Unit Subduced Cycle Indices with and without Chirality Fittingness for I_h Group. An Application to Systematic Enumeration of Dodecahedrane Derivatives

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Subduction of the coset representations of $\mathbf{I}_h$ point group produces tables of unit subduced cycle indices (USCIs) with and without chirality fittingness (CF). These indices are applied to the enumeration of dodecahedrane derivatives with respect to their molecular formulas as well as to their symmetries. The USCIs are effective to the enumeration of such derivatives as having only achiral substituents on the vertices of a dodecahedrane skeleton. On the other hand, the USCI-CFs are used for enumerating dodecahedrane derivatives with achiral and chiral substituents. Substitutions on the edges of the dodecahedrane skeleton are also discussed in terms of the present USCI approach.

Compounds of $\mathbf{I}_h$ symmetry have attracted attention of organic and inorganic chemists because of experimental and theoretical interest. Among them, dodecahedrane ($C_{20}H_{20}$), which was pointed out as a synthetic target by Kawai[1] and later by Woodward,[2], has been thoroughly investigated and recently successfully resolved by Paquette.[3] Before and after this successful synthetic elaboration, there emerged a vast number of experimental[4,5,6] and theoretical works[7] on dodecahedrane and its derivatives. Symmetrical properties of dodecahedrane have been studied by X-ray crystallographic determlnation.[8]

Total numbers of derivatives for mono to tetrasubstituted dodecahedranes have been obtained by using the Pólya-Redfield theorem.[9,10] Brocas[11] has presented a systematic enumeration of dodecahedrane derivatives, which is based on double cosets and framework groups. Hässelbarth[12] has reported an alternative method that is based on tables of marks. This method is capable of enumerating derivatives with respect to molecular formulas as well as to their symmetries and can be applied to the enumeration of dodecahedrane isomers. Mead[13] has presented an alternative method and compared these methods by using common problems.

We have reported a systematic enumeration of chemical structures in terms of unit subduced cycle indices (USCIs).[14] This method is based on an integration of point-group and permutation-group theories. The key concepts of this approach are an orbit governed by a coset representation (CR) and the subduction of such CRs. Advantages of this method, however, have not yet been proved, since tables of USCIs have been constructed only for $\mathbf{D}_2$, $\mathbf{D}_3$, $\mathbf{D}_{2h}$, $\mathbf{D}_{3h}$, $\mathbf{T}$, and $\mathbf{T}_d$. The present paper deals with a general, method of enumerating chemical structures derived from a dodecahedrane skeleton ($\mathbf{I}_h$) for the purpose of emphasizing the advantages of the USCI approach.

Results and Discussion

Table of Marks for $\mathbf{I}_h$ Point Group. We introduce the symbol $(\mathbf{G}(/\mathbf{G}_i))$ for denoting a coset representation determined by a group $\mathbf{G}$ and its subgroup $\mathbf{G}_i$.[14] Any permutation group is reduced into a sum of several coset representations. This reduction can be accomplished by using a table of marks that can go back to Burnside.[15] However, such tables have been reported only for a restricted number of point groups.[12,13,16]

The $\mathbf{I}_h$ group of order 120 posesses a set of subgroups, SSG={$\mathbf{C}_1$, $\mathbf{C}_2$, $\mathbf{C}_s$, $\mathbf{C}_i$, $\mathbf{C}_3$, $\mathbf{D}_2$, $\mathbf{C}_{2v}$, $\mathbf{C}_{2h}$, $\mathbf{C}_5$, $\mathbf{D}_3$, $\mathbf{C}_{3v}$, $\mathbf{C}_{3i}$, $\mathbf{D}_{2h}$, $\mathbf{D}_5$, $\mathbf{C}_{5v}$, $\mathbf{C}_{5i}$, $\mathbf{T}$, $\mathbf{D}_{3d}$, $\mathbf{D}_{5d}$, $\mathbf{T}_h$, $\mathbf{I}$, $\mathbf{I}_h$}. We constructed the table of marks for $\mathbf{I}_h$ point group (Table 1) by (a) obtaining a multiplication table of $\mathbf{I}$ group that is isomorphic to the alternating group of degree 5, (b) extending this table to that of the $\mathbf{I}_h$ group in terms of $\mathbf{I}_h=\mathbf{I}\otimes\mathbf{C}_s$, (c) providing a coset decomposition of each subgroup, (d) obtaining the corresponding coset representation (CR), and (e) counting fixed points in the CR with respect to every subgroup. This algorithm was programed with FORTRAN 77 and executed on a VAX-11/750 computer.[17] We then obtained the inverse of the mark table (Table 2).

Orbits of Vertices, Bonds and Faces in Dodecahedrane. Dodecahedrane has 20 vertices (CH groups), 30 C-C bonds, and 12 pentagonal faces. They respectively construct equivalence classes. These classes are called *orbits* in accord with the terminology of permutation group. Symmetry properties of each orbit is characterized by the corresponding coset representation (CR), which is determined by using a table of marks. An algorithm of the determination consists of (a) selection of a set of equivalent positions (vertices, bonds, or faces), (b) counting points (positions) fixed on symmetry operations of every subgroup in the order of the SSG, and (c) compare the resulting fixed-point vector (FPV) with every row of the table of marks. Then the row identical with the FPV indicates the CR.

For illustrating this procedure, let us examine dodecahedrane (**1**). When we count fixed objects (vertices, etc) on all the symmetry operations of a subgroup, we obtain a fixed-point vector (FPV). For example, the examination of the 20 vertices affords an FPV=(20 0 4 0 2 0 0 0 0 0 2 0 0 0 0 0 0 0 0 0 0 0), which is collected in

Table 1. The Mark Table of $\mathbf{I}_h$ Group

	$\mathbf{C}_1$	$\mathbf{C}_2$	$\mathbf{C}_s$	$\mathbf{C}_i$	$\mathbf{C}_3$	$\mathbf{D}_2$	$\mathbf{C}_{2v}$	$\mathbf{C}_{2h}$	$\mathbf{C}_5$	$\mathbf{D}_3$	$\mathbf{C}_{3v}$	$\mathbf{C}_{3i}$	$\mathbf{D}_{2h}$	$\mathbf{D}_5$	$\mathbf{C}_{5v}$	$\mathbf{C}_{5i}$	$\mathbf{T}$	$\mathbf{D}_{3d}$	$\mathbf{D}_{5d}$	$\mathbf{T}_h$	$\mathbf{I}$	$\mathbf{I}_h$
$\mathbf{I}_h(/\mathbf{C}_1)$	120	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
$\mathbf{I}_h(/\mathbf{C}_2)$	60	4	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
$\mathbf{I}_h(/\mathbf{C}_s)$	60	0	4	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
$\mathbf{I}_h(/\mathbf{C}_i)$	60	0	0	60	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
$\mathbf{I}_h(/\mathbf{C}_3)$	40	0	0	0	4	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
$\mathbf{I}_h(/\mathbf{D}_2)$	30	6	0	0	0	6	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
$\mathbf{I}_h(/\mathbf{C}_{2v})$	30	2	4	0	0	0	2	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
$\mathbf{I}_h(/\mathbf{C}_{2h})$	30	2	2	30	0	0	0	2	0	0	0	0	0	0	0	0	0	0	0	0	0	0
$\mathbf{I}_h(/\mathbf{C}_5)$	24	0	0	0	0	0	0	0	4	0	0	0	0	0	0	0	0	0	0	0	0	0
$\mathbf{I}_h(/\mathbf{D}_3)$	20	4	0	0	2	0	0	0	0	2	0	0	0	0	0	0	0	0	0	0	0	0
$\mathbf{I}_h(/\mathbf{C}_{3v})$	20	0	4	0	2	0	0	0	0	0	2	0	0	0	0	0	0	0	0	0	0	0
$\mathbf{I}_h(/\mathbf{C}_{3i})$	20	0	0	20	2	0	0	0	0	0	0	2	0	0	0	0	0	0	0	0	0	0
$\mathbf{I}_h(/\mathbf{D}_{2h})$	15	3	3	15	0	3	3	3	0	0	0	0	3	0	0	0	0	0	0	0	0	0
$\mathbf{I}_h(/\mathbf{D}_5)$	12	4	0	0	0	0	0	0	2	0	0	0	0	2	0	0	0	0	0	0	0	0
$\mathbf{I}_h(/\mathbf{C}_{5v})$	12	0	4	0	0	0	0	0	2	0	0	0	0	0	2	0	0	0	0	0	0	0
$\mathbf{I}_h(/\mathbf{C}_{5i})$	12	0	0	12	0	0	0	0	2	0	0	0	0	0	0	2	0	0	0	0	0	0
$\mathbf{I}_h(/\mathbf{T})$	10	2	0	0	4	2	0	0	0	0	0	0	0	0	0	0	2	0	0	0	0	0
$\mathbf{I}_h(/\mathbf{D}_{3d})$	10	2	2	10	1	0	0	2	0	1	1	1	0	0	0	0	0	1	0	0	0	0
$\mathbf{I}_h(/\mathbf{D}_{5d})$	6	2	2	6	0	0	0	2	1	0	0	0	0	1	1	1	0	0	1	0	0	0
$\mathbf{I}_h(/\mathbf{T}_h)$	5	1	1	5	2	1	1	1	0	0	0	2	1	0	0	0	1	0	0	1	0	0
$\mathbf{I}_h(/\mathbf{I})$	2	2	0	0	2	2	0	0	2	2	0	0	0	2	0	0	2	0	0	0	2	0
$\mathbf{I}_h(/\mathbf{I}_h)$	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1

Table 2. The Inverse of the Mark Table of $\mathbf{I}_h$ Group

	Coset representation[a)]																						
	$\mathbf{C}_1$	$\mathbf{C}_2$	$\mathbf{C}_s$	$\mathbf{C}_i$	$\mathbf{C}_3$	$\mathbf{D}_2$	$\mathbf{C}_{2v}$	$\mathbf{C}_{2h}$	$\mathbf{C}_5$	$\mathbf{D}_3$	$\mathbf{C}_{3v}$	$\mathbf{C}_{3i}$	$\mathbf{D}_{2h}$	$\mathbf{D}_5$	$\mathbf{C}_{5v}$	$\mathbf{C}_{5i}$	$\mathbf{T}$	$\mathbf{D}_{3d}$	$\mathbf{D}_{5d}$	$\mathbf{T}_h$	$\mathbf{I}$	$\mathbf{I}_h$	Sum[b)]
$\mathbf{C}_1$	$\frac{1}{120}$	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	$\frac{1}{120}$
$\mathbf{C}_2$	$-\frac{1}{8}$	$\frac{1}{4}$	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	$\frac{1}{8}$
$\mathbf{C}_s$	$-\frac{1}{8}$	0	$\frac{1}{4}$	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	$\frac{1}{8}$
$\mathbf{C}_i$	$-\frac{1}{120}$	0	0	$\frac{1}{60}$	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	$\frac{1}{120}$
$\mathbf{C}_3$	$-\frac{1}{12}$	0	0	0	$\frac{1}{4}$	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	$\frac{1}{6}$
$\mathbf{D}_2$	$\frac{1}{12}$	$-\frac{1}{4}$	0	0	0	$\frac{1}{6}$	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
$\mathbf{C}_{2v}$	$\frac{1}{4}$	$-\frac{1}{4}$	$-\frac{1}{2}$	0	0	0	$\frac{1}{2}$	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
$\mathbf{C}_{2h}$	$\frac{1}{4}$	$-\frac{1}{4}$	$-\frac{1}{4}$	$-\frac{1}{4}$	0	0	0	$\frac{1}{2}$	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
$\mathbf{C}_5$	$-\frac{1}{20}$	0	0	0	0	0	0	0	$\frac{1}{4}$	0	0	0	0	0	0	0	0	0	0	0	0	0	$\frac{1}{5}$
$\mathbf{D}_3$	$\frac{1}{4}$	$-\frac{1}{2}$	0	0	$-\frac{1}{4}$	0	0	0	0	$\frac{1}{2}$	0	0	0	0	0	0	0	0	0	0	0	0	0
$\mathbf{C}_{3v}$	$\frac{1}{4}$	0	$-\frac{1}{2}$	0	$-\frac{1}{4}$	0	0	0	0	0	$\frac{1}{2}$	0	0	0	0	0	0	0	0	0	0	0	0
$\mathbf{C}_{3i}$	$\frac{1}{12}$	0	0	$-\frac{1}{6}$	$-\frac{1}{4}$	0	0	0	0	0	0	$\frac{1}{2}$	0	0	0	0	0	0	0	0	0	0	$\frac{1}{6}$
$\mathbf{D}_{2h}$	$-\frac{1}{3}$	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{6}$	0	$-\frac{1}{6}$	$-\frac{1}{2}$	$-\frac{1}{2}$	0	0	0	0	$\frac{1}{3}$	0	0	0	0	0	0	0	0	0	0
$\mathbf{D}_5$	$\frac{1}{4}$	$-\frac{1}{2}$	0	0	0	0	0	0	$-\frac{1}{4}$	0	0	0	0	$\frac{1}{2}$	0	0	0	0	0	0	0	0	0
$\mathbf{C}_{5v}$	$\frac{1}{4}$	0	$-\frac{1}{2}$	0	0	0	0	0	$-\frac{1}{4}$	0	0	0	0	0	$\frac{1}{2}$	0	0	0	0	0	0	0	0
$\mathbf{C}_{5i}$	$\frac{1}{20}$	0	0	$-\frac{1}{10}$	0	0	0	0	$-\frac{1}{4}$	0	0	0	0	0	0	$\frac{1}{2}$	0	0	0	0	0	0	$\frac{1}{5}$
$\mathbf{T}$	$\frac{1}{6}$	0	0	0	$-\frac{1}{2}$	$-\frac{1}{6}$	0	0	0	0	0	0	0	0	0	0	$\frac{1}{2}$	0	0	0	0	0	0
$\mathbf{D}_{3d}$	$-\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$	0	0	-1	0	$-\frac{1}{2}$	$-\frac{1}{2}$	$-\frac{1}{2}$	0	0	0	0	0	1	0	0	0	0	0
$\mathbf{D}_{5d}$	$-\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$	0	0	0	-1	$\frac{1}{2}$	0	0	0	0	$-\frac{1}{2}$	$-\frac{1}{2}$	$-\frac{1}{2}$	0	0	1	0	0	0	0
$\mathbf{T}_h$	$-\frac{1}{6}$	0	0	$\frac{1}{3}$	$\frac{1}{2}$	$\frac{1}{6}$	0	0	0	0	0	-1	$-\frac{1}{3}$	0	0	0	$-\frac{1}{2}$	0	0	1	0	0	0
$\mathbf{I}$	$-\frac{1}{2}$	1	0	0	$\frac{1}{2}$	0	0	0	0	$-\frac{1}{2}$	0	0	0	$-\frac{1}{2}$	0	0	$-\frac{1}{2}$	0	0	0	$\frac{1}{2}$	0	0
$\mathbf{I}_h$	$\frac{1}{2}$	-1	0	-1	$-\frac{1}{2}$	0	0	2	0	$\frac{1}{2}$	0	1	0	$\frac{1}{2}$	0	0	$\frac{1}{2}$	-1	-1	-1	$-\frac{1}{2}$	1	0

a) The symbol $\mathbf{G}_i$ is an abbreviation of $\mathbf{I}_h(/\mathbf{G}_i)$, where $\mathbf{G}_1=\mathbf{C}_1$, $\mathbf{G}_2=\mathbf{C}_2,\cdots,\mathbf{G}_s=\mathbf{I}_h$. For example, we here use $\mathbf{C}_2$ for $\mathbf{I}_h(/\mathbf{C}_2)$. b) Sum$=\sum_{i=1}^{s}\overline{m}_{ji}$.

the order of the above SSG. This vector is identical with the $\mathbf{I}_h(/\mathbf{C}_{3v})$ row of Table 1. Hence, we conclude that the 20 methines are subject to the coset representation ($\mathbf{I}_h(/\mathbf{C}_{3v})$). In a similar way, the set of 30 bonds is concluded to be subject to the CR ($\mathbf{I}_h(/\mathbf{C}_{2v})$), while the set of 12 faces is shown to belong to $\mathbf{I}_h(/\mathbf{C}_{5v})$.

In general, the substitution positions (Δ) of a parent skeleton are classified into $\sum_{i=1}^{s}\alpha_i$ orbits ($\Delta_{i\alpha}$) each of which is subject to a CR ($\mathbf{G}(/\mathbf{G}_i)$). Here, the nonnegative integer (α_i) is the multiplicity of the CR.

Construction of a Table of Unit Subduced Cycle Indices for $\mathbf{I_h}$ Group. Let $\mathbf{G}$ be a finite group. Suppose that the group $\mathbf{G}$ has an SSG=$\{\mathbf{G}_1, \mathbf{G}_2, ..., \mathbf{G}_s\}$. Since a subduced representation ($\mathbf{G}(/\mathbf{G}_i)\downarrow\mathbf{G}_j$) is intransitive in general, this can be reduced into a sum of coset representations of $\mathbf{G}_j$ in terms of

$$\mathbf{G}(/\mathbf{G}_i)\downarrow\mathbf{G}_j=\sum_{k=1}^{v_j}\beta_k^{(ij)}\mathbf{G}_j(/\mathbf{G}_k^{(j)}), \quad (1)$$

for i=1, 2, ..., s and j=1,2, ..., s, wherein a set of subgroups of $\mathbf{G}_j$ is represented by SSG$_j$=$\{\mathbf{G}_1^{(j)}, \mathbf{G}_2^{(j)}, ..., \mathbf{G}_{v_j}^{(j)}\}$. The multiplicities ($\beta_k^{(ij)}$) are obtained by solving the following equations:

$$\nu_l=\sum_{k=1}^{v_j}\beta_k^{(ij)}m_{kl}^{(j)} \quad (2)$$

for l=1, 2, ..., v_j, where ν_l is the mark of $\mathbf{G}_l^{(j)}$ in $\mathbf{G}(/\mathbf{G}_i)\downarrow\mathbf{G}_j$.[14]

Equation 1 indicates a division of an orbit ($\Delta_{i\alpha}$) into several suborbits ($\Delta_{k\beta}^{(i\alpha)}$ for k=1, 2, ..., v_j and β=1, 2, ..., $\beta_k^{(ij)}$), each of which is subject to $\mathbf{G}_j(/\mathbf{G}_k^{(j)})$. Since the length of the suborbit ($\Delta_{k\beta}^{(i\alpha)}$) is represented by $d_{jk}=|\mathbf{G}_j|/|\mathbf{G}_k^{(j)}|$, we define a *unit subduced cycle indes with chirality fittingness* (USCI-CF) by

$$Z(\mathbf{G}(/\mathbf{G}_i)\downarrow\mathbf{G}_j;\ \$_{d_{jk}}^{(i\alpha)})=\prod_{k=1}^{v_j}(\$_{d_{jk}}^{(i\alpha)})^{\beta_k^{(ij)}}, \quad (3)$$

for each action of $\mathbf{G}(/\mathbf{G}_i)\downarrow\mathbf{G}_j$ on $\Delta_{i\alpha}$. The superscript ($i\alpha$) corresponds to the orbit ($\Delta_{i\alpha}$) that is subject to $\mathbf{G}(/\mathbf{G}_i)\downarrow\mathbf{G}_j$. The symbol ($\$$) represents a for an achiral part in which $\mathbf{G}_j$ is an achiral point group and $\mathbf{G}_k^{(j)}$ is also an achiral point group; b for a neutral part in which $\mathbf{G}_j$ is a chiral point group and $\mathbf{G}_k^{(j)}$ is also a chiral point group; or c in a chiral part in which $\mathbf{G}_j$ is an a chiral point group and $\mathbf{G}_k^{(j)}$ is a chiral point group.[18] for example, the subduction represented by

$$\mathbf{I}_h(/\mathbf{C}_{3v})\downarrow\mathbf{C}_s=4\mathbf{C}_s(/\mathbf{C}_s)+8\mathbf{C}_s(/\mathbf{C}_1) \quad (4)$$

affords a USCI ($a_1^4c_2^8$) in which a_1^4 corresponds to the achiral part ($4\mathbf{C}_s(/\mathbf{C}_s)$) and c_2^8 stems from the chiral part ($8\mathbf{C}_s(/\mathbf{C}_1)$). Note that the degree of $\mathbf{C}_s(/\mathbf{C}_s)$ is equal to 1, since this is an identity representation and that the CR ($\mathbf{C}_s(/\mathbf{C}_1)$) has a degree of 2 ($=|\mathbf{C}_s|/|\mathbf{C}_1|$).

When we substitute s for $\$$ for all the cases, we can obtain a *unit subduced cycle index* (USCI), i.e.,

$$Z(\mathbf{G}(/\mathbf{G}_i)\downarrow\mathbf{G}_j;\ s_{d_{jk}}^{(i\alpha)})=\prod_{k=1}^{v_j}s_{d_{jk}}^{(i\alpha)})^{\beta_k^{(ij)}}, \quad (5)$$

for each action of $\mathbf{G}(/\mathbf{G}_i)\downarrow\mathbf{G}_j$ on $\Delta_{i\alpha}$.

We calculated USCIs for the $\mathbf{I}_h$ point group (Table 3). The algorithm of this calculation consists of (a) subducing each CR (see above) to every subgroup, (b) calculating an FPV for the subgroup, (c) multiplying the FPV by the inverse of the table of marks for the subgroup to give multiplicities in the form of a row vector, ($\beta_1^{(ij)}$, $\beta_2^{(ij)}$, ..., $\beta_{v_j}^{(ij)}$), and (d) introducing them into Eqs. 3 and 5. This algorithm was programed with FORTRAN 77 and executed on a VAX-11/750 computer. Table 3 contains only USCI-CFs. The corresponding USCIs are easily obtained by substituting a variable (s) for every a, b, and c.

Dodecahedrane Derivatives with Achiral Substituents. A *subduced cycle index* (SCI) for every subgroup is defined as a product of USCIs over all participating orbits ($\Delta_{i\alpha}$).[14] This is expressed by

$$ZI(\mathbf{G}_j;\ s_{d_{jk}}^{(i\alpha)})=\prod_{i=1}^{s}\prod_{\alpha}Z(\mathbf{G}(/\mathbf{G}_i)\downarrow\mathbf{G}_j;\ s_{d_{jk}}^{(i\alpha)}) \quad (6)$$

for j=1,2, ..., s. Suppose that we select $|\Delta|$ of substituents from a set represented by $\mathbf{X}=\{X_1, X_2, ..., X_{|\mathbf{X}|}\}$. In order to obtain a generating function for an FPV, the $s_{d_{jk}}^{(i\alpha)}$ term is replaced by a figure-inventory which is defined as

$$s_{d_{jk}}^{(i\alpha)}=\sum_{r=1}^{|\mathbf{X}|}w_{i\alpha}(X_r)^{d_{jk}}, \quad (7)$$

where $w_{i\alpha}(X_r)^{d_{jk}}$ denotes the weight of the X_r substituent.

In order to enumerate isomers of fixed symmetry for substituted dodecahedranes with $C_{20}H_{20-p-q}X_pY_q$, we first constructed such SCIs for yielding generating functions. Since the vertices of the dodecahedrane skeleton belong to a single orbit governed by $\mathbf{I}_h(/\mathbf{C}_{3v})$, we adopted the $\mathbf{I}_h(/\mathbf{C}_{3v})$ row of Table 3 to generate the SCIs for this case. A figure inventory was selected as being

$$s_d=1+x^d+y^d, \quad (8)$$

where x and y are weights for counting X- and Y-substitutions. This was introduced into the SCIs to provide the following generating functions,

$$s_1^{20}=(1+x+y)^{20} \text{ for } \mathbf{C}_1, \quad (9)$$

$$s_2^{10}=(1+x^2+y^2)^{10} \text{ for } \mathbf{C}_2, \quad (10)$$

$$s_1^4s_2^8=(1+x+y)^4(1+x^2+y^2)^8 \text{ for } \mathbf{C}_s, \quad (11)$$

$$s_2^{10}=(1+x^2+y^2)^{10} \text{ for } \mathbf{C}_i, \quad (12)$$

$$s_1^2s_3^6=(1+x+y)^2(1+x^3+y^3)^6 \text{ for } \mathbf{C}_3, \quad (13)$$

$$s_4^5=(1+x^4+y^4)^5 \text{ for } \mathbf{D}_2, \quad (14)$$

$$s_2^4s_4^3=(1+x^2+y^2)^4(1+x^4+y^4)^3 \text{ for } \mathbf{C}_{2v}, \quad (15)$$

$$s_2^2s_4^4=(1+x^2+y^2)^2(1+x^4+y^4)^4 \text{ for } \mathbf{C}_{2h}, \quad (16)$$

$$s_4^5=(1+x^5+y^5)^4 \text{ for } \mathbf{C}_5, \quad (17)$$

$$s_2s_6^3=(1+x^2+y^2)(1+x^6+y^6)^3 \text{ for } \mathbf{D}_3, \quad (18)$$

$$s_1^2s_3^2s_6^2=(1+x+y)^2(1+x^3+y^3)^2(1+x^6+y^6)^2 \text{ for } \mathbf{C}_{3v}, \quad (19)$$

$$s_2s_6^3=(1+x^2+y^2)(1+x^6+y^6)^3 \text{ for } \mathbf{C}_{3i}, \quad (20)$$

$$s_4^3s_8=(1+x^4+y^4)^3(1+x^8+y^8) \text{ for } \mathbf{D}_{2h}, \quad (21)$$

$$s_{10}^2=(1+x^{10}+y^{10})^2 \text{ for } \mathbf{D}_5, \quad (22)$$

$$s_5^4=(1+x^5+y^5)^4 \text{ for } \mathbf{C}_{5v}, \quad (23)$$

$$s_{10}^2=(1+x^{10}+y^{10})^2 \text{ for } \mathbf{C}_{5i}, \quad (24)$$

$$s_4^2s_{12}=(1+x^4+y^4)^2(1+x^{12}+y^{12}) \text{ for } \mathbf{T}, \quad (25)$$

$$s_2s_6s_{12}=(1+x^2+y^2)(1+x^6+y^6)(1+x^{12}+y^{12}) \text{ for } \mathbf{D}_{3d}, \quad (26)$$

$$s_{10}^2=(1+x^{10}+y^{10})^2 \text{ for } \mathbf{D}_{5d}, \quad (27)$$

Table 3. Unit Subduced Cycle Indices for $\mathbf{I}_h$ Group[a)]

	$\mathbf{C}_1$	$\mathbf{C}_2$	$\mathbf{C}_s$	$\mathbf{C}_i$	$\mathbf{C}_3$	$\mathbf{D}_2$	$\mathbf{C}_{2v}$	$\mathbf{C}_{2h}$	$\mathbf{C}_5$	$\mathbf{D}_3$	$\mathbf{C}_{3v}$	$\mathbf{C}_{3i}$	$\mathbf{D}_{2h}$	$\mathbf{D}_5$	$\mathbf{C}_{5v}$	$\mathbf{C}_{5i}$	$\mathbf{T}$	$\mathbf{D}_{3d}$	$\mathbf{D}_{5d}$	$\mathbf{T}_h$	$\mathbf{I}$	$\mathbf{I}_h$
$\mathbf{I}_h(/\mathbf{C}_1)$	b_1^{120}	b_2^{60}	c_2^{60}	c_2^{60}	b_3^{40}	b_4^{30}	c_4^{30}	c_4^{30}	b_5^{24}	b_6^{20}	c_6^{20}	c_6^{20}	c_8^{15}	b_{10}^{12}	c_{10}^{12}	c_{10}^{12}	b_{12}^{10}	c_{12}^{10}	c_{20}^{6}	c_{24}^{5}	b_{60}^{2}	c_{120}
$\mathbf{I}_h(/\mathbf{C}_2)$	b_1^{60}	$b_1^4b_2^{28}$	c_2^{30}	c_2^{30}	b_2^{30}	$b_2^6b_4^{12}$	$c_2^2c_4^{14}$	$c_2^2c_4^{14}$	b_5^{12}	$b_3^4b_6^8$	c_6^{10}	c_6^{10}	$c_4^3c_8^6$	$b_5^4b_{10}^4$	c_{10}^6	c_{10}^6	$b_6^2b_{12}^4$	$c_6^2c_{12}^4$	$c_{10}^2c_{20}^2$	$c_{12}c_{24}^2$	b_{30}^2	c_{60}
$\mathbf{I}_h(/\mathbf{C}_s)$	b_1^{60}	b_2^{30}	$a_1^4c_2^{28}$	c_2^{30}	b_3^{20}	b_4^{15}	$a_2^4c_4^{13}$	$a_2^2c_4^{14}$	b_5^{15}	b_6^{10}	$a_3^4c_6^8$	c_6^{10}	$a_4^3c_6^8$	b_{10}^6	$a_5^4c_{10}^4$	c_{10}^6	b_{12}^5	$a_6^2c_{12}^4$	$a_{10}^2c_{20}^2$	$a_{12}c_{24}^2$	b_{60}	a_{60}
$\mathbf{I}_h(/\mathbf{C}_i)$	b_1^{60}	b_2^{30}	c_2^{30}	a_1^{60}	b_3^{20}	b_4^{15}	c_4^{15}	a_2^{30}	b_5^{12}	b_6^{10}	c_6^{10}	a_3^{20}	a_4^{15}	b_{10}^6	c_{10}^6	a_5^{12}	b_{12}^5	a_6^{10}	a_{10}^6	a_{12}^5	b_{60}	a_{60}
$\mathbf{I}_h(/\mathbf{C}_3)$	b_1^{40}	b_2^{20}	c_2^{20}	c_2^{20}	$b_1^4b_3^{12}$	b_4^{10}	c_4^{10}	c_4^{10}	b_5^8	$b_2^2b_6^6$	$c_2^2c_6^6$	$c_2^2c_6^6$	c_8^5	b_{10}^4	c_{10}^4	c_{10}^4	$b_4^4b_{12}^2$	$c_4c_{12}^3$	c_{20}^2	$c_8^2c_{24}$	b_{20}^2	c_{40}
$\mathbf{I}_h(/\mathbf{D}_2)$	b_1^{30}	$b_1^6b_2^{12}$	c_2^{15}	c_2^{15}	b_3^{10}	$b_1^6b_4^6$	$c_2^3c_4^6$	$c_2^3c_4^6$	b_5^6	$b_3^6c_6^2$	c_6^5	c_6^5	$c_2^3c_8^3$	b_5^6	c_{10}^3	c_{10}^3	$b_3^2b_{12}^2$	$c_6^3c_{12}$	c_{10}^3	c_6c_{24}	b_{15}^2	c_{30}
$\mathbf{I}_h(/\mathbf{C}_{2v})$	b_1^{30}	$b_1^2b_2^{14}$	$a_1^4c_2^{13}$	c_2^{15}	b_3^{10}	$b_2^3b_4^6$	$a_1^2a_2^2c_4^6$	$a_2^2c_2c_4^6$	b_5^6	$b_3^2b_6^4$	$a_3^4c_6^3$	c_6^5	$a_2^3c_8^3$	$b_5^2b_{10}^2$	$a_5^4c_{10}$	c_{10}^3	$b_6b_{12}^2$	$a_6^2c_6c_{12}$	$a_{10}^2c_{10}$	a_6c_{24}	b_{30}	a_{30}
$\mathbf{I}_h(/\mathbf{C}_{2h})$	b_1^{30}	$b_1^2b_2^{14}$	$a_1^2c_2^{14}$	a_1^{30}	b_3^{10}	$b_2^3b_4^6$	$a_2^2c_2c_4^6$	$a_1^2c_2^{14}$	b_5^6	$b_3^2b_6^4$	$a_3^2c_6^4$	a_3^{10}	$a_2^3a_4^6$	$b_5^2b_{10}^2$	$a_5^2c_{10}^2$	a_5^6	$b_6b_{12}^2$	$a_3^2a_6^4$	$a_5^2a_{10}^2$	$a_6a_{12}^2$	b_{30}	a_{30}
$\mathbf{I}_h(/\mathbf{C}_5)$	b_1^{24}	b_2^{12}	c_2^{12}	c_2^{12}	b_3^8	b_4^6	c_4^6	c_4^6	$b_1^4b_5^4$	b_6^4	c_6^4	c_6^4	c_8^3	$b_2^2b_{10}^2$	$c_2^2c_{10}^2$	$c_2^2c_{10}^2$	b_{12}^2	c_{12}^2	c_4c_{20}	c_{24}	b_{12}^2	c_{24}
$\mathbf{I}_h(/\mathbf{D}_3)$	b_1^{20}	$b_1^4b_2^8$	c_2^{10}	c_2^{10}	$b_1^2b_3^6$	$b_2^6b_4^2$	$c_2^2c_4^4$	$c_2^2c_4^4$	b_5^4	$b_1^2b_3^2b_6^2$	$c_2c_6^3$	$c_2c_6^3$	$c_4^3c_8$	b_5^4	c_{10}^2	c_{10}^2	$b_4^2b_6^2$	$c_2c_6c_{12}$	c_{10}^2	c_8c_{12}	b_{10}^2	c_{20}
$\mathbf{I}_h(/\mathbf{C}_{3v})$	b_1^{20}	b_2^{10}	$a_1^4c_2^8$	c_2^{10}	$b_1^2b_3^6$	b_4^5	$a_2^4c_4^3$	$a_2^2c_4^4$	b_5^4	$b_2b_6^3$	$a_1^2a_3^2c_6^2$	$c_2c_6^3$	$a_4^3c_8$	b_{10}^2	a_5^4	c_{10}^2	$b_4^2b_{12}$	$a_2a_6c_{12}$	a_{10}^2	c_8a_{12}	b_{20}	a_{20}
$\mathbf{I}_h(/\mathbf{C}_{3i})$	b_1^{20}	b_2^{10}	c_2^{10}	a_1^{20}	$b_1^2b_3^6$	b_4^5	c_4^5	a_2^{10}	b_5^4	$b_2b_6^3$	$c_2c_6^3$	$a_1^2c_3^6$	a_4^5	b_{10}^2	a_{10}^2	a_5^4	$b_4^2b_{12}$	$a_2a_6^3$	a_{10}^2	$a_4^2a_{12}$	b_{20}	a_{20}
$\mathbf{I}_h(/\mathbf{D}_{2h})$	b_1^{15}	$b_1^3b_2^6$	$a_1^3c_2^6$	a_1^{15}	b_3^5	$b_1^3b_4^3$	$a_1^3c_4^3$	$a_1^3a_2^6$	b_5^3	$b_3^3b_6$	$c_3^3c_6$	a_3^5	$a_1^3a_4^3$	b_5^3	a_5^3	a_5^3	b_3b_{12}	$a_3^3a_6$	a_5^3	a_3a_{12}	b_{15}	a_{15}
$\mathbf{I}_h(/\mathbf{D}_5)$	b_1^{12}	$b_1^4b_2^4$	c_2^6	c_2^6	b_3^4	b_2^6	$c_2^2c_4^2$	$c_2^2c_4^2$	$b_1^2b_5^2$	b_3^4	c_6^2	c_6^2	c_4^3	$b_1^2b_5^2$	c_2c_{10}	c_2c_{10}	b_6^2	c_6^2	c_2c_{10}	c_{12}	b_6^2	c_{12}
$\mathbf{I}_h(/\mathbf{C}_{5v})$	b_1^{12}	b_2^6	$a_1^4c_2^4$	c_2^6	b_3^4	b_4^3	$a_2^4c_4$	$a_2^2c_4^2$	$b_1^2b_5^2$	b_6^2	c_3^4	c_6^2	a_4^3	b_2b_{10}	$a_1^2a_5^2$	c_2c_{10}	b_{12}	a_6^2	a_2c_{10}	a_{12}	b_{12}	a_{12}
$\mathbf{I}_h(/\mathbf{C}_{5i})$	b_1^{12}	b_2^6	c_2^6	a_1^{12}	b_3^4	b_4^3	c_4^3	a_2^6	$b_1^2b_5^2$	b_6^2	c_6^2	a_3^4	a_4^3	b_2b_{10}	c_2c_{10}	$a_1^2a_5^2$	b_{12}	a_6^2	a_2c_{10}	a_{12}	b_{12}	a_{12}
$\mathbf{I}_h(/\mathbf{T})$	b_1^{10}	$b_1^2b_2^4$	c_2^5	c_2^5	$b_1^4b_3^2$	$b_1^2b_4^2$	$c_2c_4^2$	$c_2c_4^2$	b_5^2	$b_2^2b_3^2$	$c_2^2c_6$	$c_2^2c_6$	c_2c_8	b_5^2	c_{10}	c_{10}	$b_1^2b_4^2$	c_4c_6	c_{10}	c_2c_8	b_5^2	c_{10}
$\mathbf{I}_h(/\mathbf{D}_{3d})$	b_1^{10}	$b_1^2b_2^4$	$a_1^2c_2^4$	a_1^{10}	$b_1b_3^3$	$b_2^3b_4$	$a_2^2c_2c_4$	$a_1^2a_2^4$	b_5^2	$b_1b_3b_6$	$a_1a_3a_6$	$a_1c_3^3$	$a_2^3a_4$	b_5^2	a_5^2	a_5^2	b_4b_6	$a_1a_3a_6$	a_5^2	a_4a_6	b_{10}	a_{10}
$\mathbf{I}_h(/\mathbf{D}_{5d})$	b_1^6	$b_1^2b_2^2$	$a_1^2c_2^2$	a_1^6	b_3^2	b_2^3	$a_2^2c_2$	$a_1^2c_2^2$	b_1b_5	b_3^2	a_3^2	a_3^2	a_2^3	b_1b_5	a_1a_5	a_1c_5	b_6	a_3^2	a_1c_5	a_6	b_6	a_6
$\mathbf{I}_h(/\mathbf{T}_h)$	b_1^5	$b_1b_2^2$	$a_1c_2^2$	a_1^5	$b_1^2b_3$	b_1b_4	a_1c_4	$a_1a_2^2$	b_5	b_2b_3	c_2a_3	$a_1^2a_3$	a_1a_4	b_5	a_5	a_5	b_1b_4	a_2a_3	a_5	a_1a_4	b_5	a_5
$\mathbf{I}_h(/\mathbf{I})$	b_1^2	b_1^2	c_2	c_2	b_1^2	b_1^2	c_2	c_2	b_1^2	b_1^2	c_2	c_2	c_2	b_1^2	c_2	c_2	b_1^2	c_2	c_2	c_2	b_1^2	c_2
$\mathbf{I}_h(/\mathbf{I}_h)$	b_1	b_1	a_1	a_1	b_1	b_1	a_1	a_1	b_1	b_1	a_1	a_1	a_1	b_1	a_1	a_1	b_1	a_1	a_1	a_1	b_1	a_1
$\sum_{i=1}^{s}\overline{m}_{ji}$	$\frac{1}{120}$	$\frac{1}{8}$	$\frac{1}{8}$	$\frac{1}{120}$	$\frac{1}{6}$	0	0	0	$\frac{1}{5}$	0	0	$\frac{1}{6}$	0	0	0	$\frac{1}{5}$	0	0	0	0	0	0

a) This table lists USCIs with chirality fittingness. They can be converted into the corresponding USCIs without chirality fittingness by substituting s for a, b, and c.

Table 4. Coefficients Calculated from Generating Functions

	C_1	C_2	C_s	C_i	C_3	D_2	C_{2v}	C_{2h}	C_5	D_3	C_{3v}	C_{3i}	D_{2h}	D_5	C_{5v}	C_{5i}	T	D_{3d}	D_{5d}	T_h	I	I_h
[20,0,0]	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
[19,1,0]	20	0	4	0	0	0	0	0	0	0	2	0	0	0	0	0	0	0	0	0	0	0
[18,2,0]	190	10	14	10	1	0	4	2	0	1	1	1	0	0	0	0	0	1	0	0	0	0
[18,1,1]	380	0	12	0	2	0	0	0	0	0	2	0	0	0	0	0	0	0	0	0	0	0
[17,3,0]	1140	0	36	0	6	0	0	0	0	0	2	0	0	0	0	0	0	0	0	0	0	0
[17,2,1]	3420	0	44	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
[16,4,0]	4845	45	77	45	12	5	9	5	0	0	4	0	3	0	0	0	2	0	0	0	0	0
[16,3,1]	19380	0	100	0	12	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
[16,2,2]	29070	90	158	90	0	0	12	2	0	0	0	0	0	0	0	0	0	0	0	0	0	0
[15,5,0]	15504	0	144	0	6	0	0	0	4	0	2	0	0	0	4	0	0	0	0	0	0	0
[15,4,1]	77520	0	208	0	12	0	0	0	0	0	4	0	0	0	0	0	0	0	0	0	0	0
[15,3,2]	155040	0	352	0	6	0	0	0	0	0	2	0	0	0	0	0	0	0	0	0	0	0
[14,6,0]	38760	120	232	120	15	0	16	8	0	3	3	3	0	0	0	0	0	1	0	0	0	0
[14,5,1]	232560	0	368	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
[14,4,2]	581400	360	728	360	0	0	24	8	0	0	0	0	0	0	0	0	0	0	0	0	0	0
[14,3,3]	775200	0	736	0	30	0	0	0	0	0	2	0	0	0	0	0	0	0	0	0	0	0
[13,7,0]	77520	0	336	0	30	0	0	0	0	0	6	0	0	0	0	0	0	0	0	0	0	0
[13,6,1]	542640	0	560	0	30	0	0	0	0	0	6	0	0	0	0	0	0	0	0	0	0	0
[13,5,2]	1627920	0	1232	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
[13,4,3]	2713200	0	1456	0	60	0	0	0	0	0	4	0	0	0	0	0	0	0	0	0	0	0
[12,8,0]	125970	210	434	210	15	10	22	10	0	3	3	3	4	0	0	0	1	1	0	1	0	0
[12,7,1]	1007760	0	784	0	30	0	0	0	0	0	6	0	0	0	0	0	0	0	0	0	0	0
[12,6,2]	3527160	840	1848	840	15	0	40	8	0	3	3	3	0	0	0	0	0	1	0	0	0	0
[12,5,3]	7054320	0	2352	0	30	0	0	0	0	0	2	0	0	0	0	0	0	0	0	0	0	0
[12,4,4]	8817900	1260	2828	1260	60	20	48	20	0	0	4	0	6	0	0	0	2	0	0	0	0	0

$$s_8 s_{12} = (1+x^8+y^8)(1+x^{12}+y^{12}) \text{ for } \mathbf{T}_h, \quad (28)$$

$$s_{20} = 1+x^{20}+y^{20} \text{ for } \mathbf{I}, \quad (29)$$

and

$$s_{20} = 1+x^{20}+y^{20} \text{ for } \mathbf{I}_h. \quad (30)$$

Expansion of the right-hand side of each equation afforded a generating function, in which the coefficient of term $x^p y^q$ indicates the number of fixed points with $x^p y^q$ and the respective subsymmetry. Table 4 collects selected results of these expansions. We use an index $[20-p-q,\ p,\ q]$ for $x^p y^q$, $x^q y^p$, $x^{20-p-q} y^p$, $x^{20-p-q} y^q$, $x^p y^{20-p-q}$, and $x^q y^{20-p-q}$, since these terms have equal coefficients. This index corresponds to the molecular formulas, $C_{20}H_{20-p-q}X_pY_q$, $C_{20}H_{20-p-q}X_qY_p$, $C_{20}H_qX_{20-p-q}Y_p$, $C_{20}H_pX_{20-p-q}Y_q$, $C_{20}H_qX_pY_{20-p-q}$, and $C_{20}H_pX_qY_{20-p-q}$.

With respect to every $x^p y^q$ term, we can obtain a row vector (FPV), the elements of which are the coefficients of the $x^p y^q$ term appearing in the respective equations for the subsymmetries of $\mathbf{I}_h$. For the [12,4,4] case, we obtain an FPV=(8817900 1260 2828 1260 60 20 48 20 0 0 4 0 6 0 0 0 2 0 0 0 0 0) by collecting the coefficients of the corresponding terms (e.g. x^4y^4) appearing in the right-hand side of each generating function. Note that the elements of the FPV are aligned in the order of the SSG described above. The multiplication of the FPV by the inverse (Table 2) affords a row vector, (72974 296 679 17 13 2 21 7 0 0 2 0 2 0 0 0 1 0 0 0 0 0). This vector indicates that there emerge 72974 $\mathbf{C}_1$-isomers, 296 $\mathbf{C}_2$-isomers, 679 $\mathbf{C}_s$-isomers, 17 $\mathbf{C}_i$-isomers, 13 $\mathbf{C}_3$-isomers, 2 $\mathbf{D}_2$-isomers, 21 $\mathbf{C}_{2v}$-isomers, 7 $\mathbf{C}_{2h}$-isomers, 2 $\mathbf{C}_{3v}$-isomers, 2 $\mathbf{D}_{2h}$-isomers, and one $\mathbf{T}$-isomers. Since we count every enantiomeric pair in this enumeration, each chiral derivative and its antipode are pairwise counted in, while each achiral derivative is counted once in itself. Similarly, we enumerate isomers with every index $[20-p-q,p,q]$, as is shown in Table 5. Among the values listed in this table, the values of the $[20-p,p,0]$ cases are identical with those of Brocas' alternative enumeration.[11]

In order to verify the results collected in Table 5, we depict several chiral derivatives. Fig. 1 illustrates seven $\mathbf{D}_2$-derivatives, where the $[20-p-q,p,q]$-

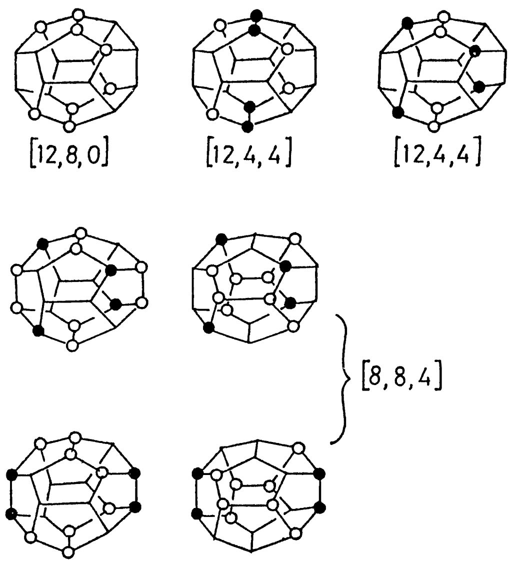

Fig. 1. $\mathbf{D}_2$-Molecules drived from **1**.

Table 5. Number of Dodecahedrane Derivatives with Achiral Substituents

	C_1	C_2	C_s	C_i	C_3	D_2	C_{2v}	C_{2h}	C_5	D_3	C_{3v}	C_{3i}	D_{2h}	D_5	C_{5v}	C_{5i}	T	D_{3d}	D_{5d}	T_h	I	I_h	Total
[20,0,0]	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	1
[19,1,0]	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	1
[18,2,0]	0	1	1	0	0	0	2	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	5
[18,1,1]	2	0	2	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	5
[17,3,0]	5	0	8	0	1	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	15
[17,2,1]	23	0	11	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	34
[16,4,0]	28	8	13	0	1	0	3	1	0	0	2	0	1	0	0	0	1	0	0	0	0	0	58
[16,3,1]	148	0	25	0	3	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	176
[16,2,2]	214	19	33	1	0	0	6	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	274
[15,5,0]	112	0	33	0	1	0	0	0	0	0	1	0	0	0	2	0	0	0	0	0	0	0	149
[15,4,1]	620	0	50	0	2	0	0	0	0	0	2	0	0	0	0	0	0	0	0	0	0	0	674
[15,3,2]	1248	0	87	0	1	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	1337
[14,6,0]	284	23	47	0	2	0	8	3	0	1	1	1	0	0	0	0	0	1	0	0	0	0	371
[14,5,1]	1892	0	92	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1984
[14,4,2]	4714	82	168	4	0	0	12	4	0	0	0	0	0	0	0	0	0	0	0	0	0	0	4984
[14,3,3]	6366	0	183	0	7	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	6557
[13,7,0]	603	0	81	0	6	0	0	0	0	0	3	0	0	0	0	0	0	0	0	0	0	0	693
[13,6,1]	4451	0	137	0	6	0	0	0	0	0	3	0	0	0	0	0	0	0	0	0	0	0	4597
[13,5,2]	13412	0	308	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	13720
[13,4,3]	22424	0	362	0	14	0	0	0	0	0	2	0	0	0	0	0	0	0	0	0	0	0	22802
[12,8,0]	975	43	96	2	2	1	9	2	0	1	1	0	1	0	0	0	0	1	0	1	0	0	1135
[12,7,1]	8299	0	193	0	6	0	0	0	0	0	3	0	0	0	0	0	0	0	0	0	0	0	8501
[12,6,2]	29062	197	439	12	2	0	20	3	0	1	1	1	0	0	0	0	0	1	0	0	0	0	29739
[12,5,3]	58490	0	587	0	7	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	59085
[12,4,4]	72974	296	679	17	13	2	21	7	0	0	2	0	2	0	0	0	1	0	0	0	0	0	74014
[11,9,0]	1336	0	124	0	4	0	0	0	0	0	2	0	0	0	0	0	0	0	0	0	0	0	1466
[11,8,1]	12478	0	238	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	12716
[11,7,2]	50080	0	616	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	50696
[11,6,3]	117148	0	838	0	14	0	0	0	0	0	2	0	0	0	0	0	0	0	0	0	0	0	118002
[11,5,4]	175812	0	1092	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	176904
[10,10,0]	1448	54	112	2	8	0	12	4	0	0	4	0	0	0	2	0	0	0	2	0	0	0	1648
[10,9,1]	15262	0	262	0	8	0	0	0	0	0	4	0	0	0	0	0	0	0	0	0	0	0	15536
[10,8,2]	68770	300	694	18	0	0	24	6	0	0	0	0	0	0	0	0	0	0	0	0	0	0	69812
[10,7,3]	184216	0	1060	0	28	0	0	0	0	0	4	0	0	0	0	0	0	0	0	0	0	0	185308
[10,6,4]	322254	606	1452	36	28	0	36	12	0	0	4	0	0	0	0	0	0	0	0	0	0	0	324428
[10,5,5]	387192	0	1590	0	0	0	0	0	0	0	0	0	0	0	6	0	0	0	0	0	0	0	388788
[9,9,2]	76596	0	768	0	4	0	0	0	0	0	2	0	0	0	0	0	0	0	0	0	0	0	77370
[9,8,3]	230345	0	1188	0	14	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	231550
[9,7,4]	460972	0	1816	0	28	0	0	0	0	0	4	0	0	0	0	0	0	0	0	0	0	0	462820
[9,6,5]	645592	0	2098	0	14	0	0	0	0	0	2	0	0	0	0	0	0	0	0	0	0	0	647706
[8,8,4]	518280	756	1864	46	0	4	36	12	0	0	0	0	2	0	0	0	0	0	0	0	0	0	521000
[8,7,5]	830212	0	2380	0	6	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	832592
[8,6,6]	968140	1017	2533	63	18	0	48	12	0	3	3	3	0	0	0	0	0	0	0	0	0	0	971840
[7,7,6]	1107124	0	2794	0	42	0	0	0	0	0	6	0	0	0	0	0	0	0	0	0	0	0	1109966

molecule is represented with p open circles and q solid circles. There appear one [12,8,0]-isomer, two [12,4,4]-isomers and four [8,8,4]-isomers, as found in the $\mathbf{D}_2$-column of Table 5. Note that such an index corresponds to several combinatorial possibilities. For example, the [12,8,0] index corresponds to $C_{20}H_{12}X_8$, $C_{20}H_{12}Y_8$, $C_{20}H_8Y_{12}$, $C_{20}H_8Y_{12}$, $C_{20}X_{12}Y_8$, and $C_{20}X_8Y_{12}$, if we select such substituents from H, X, and Y.

There are six $\mathbf{D}_3$-derivatives, as illustrated in Fig. 2. Each of these molecules holds a C_3 axis lying through a pair of vertices which, for example, are denoted by solid circles in the [12,6,2]-moleucle of Fig. 2. Figure 2 also depicts two **T**-molecules. The comparison of the **T**-[12,4,4]-molecule of Fig. 2 with the $\mathbf{D}_2$-[12,4,4]-molecules of Fig. 1 clarifies the geometrical relationship between them.

Figure 3 collects all isomers with an index [18,1,1]. This contains two asymmetric ($\mathbf{C}_1$) isomers, two $\mathbf{C}_s$-isomers and one $\mathbf{C}_{3v}$-isomer.

Figure 4 depicts achiral dodecahedrane derivatives of high symmetry. A comparison between the $\mathbf{T}_h$-[12,8,0]-molecule of Fig. 4 and the **T**-[12,4,4]-molecule of Fig. 2 clarifies the strerochemical equivalency of the respective vertices. Thus, the 8 vertices of the former molecule are subject to $\mathbf{T}_h(/\mathbf{C}_3)$, and both the sets of four equivalent vertices in the latter compound are governed by $\mathbf{T}(/\mathbf{C}_3)$. This type of correspondence will be discussed elsewhere.[19]

Table 5 indicates absence of $\mathbf{C}_5$-, $\mathbf{D}_5$-, $\mathbf{C}_{5i}$-, and **I**-derivatives in this series. These have been referred to as phantom subgroups, the absence of which was proved by a rather laborious method.[11] The present approach provides us with a simpler proof to clarify non-existence of these subgroups. Compare the USCI of the $\mathbf{C}_5$ group (s_5^4) with that of $\mathbf{C}_{5v}$ (s_5^4) for an orbit governed by $\mathbf{I}_h(/\mathbf{C}_{3v})$. The USCI ($s_5^4$) indicates an orbit occupied by atoms, $A_5B_5C_5D_5$. Even if this occupation is effected to realize $\mathbf{C}_5$, the resulting molecule has $\mathbf{C}_{5v}$ symmetry, because the two cases have the same USCI. This means non-existence of $\mathbf{C}_5$-derivatives. Similarly, the examination of USCI of the $\mathbf{I}_h(/\mathbf{C}_{3v})$ row, i.e., $\mathbf{D}_5$ (s_{10}^2) vs. $\mathbf{D}_{5d}$ (s_{10}^2), $\mathbf{C}_{5i}$ (s_{10}^2), vs. $\mathbf{D}_{5d}$ (s_{10}^2), and $\mathbf{I}$ (s_{20}) vs. $\mathbf{I}_h$ (s_{20}), indicates non-existence of $\mathbf{D}_5$-, $\mathbf{C}_{5i}$- and $\mathbf{I}$-derivatives.

The total number of isomers with each $x^p y^q$ term is obtained by summing up the corresponding row of Table 5. This value is listed in the rightmost column of Table 5. This is calculated alternatively by using a cycle index (CI). The cycle index is obtained by means of the data collected in Table 3.

$$\begin{aligned}\mathrm{CI}(\mathbf{T}_d; s_d) &= (1/120)s_1^{20}+(1/8)s_2^{10}+(1/8)s_1^4s_2^8+(1/120)s_2^{10} \\ &\quad +(1/6)s_1^2s_3^6+(1/5)s_5^4+(1/6)s_2s_6^3+(1/5)s_{10}^2 \\ &= (1/120)(s_1^{20}+16s_2^{10}+15s_1^4s_2^8+20s_1^2s_6^3+24s_5^4 \\ &\quad +20s_2s_6^3+24s_{10}^2), \end{aligned} \tag{31}$$

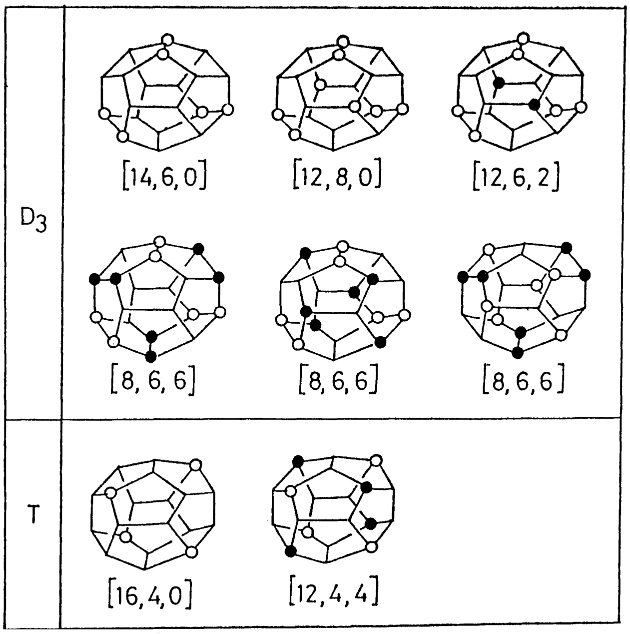

Fig. 2. $\mathbf{D}_3$- and $\mathbf{T}$-Molecules drived from **1**.

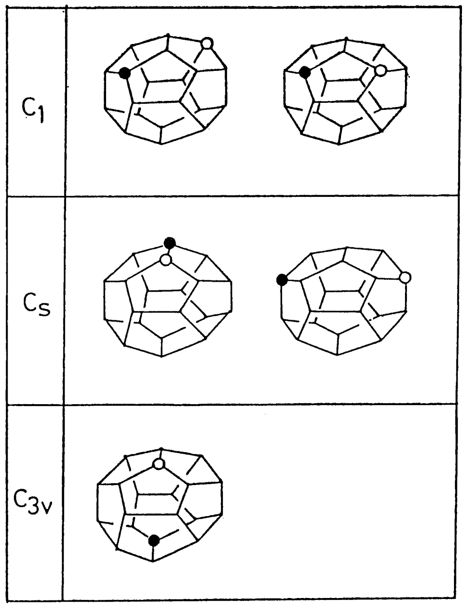

Fig. 3. [18,1,1]-Isomers drived from **1** with H, X, and Y.

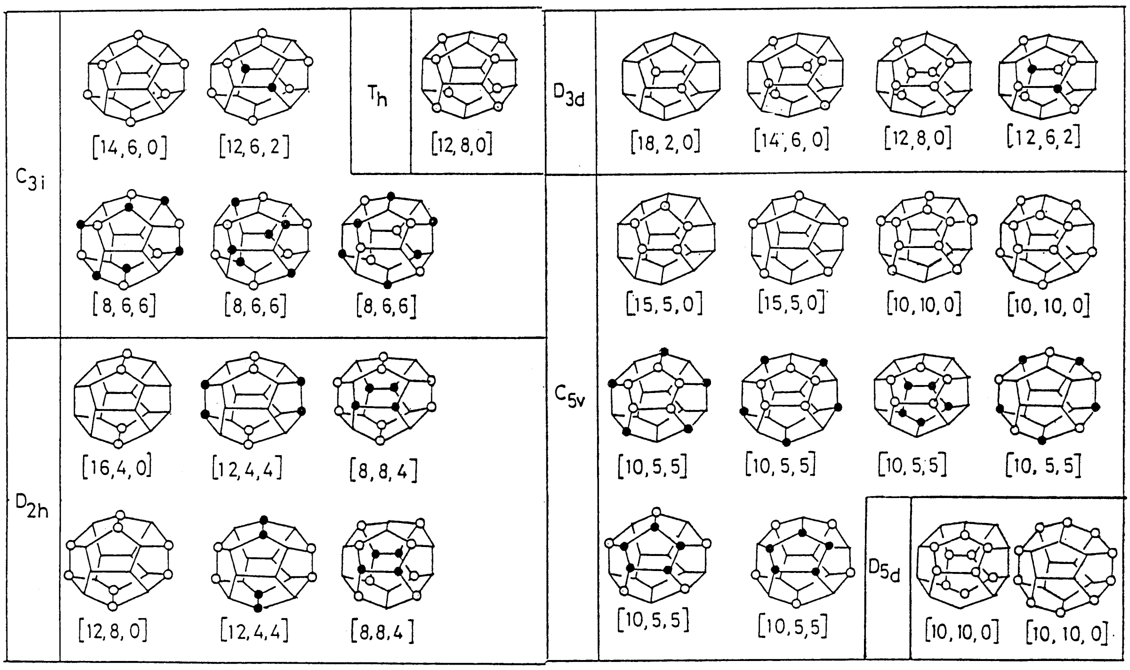

Fig. 4. Achiral dodecahedrane derivtives of high symmetries.

where each term is selected from the $\mathbf{I}_h(/\mathbf{C}_{3v})$ row; and its coefficient is the factor found in the bottom of the table. This equation can be proved to be identical with what is obtained alternatively by Pólya's theorem.[20] After introduction of the figure inventory (Eq. 8) into this CI, we expand the resulting equation to give a generating function, whose coefficients are proved to be equal to the value collected in the rightmost column of Table 5.

Dodecahedrane Derivatives with Achiral and Chiral Substituents. Substitution of chiral substituents on an achiral skeleton is one of the strategies that generate chiral compounds of high symmetry.[21,22] For example, a chiral molecule of **T** symmetry has been synthesized from an adamantane ($\mathbf{T}_d$) skeleton in light of this strategy.[23] The next question is what symmetries are realized on the basis of a dodecahedrane skeleton if chiral substituents are permitted. We are able to solve this problem by introducing a *subduced cycle index with chirality fittingness* (SCI-CF), which is defined as

$$\mathrm{ZI}(\mathbf{G}_j;\ \$_{d_{jk}}^{(i\alpha)}) = \prod_{i=1}^{s}\prod_{\alpha} \mathrm{Z}(\mathbf{G}(/\mathbf{G}_i)\downarrow\mathbf{G}_j;\ \$_{d_{jk}}^{(i\alpha)}) \tag{32}$$

for $j=1,2,\ldots,s$.[18]

In order to obtain a generating function for the FPV of each subsymmetry, we replace the $\$_{d_{jk}}^{(i\alpha)}$ term in Eq. 32 by one of the following figure inventories,

$$a_{d_{jk}}^{(i\alpha)} = \sum_{r=1}^{|\mathbf{X}|} w_{i\alpha}(X_r^{(a)})^{d_{jk}} \text{ for } \$ = a, \tag{33}$$

$$b_{d_{jk}}^{(i\alpha)} = \sum_{r=1}^{|\mathbf{X}|} w_{i\alpha}(X_r)^{d_{jk}} \text{ for } \$ = b, \tag{34}$$

and

$$b_{d_{jk}}^{(i\alpha)} = \sum_{r=1}^{|\mathbf{X}|} w_{i\alpha}(X_r^{(a)})^{d_{jk}} + 2\sum_{r=1}^{|\mathbf{X}|} [w_{i\alpha}(X_r^{(c)})^{d_{jk}} w_{i\alpha}(X_r^{(c\#)})^{d_{jk}}] \text{ for } \$=c, \tag{35}$$

where the symbol $(X_r^{(a)})$ denotes an achiral substituent; the symbol (X_r) denotes any sub-stituent; and $X_r^{(c)}$ and $X_r^{(c\#)}$ are a pair of antipodes.

For simplicity of discusssion, we consider a hydrogen atom, a chiral substituent (R) and its antipode (S) as substituents. In this case, we adopted USCI-CFs appearing in the $\mathbf{I}_h(/\mathbf{C}_{3v})$ row of Table 3. Each of the monomials in this row, by itself, is the SCI-CF of the corresponding subsymmetry, since there is only one orbit. If Eqs. 33—35 are applied to this case, figure inventories are selected to be

$$a_d = 1, \tag{36}$$

$$b_d = 1 + r^d + s^d, \tag{37}$$

and

$$c_d = 1 + 2(rs)^{d/2}, \tag{38}$$

where r and s are concerned with the substitution of R and S. They are then introduced into the SCI-CFs to provide the following generating functions,

$$b_1^{20} = (1+r+s)^{20} \text{ for } \mathbf{C}_1, \tag{39}$$

$$b_2^{10} = (1+r^2+s^2)^{10} \text{ for } \mathbf{C}_2, \tag{40}$$

$$a_1^4 c_2^8 = (1+2rs)^8 \text{ for } \mathbf{C}_s, \tag{41}$$

$$c_2^{10} = (1+2rs)^{10} \text{ for } \mathbf{C}_i, \tag{42}$$

$$b_1^2 b_3^6 = (1+r+s)^2(1+r^3+s^3)^6 \text{ for } \mathbf{C}_3, \tag{43}$$

$$b_4^5 = (1+r^4+s^4)^5 \text{ for } \mathbf{D}_2, \tag{44}$$

$$a_2^4 c_4^3 = (1+2r^2s^2)^3 \text{ for } \mathbf{C}_{2v}, \tag{45}$$

$$a_2^2 c_4^4 = (1+2r^2s^2)^4 \text{ for } \mathbf{C}_{2h}, \tag{46}$$

$$b_4^5 = (1+r^5+s^5)^4 \text{ for } \mathbf{C}_5, \tag{47}$$

$$b_2 b_6^3 = (1+r^2+s^2)(1+r^6+s^6)^3 \text{ for } \mathbf{D}_3, \tag{48}$$

$$a_1^2 a_3^2 c_6^2 = (1+2r^2s^2)^2 \text{ for } \mathbf{C}_{3v}, \tag{49}$$

$$c_2 b_6^3 = (1+2rs)(1+2r^3s^3)^3 \text{ for } \mathbf{C}_{3i}, \tag{50}$$

$$a_4^3 c_8 = 1+2r^4s^4 \text{ for } \mathbf{D}_{2h}, \tag{51}$$

$$b_{10}^2 = (1+r^{10}+s^{10})^2 \text{ for } \mathbf{D}_5, \tag{52}$$

$$a_5^4 = 1 \text{ for } \mathbf{C}_{5v}, \tag{53}$$

$$c_{10}^2 = (1+2r^5s^5)^2 \text{ for } \mathbf{C}_{5i}, \tag{54}$$

$$b_4^2 b_{12} = (1+r^4+s^4)^2(1+r^{12}+s^{12}) \text{ for } \mathbf{T}, \tag{55}$$

$$a_2 a_6 c_{12} = 1+2r^6s^6 \text{ for } \mathbf{D}_{3d}, \tag{56}$$

$$a_{10}^2 = 1 \text{ for } \mathbf{D}_{5d}, \tag{57}$$

$$c_8 a_{12} = 1+2r^4s^4 \text{ for } \mathbf{T}_h, \tag{58}$$

$$b_{20} = 1+r^{20}+s^{20} \text{ for } \mathbf{I}, \tag{59}$$

and

$$a_{20} = 1 \text{ for } \mathbf{I}_h. \tag{60}$$

The right-hand side of each equation is expanded to afford a generating function. Since terms r^ps^q and r^qs^p express a pair of antipodes, coefficients of the paired terms are summed up to give the number of fixed points. In the case of $p=q$, the coefficient of r^ps^q by itself represents the number.

In order to illustrate a procedure, we examine the coefficients of the term r^4 (and s^4) appearing in the respective expansions. Thus, we obtain the corresponding FPV as being (4845×2 45×2 0 0 12×2 5×2 0 0 0 0 0 0 0 0 0 0 2×2 0 0 0 0 0). The multiplication by 2 takes account of a pairwise appearance of antipodes. The FPV is multiplied by the inverse (Table 2) to afford a row vector, (69 20 0 0 4 1 0 0 0 0 0 0 0 0 0 0 2 0 0 0 0 0). This vector indicates that there are 69 $\mathbf{C}_1$ enantiomeric pairs, 20 $\mathbf{C}_2$ pairs, 4 $\mathbf{C}_3$ pairs, one $\mathbf{D}_2$ pair, and two **T** pairs in the case of R_4 (and S_4) subsitution. Figure 5 depicts $\mathbf{C}_3$, $\mathbf{D}_2$, and **T** isomers. The substituents (R) for $\mathbf{D}_2$ group can have any chiral symmetry; however, the respective R substituents on the C_3 axis of the $\mathbf{C}_3$ and **T**-molecules should belong to $\mathbf{C}_3$-symmetry. It should be noted that the two derivatives of **T**-symmetry in Fig. 5 are diastereomeric to each other.

Results for other terms can be obtained in a similar way. Table 6 lists the results for terms having a power of less than 5.

Bond-Modification of a Dodecahedrane Skeleton. The 30 bonds of dodecahedrane (**1**) can be regarded as

Table 6. Number of Dodecahedrane Derivatives with Achiral and Chiral Substituents

Term	$\mathbf{C}_1$	$\mathbf{C}_2$	$\mathbf{C}_s$	$\mathbf{C}_i$	$\mathbf{C}_3$	$\mathbf{D}_2$	$\mathbf{C}_{2v}$	$\mathbf{C}_{2h}$	$\mathbf{C}_5$	$\mathbf{D}_3$	$\mathbf{C}_{3v}$	$\mathbf{C}_{3i}$	$\mathbf{D}_{2h}$	$\mathbf{D}_5$	$\mathbf{C}_{5v}$	$\mathbf{C}_{5i}$	$\mathbf{T}$	$\mathbf{D}_{3d}$	$\mathbf{D}_{5d}$	$\mathbf{T}_h$	$\mathbf{I}$	$\mathbf{I}_h$
r^5s^5	387696	0	448	134	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
$r^5s^4+r^4s^5$	352716	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
$r^5s^3+r^3s^5$	117567	0	0	0	15	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
$r^5s^2+r^2s^5$	27132	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
r^5s+rs^5	3876	0	8	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
r^5+s^5	257	0	0	0	3	0	0	0	2	0	0	0	0	0	0	0	0	0	0	0	0	0
r^4s^4	73163	302	269	49	12	3	5	11	0	0	0	4	0	0	0	0	0	0	0	2	0	0
$r^4s^3+r^3s^4$	45120	0	0	0	300	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
$r^4s^2+r^2s^4$	9600	180	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
r^4s+rs^4	1290	0	0	0	6	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
r^4+s^4	69	20	0	0	4	1	0	0	0	0	0	0	0	0	0	0	2	0	0	0	0	0
r^3s^3	6395	0	110	15	5	0	0	0	0	0	2	3	0	0	0	0	0	0	0	0	0	0
$r^3s^2+r^2s^3$	2583	0	0	0	3	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
r^3s+rs^3	321	0	0	0	6	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
r^3+s^3	18	0	0	3	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
r^2s^2	219	19	23	1	0	0	3	4	0	0	0	0	0	0	0	0	0	0	0	0	0	0
r^2s+rs^2	57	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
r^2+s^2	1	4	0	0	6	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0
rs	1	0	4	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0
$r+s$	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1

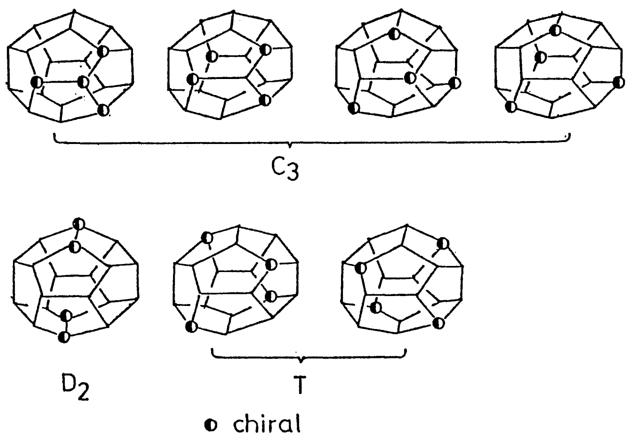

Fig. 5. Isomers drived from **1** having H_{16} and 4 chiral ligands.

substitution positions. One of such derivations is fusion of five-membered rings to an appropriate number of the bonds. If two or three of the rings meet at a vertex, they are allowed to hold a bond at the vertex in common. Thereby, we can obtain dodecahedrane derivatives that consists of five-membered rings only. Another application of the bond-modification is the retrosynthetic analysis of dodecahedrane construction.[3] If we place an appropiate number of out-bonds,[24] we can obtain possible precursors to be considered in a synthetic design.

Since the 30 bonds construct a single orbit governed by $\mathbf{I}_h(/\mathbf{C}_{2v})$, the $\mathbf{I}_h(/\mathbf{C}_{2v})$ row of Table 3 was selected for generating the SCIs of this case. A figure inventory was selected to be

$$s_d = 1 + x^d, \tag{61}$$

where x is concerned with the substitution of a five-membered ring. This figure inventory was introduced into the SCIs to provide the following generating functions,

$$s_1^{30} = (1+x)^{30} \text{ for } \mathbf{C}_1, \tag{62}$$

$$s_1^2 s_2^{14} = (1+x)^2(1+x^2)^{14} \text{ for } \mathbf{C}_2, \tag{63}$$

$$s_1^4 s_2^{13} = (1+x)^4(1+x^2)^{13} \text{ for } \mathbf{C}_s, \tag{64}$$

$$s_2^{15} = (1+x^2)^{15} \text{ for } \mathbf{C}_i, \tag{65}$$

$$s_3^{10} = (1+x^3)^{10} \text{ for } \mathbf{C}_3, \tag{66}$$

$$s_2^3 s_4^6 = (1+x^2)^3(1+x^4)^6 \text{ for } \mathbf{D}_2, \tag{67}$$

$$s_1^2 s_2^2 s_4^6 = (1+x)^2(1+x^2)^2(1+x^4)^6 \text{ for } \mathbf{C}_{2v}, \tag{68}$$

$$s_2^3 s_4^6 = (1+x^2)^3(1+x^4)^6 \text{ for } \mathbf{C}_{2h}, \tag{69}$$

$$s_5^6 = (1+x^5)^6 \text{ for } \mathbf{C}_5, \tag{70}$$

$$s_3^2 s_6^4 = (1+x^3)^2(1+x^6)^4 \text{ for } \mathbf{D}_3, \tag{71}$$

$$s_3^4 s_6^3 = (1+x^3)^4(1+x^6)^3 \text{ for } \mathbf{C}_{3v}, \tag{72}$$

$$s_6^5 = (1+x^6)^5 \text{ for } \mathbf{C}_{3i}, \tag{73}$$

$$s_2^3 s_8^3 = (1+x^2)^3(1+x^8)^3 \text{ for } \mathbf{D}_{2h}, \tag{74}$$

$$s_5^2 s_{10}^2 = (1+x^5)^2(1+x^{10})^2 \text{ for } \mathbf{D}_5, \tag{75}$$

$$s_5^4 s_{10} = (1+x^5)^4(1+x^{10}) \text{ for } \mathbf{C}_{5v}, \tag{76}$$

$$s_{10}^3 = (1+x^{10})^3 \text{ for } \mathbf{C}_{5i}, \tag{77}$$

$$s_6 s_{12}^2 = (1+x^6)(1+x^{12})^2 \text{ for } \mathbf{T}, \tag{78}$$

$$s_6^3 s_{12} = (1+x^6)^3(1+x^{12}) \text{ for } \mathbf{D}_{3d}, \tag{79}$$

$$s_{10}^3 = (1+x^{10})^3 \text{ for } \mathbf{D}_{5d}, \tag{80}$$

$$s_6 s_{24} = (1+x^6)(1+x^{24}) \text{ for } \mathbf{T}_h, \tag{81}$$

$$s_{30} = 1+x^{30} \text{ for } \mathbf{I}, \tag{82}$$

and

$$s_{30} = 1+x^{30} \text{ for } \mathbf{I}_h. \tag{83}$$

After expansion of these equations, the coefficients of terms $x^p (p=1$ to $30)$ are collected to give a 30×22 matrix. This is multiplied by the inverse (Table 2) to give numbers of derivatives. The results are found in

Table 7. Number of Derivatives due to Bond Modification

Term	C_1	C_2	C_s	C_i	C_3	D_2	C_{2v}	C_{2h}	C_5	D_3	C_{3v}	C_{3i}	D_{2h}	D_5	C_{5v}	C_{5i}	T	D_{3d}	D_{5d}	T_h	I	I_h	Total
x^{30}, 1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	1
x^{29}, x	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1
x^{28}, x^2	0	3	4	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	8
x^{27}, x^3	25	5	10	0	1	0	2	0	0	1	2	0	0	0	0	0	0	0	0	0	0	0	46
x^{26}, x^4	199	21	34	0	0	1	3	3	0	0	0	0	1	0	0	0	0	0	0	0	0	0	262
x^{25}, x^5	1124	41	82	0	0	0	7	0	0	0	0	0	0	1	2	0	0	0	0	0	0	0	1257
x^{24}, x^6	4801	99	175	4	8	3	9	6	0	1	3	0	0	0	0	0	0	3	0	1	0	0	5113
x^{23}, x^7	16698	176	352	0	0	0	12	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	17238
x^{22}, x^8	48297	318	604	15	0	5	15	15	0	0	0	0	0	1	0	0	0	0	0	0	0	0	49270
x^{21}, x^9	118482	486	972	0	24	0	21	0	0	4	8	0	0	0	0	0	0	0	0	0	0	0	119997
x^{20}, x^{10}	249269	717	1430	40	0	7	21	18	2	0	0	0	3	0	2	0	0	0	3	0	0	0	251512
x^{19}, x^{11}	453741	986	1972	0	0	0	30	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	456729
x^{18}, x^{12}	718865	1204	2485	69	43	9	28	24	0	3	9	3	3	0	0	0	1	4	0	0	0	0	422750
x^{17}, x^{13}	995764	1484	2968	0	0	0	35	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1000251
x^{16}, x^{14}	1209378	1554	3270	89	0	12	36	36	0	0	0	0	1	0	0	0	0	0	0	0	0	0	1214376
x^{15}	1290082	1688	3376	0	54	0	40	0	2	6	12	0	0	2	4	0	0	0	0	0	0	0	1295266

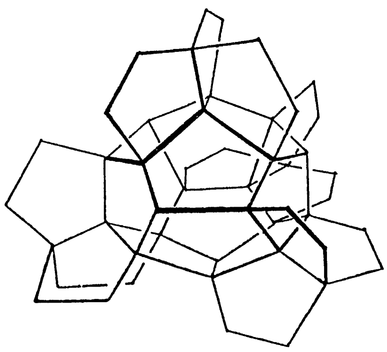

Fig. 6. A **T**-hydrocarbon by the edge substitution of **1**.

Table 7.

Figure 6 illustrates a **T**-molecule with the term (x^{12}), which is a hydrocarbon ($C_{48}H_{52}$) posessing only five-membered rings. We tentatively call this compound *dodecapentagonododecahedrane*. This is an interesting synthetic target, since it is a chiral hydrocarbon of **T**-symmetry that has a completely fixed conformation. Compare this compound with a mobile **T**-molecule reported.[23]

Table 7 indicates that a $I_h(/C_{2v})$ orbit produces derivatives of C_5 and of D_5 symmetry, whereas these symmetries are not realized in a derivation based on an $I_h(/C_{3v})$ orbit, as discussed in the case of permitting achiral substituents only (Table 5). On the other hand, derivatives of C_{5i} and of **I** symmetry are forbidden in this $I_h(/C_{2v})$ orbit as well as in the previous $I_h(/C_{3v})$ orbit. Existence and non-exsistence of these symmetries in the present $I_h(/C_{2v})$ case are rationalized by examining the $I_h(/C_{2v})$ row of the table of USCIs (Table 3).

Figure 7 illustrates the labeling of edges with outbonds (—||—),[24] which produces D_{2h}-precursors. Among them, an x^2-D_{2h}-compound can be correlated with pagodane that was reported as a precursor of dodecahedrane.[6] The number of these precursors

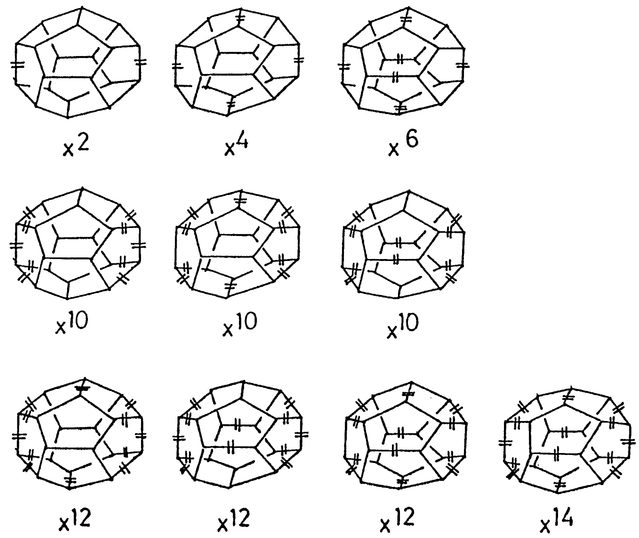

Fig. 7. D_{2h}-Precursors by the edge labeling of **1**.

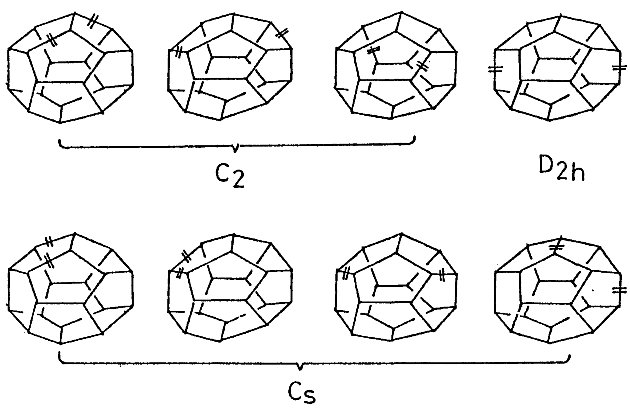

Fig. 8. Eight modes of bond scission corresponding to the x^2 term.

appears at the D_{2h} column of Table 7.

The x^2 row of Table 7 indicates the number of precursors produced by cleaving two bonds of dodecahedrane. Figure 8 depicts 8 modes of such bond scission.

Conclusion

A method based on unit subduced cycle indices (USCIs) is a versatile tool for enumerating high-symmetry molecules. This is verified by solving the enumeration problems of dodecahedrane derivatives, in which chiral as well as achiral substitution are taken into consideration, and in which bond-modification of the dodecahedrane skeleton is considered. Since the table of marks (and the inverse) and the table of USCIs for $\mathbf{I}_h$ group are given, it is possible to apply the present method to all of molecules of $\mathbf{I}_h$ symmetry.

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