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The group table for the icosahedral group I is constructed by using the isomorphism between the group I and a subgroup of the permutation group S_{12} . The single-valued irreducible representations and Clebsch-Gordan (CG) coefficients of I are calculated by a computer code based on the eigenfunction method. The irreducible matrix elements for all the 60 group elements are given explicitly in the form of $\sqrt{m/n} [\exp(i\phi)]^p [2\cos\phi]^q [2\cos2\phi]^r$, where m, n, p, q, and r are integers and $\phi = 2\pi/5$. The Clebsch-Gordan coefficients of I are all real under a new phase convention for time reverse states and tabulated in the form of $\sqrt{m/n}$.

I. INTRODUCTION

The icosahedral group I is the most complicated point group and has been the subject of many studies. 1-6 The discovery of the quasicrystal, or the icosahedral crystals,7 has revived the interest in the group. Early works²⁻⁴ are mainly concerned with the construction of the SO₃\$\pm\$I subduced basis, namely the linear combinations of the spherical harmonics adapted to the symmetry of the group I. Although the primitive character of the group has been known for a long time, its irreducible matrices are not readily available except for three generators of the group. 1,4 Using the O₃ I subduction coefficients given by McLellian, 4 Goulding 5 calculated the 3jm-symbol of the group I, and later Pooler⁶ calculated both the 3jm- and 6j-symbols of I. All the above studies are based on the fact that the group I is a subgroup of the rotation group SO₃ and use the subduction to construct the irreducible representations and 3jm-symbols of the group I from their counterparts of the group SO₃.

Conscious of the fact that there is no universal and simple method for finding characters and irreps of a finite group, Chen⁸ developed a new approach to group representation theory which, in turn, gives rise to a new method, the eigenfunction method (EFM) for calculating characters, irreps, CG coefficients, isoscalar factors, etc. The EFM has been successfully applied to point groups, permutation groups, unitary groups, and space groups (for an extensive review the reader is referred to the monograph⁸ and Ref. 9). Recently, a versatile space group program package based on the EFM has been written by two of us¹⁰ that can be used to compute ab initia the single- and double-valued irreps (projective irreps) of the 32 point groups (little cogroup of the 230 space groups), as well as the point group or space group CG coefficients. The program is written in FORTRAN-77 and implemented on the IBM-PC. The only input is the name of the space group or the point group and the wave vector to be considered [for point groups one only needs to set the wave vector to be (0,0,0)]. It is quite interesting to use the same program with minor modifications to calculate all the irreps

II. RETROSPECT ON THE EFM

The essence of the EFM is best illustrated¹¹ in the threedimensional rotation group SO₃. According to the terminology in Refs. 8 and 9, the Casimir operator J^2 of SO_3 is called the first kind of complete set of commuting operators (CSCO-I) of SO₃, which is a CSCO in the class parameter space. The eigenfunction of J^2 in the class parameter space is proportional to the complex conjugate of the primitive character. The operator set (J^2, J_z) is called the second kind of CSCO (CSCO-II) of SO₃, whose eigenfunction $|jm\rangle$ gives the $SO_3 \supset SO_2$ irreducible basis. The operator set $(J^2, J_z, \overline{J}_z)$ is called the third kind of CSCO (CSCO-III), which is a CSCO in the group parameter space, where \overline{J}_z is the Casimir operator of the subgroup SO_2 of the intrinsic group SO_3 , which is commuting and anti-isomorphic with the rotation group SO₃ and describes the rotation of a system (such as a deformed nucleus) around its intrinsic (body fixed) axes. 11 Physically, \overline{J}_{z} is the third component of the angular momentum in the intrinsic coordinate system, 11 usually denoted by J_3 . The eigenfunction of the CSCO-III is the complex conjugate of the irreducible matrix of SO₃, $D_{mk}^{j}(\alpha,\beta,\gamma)^*$.

It was shown that the above approach can be extended to any compact group.^{8,9} For a finite group G, the Casimir operator J^2 is replaced by the CSCO-I of the finite group G, denoted by C, which is a linear combination of a few class operators of G and is the analogy of the Casimir operator in Lie groups. The eigenvectors of C in the class space are proportional to the complex conjugate of the character vectors. The characters are obtained by further using the normalization condition for the character stemmed from the orthogonal theorems of the characters. Suppose G(s) is a canonical subgroup chain of G, and C(s) is an appropriate linear com-

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and CG coefficients of the most complicated point group, the icosahedral group I. In this paper, the irreducible representations and CG coefficients of the group I are constructed solely from the group table of I without invoking any knowledge of the group SO₃.

a) Permanent address.

bination of all the CSCO-I's of the subgroups contained in G(s). Then, (C,C(s)) is the CSCO-II of G and its eigenvectors give the irreducible basis of G. Similarly suppose that $\overline{\mathbf{G}}(s)$ is the corresponding subgroup chain of the intrinsic group $\overline{\mathbf{G}}$, which is commuting and anti-isomorphic with the group G. Note that $\overline{\mathbf{G}}(s)$ has the corresponding operator set $\overline{C}(s)$. Then, $(C,C(s),\overline{C}(s))$ is the CSCO-III of G, whose eigenvectors (after proper normalization and using the standard phase convention^{8,9}) in the group space give the complex conjugate of the irreducible matrix vector $\{D_{ab}^{\nu}(R_1),$ $D_{ab}^{\nu}(R_2),...,D_{ab}^{\nu}(R_{|G|})$, where ν , a, and b are the eigenval ues of C, C(s), and $\overline{C}(s)$, respectively, while $R_1, R_2, ..., R_{|G|}$ are the elements of the group G of order |G|. In practice it is very convenient to linearly combine the operators C, C(s), and $\overline{C}(s)$ into a single operator K which is a CSCO in the group space and can be served as the CSCO-III of G. Having done this, we only need to solve the eigenequation of a single operator K to find the irreducible matrices of G.

The prerequisite condition for the application of the eigenfunction method is that the group table is known. In the following section we describe a way to construct the group table of the group I.

III. GROUP TABLE

A regular icosahedron (icosahedron for short) has 12 vertices, 20 faces (which consist of identical regular triangles), and 30 edges. The rotation axes of the group I consists of 6 fivefold axes (joining the two opposite vertices), A_{5j} (j=1,2,...,6), 10 threefold axes (joining the centers of two opposite faces), A_{3j} (j=1,2,...,10), and 15 twofold axes (joining the midpoints of two opposite edges), A_{2j} (j=1,2,...,15). The vertices of the icosahedron, the centers of the triangles, and the midpoints of the edges are indexed as in Figs. 1 and 2, and the rotation axes are listed in Table I by listing the indices of the vertices, centers, or midpoints through which they pass.

The rotation operators of the group I are denoted by

$$C_{5,j}^{m}$$
 $(j = 1,2,...,6; m = 1,2,3,4),$
 $C_{3,j}^{m}$ $(j = 1,2,...,10; m = 1,2),$ (1)
 $C_{2,j}$ $(j = 1,2,...,15).$

Together with the identity, they form the group of I with order 60. The group elements are denoted by R_i , i = 1,2,...,60.

For constructing the group table, it is convenient to use the permutations of the 12 vertices fo the icosahedron under the rotations, which form a subgroup of the permutation group S_{12} , to replace the rotation operations. (The isomorphism between the group I and the subgroup of S_{12} is shown in the first table in the Appendix.) With this as input, the group table of the group I is generated by the computer by using the multiplication rule of the permutation group and is shown in the second table in the Appendix.

IV. THE CSCO-I AND CHARACTERS

From the group table, the program¹⁰ will find the class operators and the class multiplication tables, the CSCO-I and the primitive characters. For a detailed description of

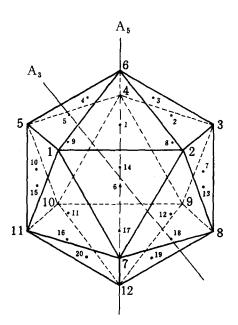


FIG. 1. The large size integers label the 12 vertices and the small size integers the centers of the 20 faces.

the program, the reader is referred to Ref. 10.

The five class operators of the group I are found as follows:

$$C_1 = E = R_1, \quad C_2 = \sum_{i=1}^{6} (C_{5,j}^1 + C_{5,j}^4) = \sum_{i=2}^{13} R_i,$$
 (2a)

$$C_{3} = \sum_{j=1}^{6} (C_{5,j}^{2} + C_{5,j}^{3}) = \sum_{i=14}^{25} R_{i},$$

$$C_{4} = \sum_{j=1}^{10} (C_{3,j}^{1} + C_{3,j}^{2}) = \sum_{i=26}^{45} R_{i},$$
(2b)

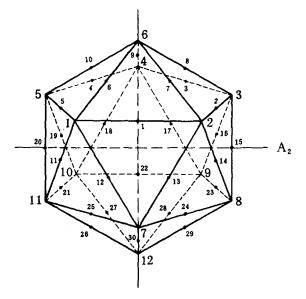


FIG. 2. The large size integers label the 12 vertices and the small size integers the midpoints of the 30 faces.

TABLE I. The rotation axes of the group I. Here $m \rightarrow n$ denotes an axis going from the point m to the point n, its positive direction being toward the point n.

Five	efold axes	Threefold axes		Twofold axes		
.1	9→1	A _{3,1}	17 → 1	A _{2,1}	22→1	
2	10→2	$A_{3,2}$	16→2	$A_{2,2}$	21 → 2	
	$11 \rightarrow 3$	$A_{3,3}$	$20 \rightarrow 3$	$A_{2,3}$	$25 \rightarrow 3$	
	7→4	$A_{3,4}$	19→4	$A_{2,4}$	24 → 4	
	8 → 5	$A_{3,5}$	18→5	A2,5	$23 \rightarrow 5$	
s	12→6	$A_{3,6}$	14→6	$A_{2,6}$	$28 \rightarrow 6$	
		$A_{3,7}$	15→7	$A_{2,7}$	$27 \rightarrow 7$	
		$A_{3,8}$	11→8	$A_{2,8}$	26→8	
		$A_{3,9}$	12→9	$A_{2,9}$	30→9	
		$A_{3,10}$	$13 \rightarrow 10$	$A_{2,10}$	29 → 1	
				$A_{2,11}$	16→1	
				$A_{2,12}$	17 → 1	
				$A_{2,13}$	18→1	
				$A_{2,14}$	19→1	
				A2,15	20 → 1	

$$C_5 = \sum_{i=1}^{15} C_{2,j} = \sum_{i=46}^{60} R_i.$$
 (2c)

The CSCO-I of the group I is found as $C = C_2$. In the class space spanned by $C_1,...,C_5$, the representation matrix of C_2 is found to be

$$D(C_2) = \begin{pmatrix} 0 & 12 & 0 & 0 & 0 \\ 1 & 5 & 1 & 5 & 0 \\ 0 & 1 & 1 & 5 & 5 \\ 0 & 3 & 3 & 3 & 3 \\ 0 & 0 & 4 & 4 & 4 \end{pmatrix}. \tag{3}$$

By diagonalizing $D(C_2)$, we obtain five distinct eigenvalues that can be served as the irrep label and five character vectors that are well known and not listed here. The corre-

spondence between the eigenvalues of C_2 and the Mülliken notation is as follows:

The eigenvalues of C_2 :

12
$$8\cos(\pi/5)$$
 $8\cos(3\pi/5)$ - 3 0.

The Mülliken notation:

$$A T_1 T_2 G H.$$

V. THE CSCO-III AND IRREDUCIBLE MATRICES

The subgroup or subgroup chain G(s) used for classifying the irreducible matrices can be specified either by the user according to one's need or by the computer. We choose the cyclic group $C_5 = (E, C_{5,1}^1, C_{5,1}^2, C_{5,1}^3, C_{5,1}^4)$ $= (R_1, R_2, R_{14}, R_{15}, R_3)$ as the subgroup G(s). Once G(s) is specified, the program will find the CSCO-I of G(s). In our case it is trivial, since any element of C_5 except the identity can be chosen as its CSCO-I. The operator $C_{5,1}^1 = R_2$ has been chosen as C(s) and its rotation axis is chosen as the z axis,

$$C(s) = R_2 = R_z (2\pi/5) = \exp(-2\pi i J_z/5).$$
 (4a)

The corresponding intrinsic operator is $\overline{C}(s) = \overline{C}_{5,1}^1 = \overline{R}_2$. The program will find a single operator as the CSCO-III K of the group I with the result

$$K = 7C + C(s) + 9\overline{C}(s). \tag{4b}$$

From (4) and (2a), and the group table, the program will find the representation matrix of the CSCO-III K in the group space, and its 60 eigenvectors corresponding to the 60 distinct eigenvalues. With proper normalization and taking complex conjugate, they yield all the irreducible matrix elements of the group I. The program contains a subroutine to check that the calculated matrices do form a representation of the group. The rows and columns of the matrices are indexed according to the eigenvalue $\exp(-2\pi\mu i/5)$ of C(s), where μ is the eigenvalue of J_z modulo 5. The values of the integer μ along with its index a for different irreps are listed below:

irreps
$$A$$
 T_1 T_2 G H μ : (0) $(1,0,-1)$ $(2,0,-2)$ $(2,1,-1,-2)$ $(2,1,0,-1,-2)$ (5) a : (1) $(1,2,3)$ $(1,2,3,)$ $(1,2,3,4)$ $(1,2,3,4,5)$.

The original output of the matrix elements are complex decimals. To convert the complex decimals to the exact values, we use the following procedure. From the character table and the matrices for the generators of the group I given in Ref. 4, we use the ansatz that the entries are of the following form:

$$\sqrt{m/n}z^p P^q Q^r, \tag{6a}$$

where m, n, p, q, and r are integers, and

$$z = \exp\left(i\frac{2\pi}{5}\right), \quad P = \frac{\sqrt{5} - 1}{2} = 2\cos\frac{2\pi}{5},$$

$$Q = -\frac{\sqrt{5} + 1}{2} = 2\cos\frac{4\pi}{5}.$$
 (6b)

Among the 60×60 entries, besides 0 and 1, there are only 30 distinct values, 10 being real and 20 complex, denoted by capital and small letters, respectively. With the help of a computer, all of the 30 decimal values are converted into the form of (6) and are listed in Table II. The irreducible matrix elements of the group I are given in Table III.

VI. THE CSCO-II AND CG COEFFICIENTS

The eigenfunction method for the CG coefficients is discussed in Refs. 8–10. Here we only give some key points. Let $|\nu_i a_i\rangle$, i=1,2, be the two irreducible bases. By using the CG coefficients they can be linearly combined into another irreducible basis,

A	В	D	E	F	G	Н	L	М	N
$\frac{1}{\sqrt{5}}$	-AQ	$-\sqrt{2}A$	AP	$-A^2$	B ²	A^2P^2	√6 <i>A</i> ²	M - 2A ² P	$-2A^2Q$
z^{-1}	b . $-Bz^2$	z^{-2}	e — Ez	f Dz^2	Dz^{-1}	h Ez²	$\stackrel{j}{\it Bz^{-1}}$	$-Az^{-1}$	m Az²
Gz^{-1}	p Hz²	$N_{z^{-1}}$	r Nz ⁻²	s Mz²	t Mz	Lz^{-1}	Lz^{-2}	<i>w</i> <i>Hz</i> ^{−1}	y Gz²

$$|\nu\tau\alpha\rangle = \sum_{a_1a_2} \langle \nu_1 a_1, \nu_2 a_2 | \nu\tau a \rangle |\nu_1 a_1 \rangle \nu_2 a_2 \rangle, \tag{7}$$

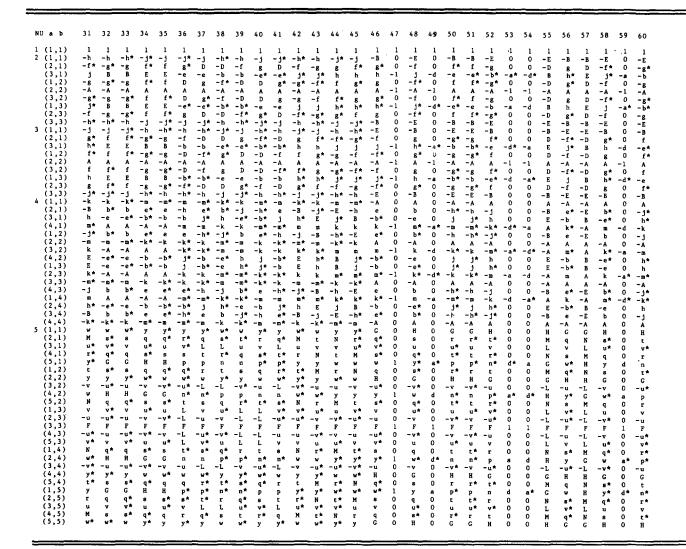
where the first factor in the right-hand side is the CG coefficient and τ is a multiplicity label, $\tau=1,2,...,(v_1v_2v)$. According to Sec. II, $|v\tau a\rangle$ is necessarily an eigenfunction of the CSCO-II, (C,C(s)), with the eigenvalues v and a. Therefore, the CG coefficients result from a diagonalization of the representative matrix of the CSCO-II in the product basis,

$$\begin{split} \sum_{a_1a_2} & \left[\left\langle v_1 a_1', v_2 a_2' \, \middle| \, \begin{matrix} C \\ C(s) \end{matrix} \middle| v_1 a_1, v_2 a_2 \right\rangle \right. \\ & \left. - \begin{pmatrix} v \\ a \end{pmatrix} \, \delta_{a_1'a_1} \delta_{a_2'a_2} \, \middle| \langle v_1 a_1, v_2 a_2 \middle| v \tau a \rangle = 0, \end{split} \tag{8}$$

where a can be understood either as the eigenvalue $\exp(-2\pi\mu i/5)$ or its index ordered in Eq. (5). Solving the eigenequation (8) we can get the eigenvalue (ν,a) and its

TABLE III. The single-valued irreducible representation of the icosahedral group.

1 (1,1) 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
(2,3) 0 0 0 f* b f D g* g g* f* f g 0 0 - g* - g - f* - f* - f - g - D - D - g* f* g - D - f - g* (3,3) 1 a* a b* b b b* b b* b b* b b* b b* b



degeneracy d, which is just the coefficients (v_1v_2v) in the CG series. For the eigenvalue (v,a) we can obtain the (v_1v_2v) orthogonal eigenvectors,

$$\{\langle v_1 a_1, v_2 a_2 | v \tau a \rangle\}, \quad \tau = 1, 2, \dots, (v_1 v_2 v). \tag{9}$$

To ensure that the CG coefficients with the same ν and τ but different a have the correct relative phase, we use the same procedure as used in Sec. III of Ref. 10 for the space group CG coefficients.

We can choose a single operator M as the CSCO-II of the group I. Once the CSCO-III, K, of a group G is found, the CSCO-II of G is readily obtained by deleting the $\overline{C}(s)$ term in K. Then the set of eigenequations (8) can be replaced by a single eigenequation of the operator M. From (4) it is known that the CSCO-II of the group I is

$$M = 7C + C(s). \tag{10}$$

The CG coefficients of the group I are calculated by the subroutine CG in the space group program package¹⁰ and the results are given in Table IV. The meaning of the table heading is as follows: NU, the index of the irrep; a, the com-

ponent index of the irrep; MUL, the multiplicity label; xx, the double index a_1a_2 .

Notice that the CG series and CG coefficients are obtained simultaneously by the EFM. Collecting the first lines in each subtable, we have the CG series for the group I listed in Table V.

As we see from Tables III and IV that although the irreducible matrices of the group I are rather complicated (i.e., the matrices are not spare ones and many matrix elements are not square roots of simple fractions), the CG coefficients are rather simple with many zeroes and the nonzero elements being square roots of simple fractions.

From Table IV, we see that the CG coefficients are all real. Besides the unitarity, they have the following properties

(1) Due to Eq. (4a), C(s) can be replaced by the operator \mathbf{J}_z with the eigenvalue μ modulo 5. Similar to the condition $m_1 + m_2 = m$ for the SO₃ CG coefficients $\langle j_1 m_1 j_2 m_2 | jm \rangle$, for the group I we have

$$\langle j_1 \mu_1 j_2 \mu_2 | j \mu \rangle = 0$$
, unless $\mu_1 + \mu_2 = \mu \pmod{5}$. (11)

```
THE CG SERIES:
                                                                                                                  THE CG SERIES:
  NU1( 2)* NU2( 2) ** + 1* NU( 1) + 1* NU( 2) + 1* NU( 5)
                                                                                                                    NU1( 3)* NU2( 3) == + 1* NU( 1) + 1* NU( 3) + 1* NU( 5)
  IRREP NU1*NU2 = 2 * 2
                                                                                                                    IRREP NU1*NU2 = 3 * 3
                                                                                                                             CG COEFFICIENTS
           CG COEFFICIÉNTS
   a MUL 11
1 1 0
2 1 0
3 1 0
1 1 1 1
2 1 0
3 1 0
4 1 0
5 1 0
                                                                                                                      a MUL 11
1 1 0
1 1 0
2 1 0
3 1 0
1 1 0
                                                                                                                                                                     31
A
0
B
                                                                                                                                                                                 33
0
0
0
0
0
 2
                            A
O
                                                                                                                    1
3
                                                                                                                  LIST OF SYMBOLS USED A=SQRT( 1/3) B=SQRT( 1/2)
                                                                                                                                                               D=SQRT( 1/6) E=-SQRT( 2/3)
LIST OF SYMBOLS USED
A=SQRT( 1/3) B=SQRT( 1/2) D=-SQRT( 1/6) E=SQRT( 2/3)
                                                                                                                  THE CG SERIES:
                                                                                                                   NU1( 3)* NU2( 4) == + 1* NU( 2) + 1* NU( 4) + 1* NU( 5)
THE CG SERIES:
                                                                                                                  IRREP NU1*NU2 = 3* 4
 NU1( 2)* NU2( 3) == + 1* NU( 4) + 1* NU( 5)
                                                                                                                             CG COEFFICIENTS
                                                                                                                  NU a MUL 11
2 1 1 0
2 1 0
3 1 -A
4 1 1 0
                                                                                                                                                                     23
0
0
                                                                                                                                                  1 4
0
                                                                                                                                                                                 31
0
8
0
0
0
0
0
                                                                                                                                                                                                     A
0
0
IRREP NU1*NU2 = 2* 3
           CG COEFFICIENTS
NU a MUL 11
4 1 1 0
2 1 0
3 1 0
4 1 -B
                    1 2
0
 5
                                                                                                                                  LIST OF SYMBOLS
                                                                                                                                                            USED
                                                                                                                                         B=-SQRT( 1/2) D=SQRT( 1/3)
G=SQRT( 1/6) H=-SQRT( 1/12)
                                                                                                                                                                                          E=-SQRT( 2/3)
LIST OF SYMBOLS USED A=SQRT( 2/3) B=SQRT( 1/3)
                                                                                                                  THE CG SERIES:
                                                                                                                    NU1( 3)* NU2( 5) == + 1* NU( 2) + 1* NU( 3) + 1* NU( 4) + 1* NU( 5)
THE CG SERIES:
                                                                                                                  IRREP NU1*NU2 = 3* 5
  NU1(2)*NU2(4) == + 1*NU(3) + 1*NU(4) + 1*NU(5)
                                                                                                                             CG CORFFICIENTS
IRREP NU1*NU2 = 2* 4
                                                                                                                                                                          23
0
D
0
                                                                                                                  NU a MUL 11
2 1 1 0
                                                                                                                                                                     2 2
B
                                                                                                                                                                                 24
0
0
8
0
0
0
0
0
0
0
0
0
0
0
           CG COEFFICIENTS
NU a MUL 11
3 1 1 0
2 1 0
3 1 A
                                                                                  34
-A
0
0
0
0
0
0
0
0
0
0
                    12
                                      21
B
O
O
E
O
                          13
                                                   23
0
                                                                                                                                                                                               0000000
                                                                                                                                                          000000
                                        0
G
O
O
              LIST OF SYMBOLS USED
                                                                                                                  LIST OF SYMBOLS USED

A-SQRT( 2/5) B--SQRT( 1/5) D-SQRT( 3/5) E-SQRT( 1/10) F-SQRT( 3/10)

G--SQRT( 8/15) H-SQRT( 1/15) J--SQRT( 2/15) K--SQRT( 4/15)

L-SQRT( 1/2) M-SQRT( 1/6) N--SQRT( 1/3) P--SQRT( 2/3)
                       B=SQRT( 1/2) D=SQRT( 2/3)
G=SQRT( 1/6) H=SQRT( 3/4)
A=SORT( 1/4)
                                                                     E=-SQRT( 1/3)
 F=SQRT( 1/12)
THE CG SERIES:
                                                                                                                  THE CG SERIES:
 NU1(2)*NU2(5) == + 1*NU(2) + 1*NU(3) + 1*NU(4) + 1*NU(5)
                                                                                                                   NU1(4)* NU2(4) == + 1* NU(1) + 1* NU(2) + 1* NU(3)
+ 1* NU(4) + 1* NU(5)
                                                                                                                   IRREP NU1*NU2 = 4* 4
                                                                                                                             CG COEFFICIENTS
NU a MUL 11
2 1 1 0
2 1 0
3 1 0
3 1 1 0
                                                        23
0
E
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-D
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0
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0
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F
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H
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                                                                                                                  NU a MUL 11
1 1 1 0
2 1 1 0
2 1 0
                                                                                                                                      12
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O
                                                                                                                                                         0 0 0 0 0 0 0 0 0 0 0 F
                                                                                                                    3
                                                                             0 K 0 0 0 L 0 0
                                                                                                                                                    0 0 0 0 0 0 0 0 0
                LIST OF SYMBOLS USED
A=SQRT( 1/10) B=-SQRT( 3/10) D=-SQRT( 3/5) E=-SQRT( 2/5)
F=SQRT( 1/5) G=SQRT( 4/15) H=SQRT( 2/15) J=-SQRT( 8/15) K=SQRT( 1/15)
L=SQRT( 1/3) H=-SQRT( 2/3) N=SQRT( 1/2) P=-SQRT( 1/6)
                                                                                                                  LIST OF SYMBOLS USED A-SQRT( 1/4) B-SQRT( 1/2) D-SQRT( 1/3) E-SQRT( 2/3) F-SQRT( 1/6)
```

```
THE CG SERIES:
 NU1 (4) * NU2(5) = = + 1* NU(2) + 1* NU(3) + 1* NU(4) + 2* NU(5)
IRREP NU1* NU2 = 4* 5
        CG COEFFICIENTS
22
0
0
0
                                     21
0
0
0
0
                                                                             34
0
0
                                               31
0
0
0
0
                                                                   32
0
G
0
                                                                        33
0
0
8
0
0
                                                                                            -A 0 0 0 H -0 0 0 0 0 0 0 0 0 0 0 0 0
                                 0 0 0 0 0 0 0 0 K 0 0
                                                                         -A 0 0 0 0 K 3 0 0 0
 L1ST OF SYMBOLS USED
A=SQRT( 1/5) B=-SQRT( 3/10) D=SQRT( 1/20) E=SQRT( 9/20)
                                                                                  F=SORT( 1/10)
 G=-SQRT( 2/5) H=SQRT( 2/15)
                                        J=-SQRT( 8/15)
                                                              K=SQRT( 1/4)
                                                                                  L=SQRT( 3/8)
 M=SQRT( 1/24) N=SQRT(2/3)
```

THE CG SERIES:

NU1(5)* NU2(5) == + 1* NU(1) + 1* NU(2) + 1* NU(3) + 2* NU(4) + 2* NU(5)

IRREP NUL*NU2 = 5* 5

CG COEFFICIENTS

LIST OF SYMBOLS USED

A=SQRT(1/5) B=SQRT(3/10) D=-SQRT(2/5) E=-SQRT(1/10) F=SQRT(8/15)

G=SQRT(1/30) H=SQRT(2/7) J=-SQRT(3/7) K=-SQRT(1/14) L=SQRT(1/70)

H=SQRT(4/105) N=-SQRT(7/15) F=-SQRT(8/35) Q=SQRT(18/35)

TABLE V. The CG series of the icosahedral group.

	A	$T_{\mathfrak{l}}$		G	Н
\overline{A} T_1	A	T_1 $A+T_1+H$	T_2 $G+H$	G $T_2 + G + H$	H $T_1 + T_2 + G + H$
G		·	$A+T_2+H$	$T_1 + G + H$ $A + T_1 + T_2 + G + H$	$T_1 + T_2 + G + H$ $T_1 + T_2 + G + 2H$
H					$A + T_1 + T_2 + 2G + 2H$

(2) Similar to the symmetries of the 3jm-symbols of the group I (Ref. 6), we have

$$\langle v_{1}\mu_{1}, v_{2}\mu_{2} | v_{3}\tau\mu_{3} \rangle$$

$$= (-)^{v_{1}+v_{2}+v_{3}} (-)^{q(v_{1}v_{2}v_{3}\tau)} \langle v_{2}\mu_{2}, v_{1}\mu_{1} | v_{3}\tau\mu_{3} \rangle$$

$$= ([v_{3}]/[v_{1}])^{1/2} (-)^{v_{1}+v_{2}+v_{3}} (-)^{q(v_{1}v_{2}v_{3}\tau)}$$

$$\times \langle v_{3}-\mu_{3}, v_{2}\mu_{2} | v_{1}\tau-\mu_{1} \rangle, \qquad (12a)$$

where $[\nu]$ is the dimension of the irrep ν , the phase $(-)^{\nu}$ is defined by

$$(-)^{\nu} = \begin{cases} -1, & \text{for } \nu = \begin{cases} T_1, & T_2, \\ A, & G, H, \end{cases}$$
 (12b)

and $(-)^{q(\nu_1\nu_2\nu_3\tau)}$ equals -1 if $(\nu_1\nu_2\nu_3\tau)$ is $(HHG\ 1)$ or any permutation of $(HHG\ 1)$.

(3) From Table IV we se that

$$\langle v_1 - \mu_1, v_2 - \mu_2 | v_3 \tau - \mu_3 \rangle$$

$$= \theta_{v_1 + v_2 + v_3} \langle v_1 \mu_1, v_2 \mu_2 | v_3 \tau \mu_3 \rangle, \tag{13a}$$

where $\theta_{\nu_1 + \nu_2 + \nu_3} = -1$, if $(\nu_1 \nu_2 \nu_3)$ is one of the following triples:

$$(T_iT_iT_i), (T_1T_2G), (HHT_i), (HHG),$$

 $(GGT_i), (GGG), \text{ for } i = 1,2,$
(13b)

and $\theta_{\nu_1 + \nu_2 + \nu_3} = 1$, otherwise. This leads us to introduce the following phase convention for the time reverse state:

$$\mathbb{T}|\mu\nu\rangle = \theta_{\nu}|\nu-\mu\rangle,\tag{14}$$

$$\theta_{\nu} = \begin{cases} -1, & \text{for } \nu = \begin{cases} T_1, T_2, G, \\ A, H. \end{cases}$$
 (13a')

Then the phase $\theta_{\nu_1 + \nu_2 + \nu_3}$ in Eq. (13a) can be expressed as

$$\theta_{\nu_1 + \nu_2 + \nu_3} = \theta_{\nu_1} \theta_{\nu_2} \theta_{\nu_3}. \tag{13b'}$$

V. DISCUSSIONS

A. The irreducible representations

Speiser¹ and McLellian⁴ have given the irreducible matrices for the three generators A, B, and C of the group I, where A is a $2\pi/5$ rotation about one of the fivefold axes that was chosen as the z axis, B is a π rotation about a twofold axis which was chosen as the x axis, and C represents the similar π rotation whose axis is perpendicular to that of B. In our notation, they are

$$A = R_2 = C_{5,1}^1 = R_z(2\pi/5),$$

$$B = R_{47} = C_{2,2} = R_x(\pi),$$

$$C = R_{57} = C_{2,12}.$$
(15)

The irrep labels A, T_1 , T_2 , G, and H are named Γ_1 , Γ_2 , Γ_3 , Γ_4 , and Γ_5 in Ref. 4, respectively. The symbols z, P, and Q in (6) are designated ϵ , α , and β in Ref. 4, respectively. Comparing our Table II with Table I and Eq. (21) in Ref. 4, we see that the matrices of the three generators for all five irreps obtained by the EFM are exactly the same as obtained by McLellian.

The irreps given here differ from that of Speiser¹ by a similarity transformation. For example, for the irrep T_1 , if we make the following basis transformation $\mathbf{e}_1 \rightarrow \mathbf{e}_1$, $\mathbf{e}_2 \rightarrow \mathbf{i}\mathbf{e}_2$, $\mathbf{e}_3 \rightarrow \mathbf{e}_3$, then the matrices for R_2 and R_{47} remain unchanged:

$$D^{T_1}(R_2) = \begin{vmatrix} z^{-1} & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & z \end{vmatrix},$$

$$D^{T_1}(R_{47}) = \begin{vmatrix} 0 & 0 & -1 \\ 0 & -1 & 0 \\ -1 & 0 & 0 \end{vmatrix},$$
(16)

while the matrix of R_{57} undergoes the following transformation:

$$D^{T_{i}}(R_{57}) = \frac{1}{\sqrt{5}} \begin{vmatrix} Q & -\sqrt{2} & P \\ -\sqrt{2}i & 1 & -\sqrt{2} \\ P & -\sqrt{2}i & Q \end{vmatrix} \rightarrow \frac{1}{\sqrt{5}} \begin{vmatrix} Q & -\sqrt{2}i & P \\ \sqrt{2}i & 1 & \sqrt{2}i \\ P & -\sqrt{2}i & Q \end{vmatrix}.$$
(17)

The transformed matrices are identical with Speiser's result.

B. The CG coefficients

The 3jm-symbols of the group I defined by Golding⁵ and Pooler⁶ are related to the CG coefficients by

$$\langle v_1 \mu_1, v_2 \mu_2 | v_3 \tau \mu_3 \rangle = [v_3]^{1/2} \begin{pmatrix} v_1 & v_2 & v_3 \\ \mu_1 & \mu_2 & -\mu_3 \end{pmatrix}^{\tau}.$$
 (18)

Comparing our results with theirs it is seen that both are identical (including the multiplicity separation) up to absolute phases. The CG coefficients here are all real, while theirs are imaginary for the triples in (13b). The discrepancy comes from the different conventions for the phase of time reverse states. Instead of (14), they impose

$$T|\mu\nu\rangle = |\nu - \mu\rangle,\tag{19}$$

which, in turn, leads to the following symmetry for the CG coefficient of I,

$$\langle v_1 - \mu_1, v_2 - \mu_2 | v_3 \tau - \mu_3 \rangle = \langle v_1 \mu_1, v_2 \mu_2 | v_3 \tau v_3 \rangle^*.$$
 (20)

Since the property (13a) is independent of absolute phase choices, the imposition of the symmetry (20) will force the CG coefficients for the triples in (13b) to be imaginary.

C. The SO₃ I subduction coefficients

The $SO_3 \supset I \supset C_5$ irreducible basis $|j\beta\nu\mu\rangle$ can be expressed in terms of the $SO_3 \supset SO_2$ basis $|jm\rangle$,

$$|j\beta\nu\mu\rangle = \sum_{m = \mu \pmod{5}} C(jm, \beta\nu\mu)|jm\rangle,$$
 (21)

where β is the label for distinguishing the multiple occurrence of the irrep ν of I in the irrep j of SO_3 and $C(jm,\beta\nu\mu)$ is called the subduction coefficient. (For j up to seven, β is

redundant.⁴) Under time reverse the basis $|jm\rangle$ transforms as

$$\mathbb{T}|jm\rangle = (-)^{j+m}|j-m\rangle. \tag{22}$$

From (14) and (22) we have

$$C(jm,\beta\nu\mu) = (-)^{j+m}\theta_{\nu}C(j-m,\beta\nu-\mu)^*$$
. (23)

McLellian calculated the subduction coefficients for j up to eight by using the projection operator method. Since the phase convention (19) is used in Refs. 4 and 6, their subduction coefficients satisfy the following relation:

$$C(jm,\beta\nu\mu) = (-)^{j+m}C(j-m,\beta\nu-\mu)^*.$$
 (24)

Therefore, their subduction coefficients differ from ours by a factor of i for the irreps T_1 , T_2 , and G. Starting from the subduction coefficients for j = 1,

$$|1T_1 \pm 1\rangle = i|1 \pm 1\rangle, |1T_1,0\rangle = |10\rangle,$$
 (25)

by using the following formula and the CG coefficients of the group I we can obtain both the subduction coefficients and $SO_3 \supset I$ isoscalar factor $\langle j_1\beta_1\nu_1, j_2\beta_2\nu_2 || j\beta\nu\tau \rangle$, recursively:

$$\sum_{\beta} \langle j_{1}\beta_{1}\nu_{1}j_{2}\beta_{2}\nu_{2} || j\beta\nu\tau\rangle^{*}C(jm,\beta\nu\mu)$$

$$= \sum_{\mu_{1}\mu_{2}m_{1}m_{2}} \langle \nu_{1}\mu_{1},\nu_{2}\mu_{2} || \nu\tau\mu\rangle$$

$$\times \langle j_{1}m_{1},j_{2}m_{2} || jm\rangle \prod_{i=1}^{2} C(j_{i}m_{i},\beta_{i}\nu_{i}\mu_{i}). \tag{26}$$

Under our phase convention, the $SO_3 \supset I$ isoscalar factors remain to be real. For example, the subduction coefficients for j = 1 - 4 and the isoscalar factors are listed below:

$$|1T_{1}, \pm 1\rangle = i|1 \pm 1\rangle, \quad |1T_{1},0\rangle = |10\rangle; \quad |2H, \pm 2\rangle = -|2 \pm 2\rangle, \quad |2H, \pm 1\rangle = i|2 \pm 1\rangle, \quad |2H,0\rangle = |20\rangle;$$

$$|3T_{2}, \pm 2\rangle = -\sqrt{3/5}|3 \pm 2\rangle + i\sqrt{2/5}|3 \mp 3\rangle, \quad |3T_{2},0\rangle = |30\rangle; \quad |3G, \pm 2\rangle = -\sqrt{2/5}|3 \pm 2\rangle - i\sqrt{3/5}|3 \mp 3\rangle,$$

$$|3G, \pm 1\rangle = -i|3 \pm 1\rangle; |4G, \pm 2\rangle = \pm\sqrt{14/15}|4 \pm 2\rangle \pm\sqrt{1/15}i|4 \mp 3\rangle, \quad |4G, \pm 1\rangle = \mp\sqrt{7/15}i|4 \pm 1\rangle \pm\sqrt{8/15}|4 \mp 4\rangle;$$

$$|4H, \pm 2\rangle = -\sqrt{1/15}|4 \pm 2\rangle + \sqrt{14/15}i|4 \pm 3\rangle, \quad |4H, \pm 1\rangle - \sqrt{8/15}i|4 \pm 1\rangle - \sqrt{7/15}|4 \mp 4\rangle, \quad |4H,0\rangle = |40\rangle;$$

$$(27)$$

$$\langle 3T_2, 1T_1 || 4G \rangle = -1/2, \quad \langle 3T_2, 1T_1 || 3G \rangle = -\sqrt{3}/2, \quad \langle 3T_2, 1T_2 || 4H \rangle = \sqrt{4/7}, \quad \langle 3T_2, 1T_1 || 2H \rangle = -\sqrt{3/7}. \tag{28}$$

The phases for the subduction coefficients $C(jm,\nu\mu)$ in (27) are more elegant than those of Refs. 4 and 6 in the sense that the coefficients $C(jm = \text{even}, \nu\mu)$ are all real, while $C(jm = \text{odd}, \nu\mu)$ are all imaginary.

In summary, with the isomorphism shown in the first table in the Appendix, the program found the CSCO-I, CSCO-II, and CSCO-III of the icosahedral group I as well as their eigenvectors that give the primitive characters, the CG

coefficients, and all the irreducible matrix elements of the group I. It once again shows the power of the eigenfunction method. With the new phase convention for the time reversal state, the CG coefficients of the group I can be made to be real even though the bases are still complex as shown in (27). The introducing of the extra phase factor $\theta_{\nu_1 + \nu_2 + \nu_3}$ in the symmetry (13a) is the only price one has to pay for real CG coefficients.

APPENDIX: THE ISOMORPHISM BETWEEN I AND A SUBGROUP OF S_{12} AND THE GROUP TABLE OF I

R_{i}	E	E	R_1	E	E
$R_2 = R_3^{-1}$	$C^{1}_{5.1}$	(265,11,7)(34,10,12,8)	$R_{40} = R_{41}^{-1}$	$C_{3.8}^{1}$	(17,11)(2,12,5)(394)(68,10)
$R_4 = R_5^{-1}$	$C^{1}_{5.2}$	(17836) (45,11,12,9)	$R_{42} = R_{43}^{-1}$	$C^{1}_{3.9}$	(13,12)(287)(4,10,5)(69,11)
$R_6 = R_7^{-1}$	$C^{1}_{5.3}$	(17,12,10,5)(28946)	$R_{44} = R_{45}^{-1}$	$C^{1}_{3.10}$	(15,11)(24,12)(398)(6,10,7)
$R_8 = R_9^{-1}$	$C^{1}_{5.4}$	(128,12,11)(39,10,56)	R ₄₆	$C_{2.1}$	(12)(3,11)(4,12)(58)(67)(9,10)
$R_{10} = R_{11}^{-1}$	$C^{1}_{5.5}$	(164,10,11)(239,12,7)	R ₄₇	$C_{\scriptscriptstyle 2.2}$	(19)(23)(47)(5,12)(68)(10,11)
$R_{12} = R_{13}^{-1}$	$C^{1}_{5.6}$	(12345)(789,10,11)	R ₄₈	$C_{2.3}$	(1,12)(2,10)(34)(58)(69)(7,11)
$R_{14} = R_{15}^{-1}$	$C_{5.1}^{2}$	(2576,11)(3,10,84,12)	R ₄₉	$C_{2.4}$	(19)(2,12)(3,11)(45)(6,10)(78)
$R_{16} = R_{17}^{-1}$	$C^{2}_{5.2}$	(18673)(4,11,95,12)	R ₅₀	$C_{2.5}$	(15)(2,10)(3,12)(47)(6,11)(89)
$R_{18} = R_{19}^{-1}$	$C_{5.3}^{2}$	(1,12,57,10)(29684)	R ₅₁	$C_{2.6}$	(16)(25)(3,11)(47)(8,10)(9,12)
$R_{20} = R_{21}^{-1}$	$C_{5.4}^{2}$	(18,11,2,12)(3,10,695)	R ₅₂	$C_{2.7}$	(13)(26)(47)(58)(9,11)(10,12)
$R_{22} = R_{23}^{-1}$	$C_{5.5}^{2}$	(14,11,6,10)(2973,12)	R ₅₃	$C_{2.8}$	(19)(24)(36)(58)(7,10)(11,12)
$R_{24} = R_{25}^{-1}$	$C_{5.6}^{2}$	(13524)(79,11,8,10)	R ₅₄	$C_{2.9}$	(19)(2,10)(35)(46)(7,12)(8,11)
$R_{26} = R_{27}^{-1}$	$C^{1}_{3.1}$	(126) (357) (4,11,8) (9,10,12)	R ₅₅	$C_{2.10}$	(14)(2,10)(3,11)(56)(70)(8,12)
$R_{28} = R_{29}^{-1}$	$C^{1}_{3.2}$	(184)(236)(579)(10,11,12)	R ₅₆	$C_{2.11}$	(1,11)(2,10)(39)(48)(57)(6,12)
$R_{30} = R_{31}^{-1}$	$C^{1}_{3.3}$	(18,10)(295)(346)(7,12,11)	R ₅₇	$C_{\scriptscriptstyle 2.12}$	(17)(2,11)(3,10)(49)(58)(6,12)
$R_{32} = R_{33}^{-1}$	$C^{1}_{3.4}$	(13,10)(29,11)(456)(78,12)	R ₅₈	$C_{2.13}$	(18)(27)(3,11)(4,10)(59)(6,12)
$R_{34} = R_{35}^{-1}$	$C_{3.5}^{1}$	(165)(24,11)(3,10,7)(89,12)	R ₅₉	$C_{2.14}$	(19)(28)(37)(4,11)(5,10)(6,12)
$R_{36} = R_{37}^{-1}$	$C_{3.6}^{1}$	(172)(35,12)(4,10,9)(6,11,8)	R ₆₀	$C_{2.15}$	(1,10)(29)(38)(47)(5,11)(6,12)
$R_{38} = R_{39}^{-1}$	$C^{1}_{3.7}$	(1,12,4)(283)(5,11,10)(679)			

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