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# Unified analytical treatment of multicentre electron attraction, electric field and electric field gradient integrals over Slater orbitals

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## Abstract

The new central and noncentral potential functions (CPFs and NCPFs) of a molecule depending on the coordinates of the nuclei are introduced. Using complete orthonormal sets of  $\Psi^\alpha$ -exponential-type orbitals ( $\Psi^\alpha$ -ETOs) introduced by the author, the series expansion formulae for the multicentre electronic attraction (EA), electric field (EF) and electric field gradient (EFG) integrals over Slater-type orbitals (STOs) in terms of CPFs and NCPFs are derived. The relationships obtained are valid for the arbitrary location, quantum numbers and screening constants of STOs.

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## 1. Introduction

The electric field induced within a molecule by its electrons determines a whole series of important physical properties of the molecule. In particular, the values of the potential of this field at the nuclei determine the nuclear dynamic shielding constants, the values of the strength of this field at the nuclei determine the forces exerted by the electrons on them and the values of the gradient of this field at the nuclei determine the interaction of their quadrupole moments with the electrons. According to the well-known Hellman–Feynman theorem of electrostatics [1], the forces exerted by the electrons on the nuclei can be found by differentiating the electronic energy (or the adiabatic potential function) of the molecule with respect to displacements of the nuclei, for which purpose it is sufficient to know the dependence of the adiabatic potential function of the molecule on the coordinates of the nuclei. The derivatives of the adiabatic potential function give the values of the electric field gradient at the nuclei which are important in the theory of electron–nuclei quadrupole interactions. It should be noted that the electric field at the nuclei, and its gradient are very sensitive to minor errors in the wavefunctions. Consequently, reliable theoretical calculations on these properties are known only for a few simple molecules (see, e.g., [2] and references

quoted therein). Older works are reviewed in [3]. There is, therefore, interest in a general investigation of the derivatives of the electrostatic potential created by the electrons and the interactions between electrons and nuclei of a molecule.

As is well known the basis sets of functions for calculations in the theory of molecular structure are of prime importance since the quality of several molecular properties may depend strongly on the nature of these basis functions. The Gaussian-type orbitals (GTOs) are used almost exclusively as the basis sets for *ab initio* quantum chemistry. However, GTOs are not able to represent important properties of the exact electronic wavefunction at nuclei and at large distances. Thus, exponential-type orbitals (ETOs) would be desirable for basis sets in molecular calculations because they satisfy the cusp condition at the nuclei [4] and the exponential decay for large distances [5] as does the exact wavefunction. It should be noted that the exact wavefunction for  $r \rightarrow \infty$ , where  $r$  is the distance to the origin, decays with  $\zeta = \sqrt{2\varepsilon}$ , where  $\zeta$  and  $\varepsilon$  are the screening parameter of ETOs and the lowest ionization potential of the molecule, respectively. Thus, the ETO basis set that is used has such a function as the most diffuse one, and may, for the smallest  $\zeta$ , become more easily nearly linear dependent. The use of these approximations for a wavefunction in molecular electronic structure calculations would be highly desirable since they are capable of producing much better approximations than the exponential functions. However, the routine use of linearly dependence functions can be prevented by the fact that the efficient and reliable computation of their two electron multicentre integrals is extremely difficult. The large body of formulae of the expansion methods of ETOs about a displaced centre [6–11], the Fourier transform methods [12–14] and the *B*-function method [15–18] developed for the evaluation of multicentre molecular integrals over ETOs is not quite satisfactory in the numerical aspects of multicentre integrals, especially in the calculation of three- and four-centre electron-repulsion integrals. The reason is that so far nobody has been able to compute the complicated two electron integrals both efficiently and reliably. This would be necessary to make molecular electronic structure calculations with an ETO basis feasible. In the literature, the wide use of ETOs as basis sets has been pursued with considerable enthusiasm by a growing number of workers because of huge advances in applied mathematics and computer science (see [19–27] and references quoted therein). In [28] we introduced the new complete orthonormal sets of  $\Psi^\alpha$ -ETOs (where  $\alpha = 1, 0, -1, -2, \dots$ ). Using  $\Psi^\alpha$ -ETOs in [29] the different analytical expressions were derived for expansion of one- and two-centre electron charge density over Slater-type orbitals (STOs) in terms of STOs about a new centre. The expansion coefficients in these formulae are expressed through the overlap integrals with the same screening parameters, for the calculation of which efficient computer programs are available in our group [30, 31]. Therefore, using the computer programs for the overlap integrals based on auxiliary functions [30] and recurrence relations [31] one can calculate arbitrary multicentre integrals appearing in the determination of various properties for molecules when the Hartree–Fock–Roothaan approximation is employed. The aim of this paper is to establish the expansion formulae for the multicentre electronic attraction (EA), electric field (EF) and electric field gradient (EFG) integrals over STOs using general analytical relations for potential functions of a molecule introduced in this study and complete orthonormal sets of  $\Psi^\alpha$ -ETOs. It should be noted that the analytical formulae obtained in this work can be used for the calculation of multicentre EA, EF and EFG integrals with arbitrary ETOs.

## 2. Expressions in terms of two-centre basic integrals

The multicentre integrals examined in this work have the following form:

- EA integrals

$$U_{nlm,n'l'm'}(\zeta, \zeta'; \vec{R}_{ca}, \vec{R}_{ab}) = \int \chi_{nlm}^*(\zeta, \vec{r}_{a1}) \chi_{n'l'm'}(\zeta', \vec{r}_{c1}) O(r_{b1}) dV_1. \quad (1)$$

- EF integrals

$$U_{nlm,n'l'm'}^i(\zeta, \zeta'; \vec{R}_{ca}, \vec{R}_{ab}) = \frac{\partial}{\partial X^i} U_{nlm,n'l'm'}(\zeta, \zeta'; \vec{R}_{ca}, \vec{R}_{ab}) \quad (2a)$$

$$= \int \chi_{nlm}^*(\zeta, \vec{r}_{a1}) \chi_{n'l'm'}(\zeta', \vec{r}_{c1}) O^i(\vec{r}_{b1}) dV_1. \quad (2b)$$

- EFG integrals

$$U_{nlm,n'l'm'}^{ij}(\zeta, \zeta'; \vec{R}_{ca}, \vec{R}_{ab}) = \frac{\partial^2}{\partial X^i \partial X^j} U_{nlm,n'l'm'}(\zeta, \zeta'; \vec{R}_{ca}, \vec{R}_{ab}) \quad (3a)$$

$$= \int \chi_{nlm}^*(\zeta, \vec{r}_{a1}) \chi_{n'l'm'}(\zeta', \vec{r}_{c1}) O^{ij}(\vec{r}_{b1}) dV_1 \quad (3b)$$

where  $\vec{R}_{ca} = \vec{r}_{c1} - \vec{r}_{a1}$ ,  $\vec{R}_{ab} = \vec{r}_{a1} - \vec{r}_{b1}$  and

$$O(r_{b1}) = \frac{1}{r_{b1}} \quad (4)$$

$$O^i(\vec{r}_{b1}) = \frac{x_{b1}^i}{r_{b1}^3} \quad (5)$$

$$O^{ij}(\vec{r}_{b1}) = \frac{3x_{b1}^i x_{b1}^j - \delta_{ij} r_{b1}^2}{r_{b1}^5} - \frac{4\pi}{3} \delta_{ij} \delta(\vec{r}_{b1}). \quad (6)$$

Here  $x^1 = x$ ,  $x^{-1} = y$ ,  $x^0 = z$  and  $X^1 = X$ ,  $X^{-1} = Y$ ,  $X^0 = Z$  are the Cartesian coordinates of the electron and nucleus  $b$ , respectively;  $\delta(\vec{r})$  is the Dirac delta function;  $\chi_{nlm}(\zeta, \vec{r}_{a1})$  and  $\chi_{n'l'm'}(\zeta', \vec{r}_{b1})$  are the normalized STOs centred on the nuclei  $a$  and  $b$  which are defined by

$$\chi_{nlm}(\zeta, \vec{r}) = R_n(\zeta, r) S_{lm}(\theta, \phi) \quad (7)$$

$$R_n(\zeta, r) = (2\zeta)^{n+1/2} [(2n)!]^{-1/2} r^{n-1} e^{-\zeta r}. \quad (8)$$

The spherical harmonics in equation (7) are determined by

$$S_{lm}(\theta, \phi) = P_{l|m|}(\cos \theta) \Phi_m(\phi) \quad (9)$$

where  $P_{l|m|}$  are normalized associated Legendre functions [32].

- For complex spherical harmonics ( $S_{lm} \equiv Y_{lm}$ )

$$\Phi_m(\phi) = \frac{1}{\sqrt{2\pi}} e^{im\phi}. \quad (10)$$

- For real spherical harmonics

$$\Phi_m(\phi) = \frac{1}{\sqrt{\pi(1 + \delta_{m0})}} \begin{cases} \cos|m|\phi & \text{for } m \geq 0 \\ \sin|m|\phi & \text{for } m < 0 \end{cases}. \quad (11)$$

Now we can move to the determination of expressions for the multicentre integrals (1), (2) and (3) in terms of basic integrals. For this purpose we use in equations (1), (2) and (3) the following sets of expansion formulae for the electron charge density, obtained with the help of  $\Psi^\alpha$ -ETOs, in terms of STOs [29]:

$$\chi_p(\zeta, \vec{r}_a)\chi_{p'}^*(\zeta', \vec{r}_c) = \frac{1}{\sqrt{4\pi}} \lim_{N \rightarrow \infty} \sum_{\mu=1}^N \sum_{\nu=0}^{\mu-1} \sum_{\sigma=-\nu}^{\nu} W_{pp'q}^{\alpha N}(\zeta, \zeta', z; \vec{R}_{ca}, 0)\chi_q(z, \vec{r}_a) \quad (12)$$

where  $\alpha = 1, 0, -1, -2, \dots, p \equiv nlm, p' \equiv n'l'm', q \equiv \mu\nu\sigma$  and  $z = \zeta + \zeta'$ . The quantities  $W_{pp'q}^{\alpha N}(\zeta, \zeta', z; \vec{R}_{ca}, 0)$  in equation (12) are the two-centre expansion coefficients which can be expressed through the overlap integrals with the same screening parameters.

Taking into account equation (12) in equations (1)–(3) we obtain the series expansion formulae for the multicentre EA, EF and EFG integrals in terms of two-centre basic integrals defined by

$$J_{nlm}(\zeta, \vec{R}) = \lim_{\zeta' \rightarrow 0} \sqrt{8\pi} (2\zeta')^{-3/2} U_{nlm,100}(\zeta, \zeta'; 0, \vec{R}) \quad (13a)$$

$$= \frac{1}{\sqrt{4\pi}} \int \chi_{nlm}^*(\zeta, \vec{r}_{a1}) O(r_{b1}) dV_1 \quad (13b)$$

$$J_{nlm}^i(\zeta, \vec{R}) = \frac{\partial}{\partial X^i} J_{nlm}(\zeta, \vec{R}) \quad (14a)$$

$$= \frac{1}{\sqrt{4\pi}} \int \chi_{nlm}^*(\zeta, \vec{r}_{a1}) O^i(r_{b1}) dV_1 \quad (14b)$$

$$J_{nlm}^{ij}(\zeta, \vec{R}) = \frac{\partial^2}{\partial X^i \partial X^j} J_{nlm}(\zeta, \vec{R}) \quad (15a)$$

$$= \frac{1}{\sqrt{4\pi}} \int \chi_{nlm}^*(\zeta, \vec{r}_{a1}) O^{ij}(r_{b1}) dV_1 \quad (15b)$$

where  $\vec{R} = \vec{R}_{ab}$  and  $X^1 = X, X^{-1} = Y, X^0 = Z (i, j = 1, -1, 0)$ . Using equation (1) of [33] in equation (13a) it is easy to establish for the two-centre basic EA integral the following relation:

$$J_{nlm}(\zeta, \vec{R}) = \frac{2^{n+1}(n+l+1)!}{[(2l+1)(2n)!(2\zeta)]^{1/2}(\zeta R)^{l+1}} \left( 1 - e^{-\zeta R} \sum_{\sigma=0}^{n+l} \gamma_\sigma^l(n)(\zeta R)^\sigma \right) \bar{S}_{lm}^*(\theta, \varphi) \quad (16)$$

where

$$\bar{S}_{lm}(\theta, \varphi) = \left( \frac{4\pi}{2l+1} \right)^{1/2} S_{lm}(\theta, \varphi) \quad (17)$$

$$\gamma_\sigma^l(n) = \frac{1}{\sigma!} - \frac{(n-l)!}{(n+l+1)!(\sigma-2l-1)!}. \quad (18)$$

Here  $\gamma_\sigma^l(n) = 0$  for  $\sigma < 0$  and  $\sigma > n+l$ . In equation (18) terms with negative factorials should be equated to zero.

### 3. Use of central and noncentral potentials in evaluation of basic integrals

In order to evaluate the two-centre basic integrals (14a) and (15a) give certain formulae which are required for the derivatives of the function

$$M_{lm}(x, y, z) = r^l \bar{S}_{lm}(\theta, \varphi). \quad (19)$$

With the aid of the well-known characteristics of the spherical harmonics we can show that the derivatives of these functions with respect to Cartesian coordinates can be expressed in terms of  $M_{l-1m}$ :

$$\frac{\partial M_{lm}}{\partial x_i} = \sum_{m'=-l}^{l-1} a_{lm,m'}^i M_{l-1m'} \quad (20)$$

$$\frac{\partial^2 M_{lm}}{\partial x_i \partial x_j} = \sum_{m'=-l}^{l-2} a_{lm,m'}^{ij} M_{l-2m'}. \quad (21)$$

Here  $a_{lm,m'}^i \equiv 0$  for  $l = 0$ ,  $a_{lm,m'}^{ij} \equiv 0$  for  $l = 0, 1$  and

$$a_{lm,m'}^1 = -\frac{\varepsilon_m}{2} \{ [(1 + \delta_{m0})(1 - \delta_{m,-1})(l - m)(l - m - 1)]^{1/2} \delta_{m',m+1} - [(1 - \delta_{m0})(1 + \delta_{m1})(l + m)(l + m - 1)]^{1/2} \delta_{m',m-1} \} \quad (22)$$

$$a_{lm,m'}^{-1} = -\frac{\varepsilon_m}{2} \{ [(1 + \delta_{m0})(1 + \delta_{m,-1})(l - m)(l - m - 1)]^{1/2} \delta_{m',-m-1} + [(1 - \delta_{m0})(1 - \delta_{m1})(l + m)(l + m - 1)]^{1/2} \delta_{m',-m+1} \} \quad (23)$$

$$a_{lm,m'}^0 = [(l + m)(l - m)]^{1/2} \delta_{m',m} \quad \text{for } l \geq 1 \quad (24)$$

$$a_{lm,m'}^{ij} = a_{lm,m'}^{ji} = \sum_{m''=-l}^{l-1} a_{lm,m''}^j a_{l-1m'',m'}^i \quad \text{for } l \geq 2 \quad (25)$$

where  $\varepsilon_m = \pm 1$ . The sign of the symbol  $\varepsilon_m$  is determined by the sign of  $m$ , i.e.  $\varepsilon_m = +1$  for  $m \geq 0$  and  $\varepsilon_m = -1$  for  $m < 0$ .

In the present study we also need the following formulae for the derivatives of a product of the functions  $M_{lm}(x, y, z)$  and  $f(r)$  where  $r = (x^2 + y^2 + z^2)^{1/2}$ :

$$\frac{\partial(M_{lm}f)}{\partial x_i} = \frac{\partial M_{lm}}{\partial x_i} f + M_{lm} x_i \left( \frac{1}{r} \frac{\partial f}{\partial r} \right) \quad (26)$$

$$\begin{aligned} \frac{\partial^2(M_{lm}f)}{\partial x_i \partial x_j} &= \frac{\partial^2 M_{lm}}{\partial x_i \partial x_j} f + \frac{\partial M_{lm}}{\partial x_i} x_j \left( \frac{1}{r} \frac{\partial f}{\partial r} \right) + \frac{\partial M_{lm}}{\partial x_j} x_i \left( \frac{1}{r} \frac{\partial f}{\partial r} \right) \\ &+ M_{lm} \left[ \delta_{ij} \left( \frac{1}{r} \frac{\partial f}{\partial r} \right) + x_i x_j \frac{1}{r} \frac{\partial}{\partial r} \left( \frac{1}{r} \frac{\partial f}{\partial r} \right) \right]. \end{aligned} \quad (27)$$

Taking into account equations (16), (19)–(21), (26) and (27) in equations (13a), (14a) and (15a) we finally obtain for two-centre basic integrals the following relations in terms of central and noncentral potential functions:

- for two-centre basic EA integrals

$$J_{nlm}(\zeta, \vec{R}) = f_{nl,lm}^{00}(\zeta, \vec{R}) \quad (28)$$

- for two-centre basic EF integrals

$$J_{nlm}^i(\zeta, \vec{R}) = \sum_{m'=-l}^{l-1} a_{lm,m'}^i f_{nl,l-1m'}^{10}(\zeta, \vec{R}) - (2l + 1) \left( \frac{X^i}{R} \right) f_{nl,lm}^{11}(\zeta, \vec{R}) \quad (29)$$

- for two-centre basic EFG integrals

$$\begin{aligned}
 J_{nlm}^{ij}(\zeta, \vec{R}) = & \sum_{m'=-l-2}^{l-2} a_{lm,m'}^{ij} f_{nl,l-2m'}^{20}(\zeta, \vec{R}) - (2l+1) \sum_{m'=-l-1}^{l-1} \left[ a_{lm,m'}^i \left( \frac{X^j}{R} \right) \right. \\
 & \left. + a_{lm,m'}^j \left( \frac{X^i}{R} \right) \right] f_{nl,l-1m'}^{21}(\zeta, \vec{R}) - (2l+1) \delta_{ij} f_{nl,lm}^{21}(\zeta, \vec{R}) \\
 & + (2l+1)(2l+3) \left( \frac{X^i}{R} \right) \left( \frac{X^j}{R} \right) f_{nl,lm}^{22}(\zeta, \vec{R}) - \frac{\sqrt{4\pi}}{3} \delta_{ij} \chi_{nlm}^*(\zeta, \vec{R}). \quad (30)
 \end{aligned}$$

Here,  $f_{nl,\nu m}^{tk}(\zeta, \vec{R})$  are the potential functions determined by

$$f_{nl,\nu m}^{tk}(\zeta, \vec{R}) = f_{nl}^{tk}(\zeta, R) \bar{S}_{\nu m}(\theta, \varphi) \quad (31)$$

$$f_{nl}^{tk}(\zeta, \vec{R}) = f_{nl,00}^{tk}(\zeta, R) = \frac{N_{nl}'(2\zeta)}{(\zeta R)^{l+t+1}} \left( 1 - e^{-\zeta R} \sum_{\sigma=0}^{n+l+k} \gamma_{\sigma}^{lk}(n) (\zeta R)^{\sigma} \right) \quad (32)$$

$$N_{nl}'(2\zeta) = 2^{n-t+1} (n+l+1)! \left[ \frac{(2\zeta)^{2t-1}}{(2l+1)(2n)!} \right]^{1/2} \quad (33)$$

where  $t = 0, 1, 2$  for EA, EF and EFG integrals, respectively, and  $0 \leq k \leq t$ . The coefficients  $\gamma_{\sigma}^{lk}(n)$  in equation (32) can be determined from  $\gamma_{\sigma}^l(n)$ , equation (18), by the following relations:

$$\gamma_{\sigma}^{l0}(n) = \gamma_{\sigma}^l(n) \quad (34)$$

$$\gamma_{\sigma}^{l1}(n) = \frac{1}{2l+1} [(2l+1-\sigma)\gamma_{\sigma}^l(n) + \gamma_{\sigma-1}^l(n)] \quad (35)$$

$$\begin{aligned}
 \gamma_{\sigma}^{l2}(n) = & \frac{1}{(2l+1)(2l+3)} [(2l+1-\sigma)(2l+3-\sigma)\gamma_{\sigma}^l(n) \\
 & + (4l+5-2\sigma)\gamma_{\sigma-1}^l(n) + \gamma_{\sigma-2}^l(n)]. \quad (36)
 \end{aligned}$$

The characteristics of the potential functions are discussed in the appendix.

Now we can move to the calculation of one-centre basic integrals. For this purpose we must go to the limit in equations (28), (29) and (30) where  $R \rightarrow 0$ . Taking into account equation (A.6) of the appendix, we can convince ourselves of the accuracy of the following formulae for the one-centre basic integrals:

- for one-centre basic EA integrals

$$J_{nlm}(\zeta) = \frac{N_{n0}^0(2\zeta)}{n+1} \delta_{l0} \delta_{m0} \quad (37)$$

- for one-centre basic EF integrals

$$J_{nlm}^i(\zeta) = \frac{(n-1)!}{(n+2)!} N_{n1}^1(2\zeta) \delta_{l1} \delta_{mi} \quad (38)$$

- for one-centre basic EFG integrals

$$J_{nlm}^{ij}(\zeta) = \frac{(n-2)!}{(n+3)!} N_{n2}^2(2\zeta) a_{2m,0}^{ij} \delta_{l2} - \frac{\sqrt{2}}{6} (2\zeta)^{3/2} \delta_{ij} \delta_{n1} \delta_{l0} \delta_{m0} \quad (39)$$

where  $J_{nlm}(\zeta) = J_{nlm}(\zeta, 0)$ ,  $J_{nlm}^i(\zeta) = J_{nlm}^i(\zeta, 0)$  and  $J_{nlm}^{ij}(\zeta) = J_{nlm}^{ij}(\zeta, 0)$ . It should be noted that expressions (37), (38) and (39) can also be established by the calculation of one-centre basic integrals separately.

Taking into account the relationships for one- and two-centre basic integrals all the multicentre EA, EF and EFG integrals can be calculated using equations (A.3), (A.5) and (A.6) for potential functions. For this purpose, we need only the Cartesian coordinates of the nuclei and the quantum numbers and screening constants of STOs.

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### Appendix

We have seen above that the multicentre EA, EF and EFG integrals contain the potential functions  $f_{nl}^{tk}(\zeta, \vec{R})$ , the radial part of which is determined by equation (32). Let us rewrite equation (32) in the following form:

$$f_{nl}^{tk}(\zeta, R) = N_{nl}^t(2\zeta) \left[ \frac{1}{x^{l+t+1}} \left( 1 - e^{-x} \sum_{\sigma=0}^{l+t} \frac{x^\sigma}{\sigma!} \right) + \frac{e^{-x}}{x^{l+t+1}} \sum_{\sigma=0}^{l+t} \left( \frac{1}{\sigma!} - \gamma_\sigma^{lk}(n) \right) x^\sigma - e^{-x} \sum_{\sigma=l+t+1}^{n+l+k} \gamma_\sigma^{lk}(n) x^{\sigma-(l+t+1)} \right] \quad (\text{A.1})$$

where  $x = \zeta R$ . Using characteristics of the coefficients  $\gamma_\sigma^l(n)$  it is easy to show that

$$\frac{1}{\sigma!} - \gamma_\sigma^{lk}(n) = 0 \quad \text{for } 0 \leq \sigma \leq l+t \quad \text{and } l \geq t\delta_{k0}. \quad (\text{A.2})$$

Taking into account equation (A.2) in (A.1) we finally obtain for the radial part of potential functions the following relation:

$$f_{nl}^{tk}(\zeta, R) = N_{nl}^t(2\zeta) \left[ \frac{1}{x^{l+t+1}} \left( 1 - e^{-x} \sum_{\sigma=0}^{l+t} \frac{x^\sigma}{\sigma!} \right) - e^{-x} \sum_{\sigma=l+t+1}^{n+l+k} \gamma_\sigma^{lk}(n) x^{\sigma-(l+t+1)} \right]. \quad (\text{A.3})$$

As can be seen from equation (A.3), the potential functions  $f_{nl}^{tk}(\zeta, R)$  become numerically unstable in the case of small values of parameter  $x = \zeta R$ . In this case, taking into account the relation

$$\frac{1}{x^n} \left( 1 - e^{-x} \sum_{\sigma=0}^{n-1} \frac{x^\sigma}{\sigma!} \right) = \sum_{\sigma=0}^{\infty} \frac{(-x)^\sigma}{(n-1)!\sigma!(n+\sigma)} \quad (\text{A.4})$$

we obtain the following series expansion formula:

$$f_{nl}^{tk}(\zeta, R) = N_{nl}^t(2\zeta) \left[ \sum_{\sigma=0}^{\infty} \frac{(-x)^\sigma}{(l+t)!\sigma!(l+t+\sigma+1)} - e^{-x} \sum_{\sigma=l+t+1}^{n+l+k} \gamma_\sigma^{lk}(n) x^{\sigma-(l+t+1)} \right]. \quad (\text{A.5})$$

With the calculation of one-centre potential functions we must go to the limit in equation (A.5) where  $x \rightarrow 0$ . Then, we obtain:

$$f_{nl}^{tk}(\zeta) = \frac{(n-t)!}{(n+t+1)!} N_{nl}^t(2\zeta) \delta_{tl} \delta_{k0} \quad (\text{A.6})$$

where  $f_{nl}^{tk}(\zeta) = f_{nl}^{tk}(\zeta, 0)$ .



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