# On the cycle index of point groups 

Ivan Baraldi ${ }^{\text {a }}$, Carla Fiori ${ }^{\text {b }}$ and Davide Vanossi ${ }^{\text {a }}$<br>${ }^{a}$ Dipartimento di Chimica, Università di Modena, via Campi 183, 41100 Modena, Italy<br>${ }^{b}$ Dipartimento di Economia Politica, Università di Modena, viale Berengario 51, 41100 Modena, Italy

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#### Abstract

In this brief work we express the cycle index of the molecular point groups as a function of a limited number of initial geometrical parameters. Such parameters are the number $m$ of elements composing the domain $D$ of sites of substitutions in the molecule belonging to the point group $\mathbf{G}$, and the numbers $\left(n\left(C_{n}\right), n(\sigma), \ldots\right)$ of sites of $D$ lying on the symmetry elements $\left(C_{n}, \sigma, \ldots\right)$ for $\mathbf{G}$.


## 1. Introduction

The application of Pòlya's theorem to the enumeration of isomers of molecular compounds is based on the cycle index of a permutation group of a finite set $D$, molecular substitutional sites, which are transformed by the symmetry operations of the molecular point group $\mathbf{G}[1,2,4,6,7]$. Once $D$ and $\mathbf{G}$ are defined, the cycle index can be developed.

To our knowledge, no systematic study of the cycle index of all finite point groups as a function of $\mathbf{G}$ and $D$ has been reported; only some partial studies have appeared [5]. However, such a study can render more familiar the chemical applications of Pòlya's theorem. It is for this reason that in the present work we have derived, in a systematic way, the cycle indices corresponding to every finite point group acting on a "generic" domain $D$, all as a function of the dimension $m$ of $D$ and of the numbers of substitutional sites of the molecule that lie on the symmetry elements for $\mathbf{G}$.

## 2. Mathematical development

Let $\mathbf{G}=\left\{g_{i}, i=1,2, \ldots,|\mathbf{G}|\right\}$ be the molecular point group of order $|\mathbf{G}|$ and $D=\left\{d_{j}, j=1,2, \ldots, m\right\}$ the domain given by the set of the $m$ substitutional sites of the molecule. Obviously, $m$ is a sum of divisors of $|\mathbf{G}|$,

$$
\begin{equation*}
m=\sum_{k| | \mathbf{G} \mid} n_{k, D} \times k \tag{1}
\end{equation*}
$$

where $n_{k, D}$ is a non-negative integer that defines the number of site orbits of length $k$ present in $D$, and one supposes that there exists at least one site orbit of dimensions

[^0]appropriate to our problem. Under the action of any element of $\mathbf{G}$, the elements of $D$ are rearranged, in other words, the sites permute amongst themselves. One writes
\[

g_{i} D=\left\{d_{j}^{\prime}=g_{i} d_{j}, j=1,2, ···, m\right\}=\left($$
\begin{array}{cccc}
d_{1} & d_{2} & \ldots & d_{m}  \tag{2}\\
d_{1}^{\prime} & d_{2}^{\prime} & \ldots & d_{m}^{\prime}
\end{array}
$$\right)=P\left(g_{i}, D\right)
\]

$\forall g_{i} \in \mathbf{G}$. The set of all the distinct permutations $P\left(g_{i}, D\right)$ forms a permutation group of order $g \leqslant|\mathbf{G}|$ that is indicated as $P(\mathbf{G}, D)=\left\{P\left(g_{i}, D\right), i=1,2, \ldots, g\right\}$. Such an action is a homomorphism from $\mathbf{G}$ to $P(\mathbf{G}, D)$. Moreover, because $P(\mathbf{G}, D) \subset S_{m}$, it follows from Lagrange's theorem that $g$ is a divisor of $m$ !. In this work we consider the situation of isomorphism between $\mathbf{G}$ and $P(\mathbf{G}, D)$, i.e., $g=|\mathbf{G}|$. In the case of homomorphism, $P(\mathbf{G}, D)$ is the permutation group of a subgroup of $\mathbf{G}$ and all the following results are also valid for this subgroup.

Each one of the permutations $P\left(g_{i}, D\right)$ can be expressed as a product of disjoint cycles. If with $e_{j p}$ we indicate the number of cycles of degree $j$ in the permutation $P$, then we can identify a corresponding monomial

$$
\begin{equation*}
x_{1}^{e_{1 p}} x_{2}^{e_{2 p}} \cdots x_{m}^{e_{m p}} \tag{3}
\end{equation*}
$$

in the indeterminates $x_{j}(j=1,2, \ldots, m)$. The cycle index of the permutation group $P(\mathbf{G}, D)$ is the arithmetic mean of these monomials, i.e.,

$$
\begin{align*}
Z(P(\mathbf{G}, D)) & =Z\left(\mathbf{G}, x_{1}, x_{2}, \ldots, x_{m}\right)=\frac{1}{g} \sum_{p \in P(\mathbf{G}, D)} x_{1}^{e_{1 p}} x_{2}^{e_{2 p}} \cdots x_{m}^{e_{m p}} \\
& =\frac{1}{g} \sum_{i=1}^{r} h_{i} x_{1}^{e_{1 i}} x_{2}^{e_{2 i}} \cdots x_{m}^{e_{m i}} \tag{4}
\end{align*}
$$

where the first sum is taken over all the $g$ permutations and the second sum is over the $r$ permutation classes of $P(\mathbf{G}, D), h_{i}$ is the number of permutations of $i$ th class, and the exponent $e_{j i}$ is the number of cycles of degree $j$ in the permutations of the $i$ th class. The following relationships are satisfied:

$$
\begin{gather*}
\sum_{i=1}^{r} h_{i}=g  \tag{5}\\
\sum_{i=1}^{m} i e_{i j}=m \tag{6}
\end{gather*}
$$

Let us now develop the reasoning that allows us to obtain the expression for the cycle index of point groups as a function of the domain $D$. The elements of $\mathbf{G}$ are between the symmetry operations $E, C_{n}^{k}, \sigma, S_{n}^{k}, i$ and $C_{n}^{k} \sigma_{h}$. If with $k^{n_{k}}$ we indicate a cycle of degree $k$ contained $n_{k}$ times in the permutation, then the structures of the cycles and the expressions for the monomials of the cycle index $Z(P(\mathbf{G}, D))$ of the
permutations corresponding to the symmetry operations working on $D$, which are a function of $m$ and of the sites that lie on the symmetry elements, have the form

$$
\begin{align*}
& \left(1^{m}\right) \rightarrow x_{1}^{m} ; \quad\left(1^{n\left(C_{n}\right)},\left(\frac{n}{j}\right)^{\left[\left(m-n\left(C_{n}\right)\right) j / n\right]}\right) \rightarrow x_{1}^{n\left(C_{n}\right)} x_{n / j}^{\left(m-n\left(C_{n}\right)\right) j / n} ; \\
& \left(1^{n(\sigma)}, 2^{[(m-n(\sigma)) / 2]}\right) \rightarrow x_{1}^{n(\sigma)} x_{2}^{(m-n(\sigma)) / 2} ; \\
& \left(1^{n(i)}, 2^{n^{\prime}\left(S_{n}\right)},\left(\frac{n}{j}\right)^{\left[\left(m-n\left(S_{n}\right)\right) j / n\right]}\right) \rightarrow x_{1}^{n(i)} x_{2}^{n^{\prime}\left(S_{n}\right)} x_{n / j}^{\left(m-n\left(S_{n}\right)\right) j / n} ;  \tag{7}\\
& \left(1^{n(i)}, 2^{[(m-n(i)) / 2]}\right) \rightarrow x_{1}^{n(i)} x_{2}^{(m-n(i))) / 2} ; \\
& \left(1^{n(i)}, 2^{\left[\left(m-n\left(\sigma_{h}\right)\right) / 2\right]},\left(\frac{n}{j}\right)^{\left.\left[\left(n\left(\sigma_{h}\right)-n(i)\right)\right) j / n\right]}\right) \rightarrow x_{1}^{n(i)} x_{2}^{\left(m-n\left(\sigma_{h}\right)\right) / 2} x_{n / j}^{\left(n\left(\sigma_{h}\right)-n(i)\right) j / n}
\end{align*}
$$

for $P(E, D), P\left(C_{n}^{k}, D\right), P(\sigma, D), P\left(S_{n}^{k}, D\right), P(i, D)$, and $P\left(C_{n}^{k} \sigma_{h}, D\right)$, respectively. In these cyclic structures of the permutations and of the terms of $Z(P(\mathbf{G}, D)), j$ is the greatest common divisor of $n$ and $k(j=\operatorname{gcd}(n, k))$, respectively, the order of the rotation axis and the number of rotations of $2 \pi / n$ around the axis; $n(p)$ is the number of substitutional sites lying on the symmetry element $p \in\left(C_{n}\right.$ axis, $\sigma$ plane, $i$ inversion, $S_{n}$ axis or the corresponding proper rotation axis); and $n^{\prime}\left(S_{n}\right)=\left(n\left(S_{n}\right)-n(i)\right) / 2$. Of course, $x_{i}^{0}=1(i=1,2, \ldots, m)$.

## 3. Expression for the cycle index

It is convenient to decompose the finite point groups in the proper rotational point groups $\left(\mathbf{C}_{\mathbf{n}}, \mathbf{D}_{\mathbf{n}}, \mathbf{T}, \mathbf{O}, \mathbf{I}\right)$ and in the remaining extended point groups $\left(\mathbf{S}_{\mathbf{2 n}}, \mathbf{C}_{\mathbf{n h}}, \mathbf{C}_{\mathbf{n v}}, \mathbf{D}_{\mathrm{nd}}, \mathbf{D}_{\mathrm{nh}}, \mathbf{T}_{\mathbf{d}}, \mathbf{T}_{\mathbf{h}}, \mathbf{O}_{\mathrm{h}}, \mathbf{I}_{\mathbf{h}}\right)$. As is well known, even when a molecular skeleton exhibits a symmetry group from the second set of groups, the first set of groups may be used in enumerating stereoisomers derived from that skeleton. The cycle indices obtained using equations (7) for the proper rotational groups and for the extended groups are reported in tables 1 and 2 , respectively. The formulas of table 1 were derived by exploiting some previous results [3]. For the formulas of table 2, we used a procedure of resolution into disjoint subsets of the point groups (see table 3), as now described for the case of $\mathbf{D}_{\mathbf{n d}}$ groups. $\mathbf{D}_{\mathbf{n d}}$ can be decomposed in the following way:

$$
\begin{equation*}
\mathbf{D}_{\mathbf{n d}}=\mathbf{D}_{\mathbf{n}} \cup\left\{S_{2 n}, S_{2 n}^{3}, \ldots, S_{2 n}^{2 n-1}\right\} \cup\left\{\sigma_{d_{1}}, \sigma_{d_{2}}, \ldots, \sigma_{d_{n}}\right\}=\mathbf{D}_{\mathbf{n}} \cup \mathbf{S}_{\mathbf{2} \mathbf{n}}^{\prime} \cup\left\{n \sigma_{d}\right\} . \tag{8}
\end{equation*}
$$

A consequence of such a decomposition is that

$$
\begin{equation*}
\sum_{P \in P\left(\mathbf{D}_{\mathbf{n d}}, D\right)} \rightarrow \sum_{P \in P\left(\mathbf{(}_{\mathbf{n}}, D\right)}+\sum_{P \in P\left(\mathbf{S}_{\mathbf{2}}^{\prime}, D\right)}+\sum_{P \in P\left(n \sigma_{d}, D\right)}, \tag{9}
\end{equation*}
$$

Table 1
Expression for the cycle index of proper rotational point groups.

then using equations (7) and $n\left(\sigma_{d}\right)=n\left(\sigma_{d 1}\right)=\cdots=n\left(\sigma_{d n}\right)$ one obtains the formula for the $Z\left(P\left(\mathbf{D}_{\mathbf{n d}}, D\right)\right)$ reported in table 2 . In tables 4 and 5 , some applications for particular rotational point groups are shown.

In the formulas of tables 1,2 , it is supposed that equivalent elements of symmetry leave the same numbers of substitutional sites invariant, as symmetry imposes. Moreover, the arithmetical properties of cyclic groups enable the cycle index of tables 1 and 2 to be expressed through the Euler function $\varphi(n)$, which determines the number of positive integers $(\leqslant n)$ which are coprime to $n$. For the relationships that appear in table 1, see [3], while for those in table 2, relative to the permutations of the groups $\mathbf{S}_{\mathbf{2}}, \mathbf{C}_{\mathbf{n h}}, \mathbf{D}_{\mathbf{n d}}$ and $\mathbf{D}_{\mathbf{n h}}$, see the appendix.

To obtain the enumerator of the isomers from the cycle index $Z(P(\mathbf{G}, D))=$ $Z\left(\mathbf{G}, x_{1}, x_{2}, \ldots, x_{m}\right)$, one must make the substitution

$$
\begin{equation*}
x_{k} \rightarrow w_{1}^{k}+w_{2}^{k}+\cdots+w_{s}^{k}, \tag{10}
\end{equation*}
$$

where $s$ indicates the number of choices for elements or molecular groups that can be attached to each one of $m$ sites of substitution, and $w_{i}$ is a weight variable for the $i$ th substituent. The series counting isomers is just

$$
\begin{equation*}
Z\left(\mathbf{G}, w_{1}+w_{2}+\cdots+w_{s}, w_{1}^{2}+w_{2}^{2}+\cdots+w_{s}^{2}, \ldots, w_{1}^{m}+w_{2}^{m}+\cdots+w_{s}^{m}\right), \tag{11}
\end{equation*}
$$

and the sum of the coefficients of this series gives the total number of isomers, a number equal to

$$
\begin{equation*}
Z(\mathbf{G}, s, s, \ldots, s) . \tag{12}
\end{equation*}
$$

Expanding the isomer-counting polynomial (equation (11)) one obtains a combination of terms of the general form

$$
\begin{equation*}
w_{1}^{n_{1}} w_{2}^{n_{2}} \cdots w_{s}^{n_{s}}, \tag{13}
\end{equation*}
$$

Table 2
Expression for the cycle index of extended point groups.
$Z\left(P\left(\mathbf{S}_{\mathbf{2 n}}, D\right)\right)=\frac{1}{2} Z\left(P\left(\mathbf{C}_{\mathbf{n}}, D\right)\right)+\frac{1}{2 n} x_{1}^{n(i)} x_{2}^{n^{\prime}\left(S_{2 n}\right)} \sum_{k \mid 2 n}^{\prime} \varphi(2 n / k) x_{2 n / k}^{\left(m-n\left(S_{2 n}\right)\right) k / 2 n}$
( $\sum_{k \mid 2 n}^{\prime}$ is over the odd divisors of $2 n$ )

$$
\begin{aligned}
Z\left(P\left(\mathbf{C}_{\mathbf{n v}}, D\right)\right)= & \frac{1}{2} Z\left(P\left(\mathbf{C}_{\mathbf{n}}, D\right)\right)+\left\{\begin{array}{l}
\frac{1}{2} x_{1}^{n^{\left(\sigma_{v}\right)}} x_{2}^{\left(m-n\left(\sigma_{v}\right)\right) / 2} \quad(n \text { odd }), \\
\frac{1}{4}\left(x_{1}^{n^{\left(\sigma_{v}\right)}} x_{2}^{\left(m-n\left(\sigma_{v}\right)\right) / 2}+x_{1}^{n\left(\sigma_{d}\right)} x_{2}^{\left(m-n\left(\sigma_{d}\right)\right) / 2}\right) \quad \text { ( } n \text { even) }
\end{array}\right. \\
Z\left(P\left(\mathbf{C}_{\mathbf{n h}}, D\right)\right)= & \frac{1}{2} Z\left(P\left(\mathbf{C}_{\mathbf{n}}, D\right)\right)+\frac{1}{2 n} x_{1}^{n(i)} x_{2}^{\left(m-n\left(\sigma_{h}\right)\right) / 2} \sum_{k \mid n} \varphi(k) x_{k}^{\left(n\left(\sigma_{h}\right)-n(i)\right) / k} \\
Z\left(P\left(\mathbf{D}_{\mathbf{n d}}, D\right)==\right. & \frac{1}{2} Z\left(P\left(\mathbf{D}_{\mathbf{n}}, D\right)\right)+\frac{1}{4} x_{1}^{n\left(\sigma_{d}\right)} x_{2}^{\left(m-n\left(\sigma_{d}\right)\right) / 2} \\
& \quad+\frac{1}{4 n} x_{1}^{n(i)} x_{2}^{n^{\prime}\left(C_{n}\right)} \sum_{k \mid 2 n}^{\prime} \varphi(2 n / k) x_{2 n / k}^{\left(m-n\left(C_{n}\right)\right) k / 2 n}, \quad n^{\prime}\left(C_{n}\right)=\left(n\left(C_{n}\right)-n(i)\right) / 2
\end{aligned}
$$

$Z\left(P\left(\mathbf{D}_{\mathbf{n h}}, D\right)\right)=\frac{1}{2} Z\left(P\left(\mathbf{D}_{\mathbf{n}}, D\right)\right)$

$$
\begin{gathered}
+\left\{\begin{array}{c}
\frac{1}{4 n}\left(p x_{1}^{n\left(\sigma_{v}\right)} x_{2}^{\left(m-n\left(\sigma_{v}\right)\right) / 2}+p x_{1}^{n\left(\sigma_{d}\right)} x_{2}^{\left(m-n\left(\sigma_{d}\right)\right) / 2}+x_{1}^{n(i)} x_{2}^{\left(m-n\left(\sigma_{h}\right)\right) / 2} \sum_{k \mid n} \varphi(k) x_{k}^{\left(n\left(\sigma_{h}\right)-n(i)\right) / k}\right) \\
\frac{1}{4 n}\left(n x_{1}^{n\left(\sigma_{v}\right)} x_{2}^{\left(m-n\left(\sigma_{v}\right)\right) / 2}+x_{1}^{n(i)} x_{2}^{\left(m-n\left(\sigma_{h}\right)\right) / 2} \sum_{k \mid n} \varphi(k) x_{k}^{\left(n\left(\sigma_{h}\right)-n(i)\right) / k}\right) \quad(n \text { odd })
\end{array}\right. \\
Z\left(P\left(\mathbf{T}_{\mathbf{d}}, D\right)\right)=\frac{1}{2} Z(P(\mathbf{T}, D))+\frac{1}{24}\left(6 x_{1}^{n(i)} x_{2}^{n^{\prime}\left(S_{4}\right)} x_{4}^{\left(m-n\left(C_{2}\right)\right) / 4}+6 x_{1}^{n(\sigma)} x_{2}^{(m-n(\sigma)) / 2)}\right) \\
Z\left(P\left(\mathbf{T}_{\mathbf{h}}, D\right)\right)=\frac{1}{2} Z(P(\mathbf{T}, D))+\frac{1}{24}\left(x_{1}^{n(i)} x_{2}^{(m-n(i)) / 2}+3 x_{1}^{n(\sigma)} x_{2}^{(m-n(\sigma)) / 2}+8 x_{1}^{n(i)} x_{2}^{n^{\prime}\left(S_{6}\right)} x_{6}^{\left(m-n\left(C_{3}\right)\right) / 6}\right) \\
\begin{aligned}
Z\left(P\left(\mathbf{O}_{\mathbf{h}}, D\right)\right)=\frac{1}{2} Z(P(\mathbf{O}, D))+\frac{1}{48}\left(x_{1}^{n(i)} x_{2}^{(m-n(i)) / 2}+8 x_{1}^{n(i)} x_{2}^{n^{\prime}\left(S_{6}\right)} x_{6}^{\left(m-n\left(C_{3}\right)\right) / 6}\right. \\
+6 x_{1}^{n(i)} x_{2}^{n^{\prime}\left(S_{4}\right)} x_{4}^{\left(m-n\left(C_{4}\right)\right) / 4}+3 x_{1}^{n\left(\sigma_{h}\right)} x_{2}^{\left(m-n\left(\sigma_{h}\right)\right) / 2} \\
\left.+6 x_{1}^{n\left(\sigma_{d}\right)} x_{2}^{\left(m-n\left(\sigma_{d}\right)\right) / 2}\right)
\end{aligned}
\end{gathered}
$$

$Z\left(P\left(\mathbf{I}_{\mathbf{h}}, D\right)\right)=\frac{1}{2} Z(P(\mathbf{I}, D))+\frac{1}{120}\left(x_{1}^{n(i)} x_{2}^{(m-n(i)) / 2}+24 x_{1}^{n(i)} x_{2}^{n^{\prime}\left(S_{10}\right)} x_{10}^{\left(m-n\left(C_{5}\right)\right) / 10}\right.$

$$
\left.+20 x_{1}^{n(i)} x_{2}^{n^{\prime}\left(S_{6}\right)} x_{6}^{\left(m-n\left(C_{3}\right)\right) / 6}+15 x_{1}^{n(\sigma)} x_{2}^{(m-n(\sigma)) / 2}\right)
$$

with $n_{i}=1,2, \ldots, m$ and $\sum_{i=1}^{s} n_{i}=m$. The coefficient of this term, in the expanded form, is the number of isomers of the general formula

$$
\begin{equation*}
R A_{n_{1}} B_{n_{2}} \cdots Z_{n_{s}} \tag{14}
\end{equation*}
$$

where $R$ is the formula for the root structure on which substitutions are being made, and $A, B, \ldots, Z$ indicate elements or molecular groups corresponding to the respective weights $w_{1}, w_{2}, \ldots, w_{s}$.

Table 3
Resolution of extended groups.

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\(\mathbf{S}_{\mathbf{2 n}}=\mathbf{C}_{\mathbf{n}} \cup\left\{S_{2 n}, S_{2 n}^{3}, \ldots, S_{2 n}^{2 n-1}\right\}=\mathbf{C}_{\mathbf{n}} \cup \mathbf{S}_{\mathbf{2 n}}^{\prime}\)
\(\mathbf{C}_{\mathbf{n v}}=\left\{\begin{array}{l}\mathbf{C}_{\mathbf{n}} \cup\left\{n \sigma_{v}\right\} \quad(n \text { odd }), \\ \mathbf{C}_{\mathbf{n}} \cup\left\{p \sigma_{v}\right\} \cup\left\{p \sigma_{v}^{\prime}\right\} \quad(n=2 p, \text { even })\end{array}\right.\)
\(\mathbf{C}_{\mathbf{n h}}=\mathbf{C}_{\mathbf{n}} \cup\left\{\sigma_{h}, C_{n} \sigma_{h}, C_{n}^{2} \sigma_{h}, \ldots, C_{n}^{n-1} \sigma_{h}\right\}=\mathbf{C}_{\mathbf{n}} \cup \mathbf{C}_{\mathbf{n}} \sigma_{h}\)
\(\mathbf{D}_{\mathbf{n h}}=\left\{\begin{array}{l}\mathbf{D}_{\mathbf{n}} \cup\left\{\sigma_{h}, C_{n} \sigma_{h}, \ldots, C_{n}^{n-1} \sigma_{h}\right\} \cup\left\{n \sigma_{v}\right\}=\mathbf{D}_{\mathbf{n}} \cup \mathbf{C}_{\mathbf{n}} \sigma_{h} \cup\left\{n \sigma_{v}\right\} \quad(n \text { odd }), \\ \mathbf{D}_{\mathbf{n}} \cup\left\{\sigma_{h}, C_{n} \sigma_{h}, \ldots, C_{n}^{n-1} \sigma_{h}\right\} \cup\left\{p \sigma_{v}\right\} \cup\left\{p \sigma_{d}\right\}=\mathbf{D}_{\mathbf{n}} \cup \mathbf{C}_{\mathbf{n}} \sigma_{h} \cup\left\{p \sigma_{v}\right\} \cup\left\{p \sigma_{d}\right\} \\ \quad(n=2 p, \text { even })\end{array}\right.\)
\(\mathbf{D}_{\mathbf{n d}}=\mathbf{D}_{\mathbf{n}} \cup\left\{S_{2 n}, S_{2 n}^{3}, \ldots, S_{2 n}^{2 n-1}\right\} \cup\left\{\sigma_{d_{1}}, \sigma_{d_{2}}, \ldots, \sigma_{d_{n}}\right\}=\mathbf{D}_{\mathbf{n}} \cup \mathbf{S}_{\mathbf{2 n}}^{\prime} \cup\left\{n \sigma_{d}\right\}\)
\(\mathbf{T}_{\mathbf{d}}=\mathbf{T} \cup\left\{S_{4 x}, S_{4 x}^{3}, S_{4 y}, S_{4 y}^{3}, S_{4 z}, S_{4 z}^{3}\right\} \cup\left\{\sigma_{1}, \ldots, \sigma_{6}\right\}\)
\(\mathbf{T}_{\mathbf{h}}=\mathbf{T} \cup\left\{i, 3 \sigma, 4 S_{6}, 4 S_{6}^{5}\right\}\)
\(\mathbf{O}_{\mathbf{h}}=\mathbf{O} \cup\left\{i, 8 S_{6}, 6 S_{4}, 3 \sigma_{h}, 6 \sigma_{d}\right\}\)
\(\mathbf{I}_{\mathbf{h}}=\mathbf{I} \cup\left\{i, 12 S_{10}, 12 S_{10}^{3}, 20 S_{6}, 15 \sigma\right\}\)
```

Table 4
Examples of the cyclic index of $\mathbf{C}_{\mathbf{n}}$ and $\mathbf{D}_{\mathbf{n}}$ point groups.
$Z\left(P\left(\mathbf{C}_{\mathbf{n}}, D\right)\right)$
$Z\left(P\left(\mathbf{C}_{2}, D\right)\right)=\frac{x_{1}^{n\left(C_{2}\right)}}{2}\left(x_{1}^{\left(m-n\left(C_{2}\right)\right)}+x_{2}^{\left(m-n\left(C_{2}\right)\right) / 2}\right)$
(a) $\mathrm{H}_{2} \mathrm{O}_{2}: m=2, n\left(C_{2}\right)=0 \quad Z\left(P\left(\mathbf{C}_{2}, D\right)\right)=\frac{1}{2}\left(x_{1}^{2}+x_{2}^{1}\right)$
(b) $\mathrm{H}_{2} \mathrm{C}\left(\mathrm{C}_{6} \mathrm{H}_{5}\right)_{2}: m=12, n\left(C_{2}\right)=0 \quad Z\left(P\left(\mathbf{C}_{2}, D\right)\right)=\frac{1}{2}\left(x_{1}^{12}+x_{2}^{6}\right)$
$Z\left(P\left(\mathbf{C}_{3}, D\right)\right)=\frac{x_{1}^{n\left(C_{3}\right)}}{3}\left(x_{1}^{m-n\left(C_{3}\right)}+2 x_{3}^{\left(m-n\left(C_{3}\right)\right) / 3}\right)$
$\mathrm{HC}\left(\mathrm{C}_{6} \mathrm{H}_{5}\right)_{3}: m=16, n\left(C_{3}\right)=1 \quad Z\left(P\left(\mathbf{C}_{3}, D\right)\right)=\frac{1}{3}\left(x_{1}^{16}+2 x_{1}^{1} x_{3}^{5}\right)$
Regular polygon of $n$ sides
Vertex: $m=n, n\left(C_{n}\right)=0 \quad Z\left(P\left(\mathbf{C}_{\mathbf{n}}, D\right)\right)=\frac{1}{n} \sum_{k \mid n} \varphi(k) x_{k}^{n / k}$
Pyramid with base a regular polygon of $n$ sides
Vertex: $m=n+1, n\left(C_{n}\right)=1 \quad Z\left(P\left(\mathbf{C}_{\mathbf{n}}, D\right)\right)=\frac{x_{1}^{1}}{n} \sum_{k \mid n} \varphi(k) x_{k}^{n / k}$

$$
Z\left(P\left(\mathbf{D}_{\mathbf{n}}, D\right)\right)
$$

$Z\left(P\left(\mathbf{D}_{\mathbf{2}}, D\right)\right)=\frac{1}{4}\left(x_{1}^{m}+x_{1}^{n\left(C_{2 x}\right)} x_{2}^{\left(m-n\left(C_{2 x}\right)\right) / 2}+x_{1}^{n\left(C_{2 y}\right)} x_{2}^{\left(m-n\left(C_{2 y}\right)\right) / 2}+x_{1}^{n\left(C_{2 z}\right)} x_{2}^{\left(m-n\left(C_{2 z}\right)\right) / 2}\right)$
$\mathrm{C}_{4 n+2} \mathrm{H}_{2 n+4}$ (acenes, $n$ is the number of condensed rings): $m=2 n+4$
$n\left(C_{2 x}\right)=n\left(C_{2 y}\right)=n\left(C_{2 z}\right)=0(n$ even $)$
$n\left(C_{2 x}\right)=n\left(C_{2 y}\right)=0, n\left(C_{2 z}\right)=2(n$ odd $)$
$Z\left(P\left(\mathbf{D}_{\mathbf{2}}, D\right)\right)=\frac{1}{4}\left(x_{1}^{2 n+4}+3 x_{2}^{n+2}\right)(n$ even $)$
$Z\left(P\left(\mathbf{D}_{\mathbf{2}}, D\right)\right)=\frac{1}{4}\left(x_{1}^{2 n+4}+2 x_{2}^{n+2}+x_{1}^{2} x_{2}^{n+1}\right)(n$ odd $)$
$Z\left(P\left(\mathbf{D}_{3}, D\right)\right)=\frac{1}{6}\left(x_{1}^{m}+2 x_{1}^{n\left(C_{3}\right)} x_{3}^{\left(m-n\left(C_{3}\right)\right) / 3}+3 x_{1}^{n\left(C_{2}\right)} x_{2}^{\left(m-n\left(C_{2}\right)\right) / 2}\right)$
$\mathrm{B}\left(\mathrm{C}_{6} \mathrm{H}_{5}\right)_{3}: m=15, n\left(C_{3}\right)=0, n\left(C_{2}\right)=1 \quad Z\left(P\left(\mathbf{D}_{3}, D\right)\right)=\frac{1}{6}\left(x_{1}^{15}+2 x_{3}^{5}+3 x_{1}^{1} x_{2}^{7}\right)$
A $n$-sided prism or antiprism
Vertex: $m=2 n, n\left(C_{n}\right)=0, n\left(C_{2}\right)=n\left(C_{3}\right)=0 \quad Z\left(P\left(\mathbf{D}_{\mathbf{n}}, D\right)\right)=\frac{1}{2 n} \sum_{k \mid n} \varphi(k) x_{k}^{2 n / k}+\frac{1}{2} x_{2}^{n}$

Table 5
Examples of the cyclic index of $\mathbf{T}, \mathbf{O}$ and $\mathbf{I}$ point groups.

$$
Z(P(\mathbf{T}, D))
$$

Tetrahedron
(a) Vertex or faces: $m=4, n\left(C_{3}\right)=1, n\left(C_{2}\right)=0$
$Z(P(\mathbf{T}, D))=\frac{1}{12}\left(x_{1}^{4}+8 x_{1}^{1} x_{3}^{1}+3 x_{2}^{2}\right)$
(b) Edges: $m=6, n\left(C_{3}\right)=0, n\left(C_{2}\right)=2$
$Z(P(\mathbf{T}, D))=\frac{1}{12}\left(x_{1}^{6}+3 x_{1}^{2} x_{2}^{2}+8 x_{3}^{2}\right)$

$$
Z(P(\mathbf{O}, D))
$$

## Octahedron and cube

(a) Vertex of octahedron or faces of cube: $m=6, n\left(C_{4}\right)=2, n\left(C_{3}\right)=n\left(C_{2}\right)=0$
$Z(P(\mathbf{O}, D))=\frac{1}{24}\left(x_{1}^{6}+6 x_{1}^{2} x_{4}^{1}+3 x_{1}^{2} x_{2}^{2}+8 x_{3}^{2}+6 x_{2}^{3}\right)$
(b) Faces of octahedron or vertex of cube: $m=8, n\left(C_{4}\right)=0, n\left(C_{3}\right)=2, n\left(C_{2}\right)=0$
$Z(P(\mathbf{O}, D))=\frac{1}{24}\left(x_{1}^{8}+6 x_{4}^{2}+3 x_{2}^{4}+8 x_{1}^{2} x_{3}^{2}+6 x_{2}^{4}\right)$
(c) Edges of octahedron and of cube: $m=12, n\left(C_{4}\right)=0, n\left(C_{3}\right)=0, n\left(C_{2}\right)=2$
$Z(P(\mathbf{O}, D))=\frac{1}{24}\left(x_{1}^{12}+6 x_{4}^{3}+3 x_{2}^{6}+8 x_{3}^{4}+6 x_{1}^{2} x_{2}^{5}\right)$

$$
Z(P(\mathbf{I}, D))
$$

Icosahedron and dodecahedron
(a) Vertex of icosahedron or faces of dodecahedron: $m=12, n\left(C_{5}\right)=2, n\left(C_{3}\right)=n\left(C_{2}\right)=0$ $Z(P(\mathbf{I}, D))=\frac{1}{60}\left(x_{1}^{12}+24 x_{1}^{2} x_{5}^{2}+20 x_{3}^{4}+15 x_{2}^{6}\right)$
(b) Vertex of dodecahedron or faces of icosahedron: $m=20, n\left(C_{5}\right)=0, n\left(C_{3}\right)=2, n\left(C_{2}\right)=0$ $Z(P(\mathbf{I}, D))=\frac{1}{60}\left(x_{1}^{20}+24 x_{5}^{4}+20 x_{1}^{2} x_{3}^{6}+15 x_{2}^{10}\right)$
(c) Edges of icosahedron and of dodecahedron: $m=30, n\left(C_{5}\right)=n\left(C_{3}\right)=0, n\left(C_{2}\right)=2$ $Z(P(\mathbf{I}, D))=\frac{1}{60}\left(x_{1}^{30}+24 x_{5}^{6}+20 x_{3}^{10}+15 x_{1}^{2} x_{2}^{14}\right)$

## Truncated icosahedron

(a) Vertex: $m=60, n\left(C_{5}\right)=n\left(C_{3}\right)=n\left(C_{2}\right)=0$
$Z(P(\mathbf{I}, D))=\frac{1}{60}\left(x_{1}^{60}+24 x_{5}^{12}+20 x_{3}^{20}+15 x_{2}^{30}\right)$
(b) Faces: $m=32, n\left(C_{5}\right)=n\left(C_{3}\right)=2, n\left(C_{2}\right)=0$
$Z(P(\mathbf{I}, D))=\frac{1}{60}\left(x_{1}^{32}+24 x_{1}^{2} x_{5}^{6}+20 x_{1}^{2} x_{3}^{10}+15 x_{2}^{16}\right)$
(c) Edges: $m=90, n\left(C_{5}\right)=n\left(C_{3}\right)=0, n\left(C_{2}\right)=2$
$Z(P(\mathbf{I}, D))=\frac{1}{60}\left(x_{1}^{90}+24 x_{5}^{18}+20 x_{3}^{30}+15 x_{1}^{2} x_{2}^{44}\right)$

## Appendix

Let $C_{r}$ be the cyclic group of order $r$, then the cycle index of $C_{r}$ is

$$
\begin{equation*}
\frac{1}{r} \sum_{d \mid r} \varphi(r / d) x_{r / d}^{d} \tag{A1}
\end{equation*}
$$

where the sum is over all the divisors of $r$. In fact, the following two properties are worth noting:
(1) called $\alpha$, a generator of $C_{r}$, for each $k \in\{1,2, \ldots, r\}$, the permutation $\alpha^{k} \in C_{r}$ is of type $x_{r / d}^{d}$ with $g=\operatorname{gcd}(r, k)$;
(2) for each $d$ divisor of $r$, the elements $k \in\{1,2, \ldots, r-1\}$ such that $k<r$, $\operatorname{gcd}(r, k)=d$ are $\varphi(r / d)$, because they are as many as the numbers $t$ such that
$k=t d, r=h d$ with $t$ and $h$ primes between them and $t<h$, or they are $\varphi(h)=\varphi(r / d)$.
From (1) and (2) it follows that

$$
\begin{equation*}
\sum_{k=1,2, \ldots, r-1} x_{r / d}^{d}=\sum_{t \mid r} \varphi(r / t) x_{r / t}^{t} \tag{A2}
\end{equation*}
$$

where in the left sum $d$ indicates the $\operatorname{gcd}(r, k)$, while in the right sum it is extended to all the proper divisors of $r$. Adding the identity permutation, the thesis is obtained.

In the case where the permutations of the group $\mathbf{S}_{\mathbf{2} \mathbf{n}}$ corresponding to the rotoreflections are considered, the sum is extended only to odd divisors of $2 n$.

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