

# Approximated computation of atomic three- and four-electron integrals over $B$ -splines

Saito Shiro L.

## Abstract

Approximated computational methods of atomic three- and four-electron integrals over  $B$ -splines which appear in Hylleraas-CI calculations are presented. The present methods represent the three- and four-electron integrals to sums of products of two-electron integrals over the  $B$ -splines. Comparison of the three- and four-electron integral values computed using the approximated methods with those given by Ruiz [J. Math. Chem. 46, 24 (2009) and J. Math. Chem. 46, 1322 (2009).] showed relative errors of  $\sim 10^{-14}$ .

## 1. INTRODUCTION

In quantum mechanical calculations for atomic systems, atomic orbitals are usually expanded with the appropriate basis functions. The most commonly used basis functions is Slater-type functions (STFs) and Gaussian-type functions (GTFs). Unfortunately, their linear dependence sometimes disturbs the calculations. The use of  $B$ -splines<sup>1,2</sup> can avoid this problem. The  $B$ -splines of order  $K$   $\{B_{i,K}(r)\}$  are piecewise polynomials of degree  $K-1$  on a knot sequence in a cavity of radius  $R$ . The knot sequence  $\{t_i\}$  is a set of points defined on an interval  $[0, R]$ .  $B_{i,K}(r)$  is nonzero in the interval  $[t_i, t_{i+K})$ . The advantage of  $B$ -splines is that they are very flexible and are relatively free from computational linear dependence. It is possible to apply a common  $B$ -spline set to all atoms, irrespective of orbital symmetry, without loss of accuracy. Atomic calculations with  $B$ -splines yield highly accurate energies and properties<sup>3-5</sup>. Therefore, the development of the atomic calculation method with  $B$ -splines is very interesting and important.

To calculate accurate atomic properties, one must calculate wave functions which are considered

electron correlation effects. There are various computational methods for dealing with such the wave functions. In particular, the configuration interaction (CI) method is extensively used. A CI wave function is expressed with a linear combination of configurations state functions (CSFs). Although the CI method can easily account for static correlation effects, it is poor at accounting for dynamic correlation effects. To effectively consider the dynamic correlation effects, wave functions must include explicitly inter-electronic distances ( $r_{ij}$ ). Hylleraas-type method<sup>6</sup> is one of the methods and gives highly accurate energy of two-electron atoms<sup>7</sup>. Unfortunately, it is difficult to apply the Hylleraas-type method to many-electronic atoms because many-electron integrals are required. The many-electron integral for the  $N$ -electronic atom is generally written as

$$\iint \dots \int d\mathbf{r}_1 d\mathbf{r}_2 \dots d\mathbf{r}_N A(\mathbf{r}_1) B(\mathbf{r}_2) \dots C(\mathbf{r}_N) r_{12}^s r_{13}^t \dots r_{N-1N}^u A'(\mathbf{r}_1) B'(\mathbf{r}_2) \dots C'(\mathbf{r}_N), \quad (1)$$

where  $A, B, C, \dots$  are atomic functions. The many-electron integrals of many-electronic atoms are expressed in complicated formulas, which are generally difficult to calculate. There is a method that retains the advantages of the Hylleraas-type method and reduces many-electron integrals. This is the method combined the Hylleraas-type method and the CI method, and is called Hylleraas-CI method.<sup>8</sup> The Hylleraas-CI method usually deals with wave functions expanded in configurations containing at most one  $r_{ij}^s$ . Therefore, the Hylleraas-CI method requires only up to four-electron integrals, even for atoms with more than four electrons. The Hylleraas-CI method was first applied by Sims and Hagstrom to the Be atom.<sup>8</sup>

The three-electron integrals<sup>9-15</sup> and four-electron integrals<sup>9,16,17</sup> over STFs have been formulated by various authors. The formulas for the three- and four-electron integrals are complicated and computationally loaded. This remains true for the integrals over the  $B$ -splines. However, it is possible to avoid this computational difficulty using an approximated computational method of many-electron integrals proposed by Kutzelnigg and Klopper<sup>18</sup>. Their method approximates a many-electron integral to sums of products of two-electron integrals by incomplete set insertion, e.g.,

$$\begin{aligned} & \iiint d\mathbf{r}_1 d\mathbf{r}_2 d\mathbf{r}_3 A(\mathbf{r}_1) B(\mathbf{r}_2) C(\mathbf{r}_3) r_{12}^s r_{13}^t A'(\mathbf{r}_1) B'(\mathbf{r}_2) C'(\mathbf{r}_3) \\ &= \sum_i \iint d\mathbf{r}_1 d\mathbf{r}_2 A(\mathbf{r}_1) B(\mathbf{r}_2) r_{12}^s \psi_i(\mathbf{r}_1) B'(\mathbf{r}_2) \\ & \times \iint d\mathbf{r}_1 d\mathbf{r}_2 \psi_i(\mathbf{r}_1) C(\mathbf{r}_2) r_{12}^s A'(\mathbf{r}_1) C'(\mathbf{r}_2), \end{aligned} \quad (2)$$

where  $\{\psi_i\}$  is an incomplete set. If  $\{\psi_i\}$  are expanded with flexible basis functions, Eq.(1) may yield highly accurate values. The  $B$ -splines are suitable for this approximation method.

Our purpose in this work is to formulate many-electron integrals over the  $B$ -splines which appear in Hylleraas-CI calculations using the approximation method and to check the accuracy of the resulting approximated formulas. There are many formulations and calculations of many-electron integrals. Most of them are for the integrals over the STFs. We check the accuracy of the approximated formulas by transforming the  $B$ -spline many-electron integrals into the STF integrals. This transformation is carried out using the  $B$ -spline expansion coefficients of the STFs. This accuracy check may be valid because the STFs should be accurately expanded with  $B$ -splines.<sup>19</sup>

Below, Section 2 provides theoretical aspects and the resulting approximated formulas of many-electron integrals. Section 3 explains computational aspects for the accuracy check. Section 4 discusses relative errors of the three- and four-electron integral values given from the approximated formulas to Ruiz's results.

## 2. THEORY

In this section, we present the formulas of approximated three- and four-electron integrals which appear in Hylleraas-CI calculations. To derive formulas of the integrals, we define a projection operator

$$p(1) = \sum_I |I(1)\rangle \langle I(1)| \quad (3)$$

using orthonormal functions  $\{I\}$ , The function  $I$  is written as

$$I(1) = i(1) Y_{l_i}^{m_i}(1), \quad (4)$$

where  $i$  is a radial function and  $Y_{l_i}^{m_i}$  is the spherical harmonics. Hereafter, the orthogonal functions that construct the projection operator  $p$  are written by  $I, J, K, \dots$ , and their radial functions are written by  $i, j, k, \dots$ . The summation of Eq.(3) is the simple notation as follows:

$$\sum_I \equiv \sum_{i=1}^N \sum_{l_i=0}^{\infty} \sum_{m_i=-l_i}^{l_i} . \quad (5)$$

The many-electron integrals are transformed by inserting the projection operators  $p$  between the inter-electronic distances, e.g.,

$$\begin{aligned} \langle ABC | r_{12}^s r_{13}^t r_{23}^u | A' B' C' \rangle &= \langle ABC | r_{12}^s p(1) r_{13}^t p(2) p(3) r_{23}^u | A' B' C' \rangle \\ &= \sum_{IJK} \langle AB | r_{12}^s | IJ \rangle \langle IC | r_{12}^t | AK \rangle \langle JK | r_{12}^u | B' C' \rangle. \end{aligned} \quad (6)$$

Here,  $A, B, C, \dots$  are atomic orbitals, and their radial functions are written by  $a, b, c, \dots$ . All the radial functions in Eq.(6) are expanded with the  $B$ -splines. We simply write integrals by omitting electronic coordinate numbers of atomic orbitals; functions in the bra and the ket are arranged in order of the electronic coordinate number:

$$\langle ABC | r_{12}^s r_{13}^t r_{23}^u | A' B' C' \rangle = \langle A(1)B(2)C(3) | r_{12}^s r_{13}^t r_{23}^u | A'(1) B'(2) C'(3) \rangle. \quad (7)$$

The three- and four-electron integrals are transformed into sums of products of two-electron integrals using the projection operators  $p$ . First, we show transformed formulas of three-electron integrals. To this end, two projection operators  $p$  are inserted between inter-electronic distances. After some manipulation, the result is as follows:

$$\begin{aligned} \langle ABC | r_{12}^s r_{13}^t r_{23}^u | A' B' C' \rangle &= \sum_{IJK} \langle AB | r_{12}^s | IJ \rangle \langle IC | r_{12}^t | AK \rangle \langle JK | r_{12}^u | B' C' \rangle \\ &= \sum_{k_1=0}^{k_{1max}} \sum_{k_2=0}^{k_{2max}} \sum_{k_3=0}^{k_{3max}} \sum_{ijk} (ai, bj)_{k_1}^s (a'i, ck)_{k_2}^t (b'j, c'k)_{k_3}^u \\ &\quad \times \sum_{l_1=\max(|k_1-l_A|, |k_2-l_A|)}^{\min(k_1+l_A, k_2+l_A)} \sum_{l_2=\max(|k_1-l_B|, |k_3-l_B|)}^{\min(k_1+l_B, k_3+l_B)} \sum_{l_3=\max(|k_2-l_C|, |k_3-l_C|)}^{\min(k_2+l_C, k_3+l_C)} \\ &\quad \times \sum_{m=\max(-l_1, -l_2+m_A+m_B, -l_3+m_A, -m_B)}^{\min(l_1, l_2+m_A+m_B, l_3+m_A, -m_C)} c^{k_1}(l_A, m_A, l_1, m) c^{k_1}(l_A, m_A, l_1, m) \\ &\quad \times c^{k_1}(l_B, m_B, l_2, m_B - m) c^{k_2}(l_2, m_A + m_B - m, l_B, m_B) \\ &\quad \times c^{k_2}(l_C, m_C, l_3, m - m_A + m_C) c^{k_3}(l_3, m - m_A + m_C, l_C, m_C) \end{aligned} \quad (8)$$

with

$$(ab, cd)_k^n = \sum_{s=0}^{\lfloor \frac{n+1}{2} \rfloor} D_{ks}^n \int dr_1 \int dr_2 a(r_1) b(r_1) \frac{r_1^{k+2s}}{r_1^{k+2s-n}} c(r_2) d(r_2), \quad (9)$$

where is  $c^k(lm, l'm')$  is Condon-Shortley coefficient and  $D_{ks}^n$  is the expansion coefficient of  $r_{12}^n$ .  $k_{1max}$  is  $s/2$  for even  $s$  values,  $\infty$  for odd  $s$  values.  $k_{2max}$  and  $k_{3max}$  are same as  $k_{1max}$ . Taking  $u = 0$  yields the three-electron integral:

$$\begin{aligned}
 \langle ABC | r_{12}^s r_{13}^t | A' B' C' \rangle &= \sum_{IJK} \langle AB | r_{12}^s | IB' \rangle \langle IC | r_{12}^t | A' C' \rangle \\
 &= \sum_{k_1=|l_B-l_{B'}|}^{l_B+l_{B'}} \sum_{k_2=|l_C-l_{C'}|}^{l_C+l_{C'}} \sum_{ijk} (ai, bb')_{k_1}^s (a'i, cc')_{k_2}^t \\
 &\quad \times \sum_{l=\max(|k_1-l_A|, |k_2-l_{A'}|)}^{\min(k_1+l_A, k_2+l_{A'})} c^{k_1}(l_{A'} m_{A'}, l m_{A'} + m_B - m_{B'}) \\
 &\quad \times c^{k_1}(l m_{A'} + m_B - m_{B'}, l_A m_A) c^{k_1}(l_B m_B, l_B m_{B'}) c^{k_2}(l_C m_C, l_C m_{C'})
 \end{aligned} \tag{10}$$

Three-electron kinetic integrals are transformed inserting the projection operator  $p$  between inter-electronic distances and the kinetic operator. The resulting formulas are as follows:

$$\begin{aligned}
 \langle ABC | r_{12}^s T_1 r_{13}^t | A' B' C' \rangle &= \sum_{IJK} \langle AB | r_{12}^s | IB' \rangle \langle I | T | J \rangle \langle JC | r_{12}^t | A' C' \rangle \\
 &= \sum_{k_1=|l_B-l_{B'}|}^{l_B+l_{B'}} \sum_{k_2=|l_C-l_{C'}|}^{l_C+l_{C'}} \sum_{l=\max(|k_1-l_A|, |k_2-l_{A'}|)}^{\min(k_1+l_A, k_2+l_{A'})} \\
 &\quad \times \sum_{ijk} (ai, bb')_{k_1}^s (i | T | j)_l (a' i, cc')_{k_2}^t \\
 &\quad \times c^{k_2}(l_A m_A, l m_A + m_B - m_{B'}) c^{k_1}(l m_A + m_B - m_{B'}, l_A m_A) \\
 &\quad \times c^{k_1}(l_B m_B, l_B m_{B'}) c^{k_2}(l_C m_C, l_C m_{C'})
 \end{aligned} \tag{11}$$

and

$$\begin{aligned}
 \langle ABC | r_{12}^s T_2 r_{13}^t | A' B' C' \rangle &= \sum_{IJ} \langle AB | r_{12}^s | IJ \rangle \langle J | T | B' \rangle \langle IC | r_{12}^t | A' C' \rangle \\
 &= \sum_{k_1=|l_B-l_{B'}|}^{l_B+l_{B'}} \sum_{k_2=|l_C-l_{C'}|}^{l_C+l_{C'}} \sum_{ij} (ai, jb)_{k_1}^s (j | T | b')_B (a' i, cc')_{k_2}^t \\
 &\quad \times \sum_{l=\max(|k_1-l_A|, |k_2-l_{A'}|)}^{\min(k_1+l_A, k_2+l_{A'})} c^{k_2}(l_{A'} m_{A'}, l m_{A'} + m_B - m_{B'}) \\
 &\quad \times c^{k_1}(l m_{A'} + m_B + m_{B'}, l_A m_A) c^{k_1}(l_B m_B, l_B m_{B'}) c^{k_2}(l_C m_C, l_C m_{C'}),
 \end{aligned} \tag{12}$$

where  $T$  is the kinetic operator:

$$T = -\frac{1}{2} \frac{d^2}{dr^2} + \frac{l(l+1)}{2r^2} \quad (13)$$

and  $(i|T|j)_l$  is a one-electron kinetic radial integral. Generally, computation of the three-electron kinetic integral is laborious. Eqs.(11) and (12) allow for easy and accurate computation of the approximated kinetic integral.

Approximated four-electron integrals are also derived in the similar way to the three-electron integrals as follows:

$$\begin{aligned} \langle ABCD | r_{12}^s r_{13}^t r_{34}^u | A' B' C' D' \rangle &= \sum_{IJ} \langle AB | r_{12}^s | IB' \rangle \langle IC | r_{12}^t | A' J \rangle \langle JD | r_{12}^u | C' D' \rangle \\ &= \sum_{k_1=|l_B-l_{B'}|}^{l_B+l_{B'}} \sum_{k_2=0}^{\infty} \sum_{k_3=|l_D-l_{D'}|}^{l_D+l_{D'}} \sum_{ij} (ai, bb')_{k_1}^s (a' i, cj)_{k_2}^t (c' j, dd')_{k_3}^u \\ &\quad \times \sum_{l_1=\max(|k_1-l_A|, |k_2-l_{A'}|)}^{\min(k_1+l_A, k_2+l_{A'})} c^{k_2}(l_A m_A, l_1 m_1) c^{k_1}(l_1 m_1, l_A m_A) \\ &\quad \times \sum_{l_2=\max(|k_2-l_C|, |k_3-l_{C'}|)}^{\min(k_2+l_C, k_3+l_{C'})} c^{k_2}(l_C m_C, l_2 m_2) c^{k_3}(l_C m_C, l_2 m_2) \\ &\quad \times c^{k_1}(l_B m_B, l_{B'} m_{B'}) c^{k_3}(l_D m_D, l_{D'} m_{D'}) \end{aligned} \quad (14)$$

and

$$\begin{aligned} \langle ABCD | r_{12}^s r_{13}^t r_{14}^u | A' B' C' D' \rangle &= \sum_{IJ} \langle AB | r_{12}^s | IB' \rangle \langle IC | r_{12}^t | JC' \rangle \langle JD | r_{12}^u | A' D' \rangle \\ &= \sum_{k_1=|l_B-l_{B'}|}^{l_B+l_{B'}} \sum_{k_2=|l_C-l_{C'}|}^{l_C+l_{C'}} \sum_{k_3=|l_D-l_{D'}|}^{l_D+l_{D'}} \sum_{ij} (ai, bb')_{k_1}^s (ij, cc')_{k_2}^t (a' j, dd')_{k_3}^u \\ &\quad \times \sum_{l_1=|k_1-l_A|}^{k_1+l_A} \sum_{l_2=|k_3-l_{A'}|}^{k_3+l_{A'}} c^{k_2}(l_A m_A, l_2 m_{A'} + m_{D'} - m_D) \\ &\quad \times c^{k_2}(l_2 m_{A'} + m_{D'} - m_D, l_1 m_A + m_B - m_{B'}) \\ &\quad \times c^{k_1}(l_1 m_A + m_B - m_{B'}, l_A m_A) c^{k_1}(l_B m_B, l_{B'} m_{B'}) \end{aligned}$$

$$\times c^{k_2}(l_C m_C, l_C' m_C') c^{k_3}(l_D m_D, l_D' m_D'). \quad (15)$$

Thus, the three- and four-electron integrals over the  $B$ -splines required for the Hylleraas-CI method are expressed as sums of products of two-electron integrals.

### 3. COMPUTATION

#### A. $B$ -splines

This work calculated all the two-electron integrals Eq.(9) and the one-electron kinetic integrals using the  $B$ -splines. The atomic radial function  $P(r)$  is expanded with the  $B$ -splines and enforces the boundary conditions  $P(0) = 0$  and  $P(R) = 0$ . Since the first and the last terms of the  $B$ -splines with  $K$ -fold multiple knots are nonzero at  $r = 0$  and  $r = R$ , respectively, they are removed from the basis function to satisfy the boundary conditions. Thus, we obtain  $N$ -term  $B$ -spline sets. We use the following two knot sequences with endpoints of  $K$ -fold multiplicity. Several methods that generate the knot sequence have been proposed by Gilbert and Bertoncini.<sup>20</sup> In atomic calculations, the knot sequence that concentrates near the nucleus is required because the atomic orbitals rapidly change near the nucleus. Hence, an exponential or a summational knot sequence is suitable for atomic calculations. The exponential knot sequence (EKS) is as follows:

$$R_1, R_1\alpha, R_1\alpha^2, \dots, R, \quad (16)$$

where  $\alpha = (R/R_1)^{1/(N-K+2)}$ ,  $R_1$  is the initial interval of the knot sequence. The other is as follows:

$$R_1, R_1(1 + \beta), R_1(1 + \beta + \beta^2), \dots, R. \quad (17)$$

Here,  $\beta$  is the parameter characterizing the distribution of the knots, and is chosen to satisfy the following condition:

$$R = R_1(1 + \beta + \beta^2 + \dots + \beta^{N-K+2}) \quad (\beta \geq 1). \quad (18)$$

This knot sequence is referred to as a ‘summational knot sequence’ (SKS).

In our previous work<sup>19</sup>, it was shown that the STF can be accurately expanded with a  $B$ -spline set. A STF can be expanded with an error of  $\sim 10^{-15}$  in a 100-term  $B$ -spline set with  $K = 15$ ,  $R = 60$  and  $10^{-4} \leq R_1 \leq 10^{-2}$ . This result was obtained for both EKS and SKS. Therefore, the present work used the parameters  $K = 15$ ,  $R = 60$  and  $R_1 = 10^{-5}$ ,  $10^{-4}$ ,  $10^{-3}$ , and  $10^{-2}$ .

#### B. Three- and four-electron integrals

The three- and four-electron integrals obtained from our approximated formulas are compared ones given by Ruiz<sup>15,17</sup>. The three- and four-electron integrals evaluated by Ruiz are as follows:

##### 1. Three-electron integral (EI3)

$$\langle ABC | r_{12}^s r_{13}^t | A' B' C' \rangle. \quad (19)$$

2. Three-electron kinetic integral (EI3K)

$$\langle ABC | r_{12} T_1 r_{13} | A' B' C' \rangle. \quad (20)$$

3. Four-electron integral type 1 (EI41)

$$\langle ABCD | r_{12} r_{13} r_{34}^{-1} | A' B' C' D' \rangle. \quad (21)$$

4. Four-electron integral type 2 (EI42)

$$\langle ABCD | r_{12} r_{13} r_{14}^{-1} | A' B' C' D' \rangle. \quad (22)$$

Here,  $A, B, C$ , and  $D$  are STFs with exponential parameters  $\zeta$ , e.g.,

$$A \equiv r_i^{n_i-1} e^{-\zeta_i r_i} Y_{l_i}^{m_i}(\theta, \varphi). \quad (23)$$

The exponential parameter of  $A$  is written by  $\zeta'_i$ . We define  $\omega_i \equiv \zeta_i + \zeta'_i$ . In this work, the radial part of STFs is expanded with the  $B$ -spline set as follows:

$$r^n e^{-\zeta r} \approx \sum_{i=2}^{N+1} C_i^{n,\zeta} B_{i,K}(r), \quad (24)$$

where  $C_i^{n,\zeta}$  are linear expansion coefficients.  $C_i^{n,\zeta}$  were determined by solving the system of linear equations:

$$\sum_{j=2}^{N+1} \left[ \int_0^R dr B_{i,K}(r) B_{j,K}(r) \right] C_j^{n,\zeta} = \int_0^R dr B_{i,K}(r) r^n e^{-\zeta r}, \quad (i = 2, \dots, N+1). \quad (25)$$

All the integrals were calculated by the Gauss integration procedure. The radial functions that construct the projection operator  $p$  were the functions obtained by dividing the eigenfunctions of the overlap matrix  $\mathbf{S}$  by the square root of its eigenvalues; the matrix element of  $\mathbf{S}$  is

$$(\mathbf{S})_{i-1,j-1} = \int_0^R dr B_{i,K}(r) B_{j,K}(r), \quad (i, j = 2, \dots, N+1). \quad (26)$$

## 4. RESULTS AND DISCUSSION

In Section 2, we showed the approximated many-electron integral formulas with  $B$ -splines which appear in Hylleraas-CI calculations. The approximated many-electron integrals require radial two-electron integrals  $(ai, bj)_\lambda^s$ ,  $(ab, ij)_\lambda^s$ , and  $(ai, bc)_\lambda^s$ . These radial two-electron integrals must be stored. The remarkable feature of this work is that the approximated three-electron kinetic integrals were obtained. The computational formulas of three-electron kinetic integrals over  $B$ -splines are very complicated. This work transformed a three-electron kinetic integral into sums of products of two-electron integrals and a one-electron kinetic integral. Hence, three-electron kinetic integrals can be



easily computed by our formulas.

Table 1 summarizes averaged relative errors of our EI3, EI3K, EI41, and EI42 values to the Ruiz's values<sup>15,17</sup>. Only the error in the EI3K value of the charge distribution ( $3d_13d_1, 2p_12p_1'', 3d_13d_1''$ ) is very large. This value given by Ruiz is probably incorrect. The averaged relative errors of EI3K were calculated excluding this value. It should be noted that the errors arise not only from the construction of the projection operator  $p$ , but also from the approximation of the STFs. The averaged relative errors are large at  $R_1 = 10^{-5}$  for both EKS and SKS. The averaged relative error depends on  $R_1$  and is larger for smaller  $R_1$  value. This is because a knot sequence with small  $R_1$  value is concentrated near the nucleus and sparse away from the nucleus. The present comparison shows that the  $B$ -spline set on the SKS with  $R_1 = 10^{-2}$  and  $R = 60$  causes small relative errors ( $\sim 10^{-14}$ ). Since the error of approximation using the  $B$ -splines of STFs is  $\sim 10^{-15}$ , the approximation using the  $B$ -splines of the projection operator  $p$  is accurate.

Table 1. Averaged relative errors of EI3, EI3K, EI41, and EI42 to Ruiz's values.

$R_1$	$10^{-5}$	$10^{-4}$	$10^{-3}$	$10^{-2}$
EI3				
EKS	8.55E-12	3.39E-13	3.67E-14	5.04E-14
SKS	4.99E-13	6.19E-14	2.57E-14	1.54E-14
EI3K				
EKS	5.23E-12	3.57E-14	4.45E-14	6.55E-14
SKS	4.44E-14	5.98E-14	3.21E-14	2.50E-14
EI41				
EKS	3.61E-12	1.60E-13	3.96E-14	4.07E-14
SKS	1.97E-13	4.88E-14	3.26E-14	2.11E-14
EI42				
EKS	3.93E-12	1.68E-13	4.52E-14	4.70E-14
SKS	2.15E-13	3.35E-14	2.79E-14	2.10E-14

Tables 2, 3, 4, and 5 respectively summarize EI3, EI3K, EI41, and EI42 values together with Ruiz's values. Our integrals are calculated using the EKS with  $R_1 = 10^{-3}$  and the SKS with  $R_1=10^{-2}$ . These knot sequences give results with small errors. Above mentioned, the EI3K value of the charge distribution ( $3d_13d_1, 2p_12p_1'', 3d_13d_1''$ ) given by Ruiz is probably incorrect. The other integrals are in good agreement with our integrals. In Ruiz's EI41 and EI42 tables, the charge distribution ( $3d_{-2}3f_0, 4f_14d_{-1}, 4d_14d_{-1}'', 4d_{-2}4f_0''$ ) is incorrect for ( $3d_{-2}3d_0, 4f_14f_{-1}, 4d_14d_{-1}'', 4d_{-2}4f_0''$ ).

Table 2. Comparison of E13 values: the charge distributions are constructed with the exponents  $\zeta = 1.40$  for STFs with " , otherwise  $\zeta = 2.86$ .

Charge distribution	$\omega_1$	$\omega_2$	$\omega_3$	$s$	$t$	EKS ( $R_1 = 10^{-3}$ )	SKS ( $R_1 = 10^{-5}$ )	Ruiz
$(1s1s, 1s2s^* 2s1s^*)$	5.72	4.26	4.26	1	1	0.43360 35040 31653 9E-05	0.43360 35040 31628 96644 48861 48030E-05	
$(2p_0^* 2p_0^*, 1s1s, 2s^* 2s^*)$	2.80	5.72	2.80	1	1	0.10739 78306 79427 9E-02	0.10739 78306 79424 68755 47273 71639E-02	
$(1s2s, 2p_1 1s^*, 2s^* 2p_1^*)$	5.72	4.26	2.80	1	1	0.59252 28510 41699 6E-06	0.59252 28510 41682 36719 83703 10602E-06	
$(3p_0^* 2p_0^*, 2p_0^* 2p_0^*, 2p_0^* 2p_0^*)$	5.72	5.72	4.26	1	1	0.49948 55683 00041 1E-06	0.49948 55683 00037 99144 99168 01541E-06	
$(1s3d_0^*, 1s1s, 1s3d_0^*)$	4.26	5.72	4.26	1	1	-0.13239 00165 89553 0E-06	-0.13239 00165 89545 99710 26215 19568E-06	
$(3d_0^* 3d_0^*, 1s1s, 3d_0^* 3d_0^*)$	5.72	5.72	4.26	1	1	0.30436 13541 39610 3E-05	0.30436 13541 39604 44980 47650 22825E-05	
$(3d_0^* 3d_0^*, 3d_0^* 4d_0^*, 4d_0^* 4d_0^*)$	5.72	5.72	4.26	1	1	0.60815 81672 25820 7E-05	0.60815 81672 25807 7E-05	
$(4f_0^* 4f_0^*, 4f_0^* 4f_0^*, 4f_0^* 4f_0^*)$	5.72	5.72	4.26	1	1	0.18668 10714 43643 3E-04	0.18668 10714 43643 30085 62633 86625E-04	
$(5g_0^* 5g_0^*, 5g_0^* 5g_0^*, 5g_0^* 5g_0^*)$	5.72	5.72	4.26	1	1	-0.38139 83741 23943 0E-06	-0.38139 83741 23940 87301 25483 13573E-06	
$(6h_0^* 6h_0^*, 6h_0^* 6h_0^*, 6h_0^* 6h_0^*)$	5.72	5.72	4.26	1	1	0.16580 01348 56814 2E+00	0.16580 01348 56801 11415 40854 65832E+00	
$(1s1s, 1s2s^* 1s2s^*)$	5.72	4.26	4.26	1	-1	0.46067 93755 92963 0E-05	0.46067 93755 92941 44439 91694 42396E-05	
$(2p_1^* 2p_1^*, 1s1s, 2s^* 2s^*)$	2.80	5.72	2.80	1	-1	0.17961 56183 43784 7E-03	0.17961 56183 43780 79836 75585 24594E-03	
$(1s2s, 1s2p_0^*, 2s^* 2p_0^*)$	5.72	4.26	2.80	1	-1	-0.29325 70321 56337 7E-06	-0.29325 70321 56326 76315 76754 18333E-06	
$(3s3s, 3p_1^* 3p_1^*, 3p_1^* 3p_1^*)$	5.72	4.26	2.80	1	-1	0.48775 40916 66589 7E-04	0.48775 40916 66583 96596 86914 74376E-04	
$(3d_1^* 3d_1^*, 1s1s, 3d_1^* 3d_1^*)$	5.72	5.72	4.26	1	-1	0.88580 21951 81444 7E-06	0.88580 21951 81417 74242 20122 35173E-06	
$(3d_0^* 3d_0^*, 3d_0^* 3d_0^*, 3d_0^* 3d_0^*)$	5.72	5.72	4.26	1	-1	0.39119 62943 71515 5E-06	0.39119 62943 71525 23817 56562 34654E-06	
$(4f_0^* 4f_0^*, 4f_0^* 4f_0^*, 4f_0^* 4f_0^*)$	5.72	5.72	4.26	1	-1	0.35801 59306 27846 2E-05	0.35801 59306 27837 55059 08860 35787E-05	
$(5g_0^* 5g_0^*, 5g_0^* 5g_0^*, 5g_0^* 5g_0^*)$	5.72	5.72	4.26	1	-1	0.13868 80908 21572 8E-03	0.13868 80908 21566 75419 70323 50220E-03	
$(6h_0^* 6h_0^*, 6h_0^* 6h_0^*, 6h_0^* 6h_0^*)$	5.72	5.72	4.26	1	-1	0.15001 30480 05948 5E-01	0.15001 30480 05940 35455 89341 87986E-01	

Table 3. Comparison of EI3K values: the charge distributions are constructed with the exponents  $\zeta = 1.40$  for STFs with ", otherwise  $\zeta = 2.86$ .

Charge distribution	$\omega_1$	$\omega_2$	$\omega_3$	EKS ( $R_1 = 10^{-3}$ )	SKS ( $R_1 = 10^{-5}$ )	Ruiz
(1s1s, 1s1s", 1s1s")	5.72	4.26	4.26	0.15659 17112 60614 7E-04	0.15659 17112 60619 2E-04	0.15659 17112 60607 62842 78921 37447 E-04
(1s1s, 1s2s", 1s2s")	5.72	4.26	4.26	0.13126 72235 19567 2E-04	0.13126 72235 19566 9E-04	0.13126 72235 19561 47025 67125 92522 E-04
(2p <sub>0</sub> 2p <sub>0</sub> , 1s1s, 2s"2s")	5.72	5.72	2.80	0.34295 19455 00138 7E-04	0.34295 19455 00116 5E-04	0.34295 19455 00106 69550 17114 73595 E-04
(1s1s, 1s2p <sub>0</sub> ", 1s2p <sub>0</sub> ")	5.72	4.26	4.26	0.45769 77948 50794 8E-06	0.45769 77948 50790 4E-06	0.45769 77948 50777 26085 44884 85868 E-06
(1s2p <sub>0</sub> , 1s1s, 1s2p <sub>0</sub> ")	5.72	5.72	4.26	-0.12906 22778 17072 8E-06	-0.12906 22778 17059 8E-06	-0.12906 22778 17056 65339 27233 71594 E-06
(1s3d <sub>0</sub> ", 1s1s, 1s3d <sub>0</sub> ")	4.26	5.72	4.26	0.79465 21564 41419 7E-07	0.79465 21564 41395 2E-07	0.79465 21564 41320 36387 60727 96090 E-07
(2p <sub>0</sub> 2p <sub>0</sub> ", 1s1s, 2p <sub>0</sub> 2p <sub>0</sub> ")	4.26	5.72	4.26	0.81495 98738 32362 9E-05	0.81495 98738 32340 8E-05	0.81495 98738 32346 11143 47248 05787 E-05
(1s1s, 2p <sub>0</sub> 2p <sub>0</sub> ", 2p <sub>0</sub> 2p <sub>0</sub> ")	5.72	4.26	4.26	0.17800 68839 29547 4E-04	0.17800 68839 29563 7E-04	0.17800 68839 29555 22718 57902 99996 E-04
(2p <sub>0</sub> 2p <sub>0</sub> , 2p <sub>0</sub> 2p <sub>0</sub> , 2p <sub>0</sub> 2p <sub>0</sub> )	5.72	5.72	5.72	0.26076 89245 48969 9E-06	0.26076 89245 48963 2E-06	0.26076 89245 48949 11133 97976 94642 E-06
(3d <sub>0</sub> 3d <sub>0</sub> ", 1s1s, 3d <sub>0</sub> 3d <sub>0</sub> ")	4.26	5.72	4.26	0.46916 53824 00630 0E-04	0.46916 53824 00611 3E-04	0.46916 53824 00611 40864 14255 65967 E-04
(3d <sub>0</sub> 3d <sub>0</sub> ", 3d <sub>0</sub> 3d <sub>0</sub> , 3d <sub>0</sub> 3d <sub>0</sub> ")	4.26	5.72	4.26	0.19195 81649 30392 9E-04	0.19195 81649 30381 7E-04	0.19195 81649 30384 83368 39585 45964 E-04
(2p <sub>1</sub> 2p <sub>1</sub> ", 1s1s, 1s1s)	4.26	5.72	5.72	0.33657 95725 13812 7E-05	0.33657 95725 13805 0E-05	0.33657 95725 13801 82596 65603 91000 E-05
(3d <sub>2</sub> 3d <sub>2</sub> , 1s1s", 2s2s")	5.72	4.26	4.26	0.11417 77154 84592 0E-04	0.11417 77154 84590 7E-04	0.11417 77154 84591 52206 92069 39983 E-04
(2p <sub>1</sub> 2p <sub>1</sub> ", 1s1s, 2p <sub>1</sub> 2p <sub>1</sub> ")	4.26	5.72	4.26	0.82384 74233 55429 5E-05	0.82384 74233 55407 0E-05	0.82384 74233 55412 57794 19375 09453 E-05
(2p <sub>1</sub> 2p <sub>1</sub> , 2p <sub>1</sub> 2p <sub>1</sub> ", 2p <sub>1</sub> 2p <sub>1</sub> ")	5.72	4.26	4.26	0.78369 38975 20385 2E-05	0.78369 38975 20371 0E-05	0.78369 38975 20372 96896 51687 01558 E-05
(3d <sub>1</sub> 3d <sub>1</sub> , 2p <sub>1</sub> 2p <sub>1</sub> ", 3d <sub>1</sub> 3d <sub>1</sub> ")	5.72	4.26	4.26	0.19549 67426 08441 8E-04	0.19549 67426 08438 3E-04	0.19218 93617 07619 19207 88728 04038 E-04
(3d <sub>2</sub> 3d <sub>2</sub> , 3d <sub>1</sub> 3d <sub>1</sub> ", 3d <sub>1</sub> 3d <sub>1</sub> )	5.72	4.26	4.26	0.40399 59434 35970 1E-04	0.40399 59434 35963 6E-04	0.40399 59434 35959 51311 79010 05972 E-04
(2p <sub>0</sub> 2p <sub>0</sub> , 2p <sub>0</sub> 2p <sub>0</sub> ", 2p <sub>0</sub> 2p <sub>0</sub> ")	5.72	4.26	4.26	-0.34528 36595 44116 5E-08	-0.34528 36595 44110 2E-08	-0.34528 36595 44116 76923 18333 94309 E-08
(3d <sub>0</sub> 3d <sub>0</sub> , 3p <sub>0</sub> 3p <sub>0</sub> ", 3d <sub>0</sub> 3d <sub>0</sub> ")	5.72	4.26	4.26	-0.58364 96884 44442 8E-08	-0.58364 96884 44424 8E-08	-0.58364 96884 44425 76337 00583 35223 E-08
(2p <sub>-1</sub> 2p <sub>-1</sub> ", 1s1s, 1s1s)	4.26	5.72	5.72	0.33657 95725 13812 7E-05	0.33657 95725 13805 0E-05	0.33657 95725 13801 82596 65603 91000 E-05
(3d <sub>-2</sub> 3d <sub>-2</sub> , 1s1s, 3d <sub>-2</sub> 3d <sub>-2</sub> )	5.72	5.72	4.26	0.87337 99889 07149 0E-05	0.87337 99889 07136 9E-05	0.87337 99889 07121 70685 75959 02696 E-05

Table 4. Comparison of E141 values: the charge distributions are constructed with the exponents  $\zeta = 0.956$  for STFs with " , otherwise  $\zeta = 3.685$ .

Charge distribution	$\omega_1$	$\omega_2$	$\omega_3$	$\omega_4$	EKS ( $R_1=10^{-3}$ )	SKS ( $R_1=10^{-3}$ )	Ruiz
(1s1s, 1s1s, 2s <sup>2</sup> 2s <sup>2</sup> , 2s <sup>2</sup> 2s <sup>2</sup> )	7.37	7.37	1.912	1.912	0.10920 77604 59568 2E-04	0.10920 77604 59567 0E-04	0.10920 77604 59562 12978 04886 77070E-04
(2s2s, 2s2s, 2s <sup>2</sup> 2s <sup>2</sup> , 2s <sup>2</sup> 2s <sup>2</sup> )	7.37	7.37	1.912	1.912	0.88667 45676 73820 4E-06	0.88667 45676 73798 7E-06	0.88667 45676 73784 06087 40018 40730E-06
(2p <sub>0</sub> 2p <sub>0</sub> , 1s1s, 2s <sup>2</sup> 2s <sup>2</sup> , 2s <sup>2</sup> 2s <sup>2</sup> )	7.37	7.37	1.912	1.912	0.33546 12747 29132 4E-05	0.33546 12747 29126 6E-05	0.33546 12747 29117 78572 92964 29862E-05
(1s1s, 1s1s, 2p <sub>0</sub> 2p <sub>0</sub> , 2p <sub>0</sub> 2p <sub>0</sub> )	7.37	7.37	1.912	1.912	0.11765 21546 23844 7E-04	0.11765 21546 23843 4E-04	0.11765 21546 23838 07738 49011 19468E-04
(2s2s, 2s2s, 2p <sub>0</sub> 2p <sub>0</sub> , 2p <sub>0</sub> 2p <sub>0</sub> )	7.37	7.37	1.912	1.912	0.95514 89489 95872 0E-06	0.95514 89489 95848 7E-06	0.95514 89489 95832 26901 42563 01884E-06
(2p <sub>0</sub> 3d <sub>0</sub> , 1s1s, 1s1s <sup>2</sup> , 2p <sub>0</sub> 2p <sub>0</sub> )	7.37	7.37	4.641	1.912	0.39691 88001 49640 5E-07	0.39691 88001 49620 0E-07	0.39691 88001 49615 94358 38215 75910E-07
(2p <sub>0</sub> 3d <sub>0</sub> , 1s1s, 1s1s <sup>2</sup> , 2p <sub>0</sub> 3d <sub>0</sub> )	7.37	7.37	4.641	1.912	-0.98344 81780 40968 4E-09	-0.98344 81780 40906 8E-09	-0.98344 81780 40909 01670 17668 17315E-09
(2p <sub>0</sub> 4f <sub>0</sub> , 1s1s, 1s1s <sup>2</sup> , 2p <sub>0</sub> 4f <sub>0</sub> )	7.37	7.37	4.641	1.912	-0.61413 29426 14986 2E-10	-0.61413 29426 14895 4E-10	-0.61413 29426 14900 02656 97377 80802E-10
(2p <sub>0</sub> 2p <sub>0</sub> , 2p <sub>0</sub> 2p <sub>0</sub> , 2p <sub>0</sub> 2p <sub>0</sub> , 2p <sub>0</sub> 2p <sub>0</sub> )	7.37	7.37	1.912	1.912	0.93556 14215 81774 2E-06	0.93556 14215 81751 5E-06	0.93556 14215 81734 86545 71520 22302E-06
(2p <sub>0</sub> 2p <sub>0</sub> , 2p <sub>0</sub> 2p <sub>0</sub> , 3d <sub>0</sub> 3d <sub>0</sub> , 3d <sub>0</sub> 3d <sub>0</sub> )	7.37	7.37	4.641	1.912	0.73879 62901 61380 7E-07	0.73879 62901 61388 5E-07	0.73879 62901 61361 90127 50795 21610E-07
(3p <sub>0</sub> 3p <sub>0</sub> , 3p <sub>0</sub> 3p <sub>0</sub> , 3d <sub>0</sub> 3d <sub>0</sub> , 3d <sub>0</sub> 3d <sub>0</sub> )	7.37	7.37	4.641	1.912	0.33286 72282 99125 4E-07	0.33286 72282 99129 8E-07	0.33286 72282 99124 06821 13613 43180E-07
(3p <sub>0</sub> 3p <sub>0</sub> , 3d <sub>0</sub> 3d <sub>0</sub> , 3d <sub>0</sub> 3d <sub>0</sub> , 3d <sub>0</sub> 3d <sub>0</sub> )	7.37	7.37	4.641	1.912	0.14388 63188 48910 6E-05	0.14388 63188 48902 9E-05	0.14388 63188 48905 80405 46675 86615E-05
(3d <sub>0</sub> 3d <sub>0</sub> , 3d <sub>0</sub> 3d <sub>0</sub> , 4d <sub>0</sub> 4d <sub>0</sub> , 4d <sub>0</sub> 4d <sub>0</sub> )	7.37	7.37	4.641	1.912	0.12238 03514 64175 6E-05	0.12238 03514 64170 6E-05	0.12238 03514 64172 07076 31777 65647E-05
(3d <sub>0</sub> 3d <sub>0</sub> , 3d <sub>0</sub> 3d <sub>0</sub> , 4f <sub>0</sub> 4f <sub>0</sub> , 4f <sub>0</sub> 4f <sub>0</sub> )	7.37	7.37	4.641	1.912	0.12180 33377 30109 7E-05	0.12180 33377 30104 7E-05	0.12180 33377 30106 38098 00606 50996E-05
(5g <sub>0</sub> 5d <sub>0</sub> , 1s1s, 6l <sub>0</sub> 6l <sub>0</sub> , 1s <sup>2</sup> 1s <sup>2</sup> )	7.37	7.37	4.641	1.912	0.26295 38179 48950 1E-05	0.26295 38179 48935 1E-05	0.26295 38179 48928 79306 19896 41088E-05
(2p <sub>-1</sub> 2p <sub>-1</sub> , 2p <sub>-1</sub> 2p <sub>-1</sub> , 2s3s <sup>2</sup> , 2s <sup>2</sup> 2s <sup>2</sup> )	7.37	7.37	4.641	1.912	0.84365 10925 65046 1E-08	0.84365 10925 65048 6E-08	0.84365 10925 65022 43129 81005 70942E-08
(2p <sub>-1</sub> 2p <sub>-1</sub> , 2p <sub>-1</sub> 2p <sub>-1</sub> , 2p <sub>-1</sub> 3p <sub>-1</sub> , 2p <sub>-1</sub> 2p <sub>-1</sub> )	7.37	7.37	4.641	1.912	0.84423 35250 59632 6E-09	0.84423 35250 59641 7E-09	0.84423 35250 59613 57835 35764 27846E-09
(3d <sub>-2</sub> 3d <sub>0</sub> , 3d <sub>-1</sub> 4d <sub>-1</sub> , 4d <sub>-1</sub> 4d <sub>-1</sub> , 4d <sub>-2</sub> 4d <sub>0</sub> )	7.37	7.37	4.641	1.912	-0.26639 13976 15675 8E-09	-0.26639 13976 15663 7E-09	-0.26639 13976 15667 34697 02989 03236E-09
(3d <sub>-2</sub> 3d <sub>0</sub> , 3d <sub>-1</sub> 3d <sub>-1</sub> , 4d <sub>-1</sub> 4d <sub>-1</sub> , 4d <sub>-2</sub> 4d <sub>0</sub> )	7.37	7.37	4.641	1.912	-0.24677 81081 89338 0E-09	-0.24677 81081 89324 3E-09	-0.24677 81081 89328 42631 12765 49502E-09
(3d <sub>-2</sub> 3d <sub>0</sub> , 4f <sub>-1</sub> 4f <sub>-1</sub> , 4d <sub>-1</sub> 4d <sub>-1</sub> , 4d <sub>-2</sub> 4f <sub>0</sub> )	7.37	7.37	4.641	1.912	-0.43715 44882 76303 2E-09	-0.43715 44882 76292 3E-09	-0.43715 44882 76299 92188 13995 57759E-09

Table 5. Comparison of EI42 values: the charge distributions are constructed with the exponents  $\zeta = 0.956$  for STFs with ", otherwise  $\zeta = 3.685$ .

Charge distribution	$\omega_1$	$\omega_2$	$\omega_3$	$\omega_4$	EKS ( $R_1=10^{-3}$ )	SKS ( $R_1=10^{-3}$ )	Ruiz
(1s1s, 1s1s, 2s <sup>*</sup> 2s <sup>*</sup> , 2s <sup>*</sup> 2s <sup>*</sup> )	7.37	7.37	1.912	1.912	0.16509 33690 91482 7E-04	0.16509 33690 91482 3E-04	0.16509 33690 91471 34726 17575 44135E-04
(2s2s, 2s2s, 2s <sup>*</sup> 2s <sup>*</sup> , 2s <sup>*</sup> 2s <sup>*</sup> )	7.37	7.37	1.912	1.912	0.13146 73615 28576 3E-05	0.13146 73615 28566 2E-05	0.13146 73615 28568 27727 38521 60655E-05
(2p <sub>0</sub> <sup>2</sup> p <sub>0</sub> , 1s1s, 2s <sup>*</sup> 2s <sup>*</sup> , 2s <sup>*</sup> 2s <sup>*</sup> )	7.37	7.37	1.912	1.912	0.49606 48449 23012 2E-05	0.49606 48449 23006 5E-05	0.49606 48449 22979 98156 05319 77607E-05
(1s1s, 1s1s, 2p <sub>0</sub> <sup>2</sup> 2p <sub>0</sub> <sup>2</sup> , 2p <sub>0</sub> <sup>2</sup> 2p <sub>0</sub> <sup>2</sup> )	7.37	7.37	1.912	1.912	0.16507 57402 75802 0E-04	0.16507 57402 75801 6E-04	0.16507 57402 75790 59750 36266 20897E-04
(2s2s, 2s2s, 2p <sub>0</sub> <sup>2</sup> 2p <sub>0</sub> <sup>2</sup> , 2p <sub>0</sub> <sup>2</sup> 2p <sub>0</sub> <sup>2</sup> )	7.37	7.37	1.912	1.912	0.13142 83133 68164 8E-05	0.13142 83133 68154 7E-05	0.13142 83133 68156 65055 41415 58624E-05
(2p <sub>0</sub> <sup>2</sup> 2p <sub>0</sub> , 1s1s, 1s1s <sup>*</sup> , 2p <sub>0</sub> <sup>2</sup> 2p <sub>0</sub> <sup>2</sup> )	7.37	7.37	4.641	1.912	0.41151 69561 68798 3E-07	0.41151 69561 68783 5E-07	0.41151 69561 68770 34211 53634 04361E-07
(2p <sub>0</sub> <sup>3</sup> d <sub>0</sub> , 1s1s, 1s1s <sup>*</sup> , 2p <sub>0</sub> <sup>3</sup> d <sub>0</sub> <sup>*</sup> )	7.37	7.37	4.641	1.912	0.96287 93608 57548 9E-08	0.96287 93608 57533 0E-08	0.96287 93608 57511 70944 44684 45982E-08
(2p <sub>0</sub> <sup>4</sup> f <sub>0</sub> , 1s1s, 1s1s <sup>*</sup> , 2p <sub>0</sub> <sup>4</sup> f <sub>0</sub> <sup>*</sup> )	7.37	7.37	4.641	1.912	0.80762 56512 90755 9E-08	0.80762 56512 90750 1E-08	0.80762 56512 90742 21860 61923 77433E-08
(2p <sub>0</sub> <sup>2</sup> p <sub>0</sub> , 2p <sub>0</sub> <sup>2</sup> p <sub>0</sub> , 2p <sub>0</sub> <sup>2</sup> 2p <sub>0</sub> <sup>*</sup> , 2p <sub>0</sub> <sup>2</sup> 2p <sub>0</sub> <sup>*</sup> )	7.37	7.37	1.912	1.912	0.13347 54141 57519 2E-05	0.13347 54141 57508 8E-05	0.13347 54141 57510 83043 91203 56254E-05
(2p <sub>0</sub> <sup>2</sup> p <sub>0</sub> , 2p <sub>0</sub> <sup>2</sup> p <sub>0</sub> , 3d <sub>0</sub> <sup>3</sup> d <sub>0</sub> <sup>*</sup> , 3d <sub>0</sub> <sup>3</sup> d <sub>0</sub> <sup>*</sup> )	7.37	7.37	4.641	1.912	0.74063 89572 95508 6E-07	0.74063 89572 95494 1E-07	0.74063 89572 95482 26588 26433 51056E-07
(3p <sub>0</sub> <sup>3</sup> p <sub>0</sub> , 3p <sub>0</sub> <sup>3</sup> p <sub>0</sub> , 3d <sub>0</sub> <sup>3</sup> d <sub>0</sub> <sup>*</sup> , 3d <sub>0</sub> <sup>3</sup> d <sub>0</sub> <sup>*</sup> )	7.37	7.37	4.641	1.912	0.33485 68986 29858 5E-07	0.33485 68986 29860 5E-07	0.33485 68986 29852 13308 55736 61429E-07
(3p <sub>0</sub> <sup>3</sup> p <sub>0</sub> , 3d <sub>0</sub> <sup>3</sup> d <sub>0</sub> , 3d <sub>0</sub> <sup>3</sup> d <sub>0</sub> <sup>*</sup> , 3d <sub>0</sub> <sup>3</sup> d <sub>0</sub> <sup>*</sup> )	7.37	7.37	4.641	1.912	0.14228 88514 01293 9E-05	0.14228 88514 01286 3E-05	0.14228 88514 01287 78023 08231 73114E-05
(3d <sub>0</sub> <sup>3</sup> d <sub>0</sub> , 3d <sub>0</sub> <sup>3</sup> d <sub>0</sub> , 4d <sub>0</sub> <sup>4</sup> d <sub>0</sub> <sup>*</sup> , 4d <sub>0</sub> <sup>4</sup> d <sub>0</sub> <sup>*</sup> )	7.37	7.37	4.641	1.912	0.12086 46488 78582 3E-05	0.12086 46488 78575 5E-05	0.12086 46488 78576 15340 42492 94343E-05
(3d <sub>0</sub> <sup>3</sup> d <sub>0</sub> , 3d <sub>0</sub> <sup>3</sup> d <sub>0</sub> , 4f <sub>0</sub> <sup>4</sup> f <sub>0</sub> <sup>*</sup> , 4f <sub>0</sub> <sup>4</sup> f <sub>0</sub> <sup>*</sup> )	7.37	7.37	4.641	1.912	0.12079 14964 05622 1E-05	0.12079 14964 05615 4E-05	0.12079 14964 05616 13393 60564 41004E-05
(5g <sub>0</sub> <sup>5</sup> g <sub>0</sub> , 1s1s, 6h <sub>0</sub> <sup>6</sup> h <sub>0</sub> <sup>*</sup> , 1s <sup>*</sup> 1s <sup>*</sup> )	7.37	7.37	4.641	1.912	0.41416 81552 13051 1E-05	0.41416 81552 13052 4E-05	0.41416 81552 13027 31066 37318 03978E-05
(2p <sub>-1</sub> 2p <sub>-1</sub> , 2p <sub>0</sub> 2p <sub>0</sub> , 2s2s <sup>*</sup> , 2s <sup>*</sup> 2s <sup>*</sup> )	7.37	7.37	4.641	1.912	0.91553 40411 05382 9E-08	0.91553 40411 05340 5E-08	0.91553 40411 05385 77879 33203 64491E-08
(2p <sub>-1</sub> 2p <sub>-1</sub> , 2p <sub>0</sub> 2p <sub>0</sub> , 2p <sub>-1</sub> 3p <sub>-1</sub> , 2p <sub>0</sub> <sup>2</sup> 2p <sub>0</sub> <sup>-1</sup> )	7.37	7.37	4.641	1.912	-0.11667 01204 88277 3E-10	-0.11667 01204 88272 1E-10	-0.11667 01204 88271 98278 93040 14812E-10
(3d <sub>-1</sub> 4d <sub>0</sub> , 3d <sub>1</sub> 4d <sub>-1</sub> , 4d <sub>1</sub> 4d <sub>-1</sub> , 4d <sub>-2</sub> 4d <sub>0</sub> <sup>*</sup> )	7.37	7.37	4.641	1.912	0.54302 68764 93281 5E-11	0.54302 68764 93270 8E-11	0.54302 68764 93278 18104 77256 87055E-11
(3d <sub>-2</sub> 3d <sub>0</sub> , 3d <sub>1</sub> 3d <sub>-1</sub> , 4d <sub>1</sub> 4d <sub>-1</sub> , 4d <sub>-2</sub> 4d <sub>0</sub> <sup>*</sup> )	7.37	7.37	4.641	1.912	0.36266 61724 30363 6E-11	0.36266 61724 30360 9E-11	0.36266 61724 30362 74379 43359 73434E-11
(3d <sub>-2</sub> 3d <sub>0</sub> , 4f <sub>1</sub> 4f <sub>-1</sub> , 4d <sub>1</sub> 4d <sub>-1</sub> , 4d <sub>-2</sub> 4f <sub>0</sub> <sup>*</sup> )	7.37	7.37	4.641	1.912	0.41870 41919 27390 7E-11	0.41870 41919 27367 4E-11	0.41870 41919 27377 18499 08741 14258E-11

There is the other approximation of three-electron integrals. It is method that constructed by sums of products of two-electron kinetic integrals and two-electron integrals:

$$\langle ABC | r_{12}^s T_1 r_{13}^t | A' B' C' \rangle = \sum_I \langle AB | r_{12}^s | IB' \rangle \langle IC | T_1 r_{12}^t | A' C' \rangle. \quad (27)$$

This approximated formula requires the two-electron kinetic integrals. Eq.(27) may be calculated more accurate than Eq.(11).

## REFERENCES

- <sup>1</sup> C. de Boor, *A practical guide to splines*, (Springer, Berlin, Heidelberg, New York, 2001).
- <sup>2</sup> J. Sapirstein and W.R. Johnson, *J. Phys. B* 29, 5213 (1996).
- <sup>3</sup> S.L. Saito, *Theor. Chem. Acc.* 109, 326 (2003).
- <sup>4</sup> S.L. Saito, *At. Data and Nucl. Data Tables* 95, 836 (2009).
- <sup>5</sup> S.L. Saito, *J. Chem. Phys.* 103, 074306 (2009).
- <sup>6</sup> E.A. Hylleraas, *Z. Phys.* 54, 347 (1929).
- <sup>7</sup> C.L. Pekeris, *Phys. Rev.* 126,1470 (1962).
- <sup>8</sup> J.S. Sims and S. Hagstrom, *Phys. Rev. A* 4, 908 (1971).
- <sup>9</sup> J.S. Sims and S. Hagstrom, *J. Chem. Phys. A* 55, 4699 (1971).
- <sup>10</sup> Öhrn and Nordling, *J. Chem. Phys.* 39, 1864 (1963).
- <sup>11</sup> F.W. King, *J. Chem. Phys.* 99, 3622 (1993).
- <sup>12</sup> Z.-C. Yan and G.W.F. Drake, *J. Phys. B* 30, 4723 (1997).
- <sup>13</sup> J.S. Sims and S.A. Hagstrom, *J. Phys. B* 37, 1519 (2004).
- <sup>14</sup> J.S. Sims and S.A. Hagstrom, *J. Phys. B* 37, 1575 (2004).
- <sup>15</sup> M.B. Ruiz, *J. Math. Chem.* 46, 24 (2009).
- <sup>16</sup> F.W. King, *Phys. Rev. A* 44, 7108 (1991).
- <sup>17</sup> M.B. Ruiz, *J. Math. Chem.* 46, 1322 (2009).
- <sup>18</sup> W. Kutzelnigg and W. Klopper, *J. Chem. Phys.* 94, 1985 (1991).
- <sup>19</sup> S.L. Saito, *Chukyo Univ. Bulletin of the School of International Liberal Studies* 9 (2), 23 (2016).
- <sup>20</sup> T. L. Gilbert and P. J. Bertocini, *J. Chem. Phys.* 61, 30265 (1974).