PHILOSOPHICAL TRANSACTIONS OF THE ROYAL SOCIETY A
MATHEMATICAL, PHYSICAL & ENGINEERING SCIENCES

Electronic Wave Functions. VII. Methods of Evaluating the Fundamental Coefficients for the Expansion of Vector-Coupled Schrodinger Integrals and Some Values of these

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Phil. Trans. R. Soc. Lond. A 1952 **245**, 116-138
doi: 10.1098/rsta.1952.0019

ELECTRONIC WAVE FUNCTIONS

VII. METHODS OF EVALUATING THE FUNDAMENTAL COEFFICIENTS FOR THE EXPANSION OF VECTOR-COUPLED SCHRÖDINGER INTEGRALS AND SOME VALUES OF THESE

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(*Communicated by Sir John Lennard-Jones, F.R.S.—Received* 8 *December* 1951)

CONTENTS

The evaluation of all types of numerical data required for the expansion of Schrödinger matrix elements between antisymmetric vector-coupled functions in terms of one- and two-electron integrals is described. Some coefficients are effectively evaluated by the defining relations, but others can be most briefly evaluated by derived procedures. The values of ranges of all the necessary coefficients are given. The expansions of a set of integrals between functions derived from p^6S^1 by single and double replacements are also given. These constitute a set which is used repeatedly in the variational treatment of all atoms more complicated than fluorine.

1. Introduction

It has been shown in parts III to VI that the evaluation of integrals of the Schrödinger Hamiltonian between antisymmetric vector-coupled functions can be reduced to a stereotyped set of changes of form using coefficients which have been denoted by U, V, W, η, Q. These coefficients are explicitly defined, but in practice they will be tabulated because the definitions are very complicated and the particular values are used repeatedly for different calculations. Effectively, these are functions of arguments which only take integral values and hence, although there are infinite numbers of values, these can be arranged in order of increasing complexity, with only the lower ranges required for the simpler atoms. The purpose of this paper is to describe the best methods of calculation of these and to report a set of values corresponding approximately to the requirements for s^n and p^n functions with one or two simple replacements.

In conjunction with these a set of actual integral expansions will be reported. These form a kind of basic set, since they correspond to the closed shells s^2S^1 and p^6S^1 with single and double replacements. They will be used in the next part for calculations on neon-like atoms, but this only constitutes a small part of their importance. The fundamental method of integral evaluation which is being used consists of a kind of resolution into contributions from component parts of the integrand and the repeated use of the integrals associated with s^2 and p^6 results from the occurrence of these as component parts of most functions for more complicated atoms. The calculation of these provides some convenient examples of the use of the numerical tables given.

It is typical of this type of calculation that if an investigation were to be performed for only one or two atomic states it might not be worth while to use the present general theory with the evaluation of all the necessary coefficients. But the same coefficients are used so repeatedly for different integrals that the prior evaluation of these would probably be well worth while for convergent variational calculations on more than two atomic states. The number of coefficients required for the first few states is completely disproportionate. Roughly, it appears that the requirements for the neon-like state approach half those required for all the atoms up to argon. Something between these two requirements is reported here.

The required coefficients were defined by explicit relations or formulas in the general theory, and when these are used for the numerical evaluation there will be no necessity for much discussion. However, in the cases of U, V, W, there are briefer methods than those given by the definitions, and these will require some explanation and justification. The integral expansions themselves will also require some explanation of the order in which the general theorems are applied. The values of the X, U, W, V coefficients calculated are given in tables 1 to 4, and in table 5 there are some particular formulas for classes of these coefficients whose values can be so simply derived that it appears needless to tabulate them. Table 6 contains the coefficients corresponding to p^n, and table 7 the composite V coefficients associated with these. Table 8 contains the Q coefficients, and tables 9 to 13 the Schrödinger integrals expansions. All tables are given in the appendix.

2. Notation and nomenclature

The notations and nomenclature used have all been used in parts III to VI, but it is probably helpful to restate the most important of these.

A set of functions $\phi(m)$ with $m = -l, -l+1, \ldots, l$ will, as previously, be called a connected set of eigangs when they satisfy the usual relations

$$(L_x \pm \mathrm{i}L_y)\,\phi(m) = \surd[(l \mp m)\,(l \pm m+1)]\,\phi(m \pm 1) \equiv N^{\pm}(m)\,\phi(m \pm 1) \tag{1}$$

for a given set of angular operators L_x, L_y, L_z.

If $\phi(m_1, m_2)$ is a doubly-connected set of eigangs under the sets of operators $\mathbf{L}_1$ and $\mathbf{L}_2$, with corresponding first eigang values l_1 and l_2, then the notation

$$\phi\theta(L, M, 1, 2) \quad \text{or} \quad \phi\theta_{12}^{LM} = \sum_m \phi(m, M-m)\,X(L, M, l_1, l_2, m) \tag{2}$$

will be used. The X's are coefficients with a formal definition chosen to make $\phi\theta_{12}^{LM}$ a connected set under the operators $(\mathbf{L}_1 + \mathbf{L}_2)$. The operator θ^{LSMU} will be used in place of the double operation $\theta^{LM}\theta^{SU}$, and M and U will be omitted when it is not necessary to specify these. Particular values of θ^{LS} will be denoted by the modified spectroscopic notations

$S^1, S^2, S^3, \ldots, P^1, P^2, \ldots$, etc., the letter denoting $L = 0, 1, 2, \ldots$, according to the code S, P, D, ..., and the suffix the value $2S+1$.

Most of the analysis of this part is concerned with changes in the particular vector couplings in the operands of integrals. It is necessary for the generality required that these integrals be treated in what is conveniently described as the selective operator form with serial and vertical notations. The fundamental variables of these integrals are sets denoted by t_i ($i = 1, 2, 3, \ldots$), and the serial notation consists of using function symbols without variables to imply that the arguments are t_i or t'_i with i increasing in a sequence from left to right throughout the whole function. The vertical notation consists of writing X above Y to denote $X(t_i)\, Y(t'_i)$ with exactly corresponding serial sequences in X and Y. The notation

$$\left(Q \middle\| \begin{matrix} X \\ Y \end{matrix}\right) \tag{3}$$

denotes the selective operator form of an integral. The operation of Q which may depend on t_i and t'_i is performed to give $QX(t_i)\, Y(t'_i)$ and then the substitutional integral operators $\int \mathrm{d}t_i\, P(t'_i \mid t_i)$ performed with respect to all the remaining t_i, t'_i variables.

Functions depending on a single t set x, y, z, v will be called single-electron functions and will always be in the form of doubly-connected sets of eigangs under **L** and **S** operators. They will be denoted by $s, s_1, s_2, \ldots, p, p_1, \ldots$, etc., the S value always being $\frac{1}{2}$ and the L value being specified by the letter of the symbol. The symbols of the type p^4P^3, etc., are used with their customary meaning, but reference may be made to part VI for the exact definition.

A terminal ω will be used to denote just a necessary set of partial antisymmetry operators to give a completely antisymmetric normalized function.

In the expansion of the integrals H_{rs} it is only necessary to consider the type of integral

$$[A^*B \mid C^*D]^L = \iint \mathrm{d}r_1\, \mathrm{d}r_2\, \bar{A}^*(r_1)\, \bar{B}(r_1)\, \bar{C}^*(r_2)\, \bar{D}(r_2)\, \{r_1, r_2\}^L, \tag{4}$$

where

$$\left.\begin{aligned} \{r_1, r_2\}^L &= r_1^{L+2}/r_2^{L-1} \quad \text{for} \quad r_2 > r_1, \\ &= r_2^{L+2}/r_1^{L-1} \quad \text{for} \quad r_1 > r_2, \end{aligned}\right\} \tag{5}$$

where $\bar{A}(r)$, etc., denote the radial variation of the respective sets of functions A, B, etc. The coefficients of the other integrals are very few and follow trivially from these. The actual functions used in all the present calculations have real radial functions so that $\bar{A}^* = \bar{A}$. In accordance with this the above integrals will be written $[AB \mid CD]^L$, but on the isolated occasions when distinction must be made the first functions in each enclosure will be referred to as A^* and C^*.

Two combinations of these integrals related to a given H_{rs} were defined and called invariants in part VI, which must be consulted for these and the related notations. The notation $qt(x_1, x_2, \ldots / y_1, y_2, \ldots)$ will denote some quantity dependent on the x_i but independent of the y_i. $\sigma(x)$ will denote i^{2x}, which is thus $(-1)^x$ when x is integral. f^* will denote the conjugate complex of f, but $\bar{f}$ will always be defined explicitly, except in the case of a connected set of eigangs, when

$$\bar{a}(m) = \sigma(m)\, a^*(-m). \tag{6}$$

3. The X coefficients

These coefficients for the expansion of vector-coupled functions are not particular to the present treatment, they have been used previously in the corresponding notation

$$X(L, M, a, b, m) = (a, b, m, M-m \mid a, b, L, M). \tag{7}$$

Condon & Shortley (1935) quote from various authors complicated explicit formulas for the dependence on l and m for special values of the other arguments. Numerical values do not appear to have been tabulated previously, but this has been found essential for the present type of analysis. It was found simplest to calculate these by recurrence relations, and the values given in table 1 were so obtained.

There is a systematic tabular method of using the recurrence relations which is so much shorter than direct substitution of numerical values in the relations that it is instructive to give details of this. Two related processes are used. The first derives the values of the $X(L, M, a, b, m)$ for given L, M, a, b from the values of $X(L, M+1, a, b, m)$ which will already have been written as a column with m decreasing downwards. A slip of paper with the values of $N^-(a, m_1)$ is placed to the left and one with $N^-(b, m_2)$ to the right, these being written and placed so that $m_1 = m$ and $m_2 = M+1-m$ for each level. Then a column $Y(m)$ is written by taking $N^-(a, m+1)$ times the adjacent X value plus $N^-(b, M+1-m)$ times the adjacent X from the row immediately below. Then from the recurrence relation

$$\begin{aligned} &N^-(L, M+1)\, X(L, M, a, b, m) \\ &\qquad = N^-(a, m+1)\, X(L, M+1, a, b, m+1) + N^-(b, M-m+1)\, X(L, M+1, a, b, m), \end{aligned} \tag{8}$$

it follows that dividing the $Y(m)$ by the value of $N^-(L, M+1)$ from a permanent table gives $X(L, M, m)$. The values are immediately checked by the normalization condition.

In the second process the $N^-(a, m)$ and $N^-(b, m)$ slips are placed alongside a variant column corresponding to $X(L, -L, m)$. Unity is entered in the lowest position $m = -a$. Then a process equivalent to deriving the values of $X(L, -L-1, m) = 0$ is followed. The value of $X(L, -L, -a+1)$ can be entered, to give $X(L, -L-1, -a) = 0$. Then the value $m = -a+2$, and so forth. However,

$$X(L, L, m) = kX(L, -L, -m), \tag{9}$$

and k is now determined to give $X(L, L, a)$ positive and the whole column normalized. Since these columns correspond to the highest possible M values, all other columns can be derived by the first process.

It has been considered simplest to calculate all the X coefficients in the form $\sigma\sqrt{(x/y)}$, where $\sigma = \pm 1$, and x and y are integers with y the same value for all m values when the other argument values are specified. The full value is given for the highest m value, but only σx is entered for the lower values of any such set. It will be seen that the coefficients for the expansion of $AB\theta^{LM}$ occur in a single vertical column and those for the inverse expansion of $A(m_1)\, B(m_2)$ in a horizontal row. In general, only the values for $a \geqslant b$ and $M \geqslant 0$ have been given, since the others can be obtained from

$$X(L, M, b, a, m) = (-1)^{a+b-L} X(L, M, a, b, M-m), \tag{10}$$

$$X(L, -M, a, b, -m) = (-1)^{a+b-L} X(L, M, a, b, m). \tag{11}$$

These rules are easily memorized in the form of the equivalent geometric procedure associating changes of sign with the even-numbered columns for both types of derivation. The following expansions provide examples for the cases $a = 2$, $b = 1$:

$$BA\theta^{21} = -BA\theta^{21}_{AB} = -\surd(\tfrac{2}{6})\,B(-1)\,A(2) - \surd(\tfrac{1}{6})\,B(0)\,A(1) + \surd(\tfrac{1}{2})\,B(1)\,A(0), \tag{12}$$

$$A(-1)\,B(0) = \surd(\tfrac{8}{15})\,AB\theta^{3,-1} - \surd(\tfrac{1}{6})\,AB\theta^{2,-1} - \surd(\tfrac{3}{10})\,AB\theta^{1,-1}. \tag{13}$$

4. The U coefficients

These coefficients which enable the order of the vector coupling of three eigang quantities to be changed were found to be more troublesome to evaluate than any of the other coefficients. Fortunately, the number of these required was the smallest, and table 2 contains most of the values required for calculations up to the $3d$ shell. A method which is fairly direct, and as good as all the others examined, is to consider a term $AB\theta(e, m_1)\,C(m_2)$, where A, B, C denote connected sets of eigangs with first values a, b, c, and to expand this numerically in two ways

$$AB\theta(e, m_1)\,C(m_2) = \sum_d X(d, m_1+m_2, e, c, m_1)\,AB\theta(e)\,C\theta(d, m_1+m_2), \tag{14}$$

and

$$\begin{aligned} AB\theta(e, m_1)\,C(m_2) &= \sum_{m_3} X(e, m_1, a, b, m_3)\,A(m_3)\,B(m_1-m_3)\,C(m_2) \\ &= \sum_{m_3, f} X(e, m_1, a, b, m_3)\,X(f, m_1+m_2-m_3, b, c, m_1-m_3)\,A(m_3)\,BC\theta(f, m_1+m_2-m_3) \\ &= \sum_{f, d} Y(f, d)\,A[BC\theta(f)]\,\theta(d, m_1+m_2). \end{aligned} \tag{15}$$

These two expressions, evaluated numerically by means of the X tables, are equal, and by theorem 2, part IV, the eigang terms with corresponding eigang values can be equated so that it follows

$$AB\theta(e)\,C\theta(d, m_1+m_2) = \sum_f Y(f, d)/X(d, m_1+m_2, e, c, m_1)\,A[BC\theta(f)]\,\theta(d, m_1+m_2). \tag{16}$$

But these coefficients are just the $U(a, b, c, d \mid e, f)$ by the definition of the latter.

Values of these coefficients are given in table 2, where it will be seen that a numerical check is provided by the fact that each subtable represents an orthogonal transformation and so different columns are orthogonal.

5. The W coefficients

The W coefficients are used in one of the most fundamental relations for the reduction of Schrödinger matrix elements between vector-coupled functions. They were defined by a formula involving a double summation of products of X coefficients, but it is simpler to evaluate them by a modification of the relation in which they are used, and which was proved to be a consequence of the definition. This is

$$\sum_f W(a, c \mid b, d \mid e, f)\,F\begin{pmatrix}\overline{A} & \overline{B} \\ C & D\end{pmatrix}\begin{matrix}\theta^{fm}_{AC} \\ \overline{\theta}^{*fm}_{BD}\end{matrix} = F\begin{pmatrix}A^* & B^* \\ C & D\end{pmatrix}\begin{matrix}\theta^{eM}_{AB} \\ \theta^{eM}_{CD}\end{matrix} \tag{17}$$

$$= F\begin{pmatrix}A^*(m_1) & B^*(M-m_1) \\ C\,D\theta^{eM}_{CD} & \end{pmatrix}\Big/ X(e, M, a, b, m_1), \tag{18}$$

where A, B, C, D denote eigangs with first values a, b, c, d, and F is some integral operator which always satisfies

$$F\begin{pmatrix} G^*(L,M) \\ H(l,m) \end{pmatrix} = \delta(L,l)\,\delta(M,m)\,qt(/M), \tag{19}$$

$$F[I(L,M)\,\mathcal{J}^*(l,m)] = \delta(L,l)\,\delta(M,m)\,qt(/M), \tag{20}$$

where G and H have been written for $AB\theta$ and $CD\theta$, and I and J for $\bar{A}C\theta$ and $\bar{B}D\theta$.

The equality (18) has not been proved previously, but it follows by the inverse expansion

$$A(m_1)\,B(M-m_1)/X(e,M,a,b,m_1) = AB\theta^{eM} + \text{other eigangs}.$$

The contribution of the other eigangs to the F operation is zero by relation (19).

The evaluation of the W coefficients for a particular set of values a, b, c, d, e is performed by carrying out the above expansion numerically in stages, when the final coefficients are the required values. In the above notation this can be represented

$$F\begin{pmatrix} G^*(e,m) \\ H(e,m) \end{pmatrix} = F\begin{pmatrix} A^*(m_1)\;B^*(m-m_1)/X(e,m,a,b,m_1) \\ \sum\limits_{m_2} C(m_2)\,D(m-m_2)\,X(e,m,c,d,m_2) \end{pmatrix} \tag{21}$$

$$= \sum_{m_2} qt(m_1,m_2)\,F\begin{pmatrix} \bar{A}(-m_1) & \bar{B}(m_1-m) \\ C(m_2) & D(m-m_2) \end{pmatrix} \tag{22}$$

$$= \sum_{f,f_1,m_2} qt_2(f,f_1,\;m_1,m_2)\,F[I(f,m_2-m_1)\,J(f_1,m_1-m_2)] \tag{23}$$

$$= \sum_{f} qt_3(f)\,F[I(f,m_5)\,\mathcal{J}^*(f,m_5)]. \tag{24}$$

The $qt_3(f)$ are the $W(a,c\,|\,b,d\,|\,e,f)$, and it is immaterial what values are used for m and m_5. Substitutions have been made by

$$\begin{aligned} A^*(m_1) &= \sigma(m_1)\,\bar{A}(-m_1), \\ J(m_4) &= [\sigma(m_4)\,\mathcal{J}(-m_4)]^* = \sigma(-m_4)\,\mathcal{J}^*(-m_4), \end{aligned} \tag{25}$$

and by the ordinary vector-coupling relations. The coefficients are evaluated as completely as possible at each stage.

The following example for $a=b=c=d=1$ and $e=0$ shows the numerical quantities written. In practice A, B, C, D and F are omitted, but, for clarity, merely the F is omitted here:

$$\begin{aligned} \begin{pmatrix} G^*(0,0) \\ H(0,0) \end{pmatrix} &= \begin{pmatrix} -A^*(0)\,B^*(0)\sqrt{3} \\ H(0,0) \end{pmatrix} = \begin{pmatrix} -A^*(0)\,B^*(0) \\ C(1)\,D(-1) - C(0)\,D(0) + C(-1)\,D(1) \end{pmatrix} \\ &= \begin{pmatrix} \bar{A}(0) & \bar{B}(0) \\ C(0) & B(0) \end{pmatrix} - \begin{pmatrix} \bar{A}(0) & \bar{B}(0) \\ C(1) & D(-1) \end{pmatrix} - \begin{pmatrix} \bar{A}(0) & \bar{B}(0) \\ C(-1) & D(1) \end{pmatrix} \\ &= \{I(2,0)\sqrt{\tfrac{4}{6}} - I(0,0)\sqrt{\tfrac{1}{3}}\}\{J(2,0)\sqrt{\tfrac{4}{6}} - J(0,0)\sqrt{\tfrac{1}{3}}\} \\ &\quad -\{I(2,1)\sqrt{\tfrac{1}{2}} - I(1,1)\sqrt{\tfrac{1}{2}}\}\{J(2,-1)\sqrt{\tfrac{1}{2}} + J(1,-1)\sqrt{\tfrac{1}{2}}\} \\ &\quad -\{I(2,-1)\sqrt{\tfrac{1}{2}} + I(1,-1)\sqrt{\tfrac{1}{2}}\}\{J(2,1)\sqrt{\tfrac{1}{2}} - J(1,1)\sqrt{\tfrac{1}{2}}\} \\ &= \tfrac{5}{3}[I(2,0)\,\mathcal{J}^*(2,0)] - 1[I(1,0)\,\mathcal{J}^*(1,0)] + \tfrac{1}{3}[I(0,0)\,\mathcal{J}^*(0,0)]. \end{aligned} \tag{26}$$

These coefficients are the $W(1,1\,|\,1,1\,|\,0,f)$ for $f = 2,1,0$.

The values of W coefficients are tabulated in table 3. In general, the related cases which can be derived by interchange of a with c and b with d have not been tabulated, because these have exactly the same values. The corresponding change of value was shown to be given by a factor $\sigma(2d-2b)$ in theorem 9, part VI, but the W coefficients are only required for integral values of $(a-c)$ and $(b-d)$, so this is unity for all values tabulated. The values for coefficients derived by interchanging a, c with b, d are obtained from the tabulating values by multiplication by $\sigma(a+b-c-d) = \pm 1$ by the same theorem.

In calculations involving many detailed substitutions it is extremely desirable to have some check such as the following, which can be applied immediately after the evaluation of a set of values. A particular F function $F[A^*(m_1)\, B^*(m_2)\, C(m_3)\, D(m_4)]$ is chosen and this is expanded two ways, in terms of the couplings $(AB)\,(CD)$ and $(AC)\,(BD)$ respectively. Then the former expression is expanded numerically in terms of the latter type of coupling by means of the calculated W coefficients. This should agree with the second expansion.

6. The V coefficients

The circumstances for the evaluation of the V coefficients are similar to those for the W coefficients. A formula involving a double summation of products of X's is given by the definition, but it is simpler to calculate the values by means of the fundamental relation in which these coefficients are used. This is

$$\begin{matrix} A \\ C \end{matrix}\left(\left\|\begin{matrix} B \\ B \end{matrix}\right)\begin{matrix} \bar{\theta}^e_{AB} \\ \theta^f_{BC} \end{matrix}\, \theta^L_{ef} = V(a, c \mid b \mid e, f \mid L) \begin{pmatrix} \bar{A} \\ C \end{pmatrix} \theta^L_{AC}, \tag{27}$$

where A, B, C are given eigangs with first values a, b, c, and the integration is performed merely over the variables of B.

The method used consists of expanding an arbitrarily chosen expansion in two ways, one involving the V coefficients and the other completely numerically. The equation of the corresponding terms determines the required values. A particular set of values a, b, c, e, f is considered at one time, but two values m_1 and m_2 can be chosen in various ways to determine the same coefficients. It is convenient to use G, H, I, J to denote

$$AB\theta, \quad CB\theta, \quad \bar{G}(t_i)\, H(t_i')\, \theta, \quad \bar{A}(t_i)\, C(t_i')\, \theta$$

respectively, and to understand that the integral operation is applied to B when it occurs explicitly or implicitly. The two expansions to be performed numerically are

$$\begin{aligned} \left(\left\|\begin{matrix} \bar{G}(e, m_1) \\ H(f, m_2) \end{matrix}\right.\right) &= \sum_g X(g, m_1+m_2, e, f, m_1)\, I(g, m_1+m_2) \\ &= \sum_g X(g, m_1+m_2, e, f, m_1)\, V(a, b \mid c \mid e, f \mid g)\, J(g, m_1+m_2) \end{aligned} \tag{28}$$

and

$$\begin{aligned} \left(\left\|\begin{matrix} \bar{G}(e, m_1) \\ H(f, m_2) \end{matrix}\right.\right) &= \left(\left\|\begin{matrix} [\sum X(e, -m_1, a, b, m_3)\, \sigma(m_1)\, A^*(m_3)\, B^*(-m_1-m_3)] \\ [\sum X(f, m_2, c, b, m_4) \qquad C(m_4)\, B(m_2-m_4)] \end{matrix}\right.\right) \\ &= \sum_{m_3} qt_1(m_3) \begin{matrix} A^*(m_3) \\ C(m_1+m_2+m_3) \end{matrix} \\ &= \sum_g qt_2(g)\, J(g, m_1+m_2). \end{aligned} \tag{29}$$

The coefficients are evaluated from the X tables at each stage. The corresponding eigang terms can be equated by theorem 2, part IV, to give the values of several V coefficients

$$V(a, c \mid b \mid e, f \mid g) = qt_2(g)/X(g, m_1+m_2, e, f, m_1).$$

The following example for the case $a=b=c=e=f=1$ shows the numerical quantities which it is convenient to record in practice:

$$\begin{matrix}\bar{G}(-1)\\ H(1)\end{matrix} = J(2,0)\, V(1,1\,|\,1\,|\,1,1\,|\,2)\sqrt{\tfrac{1}{6}} - J(1,0)\, V(1,1\,|\,1\,|\,1,1\,|\,1)\sqrt{\tfrac{1}{2}} + J(0,0)\, V(1,1\,|\,1\,|\,1,1\,|\,0)\sqrt{\tfrac{1}{3}}. \quad (30)$$

The second expansion gives

$$\begin{aligned}\begin{matrix}\bar{G}(-1)\\ H(1)\end{matrix} = \begin{matrix}-G^*(1)\\ H(1)\end{matrix} &= \begin{matrix}[-A^*(1)\,B^*(0)\sqrt{\tfrac{1}{2}}+A^*(0)\,B^*(1)\sqrt{\tfrac{1}{2}}]\\ [C(1)\,B(0)\sqrt{\tfrac{1}{2}}-C^*(0)\,B^*(1)\sqrt{\tfrac{1}{2}}]\end{matrix}\\ &= -\frac{1}{2}\left(\begin{matrix}\bar{A}(0)\\ C(0)\end{matrix} - \begin{matrix}\bar{A}(-1)\\ C(1)\end{matrix}\right)\\ &= -J(2,0)\sqrt{\tfrac{1}{24}} - J(1,0)\sqrt{\tfrac{1}{8}} + J(0,0)\sqrt{\tfrac{1}{3}}, \end{aligned} \quad (31)$$

from which the values of $-\frac{1}{2}$, $\frac{1}{2}$, 1 follow for the V coefficients shown.

The values of a moderate practical range of V coefficients are given in table 4. The values derived from these by the interchange of a with c and e with f are omitted, since these were shown to have the same values in theorem 18, part VI.

A check similar to that used for the W coefficients can be applied to a set of V values for one set of a, b, c values. An expression $A^*(m_1)\,C(m_2)\,[B(m_3)\,|\,B(m_3)]$ is expanded in terms of the functions with couplings $\bar{G}H\theta$ and then this expanded by the V coefficients in terms of the J. It is also easily expanded directly in terms of J, since $[B(m_3)\,|\,B(m_3)] = 1$ and the two expansions should be exactly the same if the correct values of the V coefficients have been used.

7. The p^n coefficients

The coefficients for the expansion

$$p^n\phi_k = \sum_l \eta_{kl}\, p^{n-1}\phi_l\, p\theta(L_k, S_k), \quad (32)$$

which is a simplification of the a^n expansion of § 3, part V, are given in table 6. It will be noted that the r variable has been omitted, since there is never more than one function with a given LS combination for any p^n. Since there is just this one LS value corresponding to each value of l, it is convenient to write this explicitly instead of a numerical value for l, and thus the table implies relations such as

$$p^3\mathrm{P}^2 = -\sqrt{(\tfrac{2}{9})}\, p^2\mathrm{S}^1 p\mathrm{P}^2 + \sqrt{(\tfrac{1}{2})}\, p^2\mathrm{P}^3 p\mathrm{P}^2 + \sqrt{(\tfrac{5}{18})}\, p^2\mathrm{D}^1 p\mathrm{P}^2. \quad (33)$$

The calculation of these coefficients will not be described, first because no alternative method shorter than the explicit application of that given by the general theory in part V is known, and secondly because these coefficients are not new, having been obtained by a different method by Racah (1943).

In conjunction with this calculation table 7 containing the V^{LS}_{ABpp} elements for $A, B = p^n\phi_k$ and some corresponding simple s and d functions has been given. This is closely connected with the p^n calculation, since it is necessary to calculate the V's corresponding to p^n from the η of p^n and then the η for p^{n+1} from these V's. It is not proposed to discuss this in detail. It has been performed explicitly by the general theory relations in several cases as a check, but the original values were obtained by special methods at early stages of these investigations and were later cross-checked by other special theorems which will be reported subsequently.

It is also convenient to tabulate at the same time the values of the expansions of $p^n\phi_k$ in terms of $p^{n-2}\phi_l p^2\phi_m\theta^{LS}$, as these are used in a similar manner in the evaluation of integrals. These were obtained by expansion of $p^n\phi_k$ in terms of $p^{n-1}\phi_l p\theta^{LS}$, and then by the further expansion of $p^{n-1}\phi$ and alteration of the coupling by the appropriate expansions with U coefficients.

It can easily be seen from considerations of antisymmetry that the $a^2\phi$ functions are always just the $aa\theta^{LS}$ with $L+S$ an even integer. Hence the s^2, p^2, d^2 have not been entered in the table.

8. The Q coefficients

The Q coefficients have been shown to be equal to simple expressions in terms of X and W coefficients containing only a very simple summation. They have been evaluated by the explicit use of these expressions (theorem 17, part VI), and are given in table 8.

For compact tabulation the $Q(ab \mid cd \mid L)$ have been written as if they were particular cases of the $Q(ab \mid cd \mid ef)$, δ being written for the value of f in this case. For reference, and to make the precise meaning of these notations clear, it is convenient to state the fundamental relation in which the Q coefficients are used:

$$\left(\sum_i \sum_j (1-yP_{ij})/r_{ij} \left\| \begin{matrix} A^* & B^*\theta^{LS} \\ C & D\theta^{LS} \end{matrix} \right.\right)$$
$$= \sum_{\bar{L}} \sum_{\bar{S}} W(L_A, L_C \mid L_B, L_D \mid L, \bar{L})\, W(S_A, S_C \mid S_B, S_D \mid S, \bar{S}) \sum_{r,s,t,u} V^{\bar{L}\bar{S}}_{ACrs} V^{\bar{L}\bar{S}}_{BDtu}$$
$$\times \{\delta(S,0)\, Q(L_r, L_s \mid L_t, L_u \mid \bar{L}, \delta)\, [x_r^* x_s \mid x_t^* x_u]^{\bar{L}} + y \sum_K Q(L_r, L_s \mid L_t, L_u \mid \bar{L}, K)\, [x_r^* x_u \mid x_t^* x_s]^K\}. \tag{34}$$

This is, in fact, a combination of theorem 18, part IV, and theorem 17, part VI. The quantity y has been included to cover the values 1 and 0 which are required for different cases.

9. The evaluation of some Schrödinger integrals

The derivation of the expansions for all the matrix elements of the Schrödinger Hamiltonian given in tables 9 to 13 will be effectively demonstrated if those between the following functions are described as examples:

$$\left.\begin{aligned} \phi_1 &= p_1^6\,\mathrm{S}^1, \\ \phi_2 &= p_1^5\,\mathrm{P}^2 p_2\,\mathrm{S}^1\,\omega, \\ \phi_3 &= p_1^4\,\mathrm{D}^1 p_2^2\,\mathrm{D}^1\,\mathrm{S}^1\,\omega, \\ \phi_4 &= p_1^4\,\mathrm{D}^1 d^2\mathrm{D}^1\,\mathrm{S}^1\,\omega, \end{aligned}\right\} \tag{35}$$

where p_1, p_2, d are electron eigang sets with $L = 1, 1, 2$ respectively. The complete set of functions for which the integrals are tabulated corresponds to single and double replacements in a $p^6\mathrm{S}^1$ function and contains two other functions with internal couplings S^1 and P^3 associated with ϕ_3 and a similar pair with ϕ_4. The few points at which the integrals of these latter functions involve special considerations will be discussed at the same time as the integrals with which they are associated. The expansions for all p^n and $s_1 s_2\mathrm{S}^1$ are well known but are retabulated here for reference. They have been rederived by the present methods chiefly as a check on the various W, V coefficients. These calculations will not be described since the same points are illustrated by those for integrals of functions (35), most of which have not previously been reported.

It will be convenient to use M_{ij} for $1/r_{ij}$, M for $\sum_{i>j} M_{ij}$, whenever the range of summation is obvious, and M_{rs} for $(\phi_r \mid M \mid \phi_s)$. It will be sufficient to examine only M_{rs}, since the coefficients of the other terms of the Schrödinger Hamiltonian matrix elements are determined by the invariant coefficient which the M_{rs} calculation provides. It must be noted that although the full expression for a particular integral will be obtained by the procedures below, these will always be subdivided into the invariant and variant terms for tabulation. This is particularly useful since the $K-ZV$ terms are correctly included when these formulas are used for H instead of M.

For the expansion of M_{12} it follows

$$M_{12} = \left(\sum_{i>j} M_{ij} \left\| \begin{matrix} p_1^5\,\mathrm{P}^2 p_1\,\mathrm{S}^1{}^* \\ p_1^5\,\mathrm{P}^2 p_2\,\mathrm{S}^1\omega \end{matrix}\right.\right) = \surd 6 \left(\sum_{i=1}^{5} M_{i6} \left\| \begin{matrix} p_1^5\,\mathrm{P}^2 p_1\,\mathrm{S}^1{}^* \\ p_1^5\,\mathrm{P}^2 p_2\,\mathrm{S}^1 \end{matrix}\right.\right)$$
$$= \surd 6 \sum_L W(1,1 \mid 1,1 \mid 0,L)\, W(\tfrac{1}{2},\tfrac{1}{2} \mid \tfrac{1}{2},\tfrac{1}{2} \mid 0,0)\, V^{LO}_{AApp}\, Q(1,1 \mid 1,1 \mid L,\delta)\, [p_1p_1 \mid p_1p_2]^L, \quad (36)$$

where A denotes $p^5\mathrm{P}^2$. The second equality follows by the removal of the ω by theorem 15, part III, for $m=5$, $n=0$. The last equality follows by the direct use of equation (34) in the special case $y=0$, so that only the terms with $S=0$ need be retained. The final expansion of table 11 is obtained by inserting the W, V, Q values from the appropriate tables. The products are conveniently found by writing the values for different L in columns and then multiplying across in each row.

For the expansion of M_{23} it is necessary to expand $p_1^5\,\mathrm{P}^2$ by table 6 and then alter the coupling so that the last p_1 is coupled directly to the p_2 in ϕ_2. This alteration can be made without any other change, since the coefficients involved are of the type $U(a,b,c,0)$ which were shown to give only one term with coefficient unity in theorem 6, part VI. By this change and the removal of the ω operators by theorem 15, part III, it follows that

$$M_{23} = \left(M \left\| \begin{matrix} [-\surd(\tfrac{1}{15})\, p_1^4\,\mathrm{S}^1 p_1p_2\,\mathrm{S}^1\mathrm{S}^1 - \surd(\tfrac{3}{5})\, p_1^4\,\mathrm{P}^3 p_1p_2\,\mathrm{P}^3\mathrm{S}^1 + \surd(\tfrac{1}{3})\, p_1^4\,\mathrm{D}^1 p_1p_2\,\mathrm{D}^1\mathrm{S}^1]^*\omega \\ p_1^4\,\mathrm{D}^1 p_2p_2\,\mathrm{D}^1\mathrm{S}^1\omega \end{matrix}\right.\right)$$
$$= \surd 10 \left(\left[\sum_{i=1}^{4} + \sum_{i=6}\right] M_{i5} \left\| \begin{matrix} [-\surd(\tfrac{1}{15})\, p_1^4\,\mathrm{S}^1 p_1p_2\,\mathrm{S}^1\mathrm{S}^1 - \surd(\tfrac{3}{5})\, p_1^4\,\mathrm{P}^3 p_1p_2\,\mathrm{P}^3\mathrm{S}^1 + \surd(\tfrac{1}{3})\, p_1^4\,\mathrm{D}^1 p_1p_2\,\mathrm{D}^1\mathrm{S}^1]^* \\ p_1^4\,\mathrm{D}^1 p_2p_2\,\mathrm{D}^1\mathrm{S}^1 \end{matrix}\right.\right). \quad (37)$$

The two ranges of summation and the three expansion terms give six contributions which must be considered separately. The three terms for the range $i=1$ to 4 must all be explicitly evaluated by the WVQ formula as quoted in equation (34) and as used in the previous case M_{12}. Inspection of the other three terms shows that the first two vanish. The first, by theorem 9, part IV, is a multiple of

$$(p_1p_2\,\mathrm{S}^1 \mid M \mid p_2p_2\,\mathrm{D}^1) = 0, \quad (38)$$

and the second vanishes similarly. The third is a multiple of

$$(p_1p_2\,\mathrm{D}^1 \mid M \mid p_2p_2\,\mathrm{D}^1).$$

In principle this could be evaluated by a WVQ expansion; in particular it is well known and can be seen to have the same expansion coefficients as $(p^2\mathrm{D}^1 \mid M \mid p^2\mathrm{D}^1)$. All four contributions have to be added together to give the value in table 11, and in actual fact this type of integral is one of the most laborious to evaluate of those which are usually required for variational problems.

The expansion of M_{24} need not be analyzed in detail. It differs from that of M_{23} only in the d^2 replacing p_2^2. Just the same p_1^5 expansion, the same changes of coupling and the same ω removal are performed. Of the resulting six terms only the last does not vanish, since in this case the first three terms vanish since the two non-coincidences cause the V_{ABpd}^{LS} coefficients of $p_1 p_2$, d^2 to be zero.

The expansion of M_{44} will be described, and this will be considered sufficient to illustrate the similar evaluations for M_{22} and M_{33}, since they are obtained by exactly the same changes of form and the resulting terms are slightly simpler. M_{44} is resolved into simpler components by the application of the first removal theorem, thus

$$M_{44} = \left(M \left\| \begin{matrix} p^4\mathrm{D}^{1*} \\ p^4\mathrm{D}^1 \end{matrix} \right.\right) + \left(M \left\| \begin{matrix} d^2\mathrm{D}^{1*} \\ d^2\mathrm{D}^1 \end{matrix} \right.\right) + \left(\sum_{i=1}^{4}\sum_{j=5}^{6}(1-P_{ij})\, M_{ij} \left\| \begin{matrix} p^4\mathrm{D}^1\, d^2\mathrm{D}^1\mathrm{S}^{1*} \\ p^4\mathrm{D}^1\, d^2\mathrm{D}^1\mathrm{S}^1 \end{matrix} \right.\right). \tag{39}$$

The first term occurs in table 9. The second term could be evaluated by a WVQ expansion but is well known. The third term follows by the direct application of the WVQ equation (34), all the necessary coefficients being in the tables in the appendix.

It may be noted that the associated integrals such as

$$(p^4\mathrm{P}^3\, d^2\mathrm{P}^3\mathrm{S}^1\, \omega \mid M \mid p^4\mathrm{D}^1\, d^2\mathrm{D}^1\mathrm{S}^1\, \omega)$$

can be evaluated by just the same expansion, but in this case the first two terms are automatically zero.

The calculations of M_{13} and M_{14} are very similar, and hence only M_{14}, which is the more complicated, will be considered. When $p^6\mathrm{S}^1$ is expanded in terms of $p^4\phi_k p^2\phi_l \mathrm{S}^1$ by table 6, it can be seen that only the last term makes a non-vanishing contribution and hence

$$M_{14} = \left(M \left\| \begin{matrix} \sqrt{(\frac{1}{3})}\, p^4\mathrm{D}^1\, p^2\mathrm{D}^1\mathrm{S}^{1*} \\ p^4\mathrm{D}^1\, d^2\mathrm{D}^1\mathrm{S}^1\, \omega \end{matrix} \right.\right) = \sqrt{5}\left(M \left\| \begin{matrix} pp\mathrm{D}^{1*} \\ dd\mathrm{D}^1 \end{matrix} \right.\right), \tag{40}$$

theorem 16, part III, having been applied to remove the ω operators and theorem 9, part IV, to remove the p^4 functions. The residual integral can be evaluated by direct application of WVQ equation but is also otherwise known.

The calculation of M_{34} with two non-coincidences follows the usual ω removal and omission of the p_1^4 functions by theorem 9, part IV. The WVQ expansion vanishes because the V associated with p^2 and d^2 vanishes:

$$M_{34} = \left(\left\| \begin{matrix} p_1^4\,\mathrm{D}^{1*} \\ p_1^4\,\mathrm{D}^1 \end{matrix} \right.\right)\left(M \left\| \begin{matrix} p_2^2\,\mathrm{D}^{1*} \\ d^2\,\mathrm{D}^1 \end{matrix} \right.\right)_{\mathrm{S}^1}^{\mathrm{S}^1} = \left(M \left\| \begin{matrix} p_2^2\,\mathrm{D}^{1*} \\ d^2\,\mathrm{D}^1 \end{matrix} \right.\right), \tag{41}$$

the evaluation of the two-electron integral being trivial. When the associated terms such as

$$(p_1^4\,\mathrm{P}^3\, p_2^2\,\mathrm{P}^3\mathrm{S}^1\, \omega \mid M \mid p_1^4\,\mathrm{D}^1\, d^2\mathrm{D}^1\mathrm{S}^1\, \omega)$$

are considered, it is seen immediately that whenever the internal couplings are different for the two functions of the integral, these must by the above expansion be zero.

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This completes the description of all the types of expansion calculations for all the integrals which can be chosen between the eight functions associated with (35). All those which do not obviously vanish are stated in tables 9 to 13. They constitute a very useful set for the variational calculation of wave functions with closed p shells when these are calculated to the accuracy of permitting other variational functions corresponding to one and two replacements by other p and d orbitals.

10. Discussion

The methods of numerical evaluation which have been described provide a complement to the previous general theory. These together provide detailed methods for all the processes necessary for the expansion of Schrödinger integrals of co-detor functions.

By these methods some hundreds of necessary coefficients have been evaluated. These form a set corresponding roughly to the atoms of the first chemical period. It appears likely that extensions to higher chemical periods will not involve as much work as this first range. By the nature of the reduction processes employed, coefficients used for the simple cases will always be used repeatedly for more complicated cases.

Rather indirect methods have been used for the evaluation of some of the coefficients, but these serve as useful examples of the repeated use of the general ideas of the fundamental theory of vector coupling.

The actual Schrödinger matrix elements which have been expanded here in terms of one- and two-electron integrals have value both as a set of examples and as very useful basic data. Among other points they show very clearly that the application of the general theory is simpler than the general notations might suggest. In the theoretical formulation it is necessary to retain explicitly all possible summations, but in practice some of those frequently disappear or reduce to single terms, though the parts which vanish alter very much from calculation to calculation. The actual results reported here will be used even more repeatedly than is usual since they correspond to the functions which will be used to express the structure of $p^6\mathrm{S}^1$ groups in variation problems and these occur in all atoms higher than fluorine.

It is perhaps worth repeating the general significance of these calculations. It is considered that the most feasible way of calculating the wave functions of atoms with convergent accuracy is to determine a linear combination, $\sum_r Y_r\Phi_r$, of co-detors (or special vector-coupled Slater determinants) by variational theory. This is a simple computation when the numerical values of the $(\Phi_r \,|\, H \,|\, \Phi_s)$ are known. For n electrons these integrals depend on $4n$ variables and correspond to many times $(n!)^2$ terms. The general theory of parts III to VI shows how these can be expanded in terms of one- and two-electron integrals by means of a set of theorems involving some precisely defined U, V, W, Q coefficients. Here the best ways of evaluating these coefficients have been examined, a set of values reported and a set of integrals expanded.

M.J.M.B. is indebted to the Department of Scientific and Industrial Research and London University for a maintenance grant and post-graduate studentship respectively, for parts of the period when this work was being performed. S.F.B. is similarly indebted to London University for an Imperial Chemical Industries Fellowship.

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Appendix

Table 1. Vector-coupling coefficients $X(L, M, a, b, m) = \sigma\sqrt{(x/y)}$, where $\sigma = \pm 1$ and only σx is given after the first entry in each range with constant M

$a, b = \frac{1}{2}, \frac{1}{2}$

m,	$M-m$ \ L	1	0
$\frac{1}{2}$,	$\frac{1}{2}$	1	—
$\frac{1}{2}$,	$-\frac{1}{2}$	$\sqrt{\frac{1}{2}}$	$\sqrt{\frac{1}{2}}$
$-\frac{1}{2}$,	$\frac{1}{2}$	1	-1
$-\frac{1}{2}$,	$-\frac{1}{2}$	1	—

$a, b = 1, 1$

m,	$M-m$ \ L	2	1	0
1,	1	1	—	—
1,	0	$\sqrt{\frac{1}{2}}$	$\sqrt{\frac{1}{2}}$	—
0,	1	1	-1	—
1,	-1	$\sqrt{\frac{1}{6}}$	$\sqrt{\frac{1}{2}}$	$\sqrt{\frac{1}{3}}$
0,	0	4	0	-1
-1,	1	1	-1	1
0,	-1	$\sqrt{\frac{1}{2}}$	$\sqrt{\frac{1}{2}}$	—
-1,	0	1	-1	—
-1,	-1	1	—	—

$a, b = \frac{3}{2}, 1$

m,	$M-m$ \ L	$\frac{5}{2}$	$\frac{3}{2}$	$\frac{1}{2}$
$\frac{3}{2}$,	1	1	—	—
$\frac{3}{2}$,	0	$\sqrt{\frac{2}{5}}$	$\sqrt{\frac{3}{5}}$	—
$\frac{1}{2}$,	1	3	-2	—
$\frac{3}{2}$,	-1	$\sqrt{\frac{1}{10}}$	$\sqrt{\frac{6}{15}}$	$\sqrt{\frac{3}{6}}$
$\frac{1}{2}$,	0	6	1	-2
$-\frac{1}{2}$,	1	3	-8	1

$a, b = \frac{3}{2}, \frac{3}{2}$

m,	$M-m$ \ L	3	2	1	0
$\frac{3}{2}$,	$\frac{3}{2}$	1	—	—	—
$\frac{3}{2}$,	$\frac{1}{2}$	$\sqrt{\frac{1}{2}}$	$\sqrt{\frac{1}{2}}$	—	—
$\frac{1}{2}$,	$\frac{3}{2}$	1	-1	—	—
$\frac{3}{2}$,	$-\frac{1}{2}$	$\sqrt{\frac{1}{5}}$	$\sqrt{\frac{1}{2}}$	$\sqrt{\frac{3}{10}}$	—
$\frac{1}{2}$,	$\frac{1}{2}$	3	0	-4	—
$-\frac{1}{2}$,	$\frac{3}{2}$	1	-1	3	—
$\frac{3}{2}$,	$-\frac{3}{2}$	$\sqrt{\frac{1}{20}}$	$\sqrt{\frac{1}{4}}$	$\sqrt{\frac{9}{20}}$	$\sqrt{\frac{1}{4}}$
$\frac{1}{2}$,	$-\frac{1}{2}$	9	1	-1	-1
$-\frac{1}{2}$,	$\frac{1}{2}$	9	-1	-1	1
$-\frac{3}{2}$,	$\frac{3}{2}$	1	-1	9	-1

$a, b = 1, \frac{1}{2}$

m,	$M-m$ \ L	$\frac{3}{2}$	$\frac{1}{2}$
1,	$\frac{1}{2}$	1	—
1,	$-\frac{1}{2}$	$\sqrt{\frac{1}{3}}$	$\sqrt{\frac{2}{3}}$
0,	$\frac{1}{2}$	2	-1
0,	$-\frac{1}{2}$	$\sqrt{\frac{2}{3}}$	$\sqrt{\frac{1}{3}}$
-1,	$\frac{1}{2}$	1	-2
-1,	$-\frac{1}{2}$	1	—

$a, b = \frac{3}{2}, \frac{1}{2}$

m,	$M-m$ \ L	2	1
$\frac{3}{2}$,	$\frac{1}{2}$	1	—
$\frac{3}{2}$,	$-\frac{1}{2}$	$\sqrt{\frac{1}{4}}$	$\sqrt{\frac{3}{4}}$
$\frac{1}{2}$,	$\frac{1}{2}$	3	-1
$\frac{1}{2}$,	$-\frac{1}{2}$	$\sqrt{\frac{1}{2}}$	$\sqrt{\frac{1}{2}}$
$-\frac{1}{2}$,	$\frac{1}{2}$	1	-1
$-\frac{1}{2}$,	$-\frac{1}{2}$	$\sqrt{\frac{3}{4}}$	$\sqrt{\frac{1}{4}}$
$-\frac{3}{2}$,	$\frac{1}{2}$	1	-3
$-\frac{3}{2}$,	$-\frac{1}{2}$	1	—

$a, b = 2, \frac{1}{2}$

m,	$M-m$ \ L	$\frac{5}{2}$	$\frac{3}{2}$
2,	$\frac{1}{2}$	1	—
2,	$-\frac{1}{2}$	$\sqrt{\frac{1}{5}}$	$\sqrt{\frac{4}{5}}$
1,	$\frac{1}{2}$	4	-1
1,	$-\frac{1}{2}$	$\sqrt{\frac{2}{5}}$	$\sqrt{\frac{3}{5}}$
0,	$\frac{1}{2}$	3	-2

$a, b = 5, \frac{1}{2}$

m,	$M-m$ \ L	2	3
$\frac{5}{2}$,	$\frac{1}{2}$	1	—
$\frac{5}{2}$,	$-\frac{1}{2}$	$\sqrt{\frac{1}{6}}$	$\sqrt{\frac{5}{6}}$
$\frac{3}{2}$,	$\frac{1}{2}$	5	-1
$\frac{3}{2}$,	$-\frac{1}{2}$	$\sqrt{\frac{1}{3}}$	$\sqrt{\frac{2}{3}}$
$\frac{1}{2}$,	$\frac{1}{2}$	2	-1
$\frac{1}{2}$,	$-\frac{1}{2}$	$\sqrt{\frac{1}{2}}$	$\sqrt{\frac{1}{2}}$
$-\frac{1}{2}$,	$\frac{1}{2}$	1	-1

TABLE 1 (*cont.*)

$a, b = 2, 1$

$m,\ M-m \backslash L$	3	2	1
2, 1	1	—	—
2, 0	$\sqrt{\frac{1}{3}}$	$\sqrt{\frac{2}{3}}$	—
1, 1	2	−1	—
2, −1	$\sqrt{\frac{1}{15}}$	$\sqrt{\frac{2}{6}}$	$\sqrt{\frac{6}{10}}$
1, 0	8	1	−3
0, 1	6	−3	1
1, −1	$\sqrt{\frac{1}{5}}$	$\sqrt{\frac{1}{2}}$	$\sqrt{\frac{3}{10}}$
0, 0	3	0	−4
−1, 1	1	−1	3

$a, b = 2, \frac{3}{2}$

$m,\ M-m \backslash L$	$\frac{7}{2}$	$\frac{5}{2}$	$\frac{3}{2}$	$\frac{1}{2}$
2, $\frac{3}{2}$	1	—	—	—
2, $\frac{1}{2}$	$\sqrt{\frac{3}{7}}$	$\sqrt{\frac{4}{7}}$	—	—
1, $\frac{3}{2}$	4	−3	—	—
2, $-\frac{1}{2}$	$\sqrt{\frac{1}{7}}$	$\sqrt{\frac{16}{35}}$	$\sqrt{\frac{2}{5}}$	—
1, $\frac{1}{2}$	4	1	−2	—
0, $\frac{3}{2}$	2	−18	1	—
2, $-\frac{3}{2}$	$\sqrt{\frac{1}{35}}$	$\sqrt{\frac{12}{70}}$	$\sqrt{\frac{6}{15}}$	$\sqrt{\frac{4}{10}}$
1, $-\frac{1}{2}$	12	25	0	−3
0, $\frac{1}{2}$	18	−6	−3	2
−1, $\frac{3}{2}$	4	−27	6	−1

$a, b = 2, 2$

$m,\ M-m \backslash L$	4	3	2	1	0
2, 2	1	—	—	—	—
2, 1	$\sqrt{\frac{1}{2}}$	$\sqrt{\frac{1}{2}}$	—	—	—
1, 2	1	−1	—	—	—
2, 0	$\sqrt{\frac{3}{14}}$	$\sqrt{\frac{1}{2}}$	$\sqrt{\frac{2}{7}}$	—	—
1, 1	8	0	−3	—	—
0, 2	3	−1	2	—	—
2, −1	$\sqrt{\frac{1}{14}}$	$\sqrt{\frac{3}{10}}$	$\sqrt{\frac{6}{14}}$	$\sqrt{\frac{2}{10}}$	—
1, 0	6	2	−1	−3	—
0, 1	6	−2	−1	3	—
−1, 2	1	−3	6	−2	—
2, −2	$\sqrt{\frac{1}{70}}$	$\sqrt{\frac{1}{10}}$	$\sqrt{\frac{4}{14}}$	$\sqrt{\frac{4}{10}}$	$\sqrt{\frac{1}{5}}$
1, −1	16	4	1	−1	−1
0, 0	36	0	−4	0	1
−1, 1	16	−4	1	1	−1
−2, 2	1	−1	4	−4	1

$a, b = 3, \frac{1}{2}$

$m,\ M-m \backslash L$	$\frac{7}{2}$	$\frac{5}{2}$
3, $\frac{1}{2}$	1	—
3, $-\frac{1}{2}$	$1/\sqrt{7}$	$\sqrt{6}/\sqrt{7}$
2, $\frac{1}{2}$	6	−1
2, $-\frac{1}{2}$	$\sqrt{2}/\sqrt{7}$	$\sqrt{5}/\sqrt{7}$
1, $\frac{1}{2}$	5	−2
1, $-\frac{1}{2}$	$\sqrt{3}/\sqrt{7}$	$\sqrt{4}/\sqrt{7}$
0, $\frac{1}{2}$	4	−3

$a, b = 3, 1$

$m,\ M-m \backslash L$	4	3	2
3, 1	1	—	—
3, 0	$1/\sqrt{4}$	$\sqrt{3}/\sqrt{4}$	—
2, 1	3	−1	—
3, −1	$1/\sqrt{28}$	$\sqrt{3}/\sqrt{12}$	$\sqrt{15}/\sqrt{21}$
2, 0	12	4	−5
1, 1	15	−5	1
2, −1	$\sqrt{3}/\sqrt{28}$	$\sqrt{5}/\sqrt{12}$	$\sqrt{10}/\sqrt{21}$
1, 0	15	1	−8
0, 1	10	−6	3
1, −1	$\sqrt{6}/\sqrt{28}$	$1/\sqrt{2}$	$\sqrt{2}/\sqrt{7}$
0, 0	16	0	−3
−1, 1	6	−1	2

TABLE 1 (*cont.*)

$a, b = 3, 2$

m, $M-m$ \ L	5	4	3	2	1
3, 2	1	—	—	—	—
3, 1	$\sqrt{2}/\sqrt{5}$	$\sqrt{3}/\sqrt{5}$	—	—	—
2, 2	3	-2	—	—	—
3, 0	$\sqrt{2}/\sqrt{15}$	$\sqrt{9}/\sqrt{20}$	$\sqrt{5}/\sqrt{12}$	—	—
2, 1	8	1	-5	—	—
1, 2	5	-10	2	—	—
3, -1	$1/\sqrt{30}$	$\sqrt{27}/\sqrt{140}$	$\sqrt{5}/\sqrt{12}$	$\sqrt{5}/\sqrt{14}$	—
2, 0	9	48	0	-5	—
1, 1	15	-5	-3	3	—
0, 2	5	-60	4	-1	—
3, -2	$1/\sqrt{210}$	$\sqrt{6}/\sqrt{140}$	$\sqrt{10}/\sqrt{60}$	$\sqrt{5}/\sqrt{14}$	$\sqrt{15}/\sqrt{35}$
2, -1	24	49	15	0	-10
1, 0	90	15	-9	-2	6
0, 1	80	-30	-2	4	-3
-1, 2	15	-40	24	-3	1
2, -2	$1/\sqrt{42}$	$\sqrt{2}/\sqrt{14}$	$\sqrt{10}/\sqrt{30}$	$\sqrt{5}/\sqrt{14}$	$\sqrt{5}/\sqrt{35}$
1, -1	10	5	1	-2	-8
0, 0	20	0	-8	0	9
-1, 1	10	-5	1	2	-8
-2, 2	1	-2	10	-5	5

$a, b = 3, 3$

m, $M-m$ \ L	6	5	4	3	2	1	0
3, 3	1	—	—	—	—	—	—
3, 2	$\sqrt{\frac{1}{2}}$	$\sqrt{\frac{1}{2}}$	—	—	—	—	—
2, 3	1	-1	—	—	—	—	—
3, 1	$\sqrt{\frac{5}{22}}$	$\sqrt{\frac{1}{2}}$	$\sqrt{\frac{3}{11}}$	—	—	—	—
2, 2	12	0	-5	—	—	—	—
1, 3	5	-1	3	—	—	—	—
3, 0	$\sqrt{\frac{2}{22}}$	$\sqrt{\frac{2}{6}}$	$\sqrt{\frac{9}{22}}$	$\sqrt{\frac{1}{6}}$	—	—	—
2, 1	9	1	-2	-2	—	—	—
1, 2	9	-1	-2	2	—	—	—
0, 3	2	-2	9	-1	—	—	—
3, -1	$\sqrt{\frac{1}{33}}$	$\sqrt{\frac{1}{6}}$	$\sqrt{\frac{54}{154}}$	$\sqrt{\frac{2}{6}}$	$\sqrt{\frac{5}{42}}$	—	—
2, 0	8	2	3	-1	-10	—	—
1, 1	15	0	-40	0	12	—	—
0, 2	8	-2	3	1	-10	—	—
-1, 3	1	-1	54	-2	5	—	—
3, -2	$\sqrt{\frac{1}{132}}$	$\sqrt{\frac{5}{84}}$	$\sqrt{\frac{30}{154}}$	$\sqrt{\frac{2}{6}}$	$\sqrt{\frac{25}{84}}$	$\sqrt{\frac{3}{28}}$	—
2, -1	15	27	32	0	-15	-5	—
1, 0	50	10	-15	-1	2	6	—
0, 1	50	-10	-15	1	2	-6	—
-1, 2	15	-27	32	0	-15	5	—
-2, 3	1	-5	30	-2	25	-3	—
3, -3	$\sqrt{\frac{1}{924}}$	$\sqrt{\frac{1}{84}}$	$\sqrt{\frac{9}{154}}$	$\sqrt{\frac{1}{6}}$	$\sqrt{\frac{25}{84}}$	$\sqrt{\frac{9}{28}}$	$\sqrt{\frac{1}{7}}$
2, -2	36	16	49	$+1$	0	-4	-1
1, -1	225	25	1	-1	-9	1	1
0, 0	400	0	-36	0	16	0	-1
-1, 1	225	-25	1	1	-9	-1	1
-2, 2	36	-16	49	-1	0	4	-1
-3, 3	1	-1	9	-1	25	-9	1

TABLE 1 (*cont.*)

$a, b = 4, 1$

m,	$M-m$ \ L	5	4	3
4,	1	1	—	—
4,	0	$1/\sqrt{5}$	$\sqrt{4}/\sqrt{5}$	—
3,	1	4	-1	—
4,	-1	1√/45	$\sqrt{4}/\sqrt{20}$	$\sqrt{28}/\sqrt{36}$
3,	0	16	9	-7
2,	1	28	-7	1
3,	-1	$1/\sqrt{15}$	$\sqrt{7}/\sqrt{20}$	$\sqrt{7}/\sqrt{12}$
2,	0	7	4	-4
1,	1	7	-9	1
2,	-1	$\sqrt{2}/\sqrt{15}$	$\sqrt{9}/\sqrt{20}$	$\sqrt{5}/\sqrt{12}$
1,	0	8	1	-5
0,	1	5	-10	2
1,	-1	$\sqrt{2}/\sqrt{9}$	$1/\sqrt{2}$	$\sqrt{5}/\sqrt{18}$
0,	0	5	0	-8
-1,	1	2	-1	5

$a, b = 4, 2$

m,	$M-m$ \ L	6	5	4	3	2
4,	2	1	—	—	—	—
4,	1	$1/\sqrt{3}$	$\sqrt{2}/\sqrt{3}$	—	—	—
3,	2	2	-1	—	—	—
4,	0	$\sqrt{3}/\sqrt{33}$	$\sqrt{6}/\sqrt{15}$	$\sqrt{28}/\sqrt{55}$	—	—
3,	1	16	2	-21	—	—
2,	2	14	-7	6	—	—
4,	-1	$\sqrt{2}/\sqrt{110}$	$\sqrt{2}/\sqrt{15}$	$\sqrt{84}/\sqrt{220}$	$\sqrt{28}/\sqrt{60}$	—
3,	0	24	6	7	-21	—
2,	1	56	0	-75	9	—
1,	2	28	-7	54	-2	—
4,	-2	$1/\sqrt{495}$	$\sqrt{2}/\sqrt{90}$	$\sqrt{168}/\sqrt{1540}$	$\sqrt{56}/\sqrt{180}$	$\sqrt{70}/\sqrt{126}$
3,	-1	32	25	525	7	-35
2,	0	168	21	-64	-48	15
1,	1	224	-7	-243	49	-5
0,	2	70	-35	540	-20	1
3,	-2	$1/\sqrt{99}$	$\sqrt{7}/\sqrt{90}$	$\sqrt{378}/\sqrt{1540}$	$\sqrt{14}/\sqrt{36}$	$\sqrt{35}/\sqrt{126}$
2,	-1	14	32	243	-1	-40
1,	0	42	6	-289	-3	30
0,	1	35	-20	-30	10	-16
-1,	2	7	-25	600	-8	5
2,	-2	$1/\sqrt{33}$	$1/\sqrt{6}$	$\sqrt{54}/\sqrt{154}$	$\sqrt{2}/\sqrt{6}$	$\sqrt{5}/\sqrt{42}$
1,	-1	8	2	3	-1	-10
0,	0	15	0	-40	0	12
-1,	1	8	-2	3	1	-10
-2,	2	1	-1	54	-2	5

TABLE 2. $U(a, b, c, d \mid e, f)$ COEFFICIENTS

$(a, b, c, d) = (\frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2})$

$e \backslash f$	0	1
0	$-1/2$	$\sqrt{3}/2$
1	$\sqrt{3}/2$	$1/2$

$(a, b, c, d) = (\frac{1}{2}, \frac{1}{2}, 1, 1)$

$e \backslash f$	$\frac{1}{2}$	$\frac{3}{2}$
0	$-1/\sqrt{3}$	$\sqrt{2}/\sqrt{3}$
1	$\sqrt{2}/\sqrt{3}$	$1/\sqrt{3}$

$(a, b, c, d) = (\frac{1}{2}, 1, \frac{1}{2}, 1)$

$e \backslash f$	$\frac{1}{2}$	$\frac{3}{2}$
$\frac{1}{2}$	$-1/3$	$2\sqrt{2}/3$
$\frac{3}{2}$	$2\sqrt{2}/3$	$1/3$

$(a, b, c, d) = (1, 1, 1, 1)$

$e \backslash f$	0	1	2
0	$1/3$	$-1/\sqrt{3}$	$\sqrt{5}/3$
1	$-1/\sqrt{3}$	$1/2$	$\sqrt{5}/2\sqrt{3}$
2	$\sqrt{5}/3$	$\sqrt{5}/2\sqrt{3}$	$1/6$

$(a, b, c, d) = (1, \frac{1}{2}, 1, \frac{3}{2})$

$e \backslash f$	$\frac{1}{2}$	$\frac{3}{2}$
$\frac{1}{2}$	$-2/3$	$\sqrt{5}/3$
$\frac{3}{2}$	$\sqrt{5}/3$	$2/3$

$(a, b, c, d) = (\frac{1}{2}, 1, 1, \frac{3}{2})$

$e \backslash f$	1	2
$\frac{1}{2}$	$-1/\sqrt{6}$	$\sqrt{5}/\sqrt{6}$
$\frac{3}{2}$	$\sqrt{5}/\sqrt{6}$	$1/\sqrt{6}$

$(a, b, c, d) = (\frac{1}{2}, \frac{1}{2}, \frac{3}{2}, \frac{3}{2})$

$e \backslash f$	1	2
0	$-\sqrt{3}/2\sqrt{2}$	$\sqrt{5}/2\sqrt{2}$
1	$\sqrt{5}/2\sqrt{2}$	$\sqrt{3}/2\sqrt{2}$

$(a, b, c, d) = (1, 1, 1, 2)$

$e \backslash f$	1	2
1	$-1/2$	$\sqrt{3}/2$
2	$\sqrt{3}/2$	$1/2$

$(a, b, c, d) = (1, 1, 2, 2)$

$e \backslash f$	1	2	3
0	$1/\sqrt{5}$	$-1/\sqrt{3}$	$\sqrt{7}/\sqrt{15}$
1	$-3/2\sqrt{5}$	$1/2\sqrt{3}$	$\sqrt{7}/\sqrt{15}$
2	$\sqrt{7}/2\sqrt{5}$	$\sqrt{7}/2\sqrt{3}$	$1/\sqrt{15}$

$(a, b, c, d) = (2, 1, 1, 3)$

$e \backslash f$	1	2
2	$-1/\sqrt{3}$	$\sqrt{2}/\sqrt{3}$
3	$\sqrt{2}/\sqrt{3}$	$1/\sqrt{3}$

$(a, b, c, d) = (2, 1, 2, 2)$

$e \backslash f$	1	2	3
1	$3/10$	$-\sqrt{7}/2\sqrt{5}$	$\sqrt{14}/5$
2	$-\sqrt{7}/2\sqrt{5}$	$1/2$	$\sqrt{2}/\sqrt{5}$
3	$\sqrt{14}/5$	$\sqrt{2}/\sqrt{5}$	$1/5$

TABLE 3. $W(a, b\,|\,c, d\,|\,e, f)$ COEFFICIENTS

$(a, b\,|\,c, d) = (\frac{1}{2}, \frac{1}{2}\,|\,\frac{1}{2}, \frac{1}{2})$

$f \backslash e$	0	1
0	$-1/2$	$-1/2$
1	$3/2$	$-1/2$

$(a, b\,|\,c, d) = (1, 1\,|\,1, 1)$

$f \backslash e$	0	1	2
0	$1/3$	$1/3$	$1/3$
1	-1	$-1/2$	$1/2$
2	$5/3$	$-5/6$	$1/6$

$(a, b\,|\,c, d) = (\frac{3}{2}, \frac{3}{2}\,|\,1, 1)$

$f \backslash e$	$\frac{1}{2}$	$\frac{3}{2}$	$\frac{5}{2}$
0	$-\mathrm{i}/2\sqrt{3}$	$-\mathrm{i}/2\sqrt{3}$	$-\mathrm{i}/2\sqrt{3}$
1	$\mathrm{i}\sqrt{10}/4$	$\mathrm{i}/\sqrt{10}$	$-\mathrm{i}\,3/2\sqrt{10}$
2	$-\mathrm{i}\,5/2\sqrt{6}$	$\mathrm{i}\,2/\sqrt{6}$	$\mathrm{i}/2\sqrt{6}$

$(a, b\,|\,c, d) = (2, 2\,|\,\frac{1}{2}, \frac{1}{2})$

$f \backslash e$	$\frac{3}{2}$	$\frac{5}{2}$
0	$-\mathrm{i}/\sqrt{10}$	$-\mathrm{i}/\sqrt{10}$
1	$\mathrm{i}\,3/2\sqrt{5}$	$-\mathrm{i}/\sqrt{5}$

$(a, b\,|\,c, d) = (\frac{3}{2}, \frac{1}{2}\,|\,\frac{3}{2}, \frac{1}{2})$

$e \backslash f$	0	1
1	$3\sqrt{2}/4$	$\sqrt{10}/4$
2	$-5\sqrt{2}/4$	$\sqrt{10}/4$

$(a, b\,|\,c, d) = (2, 1\,|\,2, 1)$

$e \backslash f$	0	1	2
1	$-\sqrt{3}/\sqrt{5}$	$-3/2\sqrt{5}$	$-\sqrt{21/10}$
2	$\sqrt{5}/\sqrt{3}$	$\sqrt{5/6}$	$-\sqrt{7}/2\sqrt{3}$
3	$-7/\sqrt{15}$	$7/3\sqrt{5}$	$-\sqrt{7/5}\sqrt{3}$

$(a, b\,|\,c, d) = (1, 1\,|\,\frac{1}{2}, \frac{1}{2})$

$f \backslash e$	$\frac{1}{2}$	$\frac{3}{2}$
0	$\mathrm{i}/\sqrt{6}$	$\mathrm{i}/\sqrt{6}$
1	$-\mathrm{i}$	$\mathrm{i}/2$

$(a, b\,|\,c, d) = (\frac{3}{2}, \frac{3}{2}\,|\,\frac{1}{2}, \frac{1}{2})$

$f \backslash e$	1	2
0	$1/2\sqrt{2}$	$1/2\sqrt{2}$
1	$-\sqrt{5}/2\sqrt{2}$	$3/2\sqrt{10}$

$(a, b\,|\,c, d) = (2, 2\,|\,1, 1)$

$f \backslash e$	1	2	3
0	$-1/\sqrt{15}$	$-1/\sqrt{15}$	$-1/\sqrt{15}$
1	$3/2\sqrt{5}$	$1/2\sqrt{5}$	$-1/\sqrt{5}$
2	$-\sqrt{7}/2\sqrt{3}$	$\sqrt{7}/2\sqrt{3}$	$-1/\sqrt{21}$

$(a, b\,|\,c, d) = (2, 2\,|\,2, 2)$

$e \backslash f$	0	1	2	3	4
0	$1/5$	$1/5$	$1/5$	$1/5$	$1/5$
1	$-3/5$	$-1/2$	$-3/10$	0	$2/5$
2	1	$1/2$	$-3/14$	$-4/7$	$2/7$
3	$-7/5$	0	$4/5$	$-1/2$	$1/10$
4	$9/5$	$-6/5$	$18/35$	$-9/70$	$1/70$

$(a, b\,|\,c, d) = (\frac{1}{2}, \frac{3}{2}\,|\,\frac{3}{2}, \frac{1}{2})$

$e \backslash f$	1	2
1	$-1/4$	$-3/4$
2	$5/4$	$-1/4$

$(a, b\,|\,c, d) = (2, 1\,|\,1, 2)$

$e \backslash f$	1	2	3
1	$1/10$	$3/10$	$3/5$
2	$-1/2$	$-5/6$	$1/3$
3	$7/5$	$-7/15$	$1/15$

TABLE 4. $V(a, b \,|\, c \,|\, e, f \,|\, g)$ COEFFICIENTS

$(a, b \,|\, c) = (0, 0 \,|\, 1)$

g \ e, f	1, 1
0	$-\sqrt{3}$

$(0, 0 \,|\, \tfrac{1}{2})$

g \ e, f	$\tfrac{1}{2}, \tfrac{1}{2}$
0	$\mathrm{i}\,\sqrt{2}$

$(a, b \,|\, c) = (\tfrac{1}{2}, \tfrac{1}{2}, \tfrac{1}{2})$

g \ e, f	0, 0	1, 0	1, 1
0	$-\mathrm{i}/\sqrt{2}$	0	$\mathrm{i}\,\sqrt{3}/\sqrt{2}$
1	0	$\mathrm{i}/\sqrt{2}$	i

$(a, b \,|\, c) = (1, 1 \,|\, \tfrac{1}{2})$

g \ e, f	$\tfrac{1}{2}, \tfrac{1}{2}$	$\tfrac{3}{2}, \tfrac{1}{2}$	$\tfrac{3}{2}, \tfrac{3}{2}$
0	$-\mathrm{i}\,\sqrt{2}/\sqrt{3}$	0	$\mathrm{i}\,2/\sqrt{3}$
1	$-\mathrm{i}\,2/3$	$\mathrm{i}\,\sqrt{2}/3$	$\mathrm{i}\,\sqrt{10}/3$
2	0	$\mathrm{i}\,\sqrt{2}/\sqrt{3}$	$\mathrm{i}\,\sqrt{2}/\sqrt{3}$

$(\tfrac{1}{2}, \tfrac{1}{2} \,|\, 1)$

g \ e, f	$\tfrac{1}{2}, \tfrac{1}{2}$	$\tfrac{3}{2}, \tfrac{1}{2}$	$\tfrac{3}{2}, \tfrac{3}{2}$
0	1	0	$-\sqrt{2}$
1	$-1/3$	$-2\sqrt{2}/3$	$-\sqrt{10}/3$
2	0	0	0

$(a, b \,|\, c) = (1, 0 \,|\, 1)$

g \ e, f	0, 1	1, 1	2, 1
1	$-1/\sqrt{3}$	-1	$-\sqrt{5}/\sqrt{3}$

$(1, 0 \,|\, \tfrac{1}{2})$

g \ e, f	$\tfrac{1}{2}, \tfrac{1}{2}$	$\tfrac{3}{2}, \tfrac{1}{2}$
1	$\mathrm{i}\,\sqrt{2}/\sqrt{3}$	$\mathrm{i}\,2/\sqrt{3}$

$(a, b \,|\, c) = (2, 0 \,|\, 1)$

g \ e, f	1, 1	2, 1	3, 1
2	$-\sqrt{3}/\sqrt{5}$	-1	$-\sqrt{7}/\sqrt{5}$

$(a, b \,|\, c) = (1, 1 \,|\, 1)$

g \ e, f	0, 0	1, 0	1, 1	2, 0	2, 1	2, 2
0	$-1/\sqrt{3}$	0	1	0	0	$-\sqrt{5}/\sqrt{3}$
1	0	$1/\sqrt{3}$	$1/2$	0	$-\sqrt{5}/2\,\sqrt{3}$	$-\sqrt{5}/2$
2	0	0	$-1/2$	$-1/\sqrt{3}$	$-\sqrt{3}/2$	$-\sqrt{7}/2\,\sqrt{3}$

$(a, b \,|\, c) = (1, 1 \,|\, 2)$

g \ e, f	1, 1	2, 1	2, 2	3, 1	3, 2	3, 3
0	1	0	$-\sqrt{5}/\sqrt{3}$	0	0	$\sqrt{7}/\sqrt{3}$
1	$-1/2$	$-\sqrt{3}/2$	$-\sqrt{5}/6$	0	$\sqrt{7}/3$	$\sqrt{14}/3$
2	$1/10$	$\sqrt{3}/2\,\sqrt{5}$	$\sqrt{7}/2\,\sqrt{3}$	$\sqrt{21}/5$	$\sqrt{14}/\sqrt{15}$	$\sqrt{14}/5$

$(a, b \,|\, c) = (2, 2 \,|\, 1)$

g \ e, f	1, 1	2, 1	2, 2	3, 1	3, 2	3, 3
0	$-\sqrt{3}/\sqrt{5}$	0	1	0	0	$-\sqrt{7}/\sqrt{5}$
1	$-3/2\,\sqrt{5}$	$\sqrt{3}/2\,\sqrt{5}$	$5/6$	0	$-\sqrt{7}/3\,\sqrt{5}$	$-2\,\sqrt{14}/3\,\sqrt{5}$
2	$-\sqrt{21}/10$	$\sqrt{7}/2\,\sqrt{5}$	$1/2$	$-1/5$	$-\sqrt{2}/\sqrt{5}$	$-2\,\sqrt{6}/5$
3	0	$\sqrt{2}/\sqrt{5}$	0	$-1/\sqrt{5}$	$-\sqrt{3}/\sqrt{5}$	$-\sqrt{3}/\sqrt{5}$
4	0	0	$-2/3$	$-\sqrt{3}/\sqrt{5}$	$-\sqrt{5}/3$	$-\sqrt{11}/3\,\sqrt{5}$

$(a, b \,|\, c) = (2, 1 \,|\, 1)$

g \ e, f	1, 0	2, 0	3, 0	1, 1	2, 1	3, 1
1	$-1/\sqrt{3}$	0	0	$1/2$	$\sqrt{3}/2$	0
2	0	$1/\sqrt{3}$	0	$3/2\,\sqrt{5}$	$1/2\,\sqrt{3}$	$-\sqrt{7}/\sqrt{15}$
3	0	0	$-1/\sqrt{3}$	0	$-1/\sqrt{3}$	$-\sqrt{2}/\sqrt{3}$

$(a, b \,|\, c) = (2, 1 \,|\, 1)$

g \ e, f	1, 2	2, 2	3, 2
1	$-1/2\,\sqrt{15}$	$-1/2$	$-\sqrt{7}/\sqrt{5}$
2	$-\sqrt{3}/2\,\sqrt{5}$	$-\sqrt{7}/2\,\sqrt{3}$	$-\sqrt{14}/\sqrt{15}$
3	$-\sqrt{3}/\sqrt{5}$	$-\sqrt{2}/\sqrt{3}$	$-\sqrt{2}/\sqrt{5}$

TABLE 5. FORMULAS FOR SOME SPECIAL SIMPLE CLASSES

$$X(L, M, a, 0, M) = 1$$
$$W(0, c\,|\,b, d\,|\,b, c) = \sigma(-d)\ \surd(2c+1)/\surd(2b+1)$$
$$U(a, b, c, 0\,|\,c, a) = 1$$
$$V(0, 0\,|\,b\,|\,b, b\,|\,0) = \sigma(b)\ \surd(2b+1)$$
$$V(a, c\,|\,0\,|\,a, c\,|\,g) = 1$$

TABLE 6. $\eta(n, \phi_k, \phi_l)$ COEFFICIENTS FOR $p^n\phi_k$ EXPANSIONS

$\phi_l \backslash \phi_k$	p^3S^4	p^3P^2	p^3D^2
p^2S^1	0	$-\sqrt{\frac{2}{9}}$	0
p^2P^3	1	$\sqrt{\frac{1}{2}}$	$-\sqrt{\frac{1}{2}}$
p^2D^1	0	$\sqrt{\frac{5}{18}}$	$\sqrt{\frac{1}{2}}$

$\phi_l \backslash \phi_k$	p^4S^1	p^4P^3	p^4D^1
p^3S^4	0	$\sqrt{\frac{1}{3}}$	0
p^3P^2	1	$-\frac{1}{2}$	$\frac{1}{2}$
p^3D^2	0	$\sqrt{\frac{5}{12}}$	$\sqrt{\frac{3}{4}}$

$\phi_l \backslash \phi_k$	p^5P^2
p^4S^1	$-\sqrt{\frac{1}{15}}$
p^4P^3	$-\sqrt{\frac{3}{5}}$
p^4D^1	$\sqrt{\frac{1}{3}}$

$\phi_l \backslash \phi_k$	p^4S^1
$p^2S^1p^2S^1$	$-\sqrt{\frac{2}{9}}$
$p^2P^3p^2P^3$	$\sqrt{\frac{1}{2}}$
$p^2D^1p^2D^1$	$\sqrt{\frac{5}{18}}$

$\phi_l \backslash \phi_k$	p^4P^3
$p^2S^1p^2P^3$	$\sqrt{\frac{1}{18}}$
$p^2P^3p^2S^1$	$\sqrt{\frac{1}{18}}$
$p^2P^3p^2P^3$	$-\sqrt{\frac{1}{3}}$
$p^2P^3p^2D^1$	$\sqrt{\frac{5}{18}}$
$p^2D^1p^2P^3$	$\sqrt{\frac{5}{18}}$

$\phi_l \backslash \phi_k$	p^4D^1
$p^2S^1p^2D^1$	$-\sqrt{\frac{1}{18}}$
$p^2P^3p^2P^3$	$-\sqrt{\frac{1}{2}}$
$p^2D^1p^2S^1$	$-\sqrt{\frac{1}{18}}$
$p^2D^1p^2D^1$	$\sqrt{\frac{7}{18}}$

$\phi_l \backslash \phi_k$	p^5P^2
$p^3S^4p^2P^3$	$-\sqrt{\frac{1}{5}}$
$p^3P^2p^2S^1$	$-\sqrt{\frac{1}{15}}$
$p^3P^2p^2P^3$	$\sqrt{\frac{3}{20}}$
$p^3P^2p^2D^1$	$\sqrt{\frac{1}{12}}$
$p^3D^2p^2P^3$	$\frac{1}{2}$
$p^3D^2p^2D^1$	$-\frac{1}{2}$

$\phi_l \backslash \phi_k$	p^6S^1
$p^4S^1p^2S^1$	$-\sqrt{\frac{1}{15}}$
$p^4P^3p^2P^3$	$-\sqrt{\frac{3}{5}}$
$p^4D^1p^2D^1$	$\sqrt{\frac{1}{3}}$

TABLE 7. V_{AB}^{LS} COEFFICIENTS

L, S \ A, B	s^2S^1, s^2S^1	p^2S^1, p^2S^1	p^2D^1, p^2D^1	p^2P^3, p^2P^3	p^2S^1, p^2D^1	p^2S^1, p^2P^3	p^2D^1, p^2P^3
0, 0	$-i\sqrt{2}$	$i\sqrt{\frac{2}{3}}$	$i\sqrt{\frac{10}{3}}$	$i\sqrt{6}$	0	0	0
0, 1	0	0	0	$2i$	0	0	0
1, 0	0	0	$i\sqrt{\frac{5}{2}}$	$i\sqrt{\frac{3}{2}}$	0	0	0
1, 1	0	0	0	i	0	$i\sqrt{\frac{2}{3}}$	$-i\sqrt{\frac{5}{6}}$
2, 0	0	0	$i\sqrt{\frac{7}{6}}$	$-i\sqrt{\frac{3}{2}}$	$i\sqrt{\frac{2}{3}}$	0	0
2, 1	0	0	0	$-i$	0	0	$-i\sqrt{\frac{3}{2}}$

L, S \ A, B	p^3P^2, p^3P^2	p^3D^2, p^3D^2	p^3S^4, p^3S^4	p^3P^2, p^3D^2	p^3P^2, p^3S^4	p^3D^2, p^3S^4
0, 0	3	$-\sqrt{15}$	$\sqrt{6}$	0	0	0
0, 1	1	$-\sqrt{\frac{5}{3}}$	$\sqrt{\frac{10}{3}}$	0	0	0
1, 0	1	$-\sqrt{5}$	0	0	0	0
1, 1	0	0	0	$\sqrt{\frac{5}{3}}$	$-\sqrt{\frac{4}{3}}$	0
2, 0	0	0	0	$-\sqrt{3}$	0	0
2, 1	1	$\sqrt{\frac{7}{3}}$	0	0	0	$\sqrt{\frac{4}{3}}$

L, S \ A, B	p^4S^1, p^4S^1	p^4D^1, p^4D^1	p^4P^3, p^4P^3	p^4S^1, p^4D^1	p^4S^1, p^4P^3	p^4D^1, p^4P^3	p^5P^2, p^5P^2
0, 0	$i\,2\sqrt{\frac{2}{3}}$	$i\,2\sqrt{\frac{10}{3}}$	$i\,2\sqrt{6}$	0	0	0	5
0, 1	0	0	$2i$	0	0	0	1, 1
1, 0	0	$i\sqrt{\frac{5}{2}}$	$i\sqrt{\frac{3}{2}}$	0	0	0	1
1, 1	0	0	$-i$	0	$-i\sqrt{\frac{2}{3}}$	$-i\sqrt{\frac{5}{6}}$	-1
2, 0	0	$-i\sqrt{\frac{7}{6}}$	$i\sqrt{\frac{3}{2}}$	$i\sqrt{\frac{2}{3}}$	0	0	-1
2, 1	0	0	$-i$	0	0	$i\sqrt{\frac{3}{2}}$	1

L, S \ A, B	d^2S^1, d^2S^1	d^2D^1, d^2D^1	d^2P^3, d^2P^3	d^2S^1, d^2D^1	d^2S^1, d^2P^3	d^2D^1, d^2P^3
0, 0	$-i\sqrt{2}/\sqrt{5}$	$-i\sqrt{2}$	$-i\,3\sqrt{2}/\sqrt{5}$	0	0	0
0, 1	0	0	$-i\,2\sqrt{3}/\sqrt{5}$	0	0	0
1, 0	0	$-i/\sqrt{2}$	$-i\sqrt{3}/\sqrt{10}$	0	0	0
1, 1	0	0	$-i/\sqrt{5}$	0	$-i\sqrt{2}/\sqrt{5}$	$i\sqrt{7}/\sqrt{10}$
2, 0	0	$i\,3/7\sqrt{2}$	$i\,3\sqrt{14/10}$	$-i\sqrt{2}/\sqrt{5}$	0	0
2, 1	0	0	$i\sqrt{21/5}$	0	0	$i\sqrt{3}/\sqrt{10}$
3, 0	0	$i\,4\sqrt{2/7}$	0	0	0	0
3, 1	0	0	0	0	0	$-i\,2\sqrt{3}/\sqrt{35}$
4, 0	0	$-i\,2\sqrt{2/7}$	0	0	0	0
4, 1	0	0	0	0	0	0

TABLE 8. $Q(a, b\,|\,c, d\,|\,e, f)$ COEFFICIENTS

$(a,b\,|\,c,d)=$	$(s,s\,|\,s,s)$			$(s,s\,|\,p,p)$			$(s,p\,|\,s,p)$	
$e \backslash f$	δ	0	e	δ	1	e	δ	1
0	-2	1	0	$2\sqrt{3}$	$-1/\sqrt{3}$	1	$-2/3$	$1/3$

$(a,b\,|\,c,d)=$	$(s,s\,|\,d,d)$			$(d,s\,|\,d,s)$			$(s,d\,|\,p,p)$	
$e \backslash f$	δ	2	e	δ	0	e	δ	1
0	$-2\sqrt{5}$	$1/\sqrt{5}$	2	$-2/5$	$1/5$	2	$-2\sqrt{6}/5\sqrt{5}$	$\sqrt{6}/3\sqrt{5}$

$(a,b\,|\,c,d)=$	$(s,p\,|\,d,p)$			$(s,p\,|\,p,d)$			$(s,d\,|\,d,d)$	
$e \backslash f$	δ	1	e	δ	2	e	δ	2
1	$2\sqrt{2}/3$	$-\sqrt{2}/3$	1	$2\sqrt{2}/3$	$-\sqrt{2}/5$	2	$2\sqrt{2}/\sqrt{35}$	$-\sqrt{2}/\sqrt{35}$

$(a,b\,|\,c,d)=$	$(p,p\,|\,p,p)$			$(d,d\,|\,p,p)$		
$e \backslash f$	δ	0	2	δ	1	3
0	-6	1	$2/5$	$2\sqrt{15}$	$-2/\sqrt{15}$	$-3\sqrt{3}/7\sqrt{5}$
1	0	1	$-1/5$	0	$-1/\sqrt{5}$	$3/7\sqrt{5}$
2	$-12/25$	1	$1/25$	$4\sqrt{3}/5\sqrt{7}$	$-\sqrt{7}/5\sqrt{3}$	$-3\sqrt{3}/35\sqrt{7}$

$(a, b\,|\,c, d) = (d, p\,|\,d, p)$

$e \backslash f$	δ	1	3
1	$-4/3$	$1/15$	$9/35$
2	0	$1/5$	$-3/35$
3	$-18/49$	$2/5$	$3/245$

$(a, b\,|\,c, d) = (d, d\,|\,d, d)$

$e \backslash f$	δ	0	2	4
0	-10	1	$2/7$	$2/7$
1	0	1	$1/7$	$-4/21$
2	$-4/7$	1	$-3/49$	$4/245$
3	0	1	$-8/49$	$-1/49$
4	$-20/63$	1	$4/49$	$1/441$

TABLE 9. VARIABLE COEFFICIENTS FOR $(\psi\omega\,|\,H\,|\,\psi\omega) = \mathrm{Inv} + CY$

$Y \backslash \psi$	$p^2\,{}^1S$	$p^2\,{}^3P$	$p^2\,{}^1D$	$p^3\,{}^4S$	$p^3\,{}^2P$	$p^3\,{}^2D$
$[pp\,|\,pp]^2$	0·4	−0·2	0·04	−0·6	0·0	−0·24

$Y \backslash \psi$	$p^4\,{}^1S$	$p^4\,{}^3P$	$p^4\,{}^1D$	$p^5\,{}^2P$	$p^6\,{}^1S$
$[pp\,|\,pp]^2$	0·0	−0·6	−0·36	−0·8	−1·2

$Y \backslash \psi$	$s_1 s_2\,{}^1S$
$[s_1 s_2\,|\,s_2 s_1]^0$	1·0

TABLE 10. VARIABLE COEFFICIENTS FOR $(\psi\omega\,|\,H\,|\,\psi\omega) = \mathrm{Inv} + \sum_r C_r Y_r$

$Y \backslash \psi$	$p_1^4\,{}^1S\;p_2^2\,{}^1S\,{}^1S$	$p_1^4\,{}^3P\;p_2^2\,{}^3P\,{}^1S$	$p_1^4\,{}^1D\;p_2^2\,{}^1D\,{}^1S$	$p_1^5\,{}^2P\;p_2\,{}^1S$
$[p_1p_1\,|\,p_1p_1]^2$	0·0	−0·6	−0·36	−0·8
$[p_2p_2\,|\,p_2p_2]^2$	0·4	−0·2	0·04	0·0
$[p_1p_1\,|\,p_2p_2]^2$	0·0	−0·4	−0·56	−0·4
$[p_1p_2\,|\,p_1p_2]^2$	−1·3333333	4·0	1·3333333	5·0
$[p_1p_2\,|\,p_1p_2]^2$	−0·5333333	−0·2	−0·7866666	−0·4

$Y \backslash \psi$	$p_1^4\,{}^1S\;d^2\,{}^1S\,{}^1S$	$p_1^4\,{}^3P\;d^2\,{}^3P\,{}^1S$	$p_1^4\,{}^1D\;d^2\,{}^1D\,{}^1S$
$[p_1p_1\,|\,p_1p_1]^2$	0·0	−0·6	−0·36
$[dd\,|\,dd]^2$	0·2857143	0·1428571	−0·0612245
$[dd\,|\,dd]^4$	0·2857143	−0·1904762	0·0816327
$[p_1p_1\,|\,dd]^2$	0·0	−0·4	0·1714286
$[p_1d\,|\,p_1d]^1$	−0·5333333	1·0	−0·3333333
$[p_1d\,|\,p_1d]^3$	−0·3428571	0·0	−0·4897959

Table 11. Coefficients for single overlap integrals
$$(\psi_1\omega|H|\psi_2\omega) = C_1 I + \sum_r C_r Y_r$$

ψ_1 / ψ_2 / Y	$p_1^6\,S^1$ / $p_1^5\,P^2\,p_2\,S^1$	$p_1^5\,P^2\,p_2\,S^1$ / $p_1^4\,S^1\,p_2^2S^1\,S^1$	$p_1^5\,P^2\,p_2\,S^1$ / $p_1^4\,P^3\,p_2^2\,P^3\,S^1$	$p_1^5\,P^2\,p_2\,S^1$ / $p_1^4\,D^1\,p_2^2D^1\,S^1$
I	2·4494897	−0·8164966	−2·4494898	1·8257418
$[p_1p_1\|p_1p_2]^2$	−0·9797959	0·6531973	0·4898979	−0·8033264
$[p_2p_2\|p_1p_2]^2$	0·0	−0·3265986	0·4898979	0·0730297

Table 12. Integral coefficients for $(\psi_1\omega|H|\psi_2\omega) = \sum_r C_r Y_r$ where $\psi = p_1^4\phi p_1^2\phi$ and $p_1^4\phi d^2\phi$: $\psi_1 \neq \psi_2$

ψ_1 / ψ_2 / Y	$p_1^4\,S^1\,p_2^2\,S^1\,S^1$ / $p_1^4\,P^3\,p_2^2\,P^3\,S^1$	$p_1^4\,S^1\,p_2^2\,S^1\,S^1$ / $p_1^4\,D^1\,p_2^2\,D^1\,S^1$	$p_1^4\,D^1\,p_2^2\,D^1\,S^1$ / $p_1^4\,P^3\,p_2^2\,P^3\,S^1$
$[p_1p_1\|p_2p_2]^2$	0·0	0·7155418	0·0
$[p_1p_2\|p_1p_2]^0$	2·0	−1·4907120	−4·4721360
$[p_1p_2\|p_1p_2]^2$	−0·4	−0·0596285	0·0894427

ψ_1 / ψ_2 / Y	$p^4S^1\,d^2S^1\,S^1$ / $p^4P^3\,d^2P^3\,S^1$	$p^4S^1\,d^2S^1\,S^1$ / $p^4D^1\,d^2D^1\,S^1$	$p^4D^1\,d^2D^1\,S^1$ / $p^4P^3\,d^2P^3\,S^1$
$[pp\|dd]^2$	0·0	0·6047432	0·0
$[pd\|pd]^1$	0·6928203	−0·3527668	−0·9165152
$[pd\|pd]^3$	−0·2969230	−0·0647939	0·1122263

Table 13. Coefficients for double overlap integrals $(\psi_1\omega|H|\psi_1\omega) = \sum_r C_r Y_r$

ψ_1 / ψ_2 / Y	$p_1^6\,S^1$ / $p_1^4\,S^1\,p_2^2\,S^1\,S^1$	$p_1^6\,S^1$ / $p_1^4\,P^3\,p_2^2\,P^3\,S^1$	$p_1^6\,S^1$ / $p_1^4\,D^1\,p_2^2\,D^1\,S^1$
$[p_1p_2\|p_1p_2]^0$	−1·0	−3·0	2·2360680
$[p_1p_2\|p_1p_2]^2$	−0·4	0·6	0·0894427

ψ_1 / ψ_2 / Y	$p_1^6\,S^1$ / $p^4S^1\,d^2S^1\,S^1$	$p_1^6\,S^1$ / $p^4P^3\,d^2P^3\,S^1$	$p_1^6\,S^1$ / $p^4D^1\,d^2D^1\,S^1$
$[pd\|pd]^1$	0·5163978	1·3416408	−0·6831300
$[pd\|pd]^3$	0·3319700	−0·5749890	−0·1254729

ψ_1 / ψ_2 / Y	$p_1^5\,P^2\,p_2\,S^1$ / $p_1^4\,S^1\,d^2S^1\,S^1$	$p_1^5\,P^2\,p_2\,S^1$ / $p_1^4\,P^3\,d^2P^3\,S^1$	$p_1^5\,P^2\,p_2\,S^1$ / $p_1^4\,D^1\,d^2D^1\,S^1$
$[p_1d\|p_2d]^1$	0·4216370	1·0954452	−0·5577732
$[p_1d\|p_2d]^3$	0·2710524	−0·4694766	−0·1024482

ψ_1 / ψ_2 / Y	$p_1^4\,S^1\,p_2^2\,S^1\,S^1$ / $p_1^4\,S^1\,d^2S^1\,S^1$	$p_1^4\,P^3\,p_2^2\,P^3\,S^1$ / $p_1^4\,P^3\,d^2P^3\,S^1$	$p_1^4\,D^1\,p_2^2\,D^1\,S^1$ / $p_1^4\,D^1\,d^2D^1\,S^1$
$[p_2d\|p_2d]$	−0·5163978	−0·4472136	−0·3055050
$[p_2d\|p_2d]^3$	−0·3319700	0·1916630	−0·0561132

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