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Convergence of Translation Formulas for the Computation of Multicenter Integrals over Slater Orbitals

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Multicenter electron-repulsion integrals are calculated using auxiliary functions and two kinds of translation formulas for Slater-type orbitals (STOs) obtained from the expansion of STOs, in terms of exponential-type orbitals at a displaced center, that form complete orthonormal sets and are represented by linear combinations of STOs. The convergence of the series for real STOs is tested by calculating concrete cases. Accuracy of the results is quite high for quantum numbers, screening constants, and location of STOs. © 2001 Elsevier Science

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1. INTRODUCTION

It is well-known that multicenter molecular integrals, appearing in the mathematical expressions of physical and chemical properties of molecules, are evaluated by using two types of orbitals: Gaussian-type orbitals (GTOs) and exponential-type orbitals (ETOs). GTOs do not allow sufficient representation of important properties of the electronic wavefunction, namely, the cusps at the nuclei [1] and exponential decay at large distances [2]. For problems in which the long part of the wavefunction or its behavier in the neighborhood of the nuclei is important, it is desirable to use ETOs, which describe the physical situation more accurately than do GTOs. Therefore GTOs are inferior to ETOs in the study of molecular properties. However, the difficulties in calculating multicenter molecular integrals has restricted the use of ETOs in quantum chemistry. As shown in the literature, there is renewed interest in developing efficient methods for calculating molecular integrals by employing ETOs as basis sets (see, e.g., Refs. [3, 4] and the bibliographies quoted in these papers). It is well-known that arbitrary ETOs can be represented by a linear combination of Slater-type orbitals (STOs) [5]. Therefore, the STOs not only arise in their own right in the study of molecular systems, they are also central to the calculation of the multicenter molecular integrals over arbitrary

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ETOs based on the expansions of orbitals at a displaced center [6–12]. Probably, this was the reason why multicenter integrals over STOs have been examined thoroughly in the literature.

Recently, one of us [13] derived the different expansion formulas for translation of STOs using so-called lambda and Coulomb Sturmian ETOs (LETOs and CETOs), which were introduced into atomic and molecular calculations in Refs. [14–16] and [17], respectively (see also Refs. [18–21]). In Ref. [22] we examined the applicability of these translation formulas to the multicenter electron-repulsion integrals using auxiliary functions. However, in Ref. [22] the auxiliary functions

$$Q_{ns}^{q}(p,\, pt) = \int_{1}^{\infty}\int_{-1}^{1} (\mu\nu)^{q}(\mu+\nu)^{n}(\mu-\nu)^{s} e^{-p\mu-pt\nu}\, d\mu\, d\nu \tag{1}$$

and

$$G_{-ns}^{q}(p_a,\, p,\, pt) = \int_{1}^{\infty}\int_{-1}^{1} \frac{(\mu\nu)^{q}(\mu-\nu)^{s}}{(\mu+\nu)^{n}} \left(1 - e^{-p_a(\mu+\nu)} \sum_{k=0}^{n-1} \frac{[p_a(\mu+\nu)]^{k}}{k!}\right) e^{-p\mu-pt\nu}\, d\mu\, d\nu \tag{2}$$

were all calculated from the recurrence relations, which are particularly unsuited to numerical computations for small values of parameters p_a and pt, because of a serious loss of significant figures in each upward recurrence step. Here $p_a > 0$, $p > 0$, $-p \le pt \le p$, and the indices n, s, and q are all non-negative integers.

In the present paper the series expansion formulas are derived for the auxiliary functions Q_{ns}^{q} and G_{-ns}^{q}, which can be used for parameters of small values, at the same time avoiding the excessive loss of significant figures occurring in the method developed in Ref. [22] for the physically important case of small p_a and pt. The multicenter electron-repulsion integrals for parameters of arbitrary values are calculated using recurrence relations and series expansion formulas for auxiliary functions Q_{ns}^{q} and G_{-ns}^{q}.

The multicenter electron-repulsion integrals over STOs with respect to the molecular coordinate system examined in the present work have the form

$$I_{p_1 p_1';\, p_2 p_2'}^{ac;\, db}(\zeta_1, \zeta_1';\, \zeta_2, \zeta_2') = \int \chi_{p_1}^{*}(\zeta_1, \mathbf{r}_{a1})\chi_{p_1'}(\zeta_1', \mathbf{r}_{c1}) \frac{1}{r_{21}} \chi_{p_2}(\zeta_2, \mathbf{r}_{d2})\chi_{p_2'}^{*}(\zeta_2', \mathbf{r}_{b2})\; dV_1\, dV_2, \tag{3}$$

where $p_i \equiv n_i l_i m_i$, $p_i' \equiv n_i' l_i' m_i'$, $\mathbf{r}_{gi} = \mathbf{r}_i - \mathbf{R}_g$ ($i = 1, 2$ and $g = a, b, c, d$), and $\chi_{nlm}(\zeta, \mathbf{r})$ are the normalized real or complex STOs determined by

$$\chi_{nlm}(\zeta, \mathbf{r}) = (2\zeta)^{n+\frac{1}{2}}[(2n)!]^{-\frac{1}{2}} r^{n-1} e^{-\zeta r} S_{lm}(\theta, \varphi). \tag{4}$$

Here the spherical harmonics S_{lm} are determined by the relation [23]

$$S_{lm}(\theta, \varphi) = P_{l|m|}(\cos\theta)\Phi_m(\varphi), \tag{5}$$

where $P_{l|m|}$ are normalized associated Legendre functions. For complex spherical harmonics $S_{lm}(\theta, \varphi) \equiv Y_{lm}(\theta, \varphi)$

$$\Phi_m(\varphi) = \frac{1}{\sqrt{2\pi}} e^{im\varphi}, \tag{6}$$

and for real spherical harmonics

$$\Phi_m(\varphi) = \frac{1}{\sqrt{\pi(1+\delta_{mo})}} \begin{cases} \cos|m|\varphi & \text{for } m \geq 0 \\ \sin|m|\varphi & \text{for } m < 0 \end{cases}. \tag{7}$$

We notice that our definition of phases for complex spherical harmonics differs from the Condon–Shortley phases [24] by the sign factor. We use phases according to Ref. [25]: $Y^*_{lm}(\theta, \varphi) = Y_{l-m}(\theta, \varphi)$.

2. CALCULATION OF MULTICENTER ELECTRON-REPULSION INTEGRALS

In order to calculate multicenter electron-repulsion integrals, we use in Eq. (3) the translation formulas for the STOs obtained using LETOs and CETOs in the form (see Eqs. (18)–(23) in Ref. [13])

$$\chi_{nlm}(\zeta, \mathbf{r}_a) = \lim_{N\to\infty} \sum_{n'=1}^{N} \sum_{l'=0}^{n'-1} \sum_{m'=-l'}^{l'} V^{N*}_{nlm,n'l'm'}(\zeta, \zeta'; \mathbf{R}) \chi_{n'l'm'}(\zeta', \mathbf{r}_b), \tag{8}$$

where $\mathbf{R} = \mathbf{R}_{ab}$ and the translation coefficients V^N are determined as follows. For LETOs,

$$V^N_{nlm,n'l'm'}(\zeta, \zeta'; \mathbf{R}) = \sum_{n''=l'+1}^{N} \Omega^{l'}_{n'n''}(N) S_{nlm,n''l'm'}(\zeta, \zeta', \mathbf{R}), \tag{9}$$

$$\Omega^l_{nk}(N) = \sum_{n'=\max(n,k)}^{N} \omega^l_{n'n} \omega^l_{n'k}, \tag{10}$$

$$\omega^l_{nn'} = (-1)^{n'-l-1} [F_{n'-l-1}(n-l-1) F_{n'-l-1}(2n') F_{n'+l+1}(n+l+1)]^{1/2}. \tag{11}$$

For CETOs,

$$V^N_{nlm,n'l'm'}(\zeta, \zeta'; \mathbf{R}) = \sum_{n''=l'+1}^{N} \Omega^{l'}_{n'n''}(N) S_{nlm,n''-1l'm'}(\zeta, \zeta', \mathbf{R}), \tag{12}$$

$$\Omega^l_{nk}(N) = \left[\frac{2}{2(2k-1)}\right]^{1/2} \sum_{n'=\max(n,k)}^{N} n' \omega^l_{n'n} \omega^l_{n'k}, \tag{13}$$

$$\omega^l_{nn'} = (-1)^{n'-l-1} \left[\frac{n'+l+1}{2n} F_{n'-l-1}(n-l-1) F_{n'-l-1}(2n') F_{n'+l}(n+l)\right]^{1/2}. \tag{14}$$

Here the quantities $S_{nlm,n'l'm'}$ are the overlap integrals over the normalized STOs:

$$S_{nlm,n'l'm'}(\zeta,\zeta';\mathbf{R}) = \int \chi^*_{nlm}(\zeta,\mathbf{r}_a)\chi_{n'l'm'}(\zeta',\mathbf{r}_b)\,dV. \tag{15}$$

Now we take into account Eq. (8) for $\zeta = \zeta'$ in Eq. (3). Then, using the auxiliary function method (see Ref. [22]) it is easy to obtain for all multicenter electron-repulsion integrals, that is, for three-center hybrid and two-, three-, and four-center exchange integrals, the following relations in terms of basic two-center Coulomb and hybrid integrals. For, three-center hybrid integrals,

$$I^{aa;db}_{p_1p'_1;p_2p'_2}(\zeta_1,\zeta'_1;\zeta_2,\zeta'_2) = \sum_{l=0}^{n-1}\sum_{m=-l}^{l} W^*_{p_1p'_1p}(\zeta_1,\zeta'_1,z)\lim_{N'\to\infty}\sum_{n'=1}^{N'}\sum_{l'=0}^{n'-1}\sum_{m'=-l'}^{l'} W^{N'}_{p_2p'_2p'} \times(\zeta_2,\zeta'_2,z';\mathbf{R}_{db},0)C_{pp'}(z,z';\mathbf{R}_{ab}). \tag{16}$$

For two-center (for $c \equiv b$) and three-center (for $c \equiv b$) exchange integrals,

$$I^{ac,ab}_{p_1p'_1;p_2p'_2}(\zeta_1,\zeta'_1;\zeta_2,\zeta'_2) = \lim_{N\to\infty}\sum_{n=1}^{N}\sum_{l=0}^{n-1}\sum_{m=-l}^{l} W^{*N}_{p_1p'_1p}(\zeta_1,\zeta'_1,z;\mathbf{R}_{ca},0)H_{pp_2p'_2}(z,\zeta_2,\zeta'_2;\mathbf{R}_{ab}). \tag{17}$$

For four-center integrals,

$$\begin{aligned} I^{ac,db}_{p_1p'_1;p_2p'_2}&(\zeta_1,\zeta'_1;\zeta_2,\zeta'_2) \\ &= \lim_{N_1,N_2\to\infty}\sum_{n=1}^{N_1}\sum_{l=0}^{n-1}\sum_{m=-l}^{l} W^{*N_1}_{p_1p'_1p}(\zeta_1,\zeta'_1,z;\mathbf{R}_{ca},0) \\ &\quad\times\sum_{n'=1}^{N_2}\sum_{l'=0}^{n'-1}\sum_{m'=-l'}^{l'} W^{N_2}_{p_2p'_2p'}\big(\zeta_2,\zeta'_2,z';\mathbf{R}_{db},0\big)C_{pp'}\big(z,z';\mathbf{R}_{ab}\big). \end{aligned} \tag{18}$$

Here $p \equiv nlm$, $p' \equiv n'l'm'$, $z \equiv \zeta_1 + \zeta'_1$, and $z' = \zeta_2 + \zeta'_2$. The quantities $C_{pp'}$, $H_{pp_2p'_2}$, and W^N are the basic two-center Coulomb and hybrid integrals and the two-center charge-density expansion coefficients, respectively (see Refs. [22, 26]):

$$C_{pp'}(z,z';\mathbf{R}_{ab}) = \frac{1}{4\pi}\int\chi^*_p(z,\mathbf{r}_{a1})\frac{1}{r_{21}}\chi_{p'}(z',\mathbf{r}_{b2})\,dV_1\,dV_2, \tag{19}$$

$$H_{pp_2p'_2}(z,\zeta_2,\zeta'_2;\mathbf{R}_{ab}) = \frac{1}{\sqrt{4\pi}}\int\chi^*_p(z,\mathbf{r}_{a1})\frac{1}{r_{21}}\chi_{p_2}(\zeta_2,\mathbf{r}_{a2})\chi_{p'_2}(\zeta'_2,\mathbf{r}_{b2})\,dV_1\,dV_2, \tag{20}$$

$$W^N_{p_1p'_1p}(\zeta_1,\zeta'_1,z;\mathbf{R}_{ca},0) = \sum_{l'=0}^{n'-1}\sum_{m'=-l'}^{l'} W_{p_1p'p}(\zeta_1,\zeta'_1,z)V^N_{p'_1p'}(\zeta'_1,\zeta'_1;\mathbf{R}_{ca}), \tag{21}$$

$$W^N_{p_1p'_1p}(\zeta_1,\zeta'_1,z;0,0) = \delta_{Nn}\delta_{n,n_1+n'_1-1}W_{p_1p'_1p}(\zeta_1,\zeta'_1,z). \tag{22}$$

See Eq. (16) in Ref. [26] for the exact definition of the one-center charge-density expansion coefficients W appearing in Eqs. (16), (21), and (22).

From Eqs. (16)–(18) it can be seen that all the multicenter electron-repulsion integrals are expressed through the basic two-center Coulomb or hybrid integrals and the two-center expansion coefficients for charge-density, which are represented in terms of auxiliary functions and translation coefficients, respectively, for STOs.

Now we can move on to the derivation of series expansion formulas for the auxiliary functions $Q^q_{ns}(p, pt)$ and $G^q_{-ns}(p_a, p, pt)$ for small values of parameters p_a and pt. In these cases, only infinite-form expressions for auxiliary functions had to be derived, which can be obtained easily from the series expansion [23]:

$$e^{-x} = \sum_{k=0}^{\infty} \frac{(-x)^k}{k!}. \tag{23}$$

Taking into account (23) in Eqs. (1) and (2), we finally obtain the following series expansion formulas:

$$Q^q_{n\,n'}(p, pt) = \sum_{k=0}^{\infty} \frac{(-pt)^k}{k!} \sum_{s=0}^{n+n'} \frac{1 + (-1)^{q+k+s}}{q + k + s + 1} F_s(n, n') A_{n+n'+q-s}(p), \tag{24}$$

$$G^q_{-n\,n'}(p_a, p, pt) = \sum_{k=0}^{\infty} \frac{(-1)^k p_a^{n+k}}{(n-1)!k!(n+k)} Q^q_{k\,n'}(p, pt). \tag{25}$$

For the derivation of Eq. (25) we have taken into account the relation

$$\frac{1}{x^n}\left(1 - e^{-x} \sum_{s=0}^{n-1} \frac{x^s}{s!}\right) = \sum_{k=0}^{\infty} \frac{(-x)^k}{(n-1)!k!(n+k)}. \tag{26}$$

3. NUMERICAL RESULTS AND DISCUSSION

As can be seen from Eqs. (16)–(18), the two-center basic Coulomb and hybrid integrals occur in the multicenter electron-repulsion integrals over STOs. For these basic integrals the formulas in terms of auxiliary functions Q^q_{ns} and G^q_{-ns}, recently established in Ref. [22], were calculated by repeated application of recurrence relations (see Eqs. (21)–(29) of Ref. [22]). As stated in Ref. [22], the recurrence relations for auxiliary functions in the case of small values of parameters p_a and pt become numerically unstable. On the basis of series expansion formulas (24) and (25) we also constructed a program for evaluating the multicenter electron-repulsion integrals for small values of these parameters. Therefore, our computer programs for basic two-center Coulomb and hybrid integrals and auxiliary functions can be used in the calculation of multicenter electron-repulsion integrals for parameters of arbitrary values.

In Fig. 1, for $\lambda = \lambda' < N - 1$ we present the convergence of the series in Eq. (18) obtained using expansion coefficients (9) and (12) for translation of real STOs. Here λ and λ' are upper limits of the indices m and m', respectively. The series accuracy $\Delta f_\lambda = f_{N-1} - f_\lambda$ for the four-center electron-repulsion integrals is shown in Fig. 1, where the quantities f_{N-1} are the values of integrals for $\lambda = \lambda' = N - 1$. We see that the convergence of the series with respect to m and m' is rapid; therefore, we can include only a few terms obtained from

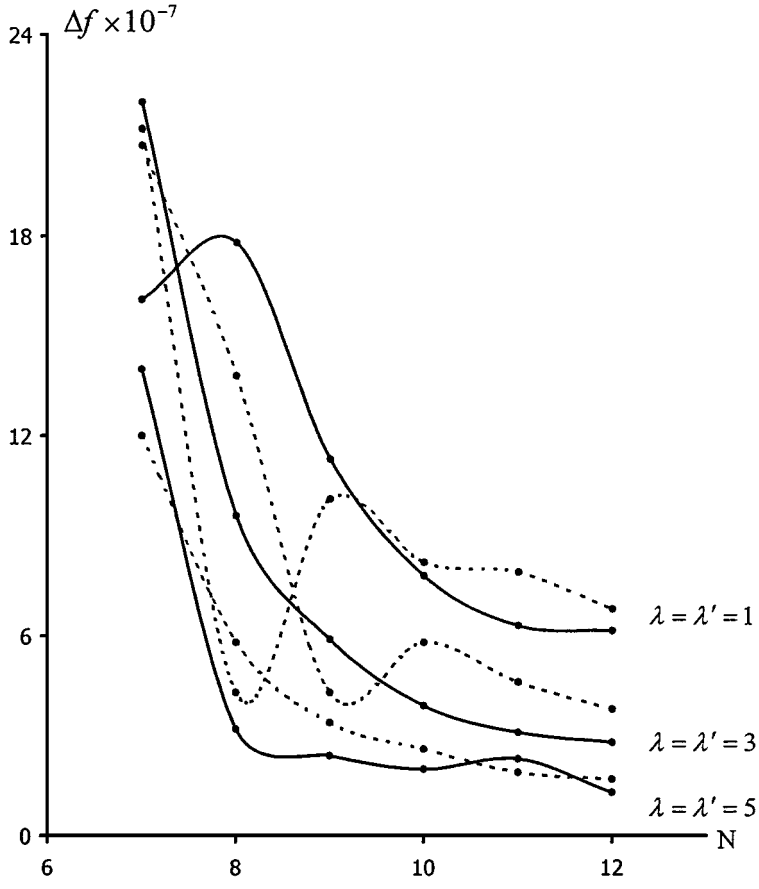

FIG. 1. The convergence of series in Eq. (18) as a function of the upper limits of the indices m and m' for the four-center electron repulsion integral $I_{211,211,211,211}$ obtained using Eqs. (9) and (12) for $\zeta_1 = 10.4$, $\zeta_1' = 9.3$, $\zeta_2 = 11.5$, $\zeta_2' = 8.1$, $R_{ab} = 0.032$, $\theta_{ab} = 45^\circ$, $\phi_{ab} = 150^\circ$, $R_{ca} = 0.23$, $\theta_{ca} = 70^\circ$, $\phi_{ca} = 180^\circ$, $R_{db} = 0.09$, $\theta_{db} = 108^\circ$, and $\phi_{db} = 120^\circ$.

the summation over indices m and m'. The full and broken lines in Fig. 1 represent the results of calculations made using Eqs. (9) and (12), obtained from LETOs and CETOs, respectively.

The results of calculations in atomic units for the three-center hybrid, the two- and three-center exchange, and the four-center exchange electron-repulsion integrals on a Pentium 233 computer (using TURBO PASCAL 7.0 language) are represented in Tables I, II, and III, respectively. The comparative values obtained from Eqs. (9) and (12) with the translations of different STOs, the number of correct decimal figures ΔI, and the central processing unit time are shown in these tables. We see from the tables that the accuracy of computer results for different translation formulas obtained from LETOs and CETOs and for translations of different STOs is satisfactory.

It should be noted that in all calculations, the convergence of expansion formulas for translation of STOs obtained using CETOs is faster than those obtained using LETOs. Therefore, it is recommended that expansion formulas for translation of STOs which are derived with the help of CETOs be used.

TABLE I

Comparison of Methods for Computing Three-Center Hybrid Integrals using Translations ($d \rightarrow b$) and ($b \rightarrow d$) for Real STOs in Eq. (16)[a]

n_1	l_1	m_1	ζ_1	n_1'	l_1'	m_1'	ζ_1'	n_2	l_2	m_2	ζ_2	n_2'	l_2'	m_2'	ζ_2'	R_{db}	R_{ab}	Eqs. (9) and (16)	(ΔI)	Eqs. (12) and (16)	(ΔI)	CPU (ms)
2	1	1	1.625	2	1	1	1.625	2	1	1	1.625	2	1	1	1.625	4.5743	2.641	−5.13451275994063E-2	(11)	−5.13451275899716E-2	(12)	295.4
2	1	1	2	2	1	1	2	2	1	1	4	1	0	0	6	0.9	0.32	−2.74646662920085E-1	(11)	−2.74646660715852E-1	(12)	304.4
2	1	1	7	2	1	1	7	1	0	0	5	1	0	0	1	1.4	2.51	6.75049985160350E-2	(12)	6.75049985202979E-2	(12)	267.1
1	0	0	2.7	1	0	0	2.7	2	1	−1	4.5	1	0	0	3.1	10.4	2.51	−5.68180065436271E-5	(7)	−5.68356903097831E-5	(7)	288.7
3	1	1	5.2	3	1	1	5.2	2	1	−1	8.4	2	1	−1	6.3	1.44	2.5	−4.34990744964696E-4	(10)	−4.34990745808048E-4	(10)	324.8
3	2	1	3.5	3	2	1	3.5	3	1	1	2.8	3	1	1	3.6	7.4	1.25	9.28725842001162E-5	(6)	9.25798998607411E-5	(7)	345
3	2	2	6.3	3	2	2	6.3	3	2	1	4.2	3	2	1	2.3	0.94	0.12	3.59478572160958E-2	(9)	3.59478573609076E-2	(8)	567.5
4	2	2	7.8	4	2	0	7.8	3	2	2	5.6	3	2	2	1.7	0.14	1.1	2.49662333569866E-1	(8)	2.4966232242652E-1	(9)	603.7

[a] For $N' = 12,\ l' = 11,\ \lambda' = 5,\ \theta_{db} = 90^\circ,\ \phi_{db} = 150^\circ,\ \theta_{ab} = 90^\circ,\ \phi_{ab} = 0^\circ$, and $\Delta I = I(d \rightarrow b) - I(b \rightarrow d)$.

TABLE II

Comparison of Methods for Computing Two-Center ($R_{ca} = R_{ab}$) and Three-Center ($R_{ca} \neq R_{ab}$) Exchange Integrals Using Translations ($c \rightarrow a$) and ($a \rightarrow c$) for Real STOs in Eq. (17)[a]

n_1	l_1	m_1	ζ_1	n_1'	l_1'	m_1'	ζ_1'	n_2	l_2	m_2	ζ_2	n_2'	l_2'	m_2'	ζ_2'	R_{ca}	R_{ab}	Eqs. (9) and (17)	(ΔI)	Eqs. (12) and (17)	(ΔI)	CPU (ms)
3	1	1	5.5	2	1	1	2.4	3	1	1	5.5	2	1	1	2.4	1.5	1.5	1.22403353933271E-1	(10)	1.22403338327418E-1	(11)	215.4
2	1	0	7.5	2	1	0	3.4	2	1	0	7.5	2	1	0	3.4	10.3	10.3	1.16231071544797E-10	(10)	1.58165683684930E-10	(10)	162.1
2	1	0	5.6	1	0	0	2.1	2	1	0	5.6	1	0	0	2.1	3.4	3.4	1.16694547668396E-5	(8)	1.166720500700857E-5	(9)	144.6
2	1	1	5.7	2	1	1	4.3	2	1	1	5.7	2	1	1	4.3	4.5	4.5	2.91819203499975E-4	(8)	2.91816235838480E-4	(9)	209.3
2	1	0	4.8	1	0	0	2.6	2	1	0	4.8	1	0	0	1.7	2.26	3.14	2.26433080531823E-5	(10)	2.26433184186111E-5	(11)	155.2
2	1	1	4.4	2	1	0	1.2	2	1	1	4.4	2	1	0	4.4	3.2	3.2	7.23509134445996E-5	(9)	7.23508107339543E-5	(9)	225
2	1	1	7.6	2	1	1	5.1	2	1	1	7.6	2	1	1	4.2	6.21	0.86	−9.51703125990969E-8	(9)	−9.72378909700860E-8	(10)	276.3
3	2	1	9.7	2	1	1	4.5	3	2	1	9.7	2	1	1	3.4	0.12	4.8	2.61859191050604E-5	(10)	2.61857831416464E-5	(9)	288.6
3	2	2	3.9	3	2	1	3.4	3	2	2	3.9	2	1	1	1.3	12	2.8	3.30134261028632E-10	(9)	2.82193349272817E-10	(9)	305.3
3	2	2	5.3	3	2	2	3.3	3	2	2	5.3	3	2	2	3.1	0.3	1.2	−1.35051623137866E-1	(9)	−1.35053892543011E-1	(10)	324.1
4	3	1	5.39	3	2	1	4.34	4	3	1	5.39	3	2	1	2.13	1.6	9	4.27418414430648E-5	(7)	4.26832262590353E-5	(7)	278.5

[a] For $N = 12,\ l = 11,\ \lambda = 5,\ \theta_{ca} = 70^\circ,\ \phi_{ca} = 180^\circ,\ \theta_{ab} = 108^\circ,\ \phi_{ab} = 120^\circ$, and $\Delta I = I(c \rightarrow a) - I(a \rightarrow c)$.

TABLE III

Comparison of Methods for Computing Four-Center Electron-Repulsion Integrals Using Translations ($c \to a, d \to b$) and ($a \to c, b \to d$) for Real STOs in Eq. (18)[a]

n_1	l_1	m_1	ζ_1	n_1'	l_1'	m_1'	ζ_1'	n_2	l_2	m_2	ζ_2	n_2'	l_2'	m_2'	ζ_2'	R_{ca}	R_{db}	R_{ab}	Eqs. (9) and (18)	(ΔI)	Eqs. (12) and (18)	(ΔI)	CPU (ms)
1	0	0	1.1	1	0	0	1.1	1	0	0	1.1	2	0	0	0.4	3.067	1.911	3.067	2.78336476913143E-2	(10)	2.78336479212079E-2	(11)	276.8
1	0	0	1.1	1	0	0	1.1	1	0	0	1.1	2	1	1	0.4	3.067	1.911	3.067	−1.08137012743966E-2	(10)	−1.08137076810082E-2	(12)	298.3
2	1	1	6.2	2	0	0	4	2	0	0	6	2	1	1	3	9.4	8.7	6.12	−1.58269572973121E-22	(22)	−1.85873656055899E-22	(22)	253.7
2	1	1	1.6	2	1	0	4.4	2	1	0	6	2	1	1	3	3.8	2.27	4.5	−1.30394501793941E-10	(11)	−1.32291414086593E-10	(11)	375.5
3	2	1	4.2	2	1	1	2.7	3	2	1	7.6	2	1	1	5	0.08	0.11	0.08	1.73324039357242E-1	(9)	1.733242386666656E-1	(10)	824.5
3	2	1	7.3	3	2	1	4.1	3	2	1	5.4	3	1	1	2.3	2.8	6.1	9.08	−8.37749228200090E-19	(19)	−7.175017556907451E-19	(19)	1378.9
3	2	2	2.7	3	2	1	1.4	3	2	1	3.5	3	1	1	1.3	1.8	3.1	3.5	1.44274257876545E-4	(6)	1.440755734100456E-4	(6)	1568.2
3	2	2	4.2	3	2	2	3.1	3	2	2	5.3	3	2	2	2.1	3.1	4.3	2.3	8.23553798110862E-7	(7)	7.735386802667405E-7	(7)	1875.4

[a] For $N = N' = 12,\ l = l' = 11,\ \lambda = \lambda' = 5,\ \theta_{ca} = 90^\circ,\ \phi_{ca} = 150^\circ,\ \theta_{db} = 112.1^\circ,\ \phi_{db} = 60^\circ,\ \theta_{ab} = 90^\circ,\ \phi_{ab} = 210^\circ$, and $\Delta I = I(c \to a,\ d \to b) - I(a \to c,\ b \to d)$.

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