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Multinomial combinatorial group representations of the octahedral and cubic symmetries

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We consider the full multinomial combinatorics of all irreducible representations of the octahedral (cubic) symmetry as a function of partitions for vertex, face and edge colorings. Full combinatorial tables for all irreducible representations and all multinomial partitions are constructed. These enumerations constitute multinomial expansions of character-based cycle index polynomials, and grow in combinatorial complexity as a function of edge or vertex coloring partitions.

KEY WORDS: group representations, combinations, multinomials, Pólya's theorem, cubic and octahedral symmetries

1. Introduction

Applications of combinatorics and graph theory to chemical problems and spectroscopy have been the topic of numerous studies in the last several decades [1–33]. These applications have ranged from simple enumeration of chemical isomers, isomerization reactions, enumeration of polyhedral ligand substitutions, chirality, use of mark groups, double cosets, combinatorics of configuration interaction computations, many-electron correlations, NMR, ESR, and so on. Both mathematical and chemical areas have enjoyed significant advances and growth as a result of this cross-fertilization. Pólya's classical paper [6, 7] on a combinatorial enumeration technique, now well known as, Pólya's theorem derived its motivation from chemistry. Enumerations of chemical isomers [1–7,8–18] including those of fullerene cages [31] have in turn been benefited by Pólya's technique and its generalization.

Advances have been made in the mathematical context by Williamson [22, 23] and Merris [24], and in the chemical context by Balasuramanian [20] to generalize Pólya's theorem to all irreducible representations of the group. Generalization of De Brujin's theorem to all characters has also been accomplished

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by Balasubramanian [9]. Balasubramanian [19,20] for the first time provided a geometric, chemical or spectroscopic interpretation to the generalization of this technique to all irreducible representations of the groups. While such techniques have been presented they were often restricted to a few kinds of substituents or colors or ligands. The algebra of applying these irreducible representations-based combinatorics becomes complex as a function of different types of partitions. Thus, these techniques have been often applied to cases of two colors for which the expressions become binomial expansions, or three or even four types of such colors. Yet a full combinational classification of these irreducible patterns requires exhaustive types of all possible distinct colors. For example, the edges of an octahedron or a cube can be colored at most with 12 different kinds of colors, vertices of a cube with eight different types of colors and so on. The computational complexity also grows exponentially as the color type partition, as represented by Young's diagram, becomes complex with many rows. Hence exhaustive generation of such combinatorial numbers can be challenging and may provide additional insight.

Many practical applications [20,32] often require such multinomially driven combinatorial expansions. Consider for example, the naturally occurring isotope of Bismuth, ^{209}Bi, has a nuclear spin of 9/2. This means that there are 10 distinct orientations of the magnetic spin vector, which we represent by $m_{\mathrm{f}} = -9/2, -7/2, -5/2, -3/2, -1/2, 1/2, 3/2, 5/2, 7/2,$ and 9/2. One can visualize each of these orientations as a distinct type of color and thus the nuclear spin statistics of bismuth clusters would require decanomial combinatorics. The challenge is simply from combinatorial explosions that occur quite rapidly with cluster size. Fullerene cages also present considerable challenge when extended for multinomial combinatorics.

In this work we consider exhaustive multinomial combinatorics of the octahedron and its close relative the cube. We have constructed exhaustive combinatorial tables for all irreducible representations of the cube vertex (octahedral face) colorings with eight different types of colors represented by the Young's tableau of eight for all irreducible representations, edge colorings with young tableau of 12, and vertex colorings of octahedron (face colorings of cube), all of which accomplished using multinomial combinatorics. This also yields some well-known results on chirality and ligand partitions [25,26,29] as special cases and isomer counts for all types of partitions exhaustively.

2. Multinomial combinatorics

Let $[n]$ be an ordered partition of n into p parts such that

$$n_1 \geq 0, n_2 \geq 0, \ldots, n_p \geq 0, \quad \sum_{i=1}^{p} n_i = n.$$

Then a multinomial expansion in λs is defined as

$$(\lambda_1 + \lambda_2 + \cdots \lambda_p)^n = \sum_{[\lambda]} \binom{n}{n_1\ n_2 \cdots n_p} \lambda_1^{n_1} \lambda_2^{n_2} \cdots \lambda_p^{np},$$

where $\binom{n}{n_1\ n_2 \cdots n_p}$ are defined as multinomial coefficients and the sum is over all such ordered partitions, also known as composition of the integer n into p parts.

The multinomial coefficients can be proven to satisfy

$$\binom{n}{n_1\ n_2 \ldots n_p} = \frac{n!}{n_1! n_2! \cdots n_p!}.$$

A few properties are that sum of all coefficients in the above expansion is p^n. It can also be proven that

$$\binom{n+q}{n_1\ n_2 \cdots n_p} = \sum_{[k]=n} \binom{n}{k_1\ k_2 \cdots k_p} \binom{q}{n_1 - k_1\ n_2 - k_2 \cdots n_p - k_p},$$

where $[k]$ stands for all ordered partitions of m such that $k_1 + k_2 + \cdots + k_p = n$, with k_i non-negative integers.

The well-known Pólya's theorem [7] provides a generating function for multinomial expansions in terms of the ordinary cycle index of a group, which is simply sum of all orbit structures of permutations of a group when it acts on a set D divided by $|G|$, the order of the group. Williamson [22,23], Merris [24] and Balasubramanian [19,20] have independently generalized the cycle index, and in particular, the current author provided a physical and geometrical interpretation of the numbers enumerated.

Define the symmetry operator T_{G}^{χ} as

$$T_G^{\chi} = \frac{1}{|G|} \sum_{g \in G} \chi(g) P(g),$$

where $\chi(g)$ be the character value of $g \in G$ for an irreducible representation Γ in the group G and $P(g)$ is a permutation operator for g. One can define a weighted permutation operator by introducing weights, which also appear in the multinomial expansion. Let D be the set of vertices, edges or faces and R be a set of colors and let us assign a weight for each color r in R. Then the weight of a function f from D to R is defined as

$$W(f) = \prod_{i=1}^{n} w(f(i)).$$

A permutational operator for each weight W is denoted by $P_W(g)$. In a matrix representation of $P_w(g)$ we can define a tensor version of Pólya's theorem for all irreducible representations in the group. In this representation the trace of $P_w(g)$ is

$$Tr(P_w(g)) = \sum_{f}^{(g)} W(f),$$

where the sum is over all f for which $gf = f$, we thus obtain:

$$T_G^{W,\chi} = \frac{1}{|G|} \sum_{g \in G} \chi(g) P_W(g).$$

$$TrT_G^{W,\chi} = \frac{1}{|G|} \sum_{g \in G} \chi(g) Tr[P_W(g)] = \frac{1}{|G|} \sum_{g \in G} \chi(g) \sum_{f}^{(g)} W(f).$$

The above generalized version Pólya's theorem can be conveniently expressed in terms of generalized character cycle index (GCCI) P_G^χ for every irreducible representation can be defined as

$$P_G^\chi = \frac{1}{|G|} \sum_{g \in G} \chi(g) s_1^{b_1} s_2^{b_2} \cdots s_n^{b_n},$$

where the sum is over all elements of the group and $s_1^{b_1} s_2^{b_2} \cdots s_n^{b_n}$ is the cyclic polynomial representation if g in G generates b_1 cycles of length 1, b_2 cycles of length $2, \ldots, b_{\mathrm{n}}$ cycles of length n when g acts on the set of elements D. The difference between Pólya's cycle index and the one above is that for each irreducible representation, we have a cycle index due to the character values multiplying the polynomial.

A multinomial combinatorial function can be obtained for each irreducible representation by substituting every s_{k} in the above expression. Let n be the number of elements in the set D. Then let R be a set of n distinct types of colors such as white, green, yellow, purple, magenta, green, red, and so on. Let $\lambda_1, \lambda_2, \ldots, \lambda_{\mathrm{n}}$ be distinct weights for these colors. The multinomial combinatorial function is obtained by substituting every s_{k} in the GCCI by $\lambda_1^k + \lambda_2^k + \cdots + \lambda_n^k$. Symbolically,

$$GF^\chi = P_G^\chi \left(S_k \to \sum_i \lambda_i^k \right).$$

Thus the above substitution generates a powerful multinomial expansion where coefficients have rich combinatorial significance for each irreducible representation of the group. For example, for the identity representation the GF enumerates isomers or equivalence classes in Pólya's term. For the anti-symmetric irreducible representation (the one which has –1 character values for all improper rotations), the index enumerates all chiral isomers. For any irreducible representation Γ whose character is χ, the GF^{χ} enumerates equivalence classes of functions from the set D to R such that they transform according to the irreducible representation Γ. We believe that this is the most powerful and general interpretation under which all enumerative combinatorics is encompassed.

The terms in the multinomial expansion would have all ordered partitions of n into various parts. First partitions of n are enumerated as provided by Young's diagram. Then for each partition all ordered tuples arising from that partition by allowing permutations of the entries correspond to the terms in the multinomial. This generates all compositions of n into p parts, and p is varied from 0 to n, to represent all terms in the multinomial expansion. The whole generating function then contains terms some of which are combinatorially equivalent. For example, the term $\lambda_1^4\lambda_2^2\lambda_3\lambda_4^1$, $\lambda_1^4\lambda_3^2\lambda_4\lambda_6^1$, $\lambda_2^4\lambda_4^2\lambda_6\lambda_7^1$, etc., are all equivalent to each other in combinatorial terms and their coefficients in the multinomial expansion would be the same. Thus the unique terms of the multinomial GF^{χ}s are simply represented by the Young diagrams of partition n.

3. Application to the octahedron (cube)

The octahedron and its relative cube present one of the most interesting cases of multinomial combinatorics since the three-dimensional octahedral group O_h of 48 operations presents interesting combinatorics, especially for the edge coloring character combinatorics. Thus as a first case, we shall consider the edge colorings of the cube and octahedron for all irreducible representations of the group. Let D be the set of 12 edges and R be a set of 12 distinct colors such as white, yellow, blue, green, red, purple, magenta, cyan, and so on. There are exactly 12^{12} such possible colorings of the edges of the cube. These 12^{12} colorings would transform as various irreducible representations of the O_h group when appropriately symmetry-adapted. In particular, the number of totally symmetric representations, i.e., number of maps among 12^{12} maps that transform as the A_{1g} representation of the group is the number of equivalence classes or positional isomers for the various distribution of colors. Likewise, the number of functions that transform as the A_{1u} representation, which has the character values of –1 for all improper rotations correspond to the patterns of chiral edge colors among 12^{12} maps, such that one function is not transformable into another chiral representation by the operation of the O_h group. Note that unlike ordinary isomer enumeration, where one considers only the rotational subgroup, we consider the entire group so that chiral, achiral, and in general all irreducible representations are covered.

We shall first construct the various cycle indices for the set D of edges. Note that the polynomials in the cycle index would depend on the set D. Hence for the 12 edges, the polynomial for the A_{1u} irreducible representation of the O_h

group is

$$P_G^{A_{1u}} = \frac{1}{48}\left[s_1^{12} - 3s_1^4 s_2^4 + (3-1)s_2^6 + (-6+6)s_1^2 s_2^5 + (-6+6)s_4^3 + 8s_3^4 - 8s_6^2\right],$$

where we have shown the terms that cancel out for clarity. By replacing every s_k by

$$\sum_i \lambda_i^k$$

in the above expression, we obtain,

$$\begin{aligned} P_{O_h}^{A_{1u}} = \frac{1}{48}\Big[&(\lambda_1+\lambda_2+\cdots+\lambda_{12})^{12} - 3(\lambda_1+\lambda_2+\cdots+\lambda_{12})^4(\lambda_1^2+\lambda_2^2+\cdots+\lambda_{12}^2)^4 \\ &+ 2(\lambda_1^2+\lambda_2^2+\cdots+\lambda_{12}^2)^6 \\ &+ 8(\lambda_1^3+\lambda_2^3+\cdots+\lambda_{12}^3)^4 - 8(\lambda_1^6+\lambda_2^6+\cdots+\lambda_{12}^6)^2\Big] \end{aligned}$$

The coefficient of a term $\lambda_1^{b_1}\lambda_2^{b_2}\cdots\lambda_{12}^{b_{12}}$ enumerates number of times the irreducible representation A_{1u} occurs in the equivalence classes of functions that contain b_1 colors of type 1, b_2 colors of type 2, …, b_{12} colors of the type 12. Since A_{1u} representation has all –1 character values for the improper rotations this also corresponds to the number of chiral edge colorings of the cube with the given distribution of colors.

Table 1 shows all the cycle index polynomials of all irreducible representations for the O_h group for edge colorings. As seen from table 1 another example of the GCCI would be that of the T_{1g} irreducible representation. The multinomial expansion is given as follows:

$$\begin{aligned} P_{O_h}^{T_{1g}} = \frac{1}{48}\Big[&3(\lambda_1+\lambda_2+\cdots+\lambda_{12})^{12} - 6(\lambda_1+\lambda_2+\cdots+\lambda_{12})^4(\lambda_1^2+\lambda_2^2+\cdots+\lambda_{12}^2)^4 \\ &- 12(\lambda_1+\lambda_2+\cdots+\lambda_{12})^2(\lambda_1^2+\lambda_2^2+\cdots+\lambda_{12}^2)^5 + 12(\lambda_1^4+\lambda_2^4+\cdots+\lambda_{12}^4)^3\Big]. \end{aligned}$$

Again the coefficient of a typical term $\lambda_1^{b_1}\lambda_2^{b_2}\cdots\lambda_{12}^{b_{12}}$ enumerates number of times the irreducible representation T_{1g} occurs in the equivalence classes of functions that contain b_1 colors of type 1, b_2 colors of type 2, …, b_{12} colors of the type 12.

Table 2 shows our complete combinatorial results for the edge colorings of the octahedron or cube for all irreducible representations. As noted above there are many more terms in the above expansions than the ones displayed in table 2, but we show only the unique terms as determined by the Young diagrams of the integer 12. For example, the very first diagram represents 12 terms, viz., λ_1^{12} or $\lambda_2^{12}\cdots\lambda_{12}^{12}$. Likewise each Young diagram represents multiple ordered partitions, and we have shown only one of them since coefficients are same for all of these. As seen from Table 2 some fascinating results are revealed about the cube for all irreducible representations of the O_h group. First non-zero A_{1u} representation occurs for the partition [10+2], which has one chiral coloring. This would

Table 1
GCCI table for the edge colorings of the cube.

	1^{12}	$1^4\ 2^4$	2^6	2^6	$1^2\ 2^5$	$1^2\ 2^5$	4^3	4^3	3^4	6^2
	1	3	3	1	6	6	6	6	8	8
A_{1g}	1	1	1	1	1	1	1	1	1	1
A_{2g}	1	1	1	1	−1	−1	−1	−1	1	1
A_{2u}	1	−1	1	−1	1	−1	−1	1	1	−1
A_{1u}	1	−1	1	−1	−1	1	1	−1	1	−1
E_g	2	2	2	2	0	0	0	0	−1	−1
E_u	2	−2	2	−2	0	0	0	0	−1	1
T_{1g}	3	−1	−1	3	−1	−1	1	1	0	0
T_{2g}	3	−1	−1	3	1	1	−1	−1	0	0
T_{1u}	3	1	−1	−3	1	−1	1	−1	0	0
T_{2u}	3	1	−1	−3	−1	1	−1	1	0	0

correspond to the term $\lambda_1^{10}\lambda_2^2$. Many other results are combinatorially complex. An important result that enables us to verify the correctness of all numbers is that the sum of all numbers for each irreducible representation multiplied by the number of times that partition occurs for the irreducible representation in a given column in table 2 is given by

$$GF^{\chi} = P_G^{\chi}(s_k \to 12)$$

For example, the above result for the $A_{1\mathrm{u}}$ representation gives

$$P_{O_h}^{A_{1u}} = \frac{1}{48}[(12^{12} - 3 \times 12^4 \times 12^4 + 2 \times 12^6 \\ + 8 \times 12^4 - 8 \times 12^2] = 185752092669 \qquad (1)$$

We have shown in table 3, all such frequencies thus obtained for all the irreducible representations. The last few rows for the edge colorings according to the irreducible representation Γ can be obtained. For example, the last row is always given by

$$\frac{1}{48}\,[12! \times \dim(\Gamma)]\,.$$

The one previous to the last row is given by

$$\frac{1}{48}\left[12! \times \frac{\dim(\Gamma)}{2}\right].$$

The last but one row is given by

$$\frac{1}{48}\left[12! \times \frac{\dim(\Gamma)}{4}\right].$$

Table 2
Octahedral edge (cube edge) combinatorics for all irreducible representations*.

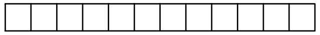
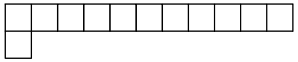
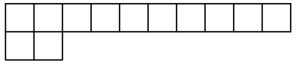
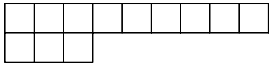
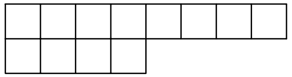
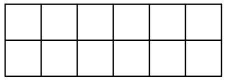
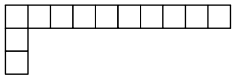
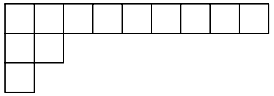
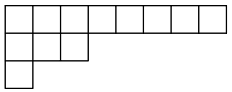
Partition	A_{1g}	A_{2g}	$A_{2u}(A_{1u})$	E_g	E_u	T_{1g}	T_{2g}	$T_{1u}=T_{2u}$
	1	0	0	0	0	0	0	0
	1	0	0	1	0	0	1	1
	4	1	1	5	2	2	5	4
	9	4	4	11	6	10	15	15
	18	9	9	27	18	26	32	31
	24	14	14	38	28	42	52	52
	30	20	18	46	34	50	60	58
	4	3	2	7	4	7	8	9
	18	13	12	31	24	37	42	43
	47	42	38	89	76	118	123	127

Table 2 Continued.

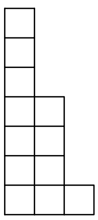
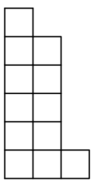
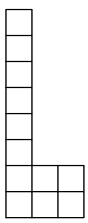
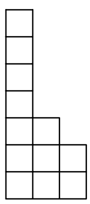
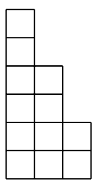
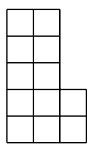
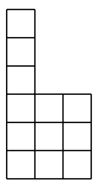
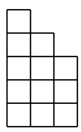
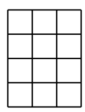
Partition	A_{1g}	A_{2g}	$A_{2u}(A_{1u})$	E_g	E_u	T_{1g}	T_{2g}	$T_{1u}=T_{2u}$
	92	82	78	174	156	238	248	252
	126	116	110	242	220	336	346	352
	76	61	59	137	118	174	189	186
	182	162	158	344	316	478	498	502
	318	288	282	606	564	842	872	868
	372	342	336	714	672	1014	1044	1050
	408	388	376	790	746	1134	1154	1166
	606	576	564	1182	1128	1704	1734	1746
	768	720	711	1488	1422	2130	2172	2169

Table 2 Continued.

Partition	A_{1g}	A_{2g}	$A_{2u}(A_{1u})$	E_g	E_u	T_{1g}	T_{2g}	$T_{1u}=T_{2u}$
(9,1,1,1)	29	29	26	58	52	81	81	84
(8,2,1,1)	130	125	120	255	240	365	370	375
(7,3,1,1)	336	336	324	672	648	984	984	996
(6,4,1,1)	590	580	570	1170	1140	172	1730	1740
(5,5,1,1)	702	702	684	1404	1368	2070	2070	2088
(7,2,2,1)	514	494	486	1008	972	1466	1486	1494
(6,3,2,1)	1178	1158	1142	2336	2284	3442	3462	3478
(5,4,2,1)	1764	1734	1716	3498	3432	5166	5196	5214
(5,3,3,1)	2328	2328	2292	4656	4584	6912	6912	6948
(4,4,3,1)	2922	2892	2868	5814	5736	8628	8658	8682
(6,2,2,2)	1792	1732	1718	3524	3436	5148	5208	5202

Table 2 Continued.

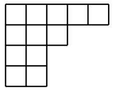
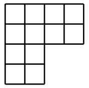
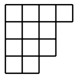
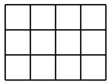
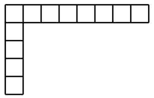
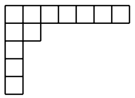
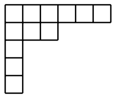
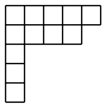
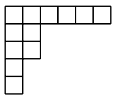
Partition	A_{1g}	A_{2g}	$A_{2u}(A_{1u})$	E_g	E_u	T_{1g}	T_{2g}	$T_{1u=}T_{2u}$
	3522	3462	3438	6984	6876	10338	1039	10422
	4422	4332	4308	8754	8616	12918	1300	13002
	5838	5778	5742	11616	11484	17262	1732	17358
 *	7740	7740	7668	15468	15324	23064	23064	23136
	248	249	246	498	492	741	741	744
	996	996	984	1992	1968	2964	2964	2976
	2316	2316	2304	4632	4608	6924	6924	6936
	3474	3474	3456	6948	6912	10386	1038	10404
	3490	3470	3450	6960	6900	10370	10390	10410

Table 2 Continued.

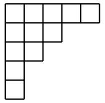
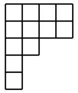
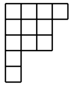
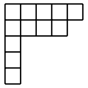
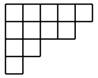
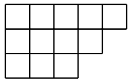
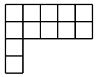
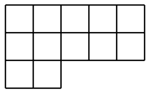
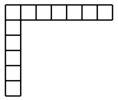
Partition	A_{1g}	A_{2g}	$A_{2u}(A_{1u})$	E_g	E_u	T_{1g}	T_{2g}	$T_{1u}=T_{2u}$
	6948	6948	6912	13896	13824	20772	20772	20808
	8700	8670	8640	17370	17280	25950	25980	26010
	11568	11568	11532	23136	23064	34632	34632	34668
	10548	10398	10362	20856	20724	31122	31182	31218
* 	17394	17334	17286	34728	34572	51906	51966	52014
* 	23136	23136	23064	46272	46128	69264	69264	69336
* 	26172	25992	25938	52164	51876	7780	77988	77982
* 	34776	34656	34584	69432	69168	103824	103944	104016
* 	1980	1980	1980	3960	3960	5940	5940	5940

Table 2 Continued.

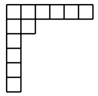
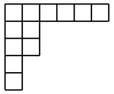
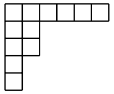
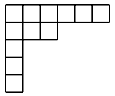
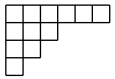
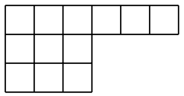
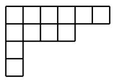
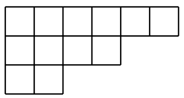
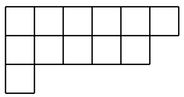
Partition	A_{1g}	A_{2g}	$A_{2u}(A_{1u})$	E_g	E_u	T_{1g}	T_{2g}	$T_{1u}=T_{2u}$
 *	6936	6936	6924	13872	13848	20784	20784	20796
 *	13860	13860	13860	27720	27720	41580	41580	41580
 *	17334	17334	17316	34668	34632	51966	51966	51984
 *	20808	20808	20772	41616	41544	62352	62352	62388
 *	34668	34668	34632	69336	69264	103932	103932	103968
 *	46200	46200	46200	92400	92400	138600	138600	138600
 *	52050	51990	51930	104040	103860	155850	155910	155970
 *	69336	69336	69264	138672	138528	207864	207864	207936
 *	104088	103968	103872	208056	207744	311712	311832	311928

Table 2 Continued.

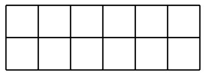
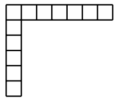
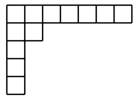
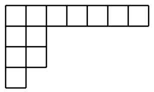
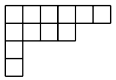
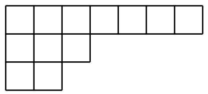
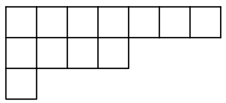
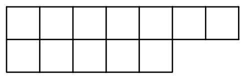
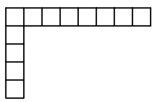
Partition	A_{1g}	A_{2g}	$A_{2u}(A_{1u})$	E_g	E_u	T_{1g}	T_{2g}	$T_{1u}=T_{2u}$
 *	156300	155940	155820	312240	311640	46746	467820	467820
 *	13860	13860	13860	27720	27720	41580	41580	41580
 *	41580	41580	41580	83160	83160	12474	124740	124740
 *	69300	69300	69300	138600	138600	20790	207900	207900
 *	103968	103968	103932	207936	207864	311832	311832	311868
 *	138600	138600	138600	277200	277200	41580	415800	415800
 *	207936	207936	207864	415872	415728	623664	623664	623736
 *	312000	311880	311760	623880	623520	935400	935520	935640
 *	83160	83160	83160	166320	166320	24948	249480	249480

Table 2 Continued.

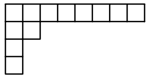
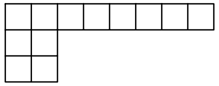
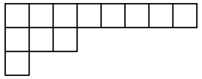
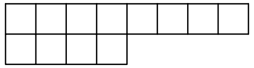
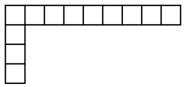
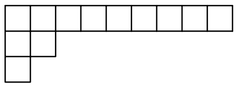
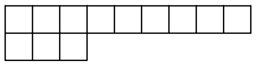
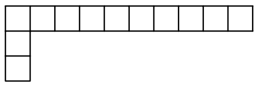
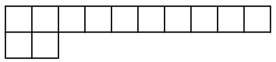
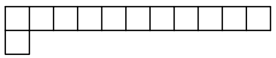
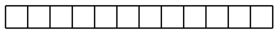
Partition	A_{1g}	A_{2g}	$A_{2u}(A_{1u})$	E_g	E_u	T_{1g}	T_{2g}	$T_{1u}=T_{2u}$
 *	207900	20790	207900	415800	415800	623700	623700	623700
 *	277200	277200	277200	554400	554400	83160	831600	831600
 *	415800	415800	415800	831600	831600	124740	1247400	1247400
 *	623736	623736	623664	1247472	1247328	187106	1871064	1871136
 *	415800	415800	415800	831600	831600	124740	1247400	1247400
 *	831600	831600	831600	1663200	1663200	249480	2494800	2494800
 *	1247400	1247400	1247400	2494800	2494800	374220	374220	374220
 *	1663200	1663200	1663200	3326400	3326400	498960	4989600	4989600
 *	2494800	2494800	2494800	4989600	4989600	748440	7484400	7484400
 *	4989600	4989600	4989600	9979200	9979200	149688	1496880	1496880
 *	9979200	9979200	9979200	19958400	19958400	299376	2993760	2993760

Table 3
Frequencies of all irreducible representations in the edge combinatorics of octahedron(cube) shown in table 2 for all multinomial terms[a].

A_{1g}	185788177224
A_{2g}	185752217877
$A_{1u}=A_{2u}$	185752092669
E_g	371504434605
E_u	371504184051
T_{1g}	557256402066
T_{2g}	557256401934
$T_{1u}=T_{2u}$	557256029616

[a] Sum of frequencies x dimension of the representation for all irreducible representations is verified to be 12^{12}.

The last minus third one row is given by

$$\frac{1}{48}\left[12! \times \frac{\dim(\Gamma)}{6}\right].$$

These results follow from the fact that the multinomial expansions that contain the terms corresponding to last four partitions for edge colorings appear only in the lead term and thus we have the result.

Table 4 shows the vertex colorings of the cube and also the face colorings of octahedron. As seen from table 4, first A_{1u} non-zero representation appears for the partition $4+4$ then 5+2+1 suggesting that to produce a chiral structure out of a cube one needs at least four colors of one kind and four colors of another kind, a result that is well known. The last two rows of numbers and the first two rows of numbers are directly predicable. The first row is non-zero for only A_{1g} or totally symmetric representation. The last row is always given by

$$\frac{1}{48}\left[8! \times \dim(\Gamma)\right].$$

The one previous to the last row is given by

$$\frac{1}{48}\left[8! \times \frac{\dim(\Gamma)}{2}\right].$$

While some of these results are well known for the A_{1g} representation in the context of isomer enumeration a full table for all irreducible representations for all partitions has not appeared before in the literature, and thus our tables provide complete multinomial combinatorics of ligand or edge partitions.

In order to complete the combinatorics of the octahedron and cube we have also considered the face colorings of the cube, which are equivalent to vertex colorings of the octahedron. Table 5 shows our complete results for this case for all

Table 4
Cube vertex(octahedral face) combinatorics for all irreducible representations[a].

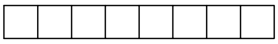
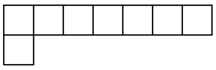
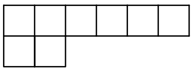
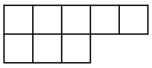
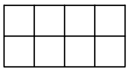
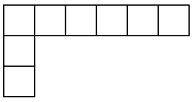
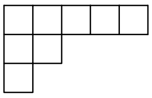
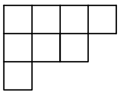
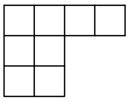
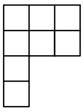
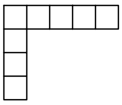
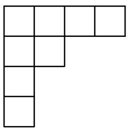
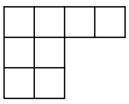
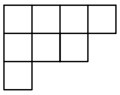
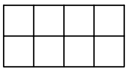
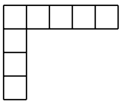
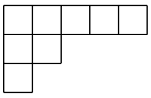
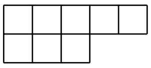
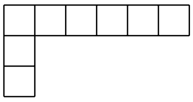
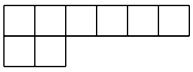
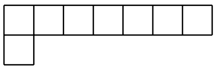
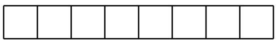
Partition	A_{1g}	A_{2g}	A_{2u}	A_{1u}	E_g	E_u	T_{1g}	T_{2g}	T_{1u}	T_{2u}
	1	0	0	0	0	0	0	0	0	0
	1	0	1	0	0	0	0	1	1	0
	3	0	1	0	2	1	0	3	2	1
	3	0	3	0	2	2		5	5	2
	6	0	3	1	4	2	2	6	5	3
	3	0	3	0	2	2	2	5	5	2
	6	1	6	1	7	7	8	13	13	8
	10	3	10	3	11	11	14	21	21	14
	16	5	11	6	21	17	20	31	28	23
	17	7	17	7	23	23	30	40	40	30
	10	4	10	4	14	14	18	24	24	18
	22	13	22	13	35	35	48	57	57	48
 *	30	18	30	18	46	46	64	76	76	64

Table 4 Continued.

Partition	A_{1g}	A_{2g}	A_{2u}	A_{1u}	E_g	E_u	T_{1g}	T_{2g}	T_{1u}	T_{2u}
 *	42	28	42	28	70	70	98	112	112	98
 *	68	44	58	46	112	104	144	168	162	150
 *	38	32	38	32	70	70	102	108	108	102
 *	76	64	76	64	140	140	204	216	216	204
 *	114	96	114	96	210	210	306	324	324	306
 *	140	140	140	140	280	280	420	420	420	420
 *	216	204	216	204	420	420	624	636	636	624
 *	420	420	420	420	840	840	1260	1260	1260	1260
 *	840	840	840	840	1680	1680	2520	2520	2520	2520

[a] Young diagrams with * must be conjugated to obtain the partition. These are shown in this way to save space.

irreducible representations. All of the results that we have obtained for the A_{1g} representation are well-known results for the vertex coloring isomers of the octahedron. The results for the $A_{1\mathrm{u}}$ representation are for the chiral isomers, while all other results for colorings that transform according to the given representation in the column.

The character cycle indices contain significantly richer and important information that could lead to powerful results in number theory and other branches of mathematics. The substitution of s_{k} by $\lambda_1^k + \lambda_2^k + \cdots + \lambda_n^k$ is one of the possibilities suggested by Pólya. If we replaces s_{k} in GCCI by other symmetric functions [34] for example

$$\lambda_1^k\lambda_2^k + \lambda_1^k\lambda_3^k + \cdots + \lambda_1^k\lambda_n^k + \lambda_2^k\lambda_3^k + \cdots + \lambda_2^k\lambda_3^k + \lambda_{n-1}^k\lambda_n^k = \sum \lambda_1^k\lambda_2^k,$$

Table 5
Octahedral vertex (cube face) combinatorics for all irreducible representations[a].

Partition	A_{1g}	A_{2g}	A_{2u}	A_{1u}	E_g	E_u	T_{1g}	T_{2g}	T_{1u}	T_{2u}
(6)	1	0	0	0	0	0	0	0	0	0
$(5,1)$	1	0	0	0	1	0	0	0	1	0
$(4,2)$	2	0	0	0	2	0	0	1	1	1
$(3,3)$	2	1	1	0	2	0	0	1	2	1
$(4,1,1)$	2	1	1	0	3	0	1	1	3	2
$(3,2,1)$	3	2	2	0	5	1	2	3	5	4
$(3,3)$ *	5	2	2	1	7	2	3	6	6	6
$(4,1,1)$ *	4	4	4	1	8	2	6	6	9	9
$(4,2)$ *	6	5	5	2	11	5	9	10	13	12
$(5,1)$ *	9	9	9	6	18	12	21	21	24	24
(6) *	15	15	15	15	30	30	45	45	45	45

[a] Young diagrams with * must be conjugated to obtain the partition. These are shown in this way to save space.

the generalized cycle indices produce new combinatorics for each irreducible representation. We may also consider the replacement by symmetric functions of the kind $\sum \lambda_1^k \lambda_2^k \lambda_3^k$ where the sum involves all possible symmetric combinations involving three terms at a time, and so on. In general it can be envisaged that the method could be generalized to a multinomial symmetric function with a multinomial expansion, which we call multinomial S-functions. Such topics can be studied separately.

Another special case of multinomial combinatorics with character theory is to choose weights $1, \mathrm{w}, \mathrm{w}^2, \ldots, \mathrm{w}^n$. Then we obtain powerful multinomial generators in ws. If we stop with weights $1, w,$ and w^2 this corresponds to filling the orbitals with zero, 1 or 2 electrons as by Pauli exclusion principle only at most 2 electrons are allowed [21]. In this case it is a special application to enumeration of electronic configurations that comply with the Pauli exclusion principle. In the general case, for example, the GF for the $\mathrm{A}_{2\mathrm{g}}$ representation of the edge group of cube for this case is given by

$$\begin{aligned} P_{O_h}^{A_{2g}} = \frac{1}{48}\big[&(1+w+w^2+w^3+\cdots+w^{12})^{12} \\ &-3(1+w+w^2+w^3+\cdots+w^{12})^4(1+w^2+w^4+w^6+\cdots+w^{24})^4 \\ &+2(1+w^2+w^4+w^6+\cdots+w^{24})^6 \\ &+8(1+w^3+w^6+w^9+\cdots+w^{36})^4 \\ &-8(1+w^{12}+w^{24}+w^{36}+\cdots+w^{72})^2\big] \end{aligned}$$

Other variations that lead to infinite power series in multinomial weights are also feasible. There is much to be desired in such powerful multinomial combinatorial theory.

4. Conclusion

In this work we obtained the full combinatorial tables for all irreducible representations of the octahedral group for the vertex, edge and face colorings of the cube and octahedron using multinomial combinatorics. The tables provided complete enumeration numbers for all possible partitions in the Young diagram for the colorings that transform according to the various irreducible representations of the group. As special cases, the chiral edge, vertex, and face colorings for all Young diagrams were generated. The results for other irreducible representations were interpreted. We believe that there is rich combinatorics in GCCIs when replacements are made for each term by a multinomial of symmetric functions as opposed to an ordinary Pólya replacement. Such topics will be studied in the future, as they seem to result in novel mathematical identities in number theory.

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