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ORIGINAL PAPER

Unified treatment of complete orthonormal sets for exponential type vector orbitals of particles with spin 1 in coordinate, momentum and four-dimensional spaces

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Abstract The new formulas are obtained for complete orthonormal sets of exponential type vector orbitals of a particle with spin 1 in coordinate, momentum and four-dimensional spaces using the properties of spherical vectors and complete orthonormal scalar basis sets of ψ^{α}-exponential type orbitals (ψ^{α}-ETO), ϕ^{α}-momentum space orbitals (ϕ^{α}-MSO) and z^{α}-hyperspherical harmonics (z^{α}-HSH) introduced by the author for particles with spin $s = 0$, where $\alpha = 1, 0, -1, -2, \ldots$ These vector orbitals are complete without the inclusion of the continuum and, therefore, their group of transformation is the four-dimensional rotation group of O(4). For overlap integrals over vector Slater orbitals with the same screening constant the analytical relations in coordinate space are also derived. It should be noted that the new idea presented in this study is the combination of spherical vectors with complete orthonormal scalar sets for radial parts of ψ^{α}-, ϕ^{α}-, z^{α}-orbitals.

Keywords Spherical vector · Exponential type vector orbitals · Overlap integral

1 Introduction

It is well known that the Schrödinger's hydrogen-like orbitals and their extensions to momentum and four-dimensional spaces by Fock [1,2] are awkward to use as basis because they are not complete unless the continuum is included. Hylleraas, Shull and Löwdin in Refs. [3–6] introduced the so-called Lambda and Coulomb Sturmian functions which are complete and orthonormal basis sets for the particles with spin s = 0 in coordinate space. These functions later were used extensively by Filter, Steinborn [7] and Weniger [8]. The method for constructing relativistic Coulomb Sturmian basis

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set has been developed and discussed by Avery and Antonsen [9]. Recently, in Refs. [10–12] we suggested in coordinate, momentum and four-dimensional spaces the scalar basis sets of ψ^{α}-ETO, ϕ^{α}-MSO and z^{α}-HSH for particles with spin $s = 0$ which are complete without the inclusion of the continuum, where $\alpha = 1, 0, -1, -2, \ldots$. In the present work, we obtain a large number of new different complete and orthonormal sets for vector wave functions, and vector Slater orbitals in coordinate, momentum and four-dimensional spaces using complete orthonormal scalar basis sets of ψ^{α}-ETO, ϕ^{α}-MSO and z^{α}-HSH functions. It should be noted that the Lambda and Coulomb Sturmian functions introduced by Hylleraas, Shull and Löwdin are the special classes of ψ^{α}-ETO for $\alpha = 0$ and $\alpha = 1$, respectively (see Ref. [10]).

2 Spherical vectors and vector wave functions

For the derivation of relations for complete orthonormal sets of vector wave functions of a particle with spin $s = 1$ in coordinate, momentum and four-dimensional spaces we use the following eigenvalue equations of spherical vectors (see Sect. 7.3. of Ref. [13]):

$$\hat{j}^2 Y^l_{jm_j}(\theta, \varphi) = j(j+1) Y^l_{jm_j}(\theta, \varphi) \tag{1}$$

$$\hat{j}_z Y^l_{jm_j}(\theta, \varphi) = m_j Y^l_{jm_j}(\theta, \varphi) \tag{2}$$

$$\hat{l}^2 Y^l_{jm_j}(\theta, \varphi) = l(l+1) Y^l_{jm_j}(\theta, \varphi) \tag{3}$$

$$\hat{s}^2 Y^l_{jm_j}(\theta, \varphi) = 2 Y^l_{jm_j}(\theta, \varphi), \tag{4}$$

Here, $\hat{l}$-orbital angular momentum operator, $\hat{s}$-spin operator for s = 1, $\hat{j} = \hat{l} + \hat{s}$-total angular momentum operator. The spherical vectors $Y^l_{jm_j}(\theta, \varphi)$ are expressed through the products of scalar spherical harmonics $Y_{lm_l}(\theta, \varphi)$ and basis spin functions u_{1m_s}, i.e.,

$$Y^l_{jm_j}(\theta, \varphi) = \sum_{m_l, m_s} (l1m_l m_s \left| l1jm_j \right.) Y_{lm_l}(\theta, \varphi) u_{1m_s}, \tag{5}$$

where $(l1m_l m_s \left| l1jm_j \right.)$ are the Clebsch–Gordan coefficients, $m_l = m_j - m_s$ and (see Sect. 6.1. of Ref. [13]):

$$u_{11} = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}, \quad u_{10} = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}, \quad u_{1-1} = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}. \tag{6}$$

The complete sets of scalar spherical harmonics, basis spin functions and spherical vectors satisfy the following orthonormality relations:

$$\int_0^{\pi} \int_0^{2\pi} Y^*_{lm_l}(\theta, \varphi) Y_{l'm'_l}(\theta, \varphi) \mathrm{Sin}\theta d\theta d\varphi = \delta_{ll'} \delta_{m_l m'_l} \tag{7}$$

$$u^{+}_{1m_s} u_{1m'_s} = \delta_{m_s m'_s} \tag{8}$$

$$\int_0^{\pi} \int_0^{2\pi} Y^{l+}_{jm_j}(\theta, \varphi) Y^{l'}_{j'm'_j}(\theta, \varphi) \mathrm{Sin}\theta d\theta d\varphi = \delta_{jj'} \delta_{m_j m'_j} \delta_{ll'}. \tag{9}$$

We notice that the spherical vectors are not eigenfunctions of the operators $\hat{l}_z$ and $\hat{s}_z$, i.e., the quantum numbers m_l and m_s cannot be used to characterize them. This is important in derivation of relations for the complete orthonormal sets of vector wave functions in coordinate, momentum and four-dimensional spaces.

Taking into account Eq. (6) for the basis spin functions u_{1m_s} in (5) we can express the spherical vectors $Y^l_{jm_j}(\theta, \varphi)$ only through the scalar spherical harmonics $Y_{lm_l}(\theta, \varphi)$, i.e.,

$$Y^l_{jm_j}(\theta, \varphi) = \begin{pmatrix} a^l_{jm_j}(0) Y_{lm_l(0)}(\theta, \varphi) \\ a^l_{jm_j}(1) Y_{lm_l(1)}(\theta, \varphi) \\ a^l_{jm_j}(2) Y_{lm_l(2)}(\theta, \varphi) \end{pmatrix}, \tag{10}$$

where $m_l(\lambda) = m_j - 1 + \lambda$, $0 \le \lambda \le 2$ and

$$a^l_{jm_j}(\lambda) = (l1m_l 1 - \lambda \left| l1jm_j \right.). \tag{11}$$

Now we move on to the derivation of vector wave functions. For this purpose we introduce the following complete and orthonormal sets of functions:

$$\psi_{nlm_l}(\vec{r}) = R_{nl}(r) Y_{lm_l}(\theta, \varphi) \tag{12}$$

These functions are complete and orthonormal with respect to an integration over the whole 3-dimensional space $\Re^3$ in a suitable Hilbert space of functions $F(\vec{r})$ by forming products of the (surface) spherical harmonics $Y_{lm_l}(\theta, \varphi)$, which are complete and orthonormal with respect to an integration over the surface of the unit sphere in $\Re^3$, and the radial functions $R_{nl}(r)$, which are complete and orthonormal with respect to an integration over the positive semiaxis $0 \le r < \infty$ in a suitable Hilbert space of radial functions $f(r)$.

It is obviously possible to expand a function $F(\vec{r})$ belonging to a suitable Hilbert space in terms of the complete and orthonormal functions $\psi_{nlm_l}(\vec{r})$ which are determined by Eq. (12):

$$F(\vec{r}) = \sum_{nlm_l} C_{nlm_l} \psi_{nlm_l}(\vec{r}) \tag{13}$$

$$C_{nlm_l} = \int \psi^*_{nlm_l}(\vec{r}) F(\vec{r}) d^3\vec{r}. \tag{14}$$

As long as the ψ_{nlm_l} are complete and orthonormal set of functions, the convergence of expansion (13) is guaranteed. Thus, the functions ψ_{nlm_l} constructed by the product of complete and orthonormal functions $R_{nl}(r)$ and $Y_{lm_l}(\theta, \varphi)$ also are the complete orthonormal functions in a suitable space of the radial functions and the (surface) spherical harmonics.

In this way, one can construct the vector wave functions. For this purpose, we multiply the scalar components of the spherical vectors by the complete orthonormal radial functions $R_{nl}(r)$. Then, we obtain the following complete orthonormal set of vector wave functions:

$$\psi^l_{njm_j}(\vec{r}) = R_{nl}(r)Y^l_{jm_j}(\theta, \varphi) = \begin{pmatrix} a^l_{jm_j}(0)\psi_{nlm_{l(0)}}(r, \theta, \varphi) \\ a^l_{jm_j}(1)\psi_{nlm_{l(1)}}(r, \theta, \varphi) \\ a^l_{jm_j}(2)\psi_{nlm_{l(2)}}(r, \theta, \varphi) \end{pmatrix}. \tag{15}$$

The vector wave functions also satisfy the orthonormality relation, i.e.,:

$$\int \psi^{l+}_{njm_j}(\vec{r})\psi^{l'}_{n'j'm'_j}(\vec{r})d^3r = \delta_{nn'}\delta_{jj'}\delta_{m_jm'_j}\delta_{ll'}. \tag{16}$$

3 Complete orthonormal sets of exponential type vector orbitals

For the derivation of relations for the complete orthonormal sets of vector orbitals in coordinate, momentum and four-dimensional spaces we use the properties of spherical vectors (see Sect. 7.3. of Ref. [13]) and scalar basis sets of ψ^α-ETO, ϕ^α-MSO, z^α-HSH functions presented in [10–12]. Then, we obtain the following results: for vector Ψ^α-ETO (Ψ^α-VETO) in coordinate space

$$\Psi^{\alpha l}_{njm_j}(\zeta, \vec{r}) = \begin{pmatrix} a^l_{jm_j}(0)\psi^\alpha_{nlm_l(0)}(\zeta, \vec{r}) \\ a^l_{jm_j}(1)\psi^\alpha_{nlm_l(1)}(\zeta, \vec{r}) \\ a^l_{jm_j}(2)\psi^\alpha_{nlm_l(2)}(\zeta, \vec{r}) \end{pmatrix} \tag{17a}$$

$$\bar{\Psi}^{\alpha l}_{njm_j}(\zeta, \vec{r}) = \begin{pmatrix} a^l_{jm_j}(0)\bar{\psi}^{\alpha l}_{nlm_l(0)}(\zeta, \vec{r}) \\ a^l_{jm_j}(1)\bar{\psi}^{\alpha l}_{nlm_l(1)}(\zeta, \vec{r}) \\ a^l_{jm_j}(2)\bar{\psi}^{\alpha l}_{nlm_l(2)}(\zeta, \vec{r}) \end{pmatrix}, \tag{17b}$$

for vector Φ^α-MSO (Φ^α-VMSO) in momentum space

$$\Phi^{\alpha l}_{njm_j}(\zeta, \vec{k}) = \begin{pmatrix} a^l_{jm_j}(0)\phi^\alpha_{nlm_l(0)}(\zeta, \vec{k}) \\ a^l_{jm_j}(1)\phi^\alpha_{nlm_l(1)}(\zeta, \vec{k}) \\ a^l_{jm_j}(2)\phi^\alpha_{nlm_l(2)}(\zeta, \vec{k}) \end{pmatrix} \tag{18a}$$

$$\bar{\Phi}^{\alpha l}_{njm_j}(\zeta,\vec{k}) = \begin{pmatrix} a^l_{jm_j}(0)\bar{\phi}^{\alpha}_{nlm_l(0)}(\zeta,\vec{k}) \\ a^l_{jm_j}(1)\bar{\phi}^{\alpha}_{nlm_l(1)}(\zeta,\vec{k}) \\ a^l_{jm_j}(2)\bar{\phi}^{\alpha}_{nlm_l(2)}(\zeta,\vec{k}) \end{pmatrix}, \tag{18b}$$

for vector Z^α-HSH (Z^α-VHSH) in four-dimensional space

$$Z^{\alpha l}_{njm_j}(\zeta,\beta\theta\varphi) = \begin{pmatrix} a^l_{jm_j}(0)z^{\alpha}_{nlm_l(0)}(\zeta,\beta\theta\varphi) \\ a^l_{jm_j}(1)z^{\alpha}_{nlm_l(1)}(\zeta,\beta\theta\varphi) \\ a^l_{jm_j}(2)z^{\alpha}_{nlm_l(2)}(\zeta,\beta\theta\varphi) \end{pmatrix} \tag{19a}$$

$$\bar{Z}^{\alpha l}_{njm_j}(\zeta,\beta\theta\varphi) = \begin{pmatrix} a^l_{jm_j}(0)\bar{z}^{\alpha}_{nlm_l(0)}(\zeta,\beta\theta\varphi) \\ a^l_{jm_j}(1)\bar{z}^{\alpha}_{nlm_l(1)}(\zeta,\beta\theta\varphi) \\ a^l_{jm_j}(2)\bar{z}^{\alpha}_{nlm_l(2)}(\zeta,\beta\theta\varphi) \end{pmatrix}. \tag{19b}$$

Here, the coefficients $a^l_{jm_j}(\lambda)$ are determined by Eq. (11) and $n \geq 1$, $1 \leq j \leq n$, $-j \leq m_j \leq j$, $j-1 \leq l \leq \min(j+1, n-1)$.

The functions $\psi^\alpha_{nlm_l}$, $\bar{\psi}^\alpha_{nlm_l}$, $\phi^\alpha_{nlm_l}$, $\bar{\phi}^\alpha_{nlm_l}$, $z^\alpha_{nlm_l}$ and $\bar{z}^\alpha_{nlm_l}$ occurring on the right-hand side of Eqs. (17a)–(19b) are the complete orthonormal sets of orbitals for particles with spin $s = 0$ in coordinate, momentum and four-dimensional spaces.

The vector wave functions Ψ^α, Φ^α and Z^α are orthonormal with respect to the $\bar{\Psi}^\alpha$, $\bar{\Phi}^\alpha$ and $\bar{Z}^\alpha$, respectively, i.e.,

$$\int \bar{\Psi}^{\alpha l+}_{njm_j}(\zeta,\vec{r})\Psi^{\alpha l'}_{n'j'm'_j}(\zeta,\vec{r})d^3\vec{r} = \delta_{nn'}\delta_{jj'}\delta_{m_jm'_j}\delta_{ll'} \tag{20}$$

$$\int \bar{\Phi}^{\alpha l+}_{njm_j}(\zeta,\vec{k})\Phi^{\alpha l'}_{n'j'm'_j}(\zeta,\vec{k})d^3\vec{k} = \delta_{nn'}\delta_{jj'}\delta_{m_jm'_j}\delta_{ll'} \tag{21}$$

$$\int \bar{Z}^{\alpha l+}_{njm_j}(\zeta,\beta\theta\varphi)Z^{\alpha l'}_{n'j'm'_j}(\zeta,\beta\theta\varphi)d\Omega(\zeta,\beta\theta\varphi) = \delta_{nn'}\delta_{jj'}\delta_{m_jm'_j}\delta_{ll'}. \tag{22}$$

4 Vector slater orbitals

Carrying through the calculations for vector slater orbitals analogous to those for the vector wave functions, we obtain the following relations through the scalar Slater orbitals:
for vector X-STO (X-VSTO) in coordinate space

$$X^l_{njm_j}(\zeta,\vec{r}) = \begin{pmatrix} a^l_{jm_j}(0)\chi_{nlm_l(0)}(\zeta,\vec{r}) \\ a^l_{jm_j}(1)\chi_{nlm_l(1)}(\zeta,\vec{r}) \\ a^l_{jm_j}(2)\chi_{nlm_l(2)}(\zeta,\vec{r}) \end{pmatrix}, \tag{23}$$

for vector U-MSO (U-VMSO) in momentum space

$$U^{l}_{njm_j}(\zeta,\vec{k})=\begin{pmatrix} a^{l}_{jm_j}(0)u_{nlm_l(0)}(\zeta,\vec{k})\\ a^{l}_{jm_j}(1)u_{nlm_l(1)}(\zeta,\vec{k})\\ a^{l}_{jm_j}(2)u_{nlm_l(2)}(\zeta,\vec{k})\end{pmatrix}, \tag{24}$$

for vector V-HSH (V-VHSH) in four-dimensional space

$$V^{l}_{njm_j}(\zeta,\beta\theta\varphi)=\begin{pmatrix} a^{l}_{jm_j}(0)v_{nlm_l(0)}(\zeta,\beta\theta\varphi)\\ a^{l}_{jm_j}(1)v_{nlm_l(1)}(\zeta,\beta\theta\varphi)\\ a^{l}_{jm_j}(2)v_{nlm_l(2)}(\zeta,\beta\theta\varphi)\end{pmatrix}, \tag{25}$$

See Ref. [12] for the exact definition of Slater orbitals χ_{nlm_l}, u_{nlm_l} and v_{nlm_l} in coordinate, momentum and four-dimensional spaces occurring on the right-hide side of Eqs. (23)–(25).

The vector Slater orbitals determined by relations (23), (24) and (25) are orthogonal with respect to the quantum numbers j, m_j and l, i.e.,

$$\int \mathrm{X}^{l+}_{njm_j}(\zeta,\vec{r})\mathrm{X}^{l'}_{n'j'm'_j}(\zeta,\vec{r})d^3\vec{r}=\frac{(n+n')!}{[(2n)!(2n')!]^{1/2}}\delta_{jj'}\delta_{m_jm'_j}\delta_{ll'} \tag{26}$$

$$\int U^{l+}_{njm_j}(\zeta,\vec{k})U^{l'}_{n'j'm'_j}(\zeta,\vec{k})d^3\vec{k}=\frac{(n+n')!}{[(2n)!(2n')!]^{1/2}}\delta_{jj'}\delta_{m_jm'_j}\delta_{ll'} \tag{27}$$

$$\int V^{l+}_{njm_j}(\zeta,\beta\theta\varphi)V^{l'}_{n'j'm'_j}(\zeta,\beta\theta\varphi)d\Omega(\zeta,\beta\theta\varphi)=\frac{(n+n')}{[(2n)!(2n')!]^{1/2}}\delta_{jj'}\delta_{m_jm'_j}\delta_{ll'}. \tag{28}$$

5 Evaluation of overlap integrals over vector STO in coordinate space

As an example of application, we evaluate the two-center overlap integrals over vector Slater orbitals with the same screening parameters in coordinate space defined by

$$S^{l,l'}_{njm_j,n'j'm'_j}(\vec{G})=\int \mathrm{X}^{l+}_{njm_j}(\zeta,\vec{r})\mathrm{X}^{l'}_{n'j'm'_j}(\zeta,\vec{r}-\vec{R})d^3\vec{r}, \tag{29}$$

where $\vec{r}=\vec{r}_a$, $\vec{r}-\vec{R}=\vec{r}_b$, $\vec{R}=\vec{R}_{ab}$ and $\vec{G}=2\zeta\vec{R}$.

Now we take into account Eq. (23) in (29). Then, we obtain for integrals (29) the following relation in terms of overlap integrals over χ-STO:

$$S^{ll'}_{njm_j,n'j'm'_j}(\vec{G}) = a^{ll'}_{jm_jj'm'_j}(0)s_{nlm_l(0),n'l'm'_l(0)}(\vec{G}) + a^{ll'}_{jm_jj'm'_j}(1)s_{nlm_l(1),n'l'm'_l(1)}(\vec{G}) + a^{ll'}_{jm_jj'm'_j}(2)s_{nlm_l(2),n'l'm'_l(2)}, \tag{30}$$

where $a^{ll'}_{jm_jj'm'_j}(\lambda) = a^{l}_{jm_j}(\lambda)a^{l'}_{j'm'_j}(\lambda)$ and

$$s_{nlm_l,n'l'm'_l}(\vec{G}) = \int \chi^*_{nlm_l}(\zeta,\vec{r})\chi_{n'l'm'_l}(\zeta,\vec{r}-\vec{R})d^3\vec{r}. \tag{31}$$

In order to evaluate the overlap integrals over scalar STO, Eq. (31), we use the following expressions for STO in terms of complete orthonormal sets of ψ^α- and $\bar{\psi}^\alpha$-ETOs:

$$\chi_{nlm_l}(\zeta,\vec{r}) = \sum_{\mu=l+1}^{n} \bar{\omega}^{\alpha l}_{n\mu}\psi^\alpha_{\mu lm_l}(\zeta,\vec{r}) \tag{32a}$$

$$= \{[2(n+\alpha)]!/(2n)!\}^{1/2} \sum_{\mu=l+1}^{n+\alpha} [\bar{\omega}^{\alpha l}_{n+\alpha\mu}/(2\mu)^\alpha]\bar{\psi}^\alpha_{\mu lm_l}(\zeta,\vec{r}), \tag{32b}$$

See Ref. [10] for the exact definition of coefficients $\bar{\omega}^{\alpha l}$. Then, we obtain:

$$s_{nlm_l,n'l'm'_l}(\vec{G}) = \{[2(n+\alpha)]!/(2n)!\}^{1/2} \sum_{\mu=l+1}^{n+\alpha} \sum_{\mu'=l'+1}^{n'} [\bar{\omega}^{\alpha l}_{n+\alpha\mu}/(2\mu)^\alpha]\bar{\omega}^{\alpha l'}_{n'\mu'} \times s^\alpha_{\mu lm_l,\mu'l'm'_l}(\vec{G}), \tag{33}$$

where $\alpha = 1, 0, -1, -2, \ldots$ and

$$s^\alpha_{\mu lm_l,\mu'l'm'}(\vec{G}) = \int \bar{\psi}^{\alpha *}_{\mu lm_l}(\zeta,\vec{r})\psi^\alpha_{\mu'l'm'_l}(\zeta,\vec{r}-\vec{R})d^3\vec{r}. \tag{34}$$

The analytical relations for the determination of integral (34) are available in Ref. [12].

The values overlap integrals over vector Slater orbitals with the same screening parameters obtained from the different complete sets of ψ^α-ETO ($\alpha = 1, 0, -1$) using Mathematica 5.0 international mathematical software are presented in Table 1. As can be seen from the table that the presented in this work approach for a particle with spin 1 guarantees a highly accurate calculation of the X-VSTO overlap integrals.

It should be noted that the overlap integrals over vector STO with the same screening parameters play a significant role in the calculation of arbitrary multicenter integrals

Table 1 The values of overlap integrals over X-VSTO obtained from the different complete sets of ψ^{α}-ETO in molecular coordinate system

n	j	m_j	l	n'	j'	m'_j	l'	θ	φ	$G = 2\zeta R$	Eqs. (30) and (33)		
											$\alpha = 1$	$\alpha = 0$	$\alpha = -1$
3	1	0	0	2	1	0	0	0	0	100	2.7703550866E-16	2.7703550866E-16	2.7703550866E-16
5	3	2	2	4	2	2	2	0	0	120	1.3671541011E-17	1.3671541011E-17	1.3671541011E-17
6	4	3	4	7	4	3	4	0	0	70	6.1423669728E-07	6.1423669728E-07	6.1423669728E-07
8	7	5	6	8	5	5	6	0	0	80	1.3572606274E-08	1.3572606274E-08	1.3572606274E-08
9	6	4	7	6	4	4	4	0	0	40	−4.9503929717E-04	−4.9503929717E-04	−4.9503929717E-04
11	8	6	9	10	7	6	9	0	0	60	1.1296567011E-05	1.1296567011E-05	1.1296567011E-05
3	2	1	1	2	1	0	0	$\pi/8$	$2\pi/3$	50	−1.5925219197E-07	−1.5925219197E-07	−1.5925219197E-07
5	4	3	3	5	2	1	1	$2\pi/5$	$5\pi/3$	60	4.1403685342E-06	4.1403685342E-06	4.1403685342E-06
7	6	3	5	6	5	1	4	$\pi/4$	π	30	2.3106531352E-04	2.3106531352E-04	2.3106531352E-04
9	8	3	7	8	7	7	6	$4\pi/5$	$\pi/7$	100	1.4852955548E-09	1.4852955548E-09	1.4852955548E-09
11	8	5	7	10	9	9	8	$\pi/8$	$9\pi/7$	90	1.8690202487E-09	1.8690202487E-09	1.8690202487E-09
13	10	8	9	12	11	11	10	$5\pi/6$	$5\pi/6$	120	8.2938717076E-12	8.2938717076E-12	8.2938717076E-12

arising in coordinate, momentum and four-dimensional spaces. Thus, in the evaluation of multicenter integrals over vector orbitals for a particle with spin 1 the relations for the two-center overlap integrals over ψ^{α}-ETO, ϕ^{α}-MSO, z^{α}-HSH and χ-STO also can be used. For this purpose, one has to use the expansion and one-range addition theorems for scalar basis sets of ψ^{α}-ETO, ϕ^{α}-MSO, z^{α}-HSH and χ-STO presented in our previous papers.

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