The Journal of Chemical Physics

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Cite as: J. Chem. Phys. **17**, 1248 (1949); https://doi.org/10.1063/1.1747150
Submitted: 27 April 1949 . Published Online: 22 December 2004

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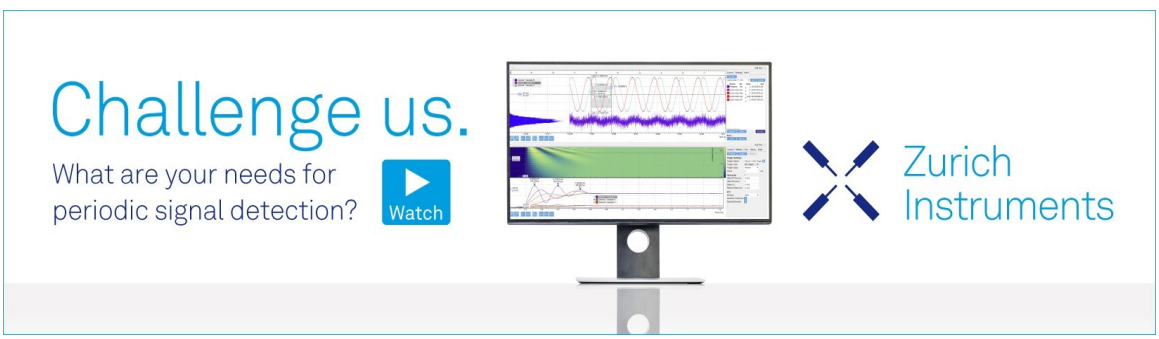

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Formulas and Numerical Tables for Overlap Integrals*

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(Received April 27, 1949)

Explicit formulas and numerical tables for the overlap integral S between AO's (atomic orbitals) of two overlapping atoms a and b are given. These cover all the most important combinations of AO pairs involving ns, $np\sigma$, and $np\pi$ AO's. They are based on approximate AO's of the Slater type, each containing two parameters μ [equal to $Z/(n-\delta)$], and $n-\delta$, where $n-\delta$ is an effective principal quantum number. The S formulas are given as functions of two parameters p and t, where $p=\frac{1}{2}(\mu_a+\mu_b)R/a_H$, R being the interatomic distance, and $t=(\mu_a-\mu_b)/(\mu_a+\mu_b)$. Master tables of computed values of S are given over wide ranges of p and t values corresponding to actual molecules, and also including the case $p=0$ (intra-atomic overlap integrals). In addition, tables of computed S values are given for several cases involving 2-quantum s, p hybrid AO's.

Hybrid S values for any desired type of hybrid can be obtained very easily from the tables as simple linear combinations of non-hybrid S values. It is shown how S values corresponding to orthogonalized Slater AO's and approximate S values for SCF (self-consistent-field) AO's can also be obtained as linear combinations of the Slater-AO S values. S values for carbon-carbon $2p\sigma$- and $2p\pi$-bonds using SCF carbon AO's have been computed (see Table in Section Vb); they correspond to stronger overlap than for Slater AO's. Non-localized MO group-orbital S values are also discussed, and are illustrated by an application to H_2O. The use of the tables to obtain dipole moments for electronic transitions in certain cases is also mentioned. The use of the tables to obtain S values for various specific atom-pairs and bond-types, and resulting conclusions, will be discussed in another paper.

I. INTRODUCTION

As is well known, the quantity known as the overlap integral is of considerable importance in the theory of molecular structure. Although the existing literature[1] contains a number of formulas and some numerical values for overlap integrals, it was thought worth while to carry through the much more systematic and comprehensive study whose results are presented below.

The overlap integral S for a pair of overlapping AO's (atomic orbitals) χ_a and χ_b of a pair of atoms a and b is defined for any value of the internuclear distance R by

$$S(\chi_a, \chi_b; R)=\int \chi_a^* \chi_b dv. \quad (1)$$

In the present paper we give formulas for S for all *AO pairs* involving ns, $np\sigma$, and $np\pi$ AO's for $n=1, 2, 3,$ and 5 using Slater AO's. We also give numerical tables for the most important of these cases, applicable to a wide variety of *atom pairs* over a wide range of R. In addition, we show how the tables, though based on Slater AO's, may be used to obtain S values for central-field AO's, as well as for hybrid AO's. Explicit tables of hybrid S values are also given for $n=2$.

In a subsequent paper, tables and figures for a variety of selected atom-pairs will be presented, together with some comments on their significance for the theory of chemical binding.

II. THE CHOICE OF ATOMIC ORBITAL FORMS

In order to evaluate overlap integrals, it is necessary first to specify the forms of the AO's. As a background, and also to obtain certain needed formulas, we first give a brief review of useful approximate AO forms. We are primarily concerned with *central-field* orbitals, classified under the familiar designations ns, np, nd, nf, $\cdots$ corresponding to $l=0, 1, 2, 3, \cdots$, with $n \geq l+1$. However, since the application of our computations is to atom-pairs in which each atom is under the influence of the cylindrically-symmetrical field of its partner, we need a sub-classification according to values of the diatomic quantum number λ ($\lambda=|m_l|$). This gives the AO types ns, $np\sigma$, $nd\sigma$, $\cdots(\lambda=0)$; $np\pi$, $nd\pi$, $\cdots(\lambda=1)$; and so on.

Let us consider an electron belonging to either of a pair of atoms a and b, using spherical polar coordinates about either center, as in Fig. 1. Intentionally, we take

* This work was assisted by the ONR under Task Order IX of Contract N6ori-20 with the University of Chicago.

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†† The work was begun before the war with computations on a considerable variety of individual atom-pairs (see abstract by R. S. Mulliken and C. A. Rieke, Rev. Mod. Phys. **14**, 259 (1942)). Recently, with the indispensable assistance of Mr. Tracy J. Kinyon in making the numerical computations, it was extended to the comprehensive effort reported here.

[1] (a) W. Heitler and F. London, Zeits. f. Physik **44**, 455 (1927), for homopolar $S(1s, 1s)$; (b) J. H. Bartlett, Jr., Phys. Rev. **37**, 507 (1931), for homopolar $S(2p\sigma, 2p\sigma)$ and $S(2p\pi, 2p\pi)$ and a table of values of the integrals A (see Eq. (15) below); (c) J. H. Bartlett, Jr. and W. H. Furry, Phys. Rev. **38**, 1615 (1931); **39** 210 (1932), especially table of values of homopolar $S(2s, 2s)$, $S(2s, 2p\sigma)$, $S(2p\sigma, 2p\sigma)$, $S(2p\pi, 2p\pi)$: Table VII, p. 222; (d) N. Rosen, Phys. Rev. **38**, 255 (1931) for formulas and extensive tables of values of the integrals A and B (see Eqs. (15), (16) below); (e) Kotani, Amemiya, and Simose, Proc. Phys. Math. Soc. Japan **20**, 1 (1938); **22**, 1 (1940). These authors give equations for S for all AO combinations with $n=1$ and 2, and (1940, p. 13) numerical tables for $S(1s, 2s)$ and $S(1s, 2p\sigma)$ for various t values. They also (1938, pp. 24–30, corrections 1940, pp. 17–18) give very complete and useful numerical tables for the integrals A and B. (f) C. A. Coulson, Proc. Camb. Phil. Soc. **38**, 210 (1941). Coulson gives very extensive formulas but no numerical tables, for integrals which differ from S only by multiplicative factors. These correspond to S for all combinations of ns, $np\sigma$, and $np\pi$ AO's with $n=1-3$ (and a few more), both for $t\neq 0$ (in our notation) and for $t=0$. (g) Several of the S formulas and a few numerical values are also given elsewhere.

the positive direction of the z axis for each atom to be directed toward the other atom, since this ensures a positive sign for S in all ordinary cases. Every central-field AO of atom a is of the form

$$\chi_a^{nl\lambda} = R_{nl}(r_a) Y_{l,\lambda}(\theta_a, \phi). \tag{2}$$

In normalized form, the Y's for the cases considered in this paper are:

$$\left.\begin{aligned} &Y_{ns} = (1/4\pi)^{\frac{1}{2}}; \\ &Y_{np\sigma} = (3/4\pi)^{\frac{1}{2}} \cos\theta_a; \\ &Y_{np\pi} = (3/4\pi)^{\frac{1}{2}} \sin\theta_a \{\cos\phi \text{ or } \sin\phi\}. \end{aligned}\right\} \tag{3}$$

Corresponding expressions hold for atom b.

When there is only one electron (hydrogenic AO's), R_{nl} takes the well-known form

$$R_{nl}(r) = \left(\sum_{k=l}^{n-1} c_{nlk} r^k\right) e^{-Zr/na_H}, \tag{4}$$

where Z is the nuclear charge, and a_H (0.529A) is the 1-quantum Bohr radius. The coefficients in Eq. (4) are those of the associated Laguerre polynomials, and the R_{nl}'s for each l form an orthogonal set.

When there is more than one electron, the best R_{nl}'s are of the SCF (self-consistent-field) type obtainable by the method of Hartree and Fock. These are not given by analytical expressions, and are usually presented in the form of numerical tables. Moreover, these SCF R_{nl}'s as tabulated are not always all orthogonal; however, it is always possible to find an equivalent set of equally good SCF R_{nl}'s which *are* orthogonal.[2] For practical computations, as Slater has shown,[3] the SCF R_{nl}'s may be approximated passably well by a finite series similar to that of Eq. (4) but with a different exponential factor in each term:

$$R_{nl}(r) = \sum_{k=l}^{n-1} d_k r^k e^{-\mu_k r/a_H}, \tag{5}$$

where the d_k's and μ_k's depend on n, l, and on the particular atom and electronic state. A considerably better series is obtained if the exponential factor in the term for which $k=n-1$ is replaced by a sum of two or three exponential terms, as follows:[3]

$$R_{nl}(r) = \sum_{\substack{k=l \\ (\neq n-1)}}^{n-2} d_k r^k e^{-\mu_k r/a_H} + r^{n-1} \sum_i d_i e^{-\mu_i r/a_H}. \tag{6}$$

For atoms containing $1s$, $2s$, and $2p$ electrons, the best approximate R_{nl}'s of the type of Eq. (5), so far as we know, are those obtained by Morse, Young, and Haurwitz, and Duncanson and Coulson.[4] These were obtained for several states of several atoms by minimizing the total energy of a complete antisymmetrized wave function built of AO's having R_{nl}'s of the type given by Eq. (5), subject also to the condition that the $2s$ AO is kept orthogonal to the $1s$. These AO's were also chosen in such a way that the virial theorem for the mean total kinetic and potential energies is satisfied.

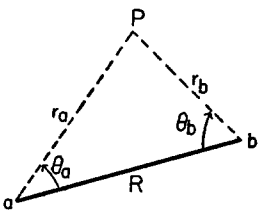

FIG. 1. Polar coordinates for an electron at P in an AO of atom a or b. In addition (not shown), $\phi = \phi_a = \phi_b$.

The well-known Slater AO's[5] are obtained by approximating the series of Eq. (5) by the single term $N_{nl} r^{n-1} e^{-\mu r/a_H}$ (or by a modification of this, $N_{nl} r^{n-1-\delta} e^{-\mu r/a_H}$). The values of μ and δ are specified by Slater for any AO of any atom by a simple recipe. This gives μ-values surprisingly close,[4b] for 2-quantum AO's, to those obtained for the r^{n-1} term by minimizing the total energy. Unlike most of the forms given by Eqs. (2)–(5), Slater's AO's have no radial nodes. This, however, does not much impair their ability to represent the *outer parts* of AO's, hence they should be especially useful for the computation of overlap integrals. Following is a summary of Slater's recipe as applied to s and p AO's in normalized form:

$$\left.\begin{aligned} &R_{nl}(r) = N_{nl} r^{n-1-\delta} e^{-\mu r/a_H}; \\ &\qquad \delta = 0 \text{ for } n = 1 \text{ to } 3;\ 0.3 \text{ for } 4s,\ 4p; \\ &\qquad\qquad 1 \text{ for } 5s,\ 5p; \\ &\mu_{ns} = \mu_{np} = Z_{a,n}/(n-\delta), \\ &1/N_{nl}^2 = \int_0^\infty r^{2n-2\delta} e^{-2\mu_{nl} r/a_H} dr, \end{aligned}\right\} \tag{7}$$

with Z values dependent on the atom a and on n. For convenience of later reference, Slater μ-values for the *valence-shell* ns and np AO's of several atoms and ions are given in Table I. Inner-electron AO's if present are assigned larger Z values.[3]

As a consequence of their nodeless character, Slater AO's of equal l and different n (e.g., $1s$ and $2s$) are very far from being orthogonal, but they can easily be orthogonalized if desired. This process restores the missing nodes, giving AO's of the form of Eq. (5), and surprisingly close to the best possible of this form.[6] As an example, if χ_{1s} and χ_{2s} refer to Slater AO's, and χ_{2s}^{or}

[2] See, e.g., C. C. J. Roothaan, forthcoming paper.
[3] J. C. Slater, Phys. Rev. **42**, 33 (1932).
[4] (a) Morse, Young, and Haurwitz, Phys. Rev. **48**, 948 (1935); (b) extended and partially corrected by W. E. Duncanson and C. A. Coulson, Proc. Roy. Soc. Edinburgh **62A**, 37 (1944).
[5] J. C. Slater, Phys. Rev. **36**, 57 (1930); C. Zener, Phys. Rev. **36**, 51 (1930).
[6] W. E. Moffitt and C. A. Coulson, Phil. Mag. [7], **38**, 634 (1937). These authors also give instructive contour diagrams of carbon atom $2te$, $2tr$, and $2di$ hybrid AO's, using orthogonalized Slater $2s$ AO's.

TABLE I. Slater μ-values[a] for valence-shell ns, np AO's.

H	1.00	C^-	1.45	O^-	2.10	Na	0.733	S	1.817
Li	0.65	C	1.625	O	2.275	Mg	0.95	Cl	2.033
Be	0.975	C^+	1.80	O^+	2.45	Al	1.167	Br	2.054
B^-	1.125	N	1.95	F	2.60	Si	1.383	I	1.90
B	1.30	N^+	2.125			P	1.60		

[a] For $1s$ inner-shell AO's, $\mu = Z - 0.3$ in all cases, where Z is the actual nuclear charge.

refers to the orthogonalized Slater $2s$ AO, we have

$$\left.\begin{aligned} \chi_{2s}^{\text{or}} &= (\chi_{2s} - Q\chi_{1s})/(1-Q^2)^{\frac{1}{2}} \\ Q &\equiv S(1s_a, 2s_a) \equiv \int \chi_{2s_a}\chi_{1s_a} d\tau. \end{aligned}\right\} \tag{8}$$

Although Q is often fairly large (for example, 0.220 if atom a is carbon), the process of orthogonalization has little effect on the computed values of overlap integrals (see Section V).

In addition to overlap integrals for pure central-field AO's, those for hybrid AO's are obviously of great interest for molecular problems. Hybrid AO's, although they can be constructed as linear combinations of central-field AO's, are not themselves central-field AO's. Hybrid overlap integrals can be obtained as simple linear combinations of Slater-AO S's (see Section V), so that no laborious new computations are required. For purposes of computing S's, approximate hybrid AO's built from Slater AO's without orthogonalization should according to our previous reasoning give satisfactory results.

The hybrid AO's which can be formed from s and p AO's are all of σ-type, that is, have cylindrical symmetry. Let χ be a normalized hybrid σ AO of the form

$$\chi = \alpha\chi_{ns} \pm (1-\alpha^2)^{\frac{1}{2}}\chi_{np\sigma}, \tag{9}$$

where $0 \leqslant \alpha \leqslant 1$, and χ_{ns} and $\chi_{np\sigma}$ are as defined by Eqs. (2)–(3) and Fig. 1, with R_{nl} given by Eqs. (7) for the case of hybrid Slater AO's. In the following, the abbreviations *te*, *tr*, and *di* (tetrahedral, trigonal, and digonal) will be used for hybrids with $\alpha^2 = \frac{1}{4}, \frac{1}{3}$, and $\frac{1}{2}$ respectively and with the plus sign in Eq. (9). A further, complementary, set of hybrid AO's *te'*, *tr'*, and *di'* is obtained by using the minus sign in Eq. (9). The hybrids *te*, *tr*, *di* of an atom give *large overlap* (large S) with corresponding or similar AO's of a second atom, while *te'*, *tr'*, and *di'* give *small overlap*.

III. NOMENCLATURE AND PARAMETERS FOR OVERLAP INTEGRALS

In discussing and tabulating overlap integrals, a careful choice of nomenclature will prove to be important. In order to characterize an overlap integral fully, we need to specify (a) the two AO's involved; (b) the two atoms involved, and which AO belongs to each atom; (c) the value of R. Two suitable types of general symbols for this purpose, also a symbol for an internal overlap or non-orthogonality integral, are indicated by the following examples. Simplified symbols can be used in special cases.

$$\left.\begin{aligned} &\text{(a) Atom-pair at any distance } R\text{:} \\ &\quad \text{general AO's and atoms: } S(n_a x, n_b y; R) \\ &\quad \text{specific AO's, general atoms:} \\ &\quad\quad S(1s_a, 2p\sigma_b; R) \text{ or } S(1s, 2p\sigma; R) \\ &\quad \text{specific AO's and atoms:} \\ &\quad\quad S(2p\pi_{\text{C}}, 3p\pi_{\text{Si}}; 1.75\text{A}) \\ &\text{(b) Atom-pair involved in specified bond at equilibrium distance:} \\ &\quad\quad S(2s, 2p\sigma; \text{C=C});\ S(2te, 3p\sigma; \text{C—Cl}); \\ &\quad\quad S(1s, 2s; \text{H—Li});\ S(2p\pi, 2p\pi, \text{O}^+ \equiv \text{C}) \\ &\text{(c) Single atom } a \text{ (internal overlap integral):} \\ &\quad\quad S(1s_a, 2s_a). \end{aligned}\right\} \tag{10}$$

In the atom-pair symbols above, it is intended to be understood that the *first AO symbol always goes with the first atom, the second with the second.* However, it is not essential here to follow any fixed rule as to which AO (or atom) symbol shall be written first. Nevertheless, in another type of notation which will be required below, it *does* become essential to adopt certain fixed conventions in this matter, and it will diminish the possibilities of error if we follow the same conventions also in using the types of notation given above. These conventions are: the AO of smaller n is to be written first, or if both n's are equal, the AO belonging to the atom of larger Z is to be written first. These rules were followed in the examples given above.

We turn now to the matter of coordinates and parameters to be used in the evaluation of the S's. The computation is best effected after transforming from polar coordinates of the two atoms (see Fig. 1) to spheroidal coordinates ξ, η, ϕ given by:

$$\xi = (r_a + r_b)/R; \quad \eta = (r_a - r_b)/R; \quad \phi = \phi_a = \phi_b. \tag{11}$$

The coordinate ξ ranges from 1 to ∞, η from -1 to $+1$.

For any given AO pair, we shall wish to obtain S values for various pairs of atoms, each for various interatomic distances R. To accomplish this, the best procedure is first to set up for each AO pair a single master formula expressed in terms of suitable parameters depending on the μ's of the two AO's and on R, and from this to compute and tabulate numerical values of S as a function of the chosen parameters. For this purpose, the two parameters p and t defined as follows are found to be appropriate for the case of Slater AO's (see Eqs. (7) and Table I).

$$\left.\begin{aligned} p &\equiv \tfrac{1}{2}(\mu_a + \mu_b)R/a_{\text{H}}, \\ t &\equiv (\mu_a - \mu_b)/(\mu_a + \mu_b). \end{aligned}\right\} \tag{12}$$

To find S for a given Slater-AO pair, atom pair and R value, one then first computes p and t for the particular case, then looks up the value of S in the master table for the given AO pair. Methods of obtaining S values for other types of AO's will be described in Section V.

Since in connection with the master tables we replace atom designations by parameters p and t, it is now necessary to introduce a type of S symbol different from those given in (10), and indicated by the following examples:

(a) Atom pair characterized by parameters p, t:
General form: $S(n_a x, n_b y; p, t)$;
Specific form: $S(2s_a, 3p\sigma_b; p, t)$,
or more briefly, but with the same meaning,
$S(2s, 3p\sigma; p, t)$.
(b) Single atom (internal overlap integral):
General form: $S(n_a x, n_a' y)$
Specific form: $S(1s, 2s; \mathrm{O}, t)$. (13)

The signs of the coordinate η in Eqs. (11) and of the parameter t in Eqs. (12) obviously depend on the assignment of the labels a and b to the two atoms in any atom pair. In order to make the master formulas and tables unambiguous with respect to the signs of η and t, it is therefore necessary to adopt suitable conventions to fix this assignment. The following two (necessarily arbitrary) conventions will be used in this paper:

(1) *In case the two AO's have unequal n, the atom whose AO has smaller n will always be identified with atom a, and its AO will always be written first in the symbol for S*, for example $S(2s_a, 3p\sigma_b; p, t)$ or more briefly $S(2s, 3p\sigma; p, t)$; but *never* $S(3p\sigma_a, 2s_b; p, t)$ or $S(3p\sigma, 2s; p, t)$. As another example, we may write $S(2p\sigma, 3s)$, but never $S(3s, 2p\sigma)$. Further examples are $S(2s, 3s)$ and $S(2p\sigma, 3p\sigma)$. In general formulations, symbols such as $S(n_a s, n_b p\sigma)$ or $S(n_a p\sigma, n_b s)$ will be used, always with the implication that $n_a < n_b$. It will be noticed that for the present case of two AO's with unequal n, both positive and negative t values are possible, depending on the sign of $\mu_a - \mu_b$. For example (see Table I),

$$t(2p\sigma_{\mathrm{F}}, 3s_{\mathrm{Mg}}) = (2.60-0.95)/(2.60+0.95) > 0,$$

but

$$t(2p\sigma_{\mathrm{Be}}, 3s_P) = (1.30-1.60)/(1.30+1.60) < 0.$$

Also, but only by accident, $t=0$ is possible. The relative practical importance of the positive and negative ranges of t varies according to what AO pair-type one considers.

(2) *In case the two AO's have equal n, the atom with larger μ will always be identified with atom a, and its AO will always be written first in the symbol for S; if the μ's are equal, either atom may be called a.* For example, $S(ns_a, np\sigma_b)$ or briefly $S(ns, np\sigma)$; $S(np\sigma_a, ns_b)$ or briefly $S(np\sigma, ns)$; and $S(2p\pi_a, 2p\pi_b)$ or briefly $S(2p\pi, 2p\pi)$, all imply $Z_a \geqslant Z_b$. Hence, according to Eqs. (12), convention (2) here restricts t to the range $t \geqslant 0$. The integrals $S(ns_a, np\sigma_b)$ and $S(np\sigma_a, ns_b)$—see Eqs. (14) below, taking $n_a = n_b$—require a little special comment because of their somewhat confusing similarity.[7] For $t>0$, the two integrals are different and have different values, but for $t=0$ they become identical. For instance, $S(2p\sigma_{\mathrm{O}}, 2s_{\mathrm{C}})$ and $S(2s_{\mathrm{O}}, 2p\sigma_{\mathrm{C}})$, which are examples of the two cases written in accordance with convention (2), have different values; but $S(2p\sigma_{\mathrm{C}}, 2s_{\mathrm{C}})$ and $S(2s_{\mathrm{C}}, 2p\sigma_{\mathrm{C}})$ are identical.

IV. MASTER FORMULAS AND COMPUTATION METHODS FOR MASTER TABLES OF SLATER-AO OVERLAP INTEGRALS

With the foregoing conventions, the S master formulas fall into five basic types. Using Eqs. (1)–(3), (7), (11)–(12), letting

$$m = n - \delta,$$

and integrating over ϕ, these five types take the forms:

$$\left.\begin{aligned}
S(n_a s, n_b s; p, t) &= \tfrac{1}{2} N_a N_b (\tfrac{1}{2}R)^{m_a+m_b+1} \int_1^\infty \int_{-1}^1 (\xi+\eta)^{m_a-1}(\xi-\eta)^{m_b-1}(\xi^2-\eta^2) e^{-p(\xi+\eta t)} d\eta d\xi, \\
S(n_a s, n_b p\sigma; p, t) &= (\tfrac{1}{2}\sqrt{3}) N_a N_b (\tfrac{1}{2}R)^{m_a+m_b+1} \int_1^\infty \int_{-1}^1 (\xi+\eta)^{m_a-1}(\xi-\eta)^{m_b-2}(-\xi\eta+1)(\xi^2-\eta^2) e^{-p(\xi+\eta t)} d\eta d\xi, \\
S(n_a p\sigma, n_b s; p, t) &= (\tfrac{1}{2}\sqrt{3}) N_a N_b (\tfrac{1}{2}R)^{m_a+m_b+1} \int_1^\infty \int_{-1}^1 (\xi+\eta)^{m_a-2}(\xi-\eta)^{m_b-1}(-\xi\eta-1)(\xi^2-\eta^2) e^{-p(\xi+\eta t)} d\eta d\xi, \\
S(n_a p\sigma, n_b p\sigma; p, t) &= (3/2) N_a N_b (\tfrac{1}{2}R)^{m_a+m_b+1} \int_1^\infty \int_{-1}^1 (\xi+\eta)^{m_a-2}(\xi-\eta)^{m_b-2}(\xi^2\eta^2-1)(\xi^2-\eta^2) e^{-p(\xi+\eta t)} d\eta d\xi, \\
S(n_a p\pi, n_b p\pi; p, t) &= (3/4) N_a N_b (\tfrac{1}{2}R)^{m_a+m_b+1} \int_1^\infty \int_{-1}^1 (\xi+\eta)^{m_a-2}(\xi-\eta)^{m_b-2}(\xi^2-1)(1-\eta^2)(\xi^2-\eta^2) e^{-p(\xi+\eta t)} d\eta d\xi.
\end{aligned}\right\} \quad (14)$$

[7] Without convention (2), $S(ns_a, np\sigma_b)$ would be defined for positive, zero, and negative values of t ($Z_a > Z_b$, $Z_a = Z_b$, $Z_a < Z_b$; see Eqs. (12)). The same would be true of $S(np\sigma_a, ns_b)$. The two integrals would then differ only in the manner in which the labels a and b are associated with the AO forms ns and $np\sigma$. Now as will be seen from Eqs. (11), (12), an exchange of the labels a and b merely changes the definitions of η and t in such a way that the positive domains of η and t for the one labeling (say η', t') become the corresponding negative domains for the other (say η'', t''). Consequently, if in Eqs. (14) for $S(ns, np\sigma)$ and $S(np\sigma, ns)$ we write η', t' in the one equation and η'', t'' in the other, and then make the substitution $\eta'' = -\eta'$, $t'' = -t'$, the two equations

The integrals over ξ and η in Eqs. (14) may be evaluated by making use of the following mathematical relations:[1]

$$A_k(p)\equiv\int_1^\infty \xi^k e^{-p\xi}d\xi = e^{-p}\sum_{\mu=1}^{k+1}[k!/p^\mu(k-\mu+1)!] \tag{15}$$

$$\left.\begin{aligned} B_k(pt)&\equiv\int_{-1}^{1}\eta^k e^{-pt\eta}d\eta \\ &=-e^{-pt}\sum_{\mu=1}^{k+1}[k!/(pt)^\mu(k-\mu+1)!]-e^{pt}\sum_{\mu=1}^{k+1}[(-1)^{k-\mu}k!/(pt)^\mu(k-\mu+1)!]; \end{aligned}\right\} \tag{16}$$

but $B_k(0)=2/(k+1)$ for k even; $=0$ for k odd. The factors N in Eqs. (14) (see N_{nl} in Eqs. (7)) may be evaluated by means of:

$$C(k,q)\equiv\int_0^\infty \lambda^k e^{-q\lambda}d\lambda = k!/q^{k+1}. \tag{17}$$

The numerical computation of the overlap integrals is comparatively simple if the A_k's and B_k's are first computed for appropriate values of the parameters p and t; here the simplest procedure (rather than using Eqs. (15), (16) directly) is to obtain the higher k A's and B's from those with lower k by using certain *recursion formulas*.[1d,1e] We first note that any particular S involves the integral of a polynomial in ξ and η. Then it is plain that each value of S is the product of a factor times a linear combination of A_k's and B_k's all computed at the same values of p and t.

For the computation of the master tables given below, the necessary A_k's and B_k's were first computed[8] for the desired values of p and t, and then combined in accordance with the following Eqs. (18)–(50) to give the S values.[9] These formulas were obtained by the use of Eqs. (15)–(17) in connection with Eqs. (14) and (7). It will be noted that a separate formula is given in each case for $t=0$, for reasons that will be understood on looking at Eqs. (16). Certain additional special formulas will now be described.

Although in general the computation of the A's and B's followed by the use of Eqs. (18)–(50) is the most expeditious procedure, an alternative set of formulas very considerably simplifies the computation in the important special case of two identical atoms ($n_a=n_b$, $t=0$), if one is interested *only* in this case. This case includes not only integrals of the type $S(nx, nx; p, 0)$, but also such integrals as $S(ns, np\sigma; p, 0)$ or $S(np\sigma, ns; p, 0)$; these are particularly important in the computation of hybrid-AO S values (see Section V). The simplified formulas were obtained by substituting for the A's in the $t=0$ formulas in Eqs. (18)–(50), using Eq. (15). Although we did not use them in computing the master tables, they are given below as Eqs. (51)–(63) for the convenience of readers who may wish to make their own computations for additional p values.[9]

One further set of special formulas is required, for the internal overlap integrals $S(n_ax, n_by; 0, t)$,—see (10) and (13). This type of integral occurs if one orthogonalizes Slater AO's, and also if one wishes to compute SCF S's from Slater S's (see Section V). The necessary formulas are given below as Eqs. (64)–(73).

MASTER FORMULAS FOR SLATER-AO OVERLAP INTEGRALS

$t=0$:

$$S(1s, 1s)=(6)^{-1}p^3[3A_2-A_0]$$

$t>0$:

$$S(1s, 1s)=(4)^{-1}p^3(1-t^2)^{+3/2}[A_2B_0-A_0B_2] \tag{18}$$

become identical except for the sign of t in the exponential, and completely identical for $t=0$. Hence $S(ns, np\sigma)$ for positive t would be equal to $S(np\sigma, ns)$ for negative t, and *vice versa*, if negative t here were not excluded by convention (2); and for $t=0$, $S(ns, np\sigma)\equiv S(np\sigma, ns)$.

[8] Most of this labor could have been avoided by the use of the A and B tables of references 1d or especially 1e. Actually, however, independent computations were made. Afterward, checks were made of some of our A and B values against those in the tables of reference 1e, and excellent agreement was found.

[9] Coulson (reference 1f) also gives formulas corresponding to the majority of the S integrals listed here. However, his formulas for $t\neq 0$ are in terms of μ_a, μ_b, and R, in a form not adapted to the present computation and tabulation. His formulas for $t=0$ are identical with our Eqs. (51)–(63) except that they are not normalized like ours to give S values directly.

$t=0$:
$$S(1s, 2s)=(12)^{-1}(3)^{-\frac{1}{2}}p^4[3A_3-A_1]$$
$t\neq 0$:
$$S(1s, 2s)=(8)^{-1}(3)^{-\frac{1}{2}}p^4(1+t)^{3/2}(1-t)^{5/2}[A_3B_0-A_2B_1-A_1B_2+A_0B_3] \tag{19}$$

$t=0$:
$$S(1s, 2p\sigma)=(12)^{-1}p^4[3A_2-A_0]$$
$t\neq 0$:
$$S(1s, 2p\sigma)=(8)^{-1}p^4(1+t)^{3/2}(1-t)^{5/2}[-A_3B_1+A_2B_0+A_1B_3-A_0B_2] \tag{20}$$

$t=0$:
$$S(1s, 3s)=(60)^{-1}(10)^{-\frac{1}{2}}p^5[5A_4-A_0]$$
$t\neq 0$:
$$S(1s, 3s)=(24)^{-1}(10)^{-\frac{1}{2}}p^5(1+t)^{3/2}(1-t)^{7/2}[A_4B_0-2A_3B_1+2A_1B_3-A_0B_4] \tag{21}$$

$t=0$:
$$S(1s, 3p\sigma)=(15)^{-1}(30)^{-\frac{1}{2}}p^5[5A_3-2A_1]$$
$t\neq 0$:
$$S(1s, 3p\sigma)=(8)^{-1}(30)^{-\frac{1}{2}}p^5(1+t)^{3/2}(1-t)^{7/2}[A_3(B_0+B_2)-A_1(B_2+B_4)-B_1(A_2+A_4)+B_3(A_0+A_2)] \tag{22}$$

$t=0$:
$$S(1s, 5s)=(720)^{-1}(35)^{-\frac{1}{2}}p^6[15A_5+10A_3-9A_1]$$
$t\neq 0$:
$$S(1s, 5s)=(96)^{-1}(35)^{-\frac{1}{2}}p^6(1+t)^{3/2}(1-t)^{9/2}[A_5B_0-3A_4B_1+2A_3B_2+2A_2B_3-3A_1B_4+A_0B_5] \tag{23}$$

$t=0$:
$$S(1s, 5p\sigma)=(240)^{-1}(105)^{-\frac{1}{2}}p^6[25A_4-6A_2-3A_0]$$
$t\neq 0$:
$$S(1s, 5p\sigma)=(32)^{-1}(105)^{-\frac{1}{2}}p^6(1+t)^{3/2}(1-t)^{9/2}[A_4(B_0+2B_2)+A_1(2B_3+B_5)-B_1(2A_3+A_5)-B_4(A_0+2A_2)] \tag{24}$$

$t=0$:
$$S(2s, 2s)=(360)^{-1}p^5[15A_4-10A_2+3A_0]$$
$t>0$:
$$S(2s, 2s)=(48)^{-1}p^5(1-t^2)^{5/2}[A_4B_0-2A_2B_2+A_0B_4] \tag{25}$$

$t=0$:
$$S(2s, 2p\sigma)=(60)^{-1}(3)^{-\frac{1}{2}}p^5[5A_3-A_1]$$
$t\neq 0$:
$$S(2s, 2p\sigma)=(16)^{-1}(3)^{-\frac{1}{2}}p^5(1-t^2)^{5/2}[A_3(B_0-B_2)+A_1(B_4-B_2)+B_1(A_2-A_4)+B_3(A_2-A_0)] \tag{26}$$
$S(2p\sigma, 2s)$: same as $S(2s, 2p\sigma)$ except each $B_k(t)$ replaced by $B_k(-t)$

$t=0$:
$$S(2s, 3s)=(360)^{-1}(30)^{-\frac{1}{2}}p^6[15A_5-10A_3+3A_1]$$
$t\neq 0$:
$$S(2s, 3s)=(48)^{-1}(30)^{-\frac{1}{2}}p^6(1+t)^{5/2}(1-t)^{7/2}[A_5B_0-A_4B_1-2A_3B_2+2A_2B_3+A_1B_4-A_0B_5] \tag{27}$$

$t=0$:
$$S(2s, 3p\sigma)=(360)^{-1}(10)^{-\frac{1}{2}}p^6[15A_4-10A_2+3A_0]$$
$t\neq 0$:
$$S(2s, 3p\sigma)=(48)^{-1}(10)^{-\frac{1}{2}}p^6(1+t)^{5/2}(1-t)^{7/2}[-A_5B_1+A_4B_0+2A_3B_3-2A_2B_2-A_1B_5+A_0B_4] \tag{28}$$

$t=0$:
$$S(2s, 5s)=(10{,}080)^{-1}(105)^{-\frac{1}{2}}p^7[105A_6-35A_4-21A_2+15A_0]$$
$t\neq 0$:
$$S(2s, 5s)=(192)^{-1}(105)^{-\frac{1}{2}}p^7(1+t)^{5/2}(1-t)^{9/2}[A_6B_0-2A_5B_1-A_4B_2+4A_3B_3-A_2B_4-2A_1B_5+A_0B_6] \tag{29}$$

$t=0$:
$$S(2s, 5p\sigma)=(2520)^{-1}(35)^{-\frac{1}{2}}p^7[35A_5-28A_3+9A_1]$$
$t\neq 0$:
$$S(2s, 5p\sigma)=(192)^{-1}(35)^{-\frac{1}{2}}p^7(1+t)^{5/2}(1-t)^{9/2}[-A_6B_1+A_5(B_0+B_2)+A_4(2B_3-B_1)-2A_3(B_2+B_4)+A_2(2B_3-B_5)+A_1(B_4+B_6)-A_0B_5] \tag{30}$$

$t=0$:
$$S(2p\sigma, 2p\sigma)=(120)^{-1}p^5[5A_4-18A_2+5A_0] \tag{31}$$
$t>0$:
$$S(2p\sigma, 2p\sigma)=(16)^{-1}p^5(1-t^2)^{5/2}[B_2(A_0+A_4)-A_2(B_0+B_4)]$$

$t=0$:
$$S(2p\sigma, 3s)=(360)^{-1}(10)^{-\frac{1}{2}}p^6[5A_4+6A_2-3A_0] \tag{32}$$
$t\neq 0$:
$$S(2p\sigma, 3s)=(48)^{-1}(10)^{-\frac{1}{2}}p^6(1+t)^{5/2}(1-t)^{7/2}[A_4(B_0-2B_2)+A_1(2B_3-B_5)+B_1(A_5-2A_3)+B_4(2A_2-A_0)]$$

$t=0$:
$$S(2p\sigma, 3p\sigma)=(120)^{-1}(30)^{-\frac{1}{2}}p^6[5A_5-18A_3+5A_1] \tag{33}$$
$t\neq 0$:
$$S(2p\sigma, 3p\sigma)=(16)^{-1}(30)^{-\frac{1}{2}}p^6(1+t)^{5/2}(1-t)^{7/2}[A_2(B_1+B_5)-A_3(B_0+B_4)-B_3(A_0+A_4)+B_2(A_1+A_5)]$$

$t=0$:
$$S(2p\sigma, 5s)=(630)^{-1}(35)^{-\frac{1}{2}}p^7[7A_3-3A_1] \tag{34}$$
$t\neq 0$:
$$S(2p\sigma, 5s)=(192)^{-1}(35)^{-\frac{1}{2}}p^7(1+t)^{5/2}(1-t)^{9/2}[A_6B_1+A_5(B_0-3B_2)+A_4(2B_3-3B_1)+2A_3(B_2+B_4)+A_2(2B_3-3B_5)+A_1(B_6-3B_4)+A_0B_5]$$

$t=0$:
$$S(2p\sigma, 5p\sigma)=(3360)^{-1}(105)^{-\frac{1}{2}}p^7[35A_6-105A_4-15A_2+21A_0] \tag{35}$$
$t\neq 0$:
$$S(2p\sigma, 5p\sigma)=(64)^{-1}(105)^{-\frac{1}{2}}p^7(1+t)^{5/2}(1-t)^{9/2}[A_6B_2-A_4B_0+2A_3(B_1+B_5)-2B_3(A_1+A_5)+B_4A_0-B_6A_2]$$

$t=0$:
$$S(3s, 3s)=(25,200)^{-1}p^7[35A_6-35A_4+21A_2-5A_0] \tag{36}$$
$t>0$:
$$S(3s, 3s)=(1440)^{-1}p^7(1-t^2)^{7/2}[A_6B_0-3A_4B_2+3A_2B_4-A_0B_6]$$

$t=0$:
$$S(3s, 3p\sigma)=(12,600)^{-1}(3)^{-\frac{1}{2}}p^7[35A_5-14A_3+3A_1]$$
$t\neq 0$:
$$S(3s, 3p\sigma)=(480)^{-1}(3)^{-\frac{1}{2}}p^7(1-t^2)^{7/2}[-A_6B_1+A_5(B_0-B_2)+A_4(B_1+2B_3)+2A_3(B_4-B_2)-A_2(2B_3+B_5)+A_1(B_4-B_6)+A_0B_5] \tag{37}$$
$S(3p\sigma, 3s)$: same as $S(3s, 3p\sigma)$ except each $B_k(t)$ replaced by $B_k(-t)$.

$t=0$:
$$S(3s, 5s)=(50,400)^{-1}(14)^{-\frac{1}{2}}p^8[35A_7-35A_5+21A_3-5A_1] \tag{38}$$
$t\neq 0$:
$$S(3s, 5s)=(2880)^{-1}(14)^{-\frac{1}{2}}p^8(1+t)^{7/2}(1-t)^{9/2}[A_7B_0-A_6B_1-3A_5B_2+3A_4B_3+3A_3B_4-3A_2B_5-A_1B_6+A_0B_7]$$

$t=0$:
$$S(3s, 5p\sigma)=(16,800)^{-1}(42)^{-\frac{1}{2}}p^8[35A_6-35A_4+21A_2-5A_0] \tag{39}$$
$t\neq 0$:
$$S(3s, 5p\sigma)=(960)^{-1}(42)^{-\frac{1}{2}}p^8(1+t)^{7/2}(1-t)^{9/2}[-A_7B_1+A_6B_0+3A_5B_3-3A_4B_2-3A_3B_5+3A_2B_4+A_1B_7-A_0B_6]$$

$t=0$:
$$S(3p\sigma, 3p\sigma)=(25,200)^{-1}p^7[35A_6-147A_4+85A_2-21A_0] \tag{40}$$
$t>0$:
$$S(3p\sigma, 3p\sigma)=(480)^{-1}p^7(1-t^2)^{7/2}[A_6B_2-A_4(B_0+2B_4)+A_2(B_6+2B_2)-A_0B_4]$$

$t=0$:
$$S(3p\sigma, 5s)=(50,400)^{-1}(42)^{-\frac{1}{2}}p^8[35A_6+49A_4-51A_2+15A_0] \tag{41}$$
$t\neq 0$:
$$S(3p\sigma, 5s)=(960)^{-1}(42)^{-\frac{1}{2}}p^8(1+t)^{7/2}(1-t)^{9/2}[A_7B_1+A_6(B_0-2B_2)-A_5(B_3+2B_1)+A_4(4B_4-B_2)+A_3(4B_3-B_5)-A_2(2B_6+B_4)+A_1(B_7-2B_5)+A_0B_6]$$
$t=0$:
$$S(3p\sigma, 5p\sigma)=(50,400)^{-1}(14)^{-\frac{1}{2}}p^8[35A_7-147A_5+85A_3-21A_1]$$

$t\neq 0$:

$$S(3p\sigma, 5p\sigma)=(960)^{-1}(14)^{-\frac{1}{2}}p^8(1+t)^{7/2}(1-t)^{9/2}[A_7B_2-A_6B_3-A_5(B_0+2B_4)+A_4(B_1+2B_5)+A_3(2B_2+B_6)-A_2(2B_3+B_7)-A_1B_4+A_0B_5] \tag{42}$$

$t=0$:

$$S(5s, 5s)=(12{,}700{,}800)^{-1}p^9[315A_8-420A_6+378A_4-180A_2+35A_0]$$

$t>0$:

$$S(5s, 5s)=(80{,}640)^{-1}p^9(1-t^2)^{9/2}[A_8B_0-4A_6B_2+6A_4B_4-4A_2B_6+A_0B_8] \tag{43}$$

$t=0$:

$$S(5s, 5p\sigma)=(2{,}116{,}800)^{-1}(3)^{-\frac{1}{2}}p^9[105A_7-63A_5+27A_3-5A_1]$$

$t\neq 0$:

$$S(5s, 5p\sigma)=(26{,}880)^{-1}(3)^{-\frac{1}{2}}p^9(1-t^2)^{9/2}[-A_8B_1+A_7(B_0-B_2)+A_6(B_1+3B_3)+3A_5(B_4-B_2)-3A_4(B_3+B_5)+3A_3(B_4-B_6)+A_2(3B_5+B_7)+A_1(B_8-B_6)-A_0B_7] \tag{44}$$

$S(5p\sigma, 5s)$: same as $S(5s, 5p\sigma)$ except each $B_k(t)$ replaced by $B_k(-t)$.

$t=0$:

$$S(5p\sigma, 5p\sigma)=(4{,}233{,}600)^{-1}p^9[105A_8-504A_6+450A_4-224A_2+45A_0]$$

$t>0$:

$$S(5p\sigma, 5p\sigma)=(26{,}880)^{-1}p^9(1-t^2)^{9/2}[A_8B_2-A_6(B_0+3B_4)+3A_4(B_2+B_6)-A_2(B_8+3B_4)+A_0B_6] \tag{45}$$

$t=0$:

$$S(2p\pi, 2p\pi)=(120)^{-1}p^5[5A_4-6A_2+A_0]$$

$t>0$:

$$S(2p\pi, 2p\pi)=(32)^{-1}p^5(1-t^2)^{5/2}[A_4(B_0-B_2)+A_2(B_4-B_0)+A_0(B_2-B_4)] \tag{46}$$

$t=0$:

$$S(2p\pi, 3p\pi)=(120)^{-1}(30)^{-\frac{1}{2}}p^6[5A_5-6A_3+A_1]$$

$t\neq 0$:

$$S(2p\pi, 3p\pi)=(32)^{-1}(30)^{-\frac{1}{2}}p^6(1+t)^{5/2}(1-t)^{7/2}[A_5(B_0-B_2)+A_4(B_3-B_1)+A_3(B_4-B_0)+A_2(B_1-B_5)+A_1(B_2-B_4)+A_0(B_5-B_3)] \tag{47}$$

$t=0$:

$$S(2p\pi, 5p\pi)=(3360)^{-1}(105)^{-\frac{1}{2}}p^7[35A_6-35A_4-3A_2+3A_0]$$

$t\neq 0$:

$$S(2p\pi, 5p\pi)=(128)^{-1}(105)^{-\frac{1}{2}}p^7(1+t)^{5/2}(1-t)^{9/2}[A_6(B_0-B_2)+2A_5(B_3-B_1)+A_4(B_2-B_0)+2A_3(B_1-B_5)+A_2(B_6-B_4)+2A_1(B_5-B_3)+A_0(B_4-B_6)] \tag{48}$$

$t=0$:

$$S(3p\pi, 3p\pi)=(25{,}200)^{-1}p^7[35A_6-49A_4+17A_2-3A_0]$$

$t>0$:

$$S(3p\pi, 3p\pi)=(960)^{-1}p^7(1-t^2)^{7/2}[A_6(B_0-B_2)+A_4(2B_4-B_0-B_2)+A_2(2B_2-B_4-B_6)+A_0(B_6-B_4)] \tag{49}$$

$t=0$:

$$S(3p\pi, 5p\pi)=(50{,}400)^{-1}(14)^{-\frac{1}{2}}p^8[35A_7-49A_5+17A_3-3A_1]$$

$t\neq 0$:

$$S(3p\pi, 5p\pi)=(1920)^{-1}(14)^{-\frac{1}{2}}p^8(1+t)^{7/2}(1-t)^{9/2}[A_7(B_0-B_2)+A_6(B_3-B_1)+A_5(2B_4-B_2-B_0)+A_4(B_1+B_3-2B_5)+A_3(2B_2-B_4-B_6)+A_2(B_5-2B_3+B_7)+A_1(B_6-B_4)+A_0(B_5-B_7)] \tag{49a}$$

$t=0$:

$$S(5p\pi, 5p\pi)=(4{,}233{,}600)^{-1}p^9[105A_8-168A_6+90A_4-32A_2+5A_0]$$

$t>0$:

$$S(5p\pi, 5p\pi)=(53{,}760)^{-1}p^9(1-t^2)^{9/2}[A_8(B_0-B_2)+A_6(3B_4-2B_2-B_0)+3A_4(B_2-B_6)+A_2(B_8+2B_6-3B_4)+A_0(B_6-B_8)] \tag{50}$$

SPECIAL FORMULAS FOR SLATER-AO OVERLAP INTEGRALS FOR $t=0$

$$S(1s, 1s)=e^{-p}[1+p+(1/3)p^2] \tag{51}$$

$$S(2s, 2s)=e^{-p}[1+p+(4/9)p^2+(1/9)p^3+(1/45)p^4] \tag{52}$$

$$S(3s, 3s)=e^{-p}[1+p+(7/15)p^2+(2/15)p^3+(2/75)p^4+(1/225)p^5+(1/1575)p^6] \tag{53}$$

$$S(5s,5s)=e^{-p}[1+p+(10/21)p^2+(1/7)p^3+(16/525)p^4+(8/1575)p^5+(8/11{,}025)p^6+(1/11{,}025)p^7+(1/99{,}225)p^8] \quad (54)$$

$$S(2p\sigma,2p\sigma)=e^{-p}[-1-p-(1/5)p^2+(2/15)p^3+(1/15)p^4] \quad (55)$$

$$S(3p\sigma,3p\sigma)=e^{-p}[-1-p-(9/25)p^2-(2/75)p^3+(34/1575)p^4+(13/1575)p^5+(1/525)p^6] \quad (56)$$

$$S(5p\sigma,5p\sigma)=e^{-p}[-1-p-(29/70)p^2-(17/210)p^3-(1/735)p^4+(1/294)p^5+(67/66{,}150)p^6+(13/66{,}150)p^7+(1/33{,}075)p^8] \quad (57)$$

$$S(2s,2p\sigma)=S(2p\sigma,2s)=(\sqrt{3}/6)e^{-p}[p+p^2+(7/15)p^3+(2/15)p^4] \quad (58)$$

$$S(3s,3p\sigma)=S(3p\sigma,3s)=(\sqrt{3}/9)e^{-p}[p+p^2+(12/25)p^3+(11/75)p^4+(17/525)p^5+(1/175)p^6] \quad (59)$$

$$S(5s,5p\sigma)=S(5p\sigma,5s)=(\sqrt{3}/12)e^{-p}[p+p^2+(17/35)p^3+(16/105)p^4+(128/3675)p^5+(23/3675)p^6+(31/33{,}075)p^7+(4/33{,}075)p^8] \quad (60)$$

$$S(2p\pi,2p\pi)=e^{-p}[1+p+(2/5)p^2+(1/15)p^3] \quad (61)$$

$$S(3p\pi,3p\pi)=e^{-p}[1+p+(34/75)p^2+(3/25)p^3+(31/1575)p^4+(1/525)p^5] \quad (62)$$

$$S(5p\pi,5p\pi)=e^{-p}[1+p+(33/70)p^2+(29/210)p^3+(41/1470)p^4+(1/245)p^5+(29/66{,}150)p^6+(1/33{,}075)p^7] \quad (63)$$

SPECIAL FORMULAS FOR SLATER-AO OVERLAP INTEGRALS FOR $p=0$

$$S(1s,1s)=(1-t^2)^{3/2} \quad (64)$$

$$S(1s,2s)=[(3/4)(1+t)^3(1-t)^5]^{\frac{1}{2}} \quad (65)$$

$$S(1s,3s)=[(2/5)(1+t)^3(1-t)^7]^{\frac{1}{2}} \quad (66)$$

$$S(1s,5s)=[(5/28)(1+t)^3(1-t)^9]^{\frac{1}{2}} \quad (67)$$

$$S(2s,2s)=-S(2p\sigma,2p\sigma)=S(2p\pi,2p\pi)=(1-t^2)^{5/2} \quad (68)$$

$$S(2s,3s)=-S(2p\sigma,3p\sigma)=S(2p\pi,3p\pi)=[(5/6)(1+t)^5(1-t)^7]^{\frac{1}{2}} \quad (69)$$

$$S(2s,5s)=-S(2p\sigma,5p\sigma)=S(2p\pi,5p\pi)=[(15/28)(1+t)^5(1-t)^9]^{\frac{1}{2}} \quad (70)$$

$$S(3s,3s)=-S(3p\sigma,3p\sigma)=S(3p\pi,3p\pi)=(1-t^2)^{7/2} \quad (71)$$

$$S(3s,5s)=-S(3p\sigma,5p\sigma)=S(3p\pi,5p\pi)=[(7/8)(1+t)^7(1-t)^9]^{\frac{1}{2}} \quad (72)$$

$$S(5s,5s)=-S(5p\sigma,5p\sigma)=S(5p\pi,5p\pi)=(1-t^2)^{9/2} \quad (73)$$

V. USE OF THE TABLES TO OBTAIN NON-SLATER OVERLAP INTEGRALS

Although the master formulas above and the master tables below are for Slater-AO overlap integrals, they can also be used in a relatively simple way to obtain S's for orthogonalized Slater AO's, for SCF AO's, for hybrid AO's, and in other ways. This follows from the definition of S in Eq. (1) and the fact that other types of AO's can be written as linear combinations of Slater AO's.

Va. Orthogonalized-Slater-AO Overlap Integrals

As a simple example for the case of orthogonalized Slater AO's, we have for $S^{or}(2s,2s)$ from Eqs. (1) and (8), using the atom-pair notation of (10):

$$S^{or}(2s_a,2s_b;R)=[S(2s_a,2s_b;R)-2QS(1s_a,2s_b;R)+Q^2S(1s_a,1s_b;R)]/(1-Q^2), \quad (74)$$

where $Q\equiv S(1s_a,2s_a)$. Using the parameter notation of (13), Eq. (74) becomes

$$S^{or}(2s,2s;p,t)=[S(2s,2s;p,t)-2QS(1s,2s;p,t)+Q^2S(1s,1s;p,t)]/(1-Q^2), \quad (75)$$

with $Q=S(1s,2s;0,t)$. It will be noted that the computation of S's corresponding to orthogonalized AO's involves the knowledge of internal Slater S's, like $S(1s_a,2s_a)$, and of other Slater S's involving inner-shell AO's, like $S(1s_a,2s_b)$ and $S(1s_a,1s_b)$ in Eq. (74). These, however, differ from like-designated outer-shell S's only in the particular ranges of p and t values needed. For internal S's we have $p=0$, but $t\neq 0$,—see Eqs. (64)–(73).

In the master tables, an effort has been made to include such ranges of p and t that orthogonalized-AO S's can be computed if desired. However, we believe that these are not likely to be important for the range

TABLE II. Comparison of Slater-AO with orthogonalized Slater-AO S's.

Integral	Slater AO's	Orthogonalized Slater AO's
$S(1s_H, 2s_C; 1.06A)$	0.575	0.572
$S(1s_H, 2s_{Li}; 1.60A)$	0.423	0.415
$S(2s_C, 2s_C; 1.20A)$	0.507	0.503
$S(2s_C, 2p\sigma_C; 1.20A)$	0.470	0.480

of R values (medium and large R) that occur for molecular problems. This conclusion is based on the sample cases in Table II, where it will be noted that the two sets of S values differ little, in spite of the rather considerable magnitude (0.220) of the integral $S(1s_C, 2s_C)$,—Q of Eq. (74),—which is involved in three of the cases. A wider variety of cases might of course sometimes disclose larger differences, but it seems unlikely that these would ever become important.

Vb. SCF-AO Overlap Integrals

We have made no extensive study of SCF-AO S's, but it is obvious from Eqs. (1) and (5) or (6) that these are approximately expressible as linear combinations of Slater S's similar to Eq. (75), although usually containing a number of terms. As an example, and for its own intrinsic interest, we have, however, computed $S^{SCF}(2p\pi_C, 2p\pi_C; R)$ and $S^{SCF}(2p\sigma_C, 2p\sigma_C; R)$. This was done after fitting the following normalized formula to the SCF $2p$ AO as given by Jucys in tabular numerical form[10] for the state $1s)^2 2s)^2 2p)^2$, ^1D:

$$\chi^{SCF}(2p_C) \approx 0.260\chi(2p; 2.694) + 0.518\chi(2p; 1.416) + 0.309\chi(2p; 0.898). \quad (76)$$

The formula applies equally to $2p\sigma$ or $2p\pi$. Each of the symbols $\chi(2p; \mu)$ denotes a $2p$ (σ or π) normalized Slater AO with R_{2p} of the form $N_\mu r e^{-\mu r/a_H}$ (see Eqs. (7)). A three-term formula (see Eq. (6)) was found necessary here to obtain a reasonably good fit to the numerical values of Jucys.

When Eq. (76), used for either $2p\sigma$ or $2p\pi$, is combined with Eq. (1), one obtains an expression for $S^{SCF}(2p\sigma_C, 2p\sigma_C; R)$ or $S^{SCF}(2p\pi_C, 2p\pi_C; R)$ as a linear combination of six terms involving Slater-AO S's. For a given R, all of these have different p values; three of them have $t=0$, the rest, other t values >0. Referring to the master tables for the necessary Slater S's, we obtained the $S^{SCF}(R)$ values given in Table III. The Table also includes comparisons with the corresponding simple Slater-AO quantities.

The foregoing example shows that good SCF AO's may give quite different S values than Slater AO's, especially at large R values.[11] When one examines the forms of SCF AO's as given by Hartree and other authors in numerical tables for such atoms as carbon and oxygen, it is seen that they differ characteristically from those of Slater and hydrogenic AO's in their more gradual decrease at large R values, especially for p AO's.[11a] This typical difference makes understandable the results set forth in Table III. For the computation of S values (and of other interatomic integrals used in molecular calculations) these results evidently raise much more serious questions than does the matter of orthogonalization. In particular, they suggest that non-neighbor interactions in polyatomic molecules may be relatively large. It might then seem that we ought to proceed to compute SCF S values for suitable parameter-ranges for the more important AO pairs. However, second thought brings to mind the fact that the best AO's for *atoms in molecules* must be very considerably different than in free atoms, even though we are not very well informed as to the exact nature of these differences and as to their variety in different molecular states. Still, for the case of AO's used in molecular states with stable binding, we would probably

TABLE III. Comparison of SCF and Slater S's for carbon-carbon $2p$ bonds.

R (A)	p (for Slater AO)	$S(2p\sigma_C, 2p\sigma_C; R)$ SCF	Slater	$S(2p\pi_C, 2p\pi_C; R)$ SCF	Slater
0.00	0.00	−1.00	−1.00	1.00	1.00
0.50	1.54	−0.53	−0.46	0.82	0.80
1.00	3.07	0.02	0.18	0.53	0.45
1.20	3.68	0.14	0.29	0.43	0.34
1.35	4.15	0.19	0.33	0.36	0.265
1.39	4.27	0.21	0.33	0.34	0.25
1.54	4.73	0.24	0.33	0.29	0.19
2.00	6.14	0.25	0.24	0.16	0.08
2.41	7.40	0.21	0.14	0.10	0.035
2.78	8.55	0.16	0.08	0.06	0.016
4.00	12.3	0.05	0.01	0.01	0.001

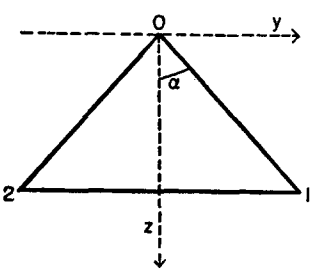

FIG. 2. Axes and notation for H_2O.

[10] A. Jucys, Proc. Roy. Soc. **173A**, 59 (1939); accurate SCF method including exchange. Jucys' $2p$ AO's are appreciably different for the states ^3P, ^1D, and ^1S, of which we have selected the ^1D, where the AO form approximates the average of those for the three cases. We should have preferred the presumably somewhat different SCF $2p$ AO for $2s2p^3$, but Jucys did not compute this.

[11] Our conclusions given above as to the smallness of the effect on S of orthogonalization (which introduces inner nodes into Slater's radially nodeless AO's) suggests that the inner nodes in SCF AO's might be dropped without much error for the computation of S values. That is, it might be adequate to retain only the outermost loop as Slater does; *provided*, however, this is represented by a sum of two or more exponential terms as in Eq. (76), instead of by a single Slater function.

[11a] *Note added in proof.* In subsequent work in this laboratory, Dr. H. Shull has found that in the case of $2s$ AO's there is little difference between SCF and Slater AO's except for small R values where the SCF AO has an inner loop. Hence S values computed using Slater ns AO's are nearly the same as using SCF ns AO's.

expect the free-atom AO's to be so modified as to correspond to *increased* rather than decreased overlap; and this increase should be relative to SCF AO's, and therefore all the more so relative to Slater AO's. Obviously the matter deserves further study. Obviously also, the exact values of Slater S's should not be taken too seriously.

Vc. Hybrid-AO Overlap Integrals

The computation of S values for hybrid AO's is a rather satisfying matter, since it is very easy to obtain these from Slater S's, and since the results are very striking. As discussed at the end of Section II, only σ-hybrid AO's can be formed from s and p AO's. The notation (see (10), (13)) and conventions of Section II for Slater-AO S's can be used without change for hybrid-Slater-AO S's.

In general, for a σ-bond between two atoms a and b, formed by AO's with respective hybridization coefficients α_a and α_b (see Eq. (9)), Eqs. (1) and (9) give

$$\begin{aligned}S^{\rm hy}(n_a x, n_b y; p, t)=&\alpha_a\alpha_b S(n_a s, n_b s; p, t)\\&+\sigma_b\alpha_a(1-\alpha_b^2)^{\frac{1}{2}}S(n_a s, n_b p\sigma; p, t)\\&+\sigma_a\alpha_b(1-\alpha_a^2)^{\frac{1}{2}}S(n_a p\sigma, n_b s; p, t)\\&+\sigma_a\sigma_b(1-\alpha_a^2)^{\frac{1}{2}}(1-\alpha_b^2)^{\frac{1}{2}}S(n_a p\sigma, n_b p\sigma; p, t),\end{aligned}\quad(77)$$

where σ_a and σ_b denote the signs before $(1-\alpha^2)^{\frac{1}{2}}$ in Eq. (9), and the parameter-pair p, t have the same values in all the integrals. For a homopolar bond this reduces to

$$\begin{aligned}S^{\rm hy}(nx, nx; p, 0)=&\alpha^2 S(ns, ns; p, 0)\\&\pm 2\alpha(1-\alpha^2)^{\frac{1}{2}}S(ns, np\sigma; p, 0)\\&+(1-\alpha^2)S(np\sigma, np\sigma; p, 0).\end{aligned}\quad(78)$$

For a bond between a $1s$ hydrogen atom AO and a hybrid σ-AO of another atom b, it becomes

$$\begin{aligned}S^{\rm hy}(1s_{\rm H}, n_b y; p, t)=&\alpha_b S(1s_{\rm H}, ns_b; p, t)\\&\pm(1-\alpha_b^2)^{\frac{1}{2}}S(1s_{\rm H}, np\sigma_b; p, t).\end{aligned}\quad(79)$$

In order to obtain numerical values of S for any given hybrid case, it is necessary only to specify α_a and α_b, then to look up the appropriate Slater-AO S values in the master tables, and finally to form linear combinations in accordance with Eqs. (77)–(79). If desired, S values corresponding to hybrid orthogonalized Slater AO's,[6] or to hybrid SCF AO's, can similarly be obtained by using Eqs. (77)–(79) in connection with orthogonalized or SCF pure-AO S values.

Since S values for any desired pair of Slater-AO hybrids can readily be obtained using Eqs. (77)–(79) and the master tables, no extensive hybrid tables will be given here. Nevertheless, two sets of Slater-AO hybrid S tables (Tables XXIV–XXVIII) have been computed explicitly in order to aid the reader in appreciating quantitatively the rather remarkable effects of hybridization on S values. Further examples of hybrid S values for specific molecules, and a discussion, will be given in a following paper.[11b]

[11b] For a preliminary report, see J. Chem. Phys. **17**, 510 (1949).

Vd. Group Overlap Integrals

A further simple application of the present tables is to the computation of overlap integrals in which one or both atoms are replaced by groups of atoms. S's of this sort frequently occur when one is working with non-localized MO's (molecular orbitals) in LCAO approximation. The non-localized MO structure of H_2O furnishes a convenient example. Neglecting s, p hybridization, the electron configuration may be written:

$$\begin{aligned}(1s_{\rm O})^2(2s_{\rm O})^2(a2py_{\rm O}+b[1s_1-1s_2])^2(c2pz_{\rm O}\\+d[1s_1+1s_2])^2(2px_{\rm O})^2.\end{aligned}\quad(80)$$

Here the two bonding MO's have been written out in LCAO form (see Fig. 2 for notation). In connection with these MO's, the overlap integrals

$$\left.\begin{aligned}S(y_{\rm O}, s-s)&\equiv\int 2py_{\rm O}[(1s_1-1s_2)/(2-2S_{1s_1 1s_2})^{\frac{1}{2}}]d\tau\\S(z_{\rm O}, s+s)&\equiv\int 2pz_{\rm O}[(1s_1+1s_2)/(2+2S_{1s_1 1s_2})^{\frac{1}{2}}]d\tau\end{aligned}\right\}\quad(81)$$

are of interest. The internal H—H group normalization factors $(2\pm 2S_{1s,\,1s})^{\frac{1}{2}}$ are obtained using the $S(1s, 1s)$ master table. The remaining integrals are easily evaluated by writing $2py_{\rm O}$ or $2pz_{\rm O}$ as a linear combination of a $2p\sigma$ and a $2p\pi$ function, relative to the axis of *either* the O—H_1 or the O—H_2 bond. Thus

$$\begin{aligned}2py_{\rm O}&=(\sin\alpha)(2p\sigma_1)+(\cos\alpha)(2p\pi_1)\\&=-(\sin\alpha)(2p\sigma_2)-(\cos\alpha)(2p\pi_2),\\2pz_{\rm O}&=(\cos\alpha)(2p\sigma_1)+(\sin\alpha)(2p\pi_1)\\&=(\cos\alpha)(2p\sigma_2)+(\sin\alpha)(2p\pi_2).\end{aligned}$$

On substituting into the expressions for $S(y_{\rm O}, s-s)$ and $S(z_{\rm O}, s+s)$ above, and noting that $\int 2p\pi_i 1s_i d\tau=0$, we obtain

$$\left.\begin{aligned}S(y_{\rm O}, s-s)&=\sqrt{2}\,\sin\alpha[1-S(1s_{\rm H}, 1s_{\rm H}; R_{12})]^{-\frac{1}{2}}\\&\quad\times S(1s, 2p\sigma; {\rm H-O}),\\S(z_{\rm O}, s+s)&=\sqrt{2}\,\cos\alpha[1+S(1s_{\rm H}, 1s_{\rm H}; R_{12})]^{-\frac{1}{2}}\\&\quad\times S(1s, 2p\sigma; {\rm H-O}).\end{aligned}\right\}\quad(82)$$

Here the notation of (10), (13) has been used in a convenient way for the S's.

Equations (82) illustrate how the computation or even the mere formulation of group overlap integrals affords added insight into the bonding characteristics of non-localized MO's. If 2α in H_2O were 90°, Eqs. (82) would give

$$S(y_{\rm O}, s-s)\approx S(z_{\rm O}, s+s)\approx S(1s, 2p\sigma; {\rm H-O}),$$

the same integral that would occur using localized MO's or using the valence-bond AO method. Actually, the experimental $2\alpha=105°$ makes $S(y_{\rm O}, s-s)$ distinctly larger and $S(z_{\rm O}, s+s)$ distinctly smaller than this; the factors $(1\mp S_{1s,\,1s})^{\frac{1}{2}}$ enhance this effect considerably. To the extent that S values can be taken as measures

of bonding strengths (see following paper), this indicates that the $y_O+(1s-1s)$ MO is more strongly bonding in H_2O than the $z_O+(1s+1s)$; also that the binding (i.e., ionization) energies of the two MO's are in the same order.

The discussion could be further elaborated by a consideration of s, p hybridization, which is undoubtedly of some importance here. For reasons of symmetry, this can affect only the $[z_O+(1s+1s)]$ MO in the non-localized MO treatment; the result must be that the $2s_O$ AO in (80) acquires some MO bonding properties and the bonding character of $[z_O+(1s+1s)]$ is further weakened; but with an over-all gain in bonding. $S(z_O, s+s)$ in Eqs. (81) now is replaced by a linear combination including $S(2s_O, s+s)$, the final S being easily computed as a function of the extent of hybridization if this were known.

Group overlap integrals can be used to obtain insight into bond strengths in many molecular problems, for example in the study of hyperconjugation. This subject will not be developed here, however, since the object of the present paper is to give methods rather than to discuss applications.

Ve. Transition Moment Integrals

Certain transition moment integrals for electronic transitions in homopolar diatomic molecules can be obtained very simply from overlap integrals,[12] for example:

$$Q_{\pi\sigma'} \equiv \int \chi_{np\pi_x} \times \chi_{np\sigma'} d\tau = \tfrac{1}{2} RS(np\pi, np\pi; p, 0). \quad (83)$$

ACKNOWLEDGMENT

We are very greatly indebted to Mr. Tracy J. Kinyon for his cooperation in the preparation of the tables. Mr. Kinyon carried through the arduous task of making all the extensive numerical computations for the tables in Sections VI and VII.

VI. MASTER TABLES FOR SLATER-AO OVERLAP INTEGRALS**

TABLE IV.

$S(1s, 1s)$

p	$t=0.0$	$t=0.1$	$t=0.2$	$t=0.3$	$t=0.4$	$t=0.5$	$t=0.6$	$t=0.7$	$t=0.8$
0.0	1.000	0.985	0.941	0.868	0.770	0.650	0.512	0.364	0.216
0.5	0.960	0.946	0.905	0.837	0.744	0.630	0.499	0.357	0.213
1.0	0.858	0.847	0.812	0.756	0.678	0.580	0.465	0.337	0.205
1.2	0.807	0.797	0.766	0.715	0.644	0.554	0.447	0.327	0.200
1.3	0.780								
1.4	0.753	0.744	0.717	0.671	0.608	0.526	0.428	0.316	0.196
1.5	0.725								
1.6	0.697	0.689	0.666	0.626	0.570	0.498	0.409	0.305	0.191
1.7	0.669								
1.8	0.641	0.635	0.615	0.581	0.533	0.469	0.388	0.293	0.185
1.9	0.614								
2.0	0.586	0.581	0.565	0.536	0.495	0.439	0.368	0.281	0.180
2.1	0.560								
2.2	0.533	0.529	0.515	0.493	0.458	0.410	0.348	0.269	0.175
2.3	0.508								
2.4	0.483	0.479	0.469	0.451	0.423	0.382	0.328	0.256	0.169
2.5	0.458								
2.6	0.435	0.432	0.425	0.411	0.388	0.355	0.308	0.244	0.164
2.7	0.412								
2.8	0.390	0.388	0.383	0.373	0.356	0.329	0.289	0.233	0.158
2.9	0.369								
3.0	0.349	0.348	0.344	0.338	0.325	0.304	0.271	0.221	0.153
3.2	0.310	0.310	0.309	0.305	0.297	0.281	0.254	0.210	0.148

$S(1s, 1s)$

p	$t=0.0$	$t=0.1$	$t=0.2$	$t=0.3$	$t=0.4$	$t=0.5$	$t=0.6$	$t=0.7$	$t=0.8$
3.4	0.275	0.276	0.276	0.274	0.270	0.259	0.237	0.200	0.143
3.5	0.259								
3.6	0.244	0.244	0.246	0.247	0.245	0.238	0.221	0.189	0.138
3.8	0.215	0.216	0.218	0.221	0.222	0.219	0.206	0.180	0.133
4.0	0.189	0.190	0.194	0.198	0.201	0.201	0.192	0.170	0.128
4.2	0.166	0.167	0.171	0.176	0.182	0.184	0.179	0.161	0.123
4.4	0.146	0.147	0.151	0.157	0.164	0.168	0.166	0.152	0.119
4.5	0.136								
4.6	0.127	0.129	0.133	0.140	0.148	0.154	0.155	0.144	0.114
5.0	0.097	0.098	0.103	0.110	0.120	0.129	0.134	0.129	0.106
5.5	0.068	0.069	0.074	0.082	0.091	0.102	0.111	0.112	0.097
6.0	0.047	0.049	0.053	0.060	0.070	0.081	0.092	0.097	0.088
6.5	0.032	0.034	0.037	0.044	0.053	0.064	0.076	0.084	0.080
7.0	0.022	0.023	0.026	0.032	0.040	0.050	0.063	0.073	0.072
7.5	0.015	0.016	0.018	0.023	0.030	0.040	0.052	0.063	0.066
8.0	0.010	0.011	0.013	0.017	0.023	0.031	0.043	0.054	0.059
9.0	0.005	0.005	0.006	0.009	0.013	0.019	0.029	0.040	0.049
10.0	0.002	0.002	0.003	0.004	0.007	0.012	0.019	0.030	0.040
12.0	0.000	0.000	0.001	0.001	0.002	0.004	0.009	0.017	0.027
15.0	0.000	0.000	0.000	0.000	0.000	0.001	0.003	0.007	0.015
20.0	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.002	0.005

TABLE V.

$S(1s, 2s)$

p	$t=-0.5$	$t=-0.4$	$t=-0.3$	$t=-0.2$	$t=-0.1$	$t=0.0$	$t=0.1$	$t=0.2$	$t=0.3$	$t=0.4$	$t=0.5$	$t=0.6$	$t=0.7$	$t=0.8$	$t=0.9$
0.0	0.844	0.933	0.977	0.978	0.938	0.866	0.768	0.652	0.526	0.400	0.281	0.177	0.095	0.037	0.007
0.5	0.829	0.916	0.959	0.960	0.923	0.854	0.760	0.647	0.525	0.401	0.284	0.180	0.097	0.039	0.007
1.0	0.787	0.866	0.906	0.907	0.875	0.814	0.730	0.628	0.516	0.400	0.288	0.186	0.102	0.042	0.008
1.5	0.722	0.790	0.823	0.825	0.799	0.749	0.679	0.593	0.496	0.393	0.290	0.192	0.109	0.046	0.009
2.0	0.644	0.697	0.722	0.723	0.702	0.664	0.610	0.542	0.463	0.376	0.285	0.195	0.114	0.050	0.011
2.2	0.611	0.657	0.679	0.679	0.661	0.627	0.579	0.519	0.447	0.367	0.282	0.196	0.116	0.051	0.011
2.4	0.577	0.617	0.635	0.635	0.619	0.589	0.547	0.494	0.430	0.357	0.277	0.195	0.117	0.053	0.012
2.6	0.543	0.578	0.592	0.591	0.576	0.550	0.514	0.468	0.411	0.345	0.272	0.194	0.119	0.054	0.012
2.8	0.510	0.539	0.550	0.547	0.534	0.512	0.481	0.441	0.392	0.333	0.265	0.192	0.119	0.055	0.013
3.0	0.478	0.501	0.508	0.505	0.493	0.474	0.448	0.414	0.372	0.320	0.258	0.190	0.120	0.057	0.013
3.2	0.446	0.464	0.468	0.464	0.453	0.437	0.416	0.388	0.352	0.306	0.251	0.187	0.120	0.058	0.014
3.4	0.416	0.428	0.430	0.425	0.415	0.402	0.384	0.361	0.331	0.292	0.243	0.184	0.120	0.058	0.014
3.6	0.386	0.395	0.394	0.388	0.379	0.368	0.354	0.336	0.311	0.278	0.234	0.180	0.119	0.059	0.014

[12] R. S. Mulliken, J. Chem. Phys. 8, 238 (1940), footnote 14. (In this footnote, Eq. (12) should read Eq. (15).)

** See Section III, especially Eqs. (12), (13), for definitions and conventions.

TABLE V.—(*Con't*)

						$S(1s, 2s)$									
p	$t=-0.5$	$t=-0.4$	$t=-0.3$	$t=-0.2$	$t=-0.1$	$t=0.0$	$t=0.1$	$t=0.2$	$t=0.3$	$t=0.4$	$t=0.5$	$t=0.6$	$t=0.7$	$t=0.8$	$t=0.9$
3.8						0.335	0.325	0.311	0.291	0.263	0.225	0.176	0.119	0.060	0.015
4.0	0.332	0.333	0.327	0.320	0.312	0.305	0.297	0.287	0.272	0.249	0.216	0.172	0.118	0.060	0.015
4.2						0.276	0.271	0.264	0.253	0.235	0.207	0.167	0.116	0.061	0.016
4.4						0.250	0.246	0.242	0.235	0.221	0.198	0.162	0.115	0.061	0.016
4.5	0.272	0.265	0.256	0.247	0.241										
4.6						0.225	0.223	0.221	0.217	0.208	0.189	0.157	0.113	0.061	0.016
5.0	0.221	0.209	0.197	0.188	0.183	0.181	0.182	0.184	0.185	0.182	0.170	0.147	0.109	0.062	0.017
5.5						0.136	0.139	0.144	0.149	0.152	0.149	0.134	0.104	0.061	0.018
6.0	0.143	0.127	0.114	0.105	0.101	0.101	0.105	0.111	0.119	0.126	0.128	0.120	0.098	0.060	0.018
6.5						0.074	0.078	0.085	0.094	0.104	0.110	0.108	0.092	0.059	0.019
7.0	0.091	0.075	0.063	0.056	0.053	0.054	0.058	0.065	0.074	0.085	0.093	0.096	0.086	0.058	0.019
7.5						0.039	0.042	0.048	0.058	0.068	0.079	0.085	0.079	0.056	0.020
8.0	0.057	0.044	0.034	0.029	0.027	0.027	0.030	0.036	0.044	0.055	0.066	0.075	0.073	0.054	0.020
9.0						0.014	0.016	0.020	0.026	0.035	0.046	0.057	0.061	0.050	0.020
10.0						0.007	0.008	0.010	0.015	0.022	0.032	0.043	0.051	0.046	0.020
12.0						0.001	0.002	0.003	0.005	0.008	0.014	0.023	0.034	0.037	0.020
15.0						0.000	0.000	0.000	0.001	0.002	0.004	0.009	0.017	0.025	0.019
20.0						0.000	0.000	0.000	0.000	0.000	0.000	0.002	0.005	0.013	0.015

TABLE VI.

						$S(1s, 2p\sigma)$							
p	$t=-0.5$	$t=-0.4$	$t=-0.3$	$t=-0.2$	$t=-0.1$	$t=0.0$	$t=0.1$	$t=0.2$	$t=0.3$	$t=0.4$	$t=0.5$	$t=0.6$	$t=0.7$	$t=0.8$
0.0	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
0.5	0.117	0.155	0.189	0.216	0.234	0.240	0.235	0.218	0.191	0.157	0.119	0.080	0.046	0.022
1.0	0.208	0.276	0.336	0.385	0.417	0.429	0.421	0.394	0.348	0.288	0.220	0.151	0.087	0.038
1.5	0.264	0.348	0.423	0.484	0.525	0.544	0.538	0.507	0.454	0.381	0.296	0.206	0.121	0.054
2.0	0.287	0.375	0.454	0.518	0.564	0.586	0.585	0.558	0.506	0.433	0.344	0.245	0.148	0.067
2.2	0.289	0.375	0.453	0.517	0.563	0.587	0.587	0.563	0.515	0.444	0.355	0.256	0.156	0.071
2.4	0.287	0.371	0.447	0.509	0.554	0.579	0.582	0.561	0.517	0.449	0.363	0.264	0.164	0.076
2.6	0.282	0.363	0.435	0.495	0.540	0.565	0.570	0.553	0.513	0.450	0.368	0.271	0.170	0.079
2.8	0.275	0.352	0.420	0.477	0.520	0.546	0.553	0.540	0.505	0.447	0.369	0.275	0.175	0.083
3.0	0.266	0.338	0.402	0.456	0.497	0.523	0.532	0.522	0.492	0.441	0.368	0.278	0.179	0.086
3.2	0.255	0.323	0.382	0.432	0.471	0.497	0.508	0.502	0.477	0.431	0.364	0.279	0.182	0.089
3.4	0.244	0.306	0.361	0.407	0.443	0.468	0.481	0.479	0.459	0.419	0.359	0.278	0.184	0.091
3.6	0.232	0.289	0.338	0.380	0.414	0.439	0.453	0.454	0.439	0.406	0.351	0.276	0.186	0.093
3.8						0.409	0.424	0.428	0.418	0.390	0.342	0.273	0.186	0.095
4.0	0.207	0.253	0.293	0.327	0.356	0.379	0.394	0.401	0.396	0.374	0.332	0.269	0.186	0.097
4.2						0.349	0.365	0.374	0.373	0.357	0.321	0.264	0.186	0.098
4.4						0.320	0.337	0.348	0.350	0.339	0.310	0.258	0.185	0.099
4.5	0.176	0.210	0.239	0.264	0.286									
4.6						0.293	0.309	0.322	0.328	0.321	0.298	0.252	0.183	0.100
5.0	0.147	0.171	0.190	0.208	0.225	0.241	0.258	0.273	0.284	0.286	0.272	0.238	0.179	0.101
5.5						0.186	0.202	0.219	0.234	0.243	0.241	0.219	0.172	0.102
6.0	0.099	0.108	0.115	0.122	0.130	0.141	0.155	0.172	0.189	0.204	0.210	0.199	0.163	0.101
6.5						0.105	0.118	0.133	0.151	0.169	0.181	0.179	0.154	0.100
7.0	0.064	0.066	0.066	0.068	0.071	0.078	0.088	0.102	0.120	0.139	0.155	0.160	0.144	0.098
7.5						0.057	0.065	0.077	0.094	0.113	0.132	0.142	0.134	0.095
8.0	0.041	0.039	0.037	0.036	0.037	0.041	0.048	0.058	0.073	0.092	0.111	0.126	0.124	0.092
9.0						0.021	0.025	0.032	0.043	0.059	0.078	0.097	0.104	0.086
10.0						0.010	0.013	0.017	0.025	0.037	0.054	0.073	0.087	0.078
12.0						0.002	0.003	0.005	0.008	0.014	0.025	0.040	0.058	0.063
15.0						0.000	0.000	0.001	0.001	0.003	0.007	0.015	0.030	0.044
20.0						0.000	0.000	0.000	0.000	0.000	0.001	0.003	0.009	0.022

TABLE VII.

					$S(1s, 3s)$				
p	$t=-0.4$	$t=-0.3$	$t=-0.2$	$t=-0.1$	$t=0.0$	$t=0.1$	$t=0.2$	$t=0.3$	$t=0.4$
0.0	0.954	0.928	0.857	0.754	0.632	0.505	0.381	0.269	0.175
0.5	0.945	0.920	0.851	0.751	0.632	0.507	0.384	0.273	0.179
1.0	0.915	0.893	0.832	0.739	0.628	0.510	0.393	0.284	0.190
1.5	0.864	0.847	0.792	0.713	0.615	0.508	0.399	0.295	0.203
2.0	0.794	0.780	0.736	0.670	0.588	0.495	0.399	0.304	0.215
2.5	0.712	0.701	0.665	0.612	0.546	0.470	0.389	0.306	0.224
3.0	0.623	0.612	0.584	0.544	0.494	0.436	0.370	0.299	0.227
3.2	0.587	0.575	0.551	0.515	0.471	0.419	0.360	0.295	0.226
3.4	0.551	0.539	0.516	0.486	0.447	0.402	0.347	0.289	0.225
3.6	0.516	0.504	0.483	0.456	0.423	0.383	0.334	0.283	0.223
3.8	0.481	0.469	0.450	0.426	0.398	0.364	0.320	0.275	0.220
4.0	0.448	0.435	0.418	0.397	0.373	0.344	0.309	0.267	0.217
4.2	0.416	0.403	0.386	0.369	0.348	0.324	0.295	0.257	0.212

					$S(1s, 3s)$				
p	$t=-0.4$	$t=-0.3$	$t=-0.2$	$t=-0.1$	$t=0.0$	$t=0.1$	$t=0.2$	$t=0.3$	$t=0.4$
4.4	0.385	0.371	0.356	0.341	0.324	0.305	0.280	0.248	0.207
4.6	0.355	0.341	0.327	0.314	0.301	0.285	0.265	0.238	0.202
4.8	0.327	0.312	0.300	0.288	0.279	0.266	0.249	0.227	0.195
5.0	0.301	0.287	0.274	0.265	0.256	0.248	0.235	0.217	0.190
5.5	0.242	0.227	0.216	0.210	0.206	0.204	0.200	0.190	0.173
6.0	0.193	0.178	0.168	0.164	0.163	0.165	0.166	0.164	0.155
6.5	0.152	0.137	0.129	0.126	0.127	0.132	0.137	0.140	0.137
7.0	0.119	0.105	0.098	0.096	0.098	0.104	0.111	0.117	0.120
7.5	0.092	0.080	0.073	0.072	0.074	0.080	0.089	0.098	0.104
8.0	0.071	0.060	0.054	0.053	0.056	0.062	0.070	0.080	0.089
9.0	0.042	0.033	0.029	0.028	0.030	0.035	0.043	0.053	0.064
10.0	0.024	0.018	0.015	0.015	0.016	0.020	0.025	0.034	0.044

TABLE VIII.

$S(1s, 3p\sigma)$

p	$t=-0.4$	$t=-0.3$	$t=-0.2$	$t=-0.1$	$t=0.0$	$t=0.1$	$t=0.2$	$t=0.3$	$t=0.4$
0.0	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
0.5	0.162	0.183	0.194	0.192	0.179	0.158	0.130	0.100	0.071
1.0	0.302	0.343	0.363	0.362	0.340	0.302	0.251	0.195	0.139
1.5	0.404	0.461	0.490	0.491	0.466	0.418	0.353	0.278	0.202
2.0	0.464	0.529	0.565	0.571	0.547	0.497	0.427	0.343	0.255
2.5	0.483	0.550	0.590	0.601	0.582	0.538	0.470	0.387	0.294
3.0	0.470	0.534	0.574	0.589	0.578	0.543	0.485	0.408	0.320
3.2	0.458	0.520	0.559	0.575	0.567	0.536	0.483	0.411	0.326
3.4	0.444	0.502	0.541	0.558	0.553	0.526	0.478	0.412	0.330
3.6	0.427	0.482	0.519	0.536	0.535	0.512	0.470	0.409	0.332
3.8	0.408	0.460	0.495	0.513	0.514	0.496	0.459	0.404	0.332
4.0	0.388	0.436	0.469	0.487	0.490	0.477	0.446	0.397	0.330
4.2	0.367	0.411	0.442	0.460	0.466	0.457	0.431	0.388	0.327
4.4	0.346	0.386	0.415	0.433	0.440	0.435	0.415	0.377	0.323
4.6	0.325	0.360	0.387	0.405	0.414	0.412	0.397	0.366	0.317
4.8	0.303	0.335	0.360	0.377	0.387	0.388	0.378	0.352	0.309
5.0	0.283	0.311	0.333	0.350	0.361	0.365	0.359	0.339	0.302
5.5	0.234	0.254	0.270	0.285	0.297	0.307	0.310	0.302	0.279
6.0	0.190	0.203	0.215	0.227	0.240	0.253	0.262	0.264	0.253
6.5	0.153	0.160	0.168	0.178	0.190	0.204	0.218	0.227	0.225
7.0	0.121	0.125	0.129	0.137	0.148	0.162	0.178	0.192	0.198
7.5	0.096	0.096	0.098	0.104	0.114	0.127	0.144	0.161	0.173
8.0	0.074	0.073	0.074	0.078	0.086	0.099	0.115	0.133	0.149
9.0	0.044	0.041	0.040	0.042	0.048	0.057	0.071	0.088	0.107
10.0	0.026	0.023	0.021	0.022	0.026	0.032	0.042	0.057	0.075

TABLE IX.

$S(1s, 5s)$

p	$t=-0.4$	$t=-0.3$	$t=-0.2$	$t=-0.1$	$t=0.0$	$t=0.1$	$t=0.2$	$t=0.3$	$t=0.4$
0.0	0.893	0.806	0.687	0.554	0.423	0.303	0.204	0.126	0.070
0.5	0.888	0.803	0.687	0.556	0.426	0.308	0.208	0.129	0.073
1.0	0.873	0.795	0.685	0.560	0.435	0.313	0.219	0.139	0.080
1.5	0.846	0.776	0.676	0.562	0.444	0.333	0.234	0.153	0.091
2.0	0.805	0.745	0.658	0.557	0.450	0.346	0.251	0.169	0.104
2.5	0.749	0.699	0.627	0.540	0.448	0.354	0.265	0.185	0.118
3.0	0.682	0.642	0.583	0.513	0.435	0.354	0.273	0.198	0.131
3.2	0.653	0.616	0.562	0.498	0.427	0.351	0.275	0.202	0.135
3.4	0.624	0.589	0.540	0.482	0.417	0.347	0.275	0.205	0.140
3.6	0.593	0.561	0.517	0.465	0.406	0.342	0.275	0.207	0.143
3.8	0.562	0.533	0.493	0.447	0.394	0.335	0.273	0.209	0.147
4.0	0.531	0.504	0.468	0.427	0.380	0.327	0.270	0.209	0.149
4.5	0.454	0.432	0.405	0.376	0.341	0.303	0.257	0.208	0.154
5.0	0.384	0.363	0.343	0.323	0.300	0.273	0.240	0.200	0.154
5.5	0.319	0.300	0.285	0.272	0.258	0.242	0.219	0.190	0.152
6.0	0.261	0.244	0.232	0.224	0.218	0.209	0.196	0.176	0.147
6.5	0.213	0.197	0.187	0.183	0.181	0.179	0.173	0.161	0.140
7.0	0.170	0.155	0.147	0.145	0.147	0.149	0.149	0.144	0.130
7.5	0.135	0.121	0.115	0.114	0.117	0.123	0.127	0.127	0.120
8.0	0.106	0.094	0.089	0.089	0.093	0.100	0.107	0.111	0.109
9.0	0.065	0.055	0.051	0.052	0.056	0.063	0.073	0.082	0.087
10.0	0.039	0.031	0.028	0.029	0.032	0.039	0.048	0.058	0.067

TABLE X.

$S(1s, 5p\sigma)$

p	$t=-0.4$	$t=-0.3$	$t=-0.2$	$t=-0.1$	$t=0.0$	$t=0.1$	$t=0.2$	$t=0.3$	$t=0.4$
0.0	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
0.5	0.153	0.161	0.157	0.143	0.121	0.096	0.071	0.047	0.029
1.0	0.293	0.310	0.304	0.278	0.238	0.190	0.141	0.096	0.059
1.5	0.409	0.435	0.429	0.397	0.344	0.279	0.210	0.146	0.091
2.0	0.493	0.526	0.524	0.490	0.431	0.355	0.273	0.194	0.124
2.5	0.540	0.580	0.581	0.550	0.493	0.414	0.326	0.238	0.157
3.0	0.553	0.596	0.603	0.579	0.526	0.453	0.366	0.274	0.186
3.2	0.550	0.593	0.603	0.581	0.532	0.462	0.377	0.286	0.197
3.4	0.543	0.586	0.597	0.578	0.534	0.467	0.385	0.296	0.207
3.6	0.532	0.574	0.587	0.572	0.531	0.470	0.392	0.304	0.215
3.8	0.518	0.559	0.573	0.561	0.526	0.469	0.395	0.311	0.223
4.0	0.501	0.541	0.556	0.548	0.516	0.465	0.396	0.316	0.230
4.5	0.453	0.488	0.504	0.502	0.482	0.445	0.390	0.321	0.242
5.0	0.396	0.426	0.442	0.445	0.436	0.412	0.372	0.316	0.247
5.5	0.339	0.363	0.377	0.384	0.383	0.371	0.345	0.303	0.246
6.0	0.285	0.302	0.315	0.324	0.328	0.326	0.313	0.285	0.240
6.5	0.237	0.248	0.258	0.268	0.277	0.282	0.279	0.263	0.230
7.0	0.192	0.199	0.206	0.216	0.227	0.237	0.242	0.237	0.216
7.5	0.155	0.158	0.163	0.172	0.184	0.197	0.208	0.211	0.200
8.0	0.123	0.124	0.127	0.135	0.147	0.161	0.175	0.185	0.182
9.0	0.076	0.074	0.074	0.080	0.090	0.104	0.121	0.137	0.147
10.0	0.046	0.042	0.042	0.045	0.052	0.064	0.079	0.098	0.114

TABLE XI.

$S(2s, 2s)$

p	$t=0.0$	$t=0.1$	$t=0.2$	$t=0.3$	$t=0.4$	$t=0.5$	$t=0.6$
0.0	1.000	0.975	0.903	0.790	0.647	0.487	0.328
0.5	0.986	0.962	0.892	0.782	0.642	0.486	0.328
1.0	0.948	0.926	0.862	0.760	0.629	0.481	0.329
1.5	0.890	0.871	0.815	0.725	0.608	0.472	0.329
2.0	0.815	0.799	0.753	0.678	0.578	0.458	0.327
2.5	0.729	0.717	0.679	0.622	0.540	0.438	0.322
3.0	0.637	0.629	0.603	0.559	0.496	0.413	0.312
3.2	0.600	0.593	0.571	0.533	0.477	0.402	0.308
3.4	0.563	0.557	0.539	0.507	0.457	0.389	0.302
3.6	0.527	0.522	0.507	0.480	0.438	0.377	0.296
3.8	0.491	0.487	0.476	0.454	0.417	0.364	0.290
4.0	0.456	0.454	0.445	0.427	0.397	0.350	0.283
4.2	0.423	0.421	0.415	0.402	0.377	0.336	0.276
4.4	0.390	0.389	0.386	0.376	0.357	0.323	0.268
4.6	0.360	0.359	0.358	0.352	0.337	0.309	0.260
4.8	0.330	0.331	0.331	0.328	0.318	0.295	0.252
5.0	0.302	0.307	0.305	0.305	0.299	0.281	0.244
5.5	0.240	0.242	0.247	0.252	0.255	0.248	0.223
6.0	0.188	0.190	0.197	0.206	0.215	0.216	0.203
6.5	0.145	0.148	0.155	0.167	0.179	0.187	0.182
7.0	0.111	0.113	0.121	0.133	0.148	0.160	0.163
7.5	0.083	0.086	0.093	0.106	0.121	0.136	0.145
8.0	0.062	0.064	0.071	0.083	0.099	0.116	0.128
8.5	0.046	0.048	0.054	0.065	0.080	0.097	0.112
9.0	0.034	0.035	0.041	0.050	0.064	0.082	0.098
9.5	0.024	0.026	0.030	0.039	0.051	0.068	0.086
10.0	0.018	0.019	0.023	0.030	0.041	0.057	0.075
10.5	0.013	0.014	0.017	0.023	0.032	0.047	0.065
11.0	0.009	0.010	0.012	0.017	0.026	0.039	0.056
11.5	0.006	0.007	0.009	0.013	0.020	0.032	0.048
12.0	0.004	0.005	0.007	0.010	0.016	0.026	0.041
12.5	0.003	0.004	0.005	0.007	0.012	0.021	0.036
13.0	0.002	0.002	0.003	0.006	0.010	0.017	0.030
13.5	0.002	0.002	0.002	0.004	0.008	0.014	0.026
14.0	0.001	0.001	0.002	0.003	0.006	0.012	0.022

TABLE XII.

	$S(2p\sigma, 2s)$						$S(2s, 2p\sigma)$						
p	$t=0.6$	$t=0.5$	$t=0.4$	$t=0.3$	$t=0.2$	$t=0.1$	$t=0.0$	$t=0.1$	$t=0.2$	$t=0.3$	$t=0.4$	$t=0.5$	$t=0.6$
0.0	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
0.5	−0.008	0.002	0.020	0.047	0.079	0.112	0.143	0.167	0.180	0.180	0.166	0.139	0.103
1.0	−0.010	0.011	0.047	0.098	0.158	0.220	0.276	0.319	0.343	0.342	0.315	0.265	0.198
1.5	−0.005	0.028	0.081	0.151	0.231	0.313	0.386	0.443	0.473	0.472	0.437	0.369	0.278
2.0	0.006	0.049	0.114	0.197	0.289	0.381	0.464	0.526	0.561	0.560	0.521	0.446	0.340
2.5	0.019	0.070	0.143	0.218	0.327	0.420	0.504	0.567	0.603	0.602	0.569	0.493	0.383
3.0	0.033	0.089	0.163	0.251	0.342	0.431	0.509	0.570	0.606	0.612	0.582	0.513	0.407
3.2	0.037	0.096	0.169	0.254	0.342	0.427	0.503	0.562	0.598	0.606	0.580	0.515	0.412
3.4	0.042	0.099	0.173	0.255	0.339	0.421	0.492	0.549	0.586	0.596	0.573	0.513	0.415
3.6	0.046	0.103	0.175	0.254	0.335	0.411	0.479	0.534	0.570	0.582	0.563	0.509	0.416
3.8	0.049	0.106	0.176	0.252	0.327	0.399	0.463	0.515	0.551	0.565	0.550	0.502	0.415
4.0	0.052	0.109	0.176	0.247	0.318	0.385	0.444	0.494	0.529	0.545	0.535	0.492	0.412
4.2	0.055	0.110	0.174	0.241	0.307	0.369	0.425	0.471	0.505	0.523	0.518	0.481	0.407
4.4	0.057	0.111	0.172	0.234	0.295	0.351	0.402	0.446	0.480	0.500	0.499	0.469	0.401
4.6	0.059	0.111	0.168	0.226	0.281	0.333	0.380	0.421	0.455	0.476	0.479	0.454	0.394
4.8	0.060	0.110	0.164	0.217	0.267	0.314	0.357	0.396	0.428	0.451	0.458	0.439	0.386
5.0	0.061	0.109	0.159	0.208	0.253	0.295	0.334	0.370	0.402	0.426	0.436	0.423	0.377
5.5	0.062	0.104	0.145	0.182	0.216	0.248	0.278	0.308	0.337	0.364	0.382	0.382	0.351
6.0	0.061	0.096	0.129	0.157	0.181	0.203	0.226	0.250	0.277	0.305	0.328	0.339	0.324
6.5	0.058	0.088	0.112	0.132	0.148	0.163	0.180	0.200	0.224	0.251	0.278	0.297	0.295
7.0	0.055	0.079	0.096	0.109	0.119	0.129	0.141	0.157	0.178	0.205	0.233	0.258	0.266
7.5	0.051	0.070	0.082	0.089	0.095	0.101	0.109	0.122	0.140	0.165	0.193	0.222	0.238
8.0	0.047	0.061	0.068	0.072	0.074	0.077	0.083	0.093	0.109	0.131	0.159	0.189	0.212
8.5	0.043	0.053	0.057	0.057	0.057	0.059	0.063	0.070	0.084	0.103	0.130	0.160	0.187
9.0	0.039	0.045	0.047	0.045	0.044	0.044	0.046	0.053	0.064	0.081	0.105	0.135	0.165
9.5	0.035	0.038	0.038	0.036	0.033	0.033	0.034	0.039	0.048	0.063	0.085	0.113	0.144
10.0	0.031	0.033	0.031	0.028	0.025	0.024	0.025	0.029	0.036	0.048	0.068	0.095	0.126
10.5							0.018	0.021	0.027	0.037	0.054	0.079	0.109
11.0	0.024	0.023	0.020	0.016	0.014	0.013	0.013	0.015	0.020	0.028	0.043	0.065	0.095
11.5							0.009	0.011	0.015	0.022	0.034	0.054	0.082
12.0	0.018	0.016	0.012	0.010	0.008	0.007	0.007	0.008	0.011	0.016	0.027	0.044	0.070
12.5							0.005	0.006	0.008	0.012	0.021	0.036	0.060
13.0							0.003	0.004	0.006	0.009	0.016	0.030	0.052
13.5							0.002	0.003	0.004	0.007	0.013	0.024	0.044
14.0							0.002	0.002	0.003	0.005	0.010	0.020	0.038

TABLE XIII.

	$S(2s, 3s)$												
p	$t=-0.6$	$t=-0.5$	$t=-0.4$	$t=-0.3$	$t=-0.2$	$t=-0.1$	$t=0.0$	$t=0.1$	$t=0.2$	$t=0.3$	$t=0.4$	$t=0.5$	$t=0.6$
0.0	0.479	0.667	0.826	0.937	0.989	0.979	0.913	0.801	0.659	0.505	0.354	0.222	0.120
0.5	0.477	0.663	0.820	0.929	0.979	0.970	0.905	0.796	0.657	0.505	0.356	0.225	0.122
1.0	0.473	0.651	0.801	0.904	0.952	0.943	0.884	0.782	0.650	0.505	0.361	0.231	0.127
1.5	0.466	0.634	0.771	0.865	0.909	0.902	0.849	0.758	0.638	0.504	0.367	0.240	0.136
2.0	0.457	0.611	0.733	0.815	0.853	0.847	0.803	0.725	0.620	0.499	0.372	0.250	0.146
2.5	0.445	0.582	0.688	0.756	0.789	0.785	0.747	0.682	0.594	0.488	0.373	0.258	0.156
3.0	0.430	0.549	0.637	0.692	0.716	0.712	0.684	0.632	0.560	0.472	0.371	0.265	0.165
3.5	0.411	0.512	0.582	0.623	0.639	0.636	0.614	0.575	0.519	0.448	0.362	0.268	0.173
4.0	0.390	0.472	0.524	0.552	0.562	0.557	0.541	0.514	0.473	0.418	0.349	0.267	0.178
4.5	0.365	0.429	0.466	0.483	0.485	0.481	0.469	0.451	0.423	0.384	0.329	0.261	0.181
5.0	0.339	0.387	0.408	0.415	0.413	0.407	0.395	0.389	0.372	0.347	0.307	0.252	0.182
5.5	0.312	0.344	0.354	0.352	0.346	0.339	0.334	0.329	0.322	0.308	0.282	0.239	0.180
6.0	0.285	0.304	0.303	0.295	0.285	0.278	0.275	0.275	0.275	0.270	0.255	0.225	0.175
6.5	0.259	0.266	0.258	0.245	0.233	0.226	0.225	0.227	0.232	0.234	0.229	0.209	0.170
7.0	0.232	0.230	0.216	0.200	0.187	0.180	0.179	0.184	0.191	0.199	0.201	0.191	0.162
7.5	0.207	0.198	0.180	0.162	0.149	0.142	0.142	0.147	0.157	0.168	0.176	0.173	0.153
8.0	0.184	0.169	0.148	0.130	0.117	0.111	0.111	0.117	0.127	0.140	0.152	0.156	0.144
9.0	0.143	0.121	0.099	0.082	0.071	0.065	0.066	0.071	0.081	0.095	0.111	0.123	0.124
10.0	0.110	0.085	0.065	0.050	0.041	0.037	0.037	0.042	0.050	0.062	0.079	0.095	0.104

TABLE XIV.

	$S(2s, 3p\sigma)$												
p	$t=-0.6$	$t=-0.5$	$t=-0.4$	$t=-0.3$	$t=-0.2$	$t=-0.1$	$t=0.0$	$t=0.1$	$t=0.2$	$t=0.3$	$t=0.4$	$t=0.5$	$t=0.6$
0.0	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
0.5	0.001	0.020	0.048	0.081	0.113	0.140	0.156	0.160	0.150	0.130	0.101	0.070	0.041
1.0	0.004	0.042	0.096	0.158	0.219	0.269	0.300	0.307	0.290	0.251	0.198	0.138	0.082
1.5	0.013	0.067	0.143	0.229	0.312	0.380	0.422	0.433	0.410	0.358	0.285	0.201	0.122
2.0	0.027	0.095	0.187	0.289	0.386	0.465	0.515	0.529	0.505	0.445	0.359	0.258	0.159
2.5	0.044	0.122	0.224	0.334	0.438	0.522	0.576	0.593	0.570	0.509	0.416	0.306	0.193
3.0	0.060	0.146	0.252	0.363	0.466	0.550	0.605	0.624	0.605	0.548	0.457	0.343	0.222
3.5	0.076	0.164	0.267	0.374	0.470	0.549	0.603	0.625	0.612	0.563	0.480	0.369	0.246
4.0	0.088	0.175	0.273	0.370	0.456	0.527	0.577	0.601	0.596	0.558	0.486	0.384	0.264
4.5	0.098	0.180	0.268	0.352	0.427	0.488	0.533	0.558	0.561	0.535	0.478	0.390	0.277
5.0	0.102	0.178	0.255	0.326	0.387	0.438	0.478	0.505	0.514	0.500	0.459	0.385	0.283
5.5	0.104	0.172	0.236	0.293	0.342	0.383	0.418	0.444	0.459	0.457	0.430	0.373	0.285
6.0	0.103	0.162	0.214	0.258	0.295	0.328	0.356	0.382	0.401	0.409	0.397	0.356	0.282
6.5	0.101	9.150	0.191	0.224	0.251	0.275	0.299	0.323	0.346	0.361	0.361	0.335	0.276
7.0	0.095	0.135	0.166	0.189	0.207	0.225	0.245	0.267	0.291	0.311	0.321	0.309	0.265
7.5	0.089	0.121	0.143	0.158	0.170	0.182	0.198	0.218	0.242	0.266	0.283	0.283	0.252
8.0	0.083	0.107	0.122	0.130	0.137	0.145	0.157	0.175	0.198	0.224	0.247	0.257	0.238
9.0	0.069	0.081	0.085	0.085	0.086	0.088	0.096	0.109	0.129	0.154	0.183	0.205	0.207
10.0	0.055	0.059	0.059	0.054	0.051	0.052	0.056	0.065	0.080	0.103	0.131	0.159	0.175

TABLE XV.

	$S(2p\sigma, 2p\sigma)$						
p	$t=0.0$	$t=0.1$	$t=0.2$	$t=0.3$	$t=0.4$	$t=0.5$	$t=0.6$
0.0	−1.000	−0.975	−0.903	−0.790	−0.647	−0.487	−0.328
0.5	−0.927	−0.906	−0.840	−0.738	−0.607	−0.461	−0.312
1.0	−0.736	−0.720	−0.673	−0.599	−0.502	−0.389	−0.271
1.5	−0.483	−0.475	−0.452	−0.416	−0.360	−0.292	−0.214
2.0	−0.226	−0.226	−0.226	−0.222	−0.211	−0.188	−0.150
2.5	0.005	−0.007	−0.029	−0.053	−0.076	−0.092	−0.092
3.0	0.159	0.148	0.121	0.079	0.032	−0.011	−0.040
3.2	0.208	0.196	0.167	0.120	0.067	0.016	−0.022
3.4	0.248	0.237	0.204	0.155	0.097	0.040	−0.005
3.6	0.279	0.268	0.235	0.184	0.123	0.061	0.010
3.8	0.303	0.291	0.258	0.207	0.144	0.079	0.023
4.0	0.319	0.308	0.275	0.224	0.161	0.094	0.035
4.2	0.328	0.318	0.286	0.237	0.175	0.107	0.045
4.4	0.332	0.322	0.293	0.245	0.185	0.117	0.054
4.6	0.332	0.322	0.294	0.250	0.191	0.126	0.062
4.8	0.327	0.318	0.293	0.251	0.196	0.132	0.068
5.0	0.319	0.311	0.288	0.249	0.197	0.136	0.074
5.5	0.289	0.282	0.266	0.236	0.193	0.141	0.083

	$S(2p\sigma, 2p\sigma)$						
p	$t=0.0$	$t=0.1$	$t=0.2$	$t=0.3$	$t=0.4$	$t=0.5$	$t=0.6$
6.0	0.250	0.247	0.235	0.214	0.181	0.138	0.087
6.5	0.210	0.208	0.201	0.187	0.164	0.131	0.087
7.0	0.171	0.171	0.167	0.160	0.145	0.120	0.085
7.5	0.137	0.137	0.137	0.134	0.126	0.109	0.081
8.0	0.107	0.108	0.109	0.110	0.107	0.096	0.075
8.5	0.083	0.084	0.086	0.089	0.090	0.085	0.069
9.0	0.063	0.064	0.067	0.071	0.075	0.073	0.063
9.5	0.047	0.048	0.052	0.057	0.061	0.063	0.057
10.0	0.035	0.036	0.039	0.045	0.050	0.054	0.051
10.5	0.026	0.027	0.030	0.035	0.041	0.045	0.045
11.0	0.019	0.020	0.021	0.027	0.033	0.038	0.040
11.5	0.013	0.014	0.017	0.021	0.026	0.032	0.035
12.0	0.010	0.010	0.012	0.016	0.021	0.027	0.031
12.5	0.007	0.007	0.009	0.012	0.017	0.022	0.027
13.0	0.005	0.005	0.007	0.009	0.013	0.018	0.023
13.5	0.003	0.004	0.005	0.007	0.010	0.015	0.020
14.0	0.002	0.003	0.003	0.005	0.008	0.012	0.017

TABLE XVI.

	$S(2p\sigma, 3s)$												
p	$t=-0.6$	$t=-0.5$	$t=-0.4$	$t=-0.3$	$t=-0.2$	$t=-0.1$	$t=0.0$	$t=0.1$	$t=0.2$	$t=0.3$	$t=0.4$	$t=0.5$	$t=0.6$
0.0	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
0.5	0.110	0.134	0.142	0.135	0.114	0.085	0.054	0.025	0.002	−0.013	−0.019	−0.018	−0.013
1.0	0.214	0.261	0.278	0.265	0.227	0.173	0.114	0.058	0.013	−0.017	−0.032	−0.032	−0.024
1.5	0.307	0.374	0.399	0.383	0.333	0.261	0.179	0.102	0.034	−0.009	−0.034	−0.039	−0.031
2.0	0.385	0.466	0.497	0.480	0.424	0.340	0.245	0.152	0.071	+0.011	−0.025	−0.038	−0.034
2.5	0.445	0.534	0.569	0.551	0.492	0.405	0.303	0.201	0.111	0.039	−0.008	−0.030	−0.033
3.0	0.486	0.576	0.609	0.591	0.533	0.447	0.346	0.243	0.148	0.069	+0.013	−0.019	−0.028
3.5	0.509	0.594	0.622	0.603	0.547	0.466	0.371	0.272	0.179	0.097	0.035	−0.005	−0.021
4.0	0.515	0.590	0.611	0.589	0.535	0.462	0.376	0.287	0.199	0.120	0.055	+0.010	−0.014
4.5	0.508	0.569	0.580	0.555	0.505	0.439	0.365	0.287	0.208	0.135	0.061	0.023	−0.005
5.0	0.490	0.536	0.537	0.508	0.461	0.404	0.341	0.275	0.208	0.143	0.083	0.034	+0.002
5.5	0.465	0.495	0.485	0.453	0.409	0.360	0.308	0.255	0.199	0.144	0.090	0.043	0.009
6.0	0.434	0.449	0.430	0.395	0.354	0.314	0.271	0.230	0.185	0.139	0.093	0.050	0.015
6.5	0.402	0.403	0.376	0.339	0.301	0.266	0.233	0.201	0.167	0.131	0.093	0.054	0.020
7.0	0.366	0.354	0.322	0.284	0.250	0.220	0.194	0.171	0.147	0.120	0.089	0.055	0.024
7.5	0.331	0.310	0.273	0.236	0.204	0.180	0.160	0.143	0.126	0.107	0.083	0.055	0.027
8.0	0.297	0.268	0.229	0.193	0.165	0.144	0.129	0.118	0.107	0.094	0.076	0.054	0.028
9.0	0.235	0.197	0.157	0.125	0.103	0.089	0.081	0.076	0.073	0.069	0.061	0.048	0.029
10.0	0.182	0.140	0.104	0.078	0.062	0.053	0.048	0.047	0.047	0.048	0.047	0.040	0.028

TABLE XVII.

						$S(2p\sigma, 3p\sigma)$						
p	$t=-0.6$	$t=-0.5$	$t=-0.4$	$t=-0.3$	$t=-0.2$	$t=-0.1$	$t=0.0$	$t=0.1$	$t=0.2$	$t=0.3$	$t=0.4$	$t=0.5$	$t=0.6$
0.0	−0.479	−0.667	−0.826	−0.937	−0.989	−0.979	−0.913	−0.801	−0.659	−0.505	−0.354	−0.222	−0.120
0.5	−0.462	−0.640	−0.790	−0.894	−0.942	−0.934	−0.872	−0.768	−0.636	−0.490	−0.347	−0.220	−0.120
1.0	−0.414	−0.564	−0.687	−0.771	−0.811	−0.805	−0.757	−0.674	−0.567	−0.446	−0.323	−0.211	−0.118
1.5	−0.343	−0.453	−0.537	−0.593	−0.618	−0.615	−0.585	−0.531	−0.460	−0.375	−0.284	−0.194	−0.114
2.0	−0.261	−0.324	−0.365	−0.389	−0.398	−0.396	−0.384	−0.362	−0.330	−0.285	−0.230	−0.168	−0.107
2.5	−0.177	−0.194	−0.195	−0.187	−0.180	−0.178	−0.181	−0.188	−0.192	−0.187	−0.169	−0.136	−0.094
3.0	−0.097	−0.076	−0.042	−0.010	+0.010	+0.013	−0.002	−0.029	−0.062	−0.089	−0.104	−0.101	−0.080
3.5	−0.028	+0.022	+0.081	+0.130	0.159	0.163	+0.142	+0.102	+0.050	−0.002	−0.043	−0.064	−0.063
4.0	+0.027	0.099	0.172	0.230	0.264	0.268	0.245	0.198	0.136	+0.070	+0.012	−0.029	−0.045
4.5	0.070	0.153	0.232	0.292	0.326	0.330	0.307	0.260	0.196	0.124	0.056	+0.003	−0.027
5.0	0.101	0.187	0.264	0.321	0.351	0.355	0.334	0.291	0.231	0.161	0.090	0.029	−0.011
5.5	0.122	0.205	0.275	0.324	0.350	0.353	0.335	0.298	0.246	0.182	0.113	0.050	+0.004
6.0	0.134	0.210	0.270	0.310	0.330	0.331	0.317	0.287	0.244	0.189	0.127	0.066	0.016
6.5	0.139	0.206	0.256	0.286	0.299	0.299	0.288	0.265	0.232	0.187	0.133	0.077	0.026
7.0	0.138	0.194	0.232	0.253	0.261	0.259	0.251	0.235	0.211	0.177	0.133	0.082	0.034
7.5	0.134	0.179	0.207	0.220	0.222	0.220	0.213	0.203	0.186	0.162	0.128	0.085	0.040
8.0	0.127	0.162	0.181	0.186	0.185	0.182	0.177	0.171	0.161	0.145	0.120	0.084	0.044
9.0	0.109	0.127	0.131	0.128	0.122	0.118	0.115	0.115	0.114	0.110	0.099	0.078	0.047
10.0	0.089	0.095	0.091	0.083	0.076	0.072	0.071	0.072	0.075	0.078	0.076	0.067	0.046

TABLE XVIII.

p	$S(3s, 3s)$ $t=0.0$	$S(3p\sigma, 3p\sigma)$ $t=0.0$	$S(3s, 3p\sigma)$ $t=0.0$	p	$S(3s, 3s)$ $t=0.0$	$S(3p\sigma, 3p\sigma)$ $t=0.0$	$S(3s, 3p\sigma)$ $t=0.0$
0.0	1.000	−1.000	0.000	6.4	0.328	0.377	0.371
0.5	0.992	−0.965	0.096	6.6	0.306	0.368	0.352
1.0	0.968	−0.866	0.189	6.8	0.285	0.358	0.333
1.5	0.932	−0.715	0.276	7.0	0.264	0.346	0.314
2.0	0.885	−0.531	0.354	7.2	0.245	0.333	0.295
2.5	0.832	−0.333	0.419	7.4	0.227	0.319	0.277
3.0	0.772	−0.140	0.468	7.6	0.209	0.304	0.259
3.5	0.708	0.031	0.499	7.8	0.193	0.288	0.241
4.0	0.641	0.171	0.511	8.0	0.177	0.273	0.225
4.5	0.572	0.273	0.504	8.5	0.141	0.233	0.185
5.0	0.504	0.342	0.483	9.0	0.114	0.195	0.151
5.2	0.477	0.359	0.470	9.5	0.089	0.161	0.121
5.4	0.451	0.372	0.457	10.0	0.070	0.130	0.096
5.6	0.425	0.380	0.441	10.5	0.054	0.104	0.076
5.8	0.400	0.385	0.425	11.0	0.041	0.082	0.059
6.0	0.375	0.385	0.407	11.5	0.031	0.064	0.045
6.2	0.351	0.382	0.389	12.0	0.024	0.050	0.034

TABLE XIX.

p	$S(5s, 5s)$ $t=0.0$	$S(5p\sigma, 5p\sigma)$ $t=0.0$	$S(5s, 5p\sigma)$ $t=0.0$	p	$S(5s, 5s)$ $t=0.0$	$S(5p\sigma, 5p\sigma)$ $t=0.0$	$S(5s, 5p\sigma)$ $t=0.0$
0.0	1.000	−1.000	0.000	7.0	0.417	0.413	0.445
0.5	0.994	−0.979	0.072	7.5	0.367	0.418	0.411
1.0	0.977	−0.917	0.142	8.0	0.320	0.407	0.374
1.5	0.950	−0.819	0.210	8.5	0.276	0.384	0.334
2.0	0.915	−0.693	0.273	9.0	0.235	0.354	0.294
2.5	0.874	−0.547	0.331	9.5	0.198	0.318	0.255
3.0	0.828	−0.390	0.383	10.0	0.166	0.281	0.218
3.5	0.780	−0.231	0.427	10.5	0.137	0.244	0.185
4.0	0.730	−0.079	0.462	11.0	0.113	0.208	0.154
4.5	0.679	0.059	0.486	11.5	0.091	0.175	0.127
5.0	0.627	0.177	0.499	12.0	0.074	0.145	0.104
5.5	0.574	0.272	0.501	12.5	0.059	0.119	0.084
6.0	0.521	0.343	0.491	13.0	0.047	0.097	0.067
6.5	0.468	0.389	0.472				

TABLE XX.

	$S(2p\pi, 2p\pi)$								$S(2p\pi, 2p\pi)$						
p	$t=0.0$	$t=0.1$	$t=0.2$	$t=0.3$	$t=0.4$	$t=0.5$	$t=0.6$	p	$t=0.0$	$t=0.1$	$t=0.2$	$t=0.3$	$t=0.4$	$t=0.5$	$t=0.6$
0.0	1.000	0.975	0.903	0.790	0.647	0.487	0.328	5.0	0.164	0.163	0.162	0.157	0.149	0.134	0.111
0.5	0.976	0.951	0.882	0.772	0.633	0.478	0.323	5.2	0.146						
1.0	0.907	0.887	0.823	0.723	0.596	0.453	0.308	5.4	0.129						
1.5	0.809	0.790	0.737	0.652	0.542	0.416	0.287	5.5	0.121	0.122	0.122	0.121	0.117	0.109	0.094
2.0	0.695	0.680	0.638	0.568	0.477	0.372	0.261	5.6	0.114						
2.5	0.578	0.567	0.535	0.481	0.410	0.325	0.233	5.8	0.101						
3.0	0.468	0.460	0.437	0.398	0.345	0.279	0.205	6.0	0.089	0.089	0.091	0.092	0.092	0.089	0.079
3.2	0.427	0.420	0.401	0.367	0.320	0.262	0.194	6.2	0.078						
3.4	0.389	0.383	0.366	0.337	0.297	0.245	0.183	6.4	0.069						
3.6	0.352	0.348	0.334	0.309	0.274	0.228	0.173	6.5	0.064	0.065	0.067	0.069	0.072	0.071	0.066
3.8	0.318	0.315	0.303	0.283	0.253	0.213	0.163	7.0	0.046	0.047	0.049	0.052	0.055	0.057	0.055
4.0	0.287	0.284	0.275	0.258	0.232	0.198	0.153	7.5	0.033	0.033	0.036	0.039	0.043	0.046	0.046
4.2	0.258	0.255	0.248	0.234	0.213	0.183	0.144	8.0	0.023	0.024	0.026	0.029	0.033	0.037	0.038
4.4	0.231	0.229	0.224	0.213	0.195	0.170	0.135	9.0	0.011	0.012	0.013	0.016	0.019	0.023	0.026
4.6	0.207	0.205	0.201	0.193	0.179	0.157	0.127	10.0	0.005	0.006	0.007	0.008	0.011	0.013	0.018
4.8	0.184	0.183	0.181	0.174	0.163	0.145	0.119								

TABLE XXI.

	$S(2p\pi, 2p\pi)$												
p	$t=-0.6$	$t=-0.5$	$t=-0.4$	$t=-0.3$	$t=-0.2$	$t=-0.1$	$t=0.0$	$t=0.1$	$t=0.2$	$t=0.3$	$t=0.4$	$t=0.5$	$t=0.6$
0.0	0.479	0.667	0.826	0.937	0.989	0.979	0.913	0.801	0.659	0.505	0.354	0.222	0.120
0.5	0.473	0.658	0.814	0.923	0.973	0.963	0.899	0.786	0.652	0.500	0.352	0.221	0.120
1.0	0.456	0.632	0.779	0.881	0.928	0.920	0.860	0.758	0.628	0.485	0.344	0.219	0.119
1.5	0.431	0.591	0.724	0.816	0.858	0.851	0.798	0.708	0.591	0.461	0.331	0.213	0.118
2.0	0.399	0.541	0.656	0.735	0.771	0.765	0.720	0.643	0.542	0.429	0.313	0.206	0.117
2.5	0.363	0.484	0.581	0.645	0.676	0.672	0.633	0.569	0.486	0.390	0.290	0.195	0.114
3.0	0.325	0.426	0.503	0.554	0.575	0.571	0.542	0.492	0.426	0.348	0.264	0.182	0.109
3.5	0.287	0.369	0.428	0.466	0.480	0.477	0.454	0.416	0.366	0.303	0.237	0.168	0.104
4.0	0.251	0.315	0.359	0.384	0.394	0.389	0.373	0.345	0.308	0.262	0.209	0.153	0.097
4.5	0.218	0.266	0.297	0.313	0.316	0.312	0.301	0.282	0.255	0.222	0.182	0.137	0.090
5.0	0.187	0.222	0.241	0.250	0.251	0.246	0.238	0.225	0.208	0.185	0.157	0.122	0.083
5.2					0.228	0.223	0.216	0.205	0.191	0.172			
5.4					0.206	0.202	0.195	0.187	0.175	0.159			
5.5	0.160	0.184	0.195	0.198	0.196	0.192	0.186	0.178	0.167	0.153	0.133	0.107	0.076
5.6					0.186	0.182	0.176	0.169	0.160	0.147			
5.8					0.168	0.164	0.159	0.153	0.146	0.135			
6.0	0.136	0.151	0.156	0.155	0.151	0.147	0.143	0.139	0.133	0.125	0.112	0.093	0 069
6.5	0.115	0.123	0.124	0.120	0.115	0.112	0.109	0.107	0.104	0.101	0.093	0.081	0.062
7.0	0.097	0.100	0.097	0.092	0.087	0.084	0.082	0.081	0.081	0.080	0.077	0.069	0.055
7.5	0.082	0.081	0.076	0.070	0.065	0.062	0.061	0.061	0.062	0.064	0.063	0.059	0.049
8.0	0.068	0.065	0.059	0.053	0.049	0.046	0.045	0.046	0.048	0.050	0.052	0.050	0.043
9.0	0.048	0.042	0.036	0.030	0.026	0.024	0.024	0.025	0.027	0.030	0.034	0.035	0.033
10.0	0.033	0.027	0.021	0.017	0.014	0.012	0.012	0.013	0.015	0.018	0.022	0.025	0.025

TABLE XXII.

	$S(2p\pi, 5p\pi)$			$S(2p\pi, 5p\pi)$	
p	$t=0.0$	$t=0.1$	p	$t=0.0$	$t=0.1$
0.5	0.726	0.58	7.5	0.093	0.090
1.0	0.707	0.563	8.0	0.072	0.071
1.5	0.677	0.543	8.5	0.055	0.055
2.0	0.635	0.515	9.0	0.041	0.042
2.5	0.584	0.482	9.5	0.030	0.032
3.0	0.526	0.438	10.0	0.023	0.024
3.5	0.464	0.393	10.5	0.017	0.018
4.0	0.401	0.345	11.0	0.012	0.014
4.5	0.341	0.298	11.5	0.009	0.010
5.0	0.284	0.253	12.0	0.007	0.008
5.5	0.234	0.212	12.5	0.005	0.006
6.0	0.189	0.174	13.0	0.003	0.004
6.5	0.151	0.142	13.5	0.002	0.003
7.0	0.119	0.114	14.0	0.002	0.003

TABLE XXIII.

p	$S(3p\pi, 3p\pi)$ $t=0.0$	$S(5p\pi, 5p\pi)$ $t=0.0$	p	$S(3p\pi, 3p\pi)$ $t=0.0$	$S(5p\pi, 5p\pi)$ $t=0.0$
0.0	1.000	1.000	6.4	0.184	0.338
0.5	0.988	0.993	6.6	0.167	0.317
1.0	0.955	0.972	6.8	0.152	0.297
1.5	0.901	0.938	7.0	0.137	0.277
2.0	0.832	0.893	7.2	0.124	0.259
2.5	0.752	0.839	7.4	0.112	0.241
3.0	0.666	0.778	7.6	0.101	0.224
3.5	0.578	0.712	7.8	0.091	0.208
4.0	0.493	0.644	8.0	0.081	0.193
4.5	0.413	0.575	8.5	0.062	0.159
5.0	0.341	0.508	9.0	0.046	0.130
5.2	0.314		9.5	0.035	0.105
5.4	0.289		10.0	0.026	0.084
5.5		0.443	10.5		0.067
5.6	0.265		11.0		0.053
5.8	0.243		11.5		0.042
6.0	0.222	0.383	12.0		0.033
6.2	0.202	0.360	12.5		0.025

VII. TABLES OF SELECTED HYBRID SLATER-AO OVERLAP INTEGRALS***

TABLE XXIV.

	$S(1s, 2di\sigma)$									$S(1s, 2di\sigma)$							
p	$t=-0.5$	$t=-0.4$	$t=-0.3$	$t=-0.2$	$t=-0.1$	$t=0.0$	$t=0.1$	$t=0.2$	p	$t=-0.5$	$t=-0.4$	$t=-0.3$	$t=-0.2$	$t=-0.1$	$t=0.0$	$t=0.1$	$t=0.2$
0.0						0.612	0.543	0.461	4.0	0.381	0.414	0.439	0.457	0.472	0.483	0.489	0.486
0.5	0.669	0.757	0.812	0.832	0.818	0.773	0.704	0.611	4.2						0.442	0.450	0.451
1.0	0.704	0.807	0.878	0.914	0.913	0.879	0.814	0.723	4.4						0.403	0.412	0.417
1.5	0.697	0.804	0.881	0.925	0.936	0.914	0.860	0.778	4.5	0.317	0.336	0.350	0.362	0.372			
2.0	0.658	0.758	0.831	0.877	0.895	0.884	0.845	0.778	4.6						0.366	0.377	0.384
2.2	0.636	0.730	0.800	0.846	0.865	0.858	0.825	0.765	5.0	0.260	0.269	0.274	0.280	0.288	0.299	0.311	0.323
2.4	0.611	0.699	0.765	0.809	0.829	0.826	0.798	0.746	5.5						0.228	0.241	0.256
2.6	0.583	0.665	0.727	0.768	0.789	0.789	0.767	0.722	6.0	0.171	0.166	0.162	0.160	0.163	0.171	0.184	0.200
2.8	0.555	0.630	0.686	0.725	0.746	0.748	0.731	0.694	6.5						0.127	0.138	0.155
3.0	0.526	0.593	0.644	0.680	0.700	0.705	0.693	0.662	7.0	0.110	0.100	0.092	0.088	0.088	0.093	0.103	0.118
3.2	0.496	0.556	0.601	0.634	0.654	0.660	0.653	0.629	7.5						0.067	0.076	0.089
3.4	0.466	0.519	0.559	0.588	0.607	0.615	0.612	0.594	8.0	0.070	0.058	0.050	0.046	0.045	0.048	0.055	0.067
3.6	0.437	0.483	0.518	0.543	0.561	0.570	0.570	0.558	9.0						0.024	0.029	0.037
3.8						0.526	0.529	0.522	10.0						0.012	0.014	0.020

TABLE XXV.

	$S(1s, 2tr\sigma)$									$S(1s, 2tr\sigma)$							
p	$t=-0.5$	$t=-0.4$	$t=-0.3$	$t=-0.2$	$t=-0.1$	$t=0.0$	$t=0.1$	$t=0.2$	p	$t=-0.5$	$t=-0.4$	$t=-0.3$	$t=-0.2$	$t=-0.1$	$t=0.0$	$t=0.1$	$t=0.2$
0.0						0.500	0.443	0.376	4.0	0.360	0.399	0.428	0.452	0.471	0.485	0.493	0.493
0.5	0.574	0.655	0.708	0.731	0.727	0.689	0.631	0.551	4.2						0.444	0.455	0.458
1.0	0.624	0.725	0.797	0.838	0.845	0.821	0.765	0.684	4.4						0.405	0.417	0.424
1.5	0.633	0.740	0.821	0.871	0.890	0.876	0.831	0.756	4.5	0.301	0.325	0.343	0.358	0.372			
2.0	0.606	0.708	0.788	0.840	0.866	0.862	0.830	0.769	4.6						0.369	0.381	0.391
2.2	0.588	0.686	0.762	0.814	0.841	0.841	0.814	0.759	5.0	0.247	0.260	0.270	0.278	0.289	0.302	0.316	0.329
2.4	0.567	0.659	0.732	0.782	0.810	0.813	0.791	0.743	5.5						0.231	0.245	0.262
2.6	0.544	0.630	0.697	0.746	0.773	0.779	0.762	0.722	6.0	0.163	0.162	0.160	0.160	0.165	0.174	0.187	0.205
2.8	0.519	0.598	0.661	0.706	0.733	0.741	0.729	0.696	6.5						0.129	0.141	0.158
3.0	0.493	0.565	0.622	0.664	0.690	0.701	0.693	0.666	7.0	0.105	0.097	0.091	0.088	0.089	0.094	0.105	0.121
3.2	0.466	0.531	0.583	0.621	0.646	0.658	0.655	0.634	7.5						0.068	0.077	0.091
3.4	0.439	0.497	0.543	0.577	0.601	0.614	0.615	0.599	8.0	0.067	0.057	0.050	0.046	0.046	0.049	0.056	0.068
3.6	0.412	0.463	0.504	0.534	0.557	0.571	0.574	0.564	9.0						0.025	0.029	0.038
3.8						0.527	0.534	0.529	10.0						0.012	0.015	0.020

*** See Section III, especially Eqs. (12), (13), for definitions and conventions, and Eqs. (9), (78), (79) for the hybrid S formulas.

TABLE XXVI.

$S(1s, 2te\sigma)$

p	$t=-0.5$	$t=-0.4$	$t=-0.3$	$t=-0.2$	$t=-0.1$	$t=0.0$	$t=0.1$	$t=0.2$
0.0						0.433	0.384	0.326
0.5	0.516	0.592	0.643	0.667	0.664	0.635	0.584	0.512
1.0	0.574	0.672	0.744	0.787	0.798	0.779	0.730	0.655
1.5	0.590	0.696	0.778	0.832	0.854	0.845	0.805	0.736
2.0	0.570	0.673	0.754	0.810	0.839	0.840	0.811	0.754
2.2	0.555	0.654	0.732	0.787	0.818	0.822	0.798	0.747
2.4	0.537	0.630	0.705	0.758	0.789	0.796	0.777	0.733
2.6	0.516	0.603	0.673	0.724	0.755	0.765	0.751	0.713
2.8	0.493	0.574	0.639	0.687	0.718	0.729	0.720	0.688
3.0	0.469	0.543	0.603	0.647	0.677	0.690	0.685	0.660
3.2	0.444	0.511	0.565	0.606	0.634	0.649	0.648	0.628
3.4	0.419	0.479	0.527	0.565	0.591	0.606	0.609	0.595
3.6	0.394	0.447	0.490	0.523	0.548	0.564	0.569	0.561
3.8						0.522	0.530	0.526

$S(1s, 2te\sigma)$

p	$t=-0.5$	$t=-0.4$	$t=-0.3$	$t=-0.2$	$t=-0.1$	$t=0.0$	$t=0.1$	$t=0.2$
4.0	0.345	0.385	0.417	0.443	0.464	0.480	0.490	0.491
4.2						0.440	0.452	0.456
4.4						0.402	0.415	0.422
4.5	0.288	0.314	0.335	0.352	0.368			
4.6						0.366	0.380	0.390
5.0	0.238	0.252	0.264	0.274	0.286	0.300	0.314	0.329
5.5						0.229	0.244	0.261
6.0	0.157	0.157	0.157	0.158	0.163	0.173	0.187	0.205
6.5						0.128	0.141	0.158
7.0	0.101	0.094	0.089	0.087	0.088	0.094	0.105	0.121
7.5						0.068	0.077	0.091
8.0	0.064	0.056	0.049	0.046	0.046	0.049	0.056	0.068
9.0						0.025	0.029	0.038
10.0						0.012	0.015	0.020

TABLE XXVII.

$S[1s, 2(\alpha=\frac{1}{3})]$

p	$t=-0.5$	$t=-0.4$	$t=-0.3$	$t=-0.2$	$t=-0.1$	$t=0.0$	$t=0.1$	$t=0.2$
0.0						0.289	0.256	0.217
0.5	0.386	0.451	0.498	0.524	0.528	0.511	0.475	0.421
1.0	0.459	0.549	0.619	0.665	0.684	0.676	0.641	0.581
1.5	0.490	0.591	0.673	0.731	0.762	0.762	0.733	0.676
2.0	0.485	0.586	0.668	0.730	0.766	0.774	0.755	0.707
2.2	0.476	0.573	0.653	0.714	0.751	0.762	0.747	0.704
2.4	0.462	0.556	0.633	0.691	0.729	0.742	0.731	0.694
2.6	0.447	0.535	0.608	0.664	0.701	0.716	0.709	0.677
2.8	0.429	0.511	0.580	0.633	0.668	0.685	0.682	0.656
3.0	0.410	0.486	0.549	0.598	0.633	0.651	0.651	0.631
3.2	0.389	0.459	0.517	0.562	0.595	0.614	0.617	0.602
3.4	0.369	0.431	0.483	0.525	0.556	0.575	0.581	0.572
3.6	0.347	0.404	0.450	0.488	0.517	0.536	0.545	0.540
3.8						0.497	0.507	0.507

$S[1s, 2(\alpha=\frac{1}{3})]$

p	$t=-0.5$	$t=-0.4$	$t=-0.3$	$t=-0.2$	$t=-0.1$	$t=0.0$	$t=0.1$	$t=0.2$
4.0	0.306	0.349	0.385	0.415	0.440	0.459	0.471	0.471
4.2						0.421	0.435	0.440
4.4						0.385	0.400	0.449
4.5	0.256	0.286	0.311	0.331	0.350			
4.6						0.351	0.366	0.378
5.0	0.212	0.231	0.245	0.259	0.273	0.288	0.304	0.319
5.5						0.221	0.237	0.254
6.0	0.141	0.144	0.146	0.150	0.156	0.167	9.181	0.199
6.5						0.124	0.137	0.154
7.0	0.091	0.087	0.084	0.082	0.085	0.091	0.102	0.118
7.5						0.066	0.075	0.089
8.0	0.058	0.051	0.046	0.044	0.044	0.048	0.055	0.067
9.0						0.024	0.029	0.037
10.0						0.012	0.014	0.020

TABLE XXVIII.

p	$S(2di\sigma, 2di\sigma)$ $t=0.0$	$S(2tr\sigma, 2tr\sigma)$ $t=0.0$	$S(2te\sigma, 2te\sigma)$ $t=0.0$	$S[2(\alpha=\frac{1}{3}), 2(\alpha=\frac{1}{3})]$ $t=0.0$
0.0	0.000	−0.333	−0.500	−0.778
0.5	0.172	−0.155	−0.325	−0.625
1.0	0.382	+0.086	−0.076	−0.375
1.5	0.590	0.339	+0.195	−0.087
2.0	0.758	0.558	0.436	+0.181
2.5	0.871	0.721	0.622	0.402
3.0	0.907	0.798	0.719	0.532
3.2	0.907	0.813	0.742	0.568
3.4	0.898	0.818	0.753	0.593
3.6	0.882	0.813	0.756	0.608
3.8	0.860	0.802	0.750	0.614
4.0	0.832	0.783	0.738	0.613
4.2	0.801	0.761	0.720	0.606
4.4	0.765	0.733	0.696	0.592
4.6	0.725	0.699	0.668	0.573
4.8	0.685	0.664	0.637	0.552
5.0	0.645	0.628	0.604	0.527
5.5	0.542	0.534	0.517	0.458
6.0	0.445	0.443	0.430	0.385
6.5	0.358	0.358	0.350	0.316
7.0	0.282	0.284	0.278	0.253
7.5	0.219	0.222	0.218	0.199
8.0	0.168	0.170	0.168	0.154
8.5	0.127	0.129	0.128	0.118
9.0	0.095	0.097	0.096	0.089
9.5	0.070	0.072	0.071	0.066
10.0	0.051	0.053	0.052	0.049