FEN FAKÜLTESİ FEN DERGİSİ

Nisan(2017) 43 (1): 65-74

Araştırma Makalesi

SELÇUK ÜNİVERSİTESİ

Geliş (Recieved) :14/01/2016
Kabul (Accepted) :21/03/2016

Slater-Tipi Orbitaller Üzerinden İki-Merkezli Moleküler İntegrallerin Eliptik Koordinatlar Kullanılarak Hesaplanması için Kullanılan Yadımcı Fonksiyonlar

Erhan AKIN

Selçuk Üniversitesi, Fen Fakültesi, Fizik Bölümü, KONYA
e-mail: eakin@selcuk.edu.tr

Öz: Bu çalışmada bir- ve iki-elektron iki-merkezli moleküler integrallerin eliptik koordinatlar kullanılarak hesaplanmasında Yakar ve ark. tarafından önerilen *I* yardımcı fonksiyonlarının yalnızca binom katsayılarını içeren yeni bir formu elde edilmiştir. Aynı zamanda *I* yardımcı fonksiyonlarında görülen *J* ve *K* fonksiyonlarının analitik ifadeleri için negatif *n* değerleri durumunda seri açılım şeklinde yeni analitik ifadeler verilmiştir. Bu çalışmada elde edilen analitik ifadeler ile Yakar ve ark. tarafından verilen analitik ifadelerin hesaplamaları karşılaştırılmış ve her iki ifadenin sonuçlarının iyi uyum içinde olduğu görülmüştür. Slater-tipi atom orbitalleri üzerinden iki-merkezli elektrik alan gradyenti integrallerinin eliptik koordinatlar kullanılarak hesaplanması bazı zorluklar içerir, bununla birlikte bu integraller bu çalışmada elde edilen *I*, *J* ve *K* yardımcı fonksiyonları kullanılarak kolaylıkla hesaplanabilir. Bu hesaplamanın sonuçlarının da literatürle iyi uyum içinde olduğu görülmüştür.

Anahtar kelimeler: Slater-tipi atom orbitalleri - Çokmerkezli moleküler integraller – Eliptik koordinatlar yöntemi

On the Auxiliary Functions Used for the Evaluation of Two-Center Molecular Integrals over Slater-Type Orbitals using Elliptical Coordinates

Abstract: In this study, a new form containing only binomial coefficients have been obtained for I auxiliary functions proposed by Yakar et al. (Yakar et al., 2006)(Yakar et al., 2006)in the calculation of one- and two-electron two-center molecular integrals by using elliptical coordinates. Also new analytical expressions in the form of serial expansion have been given for the analytical expressions of J and K functions for negative n values which appears in the I auxiliary function. Calculations of the analytical expressions obtained in this work and the analytical expressions given by Yakar et al. (Yakar et al., 2006)(Yakar et al., 2006)have been compared and it has been seen that the results from both expressions are in well agreement. Evaluation of two-center electric field gradient (EFG) integrals over Slater-type orbitals by using elliptical coordinates poses some difficulties, however these integrals have been easily evaluated by using the I, J and K auxiliary function obtained in this study. It has been seen that the results of this calculation are in good agreement with the results in the literature, too.

Keywords: Slater-type orbitals - Multicenter molecular integrals - Elliptical coordinates method

1. Introduction

In order to calculate the physical properties of a molecule theoretically, the wave function of the molecule has to be known. Hartree-Fock-Roothaan method (HFR) is the most used approximation method to determine the molecular wave function (Roothaan, 1951). This method uses the multicenter integrals over the slater type orbitals (STO's). The wave function of molecule obtained using HFR approximation is a function called the slater determinant whose elements are the one-electron molecular spin orbitals (Slater, 1960). Multicenter integrals appear both in the solution of HFR equations and in the

evaluation of physical properties of the molecule by using the wave function obtained from solution of HFR equations. Integrals having more than two-center can be reduced into two-center integrals by using expansion of an STO about a displaced center (Guseinov, 1985; Jones, 1987). The solution of such two-center integrals can be succeeded by using Fourier Convolution theorem (Zeroka, 1966), expansion by Löwdin's α coefficient (Jones, 1987), expansion by Guseinov's V coefficients (Guseinov, 1985) and the methods employing elliptical coordinates (Guseinov et al., 1998; Mekelleche and BabaAhmed, 1997; Yakar et al., 2006; Ozmen et al., 2003; Akin, 2008).

A, B, J and K auxiliary functions arise in the evaluation of two-center molecular integrals by using elliptical coordinates. Analytical expressions in the recursive form have been given for auxiliary functions A and B in the works of Mekelleche et al.(Mekelleche and BabaAhmed, 1997) and Guseinov et al. (Mekelleche and BabaAhmed, 1997; Guseinov et al., 1998) and for auxiliary functions J and K in the works of and Özmen et al. (2003) and Yakar et al. (Ozmen et al., 2003; Yakar et al., 2006). It has been stated in the works of Mekelleche et al. (1997) and Guseinov et al. (Mekelleche and BabaAhmed, 1997; Guseinov et al., 1998) that the analytical expressions used for calculation of auxiliary function A has given stable results but it has not always given stable results for B. Moreover, it has also been stated in the works of Özmen et al. (2003) and Yakar et al. (Ozmen et al., 2003; Yakar et al., 2006). that auxiliary function J has not given stable results in some cases while auxiliary function K has given stable results in all cases.

In order to overcome the instability in the auxiliary function B, Mekelleche and Baba-Ahmed (Mekelleche and BabaAhmed, 1997) have used an analytical expression in the serial expansion form instead of the recursive form while Guseinov et al. (1998) have used an analytical expression in the downward recursion. In the case of $n \geq 0$ and $n < \alpha$, Ozmen et al. (Ozmen et al., 2003) and Yakar et al. (Yakar et al., 2006) have overcome the instability of J by performing the recursion downward. In this study, analytical expressions in the serial expansion form have been obtained for the case of instability of J such as Mekelleche and Baba-Ahmed (1997) have done for B. These analytical expressions are completely stable. Although other recursive relations in the works of Özmen et al. (2003) and Yakar et al. (Ozmen et al., 2003; Yakar et al., 2006) are stable, new analytical expressions in serial expansion form can also be obtained for them.

In the evaluation of one- and two-electron two-center molecular integrals over Slater-type orbitals using elliptical coordinates, an integral appears in the form

$$\int_{1}^{\infty}\int_{-1}^{1}(\mu+\nu)^{n}(\mu-\nu)^{n'}(\mu\nu)^{q}e^{-p\mu}e^{-pt\nu}d\mu d\nu\,. \qquad (1)$$

n value in this integral is always positive for overlap, nuclear attraction, electric multipole moment and magnetic multipole moment integrals while it is negative for kinetic energy integrals with s-orbital, Coulomb and exchange integrals with $\ell > 0$, electric field gradient integrals and spin-spin nuclear attraction integrals. For the negative values of *n*, the binomial expansion gives infinite series for integral (1). However, the convergence of the infinite series is too slow. In these cases, abovementioned integrals can be calculated with high precision by using auxiliary function I containing J and K auxiliary functions. For example Ozmen et al. (Ozmen et al., 2003) have calculated two-center Coulomb integrals, and Akin (Akin, 2008) have calculated two-center electric field gradient integrals by using auxiliary functions J and K.

2. Material and Method

The two-center molecular integrals have the following form in which the STOs are taken to be complex

$$\int_{\tau}\chi^{*}_{n_a\ell_a m_a}(\zeta_a,\vec{r}_a)\hat{F}\,\chi_{n_b\ell_b m_b}(\zeta_b,\vec{r}_b)d\tau\,. \qquad (2)$$

Where $\hat{F}$ is an operator corresponding to an observable centered at a or b nucleus of the molecule, $\chi_{n_a\ell_a m_a}(\zeta_a,\vec{r}_a)$ and $\chi_{n_b\ell_b m_b}(\zeta_b,\vec{r}_b)$ are STOs centered at a and b nuclei of the molecule, respectively. STOs have the general form

$$\chi_{n\ell m}(\zeta,\vec{r})=\frac{(2\zeta)^{n+\frac{1}{2}}}{\sqrt{(2n)!}}r^{n-1}e^{-\zeta r}Y_{\ell m}(\theta,\varphi)\,. \qquad (3)$$

Here, $n\ell m$ are quantum numbers, ζ is the screening constant and $Y_{\ell m}$ are complex spherical harmonics. When the coordinate system is transformed from spherical to elliptical coordinates by placing STOs of (3) into (2) and by using the relations

$$r_a=\frac{R_{ab}}{2}(\mu+\nu)\quad r_b=\frac{R_{ab}}{2}(\mu-\nu)\quad d\tau=\frac{R_{ab}^{3}}{8}(\mu^{2}-\nu^{2})d\mu d\nu d\varphi \qquad (4)$$

and then integrating over φ, an integral in the form

$$\int_{1}^{\infty}\int_{-1}^{1}(\mu+\nu)^{n}(\mu-\nu)^{n'}(\mu\nu)^{q}e^{-p\mu}e^{-pt\nu}d\mu d\nu \qquad (5)$$

appears. Where R_{ab} is the distance between the nuclei a and b and the new variables p and t are defined to be

$$p = \frac{R_{ab}}{2}(\zeta_a + \zeta_b) \qquad t = \frac{(\zeta_a - \zeta_b)}{(\zeta_a + \zeta_b)} \ .$$

n' and q in eq.(5) have always positive values while n sometimes may have negative values. Integral in (5) is labelled as $Q^q_{nn'}(p,t)$ for positive n and $Q^q_{-nn'}(p,t)$ for negative n by Guseinov (Guseinov, 1970) and as $I(n,n',q,p,t)$ for either case by Yakar et al. (Yakar et al., 2006) and Ozmen *et al.* (Ozmen et al., 2003). Guseinov et al. (Guseinov et al., 1998) have calculated two-center overlap integrals over Slater-type orbitals using $Q^q_{nn'}$ auxiliary functions. Furthermore, Pashaev (Pashaev, 2009) has calculated two-center overlap integrals over Slater-type orbitals based on the B Filter-Steinborn and Guseinov $Q^q_{nn'}$.

The analytical solution of integral of (5) for the positive case of n in both of these works were given as

$$I(n,n',q,p,t) = Q^q_{nn'}(p,t) = \sum_{m=0}^{n+n'} F_m(n,n') A_{n+n'+q-m}(p) B_{q+m}(pt) \tag{6}$$

in terms of A and B auxiliary functions. Here, auxiliary functions A and B are defined by the integrals (Mulliken, 1949).

$$A_n(p) = \int_1^\infty \mu^n e^{-p\mu} d\mu \qquad B_n(pt) = \int_{-1}^1 \nu^n e^{-pt\nu} d\nu \ . \tag{7}$$

p constants are always different than zero but $pt = 0$ occurs in the case of $\zeta_a = \zeta_b$. In this case, the solution of B integral is quite simple. Therefore, the case of $pt = 0$ is not in the scope of this work. Analytical solutions of A and B integrals are given in the works of Guseinov et al. (Guseinov et al., 1998) in the following recursive form

$$A_n(p) = \frac{n}{p} A_{n-1}(p) + \frac{e^{-p}}{p} \tag{8}$$

and

$$B_n(pt) = \frac{1}{pt}[nB_{n-1}(pt) + c] \tag{9}$$

for $pt \neq 0$. If n is an even number in equation of (9) , $c = 2\sinh(pt)$, otherwise $c = 2\cosh(pt)$. The starting values for recursion relations (8) and (9) are $A_0(p) = e^{-p}/p$ and $B_0(pt) = (e^{pt} - e^{-pt})/pt$. In the case of negative n, Ozmen *et al.* (2003) and Yakar et.al. (Ozmen et al., 2003; Yakar et al., 2006) have again labeled the analytical solution of the integral (5) as

$I(n,n',q,p,t)$. In this case, a different analytical expression for I has been given as

$$I(n,n',q,p,t)=\sum_{i=0}^{2q}{}^{(2)}F_i(q,q)(n'+i)!\sum_{j=0}^{n'+i}\frac{[p(1-t)^{j-n'-i-1}}{j!}\sum_{k=0}^{j}2^{n'-2q+i-k}F_k(j,0)$$
$$\times\left\{e^{-p(1-t)}\left[(-1)^k J_{2q-i+n+k}(pt)-J_{2q-i+n+k}(p)\right]\right.$$
$$\left.+\left[(-1)^{j-k}e^{p(1-t)}-e^{-p(1-t)}\right]K_{2q-i+n+k}(p)\right\} \quad (10)$$

Here J_n and K_n are defined to be

$$J_n(\alpha)=\int_0^2 x^n e^{-\alpha x}dx \qquad K_n(\alpha)=\int_2^\infty x^n e^{-\alpha x}dx \quad (11)$$

and in the case of $\alpha\neq 0$, analytical solutions of these integrals have been given by the recursive relations

$$J_n(\alpha)=-\frac{2^n}{\alpha e^{2\alpha}}+\frac{n}{\alpha}J_{n-1}(\alpha) \quad (12)$$

$$K_n(\alpha)=\frac{2^n}{\alpha e^{2\alpha}}+\frac{n}{\alpha}K_{n-1}(\alpha) \quad (13)$$

for $n\geq 0$ and

$$J_n(\alpha)=-\frac{\alpha}{(n-1)}\left[J_{n-1}(\alpha)+\frac{(-\alpha)^{n-2}}{(n-1)!}\right]-\frac{1}{e^{2\alpha}(n-1)2^{n-1}} \quad (14)$$

$$K_n(\alpha)=\frac{1}{e^{2\alpha}(n-1)2^{n-1}}-\frac{\alpha}{(n-1)}K_{n-1}(\alpha) \quad (15)$$

for $n<0$. The starting values of J and K in eqs. (12-15) are

$$J_0(\alpha)=(1-e^{-2\alpha})/\alpha \qquad K_0=e^{-2\alpha}/\alpha \quad (16)$$

$$J_{-1}(\alpha)=Ei(-2\alpha)-\ell og(|\alpha|)-\gamma \qquad K_{-1}=-Ei(-2\alpha) \quad (17)$$

where $Ei(-2\alpha)$ is the well-known exponential integral (Arfken, 2011) and $\gamma=0.577215664901532860$. Furthermore, for $\alpha=0$ and $n\neq -1$, $J_n(0)=\frac{2^{n+1}}{n+1}$ and $J_{-1}(0)=\ell n(2)$.

J and K auxiliary functions can easily be evaluated for positive n values and

they can be expressed in a series expansion as follows

$$J_n(\alpha) = \lim_{N\to\infty} \sum_{i=0}^{N} \frac{(-\alpha)^i}{i!} \frac{2^{n+i+1}}{n+i+1} \tag{18}$$

$$K_n(\alpha) = \frac{n!}{\alpha^{n+1}} - J_n(\alpha). \tag{19}$$

However, the case for negative n values is a little more complicated and we have obtained the following series expressions

$$J_n(\alpha) = \lim_{N\to\infty} \sum_{\substack{i=0 \\ \neq n-1}}^{N} \frac{(-\alpha)^i 2^{i-n+1}}{i!(i-n+1)} + \frac{(-\alpha)^{n-1}}{(n-1)!} \ell n(2) \tag{20}$$

$$K_n(\alpha) = E_n(\alpha) - J_n(\alpha) \tag{21}$$

Here E is the integral

$$E_n(\alpha) = \int_0^{\infty} x^n e^{-\alpha x} dx \tag{22}$$

for $n < 0$. We note that E is the well-known Gamma function for $n \geq 0$.

For $n < 0$ the E integral diverges, however in the evaluation of molecular integrals the diverging parts of negative and positive terms cancels and in this work we have obtained the net contribution of E integral to the I integral as

$$E_n(\alpha) = -\frac{\alpha}{n-1}\left[E_{n-1}(\alpha) + \frac{(-\alpha)^{n-2}}{(n-1)!} \right] \tag{23}$$

for $n < 0$. This newly introduced $E_n(\alpha)$ expression is essentially a sum of $J_n(\alpha)$ and $K_n(\alpha)$ auxiliary functions of Özmen et al. (2003) and Yakar et al. (Ozmen et al., 2003; Yakar et al., 2006). The starting value of E is $E_{-1}(\alpha) = -\ell og(|\alpha|) - 0.577215664901532860$ Using E auxiliary function and binomial coefficients, another version of I function in eq.(16) of the works of Yakar et al. (Yakar et al., 2006) has been obtained as

$$I(n,n',q,p,t) = \frac{1}{2^{2q+1}} \sum_{i=0}^{q} (-1)^{q-i} F_i(q) M(2i+n, 2q-2i+n', p, t) \tag{24}$$

where

$$M(m,n,p,t) = \sum_{i=0}^{n} F_i(n) \frac{j!}{[p(1-t)]^{i+1}} \sum_{j=0}^{n-i} F_j(n-i) 2^{n-i-j}$$

$$\times \left\{(-1)^j e^{-p(1-t)} J_{m+j}(pt) + (-1)^{n-i-j} e^{p(1-t)} K_{m+j}(p) - e^{-p(1-t)} E_{m+j}(p)\right\}. \quad (25)$$

3. Results and Discussion

In this work, analytical expressions for J and K auxiliary functions occuring in the calculation of two-center molecular integrals using elliptical coordinates have been obtained. Available analytical expressions of B and J are unstable for $n \geq 0$ and their accurate calculation need a demanding process (Ozmen et al., 2003). In order to overcome this instability some researchers have employed a downward recursive approach (Guseinov et al., 1998; Ozmen et al., 2003; Yakar et al., 2006). When n>α the downward recursion has been started from a certain value of n_{top} and eqs.(9) and (12) have been rewritten in the form of downward recursion. Thus authors have accurately computed two-center overlap integrals and two-center Coulomb integrals. Also, Mekelleche and Baba-Ahmed (Mekelleche and BabaAhmed, 1997) have given an analytical expression in the form of serial expansion for B. Our main aim in this work is to give new analytical expressions for auxiliary functions J, K and I to compare them with other analytical expressions in the literature. For this purpose, Eq.(24) obtained in this work and eq.(16) of the works of Yakar et al. (Yakar et al., 2006) for I integral are given in Table 1. Furthermore, we have tested our expressions by calculating two-center electric field gradient integrals with large negative n values over STO's by using J, K and I auxiliary functions obtained in this study. One reason for choosing the EFG integrals to test our analytical expressions is the evaluation of these integrals involves using of I integrals given in eq.(5) with negative n values up to $n = -3$. Another one is that there are only a few works in the literature dealing with these integrals. In the two of these works (Pietrovito et al., 1984; Kim et al., 1986) authors have used the Fourier Convolution theorem to evaluate EFG integrals. In another work, Guseinov and Görgün have employed unsymmetrical one-range addition theorem (Guseinov, 2011). $\zeta - function\ method$ was also used by Fernandez et al. (Fernandez et al., 2006) and Ema et al. (Ema et al., 2008). However we have calculated these integrals by using recursive J, K and I given in the works of Özmen et al. (Ozmen et al., 2003), Yakar et al. (Yakar et al., 2006) and Akin (Akin, 2008). We have done same calculations by using J, K, E and I auxiliary functions given in this work.

In Table 2 we have compared our results with the results obtained by using the

auxiliary function J , K and I given in the works of Özmen et al. (Ozmen et al., 2003) and Yakar et al. (Yakar et al., 2006)2006) and the values given in the literature. The values in 10th and 11th columns of Table 2 are obtained by using J, K and I expressions given in the works of Özmen et al. (Ozmen et al., 2003) and Yakar et al. (Yakar et al., 2006) and the expressions obtained in this work, respectively. The values in the last column are calculated in the works of Fernandez et al. (Fernandez et al., 2006) and Ema et al. (Ema et al., 2008) by using Fourier convolution method. The calculations were performed by using a computer program written in Fortran. As it is seen from these tables, the results obtained from both expressions are in good agreement with each other and the literature.

4. Conclusions

There are many methods in the literature to evaluate one- and two-electron multicenter molecular integrals over Slater-type orbitals (for example, Fourier convolution method, zeta-function method). However, these methods requires tiresome and extensive mathematical work. I auxiliary function obtained in this work is quite useful for the calculation of abovementioned integrals since it is valid for negative n values and has a simple form. In the methods as Guseinov's serial expansion method (Guseinov, 1985), multicenter molecular integrals over Slater-type orbitals are reduced to one-center integrals over Slater-type orbitals by the expansion of Slater-type orbitals about a displaced center. Such multicenter molecular integrals can be reduced to two-center molecular integrals and these integrals can easily be calculated by I auxiliary functions obtained in this work.

Table 1. Values of $I(n,n',q,p,t)$ auxiliary functions ($n'=2$, $q=1$, $p=0.8$, $t=0.5$)

n	Eq.(24) of this work	Eq.(16) of Ref.[8,9]
-5	0.389416765515819048021022100192 79	0.389416765515819048021022100192 79
-4	-0.621626280751972823915089089605 22	-0.621626280751972823915089089605 22
-3	1.077087324015408863673774927150 20	1.077087324015408863673774927150 20
-2	-0.274461826906081603883782772827 55	-0.274461826906081603883782772827 55
-1	-5.294138709228672682206696410065 07	-5.294138709228672682206696410065 07
0	-9.340905197006674379254617088083 44	-9.340905197006674379254617088083 44
1	-28.821970028568407692402381000677 1	-28.821970028568407692402381000677 1
2	-119.425243440923029382409224664043	-119.425243440923029382409224664043
3	-598.815281744536476379448764400859	-598.815281744536476379448764400859
4	-3385.698686474773018263121834560 09	-3385.698686474773018263121834560 09
5	-19886.551403458812577337363209203 3	-19886.551403458812577337363209203 3

Table 2. Values of two-center EFG integrals over STOs for various quantum numbers, screening parameters and internuclei distances (in a.u.)

n	ℓ	m	ζ	n'	ℓ'	m'	ζ'	R_{ab}	With J, K and I in this work	With J, K and I in the works of Yakar et al.(Yakar et al., 2006)	Literature
1	0	0	2.6909	1	0	0	2.6909	3.0150	7.29683432097278895314777370217658 5E-02	7.29683432097278895314777370217658 5E-02	0.07296834 (*)
1	0	0	2.6909	2	0	0	0.7075	3.0150	1.36613744414284751848345737130303 6E-02	1.36613744414284751848345737130303 6E-02	0.01366137 (*)
1	0	0	2.6909	2	1	0	0.8449	3.0150	1.14007850892520595944185914591845 1E-02	1.14007850892520595944185914591845 1E-02	0.01140079 (*)
1	0	0	8.6533	2	1	0	2.6693	1.7330	3.38906180711127806925841588479981 7E-02	3.38906180711127806925841588479981 7E-02	0.03389062 (**)
2	1	0	2.6693	2	1	0	2.6693	1.7330	0.53055649236204726567490361552320 3E-00	0.53055649236204726567490361552320 3E-00	0.5305565 (**)
2	1	1	2.4965	2	1	1	2.4965	1.7330	0.21431805669485109676200384568024 0E-00	0.21431805669485109676200384568024 0E-00	0.2143181 (**)

(*) (Pietrovito et al., 1984)

(**)(Kim et al., 1986)

References

Akin E (2008). Evaluation of two-center electric field gradient integrals over STOs using elliptical coordinates. *Eur Phys J D* 49: 305-310.

Arfken GB, Weber HJ, Harris FE (2011). *Mathematical methods for physicists,* Academic Press, New York.

Ema I, Lopez R, Fernandez JJ, Ramirez G, Rico JF (2008). Auxiliary functions for molecular integrals with Slater-type orbitals. II. Gauss transform methods. *International Journal of Quantum Chemistry* 108: 25-39.

Fernandez JJ, Lopez R, Ema I, Ramirez G, Rico JF (2006). Auxiliary functions for molecular integrals with slater-type orbitals. I. translation methods. *International Journal of Quantum Chemistry* 106: 1986-1997.

Guseinov II (1970). Analytical evaluation of two-centre Coulomb, hybrid and one-electron integrals for Slater-type orbitals. *Journal of Physics B: Atomic and Molecular Physics* 3: 1399-1406.

Guseinov II (1985). Expansion of Slater-type orbitals about a displaced center and the evaluation of multicenter electron-repulsion integrals. *Physical Review A* 31: 2851.

Guseinov II, Görgün NS (2011). Calculation of multicenter electric field gradient integrals over Slater-type orbitals using unsymmetrical one-range addition theorems. *J Mol Model* 17.

Guseinov II, Ozmen A, Atav U, Yuksel H (1998). Computation of overlap integrals over Slater-type orbitals using auxiliary functions. *International Journal of Quantum Chemistry* 67: 199-204.

Jones HW (1987). Exact formulas and their evaluation for slater-type-orbital overlap integrals with large quantum numbers. *Physical Review A* 35: 1923-1926.

Kim HW, Hameka HF Zeroka D (1986). Calculation of the deuterium electric-field gradient in Df. *J Chem Phys* 84: 5639-5644.

Mekelleche SM, BabaAhmed A (1997). Calculation of the one-electron two-center integrals over Slater-type orbitals by means of the ellipsoidal coordinates method. *International Journal of Quantum Chemistry* 63: 843-852.

Mulliken RS, Rieke CA, Orlof D, Orlof H (1949). Formulas and numerical tables for overlap integrals. *J Chem Phys* 17.

Ozmen A, Karakas A, Atav U, Yakar Y (2003). Computation of two-center coulomb integrals over Slater-type orbitals using elliptical coordinates. *International Journal of Quantum Chemistry* 91: 13-19.

Pashaev FG (2009). Use of filter-steinborn b and guseinov Q(ns)(q) auxiliary functions in evaluation of two-center overlap integrals over Slater type orbitals. *J Math Chem* 45: 884-890.

Pietrovito AJ, Hameka HF, Zeroka D (1984). Calculation of the deuterium electric-field gradient in Lid. *J Chem Phys* 81: 1960-1965.

Roothaan CCJ (1951). New developments in molecular orbital theory. *Rev Mod Phys* 23: 69-89.

Slater C (1960). *Quantum Theory of Atomic Structure,* London:McGraw-Hill Book Company Inc., London.

Yakar Y, Ozmen A, Atav U (2006). Evaluation of two-center one- and two-electron integrals over Slater type orbitals. *Chinese J Chem* 24: 603-608.

Zeroka D, Hameka, H.F. (1966). Calculation of magnetic shielding constants of diatomic molecules. I. General theory and application to HF molecule. *J Chem Phys* 45: 300-311.