INTEGRAL EXPRESSIONS FOR (nl|n'l') WITH n, n' = 3, 4

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(Received February 1, 1976)

In this paper we give integral expressions for overlap integrals (nl|n'l') with n, n' = 3, 4 using SLATER type orbitals for 3*d*, 4*s* and 4*p* atomic orbitals and an approximate function for the radial part of 4*s* and 4*p*.

In LCAO—MO calculations on polynuclear complexes of transition metal ions have to be calculated overlap integrals between 2*s*, 2*p*, 3*d*, 4*s* and 4*p* atomic orbitals. From these integrals the expressions of (nl|n'l') with $n=2, 3, 4$; $n'=2, 3$ are available in literature [1-4] but expressions of the other integrals — to our knowledge — have not been published until now. As these integrals are important in theoretical investigations of polynuclear complexes and similar molecular problems, we give in the following expressions for these integrals using SLATER type orbitals.

The calculation of overlap integrals

The radial part of SLATER type orbitals is of the form

$$r^{n^*-1} \cdot e^{-\alpha r},$$

where

$$\alpha = \frac{Z-\sigma}{n^* a_0};$$

n^* is the effective principal quantum number and $Z-\sigma$ is the effective nuclear charge. If the principal quantum number is $n=1, 2, 3, 4, \ldots$, n^* has the following values: $n^*=1, 2, 3, 3.7, \ldots$. The constant α can be determined with the help of SLATER's rules.

The overlap integrals of the real SLATER type orbitals can be divided into three classes:

1. The overlap integrals (nl|n'l') with $n=2, 3$; $n'=2, 3$ can be calculated in elliptical coordinates (μ, ν, φ) defined by

$$\mu = \frac{r+r'}{R}, \qquad \nu = \frac{r-r'}{R}, \qquad \varphi = \varphi',$$

where $1 \leq \mu \leq \infty$, $-1 \leq \nu \leq 1$, $0 \leq \varphi \leq 2\pi$ and the meaning of r, r', φ and R can be seen in Fig. 1 (the coordinate system (2) is left-handed).

In these elliptical coordinates the overlap integrals (3*d*, 2*s*), (3*d*, 2*p*) and (3*d*, 3*d*) can be expressed by the integrals

$$A_n(a) = \int_1^\infty \mu^n e^{-a\mu} d\mu$$

$$B_n(b) = \int_{-1}^1 \nu^n e^{-b\nu} d\nu$$

where $a = \frac{R}{2}(\alpha+\beta)$, $b = \frac{R}{2}(\alpha-\beta)$ and α, β are orbital exponents. The values of $A_n(a)$ and $B_n(b)$ for various a and b can be found for example in [5] but it is inconvenient

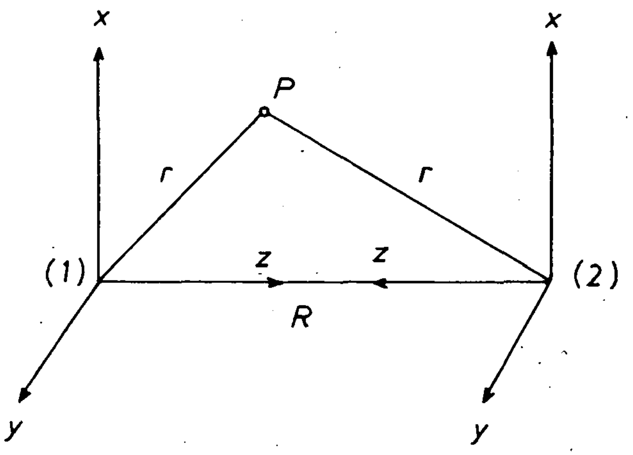

Fig. 1

to use this table in practice. It seems more practical to calculate these integrals with the help of the following recurrence relations:

$$A_n = \frac{1}{a}[nA_{n-1} + e^{-a}],$$

$$B_n = \frac{1}{b}[nB_{n-1} + (-1)^n e^b - e^{-b}].$$

2. The overlap integrals (nl|n'l') with n=4; n'=2, 3 can be expressed with the help of integrals

$$I(n|y \pm x) = \frac{(n|y \pm x)!}{(y \pm x)^{n+1}}, \qquad G(n|y+x) = \frac{\Gamma(n)}{(y+x)^n},$$

where $x = \alpha R$, $y = \beta R$ and

$$(n|y\pm x)! = \int_0^{y\pm x} t^n e^{-t}\,dt, \qquad \Gamma(n) = \int_0^{\infty} t^{n-1} e^{-t}\,dt.$$

For the calculation of these integrals it is necessary to know the values of the incomplete Γ-function, which are available in [6].

3. The overlap integrals (nl/n'l') with n, n'=4 cannot be expressed by any closed formulas. For this reason we approximated the radial part of $4s$ and $4p$ by the function

$$\tilde{\psi} = \sum_{k=1}^{4} c_k r^k e^{-\alpha' r}$$

where c_k-s and α' are constants. These constants can be determined in various ways, for example under the condition

$$\int (\psi - \tilde{\psi})^2\, dV = min.$$

From this condition for c_k-s (if $\alpha' = \alpha_{4s}$), we get for the Co atom the following results:

$$c_1 = -0.047\,530\,507,$$

$$c_2 = 0.360\,145\,640,$$

$$c_3 = 0.728\,294\,860,$$

$$c_4 = -0.041\,616\,865.$$

Naturally the coefficients c_k-s depend on α. We intend to determine these c_k-s and α' for all transition elements.

Using the approximate function, the overlap integrals $(4s, 4s)$, $(4s, 4p)$, $(4p, 4p)$ as well as (nl|n'l') with n=4; n'=2, 3 can already be expressed with integrals $A_n(a)$ and $B_n(b)$.

Expressions for integrals

1. $(3d_{xy}, 3d_{xy}) = (3d_{x^2-y^2}, 3d_{x^2-y^2}) =$

$$= \frac{1}{6}\frac{(ab)^{3.5}}{128}\{A_6 B_0 - 2A_6 B_2 + A_6 B_4 - 2A_4 B_0 + 3A_4 B_2 - A_4 B_6 + A_2 B_0 - 3A_2 B_4 + 2A_2 B_6 - A_0 B_2 + 2A_0 B_4 - A_0 B_6\}$$

2. $(3d_{xz}, 3d_{xz}) = (3d_{yz}, 3d_{yz}) =$

$$= \frac{2}{3}\frac{(ab)^{3.5}}{128}\{-A_6 B_2 + A_6 B_4 + A_4 B_0 - A_4 B_6 - A_2 B_0 + A_2 B_6 + A_0 B_2 - A_0 B_4\}$$

3. $(3d_{z^2}, 3d_{z^2}) =$

$$= \frac{1}{9}\frac{(ab)^{3.5}}{128}\{A_6 B_0 - 6A_6 B_2 + 9A_6 B_4 - 6A_4 B_0 + 3A_4 B_2 - 9A_4 B_6 + 9A_2 B_0 - 3A_2 B_4 + 6A_2 B_6 - 9A_0 B_2 + 6A_0 B_4 - A_0 B_6\}$$

4. $$(4s, 3d_{z^2}) = \frac{2^{1.7}}{3(7.4!)^{0.7}} \frac{y^{4.2}}{x^{2.5}} \times$$

$$\times e^x [(360-360x+192x^2-72x^3+24x^4-8x^5)\{G(4.7|y+x)-$$
$$-I(3.7|y+x)\}+(360x-360x^2+192x^3-72x^4+24x^5)\{G(5.7|y+x)-$$
$$-I(4.7|y+x)\}+(144x^2-144x^3+72x^4-24x^5)\{G(6.7|y+x)-$$
$$-I(5.7|y+x)\}+(24x^3-24x^4+8x^5)\{G(7.7|y+x)-I(6.7|y+x)\}]+$$
$$+e^{-x}[(360+360x+192x^2+72x^3+24x^4+8x^5)\{I(3.7|y-x)-$$
$$-G(4.7|y+x)\}-(360x+360x^2+192x^3+72x^4+24x^5)\{I(4.7|y-x)+$$
$$+G(5.7|y+x)\}+(144x^2+144x^3+72x^4+24x^5)\{I(5.7|y-x)-$$
$$-G(6.7|y+x)\}-(24x^3+24x^4+8x^5)\{I(6.7|y-x)+G(7.7|y+x)\}]$$

5. $$(4p_x, 3d_{xz}) = (4p_y, 3d_{yz}) = \frac{2^{1.7}}{(7.4!)^{0.5}} \frac{y^{4.2}}{x^{3.5}} \times$$

$$\times\{e^x[(720-720x+312x^2-72x^3+8x^4)\{I(2.7|y+x)-G(3.7|y+x)\}+$$
$$+(720x-720x^2+312x^3-72x^4+8x^5)\{I(3.7|y+x)-G(4.7|y+x)\}+$$
$$+(312x^2-312x^3+128x^4-24x^5)\{I(4.7|y+x)-G(5.7|y+x)\}+$$
$$+(72x^3-72x^4+24x^5)\{I(5.7|y+x)-G(6.7|y+x)\}+$$
$$+(8x^4-8x^5)\{I(6.7|y+x)-G(7.7|y+x)\}]+$$
$$+e^{-x}[(720+720x+312x^2+72x^3+8x^4)\{G(3.7|y+x)-I(2.7|y-x)\}+$$
$$+(720x+720x^2+312x^3+72x^4+8x^4)\{G(4.7|y+x)+I(3.7|y-x)\}+$$
$$+(312x^2+312x^3+128x^4+24x^5)\{G(5.7|y+x)-I(4.7|y-x)\}+$$
$$+(72x^3+72x^4+24x^5)\{G(6.7|y+x)+I(5.7|y-x)\}+$$
$$+(8x^4+8x^5)\{G(7.7|y+x)-I(6.7|y-x)\}]$$

6. $$(4p_z, 3d_{z^2}) = \frac{\sqrt{3}}{3} \frac{2^{0.7}}{(7.4!)^{0.5}} \frac{y^{4.2}}{x^{4.5}} \times$$

$$\times\{e^x[(15120-15120x+7440x^2-2400x^3+576x^4-112x^5+16x^6)\{I(2.7|y+x)-$$
$$-G(3.7|y+x)\}+(15120x-15120x^2+7440x^3-2400x^4+576x^5-112x^6+$$
$$+16x^7)\{I(3.7|y+x)-G(4.7|y+x)\}+(6480x^2-6480x^3+3168x^4-$$
$$-1008x^5+240x^6-48x^7)\{I(4.7|y+x)-G(5.7|y+x)\}+(1440x^3-$$
$$-1440x^4+688x^5-208x^6+46x^7)\{I(5.7|y+x)-G(6.7|y+x)\}+$$
$$+(144x^4-144x^5+64x^6-16x^7)\{I(6.7|y+x)-G(7.7|y+x)\}]+$$
$$+e^{-x}[(15120+15120x+7440x^2+2400x^3+576x^4+112x^5+16x^6)\{G(3.7|y+x)-$$
$$-I(2.7|y-x)\}+(15120x+15120x^2+7440x^3+2400x^4+576x^5+112x^6+$$
$$+16x^7)\{G(4.7|y+x)+I(3.7|y-x)\}+(6480x^2+6480x^3+3168x^4+$$
$$+1008x^5+240x^6+48x^7)\{G(5.7|y+x)-I(4.7|y-x)\}+(1440x^3+$$
$$+1440x^4+688x^5+208x^6+46x^7)\{G(6.7|y+x)+I(5.7|y-x)\}+$$
$$+(144x^4+144x^5+64x^6+16x^7)\{G(7.7|y+x)-I(6.7|y-x)\}]$$

7. $(4s, 4s) = 2\pi \left(\frac{R}{2}\right)^5 N_{4s}(\alpha) N_{4s}(\beta) \times$

$$\times \{a_1 b_1 [A_4 B_0 - 2A_2 B_2 + A_0 B_4] +$$

$$+ a_1 b_2 \frac{R}{2} [A_5 B_0 - A_4 B_1 - 2A_3 B_2 + 2A_2 B_3 + A_1 B_4 - A_0 B_5] +$$

$$+ a_1 b_3 \left(\frac{R}{2}\right)^2 [A_6 B_0 - 2A_5 B_1 - A_4 B_2 + A_3 B_3 - A_2 B_4 - 2A_1 B_5 + A_0 B_6] +$$

$$+ a_1 b_4 \left(\frac{R}{2}\right)^3 [A_7 B_0 - 3A_6 B_1 + A_5 B_2 + 5A_4 B_3 - 5A_3 B_4 - A_2 B_5 + 3A_1 B_6 - A_0 B_7] +$$

$$+ a_2 b_1 \frac{R}{2} [A_5 B_0 + A_4 B_1 - 2A_3 B_2 - 2A_2 B_3 + A_1 B_4 + A_0 B_5] +$$

$$+ a_2 b_2 \left(\frac{R}{2}\right)^2 [A_6 B_0 - 3A_4 B_2 + 3A_2 B_4 - A_0 B_6] +$$

$$+ a_2 b_3 \left(\frac{R}{2}\right)^3 [A_7 B_0 - A_6 B_1 - 3A_5 B_2 + 3A_4 B_3 + 3A_3 B_4 - 3A_2 B_5 - A_1 B_6 + A_0 B_7] +$$

$$+ a_2 b_4 \left(\frac{R}{2}\right)^4 [A_8 B_0 - 2A_7 B_1 - 2A_6 B_2 + 6A_5 B_3 - 6A_3 B_5 + 2A_2 B_6 + 2A_1 B_7 - A_0 B_8] +$$

$$+ a_3 b_1 \left(\frac{R}{2}\right)^2 [A_6 B_0 + 2A_5 B_1 - A_4 B_2 - 4A_3 B_3 - A_2 B_4 + 2A_1 B_5 + A_0 B_6] +$$

$$+ a_3 b_2 \left(\frac{R}{2}\right)^3 [A_7 B_0 + A_6 B_1 - 3A_5 B_2 - 3A_4 B_3 + 3A_3 B_4 + 3A_2 B_5 - A_1 B_6 - A_0 B_7] +$$

$$+ a_3 b_3 \left(\frac{R}{2}\right)^4 [A_8 B_0 - 4A_6 B_2 + 6A_4 B_4 - 4A_2 B_6 + A_0 B_8] +$$

$$+ a_3 b_4 \left(\frac{R}{2}\right)^5 [A_9 B_0 - A_8 B_1 - 4A_7 B_2 + 4A_6 B_3 + 6A_5 B_4 - 6A_4 B_5 - 4A_3 B_6 + 4A_2 B_7 +$$
$$+ A_1 B_8 - A_0 B_9] +$$

$$+ a_4 b_1 \left(\frac{R}{2}\right)^3 [A_7 B_0 + 3A_6 B_1 + A_5 B_2 - 5A_4 B_3 - 5A_3 B_4 + A_2 B_5 + 3A_1 B_6 + A_0 B_7] +$$

$$+ a_4 b_2 \left(\frac{R}{2}\right)^4 [A_8 B_0 + 2A_7 B_1 - 2A_6 B_2 - 6A_5 B_3 + 6A_3 B_5 + 2A_2 B_6 - 2A_1 B_7 - A_0 B_8] +$$

$$+ a_4 b_3 \left(\frac{R}{2}\right)^5 [A_9 B_0 + A_8 B_1 - 4A_7 B_2 - 4A_6 B_3 + 6A_5 B_4 + 6A_4 B_5 - 4A_3 B_6 - 4A_2 B_7 +$$
$$+ A_1 B_8 + A_0 B_9] +$$

$$+ a_4 b_4 \left(\frac{R}{2}\right)^6 [A_{10} B_0 - 5A_8 B_2 + 10A_6 B_4 - 10A_4 B_6 + 5A_2 B_8 - A_0 B_{10}]\}$$

8. $(4s, 4p_z) = 2\pi \left(\frac{R}{2}\right)^5 N_{4s}(\alpha) N_{4p_z}(\beta) \times$

$$\times \{a_1 b_1 [-A_4 B_1 + A_3 B_0 - A_3 B_2 + A_2 B_1 + A_2 B_3 - A_1 B_2 + A_1 B_4] +$$

$$+a_1 b_2 \frac{R}{2}[-A_5B_1+A_4B_0+2A_3B_3-2A_2B_2-A_1B_5+A_0B_4]+$$

$$+a_1 b_3 \left(\frac{R}{2}\right)^2[-A_6B_1+A_5B_0+A_5B_2-A_4B_1+2A_4B_3-2A_3B_2-2A_3B_4+$$

$$+2A_2B_3-A_2B_5+A_1B_4+A_1B_6-A_0B_5]+$$

$$+a_1 b_4 \left(\frac{R}{2}\right)^3[-A_7B_1+A_6B_0+2A_6B_2-2A_5B_1+A_5B_3-A_4B_2-4A_4B_4+4A_3B_3+$$

$$+A_3B_5-A_2B_4+2A_2B_6-2A_1B_5-A_1B_7+A_0B_6]+$$

$$+a_2 b_1 \frac{R}{2}[-A_5B_1+A_4B_0-2A_4B_2+2A_3B_1+2A_2B_4-2A_1B_3+A_1B_5-A_0B_4]+$$

$$+a_2 b_2 \left(\frac{R}{2}\right)^2[-A_6B_1+A_5B_0-A_5B_2+A_4B_1+2A_4B_3-2A_3B_2+2A_3B_4-2A_2B_3-A_2B_5+$$

$$+A_1B_4-A_1B_6+A_0B_5]+$$

$$+a_2 b_3 \left(\frac{R}{2}\right)^3[-A_7B_1+A_6B_0+3A_5B_3-3A_4B_2-3A_3B_5+3A_2B_4+A_1B_7-A_0B_6]+$$

$$+a_2 b_4 \left(\frac{R}{2}\right)^4[-A_8B_1+A_7B_0+A_7B_2-A_6B_1+3A_6B_3-3A_5B_2-3A_5B_4+$$

$$+3A_4B_3-3A_4B_5+3A_3B_4+3A_3B_6-3A_2B_5+A_2B_7-A_1B_6-A_1B_8+A_0B_7]+$$

$$+a_3 b_1 \left(\frac{R}{2}\right)^2[-A_6B_1+A_5B_0-3A_5B_2+3A_4B_1-2A_4B_3+2A_3B_2+2A_3B_4-2A_2B_3+$$

$$+3A_2B_5-3A_1B_4+A_1B_6-A_0B_5]+$$

$$+a_3 b_2 \left(\frac{R}{2}\right)^3[-A_7B_1+A_6B_0-2A_6B_2+2A_5B_1+A_5B_3-A_4B_2+4A_4B_4-4A_3B_3+$$

$$+A_3B_5-A_2B_2-2A_2B_6+2A_1B_5-A_1B_6+A_1B_7+A_0B_6]+$$

$$+a_3 b_3 \left(\frac{R}{2}\right)^4[-A_8B_1+A_7B_0-A_7B_2+A_6B_1+3A_6B_3-3A_5B_2+3A_5B_4-3A_4B_3-3A_4B_5+$$

$$+3A_3B_4-3A_3B_6+3A_2B_5+A_2B_7-A_1B_8-A_0B_7]+$$

$$+a_3 b_4 \left(\frac{R}{2}\right)^5[-A_9B_1+A_8B_0+4A_7B_3-4A_6B_2-6A_5B_5+6A_4B_4+4A_3B_7-4A_2B_6-$$

$$-A_1B_9+A_0B_8]+$$

$$+a_4 b_1 \left(\frac{R}{2}\right)^3[-A_7B_1+A_6B_0-4A_6B_2+4A_5B_1-5A_5B_3+5A_4B_2+5A_3B_5-5A_2B_4+4A_2B_6-$$

$$-4A_1B_5+A_1B_7-A_0B_6]+$$

$$+a_4 b_2 \left(\frac{R}{2}\right)^4[-A_8B_1+A_7B_0-3A_7B_2+3A_6B_1-A_6B_3+A_5B_2+5A_5B_4-5A_4B_3+$$

$$+5A_4B_5-5A_3B_4-A_3B_6+A_2B_5-3A_2B_7+3A_1B_6-A_1B_8+A_0B_7]+$$

$$+a_4 b_3 \left(\frac{R}{2}\right)^5 [-A_9 B_1 + A_8 B_0 - 2A_8 B_2 + 2A_7 B_1 + 2A_7 B_3 - 2A_6 B_2 + 6A_6 B_4 - 6A_5 B_3 - 6A_4 B_6 +$$

$$+6A_3 B_5 - 2A_3 B_7 + 2A_2 B_6 + 2A_2 B_8 - 2A_1 B_7 + A_1 B_9 - A_0 B_8] +$$

$$+a_4 b_4 \left(\frac{R}{2}\right)^6 [-A_{10} B_1 + A_9 B_0 - A_9 B_2 + A_8 B_1 + 4A_8 B_3 - 4A_7 B_2 + 4A_7 B_4 - 4A_6 B_3 - 6A_6 B_5 +$$

$$+6A_5 B_4 - 6A_5 B_6 + 6A_4 B_5 + 4A_4 B_7 - 4A_3 B_6 + 4A_3 B_8 - 4A_2 B_7 - A_2 B_9 +$$

$$+A_1 B_8 - A_1 B_{10} + A_0 B_9]\}$$

9. $$(4p_x, 4p_x) = (4p_y, 4p_y) = \pi \left(\frac{R}{2}\right)^5 N_{4p_x}(\alpha) N_{4p_x}(\beta) \times$$

$$\times \{a_1 b_1 [A_4 B_0 - A_4 B_2 - A_2 B_0 + A_2 B_4 + A_0 B_2 - A_0 B_4] +$$

$$+a_1 b_2 \frac{R}{2} [A_5 B_0 - A_5 B_2 - A_4 B_1 + A_4 B_3 - A_3 B_0 + A_3 B_4 + A_2 B_1 - A_2 B_5 + A_1 B_2 -$$

$$-A_1 B_4 - A_0 B_3 + A_0 B_5] +$$

$$+a_1 b_3 \left(\frac{R}{2}\right)^2 [A_6 B_0 - A_6 B_2 - 2A_5 B_1 + 2A_5 B_3 - A_4 B_0 + A_4 B_2 + 2A_3 B_1 - 2A_3 B_5 - A_2 B_4 +$$

$$+A_2 B_6 - 2A_1 B_3 + 2A_1 B_5 + A_0 B_4 - A_0 B_6] +$$

$$+a_1 b_4 \left(\frac{R}{2}\right)^3 [A_7 B_0 - A_7 B_2 - 3A_6 B_1 + 3A_6 B_3 - A_5 B_0 + 3A_5 B_2 - 2A_5 B_4 + 3A_4 B_1 - A_4 B_3 -$$

$$-2A_4 B_5 - 2A_3 B_2 - A_3 B_4 + 3A_3 B_6 - 2A_2 B_3 + 3A_2 B_5 - A_2 B_7 + 3A_1 B_4 -$$

$$-3A_1 B_6 + A_0 B_7] +$$

$$+a_2 b_1 \frac{R}{2} A_5 B_0 - A_5 B_2 + A_4 B_1 - A_4 B_3 - A_3 B_0 + A_3 B_4 - A_2 B_1 + A_2 B_5 +$$

$$+A_1 B_2 - A_1 B_4 + A_0 B_3 - A_0 B_5] +$$

$$+a_2 b_2 \left(\frac{R}{2}\right)^2 [A_6 B_0 - A_6 B_2 - A_4 B_0 - A_4 B_2 + 2A_4 B_4 + 2A_2 B_2 - A_2 B_4 - A_2 B_6 -$$

$$-A_0 B_4 + A_0 B_6] +$$

$$+a_2 b_3 \left(\frac{R}{2}\right)^3 [A_7 B_0 - A_7 B_2 - A_6 B_1 + A_6 B_3 - A_5 B_0 - A_5 B_2 + 2A_5 B_4 + 2A_3 B_2 -$$

$$-A_3 B_4 - A_3 B_6 + A_4 B_1 + A_4 B_3 - 2A_4 B_5 - 2A_2 B_3 + A_2 B_5 + A_2 B_7 -$$

$$-A_1 B_4 + A_1 B_6 + A_0 B_5 - A_0 B_7] +$$

$$+a_3 b_4 \left(\frac{R}{2}\right)^4 [A_8 B_0 - A_8 B_2 - 2A_7 B_1 + 2A_7 B_3 - A_6 B_0 + A_6 B_4 + 2A_5 B_1 + 2A_5 B_3 -$$

$$-4A_5 B_5 + A_4 B_2 - 2A_4 B_4 + A_4 B_6 - 4A_3 B_3 + 2A_3 B_5 + 2A_3 B_7 + A_2 B_4 -$$

$$-A_2 B_8 + 2A_1 B_5 - 2A_1 B_7 - A_0 B_6 + A_0 B_8] +$$

$$+a_3 b_1 \left(\frac{R}{2}\right)^2 [A_6 B_0 - A_6 B_2 + 2A_5 B_1 - 2A_5 B_3 - A_4 B_0 + A_4 B_2 - 2A_3 B_1 + 2A_3 B_5 - A_2 B_4 +$$

$$+A_2B_6+2A_1B_3-2A_1B_5+A_0B_4-A_0B_6]+$$

$$+a_3b_2\left(\frac{R}{2}\right)^3[A_7B_0-A_7B_2+A_6B_1-A_6B_3-A_5B_2+2A_5B_4-A_4B_1-A_4B_3+2A_4B_5+$$

$$+2A_3B_2-A_3B_4-A_3B_6+2A_2B_3-A_2B_5-A_2B_7-A_1B_4+A_1B_6-A_0B_5+$$

$$+A_0B_7+A_5B_0]+$$

$$+a_3b_3\left(\frac{R}{2}\right)^4[A_8B_0-A_8B_2-A_6B_0-2A_6B_2+3A_6B_4+3A_4B_2-3A_4B_6-3A_2B_4+$$

$$+2A_2B_6+A_2B_8+A_0B_6-A_0B_8]+$$

$$+a_3b_4\left(\frac{R}{2}\right)^5[A_9B_0-A_9B_2-A_8B_1+A_8B_3-A_7B_0-2A_7B_2+3A_7B_4+A_6B_1+2A_6B_3-$$

$$-3A_6B_5+3A_5B_2-3A_5B_6-3A_4B_3+3A_4B_7-3A_3B_4+2A_3B_6+$$

$$+A_3B_8+3A_2B_5-2A_2B_7-A_2B_9+A_1B_6-A_1B_8-A_0B_7+A_0B_9]+$$

$$+a_4b_1\left(\frac{R}{2}\right)^3[A_7B_0-A_7B_2+3A_6B_1-3A_6B_3-A_5B_0+3A_5B_2-2A_5B_4-2A_3B_2-A_3B_4+$$

$$+3A_3B_6+2A_2B_3-3A_2B_5+A_2B_7-3A_4B_1+A_4B_3+2A_4B_5+3A_1B_4-$$

$$-3A_1B_6+A_0B_5-A_0B_7]+$$

$$+a_4b_2\left(\frac{R}{2}\right)^4[A_8B_0-A_8B_2+2A_7B_1-2A_7B_3-A_6B_0+A_6B_4-2A_5B_1-2A_5B_3+$$

$$+4A_5B_5+A_4B_2-2A_4B_4+A_4B_6+4A_3B_3-2A_3B_5-2A_3B_7+A_2B_4-$$

$$-A_2B_8-2A_1B_5+2A_1B_7-A_0B_6+A_0B_8]+$$

$$+a_4b_3\left(\frac{R}{2}\right)^5[A_9B_0-A_9B_2+A_8B_1-A_8B_3-A_7B_0-2A_7B_2+3A_7B_4-A_6B_1-$$

$$-2A_6B_3+3A_6B_5+3A_5B_2-3A_5B_6+3A_4B_3-3A_4B_7-3A_3B_4+$$

$$+2A_3B_6+A_3B_8-3A_2B_5+2A_2B_7+A_2B_9+A_1B_6-A_1B_8+A_0B_7-A_0B_9]+$$

$$+a_4b_4\left(\frac{R}{2}\right)^6[A_{10}B_0-A_{10}B_2-A_8B_0-3A_8B_2+4A_8B_4+4A_6B_2+2A_6B_4-6A_6B_6-$$

$$-6A_4B_4+2A_4B_6+4A_4B_8+4A_2B_6-3A_2B_8-A_2B_{10}-A_0B_8+A_0B_{10}]\}$$

10. $(4p_z, 4p_z) = 2\pi\left(\frac{R}{2}\right)^5 N_{4p_z}(\alpha)N_{4p_z}(\beta)\times$

$$\times\{a_1b_1[-A_4B_2+A_2B_0+A_2B_4-A_0B_2]+$$

$$+a_1b_2\frac{R}{2}[-A_5B_2+A_4B_3+A_3B_0+A_3B_4-A_2B_1-A_2B_5-A_1B_2+A_0B_3]+$$

$$+a_1b_3\left(\frac{R}{2}\right)^2[-A_6B_2+2A_5B_3+A_4B_0-2A_3B_1-2A_3B_5+A_2B_6+2A_1B_3-A_0B_4]+$$

$$+a_1b_4\left(\frac{R}{2}\right)^3[-A_7B_2+3A_6B_3+A_5B_0-2A_5B_4-3A_4B_1-2A_4B_5+2A_3B_2+3A_3B_6+$$

$$+2A_2B_3-A_2B_7-3A_1B_4+A_0B_5]+$$

$$+a_2b_1\frac{R}{2}[-A_5B_2-A_4B_3+A_3B_4+A_2B_1-A_1B_2-A_0B_3+A_2B_5+A_3B_0]+$$

$$+a_2b_2\left(\frac{R}{2}\right)^2[-A_6B_2+A_4B_0+2A_4B_4-2A_2B_2-A_2B_6+A_0B_4]+$$

$$+a_2b_3\left(\frac{R}{2}\right)^3[-A_7B_2+A_6B_3+A_5B_0+2A_5B_4-A_4B_1-2A_4B_5-2A_3B_2-A_3B_6+$$

$$+2A_2B_3+A_2B_7+A_1B_4-A_0B_5]+$$

$$+a_2b_4\left(\frac{R}{2}\right)^4[-A_8B_2+2A_7B_3+A_6B_0+A_6B_4-2A_5B_1-4A_5B_5-A_4B_2+A_4B_6+4A_3B_3+$$

$$+2A_3B_7-A_2B_4-A_2B_8-2A_1B_5+A_0B_6]+$$

$$+a_3b_1\left(\frac{R}{2}\right)^2[-A_6B_2-2A_5B_3+A_4B_0+2A_3B_1+2A_3B_5+A_2B_6-2A_1B_3-A_0B_4]+$$

$$+a_3b_2\left(\frac{R}{2}\right)^3[-A_7B_2-A_6B_3+A_5B_0+2A_5B_4+A_4B_1+2A_4B_5-2A_3B_2-A_3B_6-2A_2B_3-$$

$$-A_2B_7+A_1B_4+A_0B_5]+$$

$$+a_3b_3\left(\frac{R}{2}\right)^4[-A_8B_2+A_6B_0+3A_6B_4-3A_4B_2-3A_4B_6+3A_2B_4+A_2B_8-A_0B_6]+$$

$$+a_3b_4\left(\frac{R}{2}\right)^5[-A_9B_2+A_8B_3+A_7B_0+3A_7B_4-A_6B_1-[3A_6B_5-3A_5B_2-3A_5B_6+3A_4B_3+$$

$$+3A_4B_7+3A_3B_4+A_3B_8-3A_2B_5-A_2B_9-A_1B_6+A_0B_7]+$$

$$+a_4b_1\left(\frac{R}{2}\right)^3[-A_7B_2-3A_6B_3+A_5B_0-2A_5B_4+3A_4B_1+2A_4B_5+2A_3B_2+3A_3B_6-$$

$$-2A_2B_3+A_2B_7-3A_1B_4-A_0B_5]+$$

$$+a_4b_2\left(\frac{R}{2}\right)^4[-A_8B_2-2A_7B_3+A_6B_0+A_6B_4+2A_5B_1+4A_5B_5-A_4B_2+A_4B_6-$$

$$-4A_3B_3-2A_3B_7-A_2B_4-A_2B_8+2A_1B_5+A_0B_6]+$$

$$+a_4b_3\left(\frac{R}{2}\right)^5[-A_9B_2-A_8B_3+A_7B_0+3A_7B_4+A_6B_1+3A_6B_5-3A_5B_2-3A_5B_6-$$

$$A_4B_3-3A_4B_7+3A_3B_4+A_3B_8+3A_2B_5+A_2B_9-A_1B_6-A_0B_7]+$$

$$+a_4b_4\left(\frac{R}{2}\right)^6[-A_{10}B_2+A_8B_0+4A_8B_4-4A_6B_2-6A_6B_6+6A_4B_4+4A_4B_8-$$

$$-4A_2B_6-A_2B_{10}+A_0B_8]\}$$

References

[1] *Mulliken, R. S., C. A. Riecke, D. Orloff, H. Orloff:* J. Chem. Phys. **17**, 1248 (1949).
[2] *Jaffé, H. H.:* J. Chem. Phys. **21**, 198, 258 (1953).
[3] *Preuss, H.:* Integraltafeln zur Quantenchemie, Springer Verl., Berlin, 1957.
[4] *Gilde, F. J.:* Acta Phys. et Chem. Szeged 7, 83 (1961).
[5] *Miller, J. J. M. Gerhauser, F. A. Matsen:* Quantum Chemistry Integrals and Tables, University of Texas Press, Austin, 1959.
[6] *Pearson, K.:* Tables of the Incomplete Γ-function, Ed: K. Pearson, London, 1922.

ИНТЕГРАЛЬНЫЕ ВЫРАЖЕНИЯ ДЛЯ (nl | n'l') с n, n' = 3, 4

В. Мараз

Представлены интегральные выражения для интеграла перекрытия (nl | n'l') с n, n' = 3, 4 с помощю орбиталей типа СЛЕТЕРА для атомных орбиталей 3*d*, 4*s* и 4*p*, и приблизительная функцая для радиальной части 4*s* и 4*p*.