ l_2 & l_2 & L_2' \end{Bmatrix} \begin{Bmatrix} l_0 & l & t \\ L_1' & L'' & L_1'' \end{Bmatrix} \begin{Bmatrix} S_1 & S'' & \kappa \\ 1/2 & 1/2 & S_1'' \end{Bmatrix} \begin{Bmatrix} L_1 & L'' & k \\ l_0 & l & L_1'' \end{Bmatrix} \begin{Bmatrix} S & S' & \kappa \\ S'' & S_1 & S_3 \end{Bmatrix} \begin{Bmatrix} L & L' & k \\ L'' & L_1 & L_3 \end{Bmatrix} \Bigg]$$
$$\times (l_0\|\mathbf{C}^t\|l)(l_2\|\mathbf{C}^t\|l_2)\sum_{n_0l_0} R^t\left(n_0l_0n_2l_2,nln_2l_2\right)\langle n_0l_0|r^{-3}|nl\rangle^{\kappa k}/\Delta E$$
$$+\,(N+1)\;[S,L,S',L']^{1/2}\sum_{\psi''}\left(nl^{N+1}\alpha_1''S_1''L_1''\{|nl^N\alpha_1S_1L_1\right)\left(nl^{N+1}\alpha_1''S_1''L_1''\{|nl^N\alpha_1'S_1'L_1'\right)[S_1'',L_1'',S'',L'']$$
$$\times\,\delta(\alpha_2S_2L_2,\alpha_2''S_2''L_2'')\;\delta(\alpha_2'S_2'L_2',\alpha_2''S_2''L_2'')$$
$$\times \Bigg[\delta(S_3'L_3',S_3''L_3'')\;[S_3,L_3,S_3'',L_3'']^{1/2}(-1)^{3S_1+2S_2+3S_3+3S_3''+2S''+L''+S'+L'+S_3'+L_3'+3S_1''+L_1''+3S_1'+L_1'+l_0+l_2+l+\kappa+k+1/2}$$
$$\times \begin{Bmatrix} S_1' & S'' & \kappa \\ 1/2 & 1/2 & S_1'' \end{Bmatrix} \begin{Bmatrix} L_1' & L'' & k \\ l_0 & l & L_1'' \end{Bmatrix} \begin{Bmatrix} S & S' & \kappa \\ S_1' & S'' & S_3' \end{Bmatrix} \begin{Bmatrix} L & L' & k \\ L_1' & L'' & L_3' \end{Bmatrix} \begin{Bmatrix} S_1'' & S'' & 1/2 \\ S_3'' & S_2 & S \end{Bmatrix} \begin{Bmatrix} S_1 & S & S_3 \\ S_2 & 1/2 & S_1'' \end{Bmatrix} \begin{bmatrix} L_3'' & l_0 & L_3 & l \\ L_2 & L & t & L_1'' \\ l_2 & l_2 & L'' & L_1 \end{bmatrix}$$
$$+\,\delta(S_3L_3,S_3''L_3'')\;[S_3',L_3',S_3'',L_3'']^{1/2}(-1)^{3S_1'+2S_2'+3S_3'+3S_3''+L''+S_1''+L_1''+3S_1+L_1+S_3+L_3+S'+L'+l_2+\kappa+k+3/2}$$
$$\times \begin{Bmatrix} S_1 & S'' & \kappa \\ 1/2 & 1/2 & S_1'' \end{Bmatrix} \begin{Bmatrix} L_1 & L'' & k \\ l_0 & l & L_1'' \end{Bmatrix} \begin{Bmatrix} S & S' & \kappa \\ S'' & S_1 & S_3 \end{Bmatrix} \begin{Bmatrix} L & L' & k \\ L'' & L_1 & L_3 \end{Bmatrix} \begin{Bmatrix} S_1'' & S'' & 1/2 \\ S_3'' & S_2' & S \end{Bmatrix} \begin{Bmatrix} S_1' & S' & S_3' \\ S_2' & 1/2 & S_1'' \end{Bmatrix} \begin{bmatrix} L_3'' & l_0 & L_3' & l \\ L_2' & L' & t & L_1'' \\ l_2 & l_2 & L'' & L_1' \end{bmatrix} \Bigg]$$
$$\times (l_0\|\mathbf{C}^t\|l_2)(l_2\|\mathbf{C}^t\|l)\sum_{n_0l_0} R^t\left(n_0l_0n_2l_2,n_2l_2nl\right)\langle n_0l_0|r^{-3}|nl\rangle^{\kappa k}/\Delta E. \tag{36}$$

5.3.2 Excitation of one electron from a closed $n_0l_0^{4l_0+2}$ shell to an open $n_1l_1^{N_1}$ shell

In this case the perturbing virtual states are defined as

$$\psi''=(n_0l_0^{4l_0+1}\;{}^2l_0,nl^N\alpha_1''S_1''L_1'')S''L'',(n_1l_1^{N_1+1}\alpha_2''S_2''L_2'',n_2l_2)S_3''L_3'';S'''L'''.$$

The first type of electrostatic integrals:

$$-\sum_{\psi''\neq\psi,\psi'}\Big[\langle\psi|\mathbf{G}|\psi''\rangle\times\langle\psi''\|\mathbf{T}^{(\kappa\mathbf{k})\mathbf{K}}\|\psi'\rangle+\langle\psi\|\mathbf{T}^{(\kappa\mathbf{k})\mathbf{K}}\|\psi''\rangle\times\langle\psi''|\mathbf{G}|\psi'\rangle\Big]/\Delta E=$$
$$(N_1+1)\;N_1\;[S,L,S',L']^{1/2}\sum_{\psi''}\;\delta(\alpha_1S_1L_1,\alpha_1''S_1''L_1'')\;\delta(\alpha_1'S_1'L_1',\alpha_1''S_1''L_1'')\;[S'',L'',S_2'',L_2'',S_3'',L_3'']$$
$$\Bigg[\left(n_1l_1^{N_1+1}\alpha_2''S_2''L_2''\{|n_1l_1^{N_1}\alpha_2'S_2'L_2'\right)\;[S_2,L_2,S_3,L_3,S_3',L_3']^{1/2}\begin{Bmatrix} S'' & 1/2 & S_1'' \\ S_3 & S & S_3'' \end{Bmatrix}\begin{Bmatrix} L'' & l_0 & L_1'' \\ L_3 & L & L_3'' \end{Bmatrix}$$
$$\times\begin{Bmatrix} S_3 & 1/2 & S_3'' \\ S_2'' & 1/2 & S_2 \end{Bmatrix}\begin{Bmatrix} L_3 & l_0 & L_3'' \\ L_2'' & l_2 & L_2 \end{Bmatrix}\begin{Bmatrix} 1/2 & S_2' & S_2'' \\ 1/2 & S_3'' & S_3' \end{Bmatrix}\begin{Bmatrix} l_1 & L_2' & L_2'' \\ l_2 & L_3'' & L_3' \end{Bmatrix}\begin{Bmatrix} S & S_3'' & S'' \\ S' & S_3' & S_1' \\ \kappa & 1/2 & 1/2 \end{Bmatrix}\begin{Bmatrix} L & L_3'' & L'' \\ L' & L_3' & L_1' \\ k & l_1 & l_0 \end{Bmatrix}$$
$$\times\sum_{\bar\alpha\bar S\bar L,\hat\alpha\hat S\hat L}(-1)^{2S+S'+L'+3S''+L''+3S_2''+L_2''+2S_2+2S_2'+3S_3+L_3+2S_3'+\bar S+\bar L+\hat L+l_0+3/2}\;[\hat S,\hat L]^{1/2}\begin{Bmatrix} l_1 & l_1 & t \\ l_0 & l_1 & \hat L \end{Bmatrix}$$
$$\times\left(n_1l_1^{N_1+1}\alpha_2''S_2''L_2''\{|n_1l_1^{N_1-1}\bar\alpha\bar S\bar L,n_1l_1^2\hat\alpha\hat S\hat L\right)\left(n_1l_1^{N_1}\alpha_2S_2L_2\{|n_1l_1^{N_1-1}\bar\alpha\bar S\bar L\right)\begin{Bmatrix} \bar S & 1/2 & S_2 \\ 1/2 & S_2'' & \hat S \end{Bmatrix}\begin{Bmatrix} \bar L & l_1 & L_2 \\ l_0 & L_2'' & \hat L \end{Bmatrix}$$

$$+\left(n_1 l_1^{N_1+1}\alpha_2'' S_2'' L_2''\{|n_1 l_1^{N_1}\alpha_2 S_2 L_2\right)\ [S_2', L_2', S_3, L_3, S_3', L_3']^{1/2}\begin{Bmatrix} S'' & 1/2 & S_1'' \\ S_3' & S' & S_3'' \end{Bmatrix}\begin{Bmatrix} L'' & l_0 & L_1'' \\ L_3' & L' & L_3'' \end{Bmatrix}$$

$$\times\begin{Bmatrix} S_3' & 1/2 & S_3'' \\ S_2'' & 1/2 & S_2' \end{Bmatrix}\begin{Bmatrix} L_3' & l_0 & L_3'' \\ L_2'' & l_2 & L_2' \end{Bmatrix}\begin{Bmatrix} 1/2 & S_2 & S_2'' \\ 1/2 & S_3'' & S_3 \end{Bmatrix}\begin{Bmatrix} l_1 & L_2 & L_2'' \\ l_2 & L_3'' & L_3 \end{Bmatrix}\begin{Bmatrix} S' & S_3'' & S'' \\ S & S_3 & S_1 \\ \kappa & 1/2 & 1/2 \end{Bmatrix}\begin{Bmatrix} L' & L_3'' & L'' \\ L & L_3 & L_1 \\ k & l_1 & l_0 \end{Bmatrix}$$

$$\times\sum_{\bar\alpha'\bar S'\bar L',\hat\alpha'\hat S'\hat L'}(-1)^{2S_1+2S_3+3S'+L'+S''+L''+3S_2''+L_2''+2S_2+2S_2'+3S_3'+L_3'+\bar S'+\bar L'+\hat L'+l_1+1/2}\ [\hat S', \hat L']^{1/2}\begin{Bmatrix} l_1 & l_1 & t \\ l_0 & l_1 & \hat L' \end{Bmatrix}$$

$$\times\ \left(n_1 l_1^{N_1+1}\alpha_2'' S_2'' L_2''\{|n_1 l_1^{N_1-1}\bar\alpha'\bar S'\bar L', n_1 l_1^2\hat\alpha'\hat S'\hat L'\right)\left(n_1 l_1^{N_1}\alpha_2' S_2' L_2'\{|n_1 l_1^{N_1-1}\bar\alpha'\bar S'\bar L'\right)\begin{Bmatrix} \bar S' & 1/2 & S_2' \\ 1/2 & S_2'' & \hat S' \end{Bmatrix}\begin{Bmatrix} \bar L' & l_1 & L_2' \\ l_0 & L_2'' & \hat L' \end{Bmatrix}\Bigg]$$

$$\times(l_0\|\mathbf{C}^t\|l_1)(l_1\|\mathbf{C}^t\|l_1)\sum_{n_0 l_0}R^t\left(n_0 l_0 n_1 l_1, n_1 l_1 n_1 l_1\right)\langle n_0 l_0|r^{-3}|n_1 l_1\rangle^{\kappa k}/\Delta E. \tag{37}$$

The second type of electrostatic integrals:

$$-\sum_{\psi''\neq\psi,\psi'}\Big[\langle\psi|\mathbf{G}|\psi''\rangle\times\langle\psi''\|\mathbf{T}^{(\kappa\mathbf{k})\mathbf{K}}\|\psi'\rangle+\langle\psi\|\mathbf{T}^{(\kappa\mathbf{k})\mathbf{K}}\|\psi''\rangle\times\langle\psi''|\mathbf{G}|\psi'\rangle\Big]/\Delta E=$$

$$(N_1+1)\ N\ [S,L,S',L']^{1/2}\sum_{\psi''}\left(n_1 l_1^{N_1+1}\alpha_2'' S_2'' L_2''\{|n_1 l_1^{N_1}\alpha_2 S_2 L_2\right)\left(n_1 l_1^{N_1+1}\alpha_2'' S_2'' L_2''\{|n_1 l_1^{N_1}\alpha_2' S_2' L_2'\right)$$

$$\times[S'', L'', S_2'', L_2'', S_3'', L_3'']\ [S_3, L_3, S_3', L_3']^{1/2}$$

$$\times\Bigg[\delta(\alpha_1' S_1' L_1', \alpha_1'' S_1'' L_1'')\ \delta(S_1, S_1'')\ (-1)^{2S_1+2S_2+2S+2S_2'+2S_3'+2S_2''+2S_3''+S''+S_3+L_3+S'+L'+l_0+l+l_1+1/2}\ [L_1, L_1'']^{1/2}$$

$$\times\begin{Bmatrix} 1/2 & S_2 & S_2'' \\ 1/2 & S_3'' & S_3 \end{Bmatrix}\begin{Bmatrix} l_1 & L_2 & L_2'' \\ l_2 & L_3'' & L_3 \end{Bmatrix}\begin{Bmatrix} S_3 & S & S_1 \\ S'' & 1/2 & S_3'' \end{Bmatrix}\begin{Bmatrix} L_3 & L & L_1 \\ L'' & l_1 & L_3'' \end{Bmatrix}\begin{Bmatrix} 1/2 & S_2' & S_2'' \\ 1/2 & S_3'' & S_3' \end{Bmatrix}\begin{Bmatrix} l_1 & L_2' & L_2'' \\ l_2 & L_3'' & L_3' \end{Bmatrix}\begin{Bmatrix} l_0 & L_1'' & L'' \\ L_1 & l_1 & t \end{Bmatrix}\begin{Bmatrix} S & S_3'' & S'' \\ S' & S_3' & S_1' \\ \kappa & 1/2 & 1/2 \end{Bmatrix}$$

$$\times\begin{Bmatrix} L & L_3'' & L'' \\ L' & L_3' & L_1' \\ k & l_1 & l_0 \end{Bmatrix}\sum_{\bar\alpha\bar S\bar L}(-1)^{\bar L}\left(nl^N\alpha_1 S_1 L_1\{|nl^{N-1}\bar\alpha\bar S\bar L\right)\left(nl^N\alpha_1'' S_1'' L_1''\{|nl^{N-1}\bar\alpha\bar S\bar L\right)\begin{Bmatrix} t & l & l \\ \bar L & L_1'' & L_1 \end{Bmatrix}$$

$$+\delta(\alpha_1 S_1 L_1, \alpha_1'' S_1'' L_1'')\delta(S_1', S_1'')\ (-1)^{2S_2+2S_1+2S_3+2S_1'+2S_2'+2S_2''+2S_3''+3S''+3S'+L'+S_3'+L_3'+l+3/2}\ [L_1', L_1'']^{1/2}$$

$$\times\begin{Bmatrix} 1/2 & S_2' & S_2'' \\ 1/2 & S_3'' & S_3' \end{Bmatrix}\begin{Bmatrix} l_1 & L_2' & L_2'' \\ l_2 & L_3'' & L_3' \end{Bmatrix}\begin{Bmatrix} S_3' & S' & S_1' \\ S'' & 1/2 & S_3'' \end{Bmatrix}\begin{Bmatrix} L_3' & L' & L_1' \\ L'' & l_1 & L_3'' \end{Bmatrix}\begin{Bmatrix} 1/2 & S_2 & S_2'' \\ 1/2 & S_3'' & S_3 \end{Bmatrix}\begin{Bmatrix} l_1 & L_2 & L_2'' \\ l_2 & L_3'' & L_3 \end{Bmatrix}\begin{Bmatrix} l_0 & L_1'' & L'' \\ L_1' & l_1 & t \end{Bmatrix}\begin{Bmatrix} S' & S_3'' & S'' \\ S & S_3 & S_1 \\ \kappa & 1/2 & 1/2 \end{Bmatrix}$$

$$\times\begin{Bmatrix} L' & L_3'' & L'' \\ L & L_3 & L_1 \\ k & l_1 & l_0 \end{Bmatrix}\sum_{\bar\alpha'\bar S'\bar L'}(-1)^{\bar L'}\left(nl^N\alpha_1' S_1' L_1'\{|nl^{N-1}\bar\alpha'\bar S'\bar L'\right)\left(nl^N\alpha_1'' S_1'' L_1''\{|nl^{N-1}\bar\alpha'\bar S'\bar L'\right)\begin{Bmatrix} t & l & l \\ \bar L' & L_1'' & L_1' \end{Bmatrix}\Bigg]$$

$$\times(l_0\|\mathbf{C}^t\|l_1)(l\|\mathbf{C}^t\|l)\sum_{n_0 l_0}R^t\left(n_0 l_0 nl, n_1 l_1 nl\right)\langle n_0 l_0|r^{-3}|n_1 l_1\rangle^{\kappa k}/\Delta E$$

$$+\ (N_1+1)\ N\ [S,L,S',L']^{1/2}\sum_{\psi''}\left(n_1 l_1^{N_1+1}\alpha_2'' S_2'' L_2''\{|n_1 l_1^{N_1}\alpha_2 S_2 L_2\right)\left(n_1 l_1^{N_1+1}\alpha_2'' S_2'' L_2''\{|n_1 l_1^{N_1}\alpha_2' S_2' L_2'\right)$$

$$\times[S_2'', L_2'', S_3'', L_3'', L'']\ [S_3, L_3, S_3', L_3']^{1/2}$$

$$\times\Bigg[\delta(\alpha_1' S_1' L_1', \alpha_1'' S_1'' L_1'')\ (-1)^{2S+2S_3'+2S_3''+2S_2+2S_2'+2S_2''+L_1+L_1''+3S''+L''+S_3+L_3+S'+L'+l+1/2}\ [S_1'', L_1'', S_1, L_1]^{1/2}$$

$$\times\begin{Bmatrix} 1/2 & S_2 & S_2'' \\ 1/2 & S_3'' & S_3 \end{Bmatrix}\begin{Bmatrix} l_1 & L_2 & L_2'' \\ l_2 & L_3'' & L_3 \end{Bmatrix}\begin{Bmatrix} S_3 & S & S_1 \\ S'' & 1/2 & S_3'' \end{Bmatrix}\begin{Bmatrix} L_3 & L & L_1 \\ L'' & l_1 & L_3'' \end{Bmatrix}\begin{Bmatrix} 1/2 & S_2' & S_2'' \\ 1/2 & S_3'' & S_3' \end{Bmatrix}\begin{Bmatrix} l_1 & L_2' & L_2'' \\ l_2 & L_3'' & L_3' \end{Bmatrix}\begin{Bmatrix} S & S_3'' & S'' \\ S' & S_3' & S_1' \\ \kappa & 1/2 & 1/2 \end{Bmatrix}\begin{Bmatrix} L & L_3'' & L'' \\ L' & L_3' & L_1' \\ k & l_1 & l_0 \end{Bmatrix}$$

$$\times \sum_{\bar{\alpha}\bar{S}\bar{L}} \delta(\bar{S},S'')\left(nl^N\alpha_1 S_1 L_1\{|nl^{N-1}\bar{\alpha}\bar{S}\bar{L}\right)\left(nl^N\alpha_1'' S_1'' L_1''\{|nl^{N-1}\bar{\alpha}\bar{S}\bar{L}\right)\begin{Bmatrix}\bar{L} & l & L_1''\\ l_0 & L'' & t\end{Bmatrix}\begin{Bmatrix} l & t & l_1\\ L'' & L_1 & \bar{L}\end{Bmatrix}$$

$$+\,\delta(\alpha_1 S_1 L_1,\alpha_1'' S_1'' L_1'')\,(-1)^{2S_1+2S_2+2S_3+3S'+S''+S_3'+2S_3''+2S_2'+2S_2''+L'+L_1'+L_1''+L''+L_3'+l_0+l+l_1+3/2}\,[S_1'',L_1'',S_1',L_1']^{1/2}$$

$$\times\begin{Bmatrix}1/2 & S_2' & S_2''\\ 1/2 & S_3'' & S_3'\end{Bmatrix}\begin{Bmatrix}l_1 & L_2' & L_2''\\ l_2 & L_3'' & L_3'\end{Bmatrix}\begin{Bmatrix}S_3' & S' & S_1'\\ S'' & 1/2 & S_3''\end{Bmatrix}\begin{Bmatrix}L_3' & L' & L_1'\\ L'' & l_1 & L_3''\end{Bmatrix}\begin{Bmatrix}1/2 & S_2 & S_2''\\ 1/2 & S_3'' & S_3\end{Bmatrix}\begin{Bmatrix}l_1 & L_2 & L_2''\\ l_2 & L_3'' & L_3\end{Bmatrix}\begin{Bmatrix}S' & S_3'' & S''\\ S & S_3 & S_1\\ \kappa & 1/2 & 1/2\end{Bmatrix}\begin{Bmatrix}L' & L_3'' & L''\\ L & L_3 & L_1\\ k & l_1 & l_0\end{Bmatrix}$$

$$\times\sum_{\bar{\alpha}'\bar{S}'\bar{L}'}\delta(\bar{S}',S'')\left(nl^N\alpha_1' S_1' L_1'\{|nl^{N-1}\bar{\alpha}'\bar{S}'\bar{L}'\right)\left(nl^N\alpha_1'' S_1'' L_1''\{|nl^{N-1}\bar{\alpha}'\bar{S}'\bar{L}'\right)\begin{Bmatrix}\bar{L}' & l & L_1''\\ l_0 & L'' & t\end{Bmatrix}\begin{Bmatrix} l & t & l_1\\ L'' & L_1' & \bar{L}'\end{Bmatrix}\Bigg]$$

$$\times(l_0\|\mathbf{C}^t\|l)(l\|\mathbf{C}^t\|l_1)\sum_{n_0 l_0} R^t\left(n_0 l_0 nl, nln_1 l_1\right)\langle n_0 l_0|r^{-3}|n_1 l_1\rangle^{\kappa k}/\Delta E. \tag{38}$$

The third type of electrostatic integrals:

$$-\sum_{\psi''\neq\psi,\psi'}\Big[\langle\psi|\mathbf{G}|\psi''\rangle\times\langle\psi''\|\mathbf{T}^{(\kappa\mathbf{k})\mathbf{K}}\|\psi'\rangle+\langle\psi\|\mathbf{T}^{(\kappa\mathbf{k})\mathbf{K}}\|\psi''\rangle\times\langle\psi''|\mathbf{G}|\psi'\rangle\Big]/\Delta E=$$

$$(N_1+1)\,[S,L,S',L',S_3,L_3,S_3',L_3']^{1/2}\sum_{\psi''}\delta(\alpha_1' S_1' L_1',\alpha_1'' S_1'' L_1'')\,\delta(\alpha_1 S_1 L_1,\alpha_1'' S_1'' L_1'')$$

$$\times\left(n_1 l_1^{N_1+1}\alpha_2'' S_2'' L_2''\{|n_1 l_1^{N_1}\alpha_2 S_2 L_2\right)\left(n_1 l_1^{N_1+1}\alpha_2'' S_2'' L_2''\{|n_1 l_1^{N_1}\alpha_2' S_2' L_2'\right)[S'',L'',S_2'',L_2'',S_3'',L_3'']$$

$$\times\Bigg[(-1)^{2S+2S_2+3S_3+2S_2'+2S_3'+2S_3''+S'+L'+3S''+L''+L_2''+l_0+l_1+l_2+3/2}\begin{Bmatrix}1/2 & S'' & S_1\\ S & S_3 & S_3''\end{Bmatrix}\begin{Bmatrix}S_2'' & S_3'' & 1/2\\ S_3 & S_2 & 1/2\end{Bmatrix}$$

$$\times\begin{Bmatrix}l_0 & L'' & L_1\\ L & L_3 & L_3''\end{Bmatrix}\begin{Bmatrix}1/2 & S_2' & S_2''\\ 1/2 & S_3'' & S_3'\end{Bmatrix}\begin{Bmatrix}l_1 & L_2' & L_2''\\ l_2 & L_3'' & L_3'\end{Bmatrix}\begin{Bmatrix}L_3 & l_0 & L_3''\\ L_2 & l_1 & L_2''\\ l_2 & t & l_2\end{Bmatrix}\begin{Bmatrix}S & S_3'' & S''\\ S' & S_3' & S_1'\\ \kappa & 1/2 & 1/2\end{Bmatrix}\begin{Bmatrix}L & L_3'' & L''\\ L' & L_3' & L_1'\\ k & l_1 & l_0\end{Bmatrix}$$

$$+\,(-1)^{2S_1+2S_2+2S_3+2S_2'+3S_3'+2S_3''+S''+L''+3S'+L'+L_2''+l_2+1/2}\begin{Bmatrix}1/2 & S'' & S_1'\\ S' & S_3' & S_3''\end{Bmatrix}\begin{Bmatrix}S_2'' & S_3'' & 1/2\\ S_3' & S_2' & 1/2\end{Bmatrix}$$

$$\times\begin{Bmatrix}l_0 & L'' & L_1'\\ L' & L_3' & L_3''\end{Bmatrix}\begin{Bmatrix}1/2 & S_2 & S_2''\\ 1/2 & S_3'' & S_3\end{Bmatrix}\begin{Bmatrix}l_1 & L_2 & L_2''\\ l_2 & L_3'' & L_3\end{Bmatrix}\begin{Bmatrix}L_3' & l_0 & L_3''\\ L_2' & l_1 & L_2''\\ l_2 & t & l_2\end{Bmatrix}\begin{Bmatrix}S' & S_3'' & S''\\ S & S_3 & S_1\\ \kappa & 1/2 & 1/2\end{Bmatrix}\begin{Bmatrix}L' & L_3'' & L''\\ L & L_3 & L_1\\ k & l_1 & l_0\end{Bmatrix}\Bigg]$$

$$\times(l_0\|\mathbf{C}^t\|l_1)(l_2\|\mathbf{C}^t\|l_2)\sum_{n_0 l_0} R^t\left(n_0 l_0 n_2 l_2, n_1 l_1 n_2 l_2\right)\langle n_0 l_0|r^{-3}|n_1 l_1\rangle^{\kappa k}/\Delta E$$

$$+\;\;(N_1+1)\,[S,L,S',L',S_3,L_3,S_3',L_3']^{1/2}\sum_{\psi''}\delta(\alpha_1' S_1' L_1',\alpha_1'' S_1'' L_1'')\,\delta(\alpha_1 S_1 L_1,\alpha_1'' S_1'' L_1'')$$

$$\times\left(n_1 l_1^{N_1+1}\alpha_2'' S_2'' L_2''\{|n_1 l_1^{N_1}\alpha_2 S_2 L_2\right)\left(n_1 l_1^{N_1+1}\alpha_2'' S_2'' L_2''\{|n_1 l_1^{N_1}\alpha_2' S_2' L_2'\right)[S'',L'',S_3'',L_3'',L_2'']$$

$$\times\Bigg[\delta(S_3,S_2'')\,(-1)^{3S''+2S_1+2S_2'+2S_3'+3S_2''+L_3''+S'+L'+L_2+L_3+L''+l_0+3/2}\begin{Bmatrix}1/2 & S'' & S_1\\ S & S_2'' & S_3''\end{Bmatrix}\begin{Bmatrix}l_0 & L'' & L_1\\ L & L_3 & L_3''\end{Bmatrix}$$

$$\times\begin{Bmatrix}L_2 & l_2 & L_3\\ t & L_2'' & l_1\end{Bmatrix}\begin{Bmatrix}L_3 & l_0 & L_3''\\ l_2 & L_2'' & t\end{Bmatrix}\begin{Bmatrix}1/2 & S_2' & S_2''\\ 1/2 & S_3'' & S_3'\end{Bmatrix}\begin{Bmatrix}l_1 & L_2' & L_2''\\ l_2 & L_3'' & L_3'\end{Bmatrix}\begin{Bmatrix}S & S_3'' & S''\\ S' & S_3' & S_1'\\ \kappa & 1/2 & 1/2\end{Bmatrix}\begin{Bmatrix}L & L_3'' & L''\\ L' & L_3' & L_1'\\ k & l_1 & l_0\end{Bmatrix}$$

$$+\,\delta(S_3',S_2'')\,(-1)^{2S_1+2S_2+2S_3+S'+S''+3S_2''+2S_1'+L_3''+L'+L_2'+L_3'+L''+l_1+1/2}\begin{Bmatrix}1/2 & S'' & S_1'\\ S' & S_2'' & S_3''\end{Bmatrix}\begin{Bmatrix}l_0 & L'' & L_1'\\ L' & L_3' & L_3''\end{Bmatrix}$$

$$\times\begin{Bmatrix}L_2' & l_2 & L_3'\\ t & L_2'' & l_1\end{Bmatrix}\begin{Bmatrix}L_3' & l_0 & L_3''\\ l_2 & L_2'' & t\end{Bmatrix}\begin{Bmatrix}1/2 & S_2 & S_2''\\ 1/2 & S_3'' & S_3\end{Bmatrix}\begin{Bmatrix}l_1 & L_2 & L_2''\\ l_2 & L_3'' & L_3\end{Bmatrix}\begin{Bmatrix}S' & S_3'' & S''\\ S & S_3 & S_1\\ \kappa & 1/2 & 1/2\end{Bmatrix}\begin{Bmatrix}L' & L_3'' & L''\\ L & L_3 & L_1\\ k & l_1 & l_0\end{Bmatrix}\Bigg]$$

$$\times (l_0\|\mathbf{C}^t\|l_2)(l_2\|\mathbf{C}^t\|l_1)\sum_{n_0l_0} R^t\left(n_0l_0n_2l_2,n_2l_2n_1l_1\right)\langle n_0l_0|r^{-3}|n_1l_1\rangle^{\kappa k}/\Delta E. \tag{39}$$

5.3.3 Excitation of one electron from a closed $n_0l_0^{4l_0+2}$ shell to an open n_2l_2 shell

In this case the perturbing virtual states are defined as

$$\psi''=(n_0l_0^{4l_0+1}\ ^2l_0,nl^N\alpha_1''S_1''L_1'')S''L'',(n_1l_1^{N_1}\alpha_2''S_2''L_2'',n_2l_2^2\ \alpha_4''S_4''L_4'')S_3''L_3'';S'''L'''.$$

The first type of electrostatic integrals:

$$-\sum_{\psi''\neq\psi,\psi'}\left[\langle\psi|\mathbf{G}|\psi''\rangle\times\langle\psi''\|\mathbf{T}^{(\kappa\mathbf{k})\mathbf{K}}\|\psi'\rangle+\langle\psi\|\mathbf{T}^{(\kappa\mathbf{k})\mathbf{K}}\|\psi''\rangle\times\langle\psi''|\mathbf{G}|\psi'\rangle\right]/\Delta E=$$

$$2\ [S,L,S',L',S_3,L_3,S_3',L_3']^{1/2}$$

$$\times\sum_{\psi''}\ \delta(\alpha_1S_1L_1,\alpha_1''S_1''L_1'')\ \delta(\alpha_1'S_1'L_1',\alpha_1''S_1''L_1'')\ \delta(\alpha_2S_2L_2,\alpha_2''S_2''L_2'')\delta(\alpha_2'S_2'L_2',\alpha_2''S_2''L_2'')\ [S'',L'',S_3'',L_3'',S_4'',L_4'']$$

$$\times\Bigg[(-1)^{3S+L+2S''+S_1+L_1+2S_2+2S_3+2S_3'+S_3''+L_3''+L_4''+l_2+\kappa+k+3/2}\begin{Bmatrix}1/2&S_3''&S_3\\S&S_1&S''\end{Bmatrix}\begin{Bmatrix}l_0&L_3''&L_3\\L&L_1&L''\end{Bmatrix}$$

$$\times\begin{Bmatrix}S_2&1/2&S_3\\1/2&S_3''&S_4''\end{Bmatrix}\begin{Bmatrix}L_2&l_2&L_3\\l_0&L_3''&L_4''\end{Bmatrix}\begin{Bmatrix}l_2&l_0&t\\l_2&l_2&L_4''\end{Bmatrix}\begin{Bmatrix}1/2&S_3''&S_3'\\S_2'&1/2&S_4''\end{Bmatrix}\begin{Bmatrix}l_2&L_3''&L_3'\\L_2'&l_2&L_4''\end{Bmatrix}\begin{Bmatrix}S''&1/2&S_1'\\S&\kappa&S'\\S_3''&1/2&S_3'\end{Bmatrix}\begin{Bmatrix}L''&l_0&L_1'\\L&k&L'\\L_3''&l_2&L_3'\end{Bmatrix}$$

$$+(-1)^{S+L+2S'+2S''+S_1+L_1+2S_2+2S_3+2S_3'+S_3''+L_3''+L_4''+l_0+\kappa+k+3/2}\begin{Bmatrix}1/2&S_3''&S_3'\\S'&S_1'&S''\end{Bmatrix}\begin{Bmatrix}l_0&L_3''&L_3'\\L'&L_1'&L''\end{Bmatrix}$$

$$\times\begin{Bmatrix}S_2'&1/2&S_3'\\1/2&S_3''&S_4''\end{Bmatrix}\begin{Bmatrix}L_2'&l_2&L_3'\\l_0&L_3''&L_4''\end{Bmatrix}\begin{Bmatrix}l_2&l_0&t\\l_2&l_2&L_4''\end{Bmatrix}\begin{Bmatrix}1/2&S_3''&S_3\\S_2&1/2&S_4''\end{Bmatrix}\begin{Bmatrix}l_2&L_3''&L_3\\L_2&l_2&L_4''\end{Bmatrix}\begin{Bmatrix}S''&1/2&S_1\\S'&\kappa&S\\S_3''&1/2&S_3\end{Bmatrix}\begin{Bmatrix}L''&l_0&L_1\\L'&k&L\\L_3''&l_2&L_3\end{Bmatrix}\Bigg]$$

$$\times(l_2\|\mathbf{C}^t\|l_2)(l_2\|\mathbf{C}^t\|l_0)\sum_{n_0l_0}R^t\left(n_0l_0n_2l_2,n_2l_2n_2l_2\right)\langle n_0l_0|r^{-3}|n_2l_2\rangle^{\kappa k}/\Delta E. \tag{40}$$

The second type of electrostatic integrals:

$$-\sum_{\psi''\neq\psi,\psi'}\left[\langle\psi|\mathbf{G}|\psi''\rangle\times\langle\psi''\|\mathbf{T}^{(\kappa\mathbf{k})\mathbf{K}}\|\psi'\rangle+\langle\psi\|\mathbf{T}^{(\kappa\mathbf{k})\mathbf{K}}\|\psi''\rangle\times\langle\psi''|\mathbf{G}|\psi'\rangle\right]/\Delta E=$$

$$2\ N\ [S,L,S',L']^{1/2}\sum_{\psi''}\delta(\alpha_2S_2L_2,\alpha_2''S_2''L_2'')\ \delta(\alpha_2'S_2'L_2',\alpha_2''S_2''L_2'')\ [S'',L'',S_3'',L_3'',S_4'',L_4'']\ [S_3,L_3,S_3',L_3']^{1/2}$$

$$\times\Bigg[\delta(\alpha_1'S_1'L_1',\alpha_1''S_1''L_1'')\ \delta(S_1,S_1'')\ (-1)^{3S+L+2S_2+3S_1'+L_1'+2S_3+2S_3'+S_3''+L_3''+L''+\kappa+k+l+1/2}\ [L_1,L_1'']^{1/2}$$

$$\times\begin{Bmatrix}S_3&S&S_1\\S''&1/2&S_3''\end{Bmatrix}\begin{Bmatrix}L_3&L&L_1\\L''&l_2&L_3''\end{Bmatrix}\begin{Bmatrix}1/2&S_3''&S_3\\S_2&1/2&S_4''\end{Bmatrix}\begin{Bmatrix}l_2&L_3''&L_3\\L_2&l_2&L_4''\end{Bmatrix}\begin{Bmatrix}L_1&L''&l_2\\l_0&t&L_1''\end{Bmatrix}\begin{Bmatrix}1/2&S_3''&S_3'\\S_2'&1/2&S_4''\end{Bmatrix}\begin{Bmatrix}l_2&L_3''&L_3'\\L_2'&l_2&L_4''\end{Bmatrix}$$

$$\times\begin{Bmatrix}S''&1/2&S_1'\\S&\kappa&S'\\S_3''&1/2&S_3'\end{Bmatrix}\begin{Bmatrix}L''&l_0&L_1'\\L&k&L'\\L_3''&l_2&L_3'\end{Bmatrix}\sum_{\bar\alpha\bar S\bar L}(-1)^{\bar L}\left(nl^N\alpha_1S_1L_1\{|nl^{N-1}\bar\alpha\bar S\bar L\right)\left(nl^N\alpha_1''S_1''L_1''\{|nl^{N-1}\bar\alpha\bar S\bar L\right)\begin{Bmatrix}\bar L&L_1''&l\\t&l&L_1\end{Bmatrix}$$

$$+\delta(\alpha_1S_1L_1,\alpha_1''S_1''L_1'')\ \delta(S_1',S_1'')\ (-1)^{S+L+3S_1+L_1+2S'+2S_2+2S_3+2S_3'+S_3''+L_3''+L''+l_0+l+l_2+\kappa+k+1/2}\ [L_1',L_1'']^{1/2}$$

$$\times\begin{Bmatrix}S_3'&S'&S_1'\\S''&1/2&S_3''\end{Bmatrix}\begin{Bmatrix}L_3'&L'&L_1'\\L''&l_2&L_3''\end{Bmatrix}\begin{Bmatrix}1/2&S_3''&S_3'\\S_2'&1/2&S_4''\end{Bmatrix}\begin{Bmatrix}l_2&L_3''&L_3'\\L_2'&l_2&L_4''\end{Bmatrix}\begin{Bmatrix}L_1'&L''&l_2\\l_0&t&L_1''\end{Bmatrix}\begin{Bmatrix}1/2&S_3''&S_3\\S_2&1/2&S_4''\end{Bmatrix}\begin{Bmatrix}l_2&L_3''&L_3\\L_2&l_2&L_4''\end{Bmatrix}$$

$$\times\begin{Bmatrix}S''&1/2&S_1\\S'&\kappa&S\\S_3''&1/2&S_3\end{Bmatrix}\begin{Bmatrix}L''&l_0&L_1\\L'&k&L\\L_3''&l_2&L_3\end{Bmatrix}\sum_{\bar\alpha'\bar S'\bar L'}(-1)^{\bar L'}\left(nl^N\alpha_1'S_1'L_1'\{|nl^{N-1}\bar\alpha'\bar S'\bar L'\right)\left(nl^N\alpha_1''S_1''L_1''\{|nl^{N-1}\bar\alpha'\bar S'\bar L'\right)\begin{Bmatrix}\bar L'&L_1''&l\\t&l&L_1'\end{Bmatrix}\Bigg]$$

$$\times (l\|\mathbf{C}^t\|l)(l_0\|\mathbf{C}^t\|l_2)\sum_{n_0l_0} R^t\left(n_0l_0nl,n_2l_2nl\right)\langle n_0l_0|r^{-3}|n_2l_2\rangle^{\kappa k}/\Delta E$$

$$+\ 2\ N\ [S,L,S',L']^{1/2}\sum_{\psi''}\delta(\alpha_2S_2L_2,\alpha_2''S_2''L_2'')\ \delta(\alpha_2'S_2'L_2',\alpha_2''S_2''L_2'')\ [S_3'',L_3'',S_4'',L_4'',L'']\ [S_3,L_3,S_3',L_3']^{1/2}$$

$$\times\Bigg[\delta(\alpha_1'S_1'L_1',\alpha_1''S_1''L_1'')\ (-1)^{3S+L+2S_1+L_1+2S_2+2S_3+2S_3'+S_1'+S_3''+L_3''+l+l_0+l_2+\kappa+k+3/2}\ [S_1'',L_1'',S_1,L_1]^{1/2}$$

$$\times\begin{Bmatrix}S_3 & S & S_1\\ S'' & 1/2 & S_3''\end{Bmatrix}\begin{Bmatrix}L_3 & L & L_1\\ L'' & l_2 & L_3''\end{Bmatrix}\begin{Bmatrix}1/2 & S_3'' & S_3\\ S_2 & 1/2 & S_4''\end{Bmatrix}\begin{Bmatrix}l_2 & L_3'' & L_3\\ L_2 & l_2 & L_4''\end{Bmatrix}\begin{Bmatrix}1/2 & S_3'' & S_3'\\ S_2' & 1/2 & S_4''\end{Bmatrix}\begin{Bmatrix}l_2 & L_3'' & L_3'\\ L_2' & l_2 & L_4''\end{Bmatrix}\begin{Bmatrix}S'' & 1/2 & S_1'\\ S & \kappa & S'\\ S_3'' & 1/2 & S_3'\end{Bmatrix}\begin{Bmatrix}L'' & l_0 & L_1'\\ L & k & L'\\ L_3'' & l_2 & L_3'\end{Bmatrix}$$

$$\times\sum_{\bar\alpha\bar S\bar L}\delta(\bar S,S'')\left(nl^N\alpha_1S_1L_1\{|nl^{N-1}\bar\alpha\bar S\bar L\right)\left(nl^N\alpha_1''S_1''L_1''\{|nl^{N-1}\bar\alpha\bar S\bar L\right)\begin{Bmatrix}\bar L & L_1'' & l\\ l_0 & t & L''\end{Bmatrix}\begin{Bmatrix}L_1 & L'' & l_2\\ t & l & \bar L\end{Bmatrix}$$

$$+\delta(\alpha_1S_1L_1,\alpha_1''S_1''L_1'')\ (-1)^{S+L+S_1+2S_2+2S_3+2S'+2S_1'+L_1'+2S_3'+S_3''+L_3''+l+\kappa+k+3/2}\ [S_1'',L_1'',S_1',L_1']^{1/2}$$

$$\times\begin{Bmatrix}S_3' & S' & S_1'\\ S'' & 1/2 & S_3''\end{Bmatrix}\begin{Bmatrix}L_3' & L' & L_1'\\ L'' & l_2 & L_3''\end{Bmatrix}\begin{Bmatrix}1/2 & S_3'' & S_3'\\ S_2' & 1/2 & S_4''\end{Bmatrix}\begin{Bmatrix}l_2 & L_3'' & L_3'\\ L_2' & l_2 & L_4''\end{Bmatrix}\begin{Bmatrix}1/2 & S_3'' & S_3\\ S_2 & 1/2 & S_4''\end{Bmatrix}\begin{Bmatrix}l_2 & L_3'' & L_3\\ L_2 & l_2 & L_4''\end{Bmatrix}\begin{Bmatrix}S'' & 1/2 & S_1\\ S' & \kappa & S\\ S_3'' & 1/2 & S_3\end{Bmatrix}\begin{Bmatrix}L'' & l_0 & L_1\\ L' & k & L\\ L_3'' & l_2 & L_3\end{Bmatrix}$$

$$\times\sum_{\bar\alpha'\bar S'\bar L'}\delta(\bar S',S'')\left(nl^N\alpha_1'S_1'L_1'\{|nl^{N-1}\bar\alpha'\bar S'\bar L'\right)\left(nl^N\alpha_1''S_1''L_1''\{|nl^{N-1}\bar\alpha'\bar S'\bar L'\right)\begin{Bmatrix}\bar L' & L_1'' & l\\ l_0 & t & L''\end{Bmatrix}\begin{Bmatrix}L_1' & L'' & l_2\\ t & l & \bar L'\end{Bmatrix}\Bigg]$$

$$\times(l_0\|\mathbf{C}^t\|l)(l\|\mathbf{C}^t\|l_2)\sum_{n_0l_0}R^t\left(n_0l_0nl,nln_2l_2\right)\langle n_0l_0|r^{-3}|n_2l_2\rangle^{\kappa k}/\Delta E. \tag{41}$$

The third type of electrostatic integrals:

$$-\sum_{\psi''\neq\psi,\psi'}\Big[\langle\psi|\mathbf{G}|\psi''\rangle\times\langle\psi''\|\mathbf{T}^{(\kappa\mathbf{k})\mathbf{K}}\|\psi'\rangle+\langle\psi\|\mathbf{T}^{(\kappa\mathbf{k})\mathbf{K}}\|\psi''\rangle\times\langle\psi''|\mathbf{G}|\psi'\rangle\Big]/\Delta E=$$

$$2N_1\ [S,L,S',L',S_3,L_3,S_3',L_3']^{1/2}\ \sum_{\psi''}\delta(\alpha_1'S_1'L_1',\alpha_1''S_1''L_1'')\ \delta(\alpha_1S_1L_1,\alpha_1''S_1''L_1'')\ [S'',L'',S_3'',L_3'',S_4'',L_4'']$$

$$\times\Bigg[\delta(\alpha_2'S_2'L_2',\alpha_2''S_2''L_2'')\ \delta(S_2,S_2'')\ (-1)^{3S+L+2S_2+L_2+2S_3+L_3+3S_1'+L_1'+L_2'+2S_3'+3S_3''+L_3''+L_4''+\kappa+k+l_0+l_1+l_2+3/2}$$

$$\times\begin{Bmatrix}S'' & 1/2 & S_1\\ S_3 & S & S_3''\end{Bmatrix}\begin{Bmatrix}L'' & l_0 & L_1\\ L_3 & L & L_3''\end{Bmatrix}\begin{Bmatrix}1/2 & S_3'' & S_3'\\ S_2' & 1/2 & S_4''\end{Bmatrix}\begin{Bmatrix}l_2 & L_3'' & L_3'\\ L_2' & l_2 & L_4''\end{Bmatrix}\begin{Bmatrix}S_2 & 1/2 & S_3\\ 1/2 & S_3'' & S_4''\end{Bmatrix}\begin{Bmatrix}L_2'' & L_2 & t\\ L_3'' & L_3 & l_0\\ L_4'' & l_2 & l_2\end{Bmatrix}\begin{Bmatrix}S'' & 1/2 & S_1'\\ S & \kappa & S'\\ S_3'' & 1/2 & S_3'\end{Bmatrix}\begin{Bmatrix}L'' & l_0 & L_1'\\ L & k & L'\\ L_3'' & l_2 & L_3'\end{Bmatrix}$$

$$\times[L_2,L_2'']^{1/2}\sum_{\bar\alpha\bar S\bar L}(-1)^{2\bar S+\bar L}\left(n_1l_1^{N_1}\alpha_2S_2L_2\{|n_1l_1^{N_1-1}\bar\alpha\bar S\bar L\right)\left(n_1l_1^{N_1}\alpha_2''S_2''L_2''\{|n_1l_1^{N_1-1}\bar\alpha\bar S\bar L\right)\begin{Bmatrix}L_2'' & L_2 & t\\ l_1 & l_1 & \bar L\end{Bmatrix}$$

$$+\delta(\alpha_2S_2L_2,\alpha_2''S_2''L_2'')\ \delta(S_2',S_2'')\ (-1)^{S+L+2S'+3S_1+L_1+2S_2+L_2+2S_3+2S_3'+L_3'+3S_3''+L_3''+L_2'+L_4''+\kappa+k+l_1+3/2}$$

$$\times\begin{Bmatrix}S'' & 1/2 & S_1'\\ S_3' & S' & S_3''\end{Bmatrix}\begin{Bmatrix}L'' & l_0 & L_1'\\ L_3' & L' & L_3''\end{Bmatrix}\ \begin{Bmatrix}1/2 & S_3'' & S_3\\ S_2 & 1/2 & S_4''\end{Bmatrix}\begin{Bmatrix}l_2 & L_3'' & L_3\\ L_2 & l_2 & L_4''\end{Bmatrix}\begin{Bmatrix}S_2' & 1/2 & S_3'\\ 1/2 & S_3'' & S_4''\end{Bmatrix}\begin{Bmatrix}L_2'' & L_2' & t\\ L_3'' & L_3' & l_0\\ L_4'' & l_2 & l_2\end{Bmatrix}\begin{Bmatrix}S'' & 1/2 & S_1\\ S' & \kappa & S\\ S_3'' & 1/2 & S_3\end{Bmatrix}\begin{Bmatrix}L'' & l_0 & L_1\\ L' & k & L\\ L_3'' & l_2 & L_3\end{Bmatrix}$$

$$\times[L_2',L_2'']^{1/2}\sum_{\bar\alpha'\bar S'\bar L'}(-1)^{2\bar S'+\bar L'}\left(n_1l_1^{N_1}\alpha_2'S_2'L_2'\{|n_1l_1^{N_1-1}\bar\alpha'\bar S'\bar L'\right)\left(n_1l_1^{N_1}\alpha_2''S_2''L_2''\{|n_1l_1^{N_1-1}\bar\alpha'\bar S'\bar L'\right)\begin{Bmatrix}L_2'' & L_2' & t\\ l_1 & l_1 & \bar L'\end{Bmatrix}\Bigg]$$

$$\times(l_1\|\mathbf{C}^t\|l_1)(l_0\|\mathbf{C}^t\|l_2)\sum_{n_0l_0}R^t\left(n_0l_0n_1l_1,n_2l_2n_1l_1\right)\langle n_0l_0|r^{-3}|n_2l_2\rangle^{\kappa k}/\Delta E$$

$$+\ 2N_1\ [S,L,S',L',S_3,L_3,S_3',L_3']^{1/2}\sum_{\psi''}\delta(\alpha_1'S_1'L_1',\alpha_1''S_1''L_1'')\ \delta(\alpha_1S_1L_1,\alpha_1''S_1''L_1'')\ [S'',L'',S_3'',L_3'',S_4'',L_4'']$$

$$\times \Bigg[\delta(\alpha_2' S_2' L_2', \alpha_2'' S_2'' L_2'') \begin{Bmatrix} S'' & 1/2 & S_1 \\ S_3 & S & S_3'' \end{Bmatrix} \begin{Bmatrix} L'' & l_0 & L_1 \\ L_3 & L & L_3'' \end{Bmatrix} \begin{Bmatrix} 1/2 & S_3'' & S_3' \\ S_2' & 1/2 & S_4'' \end{Bmatrix} \begin{Bmatrix} l_2 & L_3'' & L_3' \\ L_2' & l_2 & L_4'' \end{Bmatrix} \begin{Bmatrix} S'' & 1/2 & S_1' \\ S & \kappa & S' \\ S_3'' & 1/2 & S_3' \end{Bmatrix} \begin{Bmatrix} L'' & l_0 & L_1' \\ L & k & L' \\ L_3'' & l_2 & L_3' \end{Bmatrix}$$

$$\times [S_2, L_2, S_2'', L_2'']^{1/2} \sum_{\bar{\alpha}\bar{S}\bar{L}} (-1)^{3S+L+2S_2+2S_3+L_3+3S_1'+L_1'+2S_3'+L_3''+L_4''+3\bar{S}+\bar{L}+\kappa+k+l_2+1}$$

$$\times \left(n_1 l_1^{N_1} \alpha_2 S_2 L_2 \{ | n_1 l_1^{N_1 - 1} \bar{\alpha} \bar{S} \bar{L} \right) \left(n_1 l_1^{N_1} \alpha_2'' S_2'' L_2'' \{ | n_1 l_1^{N_1 - 1} \bar{\alpha} \bar{S} \bar{L} \right) \begin{Bmatrix} S_4'' & \bar{S} & S_3 \\ S_2 & 1/2 & 1/2 \end{Bmatrix} \begin{Bmatrix} S_4'' & \bar{S} & S_3 \\ 1/2 & S_3'' & S_2'' \end{Bmatrix} \begin{Bmatrix} l_1 & t & l_0 & L_3 \\ \bar{L} & l_1 & L_2 & L_4'' \\ L_2'' & l_2 & L_3'' & l_2 \end{Bmatrix}$$

$$+ \ \delta(\alpha_2 S_2 L_2, \alpha_2'' S_2'' L_2'') \begin{Bmatrix} S'' & 1/2 & S_1' \\ S_3' & S' & S_3'' \end{Bmatrix} \begin{Bmatrix} L'' & l_0 & L_1' \\ L_3' & L' & L_3'' \end{Bmatrix} \begin{Bmatrix} 1/2 & S_3'' & S_3 \\ S_2 & 1/2 & S_4'' \end{Bmatrix} \begin{Bmatrix} l_2 & L_3'' & L_3 \\ L_2 & l_2 & L_4'' \end{Bmatrix} \begin{Bmatrix} S'' & 1/2 & S_1 \\ S' & \kappa & S \\ S_3'' & 1/2 & S_3 \end{Bmatrix} \begin{Bmatrix} L'' & l_0 & L_1 \\ L' & k & L \\ L_3'' & l_2 & L_3 \end{Bmatrix}$$

$$\times [S_2', L_2', S_2'', L_2'']^{1/2} \sum_{\bar{\alpha}'\bar{S}'\bar{L}'} (-1)^{S+L+3S_1+L_1+2S_3+2S'+2S_2'+2S_3'+L_3'+L_3''+L_4''+3\bar{S}'+\bar{L}'+l_0+\kappa+k+1}$$

$$\times \left(n_1 l_1^{N_1} \alpha_2' S_2' L_2' \{ | n_1 l_1^{N_1 - 1} \bar{\alpha}' \bar{S}' \bar{L}' \right) \left(n_1 l_1^{N_1} \alpha_2'' S_2'' L_2'' \{ | n_1 l_1^{N_1 - 1} \bar{\alpha}' \bar{S}' \bar{L}' \right) \begin{Bmatrix} S_4'' & \bar{S}' & S_3' \\ S_2' & 1/2 & 1/2 \end{Bmatrix} \begin{Bmatrix} S_4'' & \bar{S}' & S_3' \\ 1/2 & S_3'' & S_2'' \end{Bmatrix} \begin{Bmatrix} l_1 & t & l_0 & L_3' \\ \bar{L}' & l_1 & L_2' & L_4'' \\ L_2'' & l_2 & L_3'' & l_2 \end{Bmatrix} \Bigg]$$

$$\times (l_0 \| \mathbf{C}^t \| l_1)(l_1 \| \mathbf{C}^t \| l_2) \sum_{n_0 l_0} R^t (n_0 l_0 n_1 l_1, n_1 l_1 n_2 l_2) \langle n_0 l_0 | r^{-3} | n_2 l_2 \rangle^{\kappa k} / \Delta E. \tag{42}$$

5.4 $nl^N n_2 l_2 n_1 l_1^{N_1}$ configuration

The states ψ and ψ' for $nl^N n_2 l_2 n_1 l_1^{N_1}$ configuration are defined as follows:

$$\psi = (n_0 l_0^{4l_0+2}\ {}^1S, nl^N \alpha_1 S_1 L_1) S_1 L_1, (n_2 l_2, n_1 l_1^{N_1} \alpha_2 S_2 L_2) S_3 L_3; SL,$$
$$\psi' = (n_0 l_0^{4l_0+2}\ {}^1S, nl^N \alpha_1' S_1' L_1') S_1' L_1', (n_2 l_2, n_1 l_1^{N_1} \alpha_2' S_2' L_2') S_3' L_3'; S' L'.$$

5.4.1 Excitation of one electron $n_0 l_0$ from a closed $n_0 l_0^{4l_0+2}$ shell to an open nl^N shell

By means of proper recoupling procedures each of the components of the sum in eqs. (35) and (36) must be multiplied by a phase factor equal to $(-1)^{S_2+L_2+S_2'+L_2'+3S_3+L_3+3S_3'+L_3'+2S_2''+2S_3''}$; the perturbing virtual states are defined as

$$\psi'' = (n_0 l_0^{4l_0+1}\ {}^2l_0, nl^{N+1} \alpha_1'' S_1'' L_1'') S'' L'', (n_2 l_2, n_1 l_1^{N_1} \alpha_2'' S_2'' L_2'') S_3'' L_3''; S''' L'''.$$

5.4.2 Excitation of one electron $n_0 l_0$ from a closed $n_0 l_0^{4l_0+2}$ shell to a partially filled $n_1 l_1^{N_1}$ shell

By means of proper recoupling procedures each of the components of the sum in eqs. (37), (38) and (39) must be multiplied by a phase factor equal to $(-1)^{S_2+L_2+S_2'+L_2'+3S_3+L_3+3S_3'+L_3'+2S_2''+2S_3''}$; the perturbing virtual states are defined as

$$\psi'' = (n_0 l_0^{4l_0+1}\ {}^2l_0, nl^N \alpha_1'' S_1'' L_1'') S'' L'', (n_2 l_2, n_1 l_1^{N_1+1} \alpha_2'' S_2'' L_2'') S_3'' L_3''; S''' L'''.$$

5.4.3 Excitation of one electron from a closed $n_0 l_0^{4l_0+2}$ shell into an open $n_2 l_2$ shell

By means of proper recoupling procedures each of the components of the sum in eqs. (40), (41) and (42) must be multiplied by a phase factor equal to $(-1)^{S_2+L_2+S_2'+L_2'+3S_3+L_3+3S_3'+L_3'+2S_2''+2S_3''+1}$; the perturbing virtual states are defined as

$$\psi'' = (n_0 l_0^{4l_0+1}\ {}^2l_0, nl^N \alpha_1'' S_1'' L_1'') S'' L'', (n_2 l_2^2\ \alpha_4'' S_4'' L_4'', n_1 l_1^{N_1} \alpha_2'' S_2'' L_2'') S_3'' L_3''; S''' L'''.$$

5.5 $nl^N n_1 l_1 n_2 l_2^2$ configuration

The states ψ and ψ' for $nl^N n_1 l_1 n_2 l_2^2$ configuration are defined as follows:

$$\psi = n_0 l_0^{4l_0+2}\ {}^1S, (nl^N \alpha_1 S_1 L_1, n_1 l_1) S_2 L_2, n_2 l_2^2\ \alpha_3 S_3 L_3; SL,$$
$$\psi' = n_0 l_0^{4l_0+2}\ {}^1S, (nl^N \alpha_1' S_1' L_1', n_1 l_1) S_2' L_2', n_2 l_2^2\ \alpha_3' S_3' L_3'; S' L'.$$

5.5.1 Excitation of one electron from a closed $n_0 l_0^{4l_0+2}$ shell into an open nl^N shell

In this case the perturbing virtual states are defined as

$$\psi'' = (n_0 l_0^{4l_0+1}\ {}^2l_0, (nl^{N+1} \alpha_1'' S_1'' L_1'', n_1 l_1) S_2'' L_2'') S'' L'', n_2 l_2^2\ \alpha_3'' S_3'' L_3''; S''' L'''.$$

The first type of electrostatic integrals:

$$\begin{aligned}
&-\sum_{\psi''\neq\psi,\psi'} \left[\langle\psi|\mathbf{G}|\psi''\rangle \times \langle\psi''\|\mathbf{T}^{(\kappa\mathbf{k})\mathbf{K}}\|\psi'\rangle + \langle\psi\|\mathbf{T}^{(\kappa\mathbf{k})\mathbf{K}}\|\psi''\rangle \times \langle\psi''|\mathbf{G}|\psi'\rangle\right]/\Delta E = \\
&(N+1)\ [S,L,S',L']^{1/2} \sum_{\psi''} \left(nl^{N+1}\alpha_1'' S_1'' L_1''\{|nl^N \alpha_1 S_1 L_1\right) \left(nl^{N+1}\alpha_1'' S_1'' L_1''\{|nl^N \alpha_1' S_1' L_1'\right) [S_1'', L_1'', S_2'', L_2''] \\
&\times \delta(\alpha_3 S_3 L_3, \alpha_3'' S_3'' L_3'')\ \delta(\alpha_3' S_3' L_3', \alpha_3'' S_3'' L_3'') \\
&\times \Bigg[\delta(S_2 L_2, S'' L'')\ (-1)^{3S_2+S'+L'+2S_1''+L_1''+3S''+L''+3S_2''+L_2''+l_1+\kappa+k+1/2}\ [S'', L'', S_2', L_2']^{1/2} \\
&\times \begin{Bmatrix} S_1 & 1/2 & S_2 \\ S_2'' & 1/2 & S_1'' \end{Bmatrix} \begin{Bmatrix} L_1 & l & L_1'' \\ l_1 & t & l_1 \\ L_2 & l_0 & L_2'' \end{Bmatrix} \begin{Bmatrix} S_1' & 1/2 & S_1'' \\ S_2'' & 1/2 & S_2' \end{Bmatrix} \begin{Bmatrix} L_1' & l & L_1'' \\ L_2'' & l_1 & L_2' \end{Bmatrix} \begin{Bmatrix} 1/2 & \kappa & 1/2 \\ S'' & S_2'' & S_2' \end{Bmatrix} \begin{Bmatrix} l & k & l_0 \\ L'' & L_2'' & L_2' \end{Bmatrix} \begin{Bmatrix} S & S' & \kappa \\ S_2' & S'' & S_3' \end{Bmatrix} \begin{Bmatrix} L & L' & k \\ L_2' & L'' & L_3' \end{Bmatrix} \\
&+ \delta(S_2' L_2', S'' L'')\ (-1)^{2S_1+3S_2'+S'+L'+2S_1''+L_1''+S''+L''+3S_2''+L_2''+l_0+l+l_1+\kappa+k+3/2}\ [S'', L'', S_2, L_2]^{1/2} \\
&\times \begin{Bmatrix} S_1' & 1/2 & S_2' \\ S_2'' & 1/2 & S_1'' \end{Bmatrix} \begin{Bmatrix} L_1' & l & L_1'' \\ l_1 & t & l_1 \\ L_2' & l_0 & L_2'' \end{Bmatrix} \begin{Bmatrix} S_1 & 1/2 & S_1'' \\ S_2'' & 1/2 & S_2 \end{Bmatrix} \begin{Bmatrix} L_1 & l & L_1'' \\ L_2'' & l_1 & L_2 \end{Bmatrix} \begin{Bmatrix} S_2 & S'' & \kappa \\ 1/2 & 1/2 & S_2'' \end{Bmatrix} \begin{Bmatrix} L_2 & L'' & k \\ l_0 & l & L_2'' \end{Bmatrix} \begin{Bmatrix} S & S' & \kappa \\ S'' & S_2 & S_3 \end{Bmatrix} \begin{Bmatrix} L & L' & k \\ L'' & L_2 & L_3 \end{Bmatrix} \Bigg] \\
&\times (l_1\|\mathbf{C}^t\|l_1)(l_0\|\mathbf{C}^t\|l) \sum_{n_0 l_0} R^t\,(n_0 l_0 n_1 l_1, n l n_1 l_1)\,\langle n_0 l_0|r^{-3}|nl\rangle^{\kappa k}/\Delta E \\
&+ (N+1)\ [S,L,S',L']^{1/2} \sum_{\psi''} \left(nl^{N+1}\alpha_1'' S_1'' L_1''\{|nl^N \alpha_1 S_1 L_1\right) \left(nl^{N+1}\alpha_1'' S_1'' L_1''\{|nl^N \alpha_1' S_1' L_1'\right) [L_1'', S_2'', L_2''] \\
&\times \delta(\alpha_3 S_3 L_3, \alpha_3'' S_3'' L_3'')\ \delta(\alpha_3' S_3' L_3', \alpha_3'' S_3'' L_3'') \\
&\times \Bigg[\delta(S_2 L_2, S'' L'')\ \delta(S_2, S_1'')\ (-1)^{L_1+L_2+S'+L'+3S''+L''+3S_1''+3S_2''+l+\kappa+k+1/2}\ [S'', L'', S_2', L_2']^{1/2} \\
&\times \begin{Bmatrix} t & l_1 & l \\ L_1 & L_1'' & L_2 \end{Bmatrix} \begin{Bmatrix} L_2 & t & L_1'' \\ l_1 & L_2'' & l_0 \end{Bmatrix} \begin{Bmatrix} S_1' & 1/2 & S_1'' \\ S_2'' & 1/2 & S_2' \end{Bmatrix} \begin{Bmatrix} L_1' & l & L_1'' \\ L_2'' & l_1 & L_2' \end{Bmatrix} \begin{Bmatrix} 1/2 & \kappa & 1/2 \\ S'' & S_2'' & S_2' \end{Bmatrix} \begin{Bmatrix} l & k & l_0 \\ L'' & L_2'' & L_2' \end{Bmatrix} \begin{Bmatrix} S & S' & \kappa \\ S_2' & S'' & S_3' \end{Bmatrix} \begin{Bmatrix} L & L' & k \\ L_2' & L'' & L_3' \end{Bmatrix} \\
&+ \delta(S_2' L_2', S'' L'')\ \delta(S_2', S_1'')\ (-1)^{2S_1+S'+L'+S''+L''+L_1'+L_2'+3S_1''+3S_2''+l_0+\kappa+k+3/2}\ [S'', L'', S_2, L_2]^{1/2} \\
&\times \begin{Bmatrix} t & l_1 & l \\ L_1' & L_1'' & L_2' \end{Bmatrix} \begin{Bmatrix} L_2' & t & L_1'' \\ l_1 & L_2'' & l_0 \end{Bmatrix} \begin{Bmatrix} S_1 & 1/2 & S_1'' \\ S_2'' & 1/2 & S_2 \end{Bmatrix} \begin{Bmatrix} L_1 & l & L_1'' \\ L_2'' & l_1 & L_2 \end{Bmatrix} \begin{Bmatrix} S_2 & S'' & \kappa \\ 1/2 & 1/2 & S_2'' \end{Bmatrix} \begin{Bmatrix} L_2 & L'' & k \\ l_0 & l & L_2'' \end{Bmatrix} \begin{Bmatrix} S & S' & \kappa \\ S'' & S_2 & S_3 \end{Bmatrix} \begin{Bmatrix} L & L' & k \\ L'' & L_2 & L_3 \end{Bmatrix} \Bigg] \\
&\times (l_1\|\mathbf{C}^t\|l)(l_0\|\mathbf{C}^t\|l_1) \sum_{n_0 l_0} R^t\,(n_0 l_0 n_1 l_1, n_1 l_1 n l)\,\langle n_0 l_0|r^{-3}|nl\rangle^{\kappa k}/\Delta E. \qquad (43)
\end{aligned}$$

The second type of electrostatic integrals:

$$-\sum_{\psi''\neq\psi,\psi'} \left[\langle\psi|\mathbf{G}|\psi''\rangle \times \langle\psi''\|\mathbf{T}^{(\kappa\mathbf{k})\mathbf{K}}\|\psi'\rangle + \langle\psi\|\mathbf{T}^{(\kappa\mathbf{k})\mathbf{K}}\|\psi''\rangle \times \langle\psi''|\mathbf{G}|\psi'\rangle\right]/\Delta E =$$

$$
\begin{aligned}
&2(N+1)\ [S,L,S',L']^{1/2}\sum_{\psi''}\left(nl^{N+1}\alpha_1''S_1''L_1''\{|nl^N\alpha_1S_1L_1\right)\left(nl^{N+1}\alpha_1''S_1''L_1''\{|nl^N\alpha_1'S_1'L_1'\right)[S_1'',L_1'',S_2'',L_2'',L'']\\
&\times[S_2,L_2,S_2',L_2',L_3,L_3']^{1/2}\begin{Bmatrix}S_1\ 1/2\ S_1''\\ S_2''\ 1/2\ S_2\end{Bmatrix}\begin{Bmatrix}L_1\ l\ L_1''\\ L_2''\ l_1\ L_2\end{Bmatrix}\begin{Bmatrix}S_1'\ 1/2\ S_1''\\ S_2''\ 1/2\ S_2'\end{Bmatrix}\begin{Bmatrix}L_1'\ l\ L_1''\\ L_2''\ l_1\ L_2'\end{Bmatrix}\\
&\times\Bigg[\delta(\alpha_3'S_3'L_3',\alpha_3''S_3''L_3'')\ \delta(S_2,S'')\ \delta(S_3,S_3'')\ (-1)^{2S+L+2S_2+L_2+S'+L'+L''+3S_2''+\kappa+k+1/2}\\
&\times\begin{Bmatrix}t\ l_2\ l_2\\ l_2\ L_3''\ L_3\end{Bmatrix}\begin{Bmatrix}L_2\ L_2''\ l\\ l_0\ t\ L''\end{Bmatrix}\begin{Bmatrix}L\ L''\ L_3''\\ t\ L_3\ L_2\end{Bmatrix}\begin{Bmatrix}1/2\ \kappa\ 1/2\\ S''\ S_2''\ S_2'\end{Bmatrix}\begin{Bmatrix}l\ k\ l_0\\ L''\ L_2''\ L_2'\end{Bmatrix}\begin{Bmatrix}S\ S'\ \kappa\\ S_2'\ S''\ S_3'\end{Bmatrix}\begin{Bmatrix}L\ L'\ k\\ L_2'\ L''\ L_3'\end{Bmatrix}\\
&+\delta(\alpha_3S_3L_3,\alpha_3''S_3''L_3'')\ \delta(S_2',S'')\ \delta(S_3',S_3'')\ (-1)^{2S_1+2S_2'+L_2'+3S'+2S''+L''+3S_2''+l_0+l+\kappa+k+3/2}\\
&\times\begin{Bmatrix}t\ l_2\ l_2\\ l_2\ L_3''\ L_3'\end{Bmatrix}\begin{Bmatrix}L_2'\ L_2''\ l\\ l_0\ t\ L''\end{Bmatrix}\begin{Bmatrix}L'\ L''\ L_3''\\ t\ L_3'\ L_2'\end{Bmatrix}\begin{Bmatrix}S_2\ S''\ \kappa\\ 1/2\ 1/2\ S_2''\end{Bmatrix}\begin{Bmatrix}L_2\ L''\ k\\ l_0\ l\ L_2''\end{Bmatrix}\begin{Bmatrix}S\ S'\ \kappa\\ S''\ S_2\ S_3\end{Bmatrix}\begin{Bmatrix}L\ L'\ k\\ L''\ L_2\ L_3\end{Bmatrix}\Bigg]\\
&\times(l_0\|\mathbf{C}^t\|l)(l_2\|\mathbf{C}^t\|l_2)\sum_{n_0l_0}R^t\left(n_0l_0n_2l_2,nln_2l_2\right)\langle n_0l_0|r^{-3}|nl\rangle^{\kappa k}/\Delta E\\
&+2(N+1)\ [S,L,S',L']^{1/2}\sum_{\psi''}\left(nl^{N+1}\alpha_1''S_1''L_1''\{|nl^N\alpha_1S_1L_1\right)\left(nl^{N+1}\alpha_1''S_1''L_1''\{|nl^N\alpha_1'S_1'L_1'\right)\\
&\times[S_1'',L_1'',S_2'',L_2'',S'',L''][S_2,L_2,S_2',L_2',S_3,L_3,S_3',L_3']^{1/2}\begin{Bmatrix}S_1\ 1/2\ S_1''\\ S_2''\ 1/2\ S_2\end{Bmatrix}\begin{Bmatrix}L_1\ l\ L_1''\\ L_2''\ l_1\ L_2\end{Bmatrix}\begin{Bmatrix}S_1'\ 1/2\ S_1''\\ S_2''\ 1/2\ S_2'\end{Bmatrix}\begin{Bmatrix}L_1'\ l\ L_1''\\ L_2''\ l_1\ L_2'\end{Bmatrix}\\
&\times\Bigg[\delta(\alpha_3'S_3'L_3',\alpha_3''S_3''L_3'')\ (-1)^{2S+2S_2+L_2+S_3+S'+L'+3S_2''+L_2''+S_3''+L''+l_0+l+l_2+\kappa+k+3/2}\\
&\times\begin{Bmatrix}S\ S''\ S_3''\\ 1/2\ 1/2\ S_2''\end{Bmatrix}\begin{Bmatrix}S_2\ S_2''\ 1/2\\ 1/2\ S_3\ S\end{Bmatrix}\begin{bmatrix}L''\ L_2\ l_2\ l_2\\ l_0\ L_3''\ l\ L_3\\ L_2''\ t\ L\ l_2\end{bmatrix}\begin{Bmatrix}1/2\ \kappa\ 1/2\\ S''\ S_2''\ S_2'\end{Bmatrix}\begin{Bmatrix}l\ k\ l_0\\ L''\ L_2''\ L_2'\end{Bmatrix}\begin{Bmatrix}S\ S'\ \kappa\\ S_2'\ S''\ S_3'\end{Bmatrix}\begin{Bmatrix}L\ L'\ k\\ L_2'\ L''\ L_3'\end{Bmatrix}\\
&+\delta(\alpha_3S_3L_3,\alpha_3''S_3''L_3'')\ (-1)^{2S_1+3S'+L'+2S_2'+L_2'+3S_2''+L_2''+2S''+L''+S_3'+S_3''+l_2+\kappa+k+1/2}\\
&\times\begin{Bmatrix}S'\ S''\ S_3''\\ 1/2\ 1/2\ S_2''\end{Bmatrix}\begin{Bmatrix}S_2'\ S_2''\ 1/2\\ 1/2\ S_3'\ S'\end{Bmatrix}\begin{bmatrix}L''\ L_2'\ l_2\ l_2\\ l_0\ L_3''\ l\ L_3'\\ L_2''\ t\ L'\ l_2\end{bmatrix}\begin{Bmatrix}S_2\ S''\ \kappa\\ 1/2\ 1/2\ S_2''\end{Bmatrix}\begin{Bmatrix}L_2\ L''\ k\\ l_0\ l\ L_2''\end{Bmatrix}\begin{Bmatrix}S\ S'\ \kappa\\ S''\ S_2\ S_3\end{Bmatrix}\begin{Bmatrix}L\ L'\ k\\ L''\ L_2\ L_3\end{Bmatrix}\Bigg]\\
&\times(l_0\|\mathbf{C}^t\|l_2)(l_2\|\mathbf{C}^t\|l)\sum_{n_0l_0}R^t\left(n_0l_0n_2l_2,n_2l_2nl\right)\langle n_0l_0|r^{-3}|nl\rangle^{\kappa k}/\Delta E.
\end{aligned}
\tag{44}
$$

5.5.2 Excitation of one electron from a closed $n_0l_0^{4l_0+2}$ shell to an open $n_1l_1^{N_1}$ shell

In this case the perturbing virtual states are defined as

$$\psi''=[n_0l_0^{4l_0+1}\ ^2l_0,(nl^N\alpha_1''S_1''L_1'',n_1l_1^2\ \alpha_2''S_2''L_2'')S_4''L_4'']S''L'',n_2l_2^2\ \alpha_3''S_3''L_3'';S'''L'''.$$

The first type of electrostatic integrals:

$$
\begin{aligned}
&-\sum_{\psi''\neq\psi,\psi'}\left[\langle\psi|\mathbf{G}|\psi''\rangle\times\langle\psi''\|\mathbf{T}^{(\kappa\mathbf{k})\mathbf{K}}\|\psi'\rangle+\langle\psi\|\mathbf{T}^{(\kappa\mathbf{k})\mathbf{K}}\|\psi''\rangle\times\langle\psi''|\mathbf{G}|\psi'\rangle\right]/\Delta E=\\
&2\ [S,L,S',L']^{1/2}\sum_{\psi''}\ \delta(\alpha_1S_1L_1,\alpha_1''S_1''L_1'')\ \delta(\alpha_1'S_1'L_1',\alpha_1''S_1''L_1'')\ \delta(\alpha_3S_3L_3,\alpha_3''S_3''L_3'')\ \delta(\alpha_3'S_3'L_3',\alpha_3''S_3''L_3'')\\
&\times[S_2'',L_2'',S_4'',L_4'']\ [S_2,L_2,S_2',L_2']^{1/2}\ \begin{Bmatrix}l_1\ l_0\ t\\ l_1\ l_1\ L_2''\end{Bmatrix}\\
&\times\Bigg[\delta(S_2L_2,S''L'')\ (-1)^{S_1+L_1+S_1'+L_1'+2S_2+S'+L'+S_2'+L_2'+3S''+L''+3S_4''+L_4''+L_2''+l_0+\kappa+k+3/2}\ \begin{Bmatrix}1/2\ S_2\ S_4''\\ S_1\ S_2''\ 1/2\end{Bmatrix}\\
&\times\begin{Bmatrix}l_0\ L_2\ L_4''\\ L_1\ L_2''\ l_1\end{Bmatrix}\begin{Bmatrix}S\ S'\ \kappa\\ S_2'\ S''\ S_3'\end{Bmatrix}\begin{Bmatrix}L\ L'\ k\\ L_2'\ L''\ L_3'\end{Bmatrix}\begin{Bmatrix}S''\ S_2'\ \kappa\\ 1/2\ 1/2\ S_4''\end{Bmatrix}\begin{Bmatrix}L''\ L_2'\ k\\ l_1\ l_0\ L_4''\end{Bmatrix}\begin{Bmatrix}1/2\ S_4''\ S_2'\\ S_1'\ 1/2\ S_2''\end{Bmatrix}\begin{Bmatrix}l_1\ L_4''\ L_2'\\ L_1'\ l_1\ L_2''\end{Bmatrix}
\end{aligned}
$$

$$+\ \delta(S_2'L_2',S''L'')\ (-1)^{S_1+L_1+3S_2+L_2+S'+L'+S_1'+L_1'+2S_2'+3S_4''+L_4''+L_2''+S''+L''+l_1+\kappa+k+3/2}\ \begin{Bmatrix}1/2 & S_2' & S_4''\\ S_1' & S_2'' & 1/2\end{Bmatrix}$$
$$\times\begin{Bmatrix}l_0 & L_2' & L_4''\\ L_1' & L_2'' & l_1\end{Bmatrix}\begin{Bmatrix}S & S' & \kappa\\ S'' & S_2 & S_3\end{Bmatrix}\begin{Bmatrix}L & L' & k\\ L'' & L_2 & L_3\end{Bmatrix}\begin{Bmatrix}S'' & S_2 & \kappa\\ 1/2 & 1/2 & S_4''\end{Bmatrix}\begin{Bmatrix}L'' & L_2 & k\\ l_1 & l_0 & L_4''\end{Bmatrix}\begin{Bmatrix}1/2 & S_4'' & S_2\\ S_1 & 1/2 & S_2''\end{Bmatrix}\begin{Bmatrix}l_1 & L_4'' & L_2\\ L_1 & l_1 & L_2''\end{Bmatrix}\Bigg]$$
$$\times(l_0\|\mathbf{C}^t\|l_1)(l_1\|\mathbf{C}^t\|l_1)\sum_{n_0l_0}R^t\left(n_0l_0n_1l_1,n_1l_1n_1l_1\right)\langle n_0l_0|r^{-3}|n_1l_1\rangle^{\kappa k}/\Delta E. \tag{45}$$

The second type of electrostatic integrals:

$$-\sum_{\psi''\neq\psi,\psi'}\left[\langle\psi|\mathbf{G}|\psi''\rangle\times\langle\psi''\|\mathbf{T}^{(\kappa\mathbf{k})\mathbf{K}}\|\psi'\rangle+\langle\psi\|\mathbf{T}^{(\kappa\mathbf{k})\mathbf{K}}\|\psi''\rangle\times\langle\psi''|\mathbf{G}|\psi'\rangle\right]/\Delta E=$$
$$2N\ [S,L,S',L',S_2,L_2,S_2',L_2']^{1/2}\sum_{\psi''}\delta(\alpha_3S_3L_3,\alpha_3''S_3''L_3'')\ \delta(\alpha_3'S_3'L_3',\alpha_3''S_3''L_3'')\ [S_2'',L_2'',S_4'',L_4'']$$
$$\times\Bigg[\delta(\alpha_1'S_1'L_1',\alpha_1''S_1''L_1'')\ \delta(S_2L_2,S''L'')\ \delta(S_1,S_1'')\ [L_1,L_1'']^{1/2}\begin{Bmatrix}S & S' & \kappa\\ S_2' & S'' & S_3'\end{Bmatrix}\begin{Bmatrix}L & L' & k\\ L_2' & L'' & L_3'\end{Bmatrix}\begin{Bmatrix}S_1 & 1/2 & S_2\\ 1/2 & S_4'' & S_2''\end{Bmatrix}\begin{Bmatrix}L_1'' & L_1 & t\\ L_4'' & L_2 & l_0\\ L_2'' & l_1 & l_1\end{Bmatrix}$$
$$\times(-1)^{3S_1+3S_4''+L_1+L_4''+L_2+L_2''+S'+L'+S_1'+L_1'+S_2'+L_2'+3S''+L''+\kappa+k+l_0+l+l_1+1/2}\begin{Bmatrix}S'' & S_2' & \kappa\\ 1/2 & 1/2 & S_4''\end{Bmatrix}\begin{Bmatrix}L'' & L_2' & k\\ l_1 & l_0 & L_4''\end{Bmatrix}$$
$$\times\begin{Bmatrix}1/2 & S_4'' & S_2'\\ S_1' & 1/2 & S_2''\end{Bmatrix}\begin{Bmatrix}l_1 & L_4'' & L_2'\\ L_1' & l_1 & L_2''\end{Bmatrix}\sum_{\bar\alpha\bar S\bar L}(-1)^{\bar L}\left(nl^N\alpha_1S_1L_1\{|nl^{N-1}\bar\alpha\bar S\bar L\right)\left(nl^N\alpha_1''S_1''L_1''\{|nl^{N-1}\bar\alpha\bar S\bar L\right)\begin{Bmatrix}t & l & l\\ \bar L & L_1'' & L_1\end{Bmatrix}$$
$$+\delta(\alpha_1S_1L_1,\alpha_1''S_1''L_1'')\ \delta(S_2'L_2',S''L'')\ \delta(S_1',S_1'')\ [L_1',L_1'']^{1/2}\begin{Bmatrix}S & S' & \kappa\\ S'' & S_2 & S_3\end{Bmatrix}\begin{Bmatrix}L & L' & k\\ L'' & L_2 & L_3\end{Bmatrix}\begin{Bmatrix}S_1' & 1/2 & S_2'\\ 1/2 & S_4'' & S_2''\end{Bmatrix}\begin{Bmatrix}L_1'' & L_1' & t\\ L_4'' & L_2' & l_0\\ L_2'' & l_1 & l_1\end{Bmatrix}$$
$$\times(-1)^{S_1+L_1+3S_2+L_2+3S_1'+L_1'+S'+L'+L_2'+L_2''+3S_4''+L_4''+S''+L''+\kappa+k+l+1/2}\begin{Bmatrix}S'' & S_2 & \kappa\\ 1/2 & 1/2 & S_4''\end{Bmatrix}\begin{Bmatrix}L'' & L_2 & k\\ l_1 & l_0 & L_4''\end{Bmatrix}$$
$$\times\begin{Bmatrix}1/2 & S_4'' & S_2\\ S_1 & 1/2 & S_2''\end{Bmatrix}\begin{Bmatrix}l_1 & L_4'' & L_2\\ L_1 & l_1 & L_2''\end{Bmatrix}\sum_{\bar\alpha'\bar S'\bar L'}(-1)^{\bar L'}\left(nl^N\alpha_1'S_1'L_1'\{|nl^{N-1}\bar\alpha'\bar S'\bar L'\right)\left(nl^N\alpha_1''S_1''L_1''\{|nl^{N-1}\bar\alpha'\bar S'\bar L'\right)\begin{Bmatrix}t & l & l\\ \bar L' & L_1'' & L_1'\end{Bmatrix}\Bigg]$$
$$\times(l_0\|\mathbf{C}^t\|l_1)(l\|\mathbf{C}^t\|l)\sum_{n_0l_0}R^t\left(n_0l_0nl,n_1l_1nl\right)\langle n_0l_0|r^{-3}|n_1l_1\rangle^{\kappa k}/\Delta E$$
$$+\ 2N\ [S,L,S',L',S_2,L_2,S_2',L_2']^{1/2}\sum_{\psi''}\delta(\alpha_3S_3L_3,\alpha_3''S_3''L_3'')\ \delta(\alpha_3'S_3'L_3',\alpha_3''S_3''L_3'')\ [S_2'',L_2'',S_4'',L_4'']$$
$$\times\Bigg[\delta(\alpha_1'S_1'L_1',\alpha_1''S_1''L_1'')\ \delta(S_2L_2,S''L'')[S_1'',L_1'',S_1,L_1]^{1/2}\begin{Bmatrix}S & S' & \kappa\\ S_2' & S'' & S_3'\end{Bmatrix}\begin{Bmatrix}L & L' & k\\ L_2' & L'' & L_3'\end{Bmatrix}\begin{Bmatrix}S'' & S_2' & \kappa\\ 1/2 & 1/2 & S_4''\end{Bmatrix}\begin{Bmatrix}L'' & L_2' & k\\ l_1 & l_0 & L_4''\end{Bmatrix}$$
$$\times\begin{Bmatrix}1/2 & S_4'' & S_2'\\ S_1' & 1/2 & S_2''\end{Bmatrix}\begin{Bmatrix}l_1 & L_4'' & L_2'\\ L_1' & l_1 & L_2''\end{Bmatrix}\sum_{\bar\alpha\bar S\bar L}\left(nl^N\alpha_1S_1L_1\{|nl^{N-1}\bar\alpha\bar S\bar L\right)\left(nl^N\alpha_1''S_1''L_1''\{|nl^{N-1}\bar\alpha\bar S\bar L\right)$$
$$\times(-1)^{3S_2+\bar S+\bar L+3S_1''+L_1''+S'+L'+S_1'+L_1'+S_2'+L_2'+L_2''+L_4''+l_1+\kappa+k}\ \begin{Bmatrix}S_2'' & \bar S & S_2\\ S_1 & 1/2 & 1/2\end{Bmatrix}\begin{Bmatrix}S_2'' & \bar S & S_2\\ 1/2 & S_4'' & S_1''\end{Bmatrix}\begin{Bmatrix}l & t & l_0 & L_2\\ \bar L & l & L_1 & L_2''\\ L_1'' & l_1 & L_4'' & l_1\end{Bmatrix}$$
$$+\delta(\alpha_1S_1L_1,\alpha_1''S_1''L_1'')\ \delta(S_2'L_2',S''L'')[S_1'',L_1'',S_1',L_1']^{1/2}\begin{Bmatrix}S & S' & \kappa\\ S'' & S_2 & S_3\end{Bmatrix}\begin{Bmatrix}L & L' & k\\ L'' & L_2 & L_3\end{Bmatrix}\begin{Bmatrix}S'' & S_2 & \kappa\\ 1/2 & 1/2 & S_4''\end{Bmatrix}\begin{Bmatrix}L'' & L_2 & k\\ l_1 & l_0 & L_4''\end{Bmatrix}$$
$$\times\begin{Bmatrix}1/2 & S_4'' & S_2\\ S_1 & 1/2 & S_2''\end{Bmatrix}\begin{Bmatrix}l_1 & L_4'' & L_2\\ L_1 & l_1 & L_2''\end{Bmatrix}\sum_{\bar\alpha'\bar S'\bar L'}\left(nl^N\alpha_1'S_1'L_1'\{|nl^{N-1}\bar\alpha'\bar S'\bar L'\right)\left(nl^N\alpha_1''S_1''L_1''\{|nl^{N-1}\bar\alpha'\bar S'\bar L'\right)$$
$$\times(-1)^{S_1+L_1+3S_2+L_2+\bar S'+\bar L'+S'+L'+3S_1''+L_1''+S_2'+L_2''+L_4''+l_0+\kappa+k}\ \begin{Bmatrix}S_2'' & \bar S' & S_2'\\ S_1' & 1/2 & 1/2\end{Bmatrix}\begin{Bmatrix}S_2'' & \bar S' & S_2'\\ 1/2 & S_4'' & S_1''\end{Bmatrix}\begin{Bmatrix}l & t & l_0 & L_2'\\ \bar L' & l & L_1' & L_2''\\ L_1'' & l_1 & L_4'' & l_1\end{Bmatrix}\Bigg]$$

$$\times (l_0\|\mathbf{C}^t\|l)(l\|\mathbf{C}^t\|l_1)\sum_{n_0l_0} R^t\left(n_0l_0nl,nln_1l_1\right)\langle n_0l_0|r^{-3}|n_1l_1\rangle^{\kappa k}/\Delta E. \tag{46}$$

The third type of electrostatic integrals:

$$-\sum_{\psi''\neq\psi,\psi'}\left[\langle\psi|\mathbf{G}|\psi''\rangle\times\langle\psi''\|\mathbf{T}^{(\kappa\mathbf{k})\mathbf{K}}\|\psi'\rangle+\langle\psi\|\mathbf{T}^{(\kappa\mathbf{k})\mathbf{K}}\|\psi''\rangle\times\langle\psi''|\mathbf{G}|\psi'\rangle\right]/\Delta E=$$

$$4\,[S,L,S',L',S_2,L_2,S_2',L_2']^{1/2}\sum_{\psi''}\delta(\alpha_1'S_1'L_1',\alpha_1''S_1''L_1'')\,\delta(\alpha_1S_1L_1,\alpha_1''S_1''L_1'')[L'',S_2'',L_2'',S_4'',L_4'']$$

$$\times\left[\delta(\alpha_3'S_3'L_3',\alpha_3''S_3''L_3'')\,\delta(S_3,S_3'')\,\delta(S_2,S'')\,(-1)^{2S+L+S_1+L_1+2S_2+L_3+S'+L'+S_1'+L_1'+S_2'+L_2'+3S''+L''+S_4''+L_3''+\kappa+k+1/2}\right.$$

$$\times[L_3,L_3'']^{1/2}\begin{Bmatrix}S&S'&\kappa\\S_2'&S''&S_3'\end{Bmatrix}\begin{Bmatrix}L&L'&k\\L_2'&L''&L_3'\end{Bmatrix}\begin{Bmatrix}S''&S_2'&\kappa\\1/2&1/2&S_4''\end{Bmatrix}\begin{Bmatrix}L''&L_2'&k\\l_1&l_0&L_4''\end{Bmatrix}\begin{Bmatrix}1/2&S_4''&S_2\\S_1&1/2&S_2''\end{Bmatrix}\begin{Bmatrix}l_1&L_4''&L_2\\L_1&l_1&L_2''\end{Bmatrix}$$

$$\times\begin{Bmatrix}l_2&L_3''&l_2\\L_3&l_2&t\end{Bmatrix}\begin{Bmatrix}L_3''&L''&L\\L_2&L_3&t\end{Bmatrix}\begin{Bmatrix}L''&l_0&L_4''\\l_1&L_2&t\end{Bmatrix}\begin{Bmatrix}1/2&S_4''&S_2'\\S_1'&1/2&S_2''\end{Bmatrix}\begin{Bmatrix}l_1&L_4''&L_2'\\L_1'&l_1&L_2''\end{Bmatrix}$$

$$+\delta(\alpha_3S_3L_3,\alpha_3''S_3''L_3'')\,\delta(S_3',S_3'')\,\delta(S_2',S'')\,(-1)^{S_1+L_1+3S_2+L_2+3S'+S_1'+L_1'+2S_2'+L_3'+S''+L''+L_3''+S_4''+l_0+l_1+\kappa+k+1/2}$$

$$\times[L_3',L_3'']^{1/2}\begin{Bmatrix}S&S'&\kappa\\S''&S_2&S_3\end{Bmatrix}\begin{Bmatrix}L&L'&k\\L''&L_2&L_3\end{Bmatrix}\begin{Bmatrix}S''&S_2&\kappa\\1/2&1/2&S_4''\end{Bmatrix}\begin{Bmatrix}L''&L_2&k\\l_1&l_0&L_4''\end{Bmatrix}\begin{Bmatrix}1/2&S_4''&S_2'\\S_1'&1/2&S_2''\end{Bmatrix}\begin{Bmatrix}l_1&L_4''&L_2'\\L_1'&l_1&L_2''\end{Bmatrix}$$

$$\times\left.\begin{Bmatrix}l_2&L_3''&l_2\\L_3'&l_2&t\end{Bmatrix}\begin{Bmatrix}L_3''&L''&L'\\L_2'&L_3'&t\end{Bmatrix}\begin{Bmatrix}L''&l_0&L_4''\\l_1&L_2'&t\end{Bmatrix}\begin{Bmatrix}1/2&S_4''&S_2\\S_1&1/2&S_2''\end{Bmatrix}\begin{Bmatrix}l_1&L_4''&L_2\\L_1&l_1&L_2''\end{Bmatrix}\right]$$

$$\times(l_0\|\mathbf{C}^t\|l_1)(l_2\|\mathbf{C}^t\|l_2)\sum_{n_0l_0}R^t\left(n_0l_0n_2l_2,n_1l_1n_2l_2\right)\langle n_0l_0|r^{-3}|n_1l_1\rangle^{\kappa k}/\Delta E$$

$$+4\,[S,L,S',L',S_2,L_2,S_2',L_2']^{1/2}\sum_{\psi''}\delta(\alpha_1'S_1'L_1',\alpha_1''S_1''L_1'')\,\delta(\alpha_1S_1L_1,\alpha_1''S_1''L_1'')[S'',L'',S_2'',L_2'',S_4'',L_4'']$$

$$\times\left[\delta(\alpha_3'S_3'L_3',\alpha_3''S_3''L_3'')\,(-1)^{2S+S_1+L_1+S_2+L_3+S'+L'+S_1'+L_1'+S_2'+L_2'+L''+L_3''+S_4''+L_4''+l_0+l_1+l_2+\kappa+k+3/2}\right.$$

$$\times[S_3,L_3,S_3'',L_3'']^{1/2}\begin{Bmatrix}S&S'&\kappa\\S_2'&S''&S_3'\end{Bmatrix}\begin{Bmatrix}L&L'&k\\L_2'&L''&L_3'\end{Bmatrix}\begin{Bmatrix}S''&S_2'&\kappa\\1/2&1/2&S_4''\end{Bmatrix}\begin{Bmatrix}L''&L_2'&k\\l_1&l_0&L_4''\end{Bmatrix}\begin{Bmatrix}1/2&S_4''&S_2\\S_1&1/2&S_2''\end{Bmatrix}\begin{Bmatrix}l_1&L_4''&L_2\\L_1&l_1&L_2''\end{Bmatrix}$$

$$\times\begin{Bmatrix}1/2&S&S_4''\\S''&1/2&S_3''\end{Bmatrix}\begin{Bmatrix}1/2&S&S_4''\\S_2&1/2&S_3\end{Bmatrix}\begin{Bmatrix}1/2&S_4''&S_2'\\S_1'&1/2&S_2''\end{Bmatrix}\begin{Bmatrix}l_1&L_4''&L_2'\\L_1'&l_1&L_2''\end{Bmatrix}\begin{bmatrix}L_3''&l_0&L_3&l_1\\L&l_2&L_4''&t\\L''&L_2&l_2&l_2\end{bmatrix}$$

$$+\delta(\alpha_3S_3L_3,\alpha_3''S_3''L_3'')\,(-1)^{S_1+L_1+3S_2+L_2+3S'+L'+S_1'+L_1'+S_2'+L_3'+S_4''+L_4''+2S''+L''+L_3''+l_2+\kappa+k+3/2}$$

$$\times[S_3',L_3',S_3'',L_3'']^{1/2}\begin{Bmatrix}S&S'&\kappa\\S''&S_2&S_3\end{Bmatrix}\begin{Bmatrix}L&L'&k\\L''&L_2&L_3\end{Bmatrix}\begin{Bmatrix}S''&S_2&\kappa\\1/2&1/2&S_4''\end{Bmatrix}\begin{Bmatrix}L''&L_2&k\\l_1&l_0&L_4''\end{Bmatrix}\begin{Bmatrix}1/2&S_4''&S_2'\\S_1'&1/2&S_2''\end{Bmatrix}\begin{Bmatrix}l_1&L_4''&L_2'\\L_1'&l_1&L_2''\end{Bmatrix}$$

$$\times\left.\begin{Bmatrix}1/2&S'&S_4''\\S''&1/2&S_3''\end{Bmatrix}\begin{Bmatrix}1/2&S'&S_4''\\S_2'&1/2&S_3'\end{Bmatrix}\begin{Bmatrix}1/2&S_4''&S_2\\S_1&1/2&S_2''\end{Bmatrix}\begin{Bmatrix}l_1&L_4''&L_2\\L_1&l_1&L_2''\end{Bmatrix}\begin{bmatrix}L_3''&l_0&L_3'&l_1\\L'&l_2&L_4''&t\\L''&L_2'&l_2&l_2\end{bmatrix}\right]$$

$$\times(l_0\|\mathbf{C}^t\|l_2)(l_2\|\mathbf{C}^t\|l_1)\sum_{n_0l_0}R^t\left(n_0l_0n_2l_2,n_2l_2n_1l_1\right)\langle n_0l_0|r^{-3}|n_1l_1\rangle^{\kappa k}/\Delta E. \tag{47}$$

5.5.3 Excitation of one electron from a closed $n_0l_0^{4l_0+2}$ shell to an open n_2l_2 shell

In this case the perturbing virtual states are defined as

$$\psi''=[n_0l_0^{4l_0+1}\ ^2l_0,(nl^N\alpha_1''S_1''L_1'',n_1l_1)S_2''L_2'']S''L'',n_2l_2^3\alpha_3''S_3''L_3'';S'''L'''.$$

The first type of electrostatic integrals:

$$
\begin{aligned}
&-\sum_{\psi''\neq\psi,\psi'}\Big[\langle\psi|\mathbf{G}|\psi''\rangle\times\langle\psi''\|\mathbf{T}^{(\kappa\mathbf{k})\mathbf{K}}\|\psi'\rangle+\langle\psi\|\mathbf{T}^{(\kappa\mathbf{k})\mathbf{K}}\|\psi''\rangle\times\langle\psi''|\mathbf{G}|\psi'\rangle\Big]/\Delta E=\\
&6\,[S,L,S',L']^{1/2}\sum_{\psi''}\delta(\alpha_1S_1L_1,\alpha_1''S_1''L_1'')\,\delta(\alpha_1'S_1'L_1',\alpha_1''S_1''L_1'')\,\delta(S_2L_2,S_2''L_2'')\,\delta(S_2'L_2',S_2''L_2'')\,[S'',L'',S_3'',L_3'']\\
&\times\Bigg[(-1)^{3S+L+2S''+2S_3''+S_2'+L_2'+\kappa+k}\left(n_2l_2^3\;\alpha_3''S_3''L_3''\{|n_2l_2^2\;\alpha_3'S_3'L_3'\right)[S_3,L_3]^{1/2}\begin{Bmatrix}1/2&S_2&S''\\S&S_3''&S_3\end{Bmatrix}\begin{Bmatrix}l_0&L_2&L''\\L&L_3''&L_3\end{Bmatrix}\begin{Bmatrix}S&S''&S_3''\\S'&S_2'&S_3'\\\kappa&1/2&1/2\end{Bmatrix}\\
&\times\begin{Bmatrix}L&L''&L_3''\\L'&L_2'&L_3'\\k&l_0&l_2\end{Bmatrix}\sum_{\hat\alpha\hat S\hat L}(-1)^{\hat L}\;[\hat S,\hat L]^{1/2}\left(n_2l_2^3\;\alpha_3''S_3''L_3''\{|n_2l_2\;{}^2l_2,n_2l_2^2\;\hat\alpha\hat S\hat L\right)\begin{Bmatrix}1/2&S_3&1/2\\S_3''&\hat S&1/2\end{Bmatrix}\begin{Bmatrix}l_2&L_3&l_2\\L_3''&\hat L&l_0\end{Bmatrix}\begin{Bmatrix}l_2&l_0&t\\l_2&l_2&\hat L\end{Bmatrix}\\
&+(-1)^{S+L+2S'+2S''+2S_3''+S_2+L_2+l_0+l_2+\kappa+k}\left(n_2l_2^3\;\alpha_3''S_3''L_3''\{|n_2l_2^2\;\alpha_3S_3L_3\right)[S_3',L_3']^{1/2}\begin{Bmatrix}1/2&S_2'&S''\\S'&S_3''&S_3'\end{Bmatrix}\begin{Bmatrix}l_0&L_2'&L''\\L'&L_3''&L_3'\end{Bmatrix}\\
&\times\begin{Bmatrix}S&S_3&S_2\\S'&S_3''&S''\\\kappa&1/2&1/2\end{Bmatrix}\begin{Bmatrix}L&L_3&L_2\\L'&L_3''&L''\\k&l_2&l_0\end{Bmatrix}\sum_{\hat\alpha'\hat S'\hat L'}(-1)^{\hat L'}\;[\hat S',\hat L']^{1/2}\left(n_2l_2^3\;\alpha_3''S_3''L_3''\{|n_2l_2\;{}^2l_2,n_2l_2^2\;\hat\alpha'\hat S'\hat L'\right)\begin{Bmatrix}1/2&S_3'&1/2\\S_3''&\hat S'&1/2\end{Bmatrix}\\
&\times\begin{Bmatrix}l_2&L_3'&l_2\\L_3''&\hat L'&l_0\end{Bmatrix}\begin{Bmatrix}l_2&l_0&t\\l_2&l_2&\hat L'\end{Bmatrix}\Bigg]\\
&\times(l_2\|\mathbf{C}^t\|l_2)(l_2\|\mathbf{C}^t\|l_0)\sum_{n_0l_0}R^t\,(n_0l_0n_2l_2,n_2l_2n_2l_2)\,\langle n_0l_0|r^{-3}|n_2l_2\rangle^{\kappa k}/\Delta E.
\end{aligned}
\tag{48}
$$

The second type of electrostatic integrals:

$$
\begin{aligned}
&-\sum_{\psi''\neq\psi,\psi'}\Big[\langle\psi|\mathbf{G}|\psi''\rangle\times\langle\psi''\|\mathbf{T}^{(\kappa\mathbf{k})\mathbf{K}}\|\psi'\rangle+\langle\psi\|\mathbf{T}^{(\kappa\mathbf{k})\mathbf{K}}\|\psi''\rangle\times\langle\psi''|\mathbf{G}|\psi'\rangle\Big]/\Delta E=\\
&3\;N\;[S,L,S',L']^{1/2}\sum_{\psi''}\left(n_2l_2^3\;\alpha_3''S_3''L_3''\{|n_2l_2^2\;\alpha_3'S_3'L_3'\right)\left(n_2l_2^3\;\alpha_3''S_3''L_3''\{|n_2l_2^2\;\alpha_3S_3L_3\right)[S'',L'',S_3'',L_3'']\\
&\times\Bigg[\delta(\alpha_1'S_1'L_1',\alpha_1''S_1''L_1'')\,\delta(S_2'L_2',S_2''L_2'')\,\delta(S_1,S_1'')\,\delta(S_2,S_2'')\,[L_1,L_1'',L_2,L_2'']^{1/2}\\
&\times(-1)^{3S_3''+L_3''+2S''+L''+3S+L+3S_1''+3S_1+L_2+L_2''+S_2'+L_2'+\kappa+k+l+l_0+l_1+l_2+3/2}\\
&\times\begin{Bmatrix}S_3&S&S_2\\S''&1/2&S_3''\end{Bmatrix}\begin{Bmatrix}L_3&L&L_2\\L''&l_2&L_3''\end{Bmatrix}\begin{Bmatrix}L_1&L_2&l_1\\L_2''&L_1''&t\end{Bmatrix}\begin{Bmatrix}L_2&l_2&L''\\l_0&L_2''&t\end{Bmatrix}\begin{Bmatrix}S&S''&S_3''\\S'&S_2'&S_3'\\\kappa&1/2&1/2\end{Bmatrix}\begin{Bmatrix}L&L''&L_3''\\L'&L_2'&L_3'\\k&l_0&l_2\end{Bmatrix}\\
&\times\sum_{\bar\alpha\bar S\bar L}(-1)^{\bar L}\left(nl^N\alpha_1S_1L_1\{|nl^{N-1}\bar\alpha\bar S\bar L\right)\left(nl^N\alpha_1''S_1''L_1''\{|nl^{N-1}\bar\alpha\bar S\bar L\right)\begin{Bmatrix}\bar L&L_1''&l\\t&l&L_1\end{Bmatrix}\\
&+\delta(\alpha_1S_1L_1,\alpha_1''S_1''L_1'')\,\delta(S_2L_2,S_2''L_2'')\,\delta(S_1',S_1'')\,\delta(S_2',S_2'')\,[L_1',L_1'',L_2',L_2'']^{1/2}\\
&\times(-1)^{S_2+L_2+3S_3''+L_3''+2S''+L''+S+L+2S'+3S_1''+3S_1'+L_2'+L_2''+\kappa+k+l+l_1+3/2}\\
&\times\begin{Bmatrix}S_3'&S'&S_2'\\S''&1/2&S_3''\end{Bmatrix}\begin{Bmatrix}L_3'&L'&L_2'\\L''&l_2&L_3''\end{Bmatrix}\begin{Bmatrix}L_1'&L_2'&l_1\\L_2''&L_1''&t\end{Bmatrix}\begin{Bmatrix}L_2'&l_2&L''\\l_0&L_2''&t\end{Bmatrix}\begin{Bmatrix}S&S_3&S_2\\S'&S_3''&S''\\\kappa&1/2&1/2\end{Bmatrix}\begin{Bmatrix}L&L_3&L_2\\L'&L_3''&L''\\k&l_2&l_0\end{Bmatrix}\\
&\times\sum_{\bar\alpha'\bar S'\bar L'}(-1)^{\bar L'}\left(nl^N\alpha_1'S_1'L_1'\{|nl^{N-1}\bar\alpha'\bar S'\bar L'\right)\left(nl^N\alpha_1''S_1''L_1''\{|nl^{N-1}\bar\alpha'\bar S'\bar L'\right)\begin{Bmatrix}\bar L'&L_1''&l\\t&l&L_1'\end{Bmatrix}\Bigg]\\
&\times(l\|\mathbf{C}^t\|l)(l_0\|\mathbf{C}^t\|l_2)\sum_{n_0l_0}R^t\,(n_0l_0nl,n_2l_2nl)\,\langle n_0l_0|r^{-3}|n_2l_2\rangle^{\kappa k}/\Delta E
\end{aligned}
$$

$$
\begin{aligned}
&+3\ N\ [S,L,S',L']^{1/2}\sum_{\psi''}\left(n_2l_2^3\ \alpha_3''S_3''L_3''\{|n_2l_2^2\ \alpha_3'S_3'L_3'\right)\left(n_2l_2^3\ \alpha_3''S_3''L_3''\{|n_2l_2^2\ \alpha_3S_3L_3\right)\ [S'',L'',S_3'',L_3'']\\
&\times\Bigg[\delta(\alpha_1'S_1'L_1',\alpha_1''S_1''L_1'')\ \delta(S_2'L_2',S_2''L_2'')\ (-1)^{3S_3''+L_3''+2S''+3S+L+3S_1''+3S_1+L_2+L_2''+S_2'+L_2'+\kappa+k+l+1/2}\\
&\times[S_1'',L_1'',S_1,L_1,S_2'',L_2'',S_2,L_2]^{1/2}\begin{Bmatrix}S_3 & S & S_2\\ S'' & 1/2 & S_3''\end{Bmatrix}\begin{Bmatrix}L_3 & L & L_2\\ L'' & l_2 & L_3''\end{Bmatrix}\begin{Bmatrix}S & S'' & S_3''\\ S' & S_2' & S_3'\\ \kappa & 1/2 & 1/2\end{Bmatrix}\begin{Bmatrix}L & L'' & L_3''\\ L' & L_2' & L_3'\\ k & l_0 & l_2\end{Bmatrix}\\
&\times\sum_{\bar\alpha\bar S\bar L}\left(nl^N\alpha_1S_1L_1\{|nl^{N-1}\bar\alpha\bar S\bar L\right)\left(nl^N\alpha_1''S_1''L_1''\{|nl^{N-1}\bar\alpha\bar S\bar L\right)\begin{Bmatrix}\bar S & 1/2 & S''\\ S_2 & 1/2 & S_1\end{Bmatrix}\begin{Bmatrix}\bar S & 1/2 & S''\\ S_2'' & 1/2 & S_1''\end{Bmatrix}\begin{bmatrix}L_1 & l_2 & L_1'' & l_0\\ l_1 & \bar L & L'' & t\\ L_2 & L_2'' & l & l\end{bmatrix}\\
&+\delta(\alpha_1S_1L_1,\alpha_1''S_1''L_1'')\ \delta(S_2L_2,S_2''L_2'')\ (-1)^{S_2+L_2+3S_3''+L_3''+2S''+S+L+2S'+3S_1''+3S_1'+L_2'+L_2''+\kappa+k+l+l_0+l_2+1/2}\\
&\times[S_1'',L_1'',S_1',L_1',S_2'',L_2'',S_2',L_2']^{1/2}\begin{Bmatrix}S_3' & S' & S_2'\\ S'' & 1/2 & S_3''\end{Bmatrix}\begin{Bmatrix}L_3' & L' & L_2'\\ L'' & l_2 & L_3''\end{Bmatrix}\begin{Bmatrix}S & S_3 & S_2\\ S' & S_3'' & S''\\ \kappa & 1/2 & 1/2\end{Bmatrix}\begin{Bmatrix}L & L_3 & L_2\\ L' & L_3'' & L''\\ k & l_2 & l_0\end{Bmatrix}\\
&\times\sum_{\bar\alpha'\bar S'\bar L'}\left(nl^N\alpha_1'S_1'L_1'\{|nl^{N-1}\bar\alpha'\bar S'\bar L'\right)\left(nl^N\alpha_1''S_1''L_1''\{|nl^{N-1}\bar\alpha'\bar S'\bar L'\right)\begin{Bmatrix}\bar S' & 1/2 & S''\\ S_2' & 1/2 & S_1'\end{Bmatrix}\begin{Bmatrix}\bar S' & 1/2 & S''\\ S_2'' & 1/2 & S_1''\end{Bmatrix}\begin{bmatrix}L_1' & l_2 & L_1'' & l_0\\ l_1 & \bar L' & L'' & t\\ L_2' & L_2'' & l & l\end{bmatrix}\Bigg]\\
&\times(l_0\|\mathbf{C}^t\|l)(l\|\mathbf{C}^t\|l_2)\sum_{n_0l_0}\ R^t\left(n_0l_0nl,nln_2l_2\right)\langle n_0l_0|r^{-3}|n_2l_2\rangle^{\kappa k}/\Delta E. \qquad (49)
\end{aligned}
$$

The third type of electrostatic integrals:

$$
\begin{aligned}
&-\sum_{\psi''\neq\psi,\psi'}\Big[\langle\psi|\mathbf{G}|\psi''\rangle\times\langle\psi''\|\mathbf{T}^{(\kappa\mathbf{k})\mathbf{K}}\|\psi'\rangle+\langle\psi\|\mathbf{T}^{(\kappa\mathbf{k})\mathbf{K}}\|\psi''\rangle\times\langle\psi''|\mathbf{G}|\psi'\rangle\Big]/\Delta E=\\
&3\ [S,L,S',L']^{1/2}\\
&\times\sum_{\psi''}\delta(\alpha_1S_1L_1,\alpha_1''S_1''L_1'')\ \delta(\alpha_1'S_1'L_1',\alpha_1''S_1''L_1'')\ [S'',L'',S_3'',L_3'']\\
&\times\left(n_2l_2^3\ \alpha_3''S_3''L_3''\{|n_2l_2^2\ \alpha_3'S_3'L_3'\right)\left(n_2l_2^3\ \alpha_3''S_3''L_3''\{|n_2l_2^2\ \alpha_3S_3L_3\right)\\
&\times\Bigg[\delta(S_2'L_2',S_2''L_2'')\ \delta(S_2,S_2'')\ (-1)^{3S_3''+L_3''+2S''+L''+3S+L+L_1+S_2'+L_2'+\kappa+k+l_1+3/2}\ [L_2,L_2'']^{1/2}\\
&\times\begin{Bmatrix}S_3 & S & S_2\\ S'' & 1/2 & S_3''\end{Bmatrix}\begin{Bmatrix}L_3 & L & L_2\\ L'' & l_2 & L_3''\end{Bmatrix}\begin{Bmatrix}t & l_2 & l_0\\ L'' & L_2'' & L_2\end{Bmatrix}\begin{Bmatrix}l_1 & L_2 & L_1\\ L_2'' & l_1 & t\end{Bmatrix}\begin{Bmatrix}S & S'' & S_3''\\ S' & S_2' & S_3'\\ \kappa & 1/2 & 1/2\end{Bmatrix}\begin{Bmatrix}L & L'' & L_3''\\ L' & L_2' & L_3'\\ k & l_0 & l_2\end{Bmatrix}\\
&+\delta(S_2L_2,S_2''L_2'')\ \delta(S_2',S_2'')\ (-1)^{S_2+L_2+3S_3''+L_3''+2S''+L''+S+L+L_1'+2S'+\kappa+k+l_0+l_1+l_2+3/2}\ [L_2',L_2'']^{1/2}\\
&\times\begin{Bmatrix}S_3' & S' & S_2'\\ S'' & 1/2 & S_3''\end{Bmatrix}\begin{Bmatrix}L_3' & L' & L_2'\\ L'' & l_2 & L_3''\end{Bmatrix}\begin{Bmatrix}t & l_2 & l_0\\ L'' & L_2'' & L_2'\end{Bmatrix}\begin{Bmatrix}l_1 & L_2' & L_1'\\ L_2'' & l_1 & t\end{Bmatrix}\begin{Bmatrix}S & S_3 & S_2\\ S' & S_3'' & S''\\ \kappa & 1/2 & 1/2\end{Bmatrix}\begin{Bmatrix}L & L_3 & L_2\\ L' & L_3'' & L''\\ k & l_2 & l_0\end{Bmatrix}\Bigg]\\
&\times(l_1\|\mathbf{C}^t\|l_1)(l_0\|\mathbf{C}^t\|l_2)\sum_{n_0l_0}\ R^t\left(n_0l_0n_1l_1,n_2l_2n_1l_1\right)\langle n_0l_0|r^{-3}|n_2l_2\rangle^{\kappa k}/\Delta E\\
&+3\ [S,L,S',L']^{1/2}\\
&\times\sum_{\psi''}\delta(\alpha_1S_1L_1,\alpha_1''S_1''L_1'')\ \delta(\alpha_1'S_1'L_1',\alpha_1''S_1''L_1'')\ [L'',S_3'',L_3'']\\
&\times\left(n_2l_2^3\ \alpha_3''S_3''L_3''\{|n_2l_2^2\ \alpha_3'S_3'L_3'\right)\left(n_2l_2^3\ \alpha_3''S_3''L_3''\{|n_2l_2^2\ \alpha_3S_3L_3\right)
\end{aligned}
$$

$$\times \Bigg[\delta(S_2' L_2', S_2'' L_2'')\ \delta(S_1, S'')\ (-1)^{3S_3''+L_3''+3S+L+L_2+2S_2''+L_2''+S_2'+L_2'+\kappa+k+l_1+3/2}\ [S_2, L_2, S_2'', L_2'']^{1/2}$$

$$\times \begin{Bmatrix} S_3 & S & S_2 \\ S_1 & 1/2 & S_3'' \end{Bmatrix} \begin{Bmatrix} L_3 & L & L_2 \\ L'' & l_2 & L_3'' \end{Bmatrix} \begin{Bmatrix} L'' & L_2 & l_2 \\ l_1 & t & L_1 \end{Bmatrix} \begin{Bmatrix} l_1 & L_1 & L_2'' \\ L'' & l_0 & t \end{Bmatrix} \begin{Bmatrix} S & S'' & S_3'' \\ S' & S_2' & S_3' \\ \kappa & 1/2 & 1/2 \end{Bmatrix} \begin{Bmatrix} L & L'' & L_3'' \\ L' & L_2' & L_3' \\ k & l_0 & l_2 \end{Bmatrix}$$

$$+ \delta(S_2 L_2, S_2'' L_2'')\ \delta(S_1', S'')\ (-1)^{3S_3''+L_3''+S+L+2S'+L_2'+2S_2''+L_2''+S_2+L_2+\kappa+k+l_1+l_2+l_0+3/2}\ [S_2', L_2', S_2'', L_2'']^{1/2}$$

$$\times \begin{Bmatrix} S_3' & S' & S_2' \\ S_1' & 1/2 & S_3'' \end{Bmatrix} \begin{Bmatrix} L_3' & L' & L_2' \\ L'' & l_2 & L_3'' \end{Bmatrix} \begin{Bmatrix} L'' & L_2' & l_2 \\ l_1 & t & L_1' \end{Bmatrix} \begin{Bmatrix} l_1 & L_1' & L_2'' \\ L'' & l_0 & t \end{Bmatrix} \begin{Bmatrix} S & S_3 & S_2 \\ S' & S_3'' & S'' \\ \kappa & 1/2 & 1/2 \end{Bmatrix} \begin{Bmatrix} L & L_3 & L_2 \\ L' & L_3'' & L'' \\ k & l_2 & l_0 \end{Bmatrix} \Bigg]$$

$$\times (l_0 \| \mathbf{C}^t \| l)(l_1 \| \mathbf{C}^t \| l_2) \sum_{n_0 l_0} R^t\,(n_0 l_0 n_1 l_1, n_1 l_1 n_2 l_2)\, \langle n_0 l_0 | r^{-3} | n_2 l_2 \rangle^{\kappa k} / \Delta E. \tag{50}$$

5.6 Inter-configuration matrix elements

5.6.1 Configuration interaction $nl^{N+1} \leftrightarrow nl^N n_1 l_1$

The states ψ for nl^{N+1} configuration and ψ' for $nl^N n_1 l_1$ configuration are defined as follows:

$$\psi = n_0 l_0^{4l_0+2}\ {}^1S, nl^{N+1} \alpha SL; SL,$$
$$\psi' = n_0 l_0^{4l_0+2}\ {}^1S, (nl^N \alpha_1' S_1' L_1', n_1 l_1) S' L'; S' L'.$$

5.6.2 Excitation of one electron from a closed $n_0 l_0^{4l_0+2}$ shell into an open nl^{N+1}

In this case the perturbing virtual states are defined as $\psi'' = n_0 l_0^{4l_0+1}\ {}^2l_0, nl^{N+2} \alpha'' S'' L''; S''' L'''$.

For the considered excitation the first term of the sum below is equal to zero due to the spin-orbit or hyperfine interaction:

$$- \sum_{\psi'' \neq \psi, \psi'} \Big[\langle n_0 l_0^{4l_0+2}\ {}^1S, nl^{N+1} \alpha SL; SL | \mathbf{G} | n_0 l_0^{4l_0+1}\ {}^2l_0, nl^{N+2} \alpha'' S'' L''; SL \rangle$$
$$\times \langle n_0 l_0^{4l_0+1}\ {}^2l_0, nl^{N+2} \alpha'' S'' L''; SL \| \mathbf{T}^{(\kappa \mathbf{k})\mathbf{K}} \| n_0 l_0^{4l_0+2}\ {}^1S, (nl^N \alpha_1' S_1' L_1', n_1 l_1) S' L'; S' L' \rangle$$
$$+ \langle n_0 l_0^{4l_0+2}\ {}^1S, nl^{N+1} \alpha SL; SL \| \mathbf{T}^{(\kappa \mathbf{k})\mathbf{K}} \| n_0 l_0^{4l_0+1}\ {}^2l_0, nl^{N+2} \alpha'' S'' L''; S' L' \rangle$$
$$\times \langle n_0 l_0^{4l_0+1}\ {}^2l_0, nl^{N+2} \alpha'' S'' L''; S' L' | \mathbf{G} | n_0 l_0^{4l_0+2}\ {}^1S, (nl^N \alpha_1' S_1' L_1', n_1 l_1) S' L'; S' L' \rangle \Big] / \Delta E. \tag{51}$$

The second component is as follows:

$$- \sum_{\psi''} \langle \psi \| \mathbf{T}^{(\kappa \mathbf{k})\mathbf{K}} \| \psi'' \rangle \times \langle \psi'' | \mathbf{G} | \psi' \rangle / \Delta E =$$

$$(N+2)\sqrt{N+1}\ [S', L']^{1/2} \sum_{\psi''} (-1)^{S'+L'+S_1'+L_1'+2S''+l+1/2} \left(nl^{N+2} \alpha'' S'' L'' \{ | nl^{N+1} \alpha SL \right) [S'', L''] \begin{Bmatrix} S & S' & \kappa \\ 1/2 & 1/2 & S'' \end{Bmatrix}$$

$$\times \begin{Bmatrix} L & L' & k \\ l_0 & l & L'' \end{Bmatrix} \sum_{\hat{\alpha} \hat{S} \hat{L}} (-1)^{\hat{L}}\ [\hat{S}, \hat{L}]^{1/2} \left(nl^{N+2} \alpha'' S'' L'' \{ | nl^N \alpha_1' S_1' L_1', nl^2 \hat{\alpha} \hat{S} \hat{L} \right) \begin{Bmatrix} \hat{S} & S_1' & S'' \\ S' & 1/2 & 1/2 \end{Bmatrix} \begin{Bmatrix} \hat{L} & L_1' & L'' \\ L' & l_0 & l_1 \end{Bmatrix} \begin{Bmatrix} l & l_0 & t \\ l_1 & l & \hat{L} \end{Bmatrix}$$

$$\times (l \| \mathbf{C}^t \| l_0)(l \| \mathbf{C}^t \| l_1) \sum_{n_0 l_0} R^t\,(nlnl, n_0 l_0 n_1 l_1)\, \langle n_0 l_0 | r^{-3} | nl \rangle^{\kappa k} / \Delta E. \tag{52}$$

5.6.3 Excitation of one electron from a closed $n_0 l_0^{4l_0+2}$ shell into an empty $n_1 l_1$ shell

In this case the perturbing virtual states are defined as $\psi'' = n_0 l_0^{4l_0+1}\ {}^2l_0, (nl^{N+1} \alpha_1'' S_1'' L_1'', n_1 l_1) S'' L''; S''' L'''$.

For the considered excitation two components of the sum give different contributions to the spin-orbit or hyperfine interaction:

$$
\begin{aligned}
&-\sum_{\psi''\neq\psi,\psi'}\Big[\langle n_0 l_0^{4l_0+2}\ {}^1S, nl^{N+1}\alpha SL; SL|\mathbf{G}|n_0 l_0^{4l_0+1}\ {}^2l_0, (nl^{N+1}\alpha_1'' S_1'' L_1'', n_1 l_1) S'' L''; SL\rangle\\
&\times\langle n_0 l_0^{4l_0+1}\ {}^2l_0, (nl^{N+1}\alpha_1'' S_1'' L_1'', n_1 l_1) S'' L''; SL\|\mathbf{T}^{(\kappa\mathbf{k})\mathbf{K}}\|n_0 l_0^{4l_0+2}\ {}^1S, (nl^{N}\alpha_1' S_1' L_1', n_1 l_1) S' L'; S' L'\rangle\\
&+\langle n_0 l_0^{4l_0+2}\ {}^1S, nl^{N+1}\alpha SL; SL\|\mathbf{T}^{(\kappa\mathbf{k})\mathbf{K}}\|n_0 l_0^{4l_0+1}\ {}^2l_0, (nl^{N+1}\alpha_1'' S_1'' L_1'', n_1 l_1) S'' L''; S' L'\rangle\\
&\times\langle n_0 l_0^{4l_0+1}\ {}^2l_0, (nl^{N+1}\alpha_1'' S_1'' L_1'', n_1 l_1) S'' L''; S' L'|\mathbf{G}|n_0 l_0^{4l_0+2}\ {}^1S, (nl^{N}\alpha_1' S_1' L_1', n_1 l_1) S' L'; S' L'\rangle\Big]/\Delta E. \qquad (53)
\end{aligned}
$$

The first component is as follows:

$$
\begin{aligned}
&-\sum_{\psi''}\langle\psi|\mathbf{G}|\psi''\rangle\times\langle\psi''\|\mathbf{T}^{(\kappa\mathbf{k})\mathbf{K}}\|\psi'\rangle/\Delta E=\\
&\sqrt{N+1}\,[S',L']^{1/2}\sum_{\psi''}\delta(S_1'',S)\left(nl^{N+1}\alpha_1'' S_1'' L_1''\{|nl^N\alpha_1' S_1' L_1'\right)\ \langle nl^{N+1}\alpha_1'' S_1'' L_1''\left\|\mathbf{U}^t\right\|nl^{N+1}\alpha SL\rangle\,[S'',L'']\\
&\times(-1)^{3S'+L'+2S_1'+3S''+L_1''+l+l_0+3/2}\,[S_1'',L_1'']^{1/2}\begin{Bmatrix}S & S' & \kappa\\ 1/2 & 1/2 & S''\end{Bmatrix}\begin{Bmatrix}L & L' & k\\ l & l_0 & L''\end{Bmatrix}\begin{Bmatrix}S'' & S' & 1/2\\ S_1' & S_1'' & 1/2\end{Bmatrix}\begin{Bmatrix}L'' & L' & l\\ L_1' & L_1'' & l_1\end{Bmatrix}\begin{Bmatrix}l_0 & l_1 & t\\ L_1'' & L & L''\end{Bmatrix}\\
&\times(l\|\mathbf{C}^t\|l)(l_1\|\mathbf{C}^t\|l_0)\sum_{n_0l_0}R^t\,(n_0l_0nl,nln_1l_1)\,\langle n_0l_0|r^{-3}|nl\rangle^{\kappa k}/\Delta E\\
&+\ (N+1)\sqrt{N+1}\,[S,L,S',L']^{1/2}\sum_{\psi''}\left(nl^{N+1}\alpha_1'' S_1'' L_1''\{|nl^N\alpha_1' S_1' L_1'\right)\ [S'',L'',S_1'',L_1'']\begin{Bmatrix}S & S' & \kappa\\ 1/2 & 1/2 & S''\end{Bmatrix}\begin{Bmatrix}L & L' & k\\ l & l_0 & L''\end{Bmatrix}\\
&\times(-1)^{2S+L+3S'+L'+2S_1'+3S''+L''+L_1''+l_0+3/2}\begin{Bmatrix}S'' & S' & 1/2\\ S_1' & S_1'' & 1/2\end{Bmatrix}\begin{Bmatrix}L'' & L' & l\\ L_1' & L_1'' & l_1\end{Bmatrix}\\
&\times\sum_{\bar\alpha\bar S\bar L}\left(nl^{N+1}\alpha SL\{|nl^N\bar\alpha\bar S\bar L\right)\left(nl^{N+1}\alpha_1'' S_1'' L_1''\{|nl^N\bar\alpha\bar S\bar L\right)\begin{Bmatrix}1/2 & \bar S & S\\ 1/2 & S'' & S_1''\end{Bmatrix}\begin{Bmatrix}\bar L & l & L\\ l & t & l_0\\ L_1'' & l_1 & L''\end{Bmatrix}\\
&\times(l_1\|\mathbf{C}^t\|l)(l\|\mathbf{C}^t\|l_0)\sum_{n_0l_0}R^t\,(n_0l_0nl,n_1l_1nl)\,\langle n_0l_0|r^{-3}|nl\rangle^{\kappa k}/\Delta E. \qquad (54)
\end{aligned}
$$

The second component is as follows:

$$
\begin{aligned}
&-\sum_{\psi''}\langle\psi\|\mathbf{T}^{(\kappa\mathbf{k})\mathbf{K}}\|\psi''\rangle\times\langle\psi''|\mathbf{G}|\psi'\rangle/\Delta E=\\
&\sqrt{N+1}\,[S,L,S',L']^{1/2}\sum_{\psi''}\delta(\alpha_1'' S_1'' L_1'',\alpha SL)\ (-1)^{S'+L'+L_1'+3S''+L''+L+l+l_0+1/2}\,[S'',L'']\begin{Bmatrix}S & S' & \kappa\\ 1/2 & 1/2 & S''\end{Bmatrix}\\
&\times\begin{Bmatrix}L & L' & k\\ l_0 & l_1 & L''\end{Bmatrix}\begin{Bmatrix}1/2 & S' & S_1'\\ 1/2 & S & S''\end{Bmatrix}\begin{Bmatrix}l_1 & L' & L_1'\\ l_0 & L & L''\end{Bmatrix}\sum_{\bar\alpha\bar S\bar L}\delta(\bar S,S_1')\left(nl^{N+1}\alpha SL\{|nl^N\bar\alpha\bar S\bar L\right)\left\langle nl^N\bar\alpha\bar S\bar L\left\|\mathbf{U}^t\right\|nl^N\alpha_1' S_1' L_1'\right\rangle\\
&\times\begin{Bmatrix}\bar L & t & L_1'\\ l_0 & L & l\end{Bmatrix}(l\|\mathbf{C}^t\|l_0)(l\|\mathbf{C}^t\|l)\sum_{n_0l_0}R^t\,(nlnl,nln_0l_0)\,\langle n_0l_0|r^{-3}|n_1l_1\rangle^{\kappa k}/\Delta E. \qquad (55)
\end{aligned}
$$

5.6.4 Configuration interaction $nl^{N+1}\leftrightarrow nl^{N-1}n_1l_1^2$

The states ψ for nl^{N+1} configuration and ψ' for $nl^{N-1}n_1l_1^2$ configuration are defined as follows:

$$
\begin{aligned}
&\psi=n_0l_0^{4l_0+2}\ {}^1S, nl^{N+1}\ \alpha SL; SL,\\
&\psi'=n_0l_0^{4l_0+2}\ {}^1S, nl^{N-1}\ \alpha_1' S_1' L_1', n_1l_1^2\ \alpha_2' S_2' L_2'; S' L'.
\end{aligned}
$$

5.6.5 Excitation of one electron from a closed $n_0 l_0^{4l_0+2}$ shell into an open nl^{N-1}

In this case the perturbing virtual states are defined as $\psi'' = (n_0 l_0^{4l_0+1}\ ^2l_0, nl^N \alpha_1'' S_1'' L_1'')S''L'', n_1 l_1^2\ \alpha_2'' S_2'' L_2''; S'''L'''$.

For the considered excitation the second term of the sum below is equal to zero due to the spin-orbit or hyperfine interaction:

$$
\begin{aligned}
&-\sum_{\psi''\neq\psi,\psi'}\Big[\langle n_0 l_0^{4l_0+2}\ ^1S, nl^{N+1}\ \alpha SL; SL|\mathbf{G}|(n_0 l_0^{4l_0+1}\ ^2l_0, nl^N\alpha_1'' S_1'' L_1'')S''L'', n_1 l_1^2\ \alpha_2'' S_2'' L_2''; SL\rangle\\
&\times\langle n_0 l_0^{4l_0+1}\ ^2l_0, nl^N\alpha_1'' S_1'' L_1'')S''L'', n_1 l_1^2\ \alpha_2'' S_2'' L_2''; SL\|\mathbf{T}^{(\kappa\mathbf{k})\mathbf{K}}\|n_0 l_0^{4l_0+2}\ ^1S, nl^{N-1}\ \alpha_1' S_1' L_1', n_1 l_1^2\ \alpha_2' S_2' L_2'; S'L'\rangle\\
&+\langle n_0 l_0^{4l_0+2}\ ^1S, nl^{N+1}\ \alpha SL; SL\|\mathbf{T}^{(\kappa\mathbf{k})\mathbf{K}}\|(n_0 l_0^{4l_0+1}\ ^2l_0, nl^N\alpha_1'' S_1'' L_1'')S''L'', n_1 l_1^2\ \alpha_2'' S_2'' L_2''; S'L'\rangle\\
&\times\langle(n_0 l_0^{4l_0+1}\ ^2l_0, nl^N\alpha_1'' S_1'' L_1'')S''L'', n_1 l_1^2\ \alpha_2'' S_2'' L_2''; S'L'|\mathbf{G}|n_0 l_0^{4l_0+2}\ ^1S, nl^{N-1}\ \alpha_1' S_1' L_1', n_1 l_1^2\ \alpha_2' S_2' L_2'; S'L'\rangle\Big]/\Delta E. \quad (56)
\end{aligned}
$$

The first component is as follows:

$$
\begin{aligned}
&-\sum_{\psi''}\langle\psi|\mathbf{G}|\psi''\rangle\times\langle\psi''\|\mathbf{T}^{(\kappa\mathbf{k})\mathbf{K}}\|\psi'\rangle/\Delta E =\\
&\sqrt{2(N+1)N}\ [S,L,S',L']^{1/2}\sum_{\psi''}\delta(\alpha_2' S_2' L_2', \alpha_2'' S_2'' L_2'')\left(nl^{N+1}\ \alpha SL\{|nl^N\alpha_1'' S_1'' L_1''\right)\left(nl^N\alpha_1'' S_1'' L_1''\{|nl^{N-1}\alpha_1' S_1' L_1'\right)\\
&\times(-1)^{S+L+S'+L'+3S_1'+L_1'+2S''+3S_1''+L_1''+L_2''+\kappa+k+l_1+1/2}\ [S'',L'']\ [S_1'',L_1'',S_2'',L_2'']^{1/2}\begin{Bmatrix} S & S' & \kappa\\ S_1' & S'' & S_2'\end{Bmatrix}\begin{Bmatrix} L & L' & k\\ L_1' & L'' & L_2'\end{Bmatrix}\\
&\times\begin{Bmatrix} S'' & S_1' & \kappa\\ 1/2 & 1/2 & S_1''\end{Bmatrix}\begin{Bmatrix} L'' & L_1' & k\\ l & l_0 & L_1''\end{Bmatrix}\begin{Bmatrix} S_1'' & 1/2 & S\\ S_2'' & S'' & 1/2\end{Bmatrix}\begin{Bmatrix} L_1'' & l & L\\ L_2'' & L'' & l_0\end{Bmatrix}\begin{Bmatrix} l_1 & l_0 & t\\ l & l_1 & L_2''\end{Bmatrix}\\
&\times(l_1\|\mathbf{C}^t\|l_0)(l_1\|\mathbf{C}^t\|l)\sum_{n_0 l_0}R^t\left(n_1 l_1 n_1 l_1, n_0 l_0 nl\right)\langle n_0 l_0|r^{-3}|nl\rangle^{\kappa k}/\Delta E. \qquad (57)
\end{aligned}
$$

5.6.6 Configuration interaction $nl^{N+1}n_1 l_1^{N_1-1} \leftrightarrow nl^N n_1 l_1^{N_1}$

The states ψ for $nl^{N+1}n_1 l_1^{N_1-1}$ configuration and ψ' for $nl^N n_1 l_1^{N_1}$ configuration are defined as follows:

$$
\begin{aligned}
&\psi = n_0 l_0^{4l_0+2}\ ^1S, nl^{N+1}\alpha_1 S_1 L_1, n_1 l_1^{N_1-1}\ \alpha_2 S_2 L_2; SL,\\
&\psi' = n_0 l_0^{4l_0+2}\ ^1S, nl^N\alpha_1' S_1' L_1', n_1 l_1^{N_1}\alpha_2' S_2' L_2'; S'L'.
\end{aligned}
$$

5.6.7 Excitation of one electron from a closed $n_0 l_0^{4l_0+2}$ shell into an open nl^{N+1}

In this case the perturbing virtual states are defined as $\psi'' = (n_0 l_0^{4l_0+1}\ ^2l_0, nl^{N+2}\ \alpha_1'' S_1'' L_1'')S''L'', n_1 l_1^{N_1-1}\ \alpha_2'' S_2'' L_2''; S'''L'''$.

For the considered excitation the first term of the sum below is equal to zero due to the spin-orbit or hyperfine interaction:

$$
\begin{aligned}
&-\sum_{\psi''\neq\psi,\psi'}[\langle n_0 l_0^{4l_0+2}\ ^1S, nl^{N+1}\alpha_1 S_1 L_1, n_1 l_1^{N_1-1}\alpha_2 S_2 L_2; SL|\mathbf{G}|(n_0 l_0^{4l_0+1}\ ^2l_0, nl^{N+2}\ \alpha_1'' S_1'' L_1'')S''L'', n_1 l_1^{N_1-1}\alpha_2'' S_2'' L_2''; SL\rangle\\
&\times\langle(n_0 l_0^{4l_0+1}\ ^2l_0, nl^{N+2}\ \alpha_1'' S_1'' L_1'')S''L'', n_1 l_1^{N_1-1}\alpha_2'' S_2'' L_2''; SL\|\mathbf{T}^{(\kappa\mathbf{k})\mathbf{K}}\|n_0 l_0^{4l_0+2}\ ^1S, nl^N\alpha_1' S_1' L_1', n_1 l_1^{N_1}\alpha_2' S_2' L_2'; S'L'\rangle\\
&+\langle n_0 l_0^{4l_0+2}\ ^1S, nl^{N+1}\alpha_1 S_1 L_1, n_1 l_1^{N_1-1}\ \alpha_2 S_2 L_2; SL\|\mathbf{T}^{(\kappa\mathbf{k})\mathbf{K}}\|(n_0 l_0^{4l_0+1}\ ^2l_0, nl^{N+2}\alpha_1'' S_1'' L_1'')S''L'', n_1 l_1^{N_1-1}\alpha_2'' S_2'' L_2''; S'L'\rangle\\
&\times\langle(n_0 l_0^{4l_0+1}\ ^2l_0, nl^{N+2}\alpha_1'' S_1'' L_1'')S''L'', n_1 l_1^{N_1-1}\alpha_2'' S_2'' L_2''; S'L'|\mathbf{G}|n_0 l_0^{4l_0+2}\ ^1S, nl^N\alpha_1' S_1' L_1', n_1 l_1^{N_1}\alpha_2' S_2' L_2'; S'L'\rangle]/\Delta E. \qquad (58)
\end{aligned}
$$

The second component is as follows:

$$
\begin{aligned}
&-\sum_{\psi''}\langle\psi\|\mathbf{T}^{(\kappa\mathbf{k})\mathbf{K}}\|\psi''\rangle\times\langle\psi''|\mathbf{G}|\psi'\rangle/\Delta E =\\
&(N+2)\sqrt{(N+1)N_1}\ [S,L,S',L',S_2',L_2']^{1/2}\ \left(n_1 l_1^{N_1}\alpha_2' S_2' L_2'\{|n_1 l_1^{N_1-1}\alpha_2 S_2 L_2\right)
\end{aligned}
$$

$$\times \sum_{\psi''} \delta(\alpha_2 S_2 L_2, \alpha_2'' S_2'' L_2'')\ (-1)^{3S_1+L_1+3S_2+L_2+2S'+2S_1'+3S_2'+L_2'+S''+L''+N_1+l+\kappa+k+3/2}\ [S'', L'', S_1'', L_1'']$$
$$\times \left(nl^{N+2}\alpha_1'' S_1'' L_1''\{|nl^{N+1}\alpha_1 S_1 L_1\right) \begin{Bmatrix} S & S' & \kappa \\ S'' & S_1 & S_2 \end{Bmatrix} \begin{Bmatrix} L & L' & k \\ L'' & L_1 & L_2 \end{Bmatrix} \begin{Bmatrix} S_1 & S'' & \kappa \\ 1/2 & 1/2 & S_1'' \end{Bmatrix} \begin{Bmatrix} L_1 & L'' & k \\ l_0 & l & L_1'' \end{Bmatrix} \begin{Bmatrix} S_2 & S' & S'' \\ S_1' & 1/2 & S_2' \end{Bmatrix} \begin{Bmatrix} L_2 & L' & L'' \\ L_1' & l_1 & L_2' \end{Bmatrix}$$
$$\times \sum_{\hat{\alpha}\hat{S}\hat{L}} (-1)^{\hat{S}}\ [\hat{S}, \hat{L}]^{1/2} \left(nl^{N+2}\alpha_1'' S_1'' L_1''\{|nl^N \alpha_1' S_1' L_1', nl^2 \hat{\alpha}\hat{S}\hat{L}\right) \begin{Bmatrix} \hat{S} & 1/2 & 1/2 \\ S'' & S_1' & S_1'' \end{Bmatrix} \begin{Bmatrix} \hat{L} & l_0 & l_1 \\ L'' & L_1' & L_1'' \end{Bmatrix} \begin{Bmatrix} l & l_0 & t \\ l_1 & l & \hat{L} \end{Bmatrix}$$
$$\times (l\|\mathbf{C}^t\|l_0)(l\|\mathbf{C}^t\|l_1) \sum_{n_0 l_0} R^t\,(nlnl, n_0 l_0 n_1 l_1)\,\langle n_0 l_0|r^{-3}|nl\rangle^{\kappa k}/\Delta E. \tag{59}$$

5.6.8 Excitation of one electron from a closed $n_0 l_0^{4l_0+2}$ shell into an open $n_1 l_1^{N_1-1}$ shell

In this case the perturbing virtual states are defined as $\psi'' = (n_0 l_0^{4l_0+1}\ ^2 l_0, nl^{N+1}\alpha_1'' S_1'' L_1'')S''L'', n_1 l_1^{N_1}\ \alpha_2'' S_2'' L_2''; S'''L'''$.

For the considered excitation two components of the sum below give different contributions to the spin-orbit or hyperfine interaction:

$$-\sum_{\psi''\neq\psi,\psi'} [\langle n_0 l_0^{4l_0+2}\ ^1 S, nl^{N+1}\alpha_1 S_1 L_1, n_1 l_1^{N_1-1}\alpha_2 S_2 L_2; SL|\mathbf{G}|(n_0 l_0^{4l_0+1}\ ^2 l_0, nl^{N+1}\alpha_1'' S_1'' L_1'')S''L'', n_1 l_1^{N_1}\ \alpha_2'' S_2'' L_2''; SL\rangle$$
$$\times \langle (n_0 l_0^{4l_0+1}\ ^2 l_0, nl^{N+1}\alpha_1'' S_1'' L_1'')S''L'', n_1 l_1^{N_1}\ \alpha_2'' S_2'' L_2''; SL\|\mathbf{T}^{(\kappa\mathbf{k})\mathbf{K}}\|n_0 l_0^{4l_0+2}\ ^1 S, nl^N \alpha_1' S_1' L_1', n_1 l_1^{N_1}\alpha_2' S_2' L_2'; S'L'\rangle$$
$$+ \langle n_0 l_0^{4l_0+2}\ ^1 S, nl^{N+1}\alpha_1 S_1 L_1, n_1 l_1^{N_1-1}\ \alpha_2 S_2 L_2; SL\|\mathbf{T}^{(\kappa\mathbf{k})\mathbf{K}}\|(n_0 l_0^{4l_0+1}\ ^2 l_0, nl^{N+1}\alpha_1'' S_1'' L_1'')S''L'', n_1 l_1^{N_1}\ \alpha_2'' S_2'' L_2''; S'L'\rangle$$
$$\times \langle (n_0 l_0^{4l_0+1}\ ^2 l_0, nl^{N+1}\alpha_1'' S_1'' L_1'')S''L'', n_1 l_1^{N_1}\ \alpha_2'' S_2'' L_2''; S'L'|\mathbf{G}|n_0 l_0^{4l_0+2}\ ^1 S, nl^N \alpha_1' S_1' L_1', n_1 l_1^{N_1}\alpha_2' S_2' L_2'; S'L'\rangle]/\Delta E. \tag{60}$$

The first component is as follows:

$$-\sum_{\psi''} \langle\psi|\mathbf{G}|\psi''\rangle \times \langle\psi''\|\mathbf{T}^{(\kappa\mathbf{k})\mathbf{K}}\|\psi'\rangle/\Delta E =$$
$$\sqrt{(N+1)N_1}\ [S, L, S', L', S_2', L_2']^{1/2}\ \left(n_1 l_1^{N_1}\alpha_2' S_2' L_2'\{|n_1 l_1^{N_1-1}\alpha_2 S_2 L_2\right)$$
$$\times \sum_{\psi''} \delta(S_1'', S_1)\ \delta(\alpha_2'' S_2'' L_2'', \alpha_2' S_2' L_2')\ (-1)^{2S+S_1+2S_2+3S_1'+L_1'+L''+\kappa+k+N_1+1/2}\ [S'', L'']\ [S_1'', L_1'']^{1/2}$$
$$\times \left(nl^{N+1}\alpha_1'' S_1'' L_1''\{|nl^N \alpha_1' S_1' L_1'\right) \langle nl^{N+1}\alpha_1'' S_1'' L_1''\ \|\mathbf{U}^t\|\ nl^{N+1}\alpha_1 S_1 L_1\rangle \begin{Bmatrix} S' & S & \kappa \\ S'' & S_1' & S_2' \end{Bmatrix} \begin{Bmatrix} L' & L & k \\ L'' & L_1' & L_2' \end{Bmatrix}$$
$$\times \begin{Bmatrix} S'' & S_1' & \kappa \\ 1/2 & 1/2 & S_1 \end{Bmatrix} \begin{Bmatrix} L'' & L_1' & k \\ l & l_0 & L_1'' \end{Bmatrix} \begin{Bmatrix} S_2 & S & S_1 \\ S'' & 1/2 & S_2' \end{Bmatrix} \begin{Bmatrix} L_2 & L & L_1 \\ L'' & l_1 & L_2' \end{Bmatrix} \begin{Bmatrix} l_0 & L_1'' & L'' \\ L_1 & l_1 & t \end{Bmatrix}$$
$$\times (l\|\mathbf{C}^t\|l)(l_1\|\mathbf{C}^t\|l_0) \sum_{n_0 l_0} R^t\,(n_0 l_0 nl, nln_1 l_1)\,\langle n_0 l_0|r^{-3}|nl\rangle^{\kappa k}/\Delta E$$
$$+\ (N+1)\sqrt{(N+1)N_1}\ [S, L, S', L', S_1, L_1, S_2', L_2']^{1/2}\ \left(n_1 l_1^{N_1}\alpha_2' S_2' L_2'\{|n_1 l_1^{N_1-1}\alpha_2 S_2 L_2\right)$$
$$\times \sum_{\psi''} \delta(\alpha_2'' S_2'' L_2'', \alpha_2' S_2' L_2') \left(nl^{N+1}\alpha_1'' S_1'' L_1''\{|nl^N \alpha_1' S_1' L_1'\right)\ [L'', S_1'', L_1'']\ \begin{Bmatrix} L' & L & k \\ L'' & L_1' & L_2' \end{Bmatrix} \begin{Bmatrix} L'' & L_1' & k \\ l & l_0 & L_1'' \end{Bmatrix} \begin{Bmatrix} L_2 & L & L_1 \\ L'' & l_1 & L_2' \end{Bmatrix}$$
$$\times \sum_{\bar{\alpha}\bar{S}\bar{L}} \delta(S'', \bar{S})\,(-1)^{2S_1+L_1+2S_2+2S+3S_1'+L_1'+2\bar{S}+S_1''+N_1+\kappa+k+l+1/2} \left(nl^{N+1}\alpha_1 S_1 L_1\{|nl^N \bar{\alpha}\bar{S}\bar{L}\right)\left(nl^{N+1}\alpha_1'' S_1'' L_1''\{|nl^N \bar{\alpha}\bar{S}\bar{L}\right)$$
$$\times \begin{Bmatrix} S' & S & \kappa \\ \bar{S} & S_1' & S_2' \end{Bmatrix} \begin{Bmatrix} \bar{S} & S_1' & \kappa \\ 1/2 & 1/2 & S_1'' \end{Bmatrix} \begin{Bmatrix} S_2 & S & S_1 \\ \bar{S} & 1/2 & S_2' \end{Bmatrix} \begin{Bmatrix} \bar{L} & l & L_1 \\ l_1 & L'' & t \end{Bmatrix} \begin{Bmatrix} l & t & l_0 \\ L'' & L_1'' & \bar{L} \end{Bmatrix}$$
$$\times (l_1\|\mathbf{C}^t\|l)(l\|\mathbf{C}^t\|l_0) \sum_{n_0 l_0} R^t\,(n_0 l_0 nl, n_1 l_1 nl)\,\langle n_0 l_0|r^{-3}|nl\rangle^{\kappa k}/\Delta E. \tag{61}$$

The second component is as follows:

$$-\sum_{\psi''} \langle\psi\|\mathbf{T}^{(\kappa\mathbf{k})\mathbf{K}}\|\psi''\rangle \times \langle\psi''|\mathbf{G}|\psi'\rangle/\Delta E =$$

$$N\sqrt{(N+1)N_1}\ [S,L,S',L']^{1/2}\ [S_1,L_1,S_1',L_1',S_2',L_2']^{1/2}\ \left(n_1l_1^{N_1}\alpha_2'S_2'L_2'\{|n_1l_1^{N_1-1}\alpha_2S_2L_2\right)$$
$$\times\sum_{\psi''}\delta(\alpha_1''S_1''L_1'',\alpha_1S_1L_1)\ \delta(\alpha_2''S_2''L_2'',\alpha_2'S_2'L_2')\ \delta(S''L'',S_1'L_1')\ \begin{Bmatrix}S_1' & S_2' & S'\\ 1/2 & 1/2 & \kappa\\ S_1 & S_2 & S\end{Bmatrix}\begin{Bmatrix}L_1' & L_2' & L'\\ l_0 & l_1 & k\\ L_1 & L_2 & L\end{Bmatrix}$$
$$\times\sum_{\bar\alpha\bar S\bar L,\hat\alpha\hat S\hat L}(-1)^{\bar S+\bar L+\hat L+S+L+S'+L'+S_1+L_1+S_2+L_2+2S_1'+S_2'+L_2'+N_1+l_0+1/2}\ [\hat S,\hat L]^{1/2}$$
$$\times\left(nl^N\alpha_1'S_1'L_1'\{|nl^{N-1}\bar\alpha\bar S\bar L\right)\left(nl^{N+1}\alpha_1S_1L_1\{|nl^{N-1}\bar\alpha\bar S\bar L,nl^2\hat\alpha\hat S\hat L\right)\begin{Bmatrix}\hat S & 1/2 & 1/2\\ S_1' & \bar S & S_1\end{Bmatrix}\begin{Bmatrix}\hat L & l_0 & l\\ L_1' & \bar L & L_1\end{Bmatrix}\begin{Bmatrix}l & l & t\\ l_0 & l & \hat L\end{Bmatrix}$$
$$\times(l\|\mathbf{C}^t\|l_0)(l\|\mathbf{C}^t\|l)\sum_{n_0l_0}R^t\left(nlnl,nln_0l_0\right)\langle n_0l_0|r^{-3}|n_1l_1\rangle^{\kappa k}/\Delta E. \tag{62}$$

5.6.9 Configuration interaction $nl^{N-1}n_1l_1 \leftrightarrow nl^{N-2}n_2l_2n_1l_1$

The states ψ for $nl^{N-1}n_1l_1$ configuration and ψ' for $nl^{N-2}n_2l_2n_1l_1$ configuration are defined as follows:

$$\psi = n_0l_0^{4l_0+2}\ {}^1S,(nl^{N-1}\alpha_1S_1L_1,n_1l_1)SL;SL,$$
$$\psi' = (n_0l_0^{4l_0+2}\ {}^1S,nl^{N-2}\alpha_1'S_1'L_1')\alpha_1'S_1'L_1',(n_2l_2n_1l_1)S_2'L_2';S'L'.$$

For the excitation of an electron from a closed $n_0l_0^{4l_0+2}$ shell into an open nl^{N-1} shell the perturbing virtual states are defined as $\psi'' = n_0l_0^{4l_0+1}\ {}^2l_0,(nl^N\alpha_1''S_1''L_1'',n_1l_1)S''L'';S'''L'''$.

In this case the first term of the sum below is equal to zero due to the spin-orbit or hyperfine interaction:

$$-\sum_{\psi''\neq\psi,\psi'}\left[\langle\psi|\mathbf{G}|\psi''\rangle\times\langle\psi''\|\mathbf{T}^{(\kappa\mathbf{k})\mathbf{K}}\|\psi'\rangle+\langle\psi\|\mathbf{T}^{(\kappa\mathbf{k})\mathbf{K}}\|\psi''\rangle\times\langle\psi''|\mathbf{G}|\psi'\rangle\right]/\Delta E. \tag{63}$$

The second component is as follows:

$$-\sum_{\psi''}\left\langle\psi\|\mathbf{T}^{(\kappa\mathbf{k})\mathbf{K}}\|\psi''\right\rangle\times\langle\psi''|\mathbf{G}|\psi'\rangle/\Delta E=$$
$$N\sqrt{N-1}\ [S,L,S',L',S_2',L_2']^{1/2}\sum_{\psi''}(-1)^{S+L+S_1'+L_1'+S_2'+L_2'+2S_1''+l_0+l+\kappa+k+1}\ [S'',L'',S_1'',L_1'']$$
$$\times\left(nl^N\alpha_1''S_1''L_1''\{|nl^{N-1}\alpha_1S_1L_1\right)\begin{Bmatrix}1/2 & S_1 & S_1''\\ 1/2 & S'' & S\end{Bmatrix}\begin{Bmatrix}l & L_1 & L_1''\\ l_1 & L'' & L\end{Bmatrix}\begin{Bmatrix}S & S' & \kappa\\ 1/2 & 1/2 & S''\end{Bmatrix}\begin{Bmatrix}L & L' & k\\ l_0 & l & L''\end{Bmatrix}$$
$$\times\sum_{\hat\alpha'\hat S'\hat L'}(-1)^{\hat L'}\ [\hat S',\hat L']^{1/2}\left(nl^N\alpha_1''S_1''L_1''\{|nl^{N-2}\alpha_1'S_1'L_1',nl^2\hat\alpha'\hat S'\hat L'\right)\begin{Bmatrix}\hat S' & 1/2 & 1/2\\ S_1' & S_2' & S'\\ S_1'' & 1/2 & S''\end{Bmatrix}\begin{Bmatrix}\hat L' & l_2 & l_0\\ L_1' & L_2' & L'\\ L_1'' & l_1 & L''\end{Bmatrix}\begin{Bmatrix}l & l_0 & t\\ l_2 & l & \hat L'\end{Bmatrix}$$
$$\times(l\|\mathbf{C}^t\|l_0)(l\|\mathbf{C}^t\|l_2)\sum_{n_0l_0}R^t\left(nlnl,n_0l_0n_2l_2\right)\langle n_0l_0|r^{-3}|nl\rangle^{\kappa k}/\Delta E. \tag{64}$$

For the excitation of an electron from a closed $n_0l_0^{4l_0+2}$ shell into an open n_1l_1 shell the perturbing virtual states are defined as $\psi'' = n_0l_0^{4l_0+1}\ {}^2l_0,(nl^{N-1}\alpha_1''S_1''L_1'',n_1l_1^2\alpha_2''S_2''L_2'')S''L'';S'''L'''$.

In this case the first term of the sum below is equal to zero due to the spin-orbit or hyperfine interaction:

$$-\sum_{\psi''\neq\psi,\psi'}\left[\langle\psi|\mathbf{G}|\psi''\rangle\times\langle\psi''\|\mathbf{T}^{(\kappa\mathbf{k})\mathbf{K}}\|\psi'\rangle+\langle\psi\|\mathbf{T}^{(\kappa\mathbf{k})\mathbf{K}}\|\psi''\rangle\times\langle\psi''|\mathbf{G}|\psi'\rangle\right]/\Delta E. \tag{65}$$

The second component is as follows:

$$-\sum_{\psi''}\left\langle\psi\|\mathbf{T}^{(\kappa\mathbf{k})\mathbf{K}}\|\psi''\right\rangle\times\langle\psi''|\mathbf{G}|\psi'\rangle/\Delta E=$$
$$2\sqrt{N-1}\ [S,L,S',L']^{1/2}\ \sum_{\psi''}\delta(\alpha_1S_1L_1,\alpha_1''S_1''L_1'')\ \left(nl^{N-1}\alpha_1''S_1''L_1''\{|nl^{N-2}\alpha_1'S_1'L_1'\right)$$

$$\times [S'', L''] \, [S_1'', L_1'', S_2'', L_2'']^{1/2} \begin{Bmatrix} 1/2 & S'' & S \\ S_1 & 1/2 & S_2'' \end{Bmatrix} \begin{Bmatrix} l_1 & L'' & L \\ L_1 & l_1 & L_2'' \end{Bmatrix} \begin{Bmatrix} S & S' & \kappa \\ 1/2 & 1/2 & S'' \end{Bmatrix} \begin{Bmatrix} L & L' & k \\ l_0 & l_1 & L'' \end{Bmatrix}$$

$$\times \Bigg[\delta(S_2', S_2'') \, (-1)^{S_1+L_1+2S'+L'+S_1''+L_2''+L_2'+2S''+l_0+\kappa+k+1} \, [L_2', L_2'']^{1/2} \begin{Bmatrix} S_2' & S_1' & S' \\ 1/2 & S'' & S_1'' \end{Bmatrix} \begin{Bmatrix} L_2' & L_2'' & t \\ l_1 & l_2 & l_1 \end{Bmatrix} \begin{Bmatrix} L_2' & L_2'' & t \\ L_1' & L_1'' & l \\ L' & L'' & l_0 \end{Bmatrix}$$

$$\times (l_0 \| \mathbf{C}^t \| l)(l_2 \| \mathbf{C}^t \| l_1) \sum_{n_0 l_0} R^t \left(n_0 l_0 n_2 l_2, n l n_1 l_1\right) \langle n_0 l_0 | r^{-3} | n_1 l_1 \rangle^{\kappa k} / \Delta E$$

$$+ (-1)^{S_1+L_1+2S'+L'+3S''+S_1''+S_1'+l_1+\kappa+k+1/2} \, [S_2', L_2', S_2'', L_2'']^{1/2} \begin{Bmatrix} S_1' & 1/2 & S' \\ S_2' & S_1' & 1/2 \end{Bmatrix} \begin{Bmatrix} S_1' & 1/2 & S' \\ 1/2 & S'' & S_2'' \end{Bmatrix} \begin{Bmatrix} l_2 & t & l & L_1'' \\ l_1 & l_1 & L_2'' & L' \\ L_2' & l_0 & L_1' & L'' \end{Bmatrix}$$

$$\times (l_0 \| \mathbf{C}^t \| l_1)(l_2 \| \mathbf{C}^t \| l) \sum_{n_0 l_0} R^t \left(n_0 l_0 n_2 l_2, n_1 l_1 n l\right) \langle n_0 l_0 | r^{-3} | n_1 l_1 \rangle^{\kappa k} / \Delta E \Bigg]. \tag{66}$$

5.6.10 Configuration interaction $nl^{N-1}n_1l_1 \leftrightarrow nl^{N-2}n_1l_1n_2l_2$

The states ψ for $nl^{N-1}n_1l_1$ configuration and ψ' for $nl^{N-2}n_1l_1n_2l_2$ configuration are defined as follows:

$\psi = n_0 l_0^{4l_0+2} \, {}^1S, (nl^{N-1}\alpha_1 S_1 L_1, n_1 l_1) SL; SL,$
$\psi' = (n_0 l_0^{4l_0+2} \, {}^1S, nl^{N-2}\alpha_1' S_1' L_1') \alpha_1' S_1' L_1', (n_1 l_1 n_2 l_2) S_2' L_2'; S' L'.$

Excitation of an electron from a closed $n_0 l_0^{4l_0+2}$ shell into an open nl^{N-1} shell.

By means of proper recoupling procedures the eq. (52) must be multiplied by a phase factor equal to $(-1)^{l_1+l_2+3S_2'+L_2'}$; the perturbing virtual states are defined as $\psi'' = n_0 l_0^{4l_0+1} \, {}^2l_0, (nl^N \alpha_1'' S_1'' L_1'', n_1 l_1) S'' L''; S''' L'''$.

Excitation of an electron from a closed $n_0 l_0^{4l_0+2}$ shell into an open $n_1 l_1$ shell.

By means of proper recoupling procedures the eq. (66) must be multiplied by a phase factor equal to $(-1)^{l_1+l_2+3S_2'+L_2'}$; the perturbing virtual states are defined as
$\psi'' = n_0 l_0^{4l_0+1} \, {}^2l_0, (nl^{N-1}\alpha_1'' S_1'' L_1'', n_1 l_1^2 \alpha_2'' S_2'' L_2'') S'' L''; S''' L'''$.

5.6.11 Configuration interaction $nl^N n_1 l_1 n_2 l_2 \leftrightarrow nl^{N-1} n_1 l_1^2 n_2 l_2$

The states ψ for $nl^N n_1 l_1 n_2 l_2$ configuration and ψ' for $nl^{N-1} n_1 l_1^2 n_2 l_2$ configuration are defined as follows:

$\psi = (n_0 l_0^{4l_0+2} \, {}^1S, nl^N \alpha_1 S_1 L_1) \alpha_1 S_1 L_1, (n_1 l_1 n_2 l_2) S_2 L_2) SL; SL,$
$\psi' = (n_0 l_0^{4l_0+2} \, {}^1S, nl^{N-1} \alpha_1' S_1' L_1') S_1' L_1', (n_1 l_1^2 \alpha_2' S_2' L_2', n_2 l_2) S_3' L_3'; S' L'.$

For the excitation of an electron from a closed $n_0 l_0^{4l_0+2}$ shell into an open nl shell the perturbing virtual states are defined as $\psi'' = (n_0 l_0^{4l_0+1} \, {}^2l_0, nl^{N+1} \alpha_1'' S_1'' L_1'') S'' L'', (n_1 l_1, n_2 l_2) S_2'' L_2''; S''' L'''$.

In this case the first term of the sum below is equal to zero due to the spin-orbit or hyperfine interaction:

$$- \sum_{\psi'' \neq \psi, \psi'} \left[\langle \psi | \mathbf{G} | \psi'' \rangle \times \langle \psi'' \| \mathbf{T}^{(\kappa \mathbf{k}) \mathbf{K}} \| \psi' \rangle + \langle \psi \| \mathbf{T}^{(\kappa \mathbf{k}) \mathbf{K}} \| \psi'' \rangle \times \langle \psi'' | \mathbf{G} | \psi' \rangle \right] / \Delta E. \tag{67}$$

The second component is as follows:

$$- \sum_{\psi''} \langle \psi \| \mathbf{T}^{(\kappa \mathbf{k}) \mathbf{K}} \| \psi'' \rangle \times \langle \psi'' | \mathbf{G} | \psi' \rangle / \Delta E =$$

$$\sqrt{2N} \;\; (N+1) \, [S, L, S', L' S_2', L_2', S_3', L_3',]^{1/2} \sum_{\psi''} \delta(S_2 L_2, S_2'' L_2'') \;\; \left(nl^{N+1} \alpha_1'' S_1'' L_1'' \{ | nl^N \alpha_1 S_1 L_1 \right)$$

$$\times (-1)^{2S+S_1+L_1+2S_1'+S_3'+L_3'+3S''+2S_2''+L''+\kappa+k+l+l_1+l_2+3/2} \, [S'', L'', S_1'', L_1''] \, [S_2'', L_2'']^{1/2}$$

$$\times \begin{Bmatrix} S & S' & \kappa \\ S'' & S_1 & S_2'' \end{Bmatrix} \begin{Bmatrix} L & L' & k \\ L'' & L_1 & L_2'' \end{Bmatrix} \begin{Bmatrix} 1/2 & 1/2 & S_2' \\ 1/2 & S_3' & S_2'' \end{Bmatrix} \begin{Bmatrix} l_1 & l_1 & L_2' \\ l_2 & L_3' & L_2'' \end{Bmatrix} \begin{Bmatrix} S_1' & S_3' & S \\ S_2'' & S'' & 1/2 \end{Bmatrix} \begin{Bmatrix} L_1' & L_3' & L \\ L_2'' & L'' & l_1 \end{Bmatrix} \begin{Bmatrix} S_1'' & S_1 & 1/2 \\ \kappa & 1/2 & S'' \end{Bmatrix} \begin{Bmatrix} L_1'' & L_1 & l \\ k & l_0 & L'' \end{Bmatrix}$$

$$\times \sum_{\hat{\alpha}'\hat{S}'\hat{L}'} (-1)^{\hat{L}'}\ [\hat{S}',\hat{L}']^{1/2} \left(nl^{N+1}\alpha_1''S_1''L_1''\{|nl^{N-1}\alpha_1'S_1'L_1', nl^2\hat{\alpha}'\hat{S}'\hat{L}'\right) \begin{Bmatrix} 1/2 & S'' & S_1'' \\ S_1' & \hat{S}' & 1/2 \end{Bmatrix} \begin{Bmatrix} l_0 & L'' & L_1'' \\ L_1' & \hat{L}' & l_1 \end{Bmatrix}$$
$$\times \begin{Bmatrix} l & l_0 & t' \\ l_1 & l & \hat{L}' \end{Bmatrix} (l\|\mathbf{C}^t\|l_0)(l\|\mathbf{C}^t\|l_1) \sum_{n_0 l_0} R^t\left(nlnl, n_0l_0n_1l_1\right) \langle n_0l_0|r^{-3}|nl\rangle^{\kappa k}/\Delta E. \tag{68}$$

Excitation of an electron from a closed $n_0l_0^{4l_0+2}$ shell into an open n_2l_2 shell.

For the excitation of an electron from a closed $n_0l_0^{4l_0+2}$ shell into an open n_2l_2 shell the perturbing virtual states are defined as $\psi'' = (n_0l_0^{4l_0+1}\ {}^2l_0, nl^N\alpha_1''S_1''L_1'')S''L'', (n_1l_1, n_2l_2^2\alpha_2''S_2''L_2'')S_3''L_3''; S'''L'''$.

In this case the first term of the sum below is equal to zero due to the spin-orbit or hyperfine interaction:

$$-\sum_{\psi''\neq\psi,\psi'} \left[\langle\psi|\mathbf{G}|\psi''\rangle \times \langle\psi''\|\mathbf{T}^{(\kappa\mathbf{k})\mathbf{K}}\|\psi'\rangle + \langle\psi\|\mathbf{T}^{(\kappa\mathbf{k})\mathbf{K}}\|\psi''\rangle \times \langle\psi''|\mathbf{G}|\psi'\rangle\right]/\Delta E. \tag{69}$$

The second component is as follows:

$$-\sum_{\psi''}\langle\psi\|\mathbf{T}^{(\kappa\mathbf{k})\mathbf{K}}\|\psi''\rangle \times \langle\psi''|\mathbf{G}|\psi'\rangle/\Delta E =$$
$$2\sqrt{2N}\ \ [S,L,S',L',S_2,L_2,S_2',L_2']^{1/2} \sum_{\psi''} \delta(\alpha_1S_1L_1,\alpha_1''S_1''L_1'')\ [S_2'',L_2'']\ [S'',L'',S_1'',L_1'',S_3'',L_3'']^{1/2}$$
$$\times \left(nl^N\alpha_1''S_1''L_1''\{|nl^{N-1}\alpha_1'S_1'L_1'\right)\ \begin{Bmatrix} 1/2 & S_3'' & S_2 \\ 1/2 & 1/2 & S_2'' \end{Bmatrix} \begin{Bmatrix} l_2 & L_3'' & L_2 \\ l_1 & l_2 & L_2'' \end{Bmatrix} \begin{Bmatrix} 1/2 & 1/2 & \kappa \\ S_2 & S_1 & S \\ S_3'' & S'' & S' \end{Bmatrix} \begin{Bmatrix} l_2 & l_0 & k \\ L_2 & L_1 & L \\ L_3'' & L'' & L' \end{Bmatrix}$$
$$\times \Bigg[\delta(S_1',S'')\ \delta(S_3',S_3'')\ (-1)^{S+L+S_1+L_1+2S_1'+S_2'+S_2''+3S'+3S_3'+S''+L''+L_1''+S_3''+\kappa+k+l_0+l_2+1/2}\ \frac{[L'',L_3'',L_3']^{1/2}}{[S_1']^{1/2}}$$
$$\times \begin{Bmatrix} 1/2 & 1/2 & S_2'' \\ S_3' & 1/2 & S_2' \end{Bmatrix} \begin{Bmatrix} L_1' & L_1'' & l \\ l_0 & t & L'' \end{Bmatrix} \begin{Bmatrix} L' & L'' & L_3'' \\ t & L_3' & L_1' \end{Bmatrix} \begin{Bmatrix} l_2 & l_1 & t \\ l_2 & L_2' & L_3' \\ L_2'' & l_1 & L_3'' \end{Bmatrix}$$
$$\times (l_0\|\mathbf{C}^t\|l)(l_1\|\mathbf{C}^t\|l_2) \sum_{n_0l_0} R^t\left(n_0l_0n_1l_1, nln_2l_2\right) \langle n_0l_0|r^{-3}|n_2l_2\rangle^{\kappa k}/\Delta E$$
$$+ (-1)^{S+L+S_1+L_1+L'+3S''+2S_1'+S_2'+S_1''+S_2''+2S_3''+L_3''+L_1'+L_3'+\kappa+k+l_1+l_2+3/2}\ [S_3',L_3',S'',L'',S_2'',L_2'',S_3'',L_3'']^{1/2}$$
$$\times \begin{Bmatrix} S_2' & 1/2 & S_3' & S' \\ 1/2 & S_2'' & S_3'' & S_1'' \\ 1/2 & 1/2 & S_1' & S'' \end{Bmatrix} \sum_{\lambda=|L_3'-l_0|,\ldots,L_3'+l_0} (-1)^{\lambda}\ [\lambda] \begin{Bmatrix} \lambda & l_0 & L_3' \\ l & L_1'' & L_1' \\ L_3'' & L'' & L' \end{Bmatrix} \begin{Bmatrix} l_1 & L_2' & l_1 & t \\ L_2'' & l_2 & l_2 & \lambda \\ L_3'' & L_3' & l & l_0 \end{Bmatrix}$$
$$\times (l_0\|\mathbf{C}^t\|l_2)(l_1\|\mathbf{C}^t\|l) \sum_{n_0l_0} R^t\left(n_0l_0n_1l_1, n_2l_2nl\right) \langle n_0l_0|r^{-3}|n_2l_2\rangle^{\kappa k}/\Delta E\Bigg]. \tag{70}$$

6 Results

This approach was first used for the analysis of the configuration system $(5d+6s)^3$ of the lanthanum atom [33], then it was applied to the atomic structure of the tantalum atom [40], the scandium ion [41], the titanium ion [42] and the niobium atom [43]. Recently, we reported how to detect the isomeric state $I = (3/2)^+$ in ^{229}Th by means of a laser induced fluorescence method [44] and our semi-empirical calculations. Now, as a result of our studies on the structure of complex atoms, we produced high-quality wave functions for both even and odd systems of configurations of Sr I. These wave functions were used for the parametrization of oscillator strengths for electric-dipole transitions [45].

Due to the availability of new experimental data, we conducted a re-analysis of the lanthanum $(5d+6s)^3$ system. In the fine structure least-squares fit, including all 37 known experimental energy levels, 21 independent parameters were used. The mean difference between the experimental and calculated energies amounts to 21 cm^{-1}. The least-squares fit for the hyperfine structure was performed with 37 A constants and 19 B constants, respectively. Using 13 free

parameters for the A constants and 10 free parameters for the B constants, a mean deviation of 16 MHz and 0.46 MHz was achieved, respectively.

The results of the semi-empirical fine and hyperfine structure analysis for La I are shown in table 1. In the first two columns the values of experimental and calculated level energies are listed, respectively. In the following four columns the strongest and second strongest fine-structure components with the corresponding percentages are presented. In columns seven and eight, the calculated g_J values are compared with the experimental ones. The experimental hyperfine constants A and B are listed together with their experimental uncertainty in columns nine and eleven. The calculated A and B constants for all levels are listed in columns ten and twelve.

A very good agreement between all the calculated and experimental values is noticeable, which confirms the correctness of wave functions obtained.

The values of the spin-orbit, electrostatically correlated spin-orbit and hyperfine-structure radial parameters are presented in table 2.

7 Conclusions

The structure of a complex atom can be fully described if the precise eigenfunctions describing the electronic states are known. The knowledge of these functions allowed us to determine the eigenvalues (observables). Our effort focused on calculating these functions using only the experimental values of the electronic levels. The correctness of the wave functions can be verified by means of the analysis of the hyperfine structure and comparison of experimental and calculated g_J factors.

It should be strongly emphasised that the value of the energy levels of fine-structure or hyperfine-structure sublevels is the sum of all possible electromagnetic interactions appearing in the atom. We showed that it is possible to determine quantitatively and precisely the contributions of particular interactions, and provide the exact definition of the evaluated parameters describing the interactions in the atom.

As a result of our semi-empirical approach, we will be able to predict the positions of new energy levels and determine the intermediate coupling wave functions, which is necessary to understand the strength of the transitions or the observed hyperfine-structure splittings. Our analyses clearly demonstrate that calculating the precise wave functions is impossible without the contribution from electrostatic coupling with distance configurations.

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Table 1. Comparison of the experimental and calculated energy values (cm^{-1}) and hfs A and B constants (MHz) for the model space $(5d+6s)^3$ of La I.

E_{exp}	E_{calc}	%	Main comp.	%	Sec. comp.	$g_{J_{calc}}$	$g_{J_{exp}}$	A$_{exp}$	A_{calc}	B$_{exp}$	B_{calc}
$J = 1/2$											
7231.407	7242	98.70	$5d^2(^3P)6s\ ^4P$	0.79	$5d^2(^1S)6s\ ^2$S	2.655	2.653	2460.229 (70)	2438		
9044.214	9039	68.84	$5d^2(^3P)6s\ ^2P$	30.23	$5d^3\ ^2P$	0.683	0.690	226.837 (4)	234		
16617.300	16620	97.21	$5d^3\ ^4P$	1.35	$5d^2(^1S)6s\ ^2S$	2.633		−696.6 (7.1)	−724		
16991.420	16991	96.69	$5d^2(^1S)6s\ ^2S$	1.58	$5d^3\ ^4P$	2.004		4115.0 (5.0)	4121		
20392.600	20421	67.89	$5d^3\ ^2P$	30.09	$5d^2(^3P)6s\ ^2P$	0.700	0.709	258.9 (3.0)	254		
$J = 3/2$											
0.000	13	84.66	$5d\ 6s^2\ ^2D$	12.67	$5d^2(^1D)6s\ ^2D$	0.797	0.798	141.1961(16)	143.420	44.776 (14)	44.660
2668.188	2653	98.28	$5d^2(^3F)6s\ ^4F$	1.28	$5d\ 6s^2\ ^2D$	0.406	0.404	−480.208 (2)	−509.073	13.983 (17)	14.218
7490.521	7485	96.97	$5d^2(^3P)6s\ ^4P$	2.30	$5d^2(^1D)6s\ ^2D$	1.707	1.704	929.666 (5)	929.087	37.066 (30)	36.281
8446.044	8452	59.72	$5d^2(^1D)6s\ ^2D$	15.86	$5d^2(^3P)6s\ ^2P$	0.934	0.936	−422.419 (5)	−422.253	−6.964 (30)	−6.739
9719.439	9724	52.52	$5d^2(^3P)6s\ ^2P$	24.78	$5d^3\ ^2P$	1.224	1.220	−655.208 (5)	−640.915	−31.841 (30)	−31.674
12430.609	12422	98.06	$5d^3\ ^4F$	0.94	$5d^3\ ^2D$	0.407	0.411	445.098 (5)	419.980	−16.240 (30)	−16.250
16735.140	16729	93.77	$5d^3\ ^4P$	2.04	$5d^2(^3P)6s\ ^2P$	1.695	1.698	−259.4 (2.1)	−238.529		−30.844
18037.640	18055	57.76	$5d^3\ ^2D$	26.73	$5d^3\ ^2D$	0.852		227.1 (7.0)	213.068		−36.083
21037.300	21008	64.74	$5d^3\ ^2P$	27.83	$5d^2(^3P)6s\ ^2P$	1.313	1.316	−88.8 (5.0)	−60.092		−30.932
25558.770	25582	67.28	$5d^3\ ^2D$	31.83	$5d^3\ ^2D$	0.800		250 (10)	243.341		56.531
$J = 5/2$											
1053.164	1040	80.34	$5d\ 6s^2\ ^2D$	16.53	$5d^2(^1D)6s\ ^2D$	1.199	1.199	182.1702(6)	185.392	54.168 (14)	54.186
3010.002	3004	97.82	$5d^2(^3F)6s\ ^4F$	1.33	$5d\ 6s^2\ ^2D$	1.030	1.029	300.643 (1)	311.135	13.505 (25)	13.655
7011.909	7004	86.10	$5d^2(^3F)6s\ ^2F$	4.90	$5d^2(^1D)6s\ ^2D$	0.902	0.898	304.376 (2)	300.334	28.295 (30)	27.954
7679.939	7675	83.00	$5d^2(^3P)6s\ ^4P$	8.06	$5d^2(^1D)6s\ ^2D$	1.512	1.506	802.166 (5)	803.382	−34.793 (50)	−35.083
9183.797	9178	64.39	$5d^2(^1D)6s\ ^2D$	14.32	$5d^2(^3P)6s\ ^4P$	1.245	1.254	876.295 (5)	869.564	−4.474 (50)	−4.586
12787.404	12789	99.20	$5d^3\ ^4F$	0.40	$5d^3\ ^2D$	1.030	1.026	97.526 (5)	90.673	−16.141 (50)	−16.284
17099.380	17103	96.95	$5d^3\ ^4P$	1.64	$5d^3\ ^2D$	1.589		−222 (15)	−216.086		36.666
18776.620	18763	68.56	$5d^3\ ^2D$	22.03	$5d^3\ ^2D$	1.209		9.6 (5.0)	9.433		−40.199
21969.320	22001	93.62	$5d^3\ ^2F$	3.62	$5d^2(^3F)6s\ ^2F$	0.866		165.5 (3.5)	175.259		44.694
25414.630	25392	73.07	$5d^3\ ^2D$	23.38	$5d^3\ ^2D$	1.193		30 (20)	7.018		63.855
$J = 7/2$											
3494.526	3500	99.24	$5d^2(^3F)6s\ ^4F$	0.67	$5d^2(^3F)6s\ ^2F$	1.238	1.237	462.891 (1)	481.961	18.840 (24)	18.856
8052.162	8060	91.85	$5d^2(^3F)6s\ ^2F$	3.94	$5d^3\ ^2F$	1.134	1.135	−197.065 (5)	−207.607	41.896 (123)	42.419
9960.904	9968	86.81	$5d^2(^1G)6s\ ^2G$	9.42	$5d^3\ ^2G$	0.898	0.892	−293.000 (5)	−302.300	110.089 (100)	111.715
13238.323	13245	99.27	$5d^3\ ^4F$	0.42	$5d^3\ ^2G$	1.236	1.228	−19.095 (5)	−18.262	−20.545 (100)	−20.572
17023.360	17027	89.53	$5d^3\ ^2G$	9.46	$5d^2(^1G)6s\ ^2G$	0.892	0.880	161.8 (1.1)	156.748		43.296
21943.800	21910	95.37	$5d^3\ ^2F$	4.15	$5d^2(^3F)6s\ ^2F$	1.142		59.6 (3.7)	54.980		34.283
$J = 9/2$											
4121.572	4137	99.48	$5d^2(^3F)6s\ ^4F$	0.51	$5d^2(^1G)6s\ ^2G$	1.333	1.333	489.533 (1)	508.599	31.980 (24)	31.802
9919.821	9913	91.01	$5d^2(^1G)6s\ ^2G$	8.32	$5d^3\ ^2G$	1.113	1.107	559.237 (5)	565.386	129.240 (100)	127.977
13747.276	13748	97.51	$5d^3\ ^4F$	1.88	$5d^3\ ^2G$	1.328		−63.827 (5)	−59.402	−27.104 (100)	−26.845
17140.900	17132	57.10	$5d^3\ ^2G$	35.48	$5d^3\ ^2H$	1.044		111.2 (2.0)	114.535		64.868
18315.880	18319	64.43	$5d^3\ ^2H$	32.69	$5d^3\ ^2G$	0.982	0.970	111.6 (1.1)	117.104		56.847
$J = 11/2$											
18310.920	18313	100.00	$5d^3\ ^2H$	0.00	$5d^2()6s$	1.091		58.4 (1.5)	66.398		91.931

Table 2. One- and two-body fine- and hyperfine-structure radial parameters, in cm^{-1} and MHz, respectively, for the configuration system $(5d + 6s)^3$ of the lanthanum atom. (n_0 denotes the electrons of closed shells.)

Parameter	Value
Spin-orbit and electrostatically correlated spin-orbit interactions	
$\zeta_{5\mathrm{d}}$	608 (28)
$D^0(n_0d5d, 5d5d)\ \zeta_{n_0\mathrm{d},5\mathrm{d}}$	−41.3 (5.1)
$D^2(n_0d5d, 5d5d)\ \zeta_{n_0\mathrm{d},5\mathrm{d}}$	−24 (13)
$D^4(n_0d5d, 5d5d)\ \zeta_{n_0\mathrm{d},5\mathrm{d}}$	−15.6 (8.5)
$E^2(n_0d6s, 6s5d)\ \zeta_{n_0\mathrm{d},5\mathrm{d}}$	75 (28)
$D^2(n_0d5d, 5d6s)\ \zeta_{n_0\mathrm{d},5\mathrm{d}}$	−48 (32)
$E^2(n_0d5d, 6s5d)\ \zeta_{n_0\mathrm{d},5\mathrm{d}}$	−121 (60)
Magnetic-dipole hfs interactions	
$a^{01}_{5\mathrm{d}}$	199 (24)
$a^{12}_{5\mathrm{d}}$	164 (29)
a^{10}_{6s}	3817 (54)
$D^0(n_0d5d, 5d5d)\ P^{01}(n_0d, 5d) =$	
$D^0(n_0d5d, 5d5d)\ P^{12}(n_0d, 5d)$	−14.0 (4.6)
$D^2(n_0d5d, 5d5d)\ P^{01}(n_0d, 5d) =$	
$D^2(n_0d5d, 5d5d)\ P^{12}(n_0d, 5d)$	8.7 (5.4)
$D^4(n_0d5d, 5d5d)\ P^{01}(n_0d, 5d) =$	
$D^4(n_0d5d, 5d5d)\ P^{12}(n_0d, 5d)$	5.6 (3.5)
$E^2(n_0s5d, 5d6s)\ P^{10}(n_0s, 6s)$	−1026 (94)
$E^2(n_0s5d, 5dn's)\ P^{10}(n_0s, n's)$	−43 (86)
$E^2(n_0d6s, 6s5d)\ P^{01}(n_0d, 5d) =$	
$E^2(n_0d6s, 6s5d)\ P^{12}(n_0d, 5d)$	13 (22)
$E^2(5d6s, 7s5d)\ P^{10}(6s, 7s)$	54 (120)
$a^{12}_{4\mathrm{d},5\mathrm{s}}$	63 (43)
$D^2(n_0d5d, 5d5d)\ P^{10}(n_0s, 6s)$	2037 (160)
$D^2(n_0d5d, 5d6s)\ P^{01}(n_0d, 5d) =$	
$D^2(n_0d5d, 5d6s)\ P^{12}(n_0d, 5d)$	−140 (76)
$E^2(n_0d5d, 6s5d)\ P^{01}(n_0d, 5d) =$	
$E^2(n_0d5d, 6s5d)\ P^{12}(n_0d, 5d)$	−122 (90)
Electric-quadrupole hfs interactions	
$b^{02}_{5\mathrm{d}}$	237.5 (4.4)
$b^{13}_{5\mathrm{d}}$	32.1 (3.1)
$b^{11}_{5\mathrm{d}}$	−3.4 (1.5)
$D^0(n_0d5d, 5d5d)\ P^{02}(n_0d, 5d)$	−18.86 (0.72)
$D^2(n_0d5d, 5d5d)\ P^{02}(n_0d, 5d)$	17.9 (3.4)
$D^4(n_0d5d, 5d5d)\ P^{02}(n_0d, 5d)$	11.2 (2.2)
$E^2(n_0d6s, 6s5d)\ P^{02}(n_0d, 5d)$	70.2 (2.2)
$b^{02}_{4\mathrm{d},5\mathrm{s}}$	44 (17)
$D^2(n_0d5d, 5d6s)\ P^{02}(n_0d, 5d)$	102 (45)
$E^2(n_0d5d, 6s5d)\ P^{02}(n_0d, 5d)$	187 (2.2)
$D^2(n_0d5d, 6s6s)\ P^{02}(n_0d, 5d)$	174 (36)

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