Codes in Platonic, Archimedean, Catalan, and Related Polyhedra: A Model for Maximum Addition Patterns in Chemical Cages

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The notion of *d*-code is extended to general polyhedra by defining maximum sets of vertices with pairwise separation $\geq d$. Codes are enumerated and classified by symmetry for all regular and semiregular polyhedra and their duals. Partial results are also given for the series of medials of Archimedean polyhedra. In chemistry, *d*-codes give a model for maximal addition to or substitution in polyhedral frameworks by bulky groups. Some illustrative applications from the chemistry of fullerenes and boranes are described.

1. INTRODUCTION

Much of the extensive theory of error-correcting binary codes[1] consists of finding the largest *d*-code in the *n*-cube, i.e., the largest subset of vertices such that every pairwise distance between members of the set is at least *d*. Here we extend this paradigm to *d*-codes on vertex sets of three-dimensional polyhedra, with a view to applications in chemistry, where the maximum *d*-code offers a natural model for steric effects in patterns of addition to, or substitution in, polyhedral cage molecules.[2,3]

The metric space of the vertices of the *n*-cube can be visualized in several ways, each implying a definition of distance. When the *n*-cube is seen as a graph, the distances are the lengths of shortest paths (geodesics) along the edges of the skeleton. In *n*-dimensional Euclidean space, the cube vertex coordinates are the 2^n distinct binary sequences of length *n*, and the Hamming distance between any two coordinate strings (i.e. the number of places at which they differ) is just the square of the Euclidean distance. In terms of sets, any vertex can be seen as a subset of a given set of *n* elements, and distance between vertices *a* and *b* is then defined as the cardinality of the symmetric difference

$$|a\Delta b| = |a \cup b| - |a \cap b| \quad (1)$$

All three visualizations are equivalent, as all three metric spaces are isomorphic.

Codes are useful in the detection and correction of errors in messages. If $d = 2k + 1$, the *d*-code *corrects* up to *k* single-digit errors, as all received versions of a sent message lie within a distance at most *k* of the original, and so unique reconstruction of a message is possible. On the other hand, if $d = 2k$, the *d*-code in the cube *corrects* any *k*-1 single-digit errors and *detects k* errors. When $d = 2k + 1$, an upper bound on the number of vertices in the *d*-set, $|C_d|$, is given by spherical packing i.e.,

$$|C_d| \leq \left\lfloor \frac{|M|}{|B_k|} \right\rfloor \quad (2)$$

where $|M|$ is the number of elements in the metric space and $|B_k|$ the number of elements in the ball of radius *k*. A *d*-code where *d* is odd can be called *well packed* if it realizes the sphere-packing bound (i.e. attains equality in (2)). If moreover the size of the ball $|B_k|$ divides the number of vertices of the polyhedron, then the union of all such balls partitions the metric space and the well-packed code becomes *perfectly packed*, or just *perfect*.

For all values of *d*, even and odd, a trivial and well-known lower bound for nonextendable and hence also for maximum codes is

$$|C_d| \geq \left\lceil \frac{|M|}{|B_{d-1}|} \right\rceil \quad (3)$$

as, if the union of all the balls of radius *d*-1 does not provide a covering of $|M|$, the code is extendable. By analogy with (2), (3) could be called a *sphere covering* bound.

In the present paper we consider the extension of *d*-codes from the *n*-cube to other *n*-dimensional polytopes, restricting ourselves in the present instance to three dimensions. We will always be concerned with maximum *d*-codes in this paper, and any *d*-code mentioned without qualification will be assumed to be maximum. In addition to the easy case of the five Platonic polyhedra, the 13 Archimedean solids, their duals (the Catalan polyhedra), and medials are treated. The deltahedra and the four infinite series of prisms, antiprisms, and the duals of each are also considered. This selection of cases is motivated by the simplicity of the polyhedra themselves and the potential of at least some members of these series for application in chemistry.

In a chemical context, the size of the maximum *d*-code determines the limiting stoichiometry for addition of bulky groups to a polyhedral cage under the assumption that each

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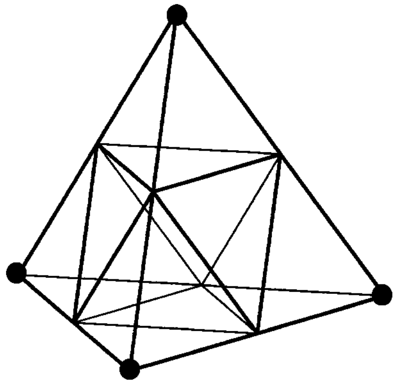


Figure 1. A 10-vertex polyhedral graph with $D = 2$ and $|C_D| = 4$ (indicated by black vertices). The graph is the dual of the chamfered tetrahedron and also arises by capping a tetrahedral subset of faces of the octahedron.

addend blocks further addition to all sites within a radius of *d*-1 edges. Further, each distinct *d*-code corresponds to a feasible chemical derivative of the original polyhedral molecule in this simplified, purely steric model. The model has been applied in conjunction with simple electronic arguments to account successfully for the ultimate product of bromination of C_{60}[2] and to predict patterns for addition of this and even larger ligands to C_{60} and C_{70} fullerenes.[3,4]

With this type of application in mind, we determine the cardinalities of the *d*-codes for all the above polyhedra and in most cases enumerate exhaustively the codes and classify them by symmetry group. The methods are mainly computational. A later paper will address the more purely mathematical case of 4-dimensional polytopes, where many of the same ideas apply.

2. COMPUTATIONAL BACKGROUND

Finding the 2-code of a graph is the classical problem of *independence number*, and finding the *d*-code for any given larger *d* can be formulated as an independence problem on a graph augmented by edges for all pairwise distances less than *d*. As *d* increases, so does the density of the augmented graph and the ease of the computation. The largest nontrivial value of *d* is *D*, where *D* is the diameter of the graph; at $d = D+1$ the augmented graph is the complete graph on *n* vertices and the *d*-code then consists of just a single vertex. For antipodal graphs the *D*-code is trivially a pair of vertices at opposite ends of a diameter. In other cases the size of the *D*-code may be larger, e.g. $|C_D|$ for the decorated tetrahedron shown in Figure 1.

A computer program for determining independence number is described by Hansen and Mladenović[5] and was used here without modification. Computation is a useful backup, but the cardinality $|C_d|$ can often be found by hand in these highly symmetrical cases. On the other hand, the number of distinct realizations of codes of the given size usually needs a computer search, and new programs were written for this task.

A given code is a subset of the vertices of the polyhedron. It is associated with a subgroup *H* of the polyhedral point group *G* such that every element of *H* leaves the code fixed in place on the polyhedron; in an exhaustive list, each distinct code would therefore occur $|G|/|H|$ times and a representive can be chosen by lexicographic ordering. Occasionally the whole orbit of $|G|/|H|$ copies is itself of interest, as it may represent a polyhedral compound.

Evaluation of $|C_d|$ is direct and fast with the program Dense Clique. Where $|C_d|$ is large, direct brute-force enumeration of all codes may be prohibitively expensive, but simple observations can often be used to cut down the work. For example, a subset of faces may cover the polyhedron, as in the case of the 20 triangles of the truncated dodecahedron, where the 2-code has exactly one vertex in each triangle. In a few cases, such as the 3-code of the great rhombicosidodecahedron where 26 of the 30 spanning squares contain exactly one vertex of the 3-code and 4 squares are empty, the numbers are still too large, and patchwise partition of the polyhedron, with solution of the independence problem within each patch, is programmed. Experimentation with subgraphs of the polyhedron will often reveal vertices or sets of vertices that must or must not be part of a given code, again enabling cheaper enumeration, or a direct proof of uniqueness.

In the following sections for the various target classes of polyhedra we list the sizes, numbers and symmetries of *d*-codes. The compilation is of direct applicability in chemical models, and some illustrative applications will be described. It may also give a starting point for further mathematical investigation.

3. RESULTS

(i) Codes in Platonic Polyhedra. As the complete graph K_4, the tetrahedron has $D = 1$, and hence its 2-code consists trivially of a single vertex. The symmetry of the polyhedron is $G = T_d$ (order 24), and the site symmetry of the code is $H = C_{3v}$ (order 6).

The octahedron has $D = 2$, $G = O_h$, $|G| = 48$ and its 2-code is a pair of antipodal vertices ($H = D_{4h}$, $|H| = 16$, hence 3 copies).

The cube has $D = 3$, $G = O_h$. Its 3-code is the antipodal pair ($H = D_{3h}$, $|H| = 12$, hence 4 copies). This is a perfect code. As the cube graph is bipartite, its 2-code is unique; the four vertices of the 2-code form an inscribed tetrahedron of site symmetry T_d and orbit size 2. The orbit of two inscribed tetrahedra forms a well-known regular compound, the *Stella Octangula* of Kepler.[6]

The icosahedron has $D = 3$, $G = I_h$, $|G| = 120$. Its 3-code is the antipodal pair ($H = D_{5h}$, $|H| = 20$) and is a perfect code correcting one error, as two disjoint sets of six vertices with radius 1 cover the polyhedron. The unique 2-code is an equilateral triangle of size 3 (site symmetry D_{3h}, 10 copies).

The dodecahedron has $D = 5$, $G = I_h$. Its 5-code is the antipodal pair ($H = D_{3d}$ $|H| = 12$). The 4-code is again of size 2 but now has 2 symmetry inequivalent versions, the antipodal pair and a pair at distance 4 ($H = C_{2v}$, $|H| = 4$, 30 copies). The 3-code has $|C_3| = 4$ and is an equilateral chiral tetrahedron, with site group *T* (the pure rotation group of the tetrahedron, $|T| = 12$) and hence has 10 copies, which together form the classical compound of 10 tetrahedra in a dodecahedron.[6] The 2-code has $|C_2| = 8$ and is a cube of T_h site symmetry; the orbit of five copies forms the classical regular compound of five cubes in a dodecahedron.[6] Each vertex of the dodecahedron belongs to two out of the five copies of the 2-code.

Table 1. Codes in Archimedean Polyhedra[a]

polyhedron	G	n	k	D	d = 2	3	4	5	6	7	8	9	10	11	12	13	14	15	16
A1: cuboctahedron	O_h	12	4	3	4	2^{+}	1												
$(3.4)^2$					(2)	(1)	(1)												
A2: truncated tetrahedron	T_d	12	3	3	4	3^{++}	1												
3.6^2					(2)	(1)	(1)												
A3: snub cube	O	24	5	4	8	3	2	1											
$3.^44$					(1)	(4)	(3)	(1)											
A4: rhombicuboctahedron	O_h	24	4	5	8	4^{+}	2	2^{++}	1										
3.4^3					(10)	(2)	(3)	(1)	(1)										
A5: truncated cube	O_h	24	3	6	8	6^{++}	4	2	2	1									
3.8^2					(23)	(1)	(2)	(3)	(1)	(1)									
A6: truncated octahedron	O_h	24	3	6	12	5	3	2^{+}	2	1									
4.6^2					(1)	(2)	(2)	(3)	(1)	(1)									
A7: icosidodecahedron	I_h	30	4	5	10	6^{++}	3	2^{+}	1										
$(3.5)^2$					(2)	(1)	(1)	(1)	(1)										
A8: truncated cuboctahedron	O_h	48	3	9	24	10	8	4	3	2	2	2^{++}	1						
4.6.8					(1)	(22)	(1)	(12)	(4)	(7)	(4)	(1)	(1)						
A9: snub dodecahedron	I	60	5	7	18	8	4	3	2	2^{+}	1								
$3^4.5$					(6)	(48)	(58)	(7)	(8)	(3)	(1)								
A10: rhombicosidodecahedron	I_h	60	4	8	20	12^{++}	6	3	2	2^{+}	2	1							
3.4.5.4					(3329)	(1)	(2)	(9)	(6)	(3)	(1)	(1)							
A11: truncated dodecahedron	I_h	60	3	10	20	14	8	7^{+}	4	3	2	2^{+}	2	1					
3.10^2					(157226)	(2)	(40)	(1)	(3)	(4)	(5)	(3)	(1)	(1)					
A12: truncated icosahedron	I_h	60	3	9	24	12	7	6^{++}	3	2	2	2^{+}	1						
5.6^2					(1085)	(12)	(2)	(1)	(6)	(6)	(3)	(1)	(1)						
A13: truncated icosidodecahedron	I_h	120	3	15	60	26	18	11	8	6	4	4^{+}	3	2	2	2^{+}	2	2^{++}	1
4.6.10					(1)	(2405)	(6)	(26)	(54)	(40)	(136)	(1)	(7)	(17)	(12)	(7)	(4)	(1)	(1)

[a] Polyhedra **A1** to **A13** are listed by name, Coxeter symbol,[10] point group G, vertex number n, valency k, and diameter D. For each $2 \le d \le D$, the first line gives the code size, and the second the number of distinct realizations. Superscripts + and ++ denote well packed and perfectly packed codes, respectively, as defined in the text.

Table 2. Codes in Catalan Polyhedra[a]

polyhedron	G	n	D	d = 2	3	4	5	6	7	8	9	10	11
C1	O_h	14	4	8	2	2	1						
				(1)	(3)	(2)	(2)						
C2	T_d	8	2	4	1								
				(1)	(2)								
C3	O	38	7	16	8	4	3	2	2	1			
				(1)	(2)	(5)	(1)	(5)	(1)	(3)			
C4	O_h	26	6	14	5	4	2	2	1				
				(1)	(2)	(1)	(2)	(1)	(3)				
C5	O_h	14	3	8	2	1							
				(1)	(1)	(2)							
C6	O_h	14	3	6	2	1							
				(1)	(2)	(2)							
C7	I_h	32	6	20	5	4	2	2	1				
				(1)	(4)	(1)	(3)	(2)	(2)				
C8	O_h	26	4	12	3	2	1						
				(1)	(1)	(3)	(3)						
C9	I	92	10	38	20	9	6	4	4	2	2	2	1
				(32)	(3)	(3)	(15)	(24)	(2)	(12)	(5)	(1)	(3)
C10	I_h	62	8	32	14	8	4	4	2	2	1		
				(1)	(1)	(3)	(6)	(1)	(2)	(1)	(3)		
C11	I_h	32	4	20	4	2	1						
				(1)	(1)	(1)	(2)						
C12	I_h	32	5	12	4	2	2	1					
				(1)	(3)	(4)	(2)	(2)					
C13	I_h	62	6	30	7	4	2	2	1				
				(1)	(1)	(2)	(7)	(3)	(3)				

[a] **Cn** is the dual of Archimedean polyhedra **An**. Other symbols are as in Table 1.

This summary of codes in the simple case of the Platonic solids already reveals some interesting features. Three well-known regular compounds occur as the geometries of orbits of d-codes. The codes also show a Russian-Doll property: the 2-code of the dodecahedron is the cube, whose 2-code is the tetrahedron, and the tetrahedron is itself the 3-code of the dodecahedron. Sequences of codes embedded in this way can also be found among the results to be presented in the remainder of this paper and will be discussed as they arise. Furthermore, there are two instances of perfect codes among the Platonic solids, albeit trivial ones, namely the 3-codes of the cube and the icosahedron.

Table 3. Codes in Medial Polyhedra[a]

				d													
polyhedron	*G*	*n*	*D*	2	3	4	5	6	7	8	9	10	11	12	13	14	15
M1	O_h	24	5	8	4	2	2	1									
M2	T_d	18	4	6	3	2	1										
M3	O	60	8	22	12	6	3	3	2	2	1						
M4	O_h	48	7	20	8	5	3	2	2	1							
M5	O_h	36	6	12	6	4	2	2	1								
M6	O_h	36	6	12	6	3	2	2	1								
M7	I_h	60	8	20	12	6	3	2	2	2	1						
M8	O_h	72	9	24	12	8	4	3	2	2	2	1					
M9	I	150	12	52	30	15	9	6	4	3	2	2	2	2	1		
M10	I_h	120	11	44	20	12	7	5	4	3	2	2	2	1			
M11	I_h	90	10	30	16	12	7	6	3	3	2	2	1				
M12	I_h	90	9	30	18	8	6	4	2	2	2	1					
				(158)	(1)	(19)	(4)	(1)	(13)	(8)	(2)	(2)					
M13	I_h	180	14	60	18	12	8	6	4	4	3	2	2	2	2	2	1

[a] **Mn** is the dual of Archimedean polyhedra **An**; other symbols are as in Table 1. Distinct codes are enumerated only for M12, the medial of the truncated icosahedron.

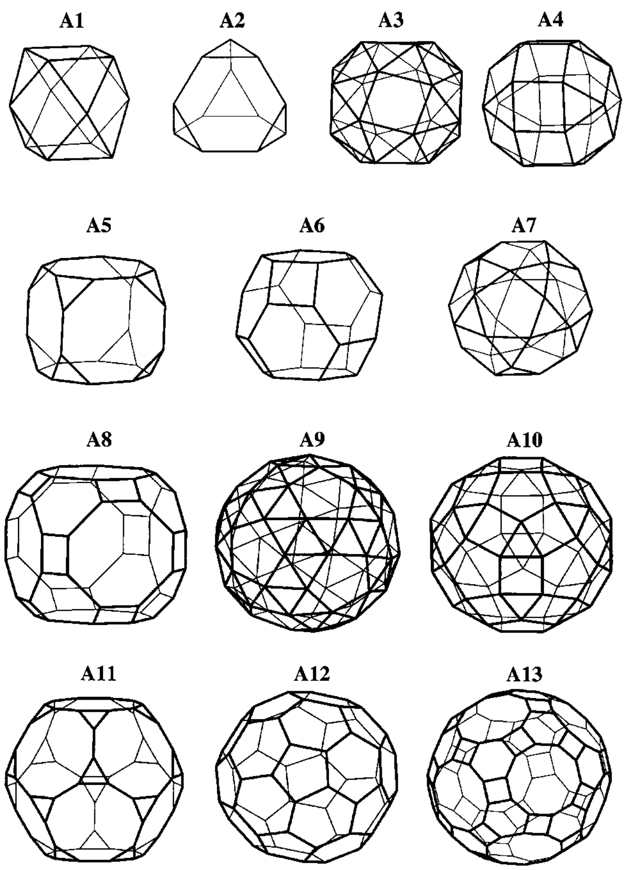


Figure 2. The 13 Archimedean polyhedra.

(ii) Codes in Archimedean Polyhedra. Table 1 lists the 13 Archimedean polyhedra, their symmetries (*G*), vertex numbers (*n*), vertex degrees (*k*), diameters (*D*), sizes of *d*-codes, and numbers of distinct codes at each *d*. The polyhedra themselves are shown in Figure 2. Tables 4−8 give the detailed breakdown of the overall counts by site subgroup for the five possible polyhedral groups T_d, O, O_h, I, and I_h.

In Table 1, all the well-packed codes are marked with + and perfectly packed codes with ++. In every case in Table 1, *perfectly packed codes are unique* (have only one distinct realization), and *each unique* (2*k*+1)-*code is well packed*.

Table 4. Symmetry Classification of Distinct Codes: T_d

polyhedron	*d*	C_1	C_2	C_s	C_{2v}	D_2	S_4	D_{2d}	C_{3v}	T	T_d
A2	2	1	.	.	.	.	1	.	.	.	.
	3	.	.	.	.	.	.	.	1	.	.
	4	.	.	1	.	.	.	.	.	.	.
C2	2	.	.	.	.	.	.	.	.	.	1
	3	.	.	.	.	.	.	.	2	.	.

Table 5. Symmetry Classification of Distinct Codes: *O*

polyhedron	*d*	C_1	C_2	C_3	C_4	D_2	D_3	D_4	T	O
A3	2	.	.	.	.	.	.	1	.	.
	3	2	.	2	.	.	.	.	.	.
	4	.	3	.	.	.	.	.	.	.
	5	1	.	.	.	.	.	.	.	.
C3	2	.	.	.	.	.	.	.	1	.
	3	.	.	.	1	.	.	.	.	1
	4	1	.	2	.	1	.	.	1	.
	5	.	.	1	.	.	.	.	.	.
	6	1	2	.	.	.	1	1	.	.
	7	.	.	.	.	.	1	.	.	.
	8	1	.	1	1	.	.	.	.	.

Perfectly packed and perhaps also well-packed codes might be expected to correspond in a chemical context to especially stable isomers, all other factors being equal, as they represent a uniform distribution of strain. Trivially, for the three bipartite polyhedra in the list, the 2-code is unique and includes exactly half the vertices. In the case of the 2-codes of the truncated dodecahedron, each code contains one marked vertex per triangular face, leading to a surprisingly large number of symmetry distinct possibilities.

To explore the relationships between codes in Archimedean and other series it is useful to define some further terms. The *contact graph* of a *d*-code has the same vertices as the code, and an edge for every pair of vertices at distance *d*. Many, but not all, contact graphs are polyhedral. A divisibility relation can be defined for two polyhedra as follows: polyhedron P_2 is a *d*-code divisor of polyhedron P_1 if the skeleton of P_2 is the contact graph of a realization of the *d*-code in P_1. For example, one of the 1085 distinct 2-codes of the truncated icosahedron (chemically realized in the T_h-symmetric $C_{60}Br_{24}$) has a contact graph that is the skeleton

Table 6. Symmetry Classification of Distinct Codes: O_h

polyhedron	*d*	C_1	C_2	C_i	C_s	C_3	D_2	C_{2v}	C_{2h}	C_4	S_4	D_3	C_{3v}	S_6	D_{2h}	D_{2d}	C_{4h}	C_{4v}	D_4	T	D_{3d}	D_{4h}	T_h	T_d	O	O_h
A1	2	.	.	.	.	.	.	.	.	.	.	.	.	.	.	1	.	.	.	.	.	1	.	.	.	.
	3	.	.	.	.	.	.	.	.	.	.	.	.	.	1	.	.	.	.	.	.	.	.	.	.	.
	4	.	.	.	.	.	.	1	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.
A4	2	2	4	.	.	.	1	.	1	.	1	.	.	.	.	.	.	.	1	.	.	.	.	.	.	.
	3	1	.	.	.	.	.	.	.	.	1	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.
	4	.	2	.	.	.	.	.	1	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.
	5	.	.	.	.	.	.	.	1	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.
	6	.	.	.	1	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.
A5	2	14	4	1	.	.	.	.	.	1	1	.	.	.	.	.	1	.	1	.	.	.	.	.	.	.
	3	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	1	.	.	.	.	.
	4	.	.	.	.	.	.	.	.	.	1	.	.	.	.	1	.	.	.	.	.	.	.	.	.	.
	5	.	1	.	.	.	.	1	1	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.
	6	.	.	.	.	.	.	.	1	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.
	7	.	.	.	1	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.
A6	2	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	1	.	.	.
	3	.	.	.	2	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.
	4	.	.	.	1	1	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.
	5	.	1	.	.	.	.	1	1	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.
	6	.	.	.	.	.	.	.	1	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.
	7	.	.	.	1	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.
A8	2	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	1	.
	3	16	5	1	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.
	4	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	1	.	.	.	.	.	.	.
	5	8	2	.	.	.	.	.	.	.	2	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.
	6	2	.	.	.	2	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.
	7	2	3	1	1	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.
	8	.	3	1	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.
	9	.	.	1	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.
	10	1	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.
C1	2	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	1
	3	.	.	.	1	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	1	1	.	.	.	.
	4	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	1	1	.	.	.	.
	5	.	.	.	.	.	.	.	.	.	.	.	1	.	.	.	.	1	.	.	.	.	.	.	.	.
C4	2	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	1
	3	.	.	.	.	.	.	1	.	.	.	1	.	.	.	.	.	.	.	.	.	.	.	.	.	.
	4	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	1	.	.
	5	.	.	.	1	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	1	.	.	.	.	.
	6	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	1	.	.	.	.	.
	7	.	.	.	.	.	.	1	.	.	.	.	1	.	.	.	.	1	.	.	.	.	.	.	.	.
C5	2	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	1
	3	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	1	.	.	.	.	.
	4	.	.	.	.	.	.	.	.	.	.	.	1	.	.	.	.	1	.	.	.	.	.	.	.	.
C6	2	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	1
	3	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	1	1	.	.	.	.
	4	.	.	.	.	.	.	.	.	.	.	.	1	.	.	.	.	1	.	.	.	.	.	.	.	.
C8	2	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	1
	3	.	.	.	.	.	.	.	.	.	.	1	.	.	.	.	.	.	.	.	.	.	.	.	.	.
	4	.	.	.	.	.	.	.	.	.	.	.	.	.	1	.	.	.	.	.	1	1	.	.	.	.
	5	.	.	.	.	.	.	1	.	.	.	.	1	.	.	.	.	1	.	.	.	.	.	.	.	.

Table 7. Symmetry Classification of Distinct Codes: *I*

polyhedron	*d*	C_1	C_2	C_3	D_2	C_5	D_3	D_5	T	I
A9	2	3	1	1	.	.	1	.	.	.
	3	35	12	.	1	.	.	.	.	.
	4	45	12	.	1	.	.	.	.	.
	5	4	.	3	.	.	.	.	.	.
	6	2	6	.	.	.	.	.	.	.
	7	.	3	.	.	.	.	.	.	.
	8	1	.	.	.	.	.	.	.	.
C9	2	28	.	4	.	.	.	.	.	.
	3	.	.	.	.	1	.	1	.	1
	4	2	.	1	.	.	.	.	.	.
	5	2	9	.	.	1	3	.	.	.
	6	14	4	4	.	.	.	.	2	.
	7	.	.	.	.	.	.	.	2	.
	8	5	5	.	.	.	1	1	.	.
	9	1	2	.	.	.	1	1	.	.
	10	.	.	.	.	.	1	.	.	.
	11	1	.	1	.	1	.	.	.	.

of the truncated cube,[3] so the truncated cube is a 2-code divisor of the truncated icosahedron. Note that divisibility is a purely combinatorial concept and so does not depend on the symmetry or actual geometries of the codes of polyhedra. Table 9 gives in a schematic format all the divisibility relationships among Archimedean, Platonic, and Catalan polyhedra. The medial of the truncated icosahedron is also studied.

Now, suppose P_2 is a d_1-code divisor of P_1. If, further, the vertices of a d_2-code in P_2 also form a d_3-code in P_1 ($d_3 > d_1$, d_2) we have a Russian Doll sequence $P_1 > P_2 > P_3$, which is, evidently, a stronger property than divisibility alone. Detailed examination of the divisibility chains in Table 9 reveals five sets of Russian Dolls, with the relevant codes displayed on Schlegel diagrams in Figure 3a−e.

Finally, a polyhedron related to the Archimedean solids and often discussed together with them is the Miller

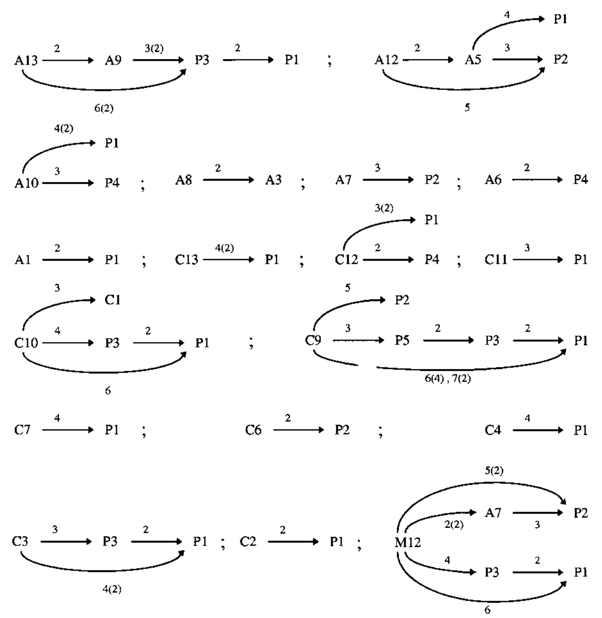
Table 8. Symmetry Classification of Distinct Codes: I_h

polyhedron	d	C_1	C_2	C_i	C_s	C_3	D_2	C_{2v}	C_{2h}	C_5	D_3	C_{3v}	S_6	D_{2h}	D_5	C_{5v}	S_{10}	T	D_{3d}	D_{5d}	T_h	I	I_h
A7	2	.	.	.	.	.	1	.	.	.	.	.	.	.	.	.	.	.	.	1	.	.	.
	3	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	1	.	.
	4	.	.	.	.	.	.	.	.	.	1	.	.	.	.	.	.	.	.	.	.	.	.
	5	.	.	.	.	.	.	.	.	.	.	.	.	1	.	.	.	.	.	.	.	.	.
	6	.	.	.	.	.	.	1	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.
A10	2	3093	215	9	.	.	7	.	1	.	.	.	.	.	2	.	2	.	.	.	.	.	.
	3	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	1	.	.
	4	.	.	.	.	.	.	.	.	.	.	.	1	.	.	.	.	.	1	.	.	.	.
	5	5	.	.	2	2	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.
	6	1	3	.	1	.	.	.	1	.	.	.	.	.	.	.	.	.	.	.	.	.	.
	7	.	2	.	.	.	.	.	1	.	.	.	.	.	.	.	.	.	.	.	.	.	.
	8	.	.	.	.	.	.	.	1	.	.	.	.	.	.	.	.	.	.	.	.	.	.
	9	.	.	.	1	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.
A11	2	156774	364	72	.	.	2	.	.	9	.	.	.	.	1	.	4	.	.	.	.	.	.
	3	.	1	.	.	.	.	.	1	.	.	.	.	.	.	.	.	.	.	.	.	.	.
	4	30	6	2	.	.	1	.	1	.	.	.	.	.	.	.	.	.	.	.	.	.	.
	5	.	.	.	1	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.
	6	2	1	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.
	7	1	.	.	2	1	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.
	8	1	2	.	.	.	.	1	1	.	.	.	.	.	.	.	.	.	.	.	.	.	.
	9	.	1	.	.	.	.	1	1	.	.	.	.	.	.	.	.	.	.	.	.	.	.
	10	.	.	.	.	.	.	.	1	.	.	.	.	.	.	.	.	.	.	.	.	.	.
	11	.	.	.	1	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.
A12	2	1037	20	5	.	17	.	.	.	.	1	.	3	.	.	.	.	1	.	.	1	.	.
	3	7	3	1	.	.	.	.	.	.	.	.	1	.	.	.	.	.	.	.	.	.	.
	4	2	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.
	5	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	1	.	.	.	.
	6	3	.	.	1	1	.	.	.	.	.	1	.	.	.	.	.	.	.	.	.	.	.
	7	1	3	.	.	.	.	1	1	.	.	.	.	.	.	.	.	.	.	.	.	.	.
	8	.	1	.	.	.	.	1	1	.	.	.	.	.	.	.	.	.	.	.	.	.	.
	9	.	.	.	.	.	.	.	1	.	.	.	.	.	.	.	.	.	.	.	.	.	.
	10	.	.	.	1	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.
A13	2	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	1	.
	3	2374	22	9	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.
	4	3	1	.	.	1	.	.	.	.	1	.	.	.	.	.	.	.	.	.	.	.	.
	5	26	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.
	6	40	13	.	.	.	1	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.
	7	32	1	2	.	1	.	.	.	.	.	.	4	.	.	.	.	.	.	.	.	.	.
	8	120	15	.	.	.	1	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.
	9	1	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.
	10	4	.	.	.	3	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.
	11	8	6	1	2	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.
	12	4	6	1	1	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.
	13	2	3	1	1	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.
	14	.	3	1	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.
	15	.	.	1	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.
	16	1	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.
C7	2	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	1
	3	.	.	.	3	.	.	.	.	.	.	1	.	.	.	.	.	.	.	.	.	.	.
	4	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	1	.	.	.	.	.
	5	.	.	.	1	.	.	.	.	.	.	.	.	.	.	.	.	.	1	1	.	.	.
	6	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	1	1	.	.	.
	7	.	.	.	.	.	.	.	.	.	.	1	.	.	.	1	.	.	.	.	.	.	.
C10	2	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	1
	3	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	1	.	.
	4	.	.	.	1	.	.	1	.	.	.	.	.	.	.	.	.	.	.	.	1	.	.
	5	1	1	.	1	.	.	1	1	.	.	.	.	.	.	.	.	1	.	.	.	.	.
	6	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	1	.	.	.	.	.
	7	.	.	.	1	.	.	.	.	.	.	.	.	.	.	.	.	.	1	.	.	.	.
	8	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	1	.	.	.	.
	9	.	.	.	.	.	.	1	.	.	.	1	.	.	.	1	.	.	.	.	.	.	.
C11	2	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	1
	3	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	1	.	.
	4	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	1	.	.	.	.
	5	.	.	.	.	.	.	.	.	.	.	1	.	.	.	1	.	.	.	.	.	.	.
C12	2	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	1
	3	.	.	.	.	.	.	1	.	.	.	1	.	.	.	.	.	1	.	.	.	.	.
	4	.	.	.	1	.	.	1	.	.	.	.	.	.	.	.	.	.	1	1	.	.	.
	5	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	1	1	.	.	.
	6	.	.	.	.	.	.	.	.	.	.	1	.	.	.	1	.	.	.	.	.	.	.

Table 8 (Continued)

polyhedron	d	C_1	C_2	C_i	C_s	C_3	D_2	C_{2v}	C_{2h}	C_5	D_3	C_{3v}	S_6	D_{2h}	D_5	C_{5v}	S_{10}	T	D_{3d}	D_{5d}	T_h	I	I_h
C13	2	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	1
	3	.	.	.	.	.	.	.	.	.	.	.	.	.	1	.	.	.	.	.	.	.	.
	4	.	.	.	.	.	.	.	.	.	.	1	.	.	.	.	.	1	.	.	.	.	.
	5	.	1	.	3	.	.	.	.	.	.	.	.	1	.	.	.	.	1	1	.	.	.
	6	.	.	.	.	.	.	.	.	.	.	.	.	1	.	.	.	.	1	1	.	.	.
	7	.	.	.	.	.	.	1	.	.	.	1	.	.	.	1	.	.	.	.	.	.	.
M12	2	70	19	.	36	7	3	5	3	.	2	3	1	.	.	1	.	1	3	2	1	.	1
	3	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	1	.	.
	4	12	5	.	1	.	1	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.
	5	.	.	.	.	.	.	.	.	.	1	.	1	1	.	.	.	.	.	.	1	.	.
	6	.	1	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.
	7	4	4	.	3	.	.	.	1	.	.	.	.	1	.	.	.	.	.	.	.	.	.
	8	1	4	.	1	.	.	.	1	.	.	.	.	1	.	.	.	.	.	.	.	.	.
	9	.	.	.	.	.	.	.	1	.	.	.	.	1	.	.	.	.	.	.	.	.	.
	10	.	.	.	1	.	.	1	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.

Table 9. Divisibility Relations within Platonic, Archimedean, and Catalan Polyhedra[a]



[a] P1 to P5 are the platonic solids in order of increasing vertex count. An arrow from P_1 to P_2 surmounted by a number d indicates a d-divisibility of P_1 by P_2, with multiplicity indicated in parentheses. The medial **M12**, i.e. the medial of the truncated icosahedron is also included as C_{60} is of chemical interest.

polyhedron, the so-called pseudorhombicuboctahedron[7] (Figure 4). This has the same number of vertices, the same face signature, and the same 1-corona of each face as the rhombicuboctahedron, but it has two orbits of vertices in the group D_{2d}. It turns out that the two polyhedra have the same set of d-code sizes; the Miller polyhedron has more distinct codes (i.e. for d increasing from 2 to 6, the values of $|C_d|$ and the number of distinct codes are as follows: 8(18), 4(5), 2(5), 2(1), 1(2)) than the true rhombicuboctahedron at most values of d, as might be expected from its lower symmetry.

(iii) Codes in Catalan Polyhedra. The Catalan solids are the duals of the Archimedean polyhedra (Figure 5). Their d-code data are displayed in Tables 2 and 4−8. Many members of the series have an orbit of vertices of high degree, and this rationalizes the relatively small size and low number of distinct codes compared with the parent Archimedean series. In every case except **C9**, the dual of the snub dodecahedron, the 2-code is unique and has the full symmetry of the polyhedron. In the dual of the Miller polyhedron, the d-code sizes show some differences from those of the dual rhombicuboctahedron: for d increasing from 2 to 6, the sizes and counts are 13(1), 5(1), 3(2), 2(4), 1(4).

(iv) Codes in Medials of the Archimedean Polyhedra. The medial of a polyhedron is constructed as follows: its vertices are the edge midpoints of the parent and its edges form an inscribed r-gon within each face of size r of the parent. Thus, the medial is the *convex hull* of the midpoints of the edges of the parents. A polyhedron and its dual share the same medial. For Platonic solids, the medials are already included in the previous lists as the medial of the tetrahedron is the octahedron, the medial of both cube and octahedron is the cuboctahedron, and the medial of both icosahedron and dodecahedron is the icosidodecahedron. Two medials of Archimedean polyhedra are themselves Archimedean; the medial of the cuboctahedron is the rhombicuboctahedron (**A4**), and the medial of the icosidodecahedron is the rhombicosidodecahedron (**A10**). Sizes of d-codes were computed for the medials of the Archimedian polyhedra (Figure 6) and are listed in Table 3. In the case of most chemical interest, the medial of the truncated icosahedron, the number of distinct d-codes were also obtained (see Table 8).

In a cubic polyhedron such as the truncated icosahedron, there is a one-to-one correspondence between the 2-codes of the medial and the Kekulé structures of the parent: C_{60} has 12,500 Kekulé structures, of which 158 are distinct and follow the symmetry classification given in Table 8 (see also ref 8).

Interestingly, the 3-code of the medial of the truncated icosahedron is unique, has T_h symmetry, and its vertices are the midpoints of the 18 double bonds edges corresponding to the T_h chemical structure of $C_{60}Br_{24}$, which is itself a 2-code of the truncated icosahedron.

(v) Codes in Prisms, Antiprisms, and Their Duals. The two infinite series of semiregular polyhedra are the prisms and antiprisms, for which complete solutions to the d-code problem are straightforwardly obtained. Draw the prism and antiprism as annular Schlegel diagrams in which the region

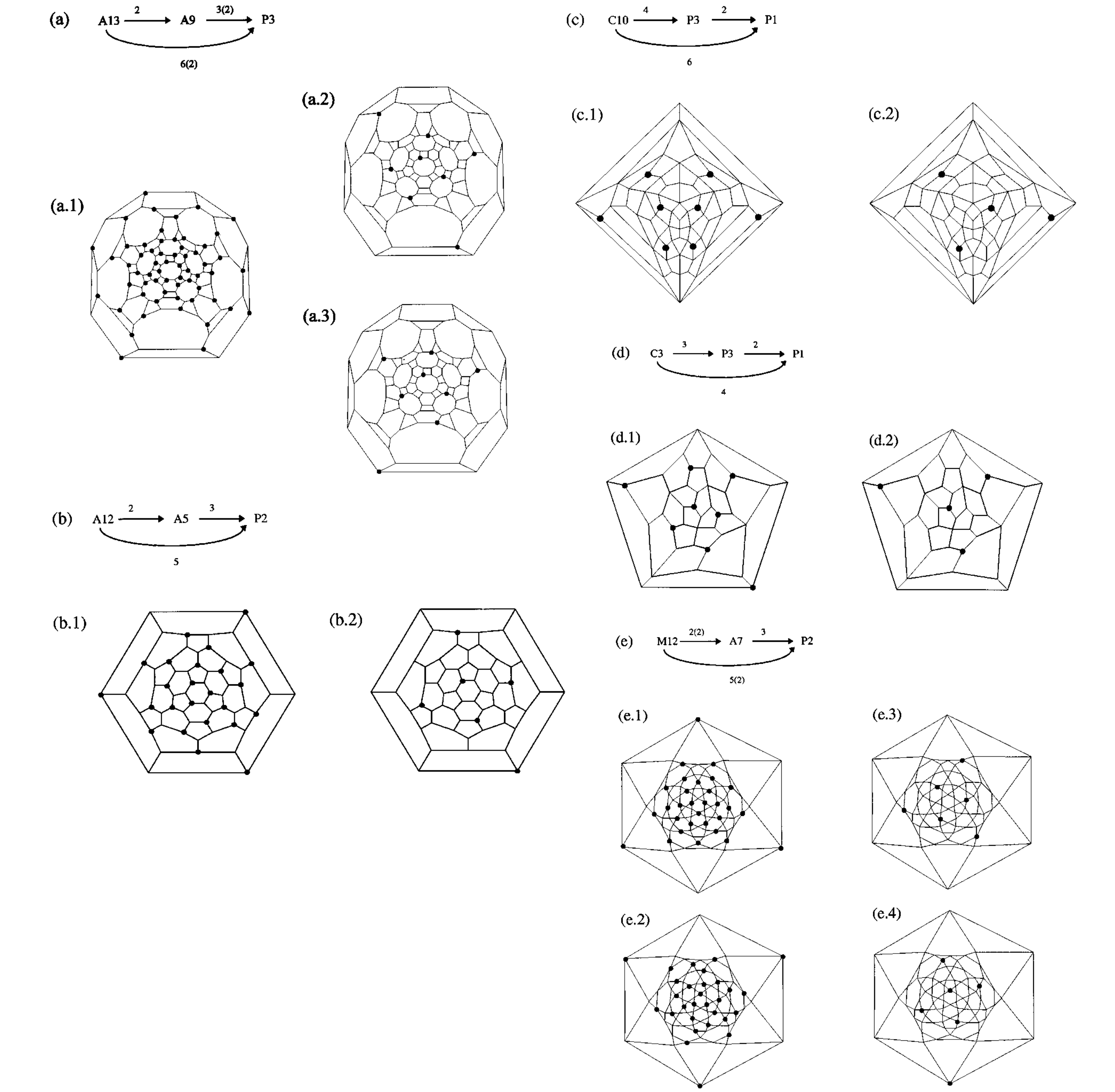


Figure 3. Russian Doll codes. (a) The 120-vertex truncated icosidodecahedron **A13** has a unique 2-code whose contact graph is the skeleton of the snub dodecahedron (vertices marked in black, figure a.1), two 3-codes of which are cubes and are also 6-codes of **A13** itself (figures a.2 and a.3). (b) The 60-vertex truncated icosahedron **A12** has a 2-code whose contact graph is the skeleton of the truncated cube (Figure b.1), the unique 3-code of which is an octahedron and also the unique 5-code of **A12** itself (Figure b.2). (c) The 62-vertex dual of the rhombicosidodecahedron **C10** has a 4-code whose contact graph is the skeleton of the cube (Figure c.1), the unique 2-code of which is the tetrahedron and one of the 6-code of **C10** itself (Figure c.2). (d) The 24-vertex dual of the snub cube **C3** has a 3-code whose contact graph is the skeleton of the cube (Figure d.1), the unique 2-code of which is the tetrahedron and also one of the 4-code of **C3** itself (Figure d.2). (e) In the 90-vertex medial of the truncated icosahedron **M12** two of the 2-codes have a contact graph whose skeleton is the icosidodecahedron (Figure e.1 and e.2). One of the two octahedra stemming from the 5-code of **M12** (Figure e.3) is embedded in the icosidodecahedron defined by Figure e.1, while both of them (Figures e.3 and e.4) are embedded in the one of Figure e.2.

bounded by the two n-cycles is either a fused strip of squares (n-prism) or fully triangulated (n-antiprism). An n-prism has diameter $\lfloor (n+2)/2 \rfloor$, and the n-antiprism has diameter $\lfloor (n+1)/2 \rfloor$. Define a *hook* movement as follows: begin from vertex j and take d-1 steps in the current cycle and then one step to reach vertex j+1 on the other cycle, always moving in a clockwise direction. Let m be the size of the maximum d-code (i.e. $|C_d| = m$). In both prisms and antiprisms a d-code of maximum size is constructed by starting from a vertex on the inner cycle, adding a hook to reach a vertex on the outer cycle, and so on, continuing until no further addition is possible. If m is odd (even) the code finishes on the inner (outer) cycle. Consecutive pairs of code-vertices (j, $j+1$) for $1 \le j < m-1$ have distance d, and pairs (j, j+2) for $1 \le j < m-2$ have distance $2d-2$ (prism) or $2d-1$ (antiprism).

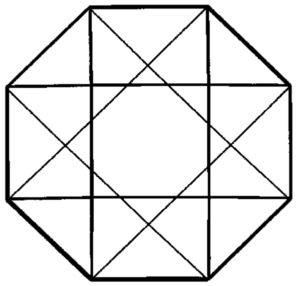


Figure 4. The Miller polyhedron.

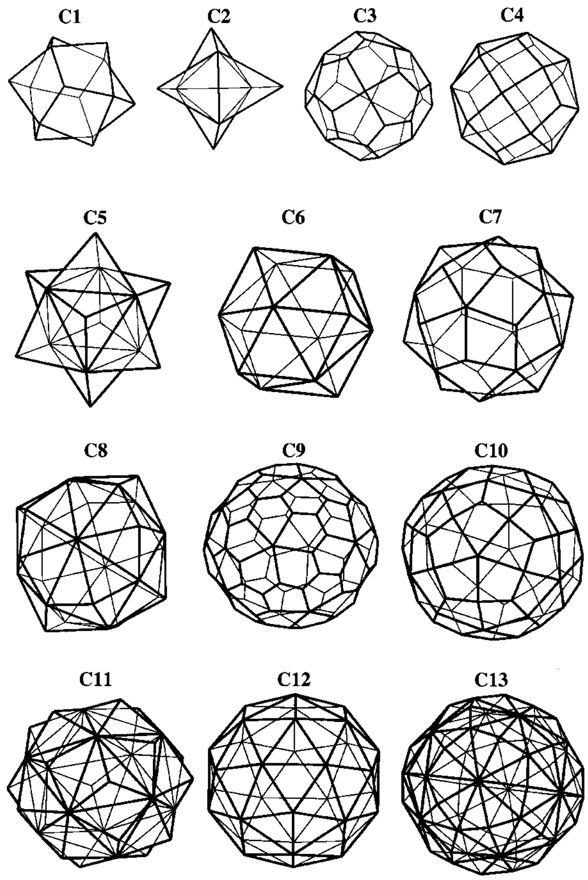


Figure 5. The Catalan polyhedra.

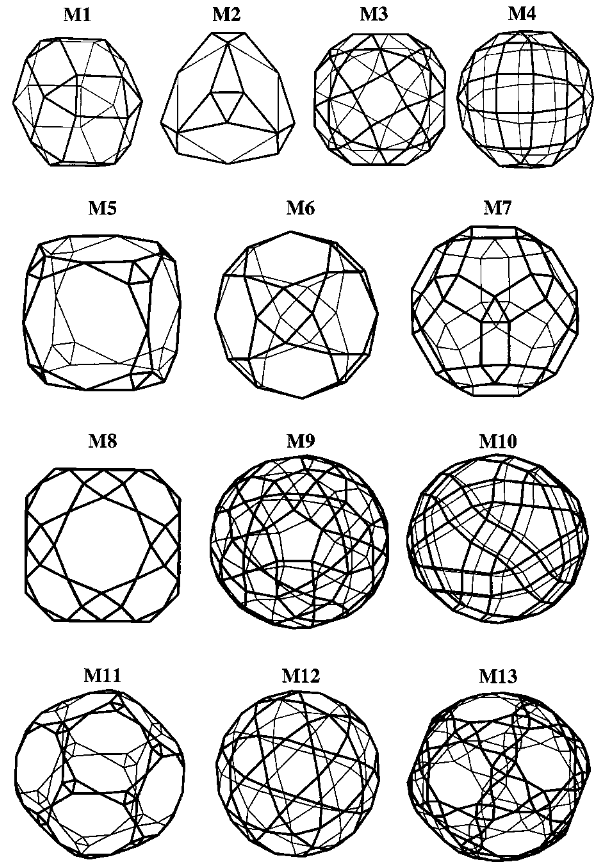


Figure 6. The medials of the Archimedean polyhedra.

For the n-gonal prism, consider the remainder i on division of n by the gap $2d$-2: $n \equiv i(\mathrm{mod}(2d - 2))$. m is odd if and only if $i > d - 1$. If m is even, then

$$m = 2\left\lfloor \frac{n}{2(d-1)} \right\rfloor = \frac{n-i}{d-1} = \begin{cases} n/(d-1) - 1 & \text{if } i = d-1 \\ \lfloor n/(d-1) \rfloor & \text{if } i < d-1 \end{cases} \quad (4)$$

If m is odd, then

$$m = 2\left\lfloor \frac{n}{2(d-1)} \right\rfloor + 1 = \frac{n-i}{d-1} + 1 = \lfloor n/(d-1) \rfloor \quad (5)$$

Hence,

$$m(n\text{-prism}) = \begin{cases} n/(d-1) - 1 & \text{if } n \equiv (d-1)(\mathrm{mod}(2d-2)) \\ \lfloor n/(d-1) \rfloor & \text{otherwise} \end{cases} \quad (6)$$

In the n-prism, the volume of the ball of radius k is $|B_k| = 4k$ and thus for $d = 2k + 1$, the code is well packed when $n \neq (d - 1)(\mathrm{mod}(2d - 2))$ and perfectly packed when $n \equiv 0(\mathrm{mod}(2d - 2))$.

For the n-gonal antiprism, consider the remainder i on division of n by the gap $2d - 1$: $n \equiv i(\mathrm{mod}(2d - 1))$. Again m is odd if and only if $i > d-1$. If m is even, then

$$m = 2\left\lfloor \frac{n}{2d-1} \right\rfloor = \frac{2(n-i)}{2d-1} \quad (7)$$

and if m is odd

$$m = \left\lfloor 2\frac{n}{2d-1} \right\rfloor + 1 \quad (8)$$

So the size of the d-code for the antiprism is

$$m(n\text{-antiprism}) = \left\lfloor \frac{2n}{2d-1} \right\rfloor \quad (9)$$

In the n-antiprism, the ball of radius k has volume $|B_k| = 4k + 1$ and thus for $d = 2k + 1$ the code is always well packed, and it is perfect for $2n \equiv 0(\mathrm{mod}(2d - 1))$.

The duals of the prisms are the bipyramids. The n-gonal bipyramid derived from the n-gonal prism as $D = 2$ and its unique 2-code consists of $\lfloor n/2 \rfloor$ points on the equator.

The dual of the n-gonal antiprism is a bipartite graph of diameter 3 consisting of 2 poles and a $2n$-gonal equator where each pole is connected to alternate equatorial points. A 3-code can be constructed in two ways, either by taking the pair of poles or any two equatorial non-neighbors of different parity making symmetry distinct codes.

Tables 10 and 11 list code sizes and numbers of distinct realizations for some small cases of prisms and antiprisms.

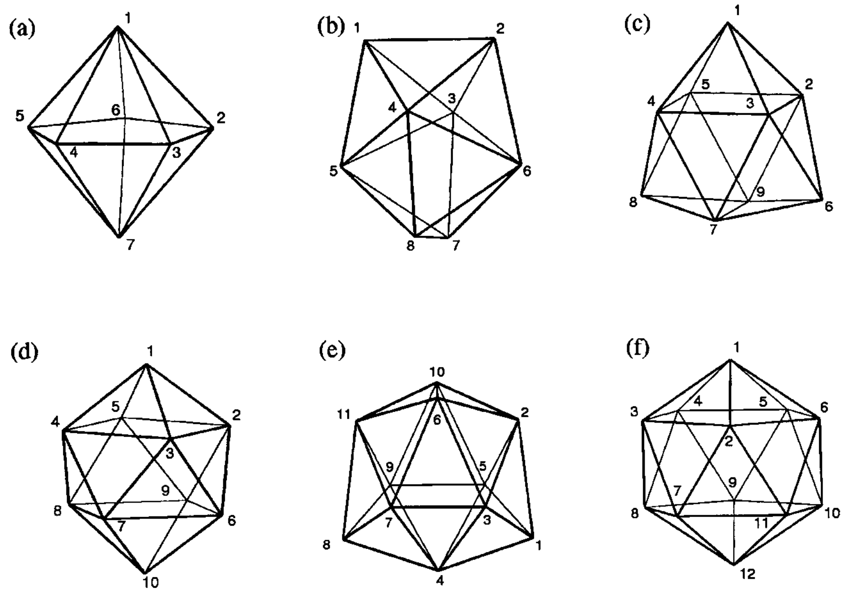


Figure 7. Deltahedral cages and chemical labeling conventions.

Table 10. Codes in Prisms[a]

	d					
n	2	3	4	5	6	7
5	4(1)	2(1)	1(1)			
6	6(1)	2(3)	2(1)	1(1)		
7	6(1)	3(1)	2(1)	1(1)		
8	8(1)	4(1)	2(3)	2(1)	1(1)	
9	8(1)	4(1)	2(3)	2(1)	1(1)	
10	10(1)	4(3)	3(1)	2(3)	2(1)	1(1)

[a] *n* is the size of the large face, and an entry *x*(*y*) denotes a *d*-code of size *x* with *y* distinct realizations.

Table 11. Codes in Antiprisms[a]

	d				
n	2	3	4	5	6
4	2(2)	1(1)			
5	3(1)	2(2)	1(1)		
6	4(1)	2(2)	1(1)		
7	4(3)	2(3)	2(1)	1(1)	
8	5(1)	3(1)	2(2)	1(1)	
9	6(1)	3(3)	2(3)	2(1)	1(1)

[a] Same conventions as in Table 10.

(vi) Chemical Significance of *d*-Codes. Two illustrations of the chemical application of *d*-codes come from the addition chemistry of C_{60} and the chemistry of carboranes. The framework of C_{60} is a truncated icosahedron. Study of *d*-codes on the truncated icosahedron, its dual, and its medial therefore correspond to models for three basic types of functionalization: addition to vertices, faces, and edges of C_{60} in sp^3, η^5, or η^6 and cyclization or bond insertion reactions, respectively.

The significance of the *d*-code as a model for $C_{60}Br_{24}$ has already been discussed, as has the connection between the 2-code of the medial and Kekulé structures. Each 2-code of the medial is also a model for maximal nonadjacent cyclopropanation of the fullerene. Although η^5 and η^6 compounds of C_{60} are as yet unknown, the unique 2-code of the dual indicates that maximal coordination to faces would not involve any η^6-hexagons; coordination to pentagons in a

Table 12. Codes in Deltahedra[a]

	d		
n	2	3	4
4	1(1)		
5	2(1)	1(2)	
6	2(1)	1(1)	
7	2(2)	1(2)	
8	2(3)	1(2)	
9	3(1)	1(2)	
10	3(1)	2(1)	1(2)
11	3(5)	2(1)	1(5)
12	3(1)	2(1)	1(1)

[a] Same conventions as in Table 10.

hypothetical molecular crystal composed of $(\eta^5)_{12}Li_{12}C_{60}$ species was considered by Andreoni et al.[9] The higher *d*-codes provide plausible candidates for more sterically hindered derivatives of all three basic types.

Deltahedral cages figure in the chemistry of the boranes and related species. In mathematics, a deltahedron is a convex polyhedron that can be constructed with all faces triangular and equilateral. Chemical usage is looser; any polyhedron all of whose faces are triangular, whether equilateral or not, is called a deltahedron. The *d*-code calculations for the *n*-vertex deltahedra ($4 \leq n \leq 12$) are listed in Table 12 and may be used to rationalize structures of derived carboranes. The 11-vertex cage is not convex when constructed with equilateral triangles but is included in Table 12 as it is realized in $B_{11}H_{11}^{2-}$ and is a deltahedron in the chemical sense.

Closo-carboranes of formula $C_2B_{n-2}H_n$ notionally derived by replacement of B^- with C in the deltahedral framework $B_nH_n^{2-}$ are known for most of the series, sometimes in more than one isomeric form.[10] As a rule, in the most stable isomer carbon atoms occupy nonadjacent sites of the cage and prefer sites of low coordination. Deltahedra with $n = 5$ and $n = 6$ are the bipyramid and the octahedron, respectively. Their 2-codes are unique and correspond to carborane structures with carbon atoms on the antipodal pair. With respect to the nomenclature given in Figure 7(a−f), at $n = 7$, there are two distinct 2-codes of size 2: a pair of polar sites (*closo* 1,7 $C_2B_5H_7$) and a pair of equatorial sites (*closo* 2,4 $C_2B_5H_7$) of which only the second obeys the low-coordination rule. The $n = 8$ deltahedron has four sites of degree 4 and four of degree 5, leading to three distinct 2-codes where two, one, or zero 4-coordinate sites are occupied, of which the first (*closo* 1,7 $C_2B_6H_8$) corresponds to the stable isomer.

In cages with $n \geq 9$, it is mathematically possible to have three nonadjacent carbon-substituted sites, and for $n \geq 10$ there is one pair of carbon sites separated by three edges. For $n = 9$, the *closo* 1,6 $C_2B_7H_9$ takes two of the three low-coordinate vertices of the unique 2-code. For $n = 10$, *closo* 1,10 $C_2B_8H_{10}$ is the unique 3-code (antipodal). For $n = 11$, the unique 3-code is not compatible with the low-coordination rule, and occupation in *closo* 1,8 $C_2B_9H_{11}$ of the two low-coordinate sites corresponds to deletion of the high-coordinate site in one of the four 2-codes. For $n = 12$, the para antipodal *closo* 1,12 is the unique 3-code of the icosahedron; the “meta” isomer 1,7 $C_2B_{10}H_{12}$ is a nonmaximal 2-code.

Many further chemical applications of *d*-code theory could be envisaged, given the wide occurrence of polyhedra in molecular and solid-state chemistry.

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