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The group-theoretical structure of the atomic g shell: connection with the alternating group A_6 as $L_2(9)$

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Abstract The special projective linear groups $PSL(2\ell + 1)$ or $L_2(2\ell + 1)$ of order $2\ell(2\ell+1)(\ell+1)$ can be used to study atomic shells of electrons with angular momentum quantum number ℓ corresponding to the atomic p, d, f, and g shells for $\ell = 1, 2, 3, 4$, respectively. For the atomic g shell the group $L_2(9)$ is isomorphic with the alternating group A_6 on six objects of order 360 or the symmetry group of the 5-dimensional simplex, a 5-dimensional analogue of the tetrahedron with 6 vertices and 15 edges. This leads to the subgroup chain $SO(9) \supset \mathrm{SO}(5) \supset L_2(9)$ for the atomic g shell analogous to the subgroup chain $SO(7) \supset G_2 \supset L_2(7) \approx^7 O$ for the atomic f shell. In the $L_2(9)$ group only the representations of spherical harmonics or sums thereof, $\Gamma(\mathrm{Y}_\ell)$, with dimensions $\dim \Gamma(\mathrm{Y}_\ell)$ or $\dim \Gamma(\mathrm{Y}_\ell) \pm 1$ divisible by 9 are found to be individually reducible to irreducible representations (irreps) or sums of irreps of $L_2(9)$. This leads to term groupings such as S, PD, G, PF, DH, L, PK, DI, FH, M, FI, PO, DN, HK, R, etc., of increasing total dimension for the irreps of $SO(9)$ for various g^n configurations in the atomic g shell.

Keywords Atomic g shell · Group theory · Alternating group A_6

1 Introduction

The detailed study of the atomic d shell was initiated by Condon and Shortley [1] in 1935 following earlier work by Slater [2] in 1929. In 1949 Racah [3] developed group-theoretical methods for study of both the atomic d and f shells and in 1966 Wybourne [4,5] extended this approach to the atomic g shell, which is of potential

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interest in the study of the chemistry of superheavy elements. Other workers [6,7] have subsequently studied the terms of the atomic g^3 configuration in greater detail.

The relevant group theory uses infinite groups of the type $SO(2\ell+1)$, which are the rotation groups in $2\ell+1$ dimensions corresponding to the $2\ell+1$ states of an electron in a shell with angular momentum quantum number ℓ. A question that was subsequently explored was the use of finite rather than infinite groups to study atomic shells. In this connection Lo and Judd [8] suggested the use of the icosahedral group to study the atomic d shell, an approach developed further in a recent paper by the present author [9]. The icosahedral group, I, which is isomorphic with the alternating group on five objects (A_5) of order 60, is a Euclidean group. This means that it corresponds to a symmetry point group in three dimensions so that the spherical harmonics S, P, D, F, G,... individually can be expressed as irreducible representations (irreps) or sums of irreps of the icosahedral group. Furthermore, the subgroup chain $SO(5) \supset SO(3) \supset I$ can be used to study the atomic d shell. An important feature of the icosahedral group that allows it to be used to study the atomic d shell is the existence of a 5-dimensional irrep, namely the H irrep, that corresponds to the five d orbital states.

The use of a similar finite group to study the atomic f shell requires a group with a 7-dimensional irrep to represent the seven f orbital states. None of the symmetry point groups in three dimensions, i.e., Euclidean groups, has any 7-dimensional representations so a non-Euclidean permutation group is required for this purpose. Judd and Lo [10] first suggested the simple group of order 168, known to mathematicians as the special projective linear group $PSL(7)$ or $L_2(7)$ and otherwise as the didodecahedral group D or the heptakisoctahedral [11] group ${}^7O$, for a study of the atomic f shell. They noted that this group has an irrep of dimension 7, which can represent the seven states of an f orbital. However, the non-Euclidean nature of ${}^7O$ means that individual spherical harmonics cannot always be expressed as irreps or sums of irreps. For example there is no way of representing the D spherical harmonic ($L = 2$) as an irrep or irrep sum in ${}^7O$, as suggested by the absence of 2- and 5-dimensional irreps in ${}^7O$.

In a recent paper [12] the present author shows how spherical harmonics can be combined to become expressible as irreps or sums of irreps of ${}^7O$. The key is to combine the spherical harmonics where $2L$, $2L + 1$, or $2L + 2$ is not divisible by seven into pairs where the sum of the two $2L + 1$ values are multiples of 7 (actually a multiple of 14 since the combined $2L + 1$ value for such a pair is always even). The combined spherical harmonics thus appear in a series S, PH, DG, F, GM, HL, I, K,... The relevant subgroup chain for the atomic f shell then becomes $SO(7) \supset G_2^7 \supset O$, where G_2 is an infinite group corresponding to an exceptional Lie algebra analogous to the $SO(3)$ group in the subgroup chain for the atomic d shell. The pairing of the spherical harmonics in the atomic f shell required by the underlying ${}^7O$ group structure corresponds to terms appearing together in an f^n state corresponding to a given irrep of $SO(7)$ or G_2.

This paper explores an analogous approach to the study of the atomic g shell. Most surprisingly, the alternating group on six objects, namely A_6 of order 360, has the irrep of dimension nine required for the nine states of a g orbital. Furthermore, A_6, when described alternatively as $L_2(9)$, is the next member of the series of special projective linear groups $L_2(5)$ ($\approx I$) and $L_2(7)$ ($\approx {}^7O$). The corresponding subgroup chain for the atomic g shell is $SO(9) \supset SO(5) \supset A_6$. This can be seen by considering A_6 as the five-dimensional symmetry point group of the analogue of the tetrahedron in five dimensions, namely a simplex with six vertices (permuted in all ways by A_6), 15 edges, 20 faces, 15 three-dimensional cells, and 6 four-dimensional hypercells.

2 The underlying finite groups

2.1 The special projective linear groups $L_2(p)$

The most familiar applications of group theory in chemistry use symmetry point groups, which describe the symmetry of molecules. The elements of symmetry point groups can include only the standard symmetry operations in 3-dimensional space, namely the identity (E), proper rotations (C_n), reflections (σ), inversion (i), and improper rotations (S_n). However, the concepts of group theory can also be applied to more abstract sets such as the permutations of a set X of n objects. A set of permutations of n objects (including the identity "permutation") with the structure of a group is called a *permutation group* of *degree n* and the number of permutations in the set is called the *order* of the group [13]. Symmetry point groups can be regarded as special cases of permutation groups, where the symmetry operations are considered to be special types of permutations when applied to discrete sets of points or lines, such as the vertices or edges of polyhedra.

Let A and X be two elements in a group. Then $X^{-1}AX = B$ is equal to some element in the group. The element B is called the *similarity transform* of A by X and A and B are said to be *conjugate*. A complete set of elements of a group which are conjugate to one another is called a *class* (or more specifically a *conjugacy class*) of the group. The number of elements in a conjugacy class is called its *order*; the orders of all conjugacy classes must be integral factors of the order of the group.

A group G in which every element commutes with every other element (i.e., $xy = yx$ for all x, y in G) is called an *Abelian* group. In an Abelian group every element is in a conjugacy class by itself, i.e., all conjugacy classes are of order one. A *normal subgroup* N of G, written $N \lhd G$, is a subgroup that consists only of *entire* conjugacy classes of G [14]. A *normal chain* of a group G is a sequence of normal subgroups $C_1 \lhd N_{a_1} \lhd N_{a_2} \lhd \ldots N_{a_s} \lhd G$, in which s is the number of normal subgroups (besides C_1 and G) in the normal chain (i.e., the length of the chain). A *simple* group is a group having no *normal* subgroups other than the identity group C_1. The only non-trivial simple group found as a symmetry point group is the icosahedral pure rotation group, I, of order 60.

The finite groups relevant to the description of the atomic shells are the so-called projective special linear groups designated as $PSL(n)$ or $L_2(n)$ of which $L_2(5)$ is the icosahedral rotation group I or the isomorphic alternating group A_5. The $L_2(n)$ groups are generated from a finite field F_p of p elements, which can be represented by the p integers $0, \ldots, p-1$. Larger integers can be converted to an element in this finite field by dividing by p and taking the remainder (i.e., the number is taken "mod p"). For example, the finite field $\mathcal{F}_5$ contains the five elements represented by the integers 0, 1, 2, 3, and 4 and other integers are converted to one of these five integers by dividing by

Table 1 Properties of the $L_2(p)$ Groups ($3 \le p \le 11$)

Group	Order	Conjugacy classes	Isomorphisms
$L_2(3)$	12	$E + 4C_3 + 4C_3^2 + 3C_2$	$A_4 \approx T$
$L_2(5)$	60	$E + 12C_5 + 12C_5^2 + 20C_3 + 15C_2$	$A_5 \approx I \approx \mathrm{L}_2(4)$
$L_2(7)$	168	$E + 24C_7 + 24C_7^3 + 42C_4 + 56C_3 + 21C_2$	^7O or D
$L_2(9)$	360	$E+72C_5+72C_5^2+90C_4+40C_3+40C_3^2+45C_2$	A_6
$L_2(11)$	660	$E + 60C_{11} + 60C_{11}^2 + 110C_6 + 132C_5 + 132C_5^2 + 110C_3 + 55C_2$	
$L_2(13)$	1092	$E + 84C_{13} + 84C_{13}^2 + 156C_7 + 156C_7^2 + 156C_7^4 + 182C_6 + 182C_3 + 91C_2$	

5 and taking the remainder, e.g., $6 \to 1$ in $\mathcal{F}_5$ (written frequently as "$6 \equiv 1$ mod 5"). The group $SL(2,p)$ is defined to be the group of all 2×2 matrices with entries in $\mathcal{F}_p$ having determinant 1 and its subgroup $PSL(2,p)$ or $L_2(p)$ for odd p is defined to be the quotient group of $SL(2,p)$ modulo its center, where the center of a group is the largest normal subgroup that is Abelian. The group $L_2(p)$ is a simple group when p is a prime number or a power of a prime number [15], e.g., $4 = 2^2$ or $9 = 3^2$. The groups $L_2(4)$ and $L_2(5)$ are isomorphic and contain 60 elements and are also isomorphic to the icosahedral pure rotation group I. The smallest non-trivial $\mathrm{L}_2(p)$ groups that are not simple groups are $L_2(6)$ and $L_2(15)$ since $6 = 2 \times 3$ and $15 = 3 \times 5$ so that they are not powers of a prime number. The group $L_2(3)$ is also not a simple group since it is merely the tetrahedral rotation group T, which is isomorphic to the alternating group A_4.

The $L_2(p)$ groups relevant to the study of the atomic shell are those groups where $p = 2\ell + 1$, i.e., the groups where $p$is a small odd number corresponding to the number of orbital states for the types of electrons under consideration. Some features of these groups for $p = 2\ell + 1$ for $\ell = 1, 2, 3, 4, 5$, and 6 are given in Table 1. The order of a $L_2(p)$ group can be determined by the following formula for odd p:

$$|L_2(p)| = (1/2)p(p^2 - 1) \tag{1}$$

The factor 1/2 in Eq. 1 is removed if p is even so $60 = 4(16 - 1) = |L_2(4)| = |L_2(5)| = (1/2)(5)(25 - 1)$ and in fact $L_2(4)$ and $L_2(5)$ are isomorphic as noted above. Also for $p = 2\ell + 1$ Eq. 1 becomes

$$|L_2(2\ell + 1)| = 2\ell(2\ell + 1)(\ell + 1) \tag{2}$$

The groups listed in Table 1 correspond to the atomic p, d, f, g, h, and i shells, respectively, and thus already go far beyond the atomic shells of obvious chemical significance.

The finite group of interest for studying the atomic g shell is the $L_2(9)$ group, which is the first $L_2(2\ell + 1)$ group where $2\ell + 1$ is not a prime number but instead the square of a prime number, namely 3. Of interest is the observation that whereas the $L_2(p)$

groups where p is a prime number have C_p operations of period p, the $L_2(9)$ group has no operations of period 9 (see Table 1).

The $L_2(p)$ groups that are isomorphic with alternating groups A_n, i.e., $L_2(3) \approx A_4$, $L_2(5) \approx A_5$, and $L_2(9) \approx A_6$, are also the analogues of symmetry point groups in $n-1$-dimensional space R^{n-1}, since they describe the proper rotations of the $(n-1)$-dimensional simplex, which has n vertices with edges connecting every pair of vertices leading to a total of $(1/2)n(n-1)$ edges. The simplest non-trivial example is the $L_2(3)$ group which is isomorphous to A_4, which thus corresponds to the proper rotations of the simplex in 3-dimensional space R^3. This, of course, is the tetrahedron ($A_4 \approx T$) with $3+1=4$ vertices and $(1/2)(4\times 3)=6$ edges. The group $L_2(5) \approx A_5$ is not only the familiar three-dimensional point group I corresponding to the proper rotations of the regular icosahedron but also a four-dimensional point group corresponding to the proper rotations in R^4 of the four-dimensional simplex with $4+1=5$ vertices and $(1/2)(5\times 4)=10$ edges. Using this approach the group $L_2(9) \approx A_6$ is a 5-dimensional point group corresponding to the proper rotations in $\mathcal{R}^5$ of the five-dimensional simplex with $5+1=6$ vertices and $(1/2)(6\times 5)=15$ edges. This defines a subgroup relationship $SO(5) \supset L_2(9)$ since $SO(5)$ is an infinite group containing all possible rotations in R^5 and $L_2(9)$ is a finite group containing only the 360 rotations in 5-dimensional space corresponding to symmetry operations of the 5-dimensional simplex.

The use of the icosahedral group to study the atomic d shell is based on the subgroup chain $SO(5) \supset SO(3) \supset\approx A_5 \approx L_2(5)$. The relationship $I \subset SO(3)$ relates to the fact that I is a symmetry point group in three dimensions, i.e., a so-called Euclidean group. The analogous subgroup chain to study the atomic f shell is $SO(7) \supset G_2 \supset {}^7O \approx L_2(7)$. The intermediate group G_2 is not one of the standard rotation groups in some space of n dimensions but instead corresponds to an exceptional rank 2 Lie algebra [16] with some mathematical resemblance to the rotation group $SO(5)$. The analysis above suggests the subgroup chain $SO(9) \supset SO(5) \supset L_2(9) \approx A_6$ to study the atomic g shell.

2.2 The spherical harmonics in $L_2(9)$

Table 2 presents the character table of the group $L_2(9) \approx A_6$. Since this is a non-Euclidean group, i.e., $L_2(9) \not\subset SO(3)$, not all of the spherical harmonics individually correspond to irreps or sums of irreps of $L_2(9)$. The following formula [17] was used to determine the irreps or sums of irreps of $L_2(9)$ corresponding to the spherical harmonics of interest:

$$\chi(\alpha) = \frac{\sin[\ell + (1/2)]\alpha}{\sin(\alpha/2)} \tag{3}$$

In this formula α is the angle corresponding to the C_n rotation, i.e., $\alpha = 2\pi/n$.

Using Eq. 3 only spherical harmonics Y_ℓ having representations $\Gamma(\mathrm{Y}_\ell)$ with dimensions $\dim \Gamma(\mathrm{Y}_\ell)$ or $\dim \Gamma(\mathrm{Y}_\ell) \pm 1$ divisible by 9 are found to be individually reducible to irreps or sums of irreps of $L_2(9) \approx A_6$ (Table 3) analogous to the case with the atomic f shell [12]. The reducible spherical harmonics in $L_2(9)$ with the lowest L values are

Table 2 Character table for the group $L_2(9) \approx A_6$

	E	$45C_2$	$40C_3$	$40C_3^2$	$90C_4$	$72C_5$	$72C_5^2$
A	1	1	1	1	1	1	1
H_1	5	1	2	−1	−1	0	0
H_2	5	1	−1	2	−1	0	0
K_1	8	0	−1	−1	0	$(1/2)(1-\sqrt{5})$	$(1/2)(1+\sqrt{5})$
K_2	8	0	−1	−1	0	$(1/2)(1+\sqrt{5})$	$(1/2)(1-\sqrt{5})$
L	9	1	0	0	1	−1	−1
M	10	−2	1	1	0	0	0

Table 3 Reduction of representations of the spherical harmonics into sums of irreps of $L_2(9)$

	E	$45C_2$	$40C_3$	$40C_3^2$	$90C_4$	$72C_5$	$72C_5^2$	
Γ(S)	1	1	1	1	1	1	1	A
Γ(P+D)	8	0	−1	−1	0	$(1/2)(1+\sqrt{5})$	$(1/2)(1-\sqrt{5})$	K_2
Γ(G)	9	1	0	0	1	−1	−1	L
Γ(P+F)	10	−2	1	1	0	0	0	M
Γ(D+H)	16	0	−2	−2	0	1	1	$K_1 + K_2$
Γ(L)	17	1	−1	−1	1	$-(1/2)(1+\sqrt{5})$	$-(1/2)(1-\sqrt{5})$	$K_1 + L$
Γ(P+K)	18	−2	0	0	0	$(1/2)(1+\sqrt{5})$	$(1/2)(1-\sqrt{5})$	$K_2 + M$
Γ(D+I)	18	2	0	0	−2	$(1/2)(1+\sqrt{5})$	$(1/2)(1-\sqrt{5})$	$H_1 + H_2 + K_2$
Γ(F+H)	18	−2	0	0	0	$(1/2)(1-\sqrt{5})$	$(1/2)(1+\sqrt{5})$	$K_1 + M$
Γ(M)	19	−1	1	1	1	−1	−1	$L + M$
Γ(F+I)	20	0	2	2	−2	0	0	$H_1 + H_2 + M$
Γ(P+O)	26	−2	−1	−1	0	$1+\sqrt{5}$	$1-\sqrt{5}$	$2K_1 + M$
Γ(D+N)	26	2	−1	−1	−2	1	1	$H_1+H_2+K_1+K_2$
Γ(H+K)	26	−2	−1	−1	0	1	1	$K_1 + K_2 + M$
Γ(R)	27	−1	0	0	1	$-(1/2)(1+\sqrt{5})$	$-(1/2)(1-\sqrt{5})$	$K_1 + L + M$
Γ(P+Q)	28	0	1	1	2	$(1/2)(1+\sqrt{5})$	$(1/2)(1-\sqrt{5})$	$A + K_2 + L + M$
Γ(F+N)	28	0	1	1	−2	$(1/2)(1-\sqrt{5})$	$(1/2)(1+\sqrt{5})$	$H_1+H_2+K_1+M$
Γ(I+K)	28	0	1	1	−2	$(1/2)(1+\sqrt{5})$	$(1/2)(1-\sqrt{5})$	$H_1+H_2+K_2+M$

the S, G, L, M, and R with the angular momentum quantum numbers $L = 0, 4, 8, 9$, and 13, respectively (Table 3). The other spherical harmonics must be combined into pairs in order for their representations $\Gamma(Y_\ell)$ to be reducible into sums of irreps of $L_2(9)$ (Table 3).

The rules determining which pairs of spherical harmonics have combined representations $\Gamma(Y_\ell)$ that are reducible to irreps or sums of irreps of $L_2(9) \approx A_6$ in the atomic g shell are more complicated than those for the atomic f shell [12]. The condition that dim $\Gamma(Y_\ell)$, dim $\Gamma(Y_\ell) \pm 1$, or dim $\Gamma(Y_\ell) \pm 2$ be divisible by 9 appears to be necessary but not sufficient. For example, when dim $\Gamma(Y_\ell) = 16$ (i.e., dim $\Gamma(Y_\ell) + 2$

is divisible by 9) the D + H combination is reducible to irreps $K_1 + K_2$ but the P + I combination cannot be reduced to a sum of irreps of $L_2(9) \approx A_6$ (Table 3). Similarly, when dim $\Gamma(\mathrm{Y}_\ell) = 20$ (i.e., dim $\Gamma(\mathrm{Y}_\ell) - 2$ is divisible by 9) the F + I combination is reducible to irreps $H_1 + H_2 + M$ whereas the D + K combination cannot be reduced to a sum of irreps of $L_2(9) \approx A_6$ (Table 3).

3 Irreps of continuous groups: root figures and their projections

3.1 Root figures and the corresponding root descriptors

The continuous groups $SO(2\ell+1)$ are used to study the atomic shells of electrons with angular momentum quantum number ℓ. They correspond to the groups of all possible proper rotations in a $(2\ell + 1)$-dimensional space with each dimension corresponding to one of the $2\ell + 1$ states of an electron with angular momentum quantum number ℓ. The groups $SO(2\ell + 1)$ also correspond to the rank ℓ Lie algebra [16] B_ℓ.

The irreps of the groups $SO(2\ell + 1)$ can be depicted on root figures. The rank of a Lie group corresponds to the dimensions of the corresponding root figure. For the groups $SO(2\ell + 1)$ relevant to the atomic d, f, and g shells, the root figures are based on a square, a cube, and a tesseract or hypercube, respectively, of dimensionalities 2, 3, and 4, respectively, corresponding to the ℓ values of the electrons under consideration. The tesseract, used for the study of g orbitals and shown in Fig. 1 as a two-dimensional projection, is a 4-dimensional hypercube with 16 vertices, 32 edges, 24 faces, and eight cubic cells. In the tesseract of Fig. 1 the cubic cell in the center shares each face with another cubic cell accounting for seven of the eight cubic cells of the tesseract. The eighth cubic cell of the tesseract has the outer faces of the large outer cube in Fig. 1 as its six faces with its center point being at infinity.

An irrep of a group corresponding to a Lie algebra, including the $SO(2\ell+1)$ groups of interest in this work, can be described by dim(Γ) points on the root figure placed so as to preserve the symmetry of the root figure including one or frequently more than one point at the origin or center of the root figure. Here dim(Γ) is the dimension of the irrep ℓ in question. The irrep of a group corresponding to a Lie algebra of rank ℓ is described by a set of small integers corresponding to the coordinates of the root

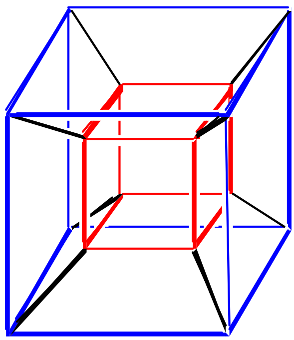


Fig. 1 A two-dimensional projection of a tesseract, the four-dimensional analogue of the cube

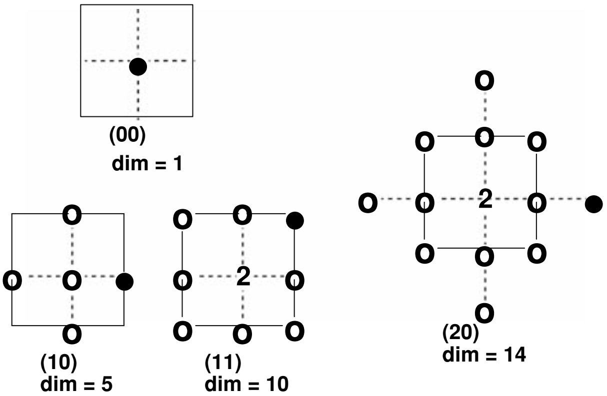


Fig. 2 Root figures corresponding to the four lowest irreps of $SO(5)$, used to study the atomic d shell. The point with the highest coordinates is indicated by a solid circle (•) and the other single points are indicated by open circles (◦). Double points in the center are indicated by **2**. The axes used to define the coordinates are indicated by dashed lines

figure point with the most positive values with the unit of measurement corresponding to the shortest distance between adjacent points. This is illustrated in Fig. 2 by the 2-dimensional root figures of the irreps (10), (11), and (20) of $SO(5)$, which are used for the study of the atomic d shell. Analogous root figures for the atomic g shell are described below. However, since they are necessarily four-dimensional based on the tesseract (Fig. 1), drawings of them on the 2-dimensional page become unintelligible.

For groups with root figures in three or more dimensions attempts to use figures analogous to Fig. 2 rapidly become confusing. It is therefore useful to use root descriptors of irreps describing the locations of points at vertices (v), at the midpoints of edges (e), at the midpoints of faces (f), at the midpoints of cells (c), at the midpoints of four-dimensional hypercells (h_4), ..., and at the center of the polytope (o) with coefficients indicating the numbers of such points and exponents indicating the number of lattice spacings of a set of points from the origin. In such root descriptors points of the root figures belonging to smaller irreps can be enclosed in brackets [] whereas "new" points for a given irrep can be enclosed in parentheses (). The sum of the coefficients of the root descriptor is the dimension of the corresponding irrep. Using this notation the root descriptors for lowest dimensional irreps of $SO(5)$ depicted in Fig. 2 for the atomic d shell are the following:

$$(00) : (o) \tag{4a}$$

$$(10) : [o] + (4e) \tag{4b}$$

$$(11) : [o] + [4e] + (o + 4v) \tag{4c}$$

$$(20) : [o] + [4e] + [o + 4v] + (4e^2) \tag{4d}$$

For the atomic f shell the three-dimensional cube root figure of the $SO(7)$ group can be projected onto a hexagon corresponding to a projection of one of the skew hexagonal Petrie polygons [18,19] of the cube corresponding to the subgroup relationship $SO(7)$

$\supset G_2$ where G_2 is a rank 2 Lie group corresponding to an exceptional Lie algebra with 14 roots [16]. In order to illustrate the shorthand further in Eq. 4 Table 4 shows the hexagonal projections of the cube root figures for the lowest dimensional irreps of $SO(7)$ along with the corresponding root descriptor using the notation above.

The study of the atomic g shell uses the group $SO(9)$ corresponding to the rank 4 Lie algebra [16] B_4. Table 5 shows the root descriptors for the locations of the points on the underlying tesseract (Fig. 1) for the root figures of the lowest dimensional irreps of $SO(9)$. Upper case letters are used to designate the locations of the points on the tesseract root figure of $SO(9)$ to differentiate such designations from the locations of the points on the cube root figure of $SO(7)$.

In these root figures the order of appearance of new types of points is the opposite of the dimensionality of the unit of which it is the center. Thus the root figure corresponding to the (00...) irrep of dimension 1 on an n-dimensional polytope contains only the center point of the polytope itself, where the coordinates are (00...). Conversely, the root figure corresponding to the (11...) irrep is the first time that the vertex points appear consistent with the fact that the highest coordinates of a vertex point are (11...). Points at distances 2 for the root figure of $SO(7)$ and even 3 for the root figure of $SO(9)$ along the midpoints of higher dimension units can appear before the vertex points appear for the first time (see Tables 4 and 5). This will occur when the dimension of the irrep (20...) is less than that of the irrep (11...), which is the case for $SO(2\ell + 1)$ where $\ell \geq 3$ (i.e., for the atomic f shell and beyond).

3.2 Projection of root figures into lower dimensional root figures: connection with subgroup relationships

Consider the subgroup chain $SO(7) \supset G_2 \supset {}^7O$ for the study of the atomic f shell. The subgroup relationship $SO(7) \supset G_2$ relates to a projection of the three-dimensional cube root figure of $SO(7)$ onto the two-dimensional hexagonal root figure of G_2 (Table 4). In this projection one of the C_3 axes of the cube (i.e., a body diagonal) is projected onto the center point (origin) of the hexagon so that both vertices passing through this axis coalesce to a single point. This projection leads to relatively little information loss since the eight points corresponding to the vertices of the cube in the root figure of $SO(7)$ are reduced only by one vertex to give seven points in the hexagonal root figure of G_2.

An alternative subgroup relationship for $SO(7)$ is $SO(7) \supset SO(5)$. This corresponds to a root figure projection of the 3-dimensional cube of $SO(7)$ to the square of $SO(5)$ (compare Fig. 2). The origin of the square of the root figure of $SO(5)$ corresponds to a C_4 axis of the cube. The eight points corresponding to the vertices of the cube root figure of $SO(7)$ coalesce pairwise into the four vertices of the square root figure of $SO(5)$. Thus in the root figure projection for $SO(7) \supset SO(5)$ eight cube vertex points become only four points in the square root figure of $SO(5)$ whereas in the root figure projection for $SO(7) \supset G_2$ the eight cube vertex points are only reduced to seven points in the hexagonal root figure of G_2. Thus the subgroup relationship $SO(7) \supset G_2$ leads to less information loss and is therefore more useful than the subgroup relationship $SO(7) \supset SO(5)$.

Table 4 The root figures corresponding to the lowest dimensional irreps of $SO(7)$ and the corresponding root descriptors [The 3-dimensional cube root figures of $SO(7)$ are viewed as projected onto the 2-dimensional hexagon root figures of G_2]

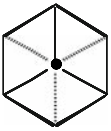
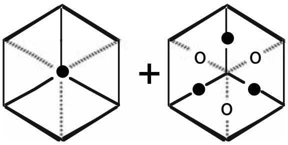
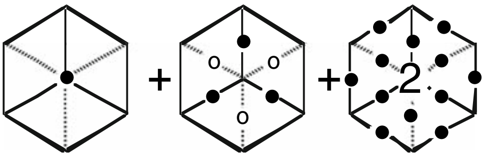
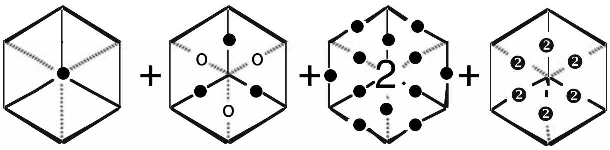
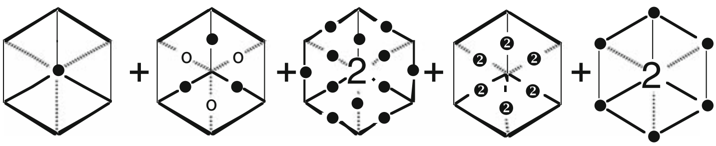
W(abc)	Dimension	Root figures
(000)		
	1	(o)
(100)		
	7	$[o] + (6f)$
(110)		
	21	$[o] + [6f] + (2o + 12e)$
(200)		
	27	$[o] + [6f] + [2o + 12e] + (6f^2)$
(111)		
	35	$[o] + [6f] + [2o + 12e] + [6f^2] + (8v)$

Table 5 The root descriptors for the lowest dimensional irreps of $SO(9)$ and the corresponding root descriptors

Irrep	Dimension	Root descriptor
(0000)	1	(O)
(1000)	9	$[O] + (8C)$
(1100)	36	$[O] + [8C] + (3O + 24F)$
(2000)	44	$[O] + [8C] + [3O + 24F] + (8C^2)$
(1110)	84	$[O] + [8C] + [3O + 24F] + [8C^2] + (32E + 8C^3)$
(1111)	126	$[O] + [8C] + [3O + 24F] + [8C^2] + [32E + 8C^3] + (2O + 24F^2 + 16V)$

Table 6 Relationships between the irreps of $SO(9)$ and those of $SO(7)$

$SO(9)$ Irrep	Dimension	Irreps of $SO(7)$	Dimensionality breakdown
(0000)	1	(000)	1 = 1
(1000)	9	(100) + 2(000)	9 = 7 + (2 × 1)
(1100)	36	(110) + 2(100) + (000)	36 = 21 + (2 × 7) + 1
(2000)	44	(200) + 2(100) + 3(000)	44 = 27 + (2 × 7) + (3 × 1)
(1110)	84	(111) + 2(110) +(100)	84 = 35 + (2 × 21) + 7
(1111)	126	3(111) + (110)	126 = (3 × 35) + 21

The cube → hexagon projection describing the subgroup relationship $SO(7) \supset G_2$ relates to the fact that the S_6 axis of the cube corresponds to a skew hexagon as a Petrie polygon in the cube. In this connection a Petrie polygon is defined by a path starting from a given vertex and taking alternating left and right turns until the original vertex is reached again [18,19]. An analogous construction in hyperspace does not appear to be useful for analogous subgroup relationships and, in any case, there do not appear to be suitable exceptional Lie algebras [16] of rank <4 to generate useful subgroups for $SO(2\ell + 1)$ for $\ell \geq 4$. Thus for the study of the atomic g shell, the best alternative is to study the subgroup relationship $SO(9) \supset SO(5)$ since the relevant finite group $L_2(9) \approx A_6$ is known to be a subgroup of $SO(5)$ being the symmetry point group of the 5-dimensional simplex (see above). For this purpose the intermediate subgroup $SO(7)$ is considered so that the corresponding projections for the resulting subgroup chain $SO(9) \supset SO(7) \supset SO(5)$ correspond to a stepwise dimension reduction from a 4-dimensional tesseract (Fig. 1) to a 3-dimensional cube and finally to a 2-dimensional square.

Considering the subgroup relationship $SO(9) \supset SO(7)$ leads to the relationships between their irreps summarized in Table 6 including the indicated dimensionality breakdown. Similarly the subgroup relationship $SO(7) \supset SO(5)$ leads to the relationships between their irreps summarized in Table 7. Taken together the information in these tables can decompose the $SO(9)$ irreps to sums of $SO(5)$ irreps for the subgroup chain $SO(9) \supset SO(5) \supset L_2(9) \approx A_6$ used for the atomic g shell.

Table 7 Relationships between the irreps of $SO(7)$ and those of $SO(5)$

$SO(7)$ Irrep	Dimension	Irreps of $SO(5)$	Dimensionality breakdown
(000)	1	(00)	1 = 1
(100)	7	(10) + 2(00)	7 = 5 + (2 × 1)
(110)	21	(11) + 2(10) + (00)	21 = 10 + (2 × 5) + 1
(200)	27	(20) + 2(10) +3(00)	27 = 14 + (2 × 5) + (3 × 1)
(111)	35	3(11) + (10)	35 = (3 × 10) + 5

The information in Tables 6 and 7 can be derived from the root descriptors for root figures of the relevant irreps. Consider, for example, one of the simplest non-trivial problems of this type, namely the decomposition of the irrep (110) of $SO(7)$ into a sum of irreps of $SO(5)$. The root descriptor for the irrep (110) is $[o] + [6f] + (2o + 12e)$. Projecting the 14 points ($2o$+ $12e$) from the cube root figure of $SO(7)$ to the square root figure of $SO(5)$ gives a collection of 14 points corresponding to the $SO(5)$ root descriptor $2o + (2 \times 4)e + 4v = 2o + 8e + 4v$. Note that four of the 12 edge midpoints of the $SO(7)$ cube are projected onto the vertices of the $SO(5)$ square and the remaining 8 edge midpoints of the $SO(7)$ cube are projected doubly onto edge midpoints of the $SO(5)$ square. The sum of the root descriptors for the (11) and (10) irreps of $SO(5)$ is seen to be the collection of 15 points on the root figure labeled $\{[o] + (4e)\} + \{[o] + [4e] + (o + 4v)\}$ from Eq. 4b and 4c, which reduces to $3o + 8e + 4v$. The "extra" point is an origin point leading to the following relationship:

$$(2o + 12e) \text{ in } SO(7) = (11) + (10) - (00) \text{ in } SO(5) \tag{5}$$

Similarly, the remaining seven points of the cube $SO(7)$ root figure for the irrep (110), namely $(o + 6f)$, project onto the square $SO(5)$ root figure as $3o + 4e$. The irrep (10) of $SO(5)$ has the root descriptor $o + 4e$ (Fig. 2) thereby leading to the following relationship:

$$(o + 6f) \text{ in } SO(7) = (3o + 4e) \text{ in } SO(5) = (10) + 2(00) \text{ in } SO(5) \tag{6}$$

Combining Eqs. 4 and 5 give the relationship (110) in $SO(7) = (11) + 2(10) + (00)$ in $SO(5)$ as indicated in Table 7.

An analogous procedure can be used to derive the more complicated relationships listed in Tables 6 and 7.

4 Applications to the atomic *g* shell

The lobal structure of *g* orbitals can become difficult to visualize since g orbitals can have up to 12 lobes when $|m| = 2$ and 3. Instead *g* orbitals are conveniently depicted as orbital graphs [20]. In this connection orbital graphs are signed bipartite graphs where the vertices correspond to the lobes of the orbitals with the corresponding signs. The edges correspond to nodes between adjacent lobes of opposite sign.

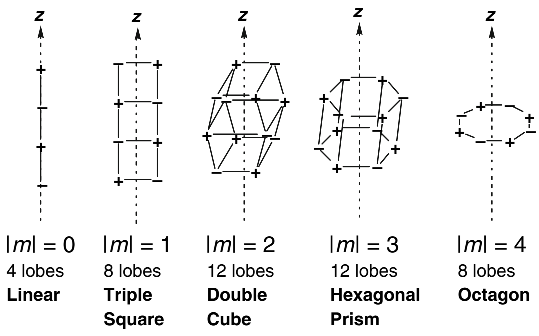


Fig. 3 Orbital graphs for the five types of g orbitals according to the values of $|m|$

The nine g orbitals can be divided into five types depending on the absolute value of m where $0 \leq |m| \leq 4$. The corresponding orbital graphs are depicted in Fig. 3 [20]. Note that $|m| = 0$ corresponds to a single g orbital, namely the $g(z^4)$ orbital, whereas the other orbital graphs correspond to pairs of g orbitals where $m = \pm1, \pm2, \pm3$, and ±4 inversely relating to their extent along the z axis. These orbital graphs have distinctive shapes, namely triple square, double cube, hexagonal prism, and octagon, respectively.

A comprehensive list of the atomic g shell terms is given by Wybourne and is too complicated to list here; the reader is referred to the Wybourne paper [4] for details. Table 8 lists the terms corresponding to the irreps of $SO(9)$ taken from the Wybourne paper, where the subscripts after a term indicate the number of times it appears in the given irrep. The sequence of letters for the Lvalues of the terms from 0 to 20 in the atomic g shell used by Wybourne [4] is S,PDFGH,IKLMN,OQRTU,VWXYZ so that the familiar letters S and P are used for the terms with $L = 0$ and 1 and the letters E and J are avoided.

The terms for the atomic g shell (Table 8) go all the way up to Z terms where $L =$ 20 for the 2772-dimensional irrep (2222) consistent with the following equation:

$$\max(L) = \ell(\ell + 1) \tag{7}$$

In Eq. 7 L refers to the term in question and ℓ refers to the angular momentum quantum number for the atomic shell in question, i.e., $\ell = 1, 2, 3, 4$ for the atomic p, d, f, and g shells, respectively. Equation 7 can be derived from the observation that the maximum L value occurs when electron pairs appear in the ℓ boxes where the m values are positive, i.e., $1 \leq m \leq \ell$ and all of the boxes are empty where the m values are negative.

The atomic g shell is seen from Table 8 to be far too complicated to discuss all of the terms in detail. Of particular interest are the terms of maximum multiplicity corresponding to the irreps with only 0's and 1's, namely (0000), (1000), ..., (1111). For g^0 to g^9 there are only unpaired electrons or empty boxes whereas from g^9 to g^{18} there is at least one electron for each $m$value from $+4$ to -4, i.e., no empty boxes. Table 9 lists these irreps with the terms grouped in parentheses according to the corresponding irreps of the finite group $L_2(9) \approx A_6$ coming from Table 3 using parentheses to define

Table 8 The terms in the atomic g shell corresponding to the irreps of $SO(9)$

Irrep	Dimension	Terms
(0000)	1	S
(1000)	9	G
(1100)	36	PFHK
(1110)	84	PF_2GHIKM
(1111)	126	$SD_2FG_2HI_2KLN$
(2000)	44	DGIL
(2100)	231	$PD_2F_2G_2H_3I_2K_2L_2MNO$
(2110)	594	$P_3D_3F_5G_5H_6I_5K_5L_4M_4N_2O_2QR$
(2111)	924	$SP_3D_6F_6G_8H_8I_8K_7L_7M_5N_4O_3Q_2RT$
(2200)	495	$S_2D_4F_2G_5H_3I_5K_3L_4M_2N_3OQ_2T$
(2210)	1650	$S_3P_4D_8F_9G_{12}H_{11}I_{13}K_{11}L_{11}M_9N_8O_5Q_5R_3T_2UV$
(2211)	2772	$SP_9D_{10}F_{17}G_{16}H_{21}I_{18}K_{20}L_{16}M_{16}N_{12}O_{11}Q_7R_6T_3U_3VW$
(2220)	1980	$S_4P_3D_8F_9G_{13}H_{10}I_{15}K_{11}L_{12}M_{10}N_{10}O_6Q_7R_4T_3U_2V_2X$
(2221)	4158	$S_2P_{10}D_{14}F_{20}G_{22}H_{25}I_{25}K_{26}L_{23}M_{22}N_{18}O_{16}Q_{12}R_{10}T_7U_5V_3W_2XY$
(2222)	2772	$S_3P_4D_{11}F_9G_{15}H_{15}I_{16}K_{14}L_{17}M_{12}N_{13}O_{10}Q_9R_6T_6U_3V_3W_2XZ$

Table 9 The terms in the atomic g shell corresponding to the irreps of $SO(9)$ for the maximum multiplicity configurations grouped according to the irreps of $L_2(9)$

g configuration	Irrep	Dimension breakdown	Terms
g^0, g^9, g^{18}	(0000)	1 = 1	S
g^1, g^8, g^{10}, g^{17}	(1000)	9 = 9	G
g^2, g^7, g^{11}, g^{16}	(1100)	36 = 10 + 26	(PF)(HK)
g^3, g^6, g^{12}, g^{15}	(1110)	84 = 10 + 18 + 9 + 28 + 19	(PF)(FH)G(IK)M
g^4, g^5, g^{13}, g^{14}	(1111)	126 = 1+18+26+18 +(2×9)+28+17	$S(DI)(DN)(FH)G_2(IK)L$

the groupings. Note that these groupings have dimensions 1, 9, 10, 17, 18, 19, 26, and 28 so that either their dimensions or their dimensions ± 1 are divisible by nine. The corresponding irreps of $L_2(9)$ for each of these groupings are listed in Table 3. In this way the subgroup chain $SO(9) \supset SO(5) \supset L_2(9) \approx A_6$ can be used to make some sense out of the otherwise complicated and forbidding list of terms for the atomic g shell given in Table 8.

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