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Molecular Integrals for Heteropolar Diatomic Molecules Based on the One-Center Expansion Method

I. One Electron Integrals

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§ 1 Introduction

One of the most serious difficulties in the theoretical investigation of molecules is the molecular integrals. The problem of solving Schrödinger equation for molecules leads us to the jungles of molecular integrals. Moreover, many physical behaviours in molecules and solids, for example, dipole-dipole interaction, spin-orbit interaction and so forth can be interpreted in terms of molecular integrals. In this respect, molecular integrals are attacked by many authors with various methods.[1]

In this series of papers, we will use the one-center expansion method developed by Barnett and Coulson[2], since it can be applied in principle for any type of molecular integrals. Further, we consider normalized 1s, 2s, 2p, 3s, 3p, 3d Slater type orbitals (STO's) as the atomic orbitals. Formulae of the molecular integrals for heteropolar diatomic molecules are given in the present paper. Though a part of these molecular integrals has already been given[2], we will give here all the considering integrals for the sake of completeness.

The coordinates (r_a, θ_a, ϕ_a) and (r_b, θ_b, ϕ_b) can be understood by **Fig. 1** and their relations are:

$$r_b \sin\theta_b = r_a \sin\theta_a\,,$$
$$r_b \cos\theta_b = \rho - r_a \cos\theta_a\,,$$
$$\phi_b = \phi_a\,, \qquad (1)$$

where ρ is the internuclear distance.

The STO's employed are given in **Table** I and are denoted by $\Psi(\mathrm{X}, n\,; \mathrm{C})$, where X is the nucleus as the origin of coordinates, n is the coordinates of the electron n and C denotes a kind of STO's including an orbital exponent. In order to express a STO at the nucleus B in terms of the coordinate system (r_a, θ_a, ϕ_a), expression (1) and the following formula are used:

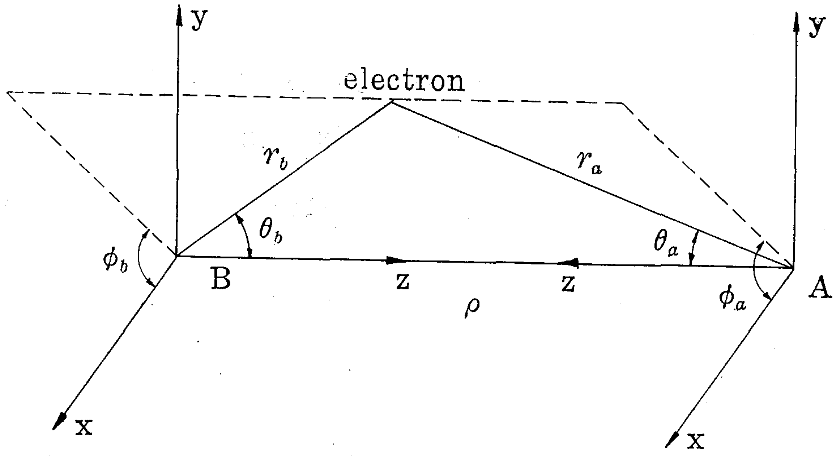

Fig. 1. Coordinates.

A, B: the nuclei

ρ: the internuclear distance

$$r_b^{m-1} \exp(-kr_b) = \sum_{n=0} (2n+1)(\rho r_a)^{-1/2} P_n(\cos\theta_a)\zeta_{m,n}(k, r_a; \rho)$$

$$= k^{-m+1} \sum_{n=0} (2n+1)(\tau t)^{-1/2} P_n(\cos\theta_a)\zeta_{m,n}(1, t; \tau), \tag{2}$$

where $t = kr_a$, $\tau = k\rho$ and P_n is the Legendre polynomial. Then molecular integrals can be expressed by the auxiliary functions $Z_{m,n,l+1/2}(\kappa, \tau)$ defined as follows:

$$Z_{m,n,l+1/2}(\kappa, \tau) = \int_0^\infty \exp(-\kappa t)\zeta_{m,n}(1, t; \tau) t^{l+1/2} dt. \tag{3}$$

Numerical calculations of them are now undertaken by the use of HITAC 5020E at *the Computer Center, the University of Tokyo* by Kobori and others[3].

§ 2 Formulae of Molecular Integrals

In the present paper, only the one electron integrals are considered and the two electron ones will be treated later. The considering one electron integrals are as follows:

a) Mononuclear integrals

i) overlap integrals

$$A(C_1, C_2) = \int \Psi(A, 1; C_1)\Psi(A, 1; C_2) dV_1, \tag{4}$$

ii) Coulomb integrals

$$B(C_1, C_2) = \rho \int \Psi(A, 1; C_1)\Psi(A, 1; C_2)(1/r_{a1}) dV_1, \tag{5}$$

b) Overlap integrals

$$S(C_1, C_2) = \int \Psi(A, 1; C_1)\Psi(B, 1; C_2) dV_1, \tag{6}$$

c) Coulomb integrals

$$C(C_1, C_2) = \rho \int \Psi(A, 1; C_1) \Psi(A, 1; C_2) (1/r_{b1}) dV_1, \tag{7}$$

d) Resonance integrals

$$R(C_1, C_2) = \rho \int \Psi(A, 1; C_1) \Psi(B, 1; C_2) (1/r_{b1}) dV_1. \tag{8}$$

Formulae of these molecular integrals are given in **Table** II to VII, where $Z_{m,n,l+1/2}$ means $Z_{m,n,l+1/2}(\tau_1/\tau_2, \tau_2)$ and $\eta = (\tau_1 + \tau_2)/2$. If the auxiliary functions are given, the molecular integrals can be computed easily by the use of the formulae in these tables.

References

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2) M.P. Barnett and C.A. Coulson, Phil. Tras. Roy. Soc. **A243** (1951) 221.
M.P. Barnett, *Methods in Computational Physics* (Academic Press, New York, 1963) Vol. 2, p. 95.
3) M. Kobori, private communication.

Table I Normalized Slater type orbitals

1s	$(k^3/\pi)^{1/2} \exp(-kr)$	$= R_1(r;k) Y_{0,0}(\theta,\phi)$
2s	$(k^5/3\pi)^{1/2} r \exp(-kr)$	$= R_2(r;k) Y_{0,0}(\theta,\phi)$
$2p_z$	$(k^5/\pi)^{1/2} z \exp(-kr)$	$= R_2(r;k) Y_{1,0}(\theta,\phi)$
$2p_x$	$(k^5/\pi)^{1/2} x \exp(-kr)$	$= R_2(r;k)\{Y_{1,1}(\theta,\phi)+Y_{1,-1}(\theta,\phi)\}/\sqrt{2}$
$2p_y$	$(k^5/\pi)^{1/2} y \exp(-kr)$	$= R_2(r;k)\{Y_{1,1}(\theta,\phi)-Y_{1,-1}(\theta,\phi)\}/\sqrt{2}\,i$
3s	$(2k^7/45\pi)^{1/2} r^2 \exp(-kr)$	$= R_3(r;k) Y_{0,0}(\theta,\phi)$
$3p_z$	$(2k^7/15\pi)^{1/2} zr \exp(-kr)$	$= R_3(r;k) Y_{1,0}(\theta,\phi)$
$3p_x$	$(2k^7/15\pi)^{1/2} xr \exp(-kr)$	$= R_3(r;k)\{Y_{1,1}(\theta,\phi)+Y_{1,-1}(\theta,\phi)\}/\sqrt{2}$
$3p_y$	$(2k^7/15\pi)^{1/2} yr \exp(-kr)$	$= R_3(r;k)\{Y_{1,1}(\theta,\phi)-Y_{1,-1}(\theta,\phi)\}/\sqrt{2}\,i$
$3d_{z^2}$	$(k^7/18\pi)^{1/2}(3z^2-r^2) \exp(-kr)$	$= R_3(r;k)\{Y_{2,0}(\theta,\phi)$
$3d_{xz}$	$(2k^7/3\pi)^{1/2} xz \exp(-kr)$	$= R_3(r;k)\{Y_{2,1}(\theta,\phi)+Y_{2,-1}(\theta,\phi)\}/\sqrt{2}$
$3d_{yz}$	$(2k^2/3\pi)^{1/2} yz \exp(-kr)$	$= R_3(r;k)\{Y_{2,1}(\theta,\phi)--Y_{2,-1}(\theta,\phi)\}/\sqrt{2}\,i$
$3d_{x^2-y^2}$	$(k^7/6\pi)^{1/2}(x^2-y^2) \exp(-kr)$	$= R_3(r;k)\{Y_{2,2}(\theta,\phi)+Y_{2,-2}(\theta,\phi)\}/\sqrt{2}$
$3d_{xy}$	$(2k^7/3\pi)^{1/2} xy \exp(-kr)$	$= R_3(r;k)\{Y_{2,2}(\theta,\phi)-Y_{2,-2}(\theta,\phi)\}/\sqrt{2}\,i$

$$R_1(r;k) = (4k^3)^{1/2} \exp(-kr)$$
$$R_2(r;k) = (4k^5/3)^{1/2} r \exp(-kr)$$
$$R_3(r;k) = (8k^7/45)^{1/2} r^2 \exp(-kr)$$

Table II Mononuclear overlap integrals

$$A(C_1,C_2) = \int \Psi(A,1;C_1)\Psi(A,1;C_2)\,dV_1$$

$A(1s, 1s) = (\tau_1^3\tau_2^3)^{1/2}/\eta^3$

$A(1s, 2s) = \sqrt{3}/2\cdot(\tau_1^3\tau_2^5)^{1/2}/\eta^4$

$A(1s, 3s) = \sqrt{10}/5\cdot(\tau_1^3\tau_2^7)^{1/2}/\eta^5$

$A(2s, 2s) = A(2p_z, 2p_z) = A(2p_x, 2p_x) = A(2p_y, 2p_y)$

$= (\tau_1^5\tau_2^5)^{1/2}/\eta^5$

$A(2s, 3s) = A(2p_z, 3p_z) = A(2p_x, 3p_x) = A(2p_y, 3p_y)$

$= \sqrt{30}/6\cdot(\tau_1^5\tau_2^7)^{1/2}/\eta^6$

$A(3s, 3s) = A(3p_z, 3p_z) = A(3p_x, 3p_x) = A(3p_y, 3p_y) = A(3d_{z^2}, 3d_{z^2})$

$= A(3d_{xz}, 3d_{xz}) = A(3d_{yz}, 3d_{yz}) = A(3d_{x^2-y^2}, 3d_{x^2-y^2}) = A(3d_{xy}, 3d_{xy})$

$= (\tau_1^7\tau_2^7)^{1/2}/\eta^7$

Table III **Mononuclear Coulomb integrals**

$$B(C_1, C_2) = \rho\int \Psi(A, 1\,; C_1)\Psi(A, 1\,; C_2)(1/r_{a1})\,dV_1$$

$B(1s, 1s) = (\tau_1^3\tau_2^3)^{1/2}/\eta^2$

$B(1s, 2s) = \sqrt{3}/3\cdot(\tau_1^3\tau_2^5)^{1/2}/\eta^3$

$B(1s, 3s) = \sqrt{10}/10\cdot(\tau_1^3\tau_2^7)^{1/2}/\eta^4$

$B(2s, 2s) = B(2p_z, 2p_z) = B(2p_x, 2p_x) = B(2p_y, 2p_y)$

$\quad = 1/2\cdot(\tau_1^5\tau_2^5)^{1/2}/\eta^4$

$B(2s, 3s) = B(2p_z, 3p_z) = B(2p_x, 3p_x) = B(2p_y, 3p_y)$

$\quad = \sqrt{30}/15\cdot(\tau_1^5\tau_2^7)^{1/2}/\eta^5$

$B(3s, 3s) = (3p_z, 3p_z) = B(3p_x, 3p_x) = B(3p_y, 3p_y) = B(3d_{z^2}, 3d_{z^2})$

$\quad = B(3d_{xz}, 3d_{xz}) = B(3d_{yz}, 3d_{yz}) = B(3d_{x^2-y^2}, 3d_{x^2-y^2}) = B(3d_{xy}, 3d_{xv})$

$\quad = 1/3\cdot(\tau_1^7\tau_2^7)^{1/2}/\eta^6$

Table IV **Overlap integrals**

$$S(C_1, C_2) = \int \Psi(A, 1\,; C_1)\Psi(B, 1\,; C_2)\,dV_1$$

$S(1s, 1s) = 4\cdot\tau_1^{3/2}/\tau_2^2\cdot Z_{1,0,3/2}$

$S(2s, 1s) = 4\sqrt{3}/3\cdot\tau_1^{5/2}/\tau_2^3\cdot Z_{1,0,5/2}$

$S(2p_z, 1s) = 4\cdot\tau_1^{5/2}/\tau_2^3\cdot Z_{1,1,5/2}$

$S(3s, 1s) = 4\sqrt{10}/15\cdot\tau_1^{7/2}/\tau_2^4\cdot Z_{1,0,7/2}$

$S(3p_z, 1s) = 4\sqrt{30}/15\cdot\tau_1^{7/2}/\tau_2^4\cdot Z_{1,1,7\cdot 2}$

$S(3d_{z^2}, 1s) = 4\sqrt{2}/3\cdot\tau_1^{7/2}/\tau_2^4\cdot Z_{1,2,7/2}$

$S(2s, 2s) = 4/3\cdot\tau_1^{5/2}/\tau_2^3\cdot Z_{2,0,5/2}$

$S(2p_z, 2s) = 4\sqrt{3}/3\cdot\tau_1^{5/2}/\tau_2^3\cdot Z_{2,1,5/2}$

$S(3s, 2s) = 4\sqrt{30}/45\cdot\tau_1^{7/2}/\tau_2^4\cdot Z_{2,0,7/2}$

$S(3p_z, 2s) = 4\sqrt{10}/15\cdot\tau_1^{7/2}/\tau_2^4\cdot Z_{2,1,7/2}$

$S(3d_{z^2}, 2s) = 4\sqrt{6}/9\cdot\tau_1^{7/2}/\tau_2^4\cdot Z_{2,2,7/2}$

$S(2p_z, 2p_z) = 4/3\cdot\tau_1^{5/2}/\tau_2^3\cdot\{3\tau_2 Z_{1,1,5/2} - Z_{1,0,7/2} - 2Z_{1,2,7/2}\}$

$S(3s, 2p_z) = 4\sqrt{10}/15\cdot\tau_1^{7/2}/\tau_2^4\cdot\{\tau_2 Z_{1,0,7/2} - Z_{1,1,9/2}\}$

$S(3p_z, 2p_z) = 4\sqrt{30}/45\cdot\tau_1^{7/2}/\tau_2^4\cdot\{3\tau_2 Z_{1,1,7/2} - Z_{1,0,9/2} - 2Z_{1,2,9/2}\}$

$S(3d_{z^2}, 2p_z) = 4\sqrt{2}/15\cdot\tau_1^{7/2}/\tau_2^4\cdot\{5\tau_2 Z_{1,2,7/2} - 2Z_{1,1,9/2} - 3Z_{1,3,9/2}\}$

$$S(2p_x, 2p_x) = S(2p_y, 2p_y)$$
$$= 4/3 \cdot \tau_1^{5/2}/\tau_2^3 \cdot \{Z_{1,0,7/2} - Z_{1,2,7/2}\}$$
$$S(3p_x, 2p_x) = S(3p_y, 2p_y)$$
$$= 4\sqrt{30}/45 \cdot \tau_1^{7/2}/\tau_2^4 \{Z_{1,0,9/2} - Z_{1,2,9/2}\}$$
$$S(3d_{xz}, 2p_x) = S(3d_{yz}, 2p_y)$$
$$= 4\sqrt{6}/15 \cdot \tau_1^{7/2}/\tau_2^4 \cdot \{Z_{1,1,9/2} - Z_{1,3,9/2}\}$$
$$S(3s, 3s) = 8/45 \cdot \tau_1^{7/2}/\tau_2^4 \cdot Z_{3,0,7/2}$$
$$S(3p_z, 3s) = 8\sqrt{3}/45 \cdot \tau_1^{7/2}/\tau_2^4 \cdot Z_{3,1,7/2}$$
$$S(3d_{z^2}, 3s) = 8\sqrt{5}/45 \cdot \tau_1^{7/2}/\tau_2^4 \cdot Z_{3,2,7/2}$$
$$S(3p_z, 3p_z) = 8/45 \cdot \tau_1^{7/2}/\tau_2^4 \cdot \{3\tau_2 Z_{2,1,7/2} - Z_{2,0,9/2} - 2Z_{2,2,9/2}\}$$
$$S(3d_{z^2}, 3p_z) = 8\sqrt{15}/225 \cdot \tau_1^{7/2}/\tau_2^4 \cdot \{5\tau_2 Z_{2,2,7/2} - 2Z_{2,1,9/2} - 3Z_{2,3,9/2}\}$$
$$S(3p_x, 3p_x) = S(3p_y, 3p_y)$$
$$= 8/45 \cdot \tau_1^{7/2}/\tau_2^4 \cdot \{Z_{2,0,9/2} - Z_{2,2,9/2}\}$$
$$S(3d_{xz}, 3p_x) = S(3d_{yz}, 3p_y)$$
$$= 8\sqrt{5}/75 \cdot \tau_1^{7/2}/\tau_2^4 \{Z_{2,1,9/2} - Z_{2,3,9/2}\}$$
$$S(3d_{z^2}, 3d_{z^2}) = 8/315 \cdot \tau_1^{7/2}/\tau_2^4 \cdot \{35\tau_2^2 Z_{1,2,7/2} - 28\tau_2 Z_{1,1,9/2} - 42\tau_2 Z_{1,3,9/2}$$
$$+ 7Z_{1,0,11/2} + 10Z_{1,2,11/2} + 18Z_{1,4,11/2}\}$$
$$S(3d_{xz}, 3d_{xz}) = S(3d_{yz}, 3d_{yz})$$
$$= 8/315 \cdot \tau_1^{7/2}/\tau_2^4 \cdot \{21\tau_2 Z_{1,1,9/2} - 21\tau_2 Z_{1,3,9/2} - 7Z_{1,0,11/2}$$
$$- 5Z_{1,2,11/2} + 12Z_{1,4,11/2}\}$$
$$S(3d_{x^2-y^2}, 3d_{x^2-y^2}) = S(3d_{xy}, 3d_{xy})$$
$$= 8/315 \cdot \tau_1^{7/2}/\tau_2^4 \cdot \{7Z_{1,0,11/2} - 10Z_{1,2,11/2} + 3Z_{1,4,11/2}\}$$

Table V Functions $\chi(n, l, a)$

$$\chi(n, l, a) = (2l+1)^{-1}[\Gamma(n+l+1) - \Gamma(n+l+1, a) + a^{2l+1}\Gamma(n-l, a)]$$
$$\chi(2, 0, a) = 2 - (2+a)\exp(-a)$$
$$\chi(3, 0, a) = 6 - (6+4a+a^2)\exp(-a)$$
$$\chi(3, 1, a) = 8 - (8+8a+4a^2+a^3)\exp(-a)$$
$$\chi(4, 0, a) = 24 - (24+18a+6a^2+a^3)\exp(-a)$$
$$\chi(4, 1, a) = 40 - (40+40a+20a^2+6a^3+a^4)\exp(-a)$$

$\chi(4,2,a)=144-(144+144a+72a^2+24a^3+6a^4+a^5)\exp(-a)$

$\chi(5,0,a)=120-(120+96a+36a^2+8a^3+a^4)\exp(-a)$

$\chi(5,1,a)=240-(240+240a+120a^2+38a^3+8a^4+a^5)\exp(-a)$

$\chi(5,2,a)=1008-(1008+1008a+504a^2+168a^3+42a^4+8a^5+a^6)\exp(-a)$

$\chi(5,3,a)=5760-(5760+5760a+2880a^2+960a^3+240a^4+48a^5+8a^6+a^7)$
$\times\exp(-a)$

$\chi(6,0,a)=720-(720+600a+240a^2+60a^3+10a^4+a^5)\exp(-a)$

$\chi(6,1,a)=1680-(1680+1680a+840a^2+272a^3+62a^4+10a^5+a^6)$
$\times\exp(-a)$

$\chi(6,2,a)=8064-(8064+8064a+4032a^2+1344a^3+336a^4+66a^5+10a^6$
$+a^7)\exp(-a)$

$\chi(6,3,a)=51840-(51840+51840a+25920a^2+8640a^3+2160a^4+432a^5$
$+72a^6+10a^7+a^8)\exp(-a)$

$\chi(6,4,a)=403200-(403200+403200a+201600a^2+67200a^3+16800a^4$
$+3360a^5+560a^6+80a^7+10a^8+a^9)\exp(-a)$

Table VI **One electron Coulomb integrals**

$$C(C_1, C_2)=\rho\int\Psi(A,1;C_1)\Psi(A,1;C_2)(1/r_{b1})\,dV_1$$

$C(1s,1s)=1/2\cdot(\tau_1^3\tau_2^3)^{1/2}/\eta^3\cdot\chi(2,0,2\eta)$
$=(\tau_1^3\tau_2^3)^{1/2}/\eta^3\cdot\{1-(1+\eta)\exp(-2\eta)\}$

$C(1s,2s)=\sqrt{3}/12\cdot(\tau_1^3\tau_2^5)^{1/2}/\eta^4\cdot\chi(3,0,2\eta)$
$=\sqrt{3}/6\cdot(\tau_1^3\tau_2^5)^{1/2}/\eta^4\cdot\{3-(3+4\eta+2\eta^2)\exp(-2\eta)\}$

$C(1s,2p_z)=1/8\cdot(\tau_1^3\tau_2^5)^{1/2}/\eta^5\cdot\chi(3,1,2\eta)$
$=(\tau_1^3\tau_2^5)^{1/2}/\eta^5\cdot\{1-(1+2\eta+2\eta^2+\eta^3)\exp(-2\eta)\}$

$C(1s,3s)=\sqrt{10}/120\cdot(\tau_1^3\tau_2^7)^{1/2}/\eta^5\cdot\chi(4,0,2\eta)$
$=\sqrt{10}/30\cdot(\tau_1^3\tau_2^7)^{1/2}/\eta^5\cdot\{6-(6+9\eta+6\eta^2+2\eta^3)\exp(-2\eta)\}$

$C(1s,3p_z)=\sqrt{30}/240\cdot(\tau_1^3\tau_2^7)^{1/2}/\eta^6\cdot\chi(4,1,2\eta)$
$=\sqrt{30}/30\cdot(\tau_1^3\tau_2^7)^{1/2}/\eta^6\cdot\{5-(5+10\eta+10\eta^2+6\eta^3+2\eta^4)\exp(-2\eta)\}$

$C(1s,3d_{z^2})=\sqrt{2}/96\cdot(\tau_1^3\tau_2^7)^{1/2}/\eta^7\cdot\chi(4,2,2\eta)$
$=\sqrt{2}/6\cdot(\tau_1^3\tau_2^7)^{1/2}/\eta^7\cdot\{9-(9+18\eta+18\eta^2+12\eta^3+6\eta^4+2\eta^5)$
$\times\exp(-2\eta)\}$

$$C(2s, 2s) = 1/24\cdot(\tau_1^5\tau_2^5)^{1/2}/\eta^5\cdot\chi(4, 0, 2\eta)$$
$$= 1/6\cdot(\tau_1^5\tau_2^5)^{1/2}/\eta^5\cdot\{6-(6+9\eta+6\eta^2+2\eta^3)\exp(-2\eta)\}$$

$$C(2s, 2p_z) = \sqrt{3}/48\cdot(\tau_1^5\tau_2^5)^{1/2}/\eta^6\cdot\chi(4, 1, 2\eta)$$
$$= \sqrt{3}/6\cdot(\tau_1^5\tau_2^5)^{1/2}/\eta^6\cdot\{5-(5+10\eta+10\eta^2+6\eta^3+2\eta^4)\exp(-2\eta)\}$$

$$C(2s, 3s) = \sqrt{30}/720\cdot(\tau_1^5\tau_2^7)^{1/2}/\eta^6\cdot\chi(5, 0, 2\eta)$$
$$= \sqrt{30}/90\cdot(\tau_1^5\tau_2^7)^{1/2}/\eta^6\cdot\{15-(15+24\eta+18\eta^2+8\eta^3+2\eta^4)$$
$$\times\exp(-2\eta)\}$$

$$C(2s, 3p_z) = \sqrt{10}/480\cdot(\tau_1^5\tau_2^7)^{1/2}/\eta^7\cdot\chi(5, 1, 2\eta)$$
$$= \sqrt{10}/30\cdot(\tau_1^5\tau_2^7)^{1/2}/\eta^7\cdot\{15-(15+30\eta+30\eta^2+19\eta^3+8\eta^4+2\eta^5)$$
$$\times\exp(-2\eta)\}$$

$$C(2s, 3d_{z^2}) = \sqrt{6}/576\cdot(\tau_1^5\tau_2^7)^{1/2}/\eta^8\cdot\chi(5, 2, 2\eta)$$
$$= \sqrt{6}/36\cdot(\tau_1^5\tau_2^7)^{1/2}/\eta^8\cdot\{63-(63+126\eta+126\eta^2+84\eta^3+42\eta^4$$
$$+16\eta^5+4\eta^6)\exp(-2\eta)\}$$

$$C(2p_z, 2p_z) = 1/48\cdot(\tau_1^5\tau_2^5)^{1/2}/\eta^7\cdot\{\chi(4, 2, 2\eta)+2\eta^2\chi(4, 0, 2\eta)\}$$
$$= 1/2\cdot(\tau_1^5\tau_2^5)^{1/2}/\eta^7\cdot\{6+2\eta^2-(6+12\eta+14\eta^2+11\eta^3+6\eta^4+2\eta^5)$$
$$\times\exp(-2\eta)\}$$

$$C(2p_z, 3s) = \sqrt{10}/480\cdot(\tau_1^5\tau_2^7)^{1/2}/\eta^7\cdot\chi(5, 1, 2\eta)$$
$$= \sqrt{10}/30\cdot(\tau_1^5\tau_2^7)^{1/2}/\eta^7\cdot\{15-(15+30\eta+30\eta^2+19\eta^3+8\eta^4+2\eta^5)$$
$$\times\exp(-2\eta)\}$$

$$C(2p_z, 3p_z) = \sqrt{30}/1440\cdot(\tau_1^5\tau_2^7)^{1/2}/\eta^8\cdot\{\chi(5, 2, 2\eta)+2\eta^2\chi(5, 0, 2\eta)\}$$
$$= \sqrt{30}/30\cdot(\tau_1^5\tau_2^7)^{1/2}/\eta^8\cdot\{21+5\eta^2-(21+42\eta+47\eta^2+36\eta^3+20\eta^4$$
$$+8\eta^5+2\eta^6)\exp(-2\eta)\}$$

$$C(2p_z, 3d_{z^2}) = \sqrt{2}/1920\cdot(\tau_1^5\tau_2^7)^{1/2}/\eta^9\cdot\{3\chi(5, 3, 2\eta)+8\eta^2\chi(5, 1, 2\eta)\}$$
$$= \sqrt{2}/3\cdot(\tau_1^5\tau_2^7)^{1/2}/\eta^9\cdot\{27+3\eta^2-(27+54\eta+57\eta^2+42\eta^3+24\eta^4$$
$$+11\eta^5+4\eta^6+\eta^7)\exp(-2\eta)\}$$

$$C(2p_x, 2p_x) = C(2p_y, 2p_y)$$
$$= 1/96\cdot(\tau_1^5\tau_2^5)^{1/2}/\eta^7\cdot\{-\chi(4, 2, 2\eta)+4\eta^2\chi(4, 0, 2\eta)\}$$
$$= 1/2\cdot(\tau_1^5\tau_2^5)^{1/2}/\eta^7\cdot\{-3+2\eta^2+(3+6\eta+4\eta^2+\eta^3)\exp(-2\eta)\}$$

$$C(2p_x, 3p_x) = C(2p_y, 3p_y)$$
$$= \sqrt{30}/2880\cdot(\tau_1^5\tau_2^7)^{1/2}/\eta^8\cdot\{-\chi(5, 2, 2\eta)+4\eta^2\chi(5, 0, 2\eta)\}$$
$$= \sqrt{30}/60\cdot(\tau_1^5\tau_2^7)^{1/2}/\eta^8\cdot\{-21+10\eta^2+(21+42\eta+32\eta^2+12\eta^3$$
$$+2\eta^4)\exp(-2\eta)\}$$

$$C(2p_x, 3d_{xz}) = C(2p_y, 3d_{yz})$$
$$= \sqrt{6}/1920\cdot(\tau_1^5\tau_2^7)^{1/2}/\eta^9\cdot\{-\chi(5, 3, 2\eta) + 4\eta^2\chi(5, 1, 2\eta)\}$$
$$= \sqrt{6}/6\cdot(\tau_1^5\tau_2^7)^{1/2}/\eta^9\cdot\{-18 + 3\eta^2 + (18 + 36\eta + 33\eta^2 + 18\eta^3 + 6\eta^4 + \eta^5)\exp(-2\eta)\}$$

$$C(3s, 3s) = 1/720\cdot(\tau_1^7\tau_2^7)^{1/2}/\eta^7\cdot\chi(6, 0, 2\eta)$$
$$= 1/45\cdot(\tau_1^7\tau_2^7)^{1/2}/\eta^7\cdot\{45 - (45 + 75\eta + 60\eta^2 + 30\eta^3 + 10\eta^4 + 2\eta^5)\times\exp(-2\eta)\}$$

$$C(3s, 3p_z) = \sqrt{3}/1440\cdot(\tau_1^7\tau_2^7)^{1/2}/\eta^8\cdot\chi(6, 1, 2\eta)$$
$$= \sqrt{3}/90\cdot(\tau_1^7\tau_2^7)^{1/2}/\eta^8\cdot\{105 - (105 + 210\eta + 210\eta^2 + 136\eta^3 + 62\eta^4 + 20\eta^5 + 4\eta^6)\exp(-2\eta)\}$$

$$C(3s, 3d_{z^2}) = \sqrt{5}/2880\cdot(\tau_1^7\tau_2^7)^{1/2}/\eta^9\cdot\chi(6, 2, 2\eta)$$
$$= \sqrt{5}/45\cdot(\tau_1^7\tau_2^7)^{1/2}/\eta^9\cdot\{126 - (126 + 252\eta + 252\eta^2 + 168\eta^3 + 84\eta^4 + 33\eta^5 + 10\eta^6 + 2\eta^7)\exp(-2\eta)\}$$

$$C(3p_z, 3p_z) = 1/1440\cdot(\tau_1^7\tau_2^7)^{1/2}/\eta^9\cdot\{\chi(6, 2, 2\eta) + 2\eta^2\chi(6, 0, 2\eta)\}$$
$$= 1/15\cdot(\tau_1^7\tau_2^7)^{1/2}/\eta^9\cdot\{84 + 15\eta^2 - (84 + 168\eta + 183\eta^2 + 137\eta^3 + 76\eta^4 + 32\eta^5 + 10\eta^6 + 2\eta^7)\exp(-2\eta)\}$$

$$C(3p_z, 3d_{z^2}) = \sqrt{15}/28800\cdot(\tau_1^7\tau_2^7)^{1/2}/\eta^{10}\cdot\{3\chi(6, 3, 2\eta) + 8\eta^2\chi(6, 1, 2\eta)\}$$
$$= \sqrt{15}/45\cdot(\tau_1^7\tau_2^7)^{1/2}/\eta^{10}\cdot\{243 + 21\eta^2 - (243 + 486\eta + 507\eta^2 + 366\eta^3 + 204\eta^4 + 92\eta^5 + 34\eta^6 + 10\eta^7 + 2\eta^8)\exp(-2\eta)\}$$

$$C(3p_x, 3p_x) = C(3p_y, 3p_y)$$
$$= 1/2880\cdot(\tau_1^7\tau_2^7)^{1/2}/\eta^9\cdot\{-\chi(6, 2, 2\eta) + 4\eta^2\chi(6, 0, 2\eta)\}$$
$$= 1/15\cdot(\tau_1^7\tau_2^7)^{1/2}/\eta^9\cdot\{-42 + 15\eta^2 + (42 + 84\eta + 69\eta^2 + 31\eta^3 + 8\eta^4 + \eta^5)\exp(-2\eta)\}$$

$$C(3p_x, 3d_{xz}) = C(3p_y, 3d_{yz})$$
$$= \sqrt{5}/9600\cdot(\tau_1^7\tau_2^7)^{1/2}/\eta^{10}\cdot\{-\chi(6, 3, 2\eta) + 4\eta^2\chi(6, 1, 2\eta)\}$$
$$= \sqrt{5}/30\cdot(\tau_1^7\tau_2^7)^{1/2}/\eta^{10}\cdot\{-162 + 21\eta^2 + (162 + 324\eta + 303\eta^2 + 174\eta^3 + 66\eta^4 + 16\eta^5 + 2\eta^6)\exp(-2\eta)\}$$

$$C(3d_{z^2}, 3d_{z^2}) = 1/40320\cdot(\tau_1^7\tau_2^7)^{1/2}/\eta^{11}\cdot\{9\chi(6, 4, 2\eta) + 20\eta^2\chi(6,2,2\eta) + 56\eta^4\chi(6, 0, 2\eta)\}$$
$$= 1/9\cdot(\tau_1^7\tau_2^7)^{1/2}/\eta^{11}\cdot\{810 + 36\eta^2 + 9\eta^4 - (810 + 1620\eta + 1656\eta^2 + 1152\eta^3 + 621\eta^4 + 279\eta^5 + 108\eta^6 + 36\eta^7 + 10\eta^8 + 2\eta^9)\times\exp(-2\eta)\}$$

$$C(3d_{xz}, 3d_{xz}) = C(3d_{yz}, 3d_{yz})$$
$$= 1/20160\cdot(\tau_1^7\tau_2^7)^{1/2}/\eta^{11}\cdot\{-3\chi(6, 4, 2\eta) + 5\eta^2\chi(6, 2\ 2\eta)$$
$$+ 28\eta^4\chi(6, 0, 2\eta)\}$$
$$= 1/3\cdot(\tau_1^7\tau_2^7)^{1/2}/\eta^{11}\cdot\{-180 + 6\eta^2 + 3\eta^4 + (180 + 360\eta + 354\eta^2$$
$$+ 228\eta^3 + 105\eta^4 + 35\eta^5 + 8\eta^6 + \eta^7)\exp(-2\eta)\}$$

$$C(3d_{x^2-y^2}, 3d_{x^2-y^2}) = C(3d_{xy}, 3d_{xy})$$
$$= 1/80640\cdot(\tau_1^7\tau_2^7)^{1/2}/\eta^{11}\cdot\{3\chi(6, 4, 2\eta) - 40\eta^2\chi(6, 2, 2\eta)$$
$$+ 112\eta^4\chi(6, 0, 2\eta)\}$$
$$= 1/3\cdot(\tau_1^7\tau_2^7)^{1/2}/\eta^{11}\cdot\{45 - 12\eta^2 + 3\eta^4 - (45 + 90\eta + 78\eta^2$$
$$+ 36\eta^3 + 9\eta^4 + \eta^5)\exp(-2\eta)\}$$

Table VI Resonance integrals

$$R(C_1, C_2) = \rho\int \Psi(A, 1; C_1)\Psi(B, 1; C_2)(1/r_{b1})\,dV_1$$

$$R(1s, 1s) = 4\cdot\tau_1^{3/2}/\tau_2\cdot Z_{0,0,3/2}$$
$$R(1s, 2s) = 4\sqrt{3}/3\cdot\tau_1^{3/2}/\tau_2\cdot Z_{1,0,3/2}$$
$$R(1s, 2p_z) = 4\cdot\tau_1^{3/2}/\tau_2\cdot\{\tau_2 Z_{0,0,3/2} - Z_{0,1,5/2}\}$$
$$R(1s, 3s) = 4\sqrt{10}/15\cdot\tau_1^{3/2}/\tau_2\cdot Z_{2,0,3/2}$$
$$R(1s, 3p_z) = 4\sqrt{30}/15\cdot\tau_1^{3/2}/\tau_2\cdot\{\tau_2 Z_{1,0,3/2} - Z_{1,1,5/2}\}$$
$$R(1s, 3d_{z^2}) = 4\sqrt{2}/3\cdot\tau_1^{3/2}/\tau_2\cdot\{\tau_2^2 Z_{0,0,3/2} - 2\tau_2 Z_{0,1,5/2} + Z_{0,2,7/2}\}$$
$$R(2s, 1s) = 4\sqrt{3}/3\cdot\tau_1^{5/2}/\tau_2^2\cdot Z_{0,0,5/2}$$
$$R(2s, 2s) = 4/3\cdot\tau_1^{5/2}/\tau_2^2\cdot Z_{1,0,5/2}$$
$$R(2s, 2p_z) = 4\sqrt{3}/3\cdot\tau_1^{5/2}/\tau_2^2\cdot\{\tau_2 Z_{0,0,5/2} - Z_{0,1,7/2}\}$$
$$R(2s, 3s) = 4\sqrt{30}/45\cdot\tau_1^{5/2}/\tau_2^2\cdot Z_{2,0,5/2}$$
$$R(2s, 3p_z) = 4\sqrt{10}/15\cdot\tau_1^{5/2}/\tau_2^2\cdot\{\tau_2 Z_{1,0,5/2} - Z_{1,1,7/2}\}$$
$$R(2s, 3d_{z^2}) = 4\sqrt{6}/9\cdot\tau_1^{5/2}/\tau_2^2\cdot\{\tau_2^2 Z_{0,0,5/2} - 2\tau_2 Z_{0,1,7/2} + Z_{0,2,9/2}\}$$
$$R(2p_z, 1s) = 4\cdot\tau_1^{5/2}/\tau_2^2\cdot Z_{0,1,5/2}$$
$$R(2p_z, 2s) = 4\sqrt{3}/3\cdot\tau_1^{5/2}/\tau_2^2\cdot Z_{1,1,5/2}$$
$$R(2p_z, 2p_z) = 4/3\cdot\tau_1^{5/2}/\tau_2^2\cdot\{3\tau_2 Z_{0,1,5/2} - Z_{0,0,7/2} - 2Z_{0,2,7/2}\}$$
$$R(2p_z, 3s) = 4\sqrt{10}/15\cdot\tau_1^{5/2}/\tau_2^2\cdot Z_{2,1,5/2}$$

$R(2p_z, 3p_z) = 4\sqrt{30}/45 \cdot \tau_1^{5/2}/\tau_2^2 \cdot \{3\tau_2 Z_{1,1,5/2} - Z_{1,0,7/2} - 2Z_{1,2,7/2}\}$

$R(2p_z, 3d_{z^2}) = 4\sqrt{2}/45 \cdot \tau_1^{5/2}/\tau_2^2 \cdot \{15\tau_2^2 Z_{0,1,5/2} - 10\tau_2 Z_{0,0,7/2}$

$\qquad - 20\tau_2 Z_{0,2,7/2} + 6Z_{0,1,9/2} + 9Z_{0,3,9/2}\}$

$R(2p_x, 2p_x) = R(2p_y, 2p_y)$

$\qquad = 4/3 \cdot \tau_1^{5/2}/\tau_2^2 \cdot \{Z_{0,0,7/2} - Z_{0,2,7/2}\}$

$R(2p_x, 3p_x) = R(2p_y, 3p_y)$

$\qquad = 4\sqrt{30}/45 \cdot \tau_1^{5/2}/\tau_2^2 \cdot \{Z_{1,0,7/2} - Z_{1,2,7/2}\}$

$R(2p_x, 3d_{xz}) = R(2p_y, 3d_{yz})$

$\qquad = 4\sqrt{6}/45 \cdot \tau_1^{5/2}/\tau_2^2 \cdot \{5\tau_2 Z_{0,0,7/2} - 5\tau_2 Z_{0,2,7/2} - 3Z_{0,1,9/2} + 3Z_{0,3,9/2}\}$

$R(3s, 1s) = 4\sqrt{10}/15 \cdot \tau_1^{7/2}/\tau_2^3 \cdot Z_{0,0,7/2}$

$R(3s, 2s) = 4\sqrt{30}/45 \cdot \tau_1^{7/2}/\tau_2^3 \cdot Z_{1,0,7/2}$

$R(3s, 2p_z) = 4\sqrt{10}/15 \cdot \tau_1^{7/2}/\tau_2^3 \cdot \{\tau_2 Z_{0,0,7/2} - Z_{0,1,9/2}\}$

$R(3s, 3s) = 8/45 \cdot \tau_1^{7/2}/\tau_2^3 \cdot Z_{2,0,7/2}$

$R(3s, 3p_z) = 8\sqrt{3}/45 \cdot \tau_1^{7/2}/\tau_2^3 \cdot \{\tau_2 Z_{1,0,7/2} - Z_{1,1,9/2}\}$

$R(3s, 3d_{z^2}) = 8\sqrt{5}/45 \cdot \tau_1^{7/2}/\tau_2^3 \cdot \{\tau_2^2 Z_{0,0,7/2} - 2\tau_2 Z_{0,1,9/2} + Z_{0,2,11/2}\}$

$R(3p_z, 1s) = 4\sqrt{30}/15 \cdot \tau_1^{7/2}/\tau_2^3 \cdot Z_{0,1,7/2}$

$R(3p_z, 2s) = 4\sqrt{10}/15 \cdot \tau_1^{7/2}/\tau_2^3 \cdot Z_{1,1,7/2}$

$R(3p_z, 2p_z) = 4\sqrt{30}/45 \cdot \tau_1^{7/2}/\tau_2^3 \cdot \{3\tau_2 Z_{0,1,7/2} - Z_{0,0,9/2} - 2Z_{0,2,9/2}\}$

$R(3p_z, 3s) = 8\sqrt{3}/45 \cdot \tau_1^{7/2}/\tau_2^3 \cdot Z_{2,1,7/2}$

$R(3p_z, 3p_z) = 8/45 \cdot \tau_1^{7/2}/\tau_2^3 \cdot \{3\tau_2 Z_{1,1,7/2} - Z_{1,0,9/2} - 2Z_{1,2,9/2}\}$

$R(3p_z, 3d_{z^2}) = 8\sqrt{15}/675 \cdot \tau_1^{7/2}/\tau_2^3 \cdot \{15\tau_2^2 Z_{0,1,7/2} - 10\tau_2 Z_{0,0,9/2}$

$\qquad - 20\tau_2 Z_{0,2,9/2} + 6Z_{0,1,11/2} + 9Z_{0,3,11/2}\}$

$R(3p_x, 2p_x) = R(3p_y, 2p_y)$

$\qquad = 4\sqrt{30}/45 \cdot \tau_1^{7/2}/\tau_2^3 \cdot \{Z_{0,0,9/2} - Z_{0,2,9/2}\}$

$R(3p_x, 3p_x) = R(3p_y, 3p_y)$

$\qquad = 8/45 \cdot \tau_1^{7/2}/\tau_2^3 \cdot \{Z_{1,0,9/2} - Z_{1,2,9/2}\}$

$R(3p_x, 3d_{xz}) = R(3p_y, 3d_{yz})$

$\qquad = 8\sqrt{5}/225 \cdot \tau_1^{7/2}/\tau_2^3 \cdot \{5\tau_2 Z_{0,0,9/2} - 5\tau_2 Z_{0,2,9/2} - 3Z_{0,1,11/2} + 3Z_{0,3,11/2}\}$

$R(3d_{z^2}, 1s) = 4\sqrt{2}/3 \cdot \tau_1^{7/2}/\tau_2^3 \cdot Z_{0,2,7/2}$

$R(3d_{z^2}, 2s) = 4\sqrt{6}/9 \cdot \tau_1^{7/2}/\tau_2^3 \cdot Z_{1,2,7/2}$

$R(3d_{z^2}, 2p_z) = 4\sqrt{2}/15 \cdot \tau_1^{7/2}/\tau_2^3 \cdot \{5\tau_2 Z_{0,2,7/2} - 2Z_{0,1,9/2} - 3Z_{0,3,9/2}\}$

$R(3d_{z^2}, 3s) = 8\sqrt{5}/45 \cdot \tau_1^{7/2}/\tau_2^3 \cdot Z_{2,2,7/2}$

$R(3d_{z^2}, 3p_z) = 8\sqrt{5}/225 \cdot \tau_1^{7/2}/\tau_2^3 \cdot \{5\tau_2 Z_{1,2,7/2} - 2Z_{1,1,9/2} - 3Z_{1,3,9/2}\}$

$$R(3d_{z^2}, 3d_{z^2}) = 8/315 \cdot \tau_1^{7/2}/\tau_2^3 \cdot \{35\tau_2^2 Z_{0,2,7/2} - 28\tau_2 Z_{0,1,9/2} - 42\tau_2 Z_{0,3,9/2} + 7Z_{0,0,11/2} + 10Z_{0,2,11/2} + 18Z_{0,4,11/2}\}$$

$$R(3d_{xz}, 2p_x) = R(3d_{yz}, 2p_y) = 4\sqrt{6}/15 \cdot \tau_1^{7/2}/\tau_2^3 \cdot \{Z_{0,1,9/2} - Z_{0,3,9/2}\}$$

$$R(3d_{xz}, 3p_x) = R(3d_{yz}, 3p_y) = 8\sqrt{5}/75 \cdot \tau_1^{7/2}/\tau_2^3 \cdot \{Z_{1,1,9/2} - Z_{1,3,9/2}\}$$

$$R(3d_{xz}, 3d_{xz}) = R(3d_{yz}, 3d_{yz}) = 8/315 \cdot \tau_1^{7/2}/\tau_2^3 \cdot \{21\tau_2 Z_{0,1,9/2} - 21\tau_2 Z_{0,3,9/2} - 7Z_{0,0,11/2} - 5Z_{0,2,11/2} + 12Z_{0,4,11/2}\}$$

$$R(3d_{x^2-y^2}, 3d_{x^2-y^2}) = R(3d_{xy}, 3d_{xy}) = 8/315 \cdot \tau_1^{7/2}/\tau_2^3 \cdot \{7Z_{0,0,11/2} - 10Z_{0,2,11/2} + 3Z_{0,4,11/2}\}$$