so that \(|g(z)| = |\Gamma(\frac{1}{2}(x + 7) + \frac{1}{2}iy)| \leq |\Gamma[\frac{1}{4}(x + 7)]|\). By the concavity of the \(\Gamma\) function, \(|g(z)| \leq \max\{\Gamma(\frac{1}{2}(a + 7)), \Gamma(\frac{1}{2}(-a + 7))\}\), \(\varepsilon \in \mathbb{D}_a\). Thus we have from (38) and (30),

\[
(46) \quad |E| < \frac{1}{2}(\pi a b)^{\frac{1}{2}} \max\{\Gamma(\frac{1}{2}(a + 7)), \Gamma(\frac{1}{2}(-a + 7))\} \sigma_{\gamma(a)}.
\]

The selection \(a = 5.0\) yields

\[
(47) \quad |E| < \frac{1}{2}(8.772)(120)(3.867 \times 10^{-15}) = 2.04 \times 10^{-12}.
\]

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NBS


**Integrals Occurring in Problems of Molecular Structure**

In theoretical work on molecular structure based either upon the valence bond method or upon the molecular orbital method, the electronic wave functions are usually built up from atomic orbitals (AO’s). The calculation of most physical and chemical quantities then reduces to the evaluation of a number of integrals involving these orbitals. It is customary to adopt SLATER\(^1\) type AO’s, defined by (cf. RÜDENBERG\(^2\))

\[
\begin{align*}
(1s) &= (\zeta^2/\pi) e^{-\zeta r} \\
(2s) &= (\zeta^4/\pi^2) e^{-\zeta r} \\
(2p\sigma) &= (\zeta^4/\pi) e^{-\zeta r} \\
(2p\pi) &= (\zeta^4/\pi) e^{-\zeta r} \\
(2p\tilde{\pi}) &= (\zeta^4/\pi) e^{-\zeta r} \\
(3d\sigma) &= (\zeta^7/2\pi) (x^2 - r^2/3) e^{-\zeta r} \\
(3d\pi) &= (\zeta^7/3\pi) x z e^{-\zeta r} \\
(3d\tilde{\pi}) &= (\zeta^7/3\pi) y x e^{-\zeta r} \\
(3d\nu) &= (\zeta^7/2\pi) (x^2 - x^2/3) e^{-\zeta r} \\
(3d\tilde{\nu}) &= (\zeta^7/3\pi) x z e^{-\zeta r} \\
(3d\tilde{\nu}) &= (\zeta^7/3\pi) y x e^{-\zeta r}
\end{align*}
\]

where \((x, y, z)\) are the cartesian coordinates of the electron referred to the nucleus as origin with the \(z\)-axis directed along the internuclear axis towards the other nucleus, \(r^2 = x^2 + y^2 + z^2\) and \(\zeta\) is a numerical screening parameter. Occasionally complex Slater type AO’s are used; however since these are simply linear combinations of the real Slater AO’s, no distinction will be made between integrals involving real and complex orbitals.

Of the distinct types of two-centre integrals that arise, six are of major
importance; if \( \chi_a, \chi_a' \) etc. denote orbitals of nucleus \( a \) and \( \chi_b, \chi_b' \) etc. orbitals of nucleus \( b \), these are*

Overlap integrals:

\[
(\chi_a | \chi_b) = \int \chi_a \chi_b \, dv.
\]

Direct Coulomb attraction integrals:

\[
(\chi_a | 1/r_b | \chi_a) = \int \chi_a (1/r_b) \chi_a \, dv.
\]

Exchange Coulomb attraction integrals:

\[
(\chi_a | 1/r_b | \chi_b) = \int \chi_a (1/r_b) \chi_b \, dv.
\]

Coulomb repulsion integrals:

\[
(\chi_a \chi_b | \chi_a' \chi_b') = \int \int \chi_a (1) \chi_b (2) (1/r_{12}) \chi_a' (1) \chi_b' (2) \, dv_1 \, dv_2.
\]

Hybrid or ionic integrals:

\[
(\chi_a \chi_a' | \chi_a'' \chi_b) = \int \int \chi_a (1) \chi_a' (2) (1/r_{12}) \chi_a'' (1) \chi_b (2) \, dv_1 \, dv_2.
\]

Exchange integrals:

\[
(\chi_a \chi_b | \chi_a' \chi_b') = \int \int \chi_a (1) \chi_b (2) (1/r_{12}) \chi_a' (1) \chi_b' (2) \, dv_1 \, dv_2.
\]

in which \( r_b \) is the distance of the electron from nucleus \( b \), (1) and (2) represent all the coordinates of electrons 1 and 2 respectively and \( r_{12} \) is the distance between these electrons. The internuclear distance \( R \) enters all the integrals as a parameter.

There are essentially only two methods of evaluating such integrals, one of which consists of using expansions of the reciprocals of the electron distances and the other expansions of the orbitals. The first method is based upon the pioneer work of Sugiura, Zener & Guillemin, Bartlett, Rosen, James and others whilst the second is largely due to Barnett & Coulson following a suggestion by Coolidge. The choice of method for any particular problem is somewhat arbitrary and will probably be decided in the future by the availability of suitable tables.

The first method as used in the past has necessitated the computation of a large number of auxiliary integrals, defined as follows:

\[
A_n(x) = \int_{-1}^{+1} e^{-x t} t^n \, dt; \quad B_n(x) = \int_{-1}^{+1} e^{-x t} t^n \, dt;
\]

\[
G_r^s(n; x) = \int_{-1}^{+1} e^{-x t} P_r^s(t) t^n (1 - t^2)^{s/2} \, dt,
\]

where \( P_r^s(t) \) is the associated Legendre function of the first kind; \( f_r^s(m; x) = \int_1^{+\infty} Q_r(t) e^{-x t} t^m \, dt, \)
where $Q_r(t)$ is the associated Legendre function of the second kind:

$$F_{k,m,n}(x,y) = \int_1^\infty dt \int_{-1}^{+1} dt'(t^2 - 1)^k(t + t')^{-(k+1)m}t^{n-1}e^{-xt}e^{-yt'};$$

$$J_n(x,y) = \int_1^\infty dt \int_{-1}^{+1} dt'(t^2 - 1)(1 - t'^2)(t^2 - t'^2)(t + t')^n e^{-xt}e^{-yt'};$$

$$K_n(x,y) = \int_1^\infty dt \int_{-1}^{+1} dt'(t^2 - 1)(1 - t'^2)(1 + t')^2(t + t')^{n-2}e^{-xt}e^{-yt'};$$

$$F_{m,n}(x,y) = \int_1^\infty dt \int_{-1}^{+1} dt'(t + t')^{-m}(-t')^n(1 - t'^2)^{m-1}e^{-xt}e^{-yt'};$$

$$S_r(m,n;x) = \int_1^\infty dt Q_r(t) e^{-xt} t^m dt \int_1^t e^{-zt'} t^n dt';$$

$$\sigma_r(m,n;x) = \int_1^\infty dt Q_r(t) e^{-xt} t^m dt \int_1^\infty e^{-zt'} t^n dt';$$

$$H_r(m,n;x) = S_r(m,n;x) + S_r(n,m;x);$$

$$W_r^*(m,n;x) = \int_1^\infty dt \int_1^\infty dt' Q^*_r(t) P^*_r(t < t') e^{-xt} t^m dt' t'^{n-1}(t'^2 - 1)^{r/2}.$$

All of these auxiliary integrals are expressable in terms of polynomials, exponentials, natural logarithms and the exponential integral $-Ei(-x) = \int_x^\infty t^{-1}e^{-t}dt$. Many of them are simply related to each other. There is a distreessing lack of uniformity not only in the choice of auxiliary integrals computed but also in the notation.

The second method, which is particularly valuable in the case of integrals involving more than two centres, requires the computation of certain so-called $\zeta$-functions which are expressable ultimately in terms of Bessel functions of half-integral orders for which the argument is pure imaginary. Several approximations to the exchange and hybrid two-centre integrals and to multi-centred integrals have been suggested and their accuracy has recently been assessed by comparison with the exact values.

This review concludes with three bibliographies:

A—Reduction of two-centre molecular integrals
B—Tables of two-centre molecular integrals
C—Multi-centre integrals.

A very large number of papers relevant to molecular integrals has been published and it is not possible (nor desirable) to describe all of them. Bibliography A is a somewhat arbitrary selection of papers chosen so that any integral that has been calculated to date may be found in at least one of them and chosen to include also those papers which the reviewer considers to be the most useful. Bibliography B describes in as much detail as space allows the tables of two-centre integrals and of auxiliary functions which
have been published since the date of inception of MTAC in 1943. Excluded from this bibliography is the multitude of published material which contains only a few isolated integrals and whose usefulness is effectively restricted to the problem concerned in the particular reference. Warning must be given that owing to the complexity of the work, the occurrence of errors is frequent, even the corrections being by no means exhaustive or completely reliable. The final bibliography C lists without description (apart from title) those papers concerned with multi-centre integrals. No systematic tabulation of multi-centre integrals has yet been published.

Information on tables published prior to 1943 may be obtained from the FMR Index14 and from the excellent bibliographies of Mulligan,15 Root-haan16 and Rüdenberg.17

Finally it seems worthwhile to mention that a discussion of future developments was reported in the proceedings of a conference on quantal methods in valence theory (QMVT).18

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**Bibliography C**

*Multicentre integrals.*


INTEGRALS OCCURRING IN PROBLEMS OF MOLECULAR STRUCTURE 211


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1 No notation has become standard yet.
Introduction. The construction of the complete character table for the symmetric group of a given degree $n$ (i.e., the group formed by the permutations of $n$ quantities) is a problem of long standing. Theoretically the problem was solved many years ago by Frobenius, who first introduced the concept of the character of a representation (thus meriting the title of founder of the theory of group representations). Frobenius' expression for the symmetric group characters as coefficients of a certain algebraic form is, however, unsuitable for practical calculation except for groups of quite low degree. Some years ago Murnaghan was able to derive a recursion scheme which permits one to calculate the characters for a given $n$ in terms of the (presumably known) characters of all the symmetric groups of lower degree. This scheme has been employed by various authors to construct character tables for all the symmetric groups of degree $n \leq 14$. The recursion scheme effectively reduces the problem to an exercise in bookkeeping, but, despite its simplicity, it suffers from two practical faults. First of all, the labor involved in computing the characters by hand becomes prohibitive for $n$ larger than, say, 14. Secondly, as mentioned above, for each $n$ the results for all lower $n$ must be used, so that errors may be expected to propagate. This, of course, is not a theoretical limitation, since in principle each table may be calculated, ab initio, and any given table can be checked for consistency by using the fact that the characters themselves satisfy certain orthogonality relations. The impracticability of proceeding by hand computation is clear when it is remembered that the number of characters of the symmetric group of degree $n$ is equal to the square of the number of unrestricted partitions of $n$; for $n = 15$, this number is 30,976.

It should be evident that the practical difficulties mentioned in the preceding paragraph can in large measure be overcome by the use of electronic computers. In fact, it seemed to us that this very calculation would provide a very good test of the speed and flexibility of such a computer with regard to the handling of purely algebraic problems. Accordingly, we set up and carried out the calculation of the complete character tables of the symmetric groups of degree $n = 15$ and 16 using the Los Alamos Electronic Computer (MANIAC). The method was checked by re-computing the tables for $n = 10$ to $n = 14$. The method of calculation is described in Sec. (III). The experience was quite encouraging, and suggests that it would be profitable to apply electronic computer techniques to a large class of quite complicated problems in algebra and group theory.

The Character Formulae. For convenience we give here a brief resume of the relevant properties of the symmetric group characters. For proofs and detailed discussion the reader is referred to the standard works of Littlewood and Murnaghan.