Finite Group Theory for Large Systems. 2. Generating Relations and Irreducible Representations for the Icosahedral Point Group, $\mathscr{I}_h$

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Generating relations and irreducible representations are given for the icosahedral point group, $\mathscr{I}_h$, that are suited to computerized projection of symmetry-adapted bases of arbitrary spaces invariant to the group. With 120 elements $\mathscr{I}_h$ is a good prototype for symmetry-adaptation to a large finite nonabelian group. The four- and five-dimensional irreducible representations are obtained by coupling direct products of the three-dimensional irreducible representations using the symmetry-adaptation algorithm. The method is applied to the Hückel treatment of icosahedral C_{20} fullerene.

I. INTRODUCTION

This article is the second in a series on the application of finite group theory to large systems in quantum chemistry.[1] Group generators and irreducible representations of the icosahedral point group, $\mathscr{I}_h$, are provided here to facilitate computerized projection of a symmetry-adapted basis for any space that is invariant to the group, given the generator transformations on a defining basis. Similar constructs have been previously tabulated elsewhere,[2,3] but the present work is original in its formulation for systematic and convenient computation on arbitrary spaces.

As used here, large systems are those that require computer-aided analysis to perform the symmetry-adaptation and to calculate reduced matrix elements. Either or both of the molecular system and its finite symmetry group are sufficiently large to make hand calculations laborious and time-consuming, if not prohibitive. For example, even the simple Hückel treatment of the smallest icosahedral fullerene, C_{20}, requires the construction of 20 × 20 matrix representations of projection operators by summing over the 120 elements of the point symmetry group. Nevertheless, group theoretical analysis facilitates calculations that otherwise might be impossible. Applying the full power of group theory to these systems requires symmetry-adapted bases and the projection operators that produce them.[4−6] A consistent set of irreducible representations for $\mathscr{I}_h$ are obtained here by the methods described by this author in reference 1. As a simple example, in section V these methods are applied to the Hückel treatment of the smallest fullerene, C_{20}.

To summarize, a basis of a state vector space, V(ω), of dimension $f(\omega)$, that is symmetry-adapted to a group G of order g is written

$$\{|\omega;\rho\alpha r\rangle, \alpha = 1, ..., M; \rho = 1, ..., f(\omega;\alpha); r = 1, ..., f(\alpha)\} \tag{1.1}$$

where α denotes the irreducible representations of G (e.g. A_g or T_{1u} of the icosahedral group); $f(\alpha)$ is the dimension of the αth irreducible representation (one for A_g and three for T_{1u}); M is the number of distinct nonequivalent irreducible representations of G as well as the number of equivalence classes (10 for the icosahedral group); ρ distinguishes repeated irreducible representations; and the frequency of repetitions, $f(\omega;\alpha)$, is given by the usual character formula:

$$f(\omega;\alpha) = \frac{1}{g}\sum_{\sigma=1}^{M} n_\sigma \chi_{\bar{\sigma}}^{\alpha} \chi_{\sigma}^{\omega} \tag{1.2}$$

Here, n_σ is the number of elements in the σth class, $\chi_{\bar{\sigma}}{}^{\alpha}$ is the character of the inverse of the σth class in the αth irreducible representation, and $\chi_{\sigma}{}^{\omega}$ is the character of the σth class in the vector space V(ω). By definition symmetry-adapted basis elements transform under elements of G according to the irreducible representations:

$$G_a|\omega;\rho\alpha r\rangle = \sum_{r'}^{f(\alpha)} [G_a]_{r'r}{}^{\alpha}|\omega;\rho\alpha r'\rangle \tag{1.3}$$

Matrix elements over symmetry-adapted vectors of any operator that commutes with G, such as the Hamiltonian, H, satisfy

$$\langle\omega;\rho\alpha r|H|\omega;\rho'\alpha' r'\rangle = \delta(\alpha,\alpha')\delta(r,r')\langle\omega,\rho\alpha\|H\|\omega;\rho'\alpha\rangle \tag{1.4}$$

The quantity on the right that is independent of the r index is termed a reduced matrix element. If the basis is ordered so that elements with the same α and r are grouped together, then for each α such that $f(\omega;\alpha) \neq 0$ the $f(\omega;\alpha) \times f(\omega;\alpha)$ reduced matrix is repeated $f(\alpha)$ times. There are therefore $f(\omega;\alpha)$ eigenvalues for α and each is $f(\alpha)$-fold degenerate.

Usually, the defining basis for V(ω) is not adapted to the symmetry group, G, so that such a basis must be constructed. The most general method for finite groups is to use the $f(\omega) \times f(\omega)$ matrices

$$[e_{rs}{}^{\alpha}]^{\omega} = \frac{f(\alpha)}{g}\sum_{a=1}^{g}[G_a^{-1}]_{sr}^{\alpha}[G_a]^{\omega}, \quad \alpha = 1, ..., M; r, s = 1, ..., f(\omega) \tag{1.5}$$

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Table 1. Character Table for Icosahedral Group, $\mathscr{I}_h$

$\mathscr{I}_h$	I	$12C_5$	$12C_5^2$	$20C_3$	$15C_2$	i	$12iC_5$	$12iC_5^2$	$20iC_3$	15σ
A_g	1	1	1	1	1	1	1	1	1	1
T_{1g}	3	τ	$(1-\tau)$	0	−1	3	τ	$(1-\tau)$	0	−1
T_{2g}	3	$(1-\tau)$	τ	0	−1	3	$(1-\tau)$	τ	0	−1
G_g	4	−1	−1	1	0	4	−1	−1	1	0
H_g	5	0	0	−1	1	5	0	0	−1	1
A_u	1	1	1	1	1	−1	−1	−1	−1	−1
T_{1u}	3	τ	$(1-\tau)$	0	−1	−3	$-\tau$	$(\tau-1)$	0	1
T_{2u}	3	$(1-\tau)$	t	0	−1	−3	$(\tau-1)$	$-\tau$	0	1
G_u	4	−1	−1	1	0	−4	1	1	−1	0
H_u	5	0	0	−1	1	−5	0	0	1	−1
C_{20}	20	0	0	2	0	0	0	0	0	4

where the sum is over all g elements of G, and $[G_a]^\omega$ is the $f(\omega) \times f(\omega)$ matrix that represents G_a on the defining basis. As detailed in reference 1, the most efficient method for computerized construction of $[e^{\alpha}_{rs}]^\omega$ is to input matrix representations of generators to calculate both $[G_a]^\alpha$ and $[G_a]^\omega$ for all elements.

A set of generating relations for all 120 elements of $\mathscr{I}_h$ in terms of two rotations and the inversion and a corresponding set of irreducible representation matrices are derived here.[7] The $\mathscr{I}_h$ character table is given in Table 1 where

$$\tau = \frac{1+\sqrt{5}}{2} \tag{1.6}$$

is sometimes called the golden mean. Cotton's notation[8] of G for the four dimensional irreducible representation and H for the five dimensional irreducible representation is used here instead of Griffith's U and V.[9]

According to Cayley's theorem, any finite group, no matter how large, is isomorphic to a group of permutations.[10] Such mapping could be particularly useful for large groups. It is well-known that the 60 element rotational subgroup, $\mathscr{I} \subset \mathscr{I}_h$, is isomorphic to the alternating group, $A(5)$, of all even permutations on five objects. This relationship is exploited here to construct the multiplication table and the generating relations.[11−13] The irreducible representations are derived by reducing direct products with projection operators, starting with the faithful irreducible representation T_{1u} of transformations on the Cartesian axes. In this way, the matrices are based on specific, well-defined assumptions.

The irreducible representations A, T_1, and T_2 are established in Section III. In Section IV the G and H irreducible representations of $\mathscr{I}$ are obtained by coupling. Symmetry-adaptation is applied to the Hückel theory of C_{20} in Section V, and Section VI is the conclusion.

II. PERMUTATIONS, MULTIPLICATION TABLE, AND GENERATING RELATIONS

Since $\mathscr{I}_h$ is the direct product $\mathscr{I} \otimes \{E, i\}$, $\mathscr{I}$ constitutes half of the elements of $\mathscr{I}_h$ and are numbered here from 1 to 60. The remaining 60 elements are products of the inversion i and the rotations. It is convenient to take

$$G_{a+60} = iG_a,\ a = 1, ..., 60 \tag{2.1}$$

Consequently, G_a, $a = 61, ..., 120$, are the improper rotations, including the inversion, reflections, and screw operations. Inversion times a C_5 rotation is an S_{10} screw and inversion times C_5^2 is an S_{10}^3. It is also convenient to take the identity to be the first element, $G_1 = E$, so that the 61st element is the inversion, $G_{61} = i$. The multiplication table and irreducible representations of $\mathscr{I}_h$ are therefore straightforward extensions from those of $\mathscr{I}$.

The isomorphism of $\mathscr{I}$ to the alternating group $A(5)$ is used here to set up the multiplication table. The specific mapping is given in Table 2 where the permutations of $A(5)$ are represented by a vector array $\{a_1, a_2, ..., a_n\}$, where a_i is the map of i as well as the conventional product of cycles.

The elements of $A(5)$ were obtained by first generating all permutations on five objects and discarding the odd ones.[14] Elements were assigned to classes by carrying out equivalence transformations. After reordering the elements to correspond to the first five classes in Table 1, the multiplication table in Table 4 was constructed.

The isomorphism of $A(5)$ to $\mathscr{I}$ was established by mapping the generators. Following Griffith, the generators of $\mathscr{I}$ were taken to be a 5-fold rotation, C_5^k about the z-axis and a 2-fold rotation, C_2^r, about an axis, r, at angles $\theta = \theta_4$ and $\varphi = 0$ to the z-axis, where θ_4 is given in Table 3. The matrices transforming the Cartesian basis elements under these two operators are designated T_1 in Table 6. An important condition on the two generators is that their product be a 3-fold rotation since $G_4G_{46} = G_{40}$ is a member of the fourth class of third-order elements, and this requirement is satisfied by the following correspondence:

$$\begin{aligned} C_5^{\hat{k}} &\leftrightarrow G_4 \\ C_2^{\vec{r}} &\leftrightarrow G_{46} \end{aligned} \tag{2.2}$$

Generating relations in terms of G_4 and G_{46} for the remaining elements of $A(5)$ are obtained from the multiplication table and are displayed in Table 5. Each relation involves elements previously generated in the table. A generating expression for the identity is unnecessary for present purposes.

With these generating relations, the Cartesian transformation matrices of the remaining rotations in $\mathscr{I}$ were calculated by matrix products. The magnitude of the rotation angle, ν, was obtained from the trace, $1 + 2\cos\nu$. Since the inverses of elements belong to the same class for this group, when two rotations with the same axis and $|\nu|$ belong to the same class, the angles must differ by sign. The polar angles of the rotation axes were determined by first transforming the matrices to the complex $D^{(1)}$ transformation matrices of the spherical harmonics, $\{Y_{1-1}, Y_{10}, Y_{11}\}$:

$$\begin{bmatrix} rY_{1,-1} \\ rY_{0,0} \\ rY_{1,1} \end{bmatrix} = \begin{bmatrix} (1/\sqrt{2}) & (-i/\sqrt{2}) & 0 \\ 0 & 0 & 1 \\ (-1/\sqrt{2}) & (-i/\sqrt{2}) & 0 \end{bmatrix} \begin{bmatrix} x \\ y \\ z \end{bmatrix} \tag{2.3}$$

where i is the imaginary. Let the 3×3 matrix in (2.3) be designated $[S]$, then transformation is

$$D(a)^{(1)} = [S][G_a]^{T_1}[\tilde{S}]^* \tag{2.4}$$

Table 2. Isomorphism of Rotational Subgroup, $\mathscr{I}$, to Alternating Group, $A(5)$, Broken Out by the Classes in Table 1[a]

1
1,2,3,4,5
(1)(2)(3)(4)(5)
E
0, 0

2	3	4	5	6	7	8	9	10	11	12	13
2,3,5,1,4	5,3,1,2,4	2,5,1,3,4	3,4,5,2,1	3,1,4,5,2	4,1,2,5,3	4,5,1,2,3	2,4,5,3,1	5,3,4,1,2	4,5,2,3,1	3,4,5,1,2	5,1,4,2,3
(12354)	(15423)	(12543)	(13245)	(13452)	(14532)	(14253)	(12435)	(15234)	(14325)	(13524)	(15342)
72	72	72	−72	−72	−72	72	72	−72	72	−72	−72
θ_1, 36	θ_1, −18	0, 0	θ_1, −18	0, 0	θ_1, 36	θ_1, 18	θ_1, 0	θ_1, −36	θ_1, −36	θ_1, 18	θ_1, 0

14	15	16	17	18	19	20	21	22	23	24	25
3,5,2,1,4	3,1,5,2,4	5,1,2,3,4	3,5,4,2,1	4,1,5,3,2	5,4,2,1,3	2,4,1,5,3	2,3,4,5,1	4,3,1,5,2	4,3,5,2,1	5,4,1,3,2	2,5,4,1,3
(13254)	(13542)	(15432)	(13425)	(14352)	(15324)	(12453)	(12345)	(14523)	(14235)	(15243)	(12543)
−144	144	−144	144	144	144	−144	144	144	−144	−144	−144
θ_1, 0	θ_1, −36	θ_1, 18	θ_1, 36	θ_1, −18	0, 0	θ_1, −36	θ_1, 18	θ_1, 0	0, 0	θ_1, 36	θ_1, −18

26	27	28	29	30	31	32	33	34	35	36	37	38	39	40	41	42	43	44	45
3,1,2,4,5	1,3,4,2,5	4,2,1,3,5	2,4,3,1,5	4,1,3,2,5	1,4,2,3,5	3,2,4,1,5	2,3,1,4,5	5,1,3,4,2	1,5,2,4,3	3,2,5,4,1	1,3,5,4,2	5,2,1,4,3	2,5,3,4,1	5,2,3,1,4	1,5,3,2,4	1,2,5,3,4	1,2,4,5,3	4,2,3,5,1	1,4,3,5,2
(132)	(234)	(143)	(124)	(142)	(243)	(134)	(123)	(152)	(253)	(135)	(235)	(153)	(125)	(154)	(254)	(354)	(345)	(145)	(245)
120	120	120	120	−120	−120	−120	−120	120	120	120	−120	−120	−120	120	120	120	−120	−120	−120
θ_2, −36	θ_3, −18	θ_2, 36	θ_3, 18	θ_3, 18	θ_3, −18	θ_2, 36	θ_2, −36	θ_2, −18	θ_3, 36	θ_3, 0	θ_3, 36	θ_3, 0	θ_2, −18	θ_3, −36	θ_2, 0	θ_2, 18	θ_2, 18	θ_3, −36	θ_2, 0

46	47	48	49	50	51	52	53	54	55	56	57	58	59	60
2,1,4,3,5	4,3,2,1,5	3,4,1,2,5	4,5,3,1,2	1,4,5,2,3	5,2,4,3,1	1,5,4,3,2	5,2,4,3,1	5,4,3,2,1	2,1,3,5,4	1,3,2,5,4	3,2,1,5,4	5,3,2,4,1	3,5,1,4,2	2,1,5,4,3
(12)(34)	(14)(23)	(13)(24)	(14)(25)	(24)(35)	(15)(34)	(25)(34)	(14)(35)	(15)(24)	(12)(45)	(23)(45)	(13)(45)	(15)(23)	(13)(25)	(12)(35)
180	180	180	180	180	180	180	180	180	180	180	180	180	180	180
θ_4, 0	θ_5, 0	90, 0	90, 36	θ_5, −36	90, −18	θ_4, −36	θ_5, −18	θ_5, 36	θ_4, 36	90, −36	θ_4, −18	θ_5, 18	θ_4, 18	90, 18

[a] Within each class the top row is an index used in the multiplication table. The second row is the ordered array representation of the permutation, and the third row is the cycle representation. The angle of rotation of the isomorphic element of $\mathscr{I}$ is given in row four, and the polar angles, θ, ϕ, of its axis of rotation are given in row five. The definitions of the five special angles are given in Table 3.

Table 3. Values of the Five Special Angles Used To Specify Rotation Axes in Table 2

θ_i:	θ_1	θ_2	θ_3	θ_4	θ_5
$\cos^{-1}\theta_i$	$1/\sqrt{5}$	$(5-2\sqrt{5})/15$	$(5+2\sqrt{5})/15$	$\tau/\sqrt{1+\tau^2}$	$1/\sqrt{1+\tau^2}$

The positive polar angle θ is obtained from the formula[15]

$$D^{(1)}_{0,0} = \cos^2\theta(1-\cos\nu) + \cos\nu \tag{2.5}$$

and the polar angle φ from

$$\phi = \frac{1}{2}\tan^{-1}\left[\frac{\mathrm{Im}(D^{(1)}_{-1,1})}{\mathrm{Re}(D^{(1)}_{-1,1})}\right] \tag{2.6}$$

The resulting mapping of permutations to the rotations of $\mathscr{I}$ is shown in Table 2. The special polar angles θ_1 through θ_5 for the rotation axes are displayed in Table 3.

III. IRREDUCIBLE REPRESENTATIONS A, T_1, AND T_2 OF $\mathscr{I}$

The rotational subgroup $\mathscr{I}$ has five irreducible representations: A, T_1, T_2, G, and H of dimension 1, 3, 3, 4, and 5, respectively. From the character table, Table 1, $\mathscr{I}_h$ has five *gerade* irreducible representations, A_g, T_{1g}, T_{2g}, G_g, and H_g, and five *ungerade* irreducible representations, A_u, T_{1u}, T_{2u}, G_u, and H_u. For the pure rotations the g and u irreducible representations are identical to the corresponding irreducible representations of $\mathscr{I}$

$$[G_a]^{\alpha_u} = [G_a]^{\alpha_g} = [G_a]^{\alpha},\ a = 1, ..., 60;\quad \alpha = A, T_1, T_2, G, H \tag{3.1}$$

and differ by sign for the remaining improper rotations:

$$[G_a]^{\alpha_g} = [G_a]^{\alpha}$$

$$[G_a]^{\alpha_u} = -[G_a]^{\alpha},\ a = 61, ..., 120;\quad \alpha = A, T_1, T_2, G, H \tag{3.2}$$

It is therefore only necessary to give generating matrices for the five irreducible representations of $\mathscr{I}$ as displayed in Table 6.

***A*:** The A irreducible representation consists entirely of ones.

***T_1*:** The Cartesian coordinates transform according to T_1 of $\mathscr{I}$ and T_{1u} of $\mathscr{I}_h$, hence the matrices $[G_4]^{T_1}$ and $[G_{46}]^{T_1}$ are given by the usual rotation matrices on the Cartesian basis where G_4 is a rotation through $2\pi/5 = 72°$ about the z-axis and G_{46} is a rotation through $\pi = 180°$ about an axis at a polar angle of

$$\theta_4 = \cos^{-1}\left(\frac{\tau}{\sqrt{1+\tau^2}}\right) \tag{3.3}$$

to the z-axis.

***T_2*:** From the character table, the character of the second class in T_2 is the same as the character of the third class in

Table 4. Multiplication Table for $A(5)$ and the Rotational Icosahedral Subgroup, $\mathscr{I}$

1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	26	27	28	29	30	31	32	33	34	35	36	37	38	39	40	41	42	43	44	45	46	47	48	49	50	51	52	53	54	55	56	57	58	59	60
2	17	11	5	34	38	1	31	6	8	45	13	28	54	51	44	24	43	30	26	59	35	52	7	48	40	4	56	15	42	55	3	14	53	29	10	25	47	12	23	9	21	33	37	60	57	41	16	50	46	22	20	27	18	36	39	58	49	19	32
3	6	18	12	1	35	39	9	32	7	29	43	11	45	52	49	31	25	44	36	26	60	46	53	5	41	16	2	57	4	40	56	15	8	54	27	13	23	48	22	24	10	58	33	38	14	55	42	20	51	47	19	21	28	59	34	37	30	50	17
4	13	7	19	37	1	36	5	10	30	12	27	44	50	43	53	45	32	23	58	34	26	6	47	54	42	55	14	3	57	2	41	16	28	9	52	46	11	24	8	20	25	39	59	33	40	15	56	48	21	49	29	17	22	38	60	35	18	31	51
5	28	1	30	25	2	10	34	8	42	13	4	37	46	33	27	60	3	52	49	53	40	38	41	18	21	36	54	11	58	17	9	44	56	6	20	57	45	7	31	26	48	12	19	14	23	51	39	16	59	50	15	24	35	47	32	29	43	55	22
6	31	29	1	8	23	3	40	35	9	38	11	2	28	47	33	53	58	4	41	50	54	19	39	42	22	12	34	52	10	59	18	45	21	57	7	5	55	43	46	32	26	15	13	17	37	24	49	51	14	60	36	16	25	27	48	30	20	44	56
7	1	32	27	4	9	24	10	41	36	3	39	12	33	29	48	2	54	59	52	42	51	40	17	37	20	53	13	35	19	8	60	43	5	22	55	44	6	56	26	47	30	18	16	11	50	38	25	58	49	15	23	34	14	31	28	46	57	21	45
8	34	6	10	42	31	9	21	40	26	2	1	5	37	45	12	56	29	36	51	16	46	55	32	58	50	7	25	38	20	53	35	13	48	23	41	30	17	3	59	22	49	11	4	28	19	60	43	33	44	14	47	39	57	24	18	52	15	27	54
9	8	35	7	10	40	32	26	22	41	6	3	1	13	38	43	34	57	27	47	49	14	59	56	30	51	39	5	23	36	21	54	11	42	46	24	4	31	18	50	60	20	29	12	2	44	17	58	15	33	45	55	48	37	53	25	19	52	16	28
10	5	9	36	30	8	41	42	26	20	1	7	4	44	11	39	28	35	55	15	48	50	31	60	57	49	24	37	6	52	34	22	12	25	40	47	19	2	32	21	51	58	3	27	13	59	45	18	43	16	33	38	56	46	17	54	23	29	53	14
11	38	43	13	2	29	12	6	3	1	15	33	45	60	20	50	55	48	37	10	40	32	57	27	34	9	44	17	58	5	23	39	51	31	18	4	28	52	16	35	7	8	49	14	47	54	36	21	26	22	41	30	59	56	19	53	25	42	46	24
12	11	39	44	13	3	27	1	7	4	43	16	33	51	58	21	38	56	46	30	8	41	35	55	28	10	59	45	18	37	6	24	49	2	32	19	14	29	53	9	36	5	48	50	15	22	52	34	42	26	20	57	31	60	23	17	54	25	40	47
13	45	12	37	28	11	4	2	1	5	33	44	14	22	49	59	47	39	57	42	31	9	29	36	56	8	19	60	43	25	38	7	50	17	3	30	54	15	27	6	10	34	16	46	51	35	20	53	21	40	26	58	55	32	52	24	18	48	23	41
14	51	44	54	60	33	37	45	13	28	50	46	22	9	21	23	20	27	18	34	38	1	43	30	24	2	57	41	16	56	15	4	40	47	12	25	32	49	19	11	5	17	59	35	26	3	42	55	31	6	8	48	52	7	58	36	39	53	29	10
15	52	49	45	38	58	33	29	43	11	20	51	47	24	10	22	19	21	28	1	35	39	25	44	31	3	14	55	42	2	57	16	41	23	48	13	17	30	50	18	12	6	26	60	36	56	4	40	9	32	7	5	46	53	37	59	34	8	54	27
16	43	53	50	33	39	59	12	27	44	48	21	49	20	25	8	29	17	22	37	1	36	32	23	45	4	40	15	56	14	3	55	42	11	24	46	51	18	31	7	19	13	34	26	58	41	57	2	5	10	30	54	6	47	35	38	60	28	9	52
17	24	45	34	53	47	2	55	38	31	60	28	56	18	22	37	7	33	42	40	19	29	20	1	16	23	5	39	51	21	36	11	54	27	15	8	48	41	13	52	6	59	14	25	32	58	9	44	46	57	35	26	4	43	10	12	49	50	30	3
18	35	25	43	3	54	48	32	56	39	57	58	29	38	19	20	40	5	33	27	41	17	14	21	1	24	49	6	37	12	22	34	52	9	28	16	11	46	42	60	53	7	30	15	23	45	59	10	36	47	55	44	26	2	50	8	13	4	51	31
19	44	36	23	46	4	52	37	30	57	27	55	59	21	39	17	33	41	6	18	28	42	1	15	22	25	38	50	7	35	13	20	53	14	10	29	40	12	47	5	58	54	24	31	16	8	43	60	56	34	48	3	45	26	11	51	9	32	2	49
20	30	26	47	52	42	51	58	49	15	10	41	36	27	1	32	37	40	17	11	18	16	34	14	23	43	60	19	8	38	25	50	7	57	21	45	55	5	22	48	33	29	9	24	4	53	13	35	3	39	12	2	54	59	28	46	31	6	56	44
21	48	31	26	49	53	40	16	59	50	34	8	42	30	28	1	18	38	41	14	12	19	24	35	15	44	9	58	17	51	39	23	5	43	55	22	20	56	6	27	46	33	2	10	25	36	54	11	13	4	37	60	3	52	32	29	47	45	7	57
22	26	46	32	41	50	54	51	14	60	40	35	9	1	31	29	42	19	39	17	15	13	16	25	36	45	18	10	59	24	49	37	6	20	44	56	7	21	57	33	28	47	23	3	8	12	34	52	38	11	2	53	58	4	48	30	27	55	43	5
23	59	52	6	40	19	29	46	57	35	55	38	31	34	24	45	16	20	1	32	14	25	4	43	26	54	11	21	36	9	44	58	17	50	30	3	8	27	15	37	18	22	47	2	53	5	39	51	60	28	56	7	33	42	12	49	10	41	13	48
24	7	60	53	27	41	17	36	47	55	32	56	39	43	35	25	1	14	21	23	30	15	26	2	44	52	34	12	22	59	10	45	18	4	51	31	16	9	28	20	38	19	54	48	3	49	6	37	57	58	29	40	5	33	8	13	50	46	42	11
25	54	5	58	18	28	42	56	34	48	37	30	57	23	44	36	22	1	15	16	24	31	45	26	3	53	20	35	13	43	60	8	19	32	2	49	29	14	10	17	21	39	4	52	46	38	50	7	27	55	59	33	41	6	51	9	11	12	47	40
26	42	40	41	20	21	22	49	50	51	8	9	10	4	2	3	25	23	24	45	43	44	53	54	52	33	32	30	31	47	48	46	1	58	59	60	36	34	35	16	14	15	6	7	5	27	28	29	11	12	13	17	18	19	56	57	55	38	39	37
27	12	24	59	44	7	55	4	36	19	39	53	16	49	18	34	11	60	40	57	5	20	9	38	14	30	31	33	32	46	1	47	48	13	41	23	50	3	17	10	52	37	56	21	43	26	29	28	25	42	58	35	2	51	6	45	22	54	8	15
28	60	13	25	56	45	5	17	2	34	14	37	54	35	50	19	41	12	58	21	55	6	15	10	39	31	30	32	33	48	47	1	46	24	11	42	18	51	4	38	8	53	44	57	22	29	26	27	59	23	40	49	36	3	20	7	43	16	52	9
29	23	58	11	6	57	43	35	18	3	52	15	38	17	36	51	59	42	13	7	22	56	37	16	8	32	33	31	30	1	46	48	47	40	25	12	2	19	49	54	39	9	20	45	55	28	27	26	41	60	24	4	50	34	44	21	5	10	14	53
30	37	10	52	57	5	20	25	42	58	4	36	19	59	12	24	14	9	38	43	56	21	2	51	35	48	47	46	1	29	28	26	27	54	8	15	23	13	41	34	49	18	7	55	44	31	33	32	39	53	16	11	60	40	45	22	6	3	17	50
31	53	38	8	21	55	6	59	23	40	17	2	34	25	60	13	39	15	10	22	44	57	36	3	49	46	1	48	47	26	27	29	28	16	52	9	42	24	11	19	35	50	45	5	56	30	32	33	14	37	54	41	12	58	7	43	20	51	4	18
32	9	54	39	7	22	56	41	60	24	35	18	3	11	23	58	8	37	16	55	20	45	50	34	4	47	48	1	46	27	26	28	29	10	14	53	12	40	25	51	17	36	57	43	6	33	31	30	52	15	38	59	42	13	21	5	44	19	49	2
33	15	16	14	45	43	44	11	12	13	49	50	51	41	42	40	52	53	54	5	6	7	18	19	17	1	46	47	48	28	29	27	26	38	39	37	60	58	59	3	4	2	21	22	20	32	30	31	8	9	10	25	23	24	57	55	56	34	35	36
34	56	2	42	48	17	8	53	31	21	28	5	25	57	14	4	32	11	20	50	27	23	47	9	43	59	10	18	45	49	24	6	37	39	38	26	58	60	1	55	40	16	13	30	54	52	22	12	44	19	46	51	7	29	41	3	15	33	36	35
35	40	57	3	9	46	18	22	54	32	23	29	6	2	55	15	21	30	12	24	51	28	44	48	10	60	43	8	19	7	50	25	38	26	37	39	1	59	58	14	56	41	52	11	31	13	53	20	47	45	17	27	49	5	16	42	4	36	33	34
36	4	41	55	19	10	47	30	20	52	7	24	27	16	3	56	13	22	31	29	25	49	8	45	46	58	17	44	9	23	5	51	39	37	26	38	59	1	60	42	15	57	32	53	12	21	11	54	18	48	43	6	28	50	2	14	40	35	34	33
37	14	4	57	54	13	30	28	5	25	44	19	46	40	16	55	51	7	29	48	17	8	11	20	32	34	52	22	12	18	45	10	59	60	1	58	35	33	36	2	42	56	27	23	50	6	49	24	53	31	21	43	47	9	15	41	3	39	38	26
38	55	15	2	31	52	11	23	29	6	47	45	17	56	41	14	27	49	5	9	46	18	30	12	21	35	13	53	20	8	19	43	60	59	58	1	34	36	33	57	3	40	51	28	24	25	7	50	22	54	32	10	44	48	4	16	42	26	37	39
39	3	56	16	12	32	53	7	24	27	18	48	43	15	57	42	6	28	50	19	10	47	22	31	13	36	21	11	54	44	9	17	58	1	60	59	33	35	34	41	55	4	25	49	29	51	23	5	30	20	52	46	8	45	40	2	14	37	26	38
40	21	23	9	26	59	35	50	46	22	31	6	8	5	17	11	48	52	7	60	33	37	27	18	20	14	3	42	55	41	16	57	2	49	19	32	10	53	29	44	54	51	38	1	34	4	56	15	45	13	28	24	43	30	39	58	36	47	12	25
41	10	22	24	36	26	60	20	51	47	9	32	7	12	6	18	5	46	53	38	58	33	21	28	19	15	56	4	40	55	42	14	3	30	50	17	27	8	54	49	45	52	35	39	1	16	2	57	29	43	11	31	25	44	34	37	59	23	48	13
42	25	8	20	58	34	26	48	21	49	5	10	30	19	13	7	54	6	47	33	39	59	17	22	29	16	41	57	2	15	56	40	4	18	31	51	52	28	9	53	50	43	1	36	37	55	14	3	12	27	44	45	32	23	60	35	38	11	24	46
43	29	48	33	11	18	16	3	39	12	58	49	15	47	30	26	23	34	14	4	9	24	54	59	2	7	50	38	25	13	35	53	20	6	56	44	45	57	21	32	27	1	42	51	52	60	19	8	10	41	36	37	40	17	46	31	28	5	22	55
44	33	27	46	14	12	19	13	4	37	16	59	50	26	48	31	15	24	35	25	2	10	3	52	60	5	23	51	39	54	11	36	21	45	7	57	22	43	55	1	30	28	53	40	49	9	58	17	34	8	42	18	38	41	29	47	32	56	6	20
45	47	33	28	17	15	13	38	11	2	51	14	60	32	26	46	36	16	25	8	23	3	58	4	53	6	37	24	49	34	52	12	22	55	43	5	56	20	44	29	1	31	50	54	41	18	10	59	40	35	9	42	19	39	30	27	48	21	57	7
46	50	19	35	22	44	57	14	37	54	59	23	40	8	53	38	49	36	3	56	45	5	12	58	41	28	29	26	27	32	33	30	31	51	4	18	9	16	52	13	25	60	55	6	21	1	48	47	17	2	34	39	15	10	43	20	7	24	11	42
47	36	51	17	55	20	45	52	15	38	41	60	24	39	9	54	4	50	34	6	57	43	42	13	59	29	28	27	26	31	30	33	32	19	49	2	53	10	14	58	11	23	22	56	7	48	1	46	35	18	3	8	37	16	5	44	21	40	25	12
48	18	34	49	43	56	21	39	53	16	25	42	58	52	37	10	35	2	51	44	7	55	60	40	11	27	26	29	28	33	32	31	30	3	17	50	15	54	8	24	59	12	5	20	57	47	46	1	4	36	19	14	9	38	22	6	45	13	41	23
49	58	21	51	15	48	50	43	16	33	42	26	20	36	5	9	57	31	60	13	3	27	56	46	38	12	22	52	34	45	18	59	10	29	53	14	47	25	40	39	44	11	8	41	30	24	37	6	1	7	4	28	35	55	54	23	17	2	32	19
50	49	59	22	51	16	46	33	44	14	21	40	26	10	34	6	58	55	32	28	11	4	39	57	47	13	35	20	53	60	43	19	8	15	27	54	41	48	23	12	37	45	31	9	42	7	25	38	2	1	5	56	29	36	18	52	24	17	3	30
51	20	50	60	47	49	14	15	33	45	26	22	41	7	8	35	30	59	56	2	29	12	48	37	55	11	54	36	21	17	58	44	9	52	16	28	24	42	46	43	13	38	40	32	10	39	5	23	6	3	1	34	57	27	25	19	53	31	18	4
52	19	20	38	23	30	15	57	58	29	36	47	55	53	7	60	44	26	2	3	54	48	5	33	40	18	45	59	10	6	37	49	24	46	42	11	31	4	51	25	43	35	41	17	27	34	12	22	32	56	39	1	14	21	13	50	8	9	28	16
53	39	17	21	16	24	31	27	55	59	56	34	48	58	54	5	3	45	26	46	4	52	41	6	33	19	8	43	60	50	7	38	25	12	47	40	49	32	2	36	23	44	28	42	18	20	35	13	37	30	57	22	1	15	9	11	51	14	10	29
54	22	37	18	32	14	25	60	28	56	46	57	35	6	59	52	26	4	43	53	47	2	33	42	7	17	58	9	44	39	51	5	23	41	13	48	3	50	30	45	34	24	19	29	40	11	21	36	55	38	31	16	20	1	49	10	12	27	15	8
55	27	47	31	59	36	38	19	52	23	24	17	53	48	32	28	12	51	8	35	37	58	10	11	50	57	2	16	41	40	4	15	56	44	20	6	21	7	45	30	29	46	60	34	39	42	3	14	54	25	18	9	13	49	1	33	26	22	5	43
56	32	28	48	39	60	34	24	17	53	54	25	18	29	46	30	9	13	49	59	36	38	51	8	12	55	42	3	14	16	41	2	57	7	45	21	43	22	5	47	31	27	37	58	35	15	40	4	19	52	23	50	10	11	26	1	33	44	20	6
57	46	30	29	35	37	58	54	25	18	19	52	23	31	27	47	50	10	11	39	60	34	13	49	9	56	15	40	4	3	14	42	55	22	5	43	6	44	20	28	48	32	36	38	59	2	16	41	24	17	53	12	51	8	33	26	1	7	45	21
58	57	42	15	29	25	49	18	48	43	30	20	52	55	4	41	46	8	45	12	32	53	28	50	6	39	51	23	5	11	54	21	36	35	34	33	38	37	26	56	16	3	10	47	19	17	44	9	7	24	27	13	22	31	14	40	2	1	60	59
59	16	55	40	50	27	23	44	19	46	53	31	21	42	56	2	43	47	9	54	13	30	7	29	51	37	6	49	24	22	12	52	34	33	36	35	26	39	38	4	57	14	17	8	48	10	18	45	28	5	25	32	11	20	3	15	41	60	1	58
60	41	14	56	24	51	28	47	45	17	22	54	32	3	40	57	10	44	48	31	52	11	49	5	27	38	25	7	50	53	20	13	35	36	33	34	39	26	37	15	2	55	46	18	9	43	8	19	23	29	6	21	30	12	42	4	16	59	58	1

Table 5. Generating Relations $G_aG_b = G_c$ for $A(5)$ and the Rotational Icosahedral Subgroup, $\mathscr{I}$, in Terms of $G_4 = C_5{}^k$ and $G_{46} = C_2{}^r$ Where r Makes an Angle of θ_4 to the z-Axis[a]

seq	a	b	c	seq	a	b	c	seq	a	b	c
1	4	4	19	20	46	27	29	39	27	12	53
2	4	19	23	21	46	59	11	40	27	14	49
3	4	23	6	22	46	50	2	41	27	22	20
4	46	19	3	23	46	26	28	42	3	27	16
5	46	23	12	24	46	10	54	43	22	27	18
6	46	6	44	25	4	57	35	44	9	27	39
7	19	46	8	26	4	2	13	45	2	2	17
8	23	46	5	27	44	44	40	46	2	29	15
9	6	46	37	28	19	3	36	47	4	18	32
10	3	46	14	29	19	12	55	48	19	17	33
11	12	46	22	30	19	44	31	49	19	18	41
12	44	46	9	31	19	14	21	50	2	18	43
13	4	3	7	32	19	22	42	51	2	11	45
14	4	12	27	33	19	9	30	52	2	38	47
15	4	44	59	34	19	7	52	53	2	25	48
16	4	14	50	35	19	27	38	54	2	15	51
17	4	22	26	36	19	50	34	55	2	28	56
18	4	9	10	37	19	26	25	56	2	57	58
19	46	7	57	38	27	3	24	57	2	45	60

[a] The relations are designed to be taken in the sequence indicated.

T_1. Since the third class consists of squares of elements in the second class, this indicates that the T_2 representation of G_4 can be taken to be the square of its T_1 representation, which is $[G_{19}]^{T_1}$. Since the characters of the fifth class are same for both T_1 and T_2, the T_2 representation of G_{46} can be any second-order matrix such that the product $[G_4]^{T_2}[G_{46}]^{T_2}$ is third order. From the multiplication table the products that yield elements in the third class are $G_{19}G_{47} = G_{43}$, $G_{19}G_{50} = G_{34}$, $G_{19}G_{53} = G_{45}$, and $G_{19}G_{54} = G_{26}$. Of these, the matrix $[G_{47}]^{T_1}$ has one of the simplest forms hence the choice $[G_{46}]^{T_2} = [G_{47}]^{T_1}$.

IV. THE G AND H IRREDUCIBLE REPRESENTATIONS

From Table 7, the direct product $T_1 \otimes T_1$ reduces to $A \oplus T_1 \oplus H$, and $T_1 \otimes T_2$ reduces to $G \oplus H$. Therefore, the appropriate coupling coefficients will block diagonalize $[G_a]^{T_1} \otimes [G_a]^{T_1}$ with the H irreducible representation as one of the blocks. Likewise, coupling coefficients will block diagonalize $[G_a]^{T_1} \otimes [G_a]^{T_2}$ with the G irreducible representation as one of the blocks. This reduction is accomplished by symmetry-adaptation through projection. Symmetry adaptation using e^{α}_{rr} is described in detail in the first article of this series; however, this approach must be modified here since, for example, the H irreducible representation is required to construct e^{H}_{rr}. Instead, the idempotent e^H is employed because it can be obtained from $E = e^{A_1} + e^{T_1} + e^{H}$. The e^{A}_{11} and $e^{T_1}_{rr}$ can be calculated, and the idempotents $e^A = e^{A}_{11}$ and $e^{T_1} = e^{T_1}_{11} + e^{T_1}_{22} + e^{T_1}_{33}$ follow directly.

***H*:** The matrix representation of the projector is then

$$[e^H]^{T_1\otimes T_1} = [E]^{T_1\otimes T_1} - [e^A]^{T_1\otimes T_1} - [e^{T_1}]^{T_1\otimes T_1} \quad (4.1)$$

This matrix is given in Table 8. Since the H irreducible representation occurs only once in this reduction, it is only necessary to select a linearly independent set of five columns of this matrix and normalize them. A number of choices are possible, each giving different forms for the representation. The selection used here are columns 1, 5, 2, 3, and 8 in that order. Since columns 1 and 5 are not orthogonal to each other, they are orthonormalized by the method described in the first article in this series. The coupling coefficients are displayed in Table 9. The first column is the normalized sum of columns 1 and 5, and the second is the normalized difference. Let this 9×5 matrix of coupling coefficients be W. Then the H irreducible representation is given by

$$[\tilde{W}]([G_a]^{T_1} \otimes [G_a]^{T_1})[W] = [G_a]^H \quad (4.2)$$

as displayed in Table 6.

***G*:** Having the H irreducible representation it is possible to construct the necessary projector:

$$[e^G]^{T_1\otimes T_2} = [E]^{T_1\otimes T_2} - [e^H]^{T_1\otimes T_2} \quad (4.3)$$

This matrix is given in Table 10. Since G occurs only once in $T_1 \otimes T_2$, only a linearly independent set of four normalized columns is required. Columns 3, 6, 7, and 8 are orthogonal to each other, hence linearly independent, and after normalization give the coupling coefficients displayed in Table 10. Let this 9×4 matrix of coupling coefficients be V. Then the G irreducible representation is given by

$$[\tilde{V}]([G_a]^{T_1} \otimes [G_a]^{T_2})[V] = [G_a]^G \quad (4.4)$$

as shown in Table 6.

V. C_{20} FULLERENE

A Hückel state space $V(\pi)$, of dimension $f(\pi)$ and invariant to the symmetry group, G, is spanned by a defining basis $B(\pi)$ of π-orbitals

$$V(\pi){:}B(\pi) = \{|\pi i\rangle,\ i = 1, ..., f(\pi)\} \quad (5.1)$$

that generates a reducible unitary representation $\Gamma(\omega)$ of G:

$$G_a|\pi i\rangle = \sum_{j}^{f(\pi)} [G_a]^{\pi}_{ji}|\pi j\rangle \quad (5.2)$$

The defining basis for the simple Hückel treatment of C_{20} fullerene is the 20-dimensional space of p_z orbitals perpendicular to the three sigma bonds at each carbon. The numbering is given in the Schlegel diagram in Figure 1. In this case, the effect of each of the rotations, reflections, and inversions of the icosahedral point group is to permute the defining basis elements among themselves. It is therefore convenient to represent the transformations by permutations. For a permutation given by the vector representation $P_a = \{a_1, a_2, ..., a_n\}$, the corresponding matrix representation is

$$[P_a]_{ij} = \delta(i,a_j) \quad (5.3)$$

i.e., if $a_j = i$ then $[P_a]_{ij} = 1$, otherwise $[P_a]_{ij} = 0$. With this convention, the operators in (1.5) become

$$[e^{\alpha}_{rs}]^{\pi}_{ij} = \frac{f(\alpha)}{g}\sum_{a}^{g}[G_a^{-1}]^{\alpha}_{sr}\delta(i,a_j) \quad (5.4)$$

The permutations corresponding to the three icosahedral generators are given in Table 12, and the characters are listed

Table 6. Irreducible Representation Matrices for the Generators G_4 and G_{46}

α	$[G_4]^\alpha = [C_5^k]^\alpha$	$[G_{46}]^\alpha = [C_2^r]^\alpha$
A	$[1]$	$[1]$
T_1	$\begin{bmatrix} \cos(72) & -\sin(72) & 0 \\ \sin(72) & \cos(72) & 0 \\ 0 & 0 & 1 \end{bmatrix}$	$\begin{bmatrix} -1/\sqrt{5} & 0 & 2/\sqrt{5} \\ 0 & -1 & 0 \\ 2/\sqrt{5} & 0 & 1/\sqrt{5} \end{bmatrix}$
T_2	$\begin{bmatrix} \cos(144) & -\sin(144) & 0 \\ \sin(144) & \cos(144) & 0 \\ 0 & 0 & 1 \end{bmatrix}$	$\begin{bmatrix} 1/\sqrt{5} & 0 & -2/\sqrt{5} \\ 0 & -1 & 0 \\ -2/\sqrt{5} & 0 & -1/\sqrt{5} \end{bmatrix}$
G	$\begin{bmatrix} \cos(72) & -\sin(72) & 0 & 0 \\ \sin(72) & \cos(72) & 0 & 0 \\ 0 & 0 & \cos(144) & -\sin(144) \\ 0 & 0 & \sin(144) & \cos(144) \end{bmatrix}$	$\begin{bmatrix} 0 & 0 & -1 & 0 \\ 0 & 2/\sqrt{5} & 0 & 1/\sqrt{5} \\ -1 & 0 & 0 & 0 \\ 0 & 1/\sqrt{5} & 0 & -2/\sqrt{5} \end{bmatrix}$
H	$\begin{bmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & \cos(144) & -\sin(144) & 0 & 0 \\ 0 & \sin(144) & \cos(144) & 0 & 0 \\ 0 & 0 & 0 & \cos(72) & -\sin(72) \\ 0 & 0 & 0 & \sin(72) & \cos(72) \end{bmatrix}$	$\begin{bmatrix} -1/5 & 2\sqrt{3}/5 & 0 & 2\sqrt{3}/5 & 0 \\ 2\sqrt{3}/5 & 3/5 & 0 & -2/5 & 0 \\ 0 & 0 & 1/\sqrt{5} & 0 & -2/\sqrt{5} \\ 2\sqrt{3}/5 & -2/5 & 0 & 3/5 & 0 \\ 0 & 0 & -2/\sqrt{5} & 0 & -1/\sqrt{5} \end{bmatrix}$

Table 7. Reductions of Direct Products of Irreducible Representations of $\mathscr{I}_h$

A	T_1	T_2	G	H
T_1	$A + T_1 + H$	$G + H$	$T_2 + G + H$	$T_1 + T_2 + G + H$
T_2	$G + H$	$A + T_2 + H$	$T_1 + G + H$	$T_1 + T_2 + G + H$
G	$T_2 + G + H$	$T_1 + G + H$	$A + T_1 + T_2 + G + H$	$T_1 + T_2 + G + 2H$
H	$T_1 + T_2 + G + H$	$T_1 + T_2 + G + H$	$T_1 + T_2 + G + 2H$	$A + T_1 + T_2 + 2G + 2H$

Table 8. Matrix Representation $[e^H]^{T_1 \otimes T_1}$ of Projection Operator e^H

2/3	0	0	0	−1/3	0	0	0	−1/3
0	1/2	0	1/2	0	0	0	0	0
0	0	1/2	0	0	0	1/2	0	0
0	1/2	0	1/2	0	0	0	0	0
−1/3	0	0	0	2/3	0	0	0	−1/3
0	0	0	0	0	1/2	0	1/2	0
0	0	1/2	0	0	0	1/2	0	0
0	0	0	0	0	1/2	0	1/2	0
−1/3	0	0	0	−1/3	0	0	0	2/3

Table 9. Coupling Coefficients To Project H from $T_1 \otimes T_1$

$T_1 \otimes T_1$	$H1$	$H2$	$H3$	$H4$	$H5$
11	$1/\sqrt{6}$	$1/\sqrt{2}$	0	0	0
12	0	0	$1/\sqrt{2}$	0	0
13	0	0	0	$1/\sqrt{2}$	0
21	0	0	$1/\sqrt{2}$	0	0
22	$1/\sqrt{6}$	$-1/\sqrt{2}$	0	0	0
23	0	0	0	0	$1/\sqrt{2}$
31	0	0	0	$1/\sqrt{2}$	0
32	0	0	0	0	$1/\sqrt{2}$
33	$-2/\sqrt{6}$	0	0	0	0

in the bottom row of Table 1. Apart from the identity, the only nonzero characters for C_{20} occur for the C_3 rotations and the reflections. The reduction frequencies for C_{20} calculated from the character formula (1.2) are

$$C_{20}{:}A_g \oplus G_g \oplus H_g \oplus T_{1u} \oplus T_{2u} \oplus G_u \tag{5.5}$$

Table 10. Matrix Representation $[e^G]^{T_1 \otimes T_2}$ of Projection Operator e^G

1/3	0	−1/3	0	0	0	−1/3	0	0
0	1/3	0	0	0	−1/3	0	1/3	0
−1/3	0	2/3	0	−1/3	0	0	0	0
0	0	0	1/3	0	1/3	0	1/3	0
0	0	−1/3	0	1/3	0	1/3	0	0
0	−1/3	0	1/3	0	2/3	0	0	0
−1/3	0	0	0	1/3	0	2/3	0	0
0	1/3	0	1/3	0	0	0	2/3	0
0	0	0	0	0	0	0	0	0

Since none of the frequencies is greater than one, the solution is completely symmetry determined, and the eigenvalues are given by the reduced matrix elements:

$$\begin{aligned} E(\alpha) &= \langle \alpha || H || \alpha \rangle \\ &= \langle \alpha 1 | H | \alpha 1 \rangle \\ &= \sum_{i=1}^{f(\alpha)} \sum_{j=1}^{f(a)} \langle \alpha 1 | \pi i \rangle \langle \pi i | H | \pi j \rangle \langle \pi j | \alpha 1 \rangle \end{aligned} \tag{5.6}$$

where the matrix $\langle \pi i | H | \pi j \rangle$ is

$$[H]^\pi = \alpha [I]^\pi + \boldsymbol{\beta} [A]^\pi \tag{5.7}$$

Here $\boldsymbol{\alpha}$ and $\boldsymbol{\beta}$ are the conventional Hückel parameters, while $[I]^\pi$ and $[A]^\pi$ are the identity and C_{20} adjacency matrices, respectively. The adjacency matrix, $[A]^\pi$, follows from the Schlegel diagram in Figure 1. The transformation coefficients

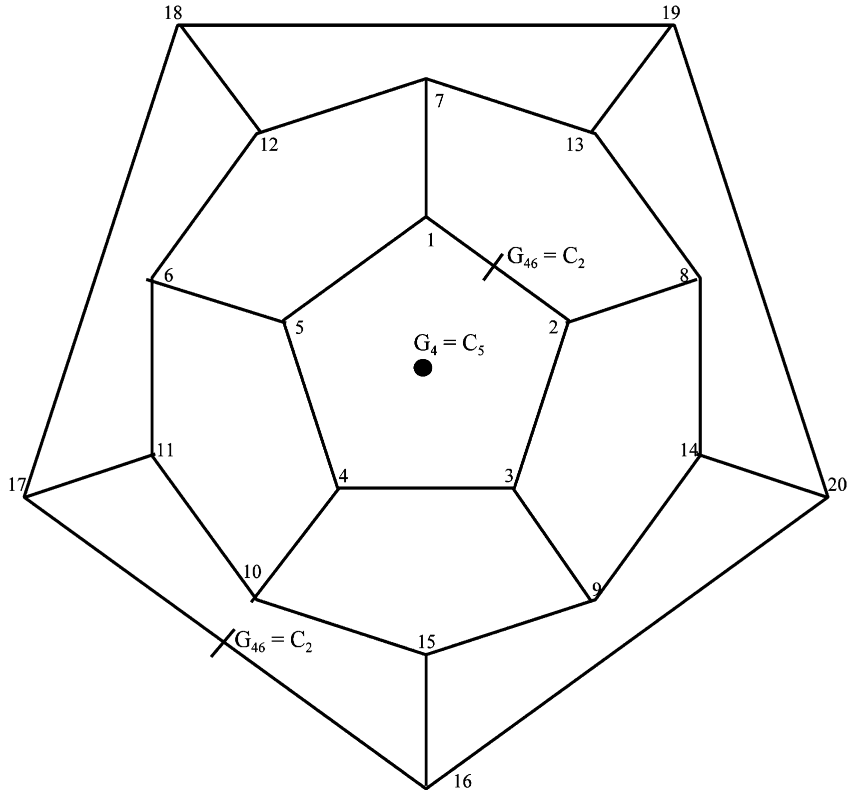

Figure 1. Schlegel diagram of icosahedral C_{20} fullerene. The axis of the $G_4 = C_5$ generator is indicated in the center of the central pentagon. The end points of the $G_{42} = C_2$ generator axis are shown at midpoints of the 1,2 and 16,17 bonds.

Table 11. Coupling Coefficients To Project G from $T_1 \otimes T_2$

$T_1 \otimes T_2$	$G1$	$G2$	$G3$	$G4$
11	$-1/\sqrt{6}$	0	$-1/\sqrt{6}$	0
12	0	$-1/\sqrt{6}$	0	$1/\sqrt{6}$
13	$2/\sqrt{6}$	0	0	0
21	0	$1/\sqrt{6}$	0	$1/\sqrt{6}$
22	$-1/\sqrt{6}$	0	$1/\sqrt{6}$	0
23	0	$2/\sqrt{6}$	0	0
31	0	0	$2/\sqrt{6}$	0
32	0	0	0	$2/\sqrt{6}$
33	0	0	0	0

Table 12. Permutational Representations in Vector Array Form of Generators G_4 and G_{46} of $\mathscr{I}$ and Inversion, G_{61}, Generated on C_{20} Fullerene as Numbered in Figure 1

G_4

5	1	2	3	4	10	6	7	8	9	15	11	12	13	14	20	16	17	18	19

G_{46}

2	1	7	13	8	14	3	5	12	19	20	9	4	6	18	17	16	15	10	11

G_{61}

16	17	18	19	20	14	15	11	12	13	8	9	10	6	7	1	2	3	4	5

in (5.6) are obtained from any nonzero column, j, of the matrix $[e_{11}^{\alpha}]^{\pi}$ according to

$$\langle \pi i | \alpha 1 \rangle = \frac{[e_{11}^{\alpha}]_{ij}^{\pi}}{\sqrt{[e_{11}^{\alpha}]_{jj}^{\pi}}} \tag{5.8}$$

Note that for this Hermitian, idempotent matrix, the element $[e_{11}^{\alpha}]_{jj}^{\pi}$ is the sum of squares of the elements in the jth column. Evidently, only one of the diagonal matrix elements of H on the symmetry-adapted basis is required for each of the six representations in (5.5) so that only a single nonzero column of each of the corresponding six matrices $[e_{11}^{\alpha}]^{\pi}$ must be calculated. As an example, the first column of the matrix $[e_{11}^{G_g}]^{\pi}$, multiplied by $g = 120$, is displayed in Table 13 with corresponding normalized transformation coefficients. The corresponding energy is

$$\langle G_g 1 | H | G_g 1 \rangle = \mathrm{E}(G_g) = \boldsymbol{\alpha} - 2.00\,\boldsymbol{\beta} \tag{5.9}$$

The rest of the eigenvalues are given in Table 14.

Table 13. First Column of Matrix $[e_{11}^{G_g}]^{\pi}$ (Center) and Corresponding Normalized Transformation Coefficients (Right)

	$120 \times [e_{11}^{G_g}]_{i1}^{\pi}$	$\langle \pi i | G_g 1 \rangle$
$\pi 1$	2.0000	0.12910
$\pi 2$	2.0000	0.12910
$\pi 3$	−0.76393	−0.049312
$\pi 4$	−2.4721	−0.15958
$\pi 5$	−0.76393	−0.049312
$\pi 6$	2.0000	0.12910
$\pi 7$	−5.2361	−0.33799
$\pi 8$	−5.2361	−0.33799
$\pi 9$	2.0000	0.12910
$\pi 10$	6.4721	0.41778
$\pi 11$	−5.2361	−0.33799
$\pi 12$	2.0000	0.12910
$\pi 13$	6.4721	0.41778
$\pi 14$	2.0000	0.12910
$\pi 15$	−5.2361	−0.33799
$\pi 16$	2.0000	0.12910
$\pi 17$	2.0000	0.12910
$\pi 18$	−0.76393	−0.049312
$\pi 19$	−2.4721	−0.15958
$\pi 20$	−0.76393	−0.049312

Table 14. Hückel Molecular Orbital Energies for C_{20}

I.R.	energy
T_{2u}	$\alpha - 2.236\beta$
G_g	$\alpha - 2.000\beta$
G_u	$\alpha + 0.000\beta$
H_g	$\alpha + 1.000\beta$
T_{1u}	$\alpha + 2.236\beta$
A_g	$\alpha + 3.000\beta$

VI. CONCLUSION

These generating relations and irreducible representations are suitable for computerized symmetry-adaptation to the icosahedral point group of any chemical system for which representations of the generators can be obtained. Although the C_{20} Hückel example is limited in that no irreducible representation occurs more than once, symmetry-adaptation for frequencies greater than one have been treated at length by this author in the first article in this series.

The next article in this series treats the Symmetry-Generation Theorem for large systems.[16] Using this theorem the reduced matrix elements of the Hamiltonian are determined from a simple generating matrix instead of the complete Hamiltonian matrix, thereby providing computational savings that increase with the size of the basis and corresponding matrix.

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