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Combined theory of one- and two-electron bipolar and polar multicenter integrals of noninteger *n* Slater functions and Coulomb-Yukawa-like potentials with noninteger indices

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By the use of one-range addition theorems suggested by the author, the combined theory for one- and two-electron multicenter integrals of χ -noninteger n Slater type orbitals (χ -NISTOs) and bipolar and polar noninteger Coulomb (C-NIBPs and C-NIPs) -Yukawa (Y-NIBPs and Y-NIPs)-like correlated potentials is presented. These multicenter integrals are expressed through the basic polar integrals of χ - integer n Slater type orbitals (χ -ISTOs) and Coulomb-Yukawa-like potentials with integer indices (C-IPs and Y-IPs). We note that the noninteger quantum number n is defined as $n*$.

Key words: Exponential type orbitals, Addition theorems, Bipolar potentials, Multicenter integrals, Self-frictional quantum numbers **PACS:** 31.10.+z; 31.15.-p

INTRODUCTION

It is well known that the main problem in the accurate electronic structure calculations arises in the evaluation of the multicenter integrals which confirms that other theories are needed instead [1, 2]. The arguments of a new theory for multicenter integrals developed in this work are based on a completely different point of view, namely, making use of the bipolar potentials (see [3-5] and refs. quoted therein). The aim of this work is to evaluate the multicenter integrals with χ -NISTOs and C-NIBPs, C-NIPs, Y-NIBPs and Y-NIPs potentials. The obtained formulas are especially useful in the accurate calculation of electronic structure properties for atoms and molecules when a χ -NISTOs basis set and explicitly correlated methods are used in the linear combination of atomic orbitals – molecular orbitals (LCAO-MO) approximation [6].

DEFINITION AND BASIC FORMULAS

The χ -NISTOs, C-NIPs (for $\eta = 0$) and Y-NIPs (for $\eta > 0$) used in this work are defined as follows:

$$\chi_{n^*lm}(\zeta,\vec{r}) = R_{n^*}(\zeta,r)S_{lm}(\theta,\varphi) \tag{1}$$

$$O_{u^*\upsilon s}(\eta,\vec{r}) = O_{u^*\upsilon}(\eta,r)S_{\upsilon s}(\theta,\varphi), \tag{2}$$

where

$$R_{n^*}(\zeta,r) = \frac{(2\zeta)^{n^*+1/2}}{\left[\Gamma(2n^*+1)\right]^{1/2}} r^{n^*-1}e^{-\zeta r} \tag{3}$$

$$O_{u^*\upsilon}(\eta,r) = \left(\frac{4\pi}{2\upsilon+1}\right)^{\frac{1}{2}} r^{u^*-1}e^{-\eta r} \tag{4}$$

Here, $S_{lm}(\theta,\varphi)$ are the complex (for $S_{lm} = Y_{lm}$) or real spherical harmonics defined as

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

where $P_{l|m|}$ are the normalized Legendre functions and for complex spherical harmonics

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

for real spherical harmonics

$$\Phi_m(\varphi) = \frac{1}{\sqrt{\pi(1+\delta_{m0})}} \begin{cases} \cos|m|\varphi & for\ m \geq 0 \\ \sin|m|\varphi & for\ m < 0. \end{cases} \tag{7}$$

Our definition of phases for the complex spherical harmonics $\left(Y_{lm}^* = Y_{l-m}\right)$ [7] differs from the Condon-Shortley phases [8] by the sign factor $(-1)^m$.

All of the one- and two-electron multicenter integrals examined in this work can be defined by the following combined formulas:

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$$U^{ij,acb;eh}_{p_1{}^*p_1'{}^*;k^*}(\zeta_1,\zeta_1';\eta)=\int \chi^*_{p_1{}^*}(\zeta_1,\vec{r}_{a1})$$

$$O^i_{k^*}\left(\eta,\vec{r}_{b1}-\vec{R}_{eh}\right)\left(-\frac{1}{2}\nabla_1^2\right)^j \chi_{p_1'{}^*}(\zeta_1',\vec{r}_{c1})\,d^3\vec{r}_1 \quad (8)$$

$$I^{ac,bd;eh}_{p_1{}^*p_1'{}^*,p_2{}^*p_2'{}^*;k^*}\left(\zeta_1,\zeta_1';\zeta_2,\zeta_2';\eta\right)$$
$$=\iint \chi^*_{p_1{}^*}(\zeta_1,\vec{r}_{a1})\,\chi_{p_1'{}^*}\left(\zeta_1',\vec{r}_{c1}\right)\chi_{p_2{}^*}(\zeta_2,\vec{r}_{b2})$$
$$\times\chi^*_{p_2'{}^*}\left(\zeta_2',\vec{r}_{d2}\right)O_{k^*}\left(\eta,\vec{r}_{21}-\vec{R}_{eh}\right)d^3\vec{r}_1 d^3\vec{r}_2, \quad (9)$$

where $p_i{}^*=n_i{}^*l_im_i$, $p'^*_i=n_i'{}^*l_i'm_i'$, $k^*=u^*\upsilon s$, $\zeta_i>0$, $\zeta_i'>0$ *and* $\eta\geq 0$. Here, the values $ij=00$, $ij=01$ *and* $ij=10$ in Eq. (8) correspond to the overlap, kinetic energy and nuclear attraction integrals,

$$S_{p_1{}^*p_1'{}^*}(\zeta_1,\zeta_1';\vec{R}_{ac})=U^{00,ac}_{p_1{}^*p_1'{}^*}(\zeta_1,\zeta_1')$$
$$=\int \chi^*_{p_1{}^*}(\zeta_1,\vec{r}_{a1})\,\chi_{p_1'{}^*}\left(\zeta_1',\vec{r}_{c1}\right)d^3\vec{r}_1 \quad (10)$$

$$K_{p_1{}^*p_1'{}^*}(\zeta_1,\zeta_1';\vec{R}_{ac})=U^{01,ac}_{p_1{}^*p_1'{}^*}(\zeta_1,\zeta_1')$$
$$=\int \chi^*_{p_1{}^*}(\zeta_1,\vec{r}_{a1})\left(-\frac{1}{2}\nabla_1^2\right)\chi_{p_1'{}^*}(\zeta_1',\vec{r}_{c1})\,d^3\vec{r}_1$$
$$=-\frac{1}{2}\zeta_1'^2\left\{S_{n_1{}^*l_1m_1,n_1'{}^*l_1'm_1'}\left(\zeta_1,\zeta_1';\vec{R}_{ac}\right)\right.$$
$$-4n_1'{}^*\left[\frac{\Gamma\left(2n_1'{}^*-1\right)}{\Gamma\left(2n_1'{}^*+1\right)}\right]^{\frac{1}{2}} S_{n_1{}^*l_1m_1,n_1'{}^*-1l_1'm_1'}\left(\zeta_1,\zeta_1';\vec{R}_{ac}\right)$$
$$+4\left(n_1'{}^*+l_1'\right)\left(n_1'{}^*-l_1'-1\right)\left[\frac{\Gamma\left(2n_1'^*-3\right)}{\Gamma\left(2n_1'^*+1\right)}\right]^{\frac{1}{2}}$$
$$\left.\times S_{n_1{}^*l_1m_1,n_1'{}^*-2l_1'm_1'}\left(\zeta_1,\zeta_1';\vec{R}_{ac}\right)\right\} \quad (11)$$

$$U^{acb;eh}_{p_1{}^*p_1'{}^*;k^*}(\zeta_1,\zeta_1';\eta)=U^{10,acb;eh}_{p_1{}^*p_1'{}^*;k^*}(\zeta_1,\zeta_1';\eta)$$
$$=\int \chi_{p_1{}^*}{}^*(\zeta_1,\vec{r}_{a1})\,\chi_{p_1'{}^*}\left(\zeta_1',\vec{r}_{c1}\right)$$
$$\times O_{k^*}\left(\eta,\vec{r}_{b1}-\vec{R}_{eh}\right)d^3\vec{r}_1. \quad (12)$$

As we see, Eqs. (9) and (12) are the bipolar (for $R_{eh}\neq 0$) and polar (for $R_{eh}=0$) nuclear attraction (see Fig. 1) and two-electron (see Fig. 2) multicenter integrals, respectively.

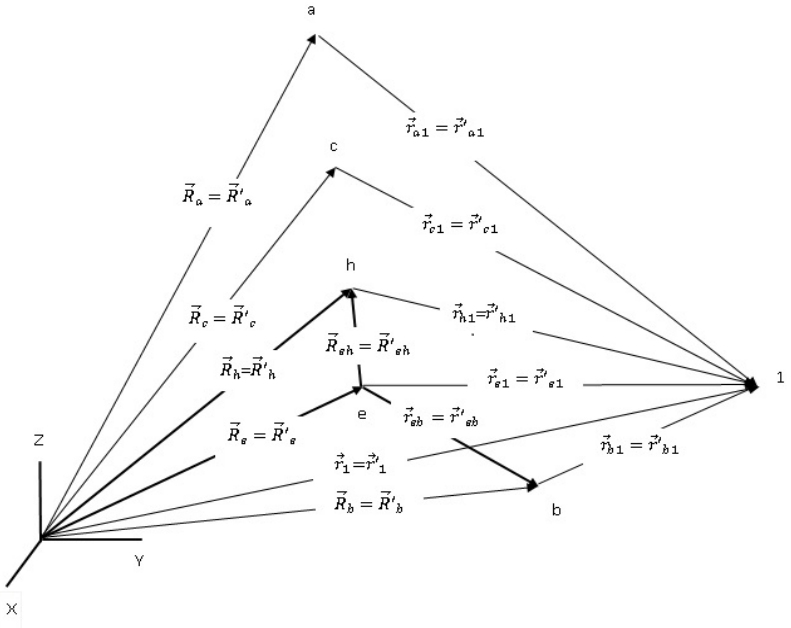

Fig. 1. Geometry of one-electron bipolar ($\vec{R}_{eh}\neq 0$) and polar ($\vec{R}_{eh}=0$) molecule.

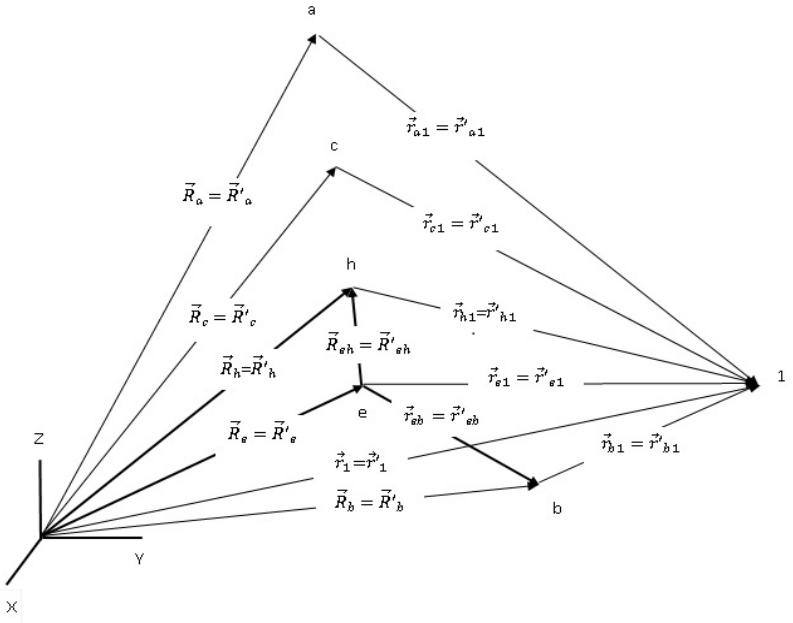

Fig. 2. Geometry of two-electron bipolar ($\vec{R}_{eh} \neq 0$) and polar ($\vec{R}_{eh} = 0$) molecule.

EVALUATION OF BIPOLAR AND POLAR MULTICENTER INTEGRALS

To evaluate the multicenter integrals (9) and (12) we use the formulas in standard convention for the two-center one-range addition theorems for χ -NISTOs in terms of χ -ISTOs in the following form [9, 10]:

$$\chi_{p^*}\left(\zeta,\vec{r}-R_{ab}\right)=\sum_{\mu=1}^{\infty}\sum_{\nu=0}^{\mu-1}\sum_{\sigma=-\nu}^{\nu}\Omega_{qp^*}^{(\alpha^*)}\left(\zeta,\zeta;\vec{R}_{ab}\right)$$

$$\times\sum_{\mu'=\nu+1}^{\mu}\tilde{\omega}_{\mu\mu'}^{(\alpha^*)\nu}\chi_{q'}\left(\zeta,\vec{r}\right), \qquad (13)$$

where $\vec{r}=\vec{r}_a$, $\vec{r}_b=\vec{r}_a-\vec{R}_{ab}=\vec{r}-\vec{R}_{ab}$, $\vec{R}_{ab}=\vec{R}_b-\vec{R}_a$, $p^*=n^*lm$, $q=\mu\nu\sigma$ and $q'=\mu'\nu\sigma$. The expansion coefficients occurring in Eq. (13) are defined as follows:

$$\Omega_{qp^*}^{(\alpha^*)}\left(\zeta,\zeta;\vec{R}_{ab}\right)=(2\mu)^{\alpha^*}\sum_{u=l+1}^{\infty}\omega_{un^*}^{(\alpha^*)l}$$

$$\times\sum_{n=\nu+1}^{\mu}\tilde{\omega}_{\mu n}^{(\alpha^*)\nu}\sum_{n'=l+1}^{u}\tilde{\omega}_{un'}^{(\alpha^*)l}S_{n\nu\sigma,n'lm}^{(\alpha^*)}\left(\zeta,\zeta;\vec{R}_{ab}\right) \qquad (14)$$

$$\omega_{un^*}^{(\alpha^*)l}=\frac{\Gamma(u-n^*)\Gamma(n^*+l-\alpha^*+2)}{\Gamma(l+1-n^*)}$$

$$\times\left[\frac{(2u)^{\alpha^*}}{\left(u-(l+1)\right)!\Gamma(2n^*+1)\Gamma(q_u{}^*+1)}\right]^{1/2} \qquad (15)$$

$$\tilde{\omega}_{\mu n}^{(\alpha^*)\nu}=\left[\frac{(2n)!\Gamma\left(q_\mu^*+1\right)}{(2\mu)^{\alpha^*}\left(\mu-\left(\nu+1\right)\right)!}\right]^{1/2}\tilde{a}_{\mu n}^{\alpha^*\nu} \qquad (16)$$

$$S_{n\nu\sigma,n'lm}^{(\alpha^*)}\left(\zeta,\zeta;\vec{R}_{ab}\right)=\int\frac{1}{(2\zeta r_a)^{\alpha^*}}$$

$$\times\chi_{n\nu\sigma}{}^*\left(\zeta,\vec{r}_a\right)\chi_{n'lm}\left(\zeta,\vec{r}_b\right)d^3\vec{r}. \qquad (17)$$

Here, $p_l{}^*=2l+2-\alpha^*$, $q_u{}^*=u+l+1-\alpha^*$, $p_\nu{}^*=2\nu+2-\alpha^*$, $q_\mu{}^*=\mu+\nu+1-\alpha^*$ and

$$\tilde{a}_{\mu n}^{\alpha^*\nu}=\frac{\left(-\left[\mu-\left(\nu+1\right)\right]\right)_{n-(\nu+1)}}{\Gamma\left(p_\nu^*+1\right)\left(p_\nu^*+1\right)_{n-(\nu+1)}\left(n-\left(\nu+1\right)\right)!}. \qquad (18)$$

$S_{n\nu\sigma,n'lm}^{(\alpha^*)}\left(\zeta,\zeta;\vec{R}_{ab}\right)$ are the modified overlap integrals (MOIs) with χ -ISTOs in molecular coordinate system; $\left(-\left[\mu-\left(\nu+1\right)\right]\right)_{n-(\nu+1)}$ and $\left(p_\nu{}^*+1\right)_{n-(\nu+1)}$ are the Pochhammer symbols. See Refs.[10,11] for the evaluation of MOIs which contain the integer $\left(\alpha^*=\alpha,\ -\infty<\alpha\le 2\right)$ or noninteger $\left(\alpha^*\neq\alpha,\ -\infty<\alpha^*<3\right)$ self-frictional quantum number.

To transform the bipolar potential in multicenter integrals (9) and (12) to the polar case we use the following relations:

$$\vec{r}_{a1}=\vec{r}_1-\vec{R}_a=\vec{r}_1'-\vec{R}_{ha},\vec{r}_{c1}=\vec{r}_1-\vec{R}_c=\vec{r}_1'-\vec{R}_{hc},$$

$$\vec{r}_{b1}=\vec{r}_1-\vec{R}_b=\vec{r}_1'-\vec{R}_{hb} \qquad (19)$$

$$\vec{r}_1' = \vec{r}_{a1} + \vec{R}_{ha} = \vec{r}_{c1} + \vec{R}_{hc} = \vec{r}_{b1} + \vec{R}_{hb} \quad (20)$$

$$\vec{r}_{b2} = \vec{r}_2 - \vec{R}_b = \vec{r}_2' - \vec{R}_{hb}, \vec{r}_{d2} = \vec{r}_2 - \vec{R}_d$$

$$= \vec{r}_2' - \vec{R}_{hd} \quad (21)$$

$$\vec{r}_2' = \vec{r}_{b2} + \vec{R}_{hb} = \vec{r}_{d2} + \vec{R}_{hd} \quad (22)$$

and

$$\vec{r}_{21} - \vec{R}_{eh} = (\vec{r}_1 - \vec{R}_h) - (\vec{r}_2 - \vec{R}_e)$$

$$= \vec{r}_1' - \vec{r}_2' = \vec{r}_{21}' \quad (23)$$

$$\vec{r}_1' = \vec{r}_1 - \vec{R}_h, \vec{r}_2' = \vec{r}_2 - \vec{R}_e . \quad (24)$$

Then, we obtain:

$$U^{acb;eh}_{p_1^* p_1'^*;k^*}\left(\zeta_1, \zeta_1';\eta\right) = \int \chi^*_{p_1^*}\left(\zeta_1, \vec{r}_1' - \vec{R}_{ha}\right)$$

$$\times \chi_{p_1'^*}\left(\zeta_1', \vec{r}_1' - \vec{R}_{hc}\right) O_{k^*}(\eta, \vec{r}_{b1}')\, d^3\vec{r}_1' \quad (25)$$

$$I^{ac,bd;eh}_{p_1^* p_1'^*, p_2^* p_2'^*;k^*}\left(\zeta_1, \zeta_1';\zeta_2, \zeta_2';\eta\right) =$$

$$\iint \chi^*_{p_1^*}\left(\zeta_1, \vec{r}_1' - \vec{R}_{ha}\right) \chi_{p_1'^*}\left(\zeta_1', \vec{r}_1' - \vec{R}_{hc}\right)$$

$$\times \chi_{p_2^*}\left(\zeta_2, \vec{r}_2' - \vec{R}_{eb}\right) \chi^*_{p_2'^*}\left(\zeta_2', \vec{r}_2' - \vec{R}_{ed}\right)$$

$$\times O_{k^*}(\eta, \vec{r}_{21}')\, d^3\vec{r}_1' d^3\vec{r}_2' . \quad (26)$$

Taking into account Eq.(13) in (25) and (26) we obtain for one- and two-electron bipolar multicenter integrals the following series of expansion relations:

$$U^{acb;eh}_{p_1^* p_1'^*;k^*}\left(\zeta_1, \zeta_1';\eta\right)$$

$$= \sum_{\kappa_1=1}^{\infty} \sum_{\upsilon_1=0}^{\kappa_1-1} \sum_{s_1=-\upsilon_1}^{\upsilon_1} \sum_{\kappa_1'=\upsilon_1+1}^{\kappa_1} \tilde{\omega}^{(\alpha^*)\upsilon_1}_{\kappa_1\kappa_1'} \Omega^{(\alpha^*)}_{\delta_1 p_1^*}\left(\zeta_1, \zeta_1; \vec{R}_{ha}\right)$$

$$\times \sum_{\gamma_1'=1}^{\infty} \sum_{\upsilon_1'=0}^{\gamma_1'-1} \sum_{s_1'=-\upsilon_1'}^{\upsilon_1'} \sum_{\gamma_1''=\upsilon_1'+1}^{\gamma_1'} \tilde{\omega}^{(\alpha^*)\upsilon_1'}_{\gamma_1'\gamma_1''} \Omega^{(\alpha^*)}_{\varepsilon_1' p_1'^*}\left(\zeta_1', \zeta_1'; \vec{R}_{hc}\right)$$

$$\times U^b_{\delta_1'\varepsilon_1'';k^*}\left(\zeta_1, \zeta_1';\eta\right) \quad (27)$$

$$I^{ac,bd;eh}_{p_1^* p_1'^*, p_2^* p_2'^*;k^*}\left(\zeta_1, \zeta_1';\zeta_2, \zeta_2';\eta\right) =$$

$$= \sum_{\kappa_1=1}^{\infty} \sum_{\upsilon_1=0}^{\kappa_1-1} \sum_{s_1=-\upsilon_1}^{\upsilon_1} \sum_{\kappa_1'=\upsilon_1+1}^{\kappa_1} \tilde{\omega}^{(\alpha^*)\upsilon_1}_{\kappa_1\kappa_1'} \Omega^{(\alpha^*)}_{\delta_1 p_1^*}\left(\zeta_1, \zeta_1; \vec{R}_{ha}\right)$$

$$\times \sum_{\gamma_1'=1}^{\infty} \sum_{\upsilon_1'=0}^{\gamma_1'-1} \sum_{s_1'=-\upsilon_1'}^{\upsilon_1'} \sum_{\gamma_1''=\upsilon_1'+1}^{\gamma_1'} \tilde{\omega}^{(\alpha^*)\upsilon_1'}_{\gamma_1'\gamma_1''} \Omega^{(\alpha^*)}_{\varepsilon_1' p_1'^*}\left(\zeta_1', \zeta_1'; \vec{R}_{hc}\right)$$

$$\times \sum_{\kappa_2=1}^{\infty} \sum_{\upsilon_2=0}^{\kappa_2-1} \sum_{s_2=-\upsilon_2}^{\upsilon_2} \sum_{\kappa_2'=\upsilon_2+1}^{\kappa_2} \tilde{\omega}^{(\alpha^*)\upsilon_2}_{\kappa_2\kappa_2'} \Omega^{(\alpha^*)}_{\delta_2 p_2^*}\left(\zeta_2, \zeta_2; \vec{R}_{eb}\right)$$

$$\times \sum_{\gamma_2'=1}^{\infty} \sum_{\upsilon_2'=0}^{\gamma_2'-1} \sum_{s_2'=-\upsilon_2'}^{\upsilon_2'} \sum_{\gamma_2''=\upsilon_2'+1}^{\gamma_2'} \tilde{\omega}^{(\alpha^*)\upsilon_2'}_{\gamma_2'\gamma_2''} \Omega^{(\alpha^*)}_{\varepsilon_2' p_2'^*}\left(\zeta_2', \zeta_2'; \vec{R}_{ed}\right)$$

$$\times J_{\delta_1'\varepsilon_1'', \delta_2'\varepsilon_2'';k^*}\left(\zeta_1, \zeta_1';\zeta_2, \zeta_2';\eta\right), \quad (28)$$

where $\delta_i = \kappa_i \upsilon_i s_i$, $\delta_i' = \kappa_i' \upsilon_i s_i$, $\varepsilon_i' = \gamma_i' \upsilon_i' s_i'$ and $\varepsilon_i'' = \gamma_i'' \upsilon_i' s_i'$. Here, $J^b_{\delta_1'\varepsilon_1'';k^*}\left(\zeta_1, \zeta_1';\eta\right)$ and $J_{\delta_1'\varepsilon_1'', \delta_2'\varepsilon_2'';k^*}\left(\zeta_1, \zeta_1';\zeta_2, \zeta_2';\eta\right)$ are the polar integrals defined as

$$J^b_{\delta_1'\varepsilon_1'';k^*}\left(\zeta_1, \zeta_1';\eta\right) = \int \chi^*_{\delta_1'}\left(\zeta_1, \vec{r}_1'\right)$$

$$\times \chi_{\varepsilon_1''}\left(\zeta_1', \vec{r}_1'\right) O_{k^*}(\eta, \vec{r}_{b1}')\, d^3\vec{r}_1' \quad (29)$$

$$J_{\delta_1'\varepsilon_1'', \delta_2'\varepsilon_2'';k^*}\left(\zeta_1, \zeta_1';\zeta_2, \zeta_2';\eta\right) = \iint \chi^*_{\delta_1'}\left(\zeta_1, \vec{r}_1'\right)$$

$$\times \chi_{\varepsilon_1''}\left(\zeta_1', \vec{r}_1'\right) \chi_{\delta_2'}\left(\zeta_2, \vec{r}_2'\right) \chi_{\varepsilon_2''}{}^*\left(\zeta_2', \vec{r}_2'\right)$$

$$\times O_{k^*}(\eta, \vec{r}_{21}')\, d^3\vec{r}_2' d^3\vec{r}_2' \quad (30)$$

Now we use in Eqs. (29) and (30) the following one-center one-range addition theorems for χ-NISTOs charge density [7, 12]:

$$\chi_{\delta_i'}\left(\zeta_i, \vec{r}_i'\right) \chi_{\varepsilon_i''}{}^*\left(\zeta_i', \vec{r}_i'\right) = \frac{1}{\sqrt{4\pi}}$$

$$\times \sum_{L_i=\left|\upsilon_i - \upsilon_i'\right|}^{\upsilon_i+\upsilon_i'}{}' \sum_{M_i=-L_i}^{Li} W_{\delta_i'\varepsilon_i'';P_i}(\zeta_i, \zeta_i'; Z_i) \chi_{p_i}(Z_i, \vec{r}_i'). \quad (31)$$

The charge density expansion coefficients occurring in (31) are determined by

$$W_{\delta_i'\varepsilon_i'';P_i}(\zeta_i, \zeta_i'; Z_i) = \frac{Z_i^{3/2}}{2^{N_i}} \left[\frac{2L_i+1}{2} \frac{\left(2N_i\right)!}{\left(2\kappa_i'\right)!\left(2\gamma_i''\right)!}\right]^{1/2}$$

$$C^{L_i|M_i|}\left(\upsilon_i s_i, \upsilon_i' s_i'\right) A^{M_i}_{s_i s_i'} \left(1+t_i\right)^{\kappa_i'+1/2} \left(1-t_i\right)^{\gamma_i''+1/2}, \quad (32)$$

where $P_i = N_i L_i M_i$, $N_i = \kappa_i + \gamma_i'' - 1$,

$$Z_i = \zeta_i + \zeta_i', \quad t_i = \frac{\zeta_i - \zeta_i'}{\zeta_i + \zeta_i'}; \quad C^{L_i|M_i|}\left(\upsilon_i s_i, \upsilon_i' s_i'\right)$$

and $A_{s_i s_i'}^{M_i}$ are the generalized Gaunt and Kronecker delta coefficients, respectively [7]. The substitution of (31) into Eqs. (29) and (30) gives:

$$J^b_{\delta_1'\varepsilon_1'';k^*}\left(\zeta_1, \zeta_1'; \eta\right)$$

$$= \sum_{L_1=\left|\upsilon_1-\upsilon_1'\right|}^{\upsilon_1+\upsilon_1'} {}' \sum_{M_1=-L_1}^{L_1} W_{\delta_1'\varepsilon_1'';P_1}(\zeta_1, \zeta_1'; Z_1)$$

$$\times J^b_{P_1;k^*}\left(Z_1; \eta\right) \qquad (33)$$

$$J_{\delta_1'\varepsilon_1'',\delta_2'\varepsilon_2'';k^*}\left(\zeta_1, \zeta_1'; \zeta_2, \zeta_2'; \eta\right)$$

$$= \sum_{L_1=\left|\upsilon_1-\upsilon_1'\right|}^{\upsilon_1+\upsilon_1'} {}' \sum_{M_1=-L_1}^{L_1} W_{\delta_1'\varepsilon_2'';P_1}(\zeta_1, \zeta_1'; Z_1)$$

$$\times \sum_{L_2=\left|\upsilon_2-\upsilon_2'\right|}^{\upsilon_2+\upsilon_2'} {}' \sum_{M_2=-L_2}^{L_2} W_{\delta_2'\varepsilon_2'';P_2}(\zeta_2, \zeta_2'; Z_2)$$

$$\times J^b_{P_1P_2;k^*}\left(Z_1, Z_2; \eta\right). \qquad (34)$$

Here, the quantities

$$J^b_{P_1;k^*}\left(Z_1; \eta\right)$$

$$= \frac{1}{\sqrt{4\pi}} \int \chi^*_{P_1}\left(Z_1, \vec{r}_1'\right) O_{k^*}(\eta, \vec{r}_{b1}') d^3\vec{r}_1' \qquad (35)$$

$$J^b_{P_1P_2;k^*}\left(Z_1, Z_2; \eta\right) = \frac{1}{4\pi} \int\int \chi_{P_1}{}^*\left(Z_1, \vec{r}_1'\right)$$

$$\times O_{k^*}(\eta, \vec{r}_{21}{}') \chi_{P_2}\left(Z_2, \vec{r}_2'\right) d^3\vec{r}_1' d^3\vec{r}_2' \qquad (36)$$

are the one- and two-electron basic polar integrals of $\chi-$ISTOs and Coulomb-Yukawa-like potential with noninteger indices, respectively.

As can be seen from the obtained formulas, the one- and two-electron bipolar multicenter integrals with the use of two-center one-range addition theorems for $\chi-$NISTOs are expressed through the basic polar integrals of $\chi-$ISTOs and Coulomb-Yukawa-like potential with noninteger indices.

The basic integrals (35) and (36) can be calculated by the use of Laguerre power series of functions with noninteger indices which can be established with the help of $L^{(p_i^*)}$–generalized and $L^{(\alpha^*)}$-modified Laguerre polynomials ($L^{(p_i^*)}$–GLPs and $L^{(\alpha^*)}$-MLPs), respectively (see Ref. [9]). For the construction of Laguerre power series, we use the potential $O_{u^*\upsilon s}$ occurring in Eqs. (35) and (36) in the following form

$$O_{u^*\upsilon s}\left(\eta, \vec{r}\right) = O_{u\upsilon s}\left(\eta, \vec{r}\right) r^{\eta^*}, \qquad (37)$$

where $u^* = u + \eta^*$, $0 < \eta^* < 1$ and u is the integer part of u^*. Then we obtain:

for $L^{(p_i^*)}$–GLPs

$$r^{\eta^*} = \sum_{\mu=\nu+1}^{\infty} \sum_{\mu'=\nu+1}^{\mu} \tilde{Y}^{\left(p_\nu^*\right)\nu}_{\mu\mu',\eta^*} r^{\mu'-(\nu+1)} \qquad (38)$$

for $L^{(\alpha^*)}$ -MLPs

$$r^{\eta^*} = \sum_{\mu=\nu+1}^{\infty} \sum_{\mu'=\nu+1}^{\mu} \tilde{\Upsilon}^{(\alpha^*)\nu}_{\mu\mu',\eta^*} r^{\mu'-1}, \qquad (39)$$

where

$$Y^{\left(p_\nu^*\right)\nu}_{\mu\mu',\eta^*} = \tilde{a}^{\left(p_\nu^*\right)\nu}_{\mu\mu'}$$

$$\times \sum_{\mu''=\nu+1}^{\mu} \tilde{a}^{\left(p_\nu^*\right)\nu}_{\mu\mu''} \frac{\Gamma(q_\mu^*+1)\Gamma(\mu''+p_\nu^*+\eta^*-\nu)}{[\mu-(\nu+1)]!} \qquad (40)$$

$$\tilde{\Upsilon}^{(\alpha^*)\nu}_{\mu\mu',\eta^*} = \tilde{a}^{(\alpha^*)\nu}_{\mu\mu'}$$

$$\times \sum_{\mu''=\nu+1}^{\mu} \tilde{a}^{(\alpha^*)\nu}_{\mu\mu''} \frac{\Gamma(q_\mu^*+1)\Gamma(\mu''-\alpha^*+\eta^*+2)}{[\mu-(\nu+1)]!}. \qquad (41)$$

Using Eqs.(38) and (39), we obtain for the one-center one-range addition theorems of O-NIPs based on the use of Laguerre power series the following relations:

$$O_{u^*\upsilon s}\left(\eta, \vec{r}\right)$$

$$= \sum_{\mu=\nu+1}^{\infty} \sum_{\mu'=u}^{\mu+u-(\nu+1)} \tilde{Y}^{\left(p_\nu^*\right)\nu}_{\mu\mu'-u+\nu+1,\eta^*} O_{\mu'\upsilon s}\left(\eta, \vec{r}\right) \qquad (42)$$

$$O_{u^*\upsilon s}\left(\eta, \vec{r}\right)$$

$$= \sum_{\mu=\nu+1}^{\infty} \sum_{\mu'=u+\nu}^{\mu+u-1} \tilde{\Upsilon}^{(\alpha^*)\nu}_{\mu\mu'-u+1,\eta^*} O_{\mu'\upsilon s}\left(\eta, \vec{r}\right). \qquad (43)$$

The substitution of Eqs.(42) and (43) into (35) and (36) gives for the basic polar integrals the following series expansions:

$$J^b_{P_1;k^*}\left(Z_1;\eta,\vec{R}'_{hb}\right) = \sum_{\mu=\nu+1}^{\infty}\sum_{\mu'=u}^{\mu+u-(\nu+1)} \tilde{Y}^{\left(p_\nu^*\right)\nu}_{\mu\mu'-u+\nu+1,\eta^*} J^b_{P_1;k'}\left(Z_1;\eta,\vec{R}'_{hb}\right) \quad (44)$$

$$J^b_{P_1P_2;k^*}\left(Z_1,Z_2;\eta\right) = \sum_{\mu=\nu+1}^{\infty}\sum_{\mu'=u+\nu}^{\mu+u-1} \tilde{\Upsilon}^{(\alpha^*)\nu}_{\mu\mu'-u+1,\eta^*} J^b_{P_1P_2;k'}\left(Z_1,Z_2;\eta\right), \quad (45)$$

where $J^b_{P_1;k^*}\left(Z_1,\eta;\vec{R}'_{hb}\right) \equiv J^b_{P_1;k^*}\left(Z_1,\eta\right)$,

$J^b_{P_1;k'}\left(Z_1,\eta;\vec{R}'_{hb}\right) = J^b_{P_1;k'}\left(Z_1,\eta\right)$, $k' = \mu'\upsilon s$ and

$$J^b_{P_1;k'}\left(Z_1,\eta;\vec{R}'_{hb}\right) = \frac{1}{\sqrt{4\pi}}\int \chi^*_{P_1}\left(Z_1,\vec{r}_1'\right) O_{k'}(\eta,\vec{r}'_{b1})d^3\vec{r}_1' = A_{\mu'\upsilon}(\eta) S_{P_1k'}(Z_1,\eta;\vec{R}'_{hb}) \quad (46)$$

$$J^b_{P_1P_2;k'}\left(Z_1,Z_2;\eta\right) = \frac{1}{4\pi}\int\int \chi_{P_1}{}^*\left(Z_1,\vec{r}_1'\right) \times O_{k'}(\eta,\vec{r}_{21}{}') \chi_{P_2}\left(Z_2,\vec{r}_2'\right) d^3\vec{r}_1' d^3\vec{r}_2' = A_{\mu'\upsilon}(\eta) \times \frac{1}{4\pi}\int S_{P_1k'}(Z_1,\eta;\vec{r}'_{h2}) \chi_{P_2}\left(Z_2,\vec{r}_{h2}{}'\right) d^3\vec{r}_{h2}{}' \quad (47)$$

The quantities $S_{P_1k'}$ occurring in Eqs. (46) and (47) are the overlap integrals over χ-ISTOs and $A_{\mu'\upsilon}(\eta)$ coefficients defined as, respectively:

$$S_{P_1k'}(Z_1,\eta;\vec{R}'_{hb}) = \int \chi^*_{P_1}\left(Z_1,\vec{r}'_{h1}\right)\chi_{k'}(\eta,\vec{r}'_{b1})d^3\vec{r}_1' , \quad (48)$$

$$A_{\mu'\upsilon}(\eta) = \left[\frac{(2\mu')!}{(2\upsilon+1)(2\eta)^{2\mu'+1}}\right]^{1/2} . \quad (49)$$

It should be noted that the two-electron integrals of $\chi-$ISTOs occurring in Eq. (47) have been studied in our previous papers [7, 16].

Table 1. The computational results of basic integral $J^b_{P_1;k'}\left(Z_1,\eta;\vec{R}'_{hb}\right)$.

N_1	L_1	M_1	Z_1	μ'	υ	s	η	R'_{hb}	θ'_{hb}	ϕ'_{hb}	Eq.(46)
1	0	0	4.1	2	1	1	1	1	108	288	0.0384304419337282709
3	0	0	9	2	0	0	3	2.3	90	180	0.001100902598119918
4	1	1	7.6	3	2	0	3.4	1.4	60	180	0.0011283910967783675
8	7	1	8.5	6	1	0	5.3	2.2	30	108	$9.760836563464515\,E-07$
9	4	1	9.6	7	3	1	6.3	1.8	120	72	$-9.12773014368389\,E-06$
9	8	8	2.5	8	6	6	1.5	1.1	30	60	-2.095067822209997817
10	6	6	3.4	9	7	7	2.3	2.9	108	120	0.677010199846579
11	7	6	8.7	8	6	6	3.5	2.1	150	108	0.0016434196671959369
12	10	10	6.1	14	8	5	7.8	2.5	108	60	-0.0000107171243862096
13	11	8	7.8	10	9	8	5.5	1.9	122	72	0.00007592144328909598
15	13	12	6.6	14	12	12	3.7	2.6	150	60	0.13030800995209336587
20	15	15	8.9	18	17	16	7.5	5.1	36	75	$8.800413162432983\,E-10$

CONCLUSION

It is shown that the one-range addition theorems for $\chi-$NISTOs, C-NIPs and Y-NIPs, based on the use of $L^{(p_i^*)}$–GLPs) and $L^{(\alpha^*)}$ -MLPs, are useful tools for the unified treatment of one- and two-electron bipolar and polar multicenter integrals when $\chi-$NISTOs basis sets and Coulomb-Yukawa-like potentials with noninteger indices are employed in electronic structure calculations. The obtained formulas can be used for the evaluation of these integrals with arbitrary values of principal and self-frictional quantum numbers, screening constants and location of orbitals and parameters of potentials. On the basis of Eq. (46), we constructed a program for the computation of $J^b_{P_1;k'}\left(Z_1,\eta;\vec{R}'_{hb}\right)$ using Mathematica 7.0 international mathematical software. The computational results are given in Table 1. It can be seen from Table 1 that the calculation results are stable for high values of quantum numbers. It is especially useful for accurate evaluation of the multicenter multielectron

molecular integrals [10]. The presented theory is especially useful in the study of different electronic structure problems dealing with atoms, molecules and solids.

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КОМБИНИРАНА ТЕОРИЯ НА ЕДНО- И ДВУ-ЕЛЕНТРОННИ БИ-ПОЛЯРНИ ИНТЕГРАЛИ ОТ НЕЦЕЛИ *n*- SLATER‘ОВИ ФУНКЦИИ И COULOMB-YUKAWA-ПОДОБНИ ПОТЕНЦИАЛИ С ДРОБНИ ИНДЕКСИ

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(Резюме)

Представена е комбинирана теория за едно- и дву-електронни многоцентрични интеграли от χ-нецели *n* – орбитали от Slater‘ов тип (χ-NISTOs) и на биполярни и полярни нецели кулонови (C-NIBPs и C-NIPs) - Юкава (Y-NIBPs и Y-NIPs)-подобните потенциали. Тези многоцентрични интеграли се представят чрез базични полярни интеграли от χ-цели *n* – орбитали от Slater‘ов тип (χ-ISTOs) и Coulomb-Yukawa-подобни потенциали с цели индекси (C-IPs и Y-IPs). Отбелязано е че не-целите квантови числа *n* се дефинират с *n**.