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Tables Useful for the Calculation of the Molecular Integrals XIV

Eiichi Ishiguro (石 黒 英 一)

Department of Physics, Faculty of Science,
Ochanomizu University, Tokyo

Michiko Sakamoto* (坂 本 三 知 子)

Department of Physics, University of Oklahoma,
Norman, Oklahoma

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The Integrals of 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, XLI, XLII and XLIII in Part XII[1] and XIII[2] 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 A and B respectively and R is the internuclear distance. The numerical tables are as follows.

Table XLIV.

$$XX+YY,\ 12=1/R^2\cdot\int(1s)_a(x^2+y^2)(2s)_b dv\,,$$

$$XX+YY,\ 13=1/R^2\cdot\int(1s)_a(x^2+y^2)(2p\sigma)_b dv\,,$$

$$ZZ,\ 12\qquad =1/R^2\cdot\int(1s)_a z^2(2s)_b dv\,,$$

$$ZZ,\ 13\qquad =1/R^2\cdot\int(1s)_a z^2(2p\sigma)_b dv\,,$$

for $A=10.00\ (0.25)\ 25.00$ 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.

17) $$XX+YY,\ 12=\frac{1}{32\sqrt{3}}\sqrt{\alpha_1^3\alpha_2'^5}\{A_5(B_0-B_2)-A_4(B_1-B_3)$$
$$-A_3(B_0-B_4)+A_2(B_1-B_5)+A_1(B_2-B_4)-A_0(B_3-B_5)\}\,,$$

* Present address: Research Institute for Fundamental Physics, Kyoto University, Kyoto.

18) $XX+YY,\ 13=\frac{1}{32}\sqrt{\alpha_1^3\alpha_2'^5}\{A_5(B_1-B_3)-A_4(B_0-B_2)$

$-A_3(B_1-B_5)+A_2(B_0-B_4)+A_1(B_3-B_5)-A_0(B_2-B_4)\}$,

19) $ZZ,\ 12=\frac{1}{32\sqrt{3}}\sqrt{\alpha_1^3\alpha_2'^5}(A_2B_5-A_3B_4-A_4B_3+A_5B_2)$,

20) $ZZ,\ 13=\frac{1}{32}\sqrt{\alpha_1^3\alpha_2'^5}(A_2B_4-A_3B_5-A_4B_2+A_5B_3)$,

where $\alpha_1=\delta_1R$, $\alpha_2'=\delta_2'R$, $A_n=A_n\left(\frac{\alpha_1+\alpha_2'}{2}\right)$ and $B_n=B_n\left(\frac{\alpha_1-\alpha_2'}{2}\right)$. A_n and B_n are the auxiliary functions explained in Part XII.

Errata to Part XII and XIII

	Page	Line	
Part XII	31	heading	Natural Science Report, Ochanomizu University, Vol. ***13***, No. 2, 1962.
	32	heading	NSR., O. U., Vol. ***13***.
		16	5) $Z,\ 13=\frac{1}{16}\sqrt{\alpha_1^3\alpha_2'^5}(A_4B_2-\cdots)$
		17	$\alpha_2'=\delta_2'R$
Part XIII	37	footnote	NSR. O. U., ***13***, 31 (1962)
	70	1	*Table XLIII.*

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References

1) Natural Science Report, Ochanomizu University, 13, 31 (1962).
2) Natural Science Report, Ochanomizu University, 14, 37 (1963).