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# Formulas for One- and Two-center Moment Integrals between Slater Type *s*, *p*-Orbitals with Integer Effective Principal Quantum Numbers of 1 to 5

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Expansion formulas are presented for one- and two-center moment integrals between Slater type *s*,*p*-orbitals with integer effective principal quantum numbers of 1 to 5, together with the procedure. These formulas are useful in the calculation of a dipole moment and a transition moment from a charge distribution calculated by LCAO-MO method. A FORTRAN subprogram containing most of these formulas, which are important in practice, occupies about 7.7*K* of the core memory of a computer, HITAC 5020.

In application of LCAO-MO calculation to the interpretation of the electronic absorption spectra of various molecules, it is useful to compare the calculated values of the intensity as well as the transition energy with the observed values. For this purpose it is necessary to evaluate one-electron moment integrals between all the possible pairs of the atomic orbitals (AO's) taken as bases. Then, these integrals can also be used to calculate the dipole moment of the molecule and to test the accuracy of the calculated charge distribution. Hence it is convenient to write a computer program for the continuous calculation of the dipole moment and the transition moments between any molecular orbitals (MO's) after solving the secular equations for molecules containing any kinds of atoms.

Two-center moment integrals between Slater-type AO's (STO's) with integer effective principal quantum number ($n^*$) are expressed by formulas similar to those for overlap integrals with auxiliary functions, $A_m$ and $B_m$ with integer $m$.*1 Some of these formulas for *s*,*p*-AO's with small values of $n^*$ (1 and 2) are found,[1,2] but, as far as we know, no adequate table has been published containing STO's with larger values of $n^*$. This paper will present many of these formulas, together with the procedure.*2

## Procedure

MO's, $\varphi$'s, are taken as linear combination of AO's, $\chi$'s, which are centered on the various atoms in the molecule:

$$\varphi_i = \sum_p C_{pi}\chi_p \tag{1}$$

Then the one-electron moment integrals between these MO's are decomposed into integrals with AO's:

$$R_{ij} = \int \varphi_i \boldsymbol{r} \varphi_j \, d\tau = \sum_{p,q} C_{pi}C_{qj}T_{pq}$$

$$T_{pq} = \int \chi_p \boldsymbol{r} \chi_q \, d\tau \tag{2}$$

$\chi_p$ and $\chi_q$ are the AO's centered on atom P and Q respectively, and $\boldsymbol{r}$ is the position vector of an electron relative to an origin fixed in the molecule. When $\boldsymbol{r}_0$ is the position vector of the middle point of P and Q, and $\boldsymbol{r}'$ is of an electron relative to this point, $\boldsymbol{r}=\boldsymbol{r}_0+\boldsymbol{r}'$, hence:

$$\begin{aligned} T_{pq} &= \int \chi_p (\boldsymbol{r}_0+\boldsymbol{r}')\chi_q \, d\tau \\ &= \int \chi_p \boldsymbol{r}_0 \chi_q \, d\tau + \int \chi_p \boldsymbol{r}' \chi_q \, d\tau \\ &= \boldsymbol{r}_0 S_{pq} + M_{pq} \end{aligned} \tag{3}$$

where $S$ is an overlap integral, and $M$ is a moment integral relative to the middle point of P and Q. In the following section, three components of $\boldsymbol{r}$, *i. e.*, $z$, $x$ and $y$ are treated.

**Two-center Integrals.** Any coordinate systems, $(z,x,y)$, with an origin on PQ, and parallel to the coordinates fixed in the molecule, are transformed by the following transformation matrix to a local coordinate system, $(Z,X,Y)$, with the positive direction of the $Z$ axis from P toward Q as is shown in Fig. 1:

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*1 In this paper, a principal quantum number, $n$, and an effective principal quantum number, $n^*$ $(=n-\delta)$, are distinguished.

*2 For the purpose of convenience some partial overlapping with the books of Miller *et al.*,[1] and Kotani *et al.*,[2] is not avoided.

1) J. Miller, J. M. Gerhauser, F. A. Matsen, "Quantum Chemistry Integrals and Tables," University of Texas Press, Austin (1959).

2) M. Kotani, A. Amemiya, E. Ishiguro and T. Kimura, "Table of Molecular Integral," II, Maruzen, Tokyo (1963).

$$\begin{pmatrix} z \\ x \\ y \end{pmatrix} = \begin{pmatrix} \gamma_z & -\gamma_z\gamma_x/\delta & -\gamma_y/\delta \\ \gamma_x & \delta & 0 \\ \gamma_y & -\gamma_x\gamma_y/\delta & \gamma_z/\delta \end{pmatrix} \begin{pmatrix} \mathcal{Z} \\ X \\ Y \end{pmatrix}$$

$$\delta = (1-\gamma_x^2)^{1/2} \tag{4}$$

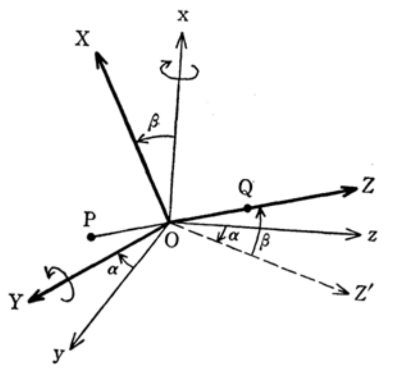


Fig. 1. Transformation to local coordinates.

where $\gamma_z$ is the direction cosine of $\mathcal{Z}$ axis relative to $z$ axis fixed in a molecule, and so on.

We take STO's as bases, which consist of appropriate combinations of $z, x, y$ and a function of $r$, where $z$, $x$ and $y$ are transformed as mentioned above, but $r$ is not. As for the two-center moment integrals relative to the local coordinate system, $(\mathcal{Z}, X, Y)$, only those integrals containing none or even numbers of $X$ and/or $Y$ respectively have non-zero values in symmetric property. When only $s$- and $p$-AO's are treated, the following nine types are all of the necessary basic two-center integrals:

$(S|\mathcal{Z}|S)$, $(S|\mathcal{Z}|P_Z)$, $(S|X|P_X)$. $(P_Z|\mathcal{Z}|S)$, $(P_X|X|S)$, $(P_Z|\mathcal{Z}|P_Z)$, $(P_Z|X|P_X)$, $(P_X|\mathcal{Z}|P_X)$, $(P_X|X|P_Z)$*3

Any two-center moment integrals between $s,p$-AO's relative to the original coordinate system are linear combinations of some of the above basic integrals (Table 1).

TABLE 1. DECOMPOSITION OF TWO-CENTER MOMENT INTEGRALS*

$$(s|i|s) = \gamma_i(S|\mathcal{Z}|S)$$
$$(s|i|p_i) = \gamma_i^2(S|\mathcal{Z}|P_Z) + (1-\gamma_i^2)(S|X|P_X)$$
$$(p_i|i|s) = \gamma_i^2(P_Z|\mathcal{Z}|S) + (1-\gamma_i^2)(P_X|X|S)$$
$$(s|i|p_j) = \gamma_i\gamma_j\{(S|\mathcal{Z}|P_Z) - (S|X|P_X)\}$$
$$(p_j|i|s) = \gamma_i\gamma_j\{(P_Z|\mathcal{Z}|S) - (P_X|X|S)\}$$
$$(p_i|i|p_i) = \gamma_i[\gamma_i^2(P_Z|\mathcal{Z}|P_Z) + (1-\gamma_i^2)\{(P_Z|X|P_X) + (P_X|\mathcal{Z}|P_X) + (P_X|X|P_Z)\}]$$
$$(p_i|j|p_j) = \gamma_i[(1-\gamma_i^2)(P_Z|X|P_X) + \gamma_i^2\{(P_Z|\mathcal{Z}|P_Z) - (P_X|\mathcal{Z}|P_X) - (P_X|X|P_Z)\}]$$
$$(p_i|j|p_i) = \gamma_j[(1-\gamma_i^2)(P_X|\mathcal{Z}|P_X) + \gamma_i^2\{(P_Z|\mathcal{Z}|P_Z) - (P_Z|X|P_X) - (P_X|X|P_Z)\}]$$
$$(p_i|i|p_j) = \gamma_j[(1-\gamma_i^2)(P_X|X|P_Z) + \gamma_i^2\{(P_Z|\mathcal{Z}|P_Z) - (P_Z|X|P_X) - (P_X|\mathcal{Z}|P_X)\}]$$
$$(p_i|j|p_k) = \gamma_i\gamma_j\gamma_k\{(P_Z|\mathcal{Z}|P_Z) - (P_Z|X|P_X) - (P_X|\mathcal{Z}|P_X) - (P_X|X|P_Z)\}$$

* Each of $i, j$ and $k$ denotes either $z$, $x$ or $y$.

*3 Integrals with $Y$ are equivalent to those with $X$.

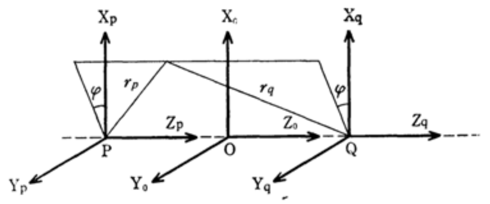


Fig. 2. Local coordinate system.*

* It should be noted that $\mathcal{Z}_p$, $\mathcal{Z}_0$ and $\mathcal{Z}_q$ axes have the same direction.

The actual calculations are performed after the transformation of the local coordinates to the spheroidal coordinate system, $(\xi, \eta, \varphi)$. By the use of the latter, each of the basic integrals is expanded into a formula with $A_m$ and $B_m$ as overlap integrals in Ref. 3. Our choice of coordinates (Fig. 2) will result in the folloinwg equations:

$$r_p = R(\xi+\eta)/2, \quad r_q = R(\xi-\eta)/2,$$
$$\mathcal{Z}_p = R(\xi\eta+1)/2, \quad \mathcal{Z}_q = R(\xi\eta-1)/2, \quad \mathcal{Z}_0 = R\xi\eta/2,$$
$$X_p = X_q = X_0 = R\{(\xi^2-1)(1-\eta^2)\}^{1/2}\cos\varphi/2,$$
$$Y_p = Y_q = Y_0 = R\{(\xi^2-1)(1-\eta^2)\}^{1/2}\sin\varphi/2 \tag{5}$$

where $R$ is the interatomic distance, and:

$$A_m(a) = \int_1^\infty \xi^m e^{-a\xi} d\xi$$
$$B_m(b) = \int_{-1}^1 \eta^m e^{-b\eta} d\eta$$
$$a = R(\mu_p+\mu_q)/2R_H = (a_p+a_q)/2$$
$$b = R(\mu_p-\mu_q)/2R_H = (a_p-a_q)/2$$
$$a = R\mu/R_H \tag{6}$$

where $R_H$ is the Bohr radius and $\mu$ denotes the exponent of STO. The parameter $a$ and $b$ correspond to $p$ and $pt$ respectively in Ref. 3. When both AO's have integer $n^*$, $m$ is also an integer, and these expansion formulas are easily obtained with a computer, given the number of each variable as input data. In this work the program was tested by obtaining the corresponding formulas of overlap integrals, in agreement with those in Ref. 3, except the difference in the direction of $\mathcal{Z}_q$ axis.*4

**One-center Integrals.** One-center moment integrals may be calculated directly in a spherical coordinate system, and only those of the type, $(s|i|p_i)$ or $(p_i|i|s)$ have non-zero values for $s,p$-AO's, where $i$ denotes either of $z, x$ or $y$.

## Results and Discussion

In Table 2, all expansion formulas of basic two-center moment integrals between $s,p$-AO's with integer $n^*$, $1 \leqq n_1^* \leqq n_2^* \leqq 5$, for $b \neq 0$, are presented. Formulas for $b=0$ are derived from the corresponding formulas for $b \neq 0$, by noting that $B_m(0) = 2/(m+1)$ for $m$ even, and $B_m(0)=0$ for $m$ odd. In practice only those for $n_1^* = n_2^*$ are important,

3) R. S. Mulliken, C. A. Rieke, D. Orloff and H. Orloff, *J. Chem. Phys.*, **17**, 1248 (1949).
4) A. Lofthus, *Mol. Phys.*, **5**, 105 (1962).

*4 In Ref. 3, all formulas for $S(n_1 p\sigma, n_2 p\sigma)$, $n_1 = n_2$, should have the opposite sign to those presented there.

TABLE 2. BASIC TWO-CENTER MOMENT INTEGRALS FOR $b \neq 0$

$n_1^* = n_2^* = 1;\ c = (a_1^3 a_2^3)^{1/2} R/8$

$(S\,|Z|\,S):\ A_3B_1 - A_1B_3$

$n_1^* = 1, n_2^* = 2;\ c = (a_1^3 a_2^5)^{1/2} R/16$

$(S\,|Z|\,S):\ (1/3)^{1/2}(A_4B_1 - A_3B_2 - A_2B_3 + A_1B_4)$

$(S\,|Z|\,P_Z):\ A_4B_2 - A_3B_1 - A_2B_4 + A_1B_3$

$(S\,|X|\,P_X):\ (1/2)\{A_4(B_0-B_2) + A_2(B_4-B_0) + A_0(B_2-B_4)\}$

$n_1^* = 1, n_2^* = 3;\ c = (a_1^3 a_2^7/30)^{1/2} R/16$

$(S\,|Z|\,S):\ (1/3)^{1/2}(A_5B_1 - 2A_4B_2 + 2A_2B_4 - A_1B_5)$

$(S\,|Z|\,P_Z):\ A_5B_2 - A_4(B_3+B_1) + A_3(B_2-B_4) + A_2(B_5+B_3) - A_1B_4$

$(S\,|X|\,P_X):\ (1/2)\{A_5(B_0-B_2) + A_4(B_3-B_1) + A_3(B_4-B_0) + A_2(B_1-B_5) + A_1(B_2-B_4) + A_0(B_5-B_3)\}$

$n_1^* = 1, n_2^* = 4;\ c = (a_1^3 a_2^9/105)^{1/2} R/64$

$(S\,|Z|\,S):\ (1/3)^{1/2}(A_6B_1 - 3A_5B_2 + 2A_4B_3 + 2A_3B_4 - 3A_2B_5 + A_1B_6)$

$(S\,|Z|\,P_Z):\ A_6B_2 - A_5(2B_3+B_1) + 2A_4B_2 + 2A_3B_5 - A_2(B_6+2B_4) + A_1B_5$

$(S\,|X|\,P_X):\ (1/2)\{A_6(B_0-B_2) + 2A_5(B_3-B_1) + A_4(B_2-B_0) + 2A_3(B_1-B_5) + A_2(B_6-B_4) + 2A_1(B_5-B_3)$
$+ A_0(B_4-B_6)\}$

$n_1^* = 1, n_2^* = 5;\ c = (a_1^3 a_2^{11}/42)^{1/2} R/960$

$(S\,|Z|\,S):\ (1/3)^{1/2}(A_7B_1 - 4A_6B_2 + 5A_5B_3 - 5A_3B_5 + 4A_2B_6 - A_1B_7)$

$(S\,|Z|\,P_Z):\ A_7B_2 - A_6(3B_3+B_1) + A_5(2B_4+3B_2) + 2A_4(B_5-B_3) - A_3(3B_6+2B_4) + A_2(B_7+3B_5)$
$- A_1B_6$

$(S\,|X|\,P_X):\ (1/2)\{A_7(B_0-B_2) + 3A_6(B_3-B_1) + A_5(3B_2-2B_4-B_0) + A_4(3B_1-B_3-2B_5)$
$+ A_3(3B_6-B_4-2B_2) + A_2(3B_5-B_7-2B_3) + 3A_1(B_4-B_6) + A_0(B_7-B_5)\}$

$n_1^* = n_2^* = 2;\ c = (a_1^5 a_2^5)^{1/2} R/32$

$(S\,|Z|\,S):\ (1/3)(A_5B_1 - 2A_3B_3 + A_1B_5)$

$(S\,|Z|\,P_Z):\ (1/3)^{1/2}\{A_5B_2 + A_4(B_3-B_1) - A_3(B_2+B_4) + A_2(B_3-B_5) + A_1B_4\}$

$(S\,|X|\,P_X):\ (1/12)^{1/2}\{A_5(B_0-B_2) + A_4(B_1-B_3) + A_3(B_4-B_0) + A_2(B_5-B_1) + A_1(B_2-B_4) + A_0(B_3-B_5)\}$

$(P_Z|Z|\,S):\ (1/3)^{1/2}\{A_5B_2 + A_4(B_1-B_3) - A_3(B_2+B_4) + A_2(B_5-B_3) + A_1B_4\}$

$(P_X|X|\,S):\ (1/12)^{1/2}\{A_5(B_0-B_2) + A_4(B_3-B_1) + A_3(B_4-B_0) + A_2(B_1-B_5) + A_1(B_2-B_4) + A_0(B_5-B_3)\}$

$(P_Z|Z|P_Z):\ A_5B_3 - A_3(B_1+B_5) + A_1B_3$

$(P_Z|X|P_X):\ (1/2)\{A_5(B_1-B_3) + A_4(B_0-B_2) + A_3(B_5-B_1) + A_2(B_4-B_0) + A_1(B_3-B_5) + A_0(B_2-B_4)\}$

$(P_X|Z|P_X):\ (1/2)\{A_5(B_1-B_3) + A_3(B_5-B_1) + A_1(B_3-B_5)\}$

$(P_X|X|P_Z):\ (1/2)\{A_5(B_1-B_3) + A_4(B_2-B_0) + A_3(B_5-B_1) + A_2(B_0-B_4) + A_1(B_3-B_5) + A_0(B_4-B_2)\}$

$n_1^* = 2, n_2^* = 3;\ c = (a_1^5 a_2^7/30)^{1/2} R/32$

$(S\,|Z|\,S):\ (1/3)(A_6B_1 - A_5B_2 - 2A_4B_3 + 2A_3B_4 + A_2B_5 - A_1B_6)$

$(S\,|Z|\,P_Z):\ (1/3)^{1/2}(A_6B_2 - A_5B_1 - 2A_4B_4 + 2A_3B_3 + A_2B_6 - A_1B_5)$

$(S\,|X|\,P_X):\ (1/12)^{1/2}\{A_6(B_0-B_2) + A_4(2B_4-B_2-B_0) + A_2(2B_2-B_4-B_6) + A_0(B_6-B_4)\}$

$(P_Z|Z|\,S):\ (1/3)^{1/2}\{A_6B_2 + A_5(B_1-2B_3) - 2A_4B_2 + 2A_3B_5 + A_2(2B_4-B_6) - A_1B_5\}$

$(P_X|X|\,S):\ (1/12)^{1/2}\{A_6(B_0-B_2) + 2A_5(B_3-B_1) + A_4(B_2-B_0) + 2A_3(B_1-B_5) + A_2(B_6-B_4) + 2A_1(B_5-B_3)$
$+ A_0(B_4-B_6)\}$

$(P_Z|Z|P_Z):\ A_6B_3 - A_5B_4 - A_4(B_1+B_5) + A_3(B_2+B_6) + A_2B_3 - A_1B_4$

$(P_Z|X|P_X):\ (1/2)\{A_6(B_1-B_3) + A_5(B_4-2B_2+B_0) + A_4(B_5+B_3-2B_1) + A_3(B_2-B_0-B_6+B_4)$
$+ A_2(B_1+B_3-2B_5) + A_1(B_6-2B_4+B_2) + A_0(B_5-B_3)\}$

$(P_X|Z|P_X):\ (1/2)\{A_6(B_1-B_3) + A_5(B_4-B_2) + A_4(B_5-B_1) + A_3(B_2-B_6) + A_2(B_3-B_5) + A_1(B_6-B_4)\}$

$(P_X|X|P_Z):\ (1/2)\{A_6(B_1-B_3) + A_5(B_4-B_0) + A_4(B_5-B_3) + A_3(B_0+B_2-B_4-B_6) + A_2(B_3-B_1)$
$+ A_1(B_6-B_2) + A_0(B_3-B_5)\}$

$n_1^* = 2, n_2^* = 4;\ c = (a_1^5 a_2^9/105)^{1/2} R/128$

$(S\,|Z|\,S):\ (1/3)(A_7B_1 - 2A_6B_2 - A_5B_3 + 4A_4B_4 - A_3B_5 - 2A_2B_6 + A_1B_7)$

$(S\,|Z|\,P_Z):\ (1/3)^{1/2}\{A_7B_2 - A_6(B_3+B_1) + A_5(B_2-2B_4) + 2A_4(B_5+B_3) + A_3(B_6-2B_4) - A_2(B_7+B_5) + A_1B_6\}$

$(S\,|X|\,P_X):\ (1/12)^{1/2}\{A_7(B_0-B_2) + A_6(B_3-B_1) + A_5(2B_4-B_2-B_0) + A_4(B_1+B_3-2B_5) + A_3(2B_2-B_4-B_6)$
$+ A_2(B_7+B_5-2B_3) + A_1(B_6-B_4) + A_0(B_5-B_7)\}$

$(P_Z|Z|\,S):\ (1/3)^{1/2}\{A_7B_2 + A_6(B_1-3B_3) + A_5(2B_4-3B_2) + 2A_4(B_3+B_5) + A_3(2B_4-3B_6) + A_2(B_7-3B_5)$
$+ A_1B_6\}$

$(P_X|X|\,S):\ (1/12)^{1/2}\{A_7(B_0-B_2) + 3A_6(B_3-B_1) + A_5(3B_2-2B_4-B_0) + A_4(3B_1-B_3-2B_5)$
$+ A_3(3B_6-B_4-2B_2) + A_2(3B_5-B_7-2B_3) + 3A_1(B_4-B_6) + A_0(B_7-B_5)\}$

$(P_Z|\mathcal{Z}|P_Z)$: $A_7B_3 - 2A_6B_4 - A_5B_1 + 2A_4(B_2+B_6) - A_3B_7 - 2A_2B_4 + A_1B_5$

$(P_Z|X|P_X)$: $(1/2)\{A_7(B_1-B_3) + A_6(2B_4-3B_2+B_0) + 3A_5(B_3-B_1) + A_4(3B_2-B_0-2B_6) + A_3(2B_1-3B_5+B_7) + 3A_2(B_6-B_4) + A_1(3B_5-2B_3-B_7) + A_0(B_4-B_6)\}$

$(P_X|\mathcal{Z}|P_X)$: $(1/2)\{A_7(B_1-B_3) + 2A_6(B_4-B_2) + A_5(B_3-B_1) + 2A_4(B_2-B_6) + A_3(B_7-B_5) + 2A_2(B_6-B_4) + A_1(B_5-B_7)\}$

$(P_X|X|P_Z)$: $(1/2)\{A_7(B_1-B_3) + A_6(2B_4-B_2-B_0) + A_5(B_1-B_3) + A_4(B_0+B_2-2B_6) + A_3(B_7+B_5-2B_1) + A_2(B_6-B_4) + A_1(2B_3-B_5-B_7) + A_0(B_6-B_4)\}$

$n_1^* = 2, n_2^* = 5$; $c = (a_1^5a_2^{11}/42)^{1/2}R/1920$

$(S|\mathcal{Z}|S)$: $(1/3)(A_8B_1 - 3A_7B_2 + A_6B_3 + 5A_5B_4 - 5A_4B_5 - A_3B_6 + 3A_2B_7 - A_1B_8)$

$(S|\mathcal{Z}|P_Z)$: $(1/3)^{1/2}\{A_8B_2 - A_7(2B_3+B_1) + A_6(2B_2-B_4) + A_5(B_3+4B_5) - A_4(B_6+4B_4) + A_3(B_5-2B_7) + A_2(B_8+2B_6) - A_1B_7\}$

$(S|X|P_X)$: $(1/12)^{1/2}\{A_8(B_0-B_2) + 2A_7(B_3-B_1) + A_6(B_4-B_0) + A_5(2B_1+2B_3-4B_5) + A_4(B_6-2B_4+B_2) + A_3(2B_7+2B_5-4B_3) + A_2(B_4-B_8) + 2A_1(B_5-B_7) + A_0(B_8-B_6)\}$

$(P_Z|\mathcal{Z}|S)$: $(1/3)^{1/2}\{A_8B_2 + A_7(B_1-4B_3) + A_6(5B_4-4B_2) + 5A_5B_3 - 5A_4B_6 + A_3(4B_7-5B_5) + A_2(4B_6-B_8) - A_1B_7\}$

$(P_X|X|S)$: $(1/12)^{1/2}\{A_8(B_0-B_2) + 4A_7(B_3-B_1) + A_6(6B_2-5B_4-B_0) + 4A_5(B_1-B_3) + 5A_4(B_6-B_2) + 4A_3(B_5-B_7) + A_2(B_8-6B_6+5B_4) + 4A_1(B_7-B_5) + A_0(B_6-B_8)\}$

$(P_Z|\mathcal{Z}|P_Z)$: $A_8B_3 - 3A_7B_4 + A_6(2B_5-B_1) + A_5(3B_2+2B_6) - A_4(2B_3+3B_7) + A_3(B_8-2B_4) + 3A_2B_5 - A_1B_6$

$(P_Z|X|P_X)$: $(1/2)\{A_8(B_1-B_3) + A_7(B_0-4B_2+3B_4) + A_6(6B_3-4B_1-2B_5) + A_5(6B_2-B_0-3B_4-2B_6) + 3A_4(B_1-B_3-B_5+B_7) + A_3(6B_6-2B_2-3B_4-B_8) + A_2(6B_5-4B_7-2B_3) + A_1(B_8-4B_6+3B_4) + A_0(B_7-B_5)\}$

$(P_X|\mathcal{Z}|P_X)$: $(1/2)\{A_8(B_1-B_3) + 3A_7(B_4-B_2) + A_6(3B_3-2B_5-B_1) + A_5(3B_2-B_4-2B_6) + A_4(3B_7-B_5-2B_3) + A_3(3B_6-B_8-2B_4) + 3A_2(B_5-B_7) + A_1(B_8-B_6)\}$

$(P_X|X|P_Z)$: $(1/2)\{A_8(B_1-B_3) + A_7(3B_4-2B_2-B_0) + 2A_6(B_1-B_5) + A_5(B_0+B_4-2B_6) + A_4(3B_7+B_5-B_3-3B_1) + A_3(2B_2-B_4-B_8) + 2A_2(B_3-B_7) + A_1(B_8+2B_6-3B_4) + A_0(B_5-B_7)\}$

$n_1^* = n_2^* = 3$; $c = (a_1^7a_2^7)^{1/2}R/960$

$(S|\mathcal{Z}|S)$: $(1/3)(A_7B_1 - 3A_5B_3 + 3A_3B_5 - A_1B_7)$

$(S|\mathcal{Z}|P_Z)$: $(1/3)^{1/2}\{A_7B_2 + A_6(B_3-B_1) - A_5(B_2+2B_4) + 2A_4(B_3-B_5) + A_3(B_6+2B_4) + A_2(B_7-B_5) - A_1B_6\}$

$(S|X|P_X)$: $(1/12)^{1/2}\{A_7(B_0-B_2) + A_6(B_1-B_3) + A_5(2B_4-B_2-B_0) + A_4(2B_5-B_3-B_1) + A_3(2B_2-B_4-B_6) + A_2(2B_3-B_5-B_7) + A_1(B_6-B_4) + A_0(B_7-B_5)\}$

$(P_Z|\mathcal{Z}|S)$: $(1/3)^{1/2}\{A_7B_2 + A_6(B_1-B_3) - A_5(2B_4+B_2) + 2A_4(B_5-B_3) + A_3(2B_4+B_6) + A_2(B_5-B_7) - A_1B_6\}$

$(P_X|X|S)$: $(1/12)^{1/2}\{A_7(B_0-B_2) + A_6(B_3-B_1) + A_5(2B_4-B_2-B_0) + A_4(B_1+B_3-2B_5) + A_3(2B_2-B_4-B_6) + A_2(B_7+B_5-2B_3) + A_1(B_6-B_4) + A_0(B_5-B_7)\}$

$(P_Z|\mathcal{Z}|P_Z)$: $A_7B_3 - A_5(2B_5+B_1) + A_3(2B_3+B_7) - A_1B_5$

$(P_Z|X|P_X)$: $(1/2)\{A_7(B_1-B_3) + A_6(B_0-B_2) + A_5(2B_5-B_3-B_1) + A_4(2B_4-B_2-B_0) + A_3(2B_3-B_5-B_7) + A_2(2B_2-B_4-B_6) + A_1(B_7-B_5) + A_0(B_6-B_4)\}$

$(P_X|\mathcal{Z}|P_X)$: $(1/2)\{A_7(B_1-B_3) + A_5(2B_5-B_3-B_1) + A_3(2B_3-B_5-B_7) + A_1(B_7-B_5)\}$

$(P_X|X|P_Z)$: $(1/2)\{A_7(B_1-B_3) + A_6(B_2-B_0) + A_5(2B_5-B_3-B_1) + A_4(B_0+B_2-2B_4) + A_3(2B_3-B_5-B_7) + A_2(B_6+B_4-2B_2) + A_1(B_7-B_5) + A_0(B_4-B_6)\}$

$n_1^* = 3, n_2^* = 4$; $c = (a_1^7a_2^9/14)^{1/2}R/1920$

$(S|\mathcal{Z}|S)$: $(1/3)(A_8B_1 - A_7B_2 - 3A_6B_3 + 3A_5B_4 + 3A_4B_5 - 3A_3B_6 - A_2B_7 + A_1B_8)$

$(S|\mathcal{Z}|P_Z)$: $(1/3)^{1/2}(A_8B_2 - A_7B_1 - 3A_6B_4 + 3A_5B_3 + 3A_4B_6 - 3A_3B_5 - A_2B_8 + A_1B_7)$

$(S|X|P_X)$: $(1/12)^{1/2}\{A_8(B_0-B_2) + A_6(3B_4-2B_2-B_0) + 3A_4(B_2-B_6) + A_2(B_8+2B_6-3B_4) + A_0(B_6-B_8)\}$

$(P_Z|\mathcal{Z}|S)$: $(1/3)^{1/2}\{A_8B_2 + A_7(B_1-2B_3) - A_6(B_4+2B_2) + A_5(4B_5-B_3) + A_4(4B_4-B_6) - A_3(B_5+2B_7) + A_2(B_8-2B_6) + A_1B_7\}$

$(P_X|X|S)$: $(1/12)^{1/2}\{A_8(B_0-B_2) + 2A_7(B_3-B_1) + A_6(B_4-B_0) + A_5(2B_1+2B_3-4B_5) + A_4(B_6-2B_4+B_2) + A_3(2B_7+2B_5-4B_3) + A_2(B_4-B_8) + 2A_1(B_5-B_7) + A_0(B_8-B_6)\}$

$(P_Z|\mathcal{Z}|P_Z)$: $A_8B_3 - A_7B_4 - A_6(2B_5+B_1) + A_5(2B_6+B_2) + A_4(2B_3+B_7) - A_3(2B_4+B_8) - A_2B_5 + A_1B_6$

$(P_Z|X|P_X)$: $(1/2)\{A_8(B_1-B_3) + A_7(B_0-2B_2+B_4) + 2A_6(B_5-B_1) + A_5(3B_4-2B_6-B_0) + A_4(B_1+3B_3-3B_5-B_7) + A_3(2B_2-3B_4+B_8) + 2A_2(B_7-B_3) + A_1(2B_6-B_8-B_4) + A_0(B_5-B_7)\}$

$(P_X|\mathcal{Z}|P_X)$: $(1/2)\{A_8(B_1-B_3) + A_7(B_4-B_2) + A_6(2B_5-B_3-B_1) + A_5(B_2+B_4-2B_6) + A_4(2B_3-B_5-B_7) + A_3(B_8+B_6-2B_4) + A_2(B_7-B_5) + A_1(B_6-B_8)\}$

$(P_X|X|P_Z)$: $(1/2)\{A_8(B_1-B_3) + A_7(B_4-B_0) + 2A_6(B_5-B_3) + A_5(B_0+2B_2-B_4-2B_6) + A_4(B_3+B_5-B_1-B_7) + A_3(B_8+2B_6-B_4-2B_2) + 2A_2(B_3-B_5) + A_1(B_4-B_8) + A_0(B_7-B_5)\}$

$n_1^* = 3, n_2^* = 5$; $c = (a_1^7a_2^{11}/35)^{1/2}R/11520$

$(S|\mathcal{Z}|S)$: $(1/3)(A_9B_1 - 2A_8B_2 - 2A_7B_3 + 6A_6B_4 - 6A_4B_6 + 2A_3B_7 + 2A_2B_8 - A_1B_9)$

$(S\,|Z|\,P_Z)$: $(1/3)^{1/2}\{A_9B_2 - A_8(B_3+B_1) + A_7(B_2-3B_4) + 3A_6(B_5+B_3) + 3A_5(B_6-B_4) - 3A_4(B_7+B_5)$
$+ A_3(3B_6-B_8) + A_2(B_9+B_7) - A_1B_8\}$

$(S\,|X|\,P_X)$: $(1/12)^{1/2}\{A_9(B_0-B_2) + A_8(B_3-B_1) + A_7(3B_4-2B_2-B_0) + A_6(B_1+2B_3-3B_5)$
$+ 3A_5(B_2-B_6) + 3A_4(B_7-B_3) + A_3(B_8+2B_6-3B_4) + A_2(3B_5-2B_7-B_9) + A_1(B_6-B_8)$
$+ A_0(B_9-B_7)\}$

$(P_Z|Z|\,S\,)$: $(1/3)^{1/2}\{A_9B_2 + A_8(B_1-3B_3) + A_7(B_4-3B_2) + A_6(5B_5+B_3) + 5A_5(B_4-B_6) - A_4(B_7+5B_5)$
$+ A_3(3B_8-B_6) + A_2(3B_7-B_9) - A_1B_8\}$

$(P_X|X|\,S\,)$: $(1/12)^{1/2}\{A_9(B_0-B_2) + 3A_8(B_3-B_1) + A_7(2B_2-B_4-B_0) + A_6(3B_1+2B_3-5B_5)$
$+ A_5(5B_6-4B_4-B_2) + A_4(B_7+4B_5-5B_3) + A_3(5B_4-2B_6-3B_8) + A_2(B_5-2B_7+B_9)$
$+ 3A_1(B_8-B_6) + A_0(B_7-B_9)\}$

$(P_Z|Z|P_Z)$: $A_9B_3 - 2A_8B_4 - A_7(B_5+B_1) + A_6(4B_6+2B_2) + A_5(B_3-B_7) - A_4(4B_4+2B_8) + A_3(B_5+B_9)$
$+ 2A_2B_6 - A_1B_7$

$(P_Z|X|P_X)$: $(1/2)\{A_9(B_1-B_3) + A_8(B_0-3B_2+2B_4) + A_7(B_5+2B_3-3B_1) + A_6(2B_2-4B_6+3B_4-B_0)$
$+ A_5(B_7-6B_5+3B_3+2B_1) + A_4(B_2-6B_4+3B_6+2B_8) + A_3(3B_5-4B_3-B_9+2B_7)$
$+ A_2(B_4+2B_6-3B_8) + A_1(B_9-3B_7+2B_5) + A_0(B_8-B_6)\}$

$(P_X|Z|P_X)$: $(1/2)\{A_9(B_1-B_3) + 2A_8(B_4-B_2) + A_7(B_5-B_1) + A_6(2B_2+2B_4-4B_6) + A_5(B_7-2B_5+B_3)$
$+ A_4(2B_8+2B_6-4B_4) + A_3(B_5-B_9) + 2A_2(B_6-B_8) + A_1(B_9-B_7)\}$

$(P_X|X|P_Z)$: $(1/2)\{A_9(B_1-B_3) + A_8(2B_4-B_2-B_0) + A_7(B_1-2B_3+B_5) + A_6(B_0+2B_2+B_4-4B_6)$
$+ A_5(B_7+2B_5-B_3-2B_1) + A_4(2B_8+B_6-2B_4-B_2) + A_3(4B_3-B_5-2B_7-B_9)$
$+ A_2(2B_6-B_4-B_8) + A_1(B_9+B_7-2B_5) + A_0(B_6-B_8)\}$

$n_1^* = n_2^* = 4;\ c = (a_1^9a_2^9)^{1/2}\,R/53760$

$(S\,|Z|\,S\,)$: $(1/3)(A_9B_1 - 4A_7B_3 + 6A_5B_5 - 4A_3B_7 + A_1B_9)$

$(S\,|Z|\,P_Z)$: $(1/3)^{1/2}\{A_9B_2 + A_8(B_3-B_1) - A_7(3B_4+B_2) + 3A_6(B_3-B_5) + 3A_5(B_4+B_6) + 3A_4(B_7-B_5)$
$- A_3(3B_6+B_8) + A_2(B_7-B_9) + A_1B_8\}$

$(S\,|X|\,P_X)$: $(1/12)^{1/2}\{A_9(B_0-B_2) + A_8(B_1-B_3) + A_7(3B_4-2B_2-B_0) + A_6(3B_5-2B_3-B_1) + 3A_5(B_2-B_6)$
$+ 3A_4(B_3-B_7) + A_3(B_8+2B_6-3B_4) + A_2(B_9+2B_7-3B_5) + A_1(B_6-B_8) + A_0(B_7-B_9)\}$

$(P_Z|Z|\,S\,)$: $(1/3)^{1/2}\{A_9B_2 + A_8(B_1-B_3) - A_7(3B_4+B_2) + 3A_6(B_5-B_3) + 3A_5(B_4+B_6) + 3A_4(B_5-B_7)$
$- A_3(B_8+3B_6) + A_2(B_9-B_7) + A_1B_8\}$

$(P_X|X|\,S\,)$: $(1/12)^{1/2}\{A_9(B_0-B_2) + A_8(B_3-B_1) + A_7(3B_4-2B_2-B_0) + A_6(B_1+2B_3-3B_5) + 3A_5(B_2-B_6)$
$+ 3A_4(B_7-B_3) + A_3(B_8+2B_6-3B_4) + A_2(3B_5-2B_7-B_9) + A_1(B_6-B_8) + A_0(B_9-B_7)\}$

$(P_Z|Z|P_Z)$: $A_9B_3 - A_7(3B_5+B_1) + 3A_5(B_3+B_7) - A_3(B_9+3B_5) + A_1B_7$

$(P_Z|X|P_X)$: $(1/2)\{A_9(B_1-B_3) + A_8(B_0-B_2) + A_7(3B_5-2B_3-B_1) + A_6(3B_4-2B_2-B_0) + 3A_5(B_3-B_7)$
$+ 3A_4(B_2-B_6) + A_3(B_9+2B_7-3B_5) + A_2(B_8+2B_6-3B_4) + A_1(B_7-B_9) + A_0(B_6-B_8)\}$

$(P_X|Z|P_X)$: $(1/2)\{A_9(B_1-B_3) + A_7(3B_5-2B_3-B_1) + 3A_5(B_3-B_7) + A_3(B_9+2B_7-3B_5) + A_1(B_7-B_9)\}$

$(P_X|X|P_Z)$: $(1/2)\{A_9(B_1-B_3) + A_8(B_2-B_0) + A_7(3B_5-2B_3-B_1) + A_6(B_0+2B_2-3B_4) + 3A_5(B_3-B_7)$
$+ 3A_4(B_6-B_2) + A_3(B_9+2B_7-3B_5) + A_2(3B_4-2B_6-B_8) + A_1(B_7-B_9) + A_0(B_8-B_6)$

$n_1^* = 4,\ n_2^* = 5;\ c = (a_1^9a_2^{11}/10)^{1/2}\,R/161280$

$(S\,|Z|\,S\,)$: $(1/3)(A_{10}B_1 - A_9B_2 - 4A_8B_3 + 4A_7B_4 + 6A_6B_5 - 6A_5B_6 - 4A_4B_7 + 4A_3B_8 + A_2B_9 - A_1B_{10})\}$

$(S\,|Z|\,P_Z)$: $(1/3)^{1/2}(A_{10}B_2 - A_9B_1 - 4A_8B_4 + 4A_7B_3 + 6A_6B_6 - 6A_5B_5 - 4A_4B_8 + 4A_3B_7 + A_2B_{10} - A_1B_9)$

$(S\,|X|\,P_X)$: $(1/12)^{1/2}\{A_{10}(B_0-B_2) + A_8(4B_4-3B_2-B_0) + A_6(4B_2+2B_4-6B_6) + A_4(4B_8+2B_6-6B_4)$
$+ A_2(4B_6-3B_8-B_{10}) + A_0(B_{10}-B_8)\}$

$(P_Z|Z|\,S\,)$: $(1/3)\{^{1/2}A_{10}B_2 + A_9(B_1-2B_3) - 2A_8(B_4+B_2) + A_7(6B_5-2B_3) + 6A_6B_4 - 6A_5B_7 + A_4(2B_8-6B_6)$
$+ 2A_3(B_9+B_7) + A_2(2B_8-B_{10}) - A_1B_9\}$

$(P_X|X|\,S\,)$: $(1/12)^{1/2}\{A_{10}(B_0-B_2) + 2A_9(B_3-B_1) + A_8(2B_4-B_2-B_0) + A_7(2B_1+4B_3-6B_5) + 2A_6(B_2-B_4)$
$+ 6A_5(B_7-B_3) + 2A_4(B_6-B_8) + A_3(6B_5-4B_7-2B_9) + A_2(B_{10}+B_8-2B_6) + 2A_1(B_9-B_7)$
$+ A_0(B_8-B_{10})\}$

$(P_Z|Z|P_Z)$: $A_{10}B_3 - A_9B_4 - A_8(3B_5+B_1) + A_7(3B_6+B_2) + 3A_6(B_3+B_7) - 3A_5(B_4+B_8) - A_4(B_9+3B_5)$
$+ A_3(B_{10}+3B_6) + A_2B_7 - A_1B_8$

$(P_Z|X|P_X)$: $(1/2)\{A_{10}(B_1-B_3) + A_9(B_0-2B_2+B_4) + A_8(3B_5-B_3-2B_1) + A_7(5B_4-B_2-3B_6-B_0)$
$+ A_6(B_1+5B_3-3B_5-3B_7) + 3A_5(B_2-B_4-B_6+B_8) + A_4(B_9+5B_7-3B_5-3B_3)$
$+ A_3(5B_6-3B_4-B_8-B_{10}) + A_2(3B_5-B_7-2B_9) + A_1(B_{10}-2B_8+B_6) + A_0(B_9-B_7)\}$

$(P_X|Z|P_X)$: $(1/2)\{A_{10}(B_1-B_3) + A_9(B_4-B_2) + A_8(3B_5-2B_3-B_1) + A_7(B_2+2B_4-3B_6) + 3A_6(B_3-B_7)$
$+ 3A_5(B_8-B_4) + A_4(B_9+2B_7-3B_5) + A_3(3B_6-2B_8-B_{10}) + A_2(B_7-B_9) + A_1(B_{10}-B_8)\}$

$(P_X|X|P_Z)$: $(1/2)\{A_{10}(B_1-B_3) + A_9(B_4-B_0) + 3A_8(B_5-B_3) + A_7(B_0+3B_2-B_4-3B_6)$
$+ A_6(B_3+3B_5-3B_7-B_1) + 3A_5(B_8+B_6-B_4-B_2) + A_4(B_9-B_7-3B_5+3B_3)$
$+ A_3(3B_4+B_6-3B_8-B_{10}) + 3A_2(B_7-B_5) + A_1(B_{10}-B_6) + A_0(B_7-B_9)\}$

$n_1^* = n_2^* = 5;\ c = (a_1^{11}a_2^{11})^{1/2}\,R/4838400$

$(S\,|Z|\,S\,)$: $(1/3)(A_{11}B_1 - 5A_9B_3 + 10A_7B_5 - 10A_5B_7 + 5A_3B_9 - A_1B_{11})$

$(S\,|Z|\,P_Z)$: $(1/3)^{1/2}\{A_{11}B_2 + A_{10}(B_3-B_1) - A_9(4B_4+B_2) + 4A_8(B_3-B_5) + A_7(4B_4+6B_6) + 6A_6(B_7-B_5) - A_5(4B_8+6B_6) + 4A_4(B_7-B_9) + A_3(4B_8+B_{10}) + A_2(B_{11}-B_9) - A_1B_{10}\}$

$(S\,|X|\,P_X)$: $(1/12)^{1/2}\{A_{11}(B_0-B_2) + A_{10}(B_1-B_3) + A_9(4B_4-3B_2-B_0) + A_8(4B_5-3B_3-B_1) + A_7(4B_2+2B_4-6B_6) + A_6(4B_3+2B_5-6B_7) + A_5(4B_8+2B_6-6B_4) + A_4(4B_9+2B_7-6B_5) + A_3(4B_6-3B_8-B_{10}) + A_2(4B_7-3B_9-B_{11}) + A_1(B_{10}-B_8) + A_0(B_{11}-B_9)\}$

$(P_Z|Z|\,S\,)$: $(1/3)^{1/2}\{A_{11}B_2+A_{10}(B_1-B_3) - A_9(4B_4+B_2) + 4A_8(B_5-B_3) + A_7(6B_6+4B_4) + 6A_6(B_5-B_7) - A_5(6B_6+4B_8) + 4A_4(B_9-B_7) + A_3(B_{10}+4B_8) + A_2(B_9-B_{11}) - A_1B_{10}\}$

$(P_X|X|\,S\,)$: $(1/12)^{1/2}\{A_{11}(B_0-B_2) + A_{10}(B_3-B_1) + A_9(4B_4-3B_2-B_0) + A_8(B_1+3B_3-4B_5) + A_7(4B_2+2B_4-6B_6) + A_6(6B_7-2B_5-4B_3) + A_5(4B_8+2B_6-6B_4) + A_4(6B_5-2B_7-4B_9) + A_3(4B_6-3B_8-B_{10}) + A_2(B_{11}+3B_9-4B_7) + A_1(B_{10}-B_8) + A_0(B_9-B_{11})\}$

$(P_Z|Z|\,P_Z)$: $A_{11}B_3 - A_9(4B_5+B_1) + A_7(6B_7+4B_3) - A_5(6B_5+4B_9) + A_3(B_{11}+4B_7) - A_1B_9$

$(P_Z|X|\,P_X)$: $(1/2)\{A_{11}(B_1-B_3) + A_{10}(B_0-B_2) + A_9(4B_5-3B_3-B_1) + A_8(4B_4-3B_2-B_0) + A_7(4B_3+2B_5-6B_7) + A_6(4B_2+2B_4-6B_6) + A_5(4B_9+2B_7-6B_5) + A_4(4B_8+2B_6-6B_4) + A_3(4B_7-3B_9-B_{11}) + A_2(4B_6-3B_8-B_{10}) + A_1(B_{11}-B_9) + A_0(B_{10}-B_8)\}$

$(P_X|Z|\,P_X)$: $(1/2)\{A_{11}(B_1-B_3) + A_9(4B_5-3B_3-B_1) + A_7(4B_3+2B_5-6B_7) + A_5(4B_9+2B_7-6B_5) + A_3(4B_7-3B_9-B_{11}) + A_1(B_{11}-B_9)\}$

$(P_X|X|\,P_Z)$: $(1/2)\{A_{11}(B_1-B_3) + A_{10}(B_2-B_0) + A_9(4B_5-3B_3-B_1) + A_8(B_0+3B_2-4B_4) + A_7(4B_3+2B_5-6B_7) + A_6(6B_6-2B_4-4B_2) + A_5(4B_9+2B_7-6B_5) + A_4(6B_4-2B_6-4B_8) + A_3(4B_7-3B_9-B_{11}) + A_2(B_{10}+3B_8-4B_6) + A_1(B_{11}-B_9)+A_0(B_8-B_{10})\}$

TABLE 3. BASIC TWO-CENTER MOMENT INTEGRALS FOR $b=0$, AND $n_1^*=n_2^*$

$n_1^*=n_2^*=2$; $c=a^5\,R/240$

- $(S\,|Z|\,P_Z)$: $(1/3)^{1/2}(5A_5-8A_3+3A_1)$
- $(S\,|X|\,P_X)$: $(1/3)^{1/2}(5A_5-6A_3+A_1)$
- $(P_Z|X|\,P_X)$: $5A_4-6A_2+A_0$

$n_1^*=n_2^*=3$; $c=a^7\,R/50400$

- $(S\,|Z|\,P_Z)$: $(1/3)^{1/2}(35A_7-77A_5+57A_3-15A_1)$
- $(S\,|X|\,P_X)$: $(1/3)^{1/2}(35A_7-49A_5+17A_3-3A_1)$
- $(P_Z|X|\,P_X)$: $35A_6-49A_4+17A_2-3A_0$

$n_1^*=n_2^*=4$; $c=a^9\,R/8467200$

- $(S\,|Z|\,P_Z)$: $(1/3)^{1/2}(105A_9-294A_7+324A_5-170A_3+35A_1)$
- $(S\,|X|\,P_X)$: $(1/3)^{1/2}(105A_9-168A_7+90A_5-32A_3+5A_1)$
- $(P_Z|X|\,P_X)$: $105A_8-168A_6+90A_4-32A_2+5A_0$

$n_1^*=n_2^*=5$; $c=a^{11}\,R/8382528000$

- $(S\,|Z|\,P_Z)$: $(1/3)^{1/2}(1155A_{11}-3927A_9+5742A_7-4510A_5+1855A_3-315A_1)$
- $(S\,|X|\,P_X)$: $(1/3)^{1/2}(1155A_{11}-2079A_9+1518A_7-814A_5+255A_3-35A_1)$
- $(P_Z|X|\,P_X)$: $1155A_{10}-2079A_8+1518A_6-814A_4+255A_2-35A_0$

TABLE 4. ONE-CENTER MOMENT INTEGRALS

| $n_1^*$ | $n_2^*$ | $M(s\,\|\,i\,\|\,p_i) = M(p_i\,\|\,i\,\|\,s)$ |
|---|---|---|
| 1 | 2 | $32(h_1^3\,h_2^5)^{1/2}/(h_1+h_2)^5$ |
| 1 | 3 | $320(h_1^3\,h_2^7/30)^{1/2}/(h_1+h_2)^6$ |
| 1 | 4 | $960(h_1^3\,h_2^9/105)^{1/2}/(h_1+h_2)^7$ |
| 1 | 5 | $896(h_1^3\,h_2^{11}/42)^{1/2}/(h_1+h_2)^8$ |
| 2 | 2 | $160(h_1^5\,h_2^5/3)^{1/2}/(h_1+h_2)^6$ |
| 2 | 3 | $640(h_1^5\,h_2^7/10)^{1/2}/(h_1+h_2)^7$ |
| 2 | 4 | $2240(h_1^5\,h_2^9/35)^{1/2}/(h_1+h_2)^8$ |
| 2 | 5 | $7168(h_1^5\,h_2^{11}/126)^{1/2}/(h_1+h_2)^9$ |
| 3 | 3 | $896(h_1^7\,h_2^7/3)^{1/2}/(h_1+h_2)^8$ |
| 3 | 4 | $7168(h_1^7\,h_2^9/42)^{1/2}/(h_1+h_2)^9$ |
| 3 | 5 | $21504(h_1^7\,h_2^{11}/105)^{1/2}/(h_1+h_2)^{10}$ |
| 4 | 4 | $4608(h_1^9\,h_2^9/3)^{1/2}/(h_1+h_2)^{10}$ |
| 4 | 5 | $30720(h_1^9\,h_2^{11}/30)^{1/2}/(h_1+h_2)^{11}$ |
| 5 | 5 | $22528(h_1^{11}\,h_2^{11}/3)^{1/2}/(h_1+h_2)^{12}$ |

which are presented in Table 3. In Tables 2 and 3, each formula is to be multiplied by a parameter $c$ which is common to formulas for a same pair of $n_1^*$ and $n_2^*$. In Table 4, one-center moment integrals are also collected, where $h=\mu/R_H$.

**For $n_1^*>n_2^*$.** According to our choice of coordinates (Fig. 2), the following two rules are derived as for basic two-center integrals.

i) Those which contain none or even number of $Z$ (type 1) do not change the sign through the exchange of two AO's with each other, and the other (type 2) change the sign.

ii) $B_m(b)=B_m(-b)$ for $m$ even, and $=-B_m(-b)$ for $m$ odd.

From the above two rules, the formulas for $n_1^*>n_2^*$ are derived in the following way. When $b\neq0$, the sign of a term with $B_m$ is changed if $m$ is odd for type 1, and even for type 2, in the formula with two exchanged AO's. When $b=0$, signs of all terms are changed for type 2, and none for type 1.
For example:

type 2: $(2S|Z|1S) = (a_1^5\,a_2^3/3)^{1/2}(R/16)(A_4B_1+A_3B_2-A_2B_3-A_1B_4)$

type 1: $(2P_z|Z|1S) = (a_1^5\,a_2^3)^{1/2}(R/16)(A_4B_2+A_3B_1-A_2B_4-A_1B_3)$

**Other Values of $n^*$.** Basic two-center integrals for larger values of $n^*$ are derived from formulas of the same type for $n^*-1$ with the rule presented by Lofthus for overlap integrals.[4] Integrals for non-integer $n^*$ may be evaluated by interpolation from the values for appropriate integer $n^*$'s, when not so high accuracy is needed.

**Programming.** Basic moment integrals may be calculated together with corresponding overlap integrals, since values of all parameters are common in both cases. A FORTRAN subprogram including all formulas of one- and two-center moment integrals for $s,p$-AO's with $n^*$ of 1 to 4 (for $b=0$, only those for $n_1^*=n_2^*$ are included), and an interpolation technique with a parabola, written for a HITAC 5020 computer at the computation center of the University of Tokyo, occupies about 7.7$K$ of the core memory, 65$K$, while a subprogram for overlap integrals in the same region of $n^*$ occupies about 5$K$.