Tables Useful for the Calculation of the Molecular Integrals XIII.

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The integrals of the type $\int \alpha_a^*(1) f(\mathbf{r}) \beta_b(1) dv$, where $f(\mathbf{r}) = x \pm iy, z, x^2+y^2$ and z^2 were calculated by using IBM 650. A part of the results was already published as Table XL and Table XLI in Part XII[1] of this series. Some of the remaining results will be given in this paper. These integrals can be expressed in terms of the parameters $A = \alpha_n = \delta_n R$ and $B = \alpha_n' = \delta_n' R$, where δ_n and δ_n' are the orbital exponents for the two atoms and R is the internuclear distance. The numerical tables are as follows.

Table XLII. $X+IY,\ 2- = 1/R \cdot \int (2s)_a (x+iy)(\pi^-)_b dv,$

$X+IY,\ 3- = 1/R \cdot \int (2p\sigma)_a (x+iy)(\pi^-)_b dv,$

$Z,\ 23 = 1/R \cdot \int (2s)_a z (2p\sigma)_b dv,$

$XX+YY,\ 22 = 1/R^2 \cdot \int (2s)_a (x^2+y^2)(2s)_b dv,$

$XX+YY,\ 23 = 1/R^2 \cdot \int (2s)_a (x^2+y^2)(2p\sigma)_b dv,$

$XX+YY,\ 33 = 1/R^2 \cdot \int (2p\sigma)_a (x^2+y^2)(2p\sigma)_b dv,$

for $A = 1.00$ (0.25) 10.00 and $B = 1.00$ (0.25) 10.00.

Table XLIII. $XX+YY,\ 44 = 1/R^2 \cdot \int (2p\pi)_a (x^2+y^2)(2p\pi)_b dv,$

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1) Natural Science Report, Ochanomizu University, 10, 31 (1962).

$$ZZ,\ 22 \qquad =1/R^2\cdot\int(2s)_a z^2(2s)_b dv\,,$$

$$ZZ,\ 23 \qquad =1/R^2\cdot\int(2s)_a z^2(2p\sigma)_b dv\,,$$

$$ZZ,\ 33 \qquad =1/R^2\cdot\int(2p\sigma)_a z^2(2p\sigma)_b dv\,,$$

$$ZZ,\ 44 \qquad =1/R^2\cdot\int(2p\pi)_a z^2(2p\pi)_b dv\,,$$

for $A=1.00$ (0.25) 10.00 and $B=1.00$ (0.25) 10.00.

In giving the numerical values, the floating digit is taken as explained in Part XII. The integrations are performed by using the following formulae.

$$6)\quad X+IY,\ 2-=\frac{\sqrt{\alpha_2{}^5\alpha'_2{}^5}}{32\sqrt{6}}\{A_5(B_0-B_2)+A_4(B_1-B_3)+A_3(B_4-B_0)$$
$$+A_2(B_5-B_1)+A_1(B_2-B_4)+A_0(B_3-B_5)\}\,,$$

$$7)\quad X+IY,\ 3-=\frac{\sqrt{\alpha_2{}^5\alpha'_2{}^5}}{32\sqrt{2}}\{A_5(B_1-B_3)+A_4(B_0-B_2)+A_3(B_5-B_1)$$
$$+A_2(B_4-B_0)+A_1(B_3-B_5)+A_0(B_2-B_4)\}\,,$$

$$8)\quad Z,\ 23=\frac{\sqrt{\alpha_2{}^5\alpha'_2{}^5}}{32\sqrt{3}}\{A_5B_2+A_4(B_3-B_1)-A_3(B_2+B_4)+A_2(B_3-B_5)+A_1B_4\}\,,$$

$$9)\quad XX+YY,\ 22=\frac{\sqrt{\alpha_2{}^5\alpha'_2{}^5}}{192}\{A_6(B_0-B_2)-A_4(B_0+B_2-2B_4)+A_2(2B_2-B_4$$
$$-B_6)-A_0(B_4-B_6)\}\,,$$

$$10)\quad XX+YY,\ 23=\frac{\sqrt{\alpha_2{}^5\alpha'_2{}^5}}{64\sqrt{3}}\{A_6(B_1-B_3)+A_5(-B_0+2B_2-B_4)+A_4(-2B_1$$
$$+B_3+B_5)+A_3(B_0-B_2-B_4+B_6)+A_2(B_1+B_3-2B_5)+A_1(-B_2+2B_4-B_6)$$
$$-A_0(B_3-B_5)\}\,,$$

$$11)\quad XX+YY,\ 33=\frac{\sqrt{\alpha_2{}^5\alpha'_2{}^5}}{64}\{(A_6-A_0)(B_2-B_4)+(A_4-A_2)(B_6-B_0)\}\,,$$

$$12)\quad XX+YY,\ 44=\frac{\sqrt{\alpha_2{}^5\alpha'_2{}^5}}{128}\{A_6(B_4-2B_2+B_0)-A_4(B_6-3B_2+2B_0)$$
$$+A_2(2B_6-3B_4+B_0)-A_0(B_6-2B_4+B_2)\}\,,$$

$$13)\quad ZZ,\ 22=\frac{\sqrt{\alpha_2{}^5\alpha'_2{}^5}}{192}(A_6B_2-2A_4B_4+A_2B_6)\,,$$

$$14)\quad ZZ,\ 23=\frac{\sqrt{\alpha_2{}^5\alpha'_2{}^5}}{64\sqrt{3}}\{A_6B_3+A_5(B_4-B_2)-A_4(B_5+B_3)+A_3(B_4-B_6)$$

$+A_2B_5\}$,

15) $ZZ,\ 33=\dfrac{\sqrt{\alpha_2{}^5\alpha'_2{}^5}}{64}\{-A_6B_4+A_4(B_6+B_2)-A_2B_4\}$,

16) $ZZ,\ 44=\dfrac{\sqrt{\alpha_2{}^5\alpha'_2{}^5}}{64}\{A_6(B_2-B_4)+A_4(B_6-B_2)+A_2(B_4-B_6)\}$,

where $\alpha_2=\delta_2R$, $\alpha'_2=\delta'_2R$, $A_n=A_n\left(\dfrac{\alpha_2+\alpha'_2}{2}\right)$ and $B_n=B_n\left(\dfrac{\alpha_2-\alpha'_2}{2}\right)$. A_n and B_n are the auxiliary functions explained in Part XII.

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