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On the complexity of Archimedean solids

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The complexity of 13 Archimedean solids via their Schlegel graphs was studied by four indices: the complexity index based on the augmented vertex-degree, and the total numbers of walks, trails and paths. All four descriptors consider the truncated tetrahedron, the truncated cube and the truncated octahedron as the least complex structures, and the rhombicuboctahedron, the icosidodecahedron, the rhombicosidodecahedron, the snub cuboctahedron and the snub icosidodecahedron the most complex structures among the 13 Archimedean solids. The ordering of remaining five Archimedean solids (the truncated icosahedron, the truncated dodecahedron, the cuboctahedron, the truncated cuboctahedron and the truncated icosidodecahedron) differs from index to index. The visualization of the complexity relationship between Archimedean solids is realized by the partial order of their indices in consonance with the Hasse diagram.

KEY WORDS: Archimeaden solids, complexity measures, Platonic solids, polyhedra

1. Introduction

Archimedean solids [1] (also known as Archimedean bodies [2] and Archimedean polyhedra [3]) came into the focus of research interest after the discovery of buckminsterfullerene, a pure carbon molecule consisting of 60 atoms [4] and assignment of its structure as that of the truncated icosahedron. As far as we know buckminsterfullerene is only real molecule whose structure resembles

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to an Archimedean solid. However, it is expected that other cage molecules will be prepared possessing structures that can be modeled by Archimedean solids. We should like to use the term *Archimedean molecules* for molecules with structures resembling Archimedean solids. At present, all Archimedean molecules, but buckminsterfullerene, are virtual molecules. Nevertheless, they are occasionally studied usually in conjunction with Platonic solids and other polyhedra [5,6]. It is anticipated that the preparation of Archimedean molecules will be difficult – these molecules are expected to be rather complex systems, but the imagination of chemists is so fertile that sooner or later they will be made or discovered. There is some work already reported in this direction [e.g., 7]. Due to the possible preparation of Archimedean molecules, it is of interest to consider the complexity of Archimedean solids.

2. Archimedean solids

Archimedean solids are semiregular convex polyhedra [8]. A semiregular polyhedron is a polyhedron whose faces are regular polygons, although not all the same, and each of whose vertices is symmetrically equivalent to every other vertex. There are 13 Archimedean solids – their names and shapes are given in figure 1. It should be noted that Archimedean solids can be generated by truncating or snubbing regular polyhedra named Platonic solids.

Graphs representing the Archimedean solids are known as of *Schlegel* graphs [8]. They are given in figure 2. Schlegel graphs of Archimedean solids (Archimedean graphs) are planar, regular, polyhedral, Hamiltonian and vertex-transitive graphs. Only *six* of Archimedean graphs (cubooctahedral graph, icosahedral graph, snub cubooctahedral graph, snub icosidodecahedral graph, rhombicuboctahedral graph and rhombicosidodecahedral graph) are the edge-transitive graphs. Note, a graph is a *planar* graph if it can be embedded in the plane. A graph is a *regular* graph if all of its vertices have the same degree. A graph is a *polyhedral* graph if each of its faces is bounded by a polygon. A graph is a *Hamiltonian* graph if possesses a spanning cycle. A graph is a *vertex-transitive* if all of its vertices are symmetrically equivalent. A graph is an *edge-transitive* if all of its edges are symmetrically equivalent. All these graph-theoretical terms are explained and illustrated in Harary's book *Graph Theory* [9] and in the book by one us (NT) *Chemical Graph Theory* [10].

The first surviving description of Archimedean solids is that of a Greek geometer Pappus of Alexandria who lived during the fourth century (around 320) [11,12]. Pappus of Alexandria attributes the invention of truncated and snubbed Platonic solids to Archimedes (287–212 B.C.). Hence, the name *Archimedean solids*. The painter–mathematicians of the Renaissance were interested in the Golden Cut and in its appearance in the Platonic solids and Archimedean solids [13]. In 1492, the Archimedean solids were rediscovered by the painter

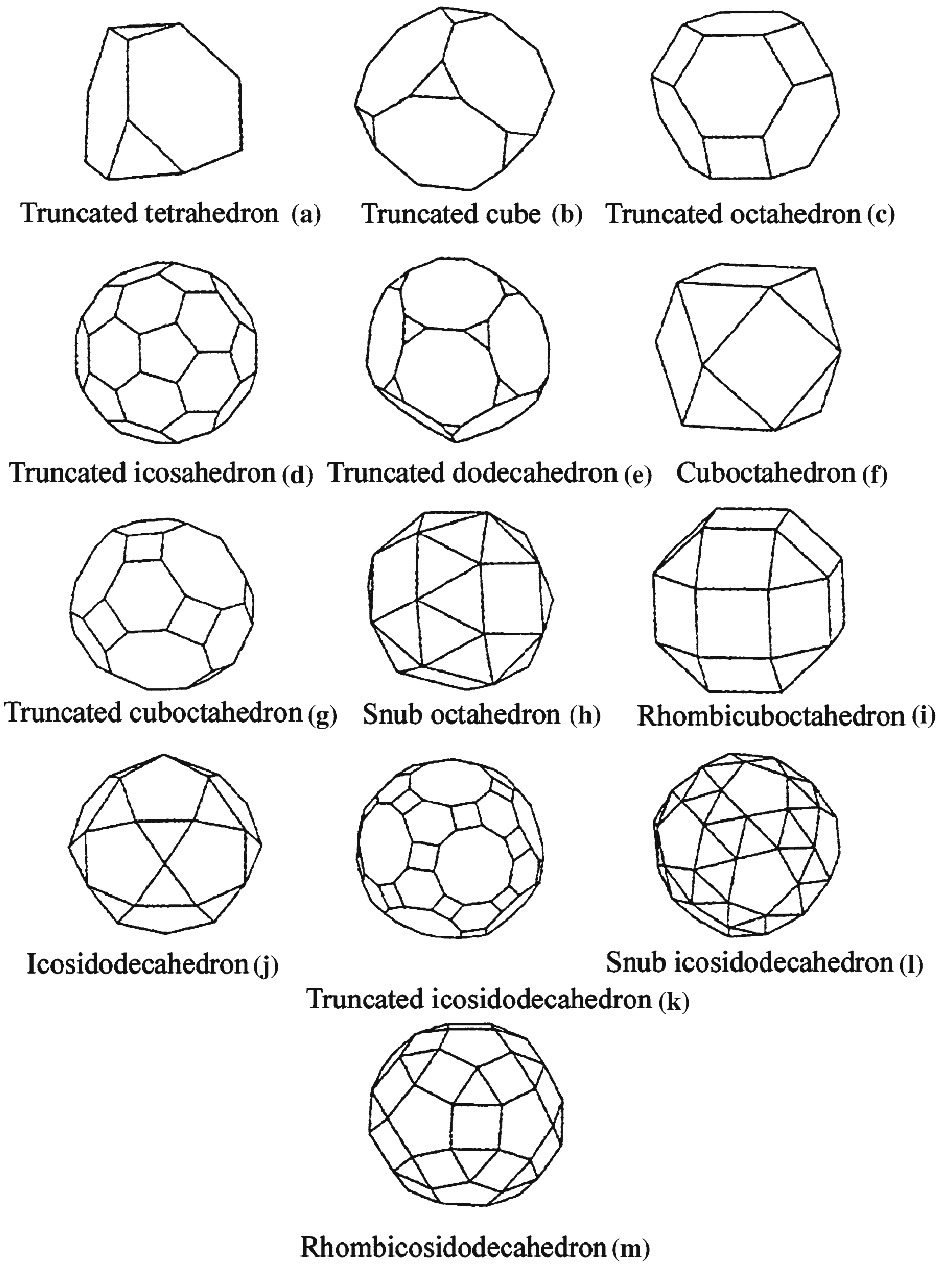

Figure 1. The shapes of Archimedean solids.

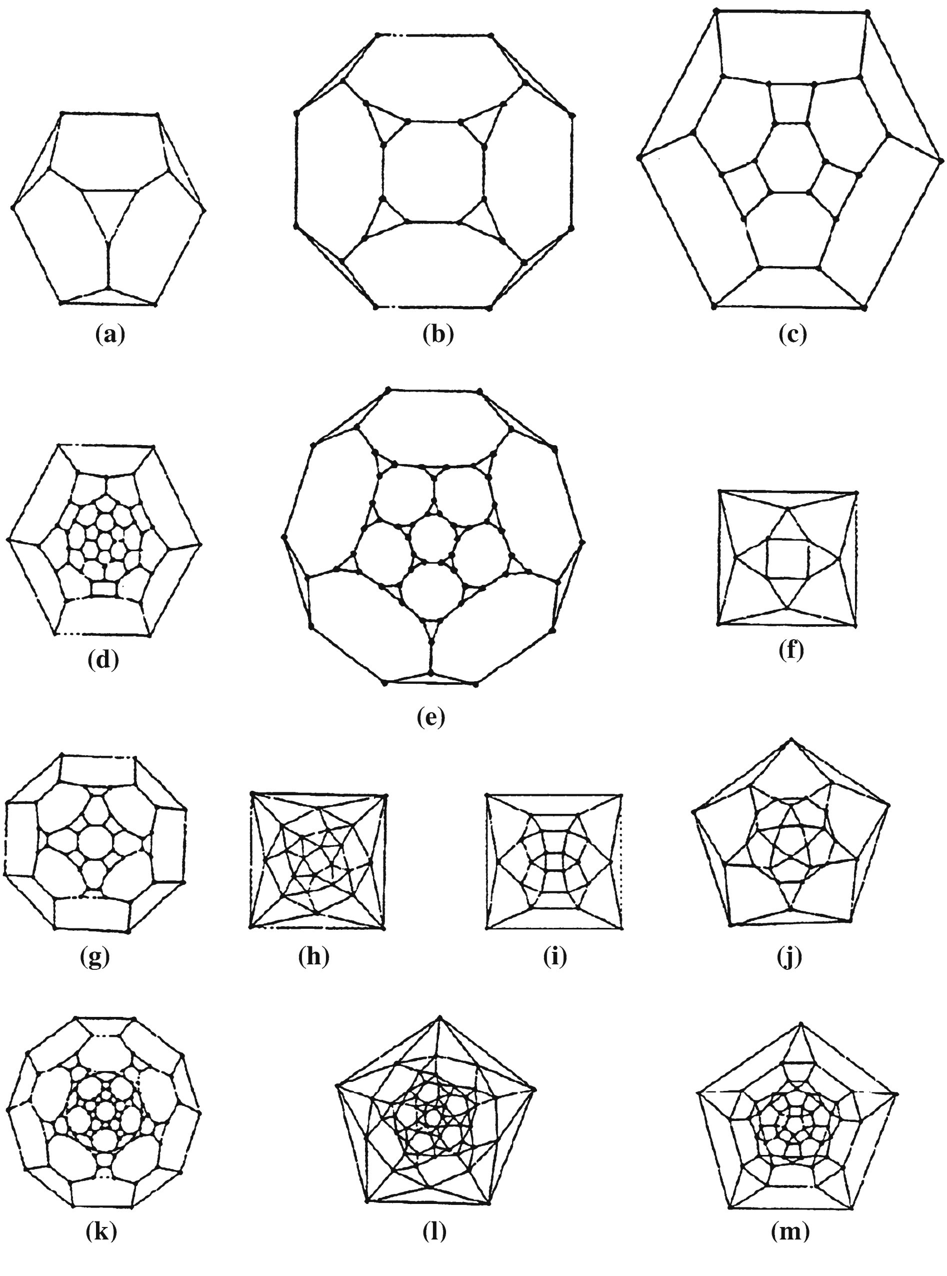

Figure 2. The Schlegel graphs of Archimedean solids.

and mathematician Piero della Francesca [14]. Luca Pacioli in his masterpiece *De Divina Proportione* (1509, reproduced in 1956) examined besides the Platonic solids some of the Archimedean solids, in particular the cubooctahedron. But the Renaissance author who was perhaps most interested in the Archimedean solids was Daniel Barbaro, as can be seen in his book *Prattica de la Perspectiva* (1569). It was, however, Johannes Keppler (1571–1630) who catalogued the 13 Archimedean solids in 1619 and gave them their now generally accepted names [15].

The surface of Archimedean solids (or of any polyhedron) in 3D space is made up of 0-, 1- and 2-dimensional faces. The formula that relates the number of faces F, the number of edges E and the number of vertices V of polyhedra, called the *Euler formula* [e.g., 16] after its inventor [17], is given by:

$$F - E + V = 2. \tag{1}$$

This beautifully simple formula is the first formula of topology. Another simple topological formula relates the number of edges to the number of n-sided faces F_n of polyhedra:

$$2E = \sum_n nF_n. \tag{2}$$

The smallest face is the triangular face F_3. Since no face can have fewer edges than 3, the following inequality must hold in all cases:

$$2E \geqslant 3F. \tag{3}$$

There is also a formula that relates the number of vertices of a degree d, V_d, to the number of edges E in a polyhedron:

$$2E = \sum_d dV_\mathrm{d}. \tag{4}$$

Since no vertex of a polyhedron can have a degree less than 3, the following inequality must hold in all cases:

$$2E \geqslant 3V. \tag{5}$$

The topological parameters F, E, V, d and the cycle-rank (or the cyclomatic number) of Archimedean solids are given in table 1. The *cycle-rank* of a polycyclic graph G, denoted by γ, is equal to the minimum number of edges necessary to be removed from G to convert it to a spanning tree [18]. It can be computed as follows:

$$\gamma = E - V + 1. \tag{6}$$

Note, the cycle-rank of a tree is zero and of a monocyclic graph is one.

Table 1
Topological parameters of the Archimedean solids.

Archimedean solid	Regular polygon	V	E	F	d	γ
Truncated tetrahedron (**A**)	Triangle	12	18	4	3	7
	Hexagon			4		
Truncated cube (**B**)	Triangle	24	36	8	3	13
	Octagon			6		
Truncated octahedron (**C**)	Square	24	36	6	3	13
	Hexagon			8		
Truncated icosahedron (**D**)	Pentagon	60	90	12	3	31
	Hexagon			20		
Truncated dodecahedron (**E**)	Triangle	60	90	20	3	31
	Decagon			12		
Cuboctahedron (**F**)	Triangle	12	24	8	4	13
	Square			6		
Truncated cuboctahedron (**G**)	Square	48	72	12	3	25
	Hexagon			8		
	Octagon			6		
Snub cuboctahedron (**H**)	Triangle	24	60	32	5	37
	Square			6		
Rhombicuboctahedron (**I**)	Triangle	24	48	8	4	25
	Square			18		
Icosidodecahedron (**J**)	Triangle	30	60	20	4	31
	Pentagon			12		
Truncated icosidodecahedron (**K**)	Square	120	180	30	3	61
	Hexagon			20		
	Decagon			12		
Snub icosidodecahedron (**L**)	Triangle	60	150	80	5	91
	Pentagon			12		
Rhombicosidodecahedron (**M**)	Triangle	60	120	20	4	61
	Square			30		
	Pentagon			12		

3. Complexity indices of Archimedean solids

We used four indices to assess the complexity of Archimedean solids: the index based on the concept of the augmented vertex-degree, and three indices based on the total numbers of walks, paths and trails. Indices based on the concept of the augmented vertex-degree and on the number of walks are currently used in the literature to study the complexity of molecules via their graphs [19–23] whilst the numbers of and paths trails to our knowledge have not been previously used for this purpose.

3.1. Augmented vertex-degree as a measure of complexity

The complexity index ξ, based on the concept of the augmented vertex-degree, was introduced recently by Randić et al. [24–27] and reviewed by several groups [20,23,28]. This concept is based on the notion of partial additivity of vertex-degrees. The degree of a vertex in a graph is the number of edges incident with this vertex. The augmented degree of a given vertex i, $(\mathrm{AVD})_i$, is obtained by adding to its degree, the degrees of vertices with the weight that depends on their distances from this vertex. This can be formalized as:

$$(\mathrm{AVD})_i = \sum_{i=1}^{\lambda_{\max}} d_i / 2^{\lambda(ij)}, \tag{7}$$

where d_i is the degree of the vertex $i, \lambda(ij)$ is the shortest distance in terms of the number of edges between vertices i and j, and $\lambda_{\max}$ is the value of the maximal shortest distance. The complexity index is then given as the sum of the augmented degrees of all vertices in a graph not equivalent by symmetry:

$$\xi = \sum_{i=1}^{V} \sum_{j=1}^{\lambda_{\max}} d_i / 2^{\lambda(ij)}. \tag{8}$$

In the case of vertex-transitive graphs such as Schlegel graphs representing Archimeaden solids, equation. (8) reduces to equation. (7), that is:

$$\xi = \sum_{i} (\mathrm{AVD})_i. \tag{9}$$

The greater values of ξ, the greater complexity of an Archimeden solid. The values of ξ are given in table 2.

3.2. The numbers walks, paths and trails as complexity indices

A *walk* in a grah is an alternating sequence of vertices and edges, such that each edge is both, immediately preceded and followed by vertices. A walk is a *trail* if all the edges are distinct and a *path* if all vertices are distinct. The length of the walk (trail, path) is the number of edges in it. The total walk count was used, for example, by Rücker and Rücker [29] and by us [30] as a measure of the complexity of graphs and molecules.

3.2.1. The number of walks in the graph

Since all the observed graphs are regular graphs, the number of walks of length q, $w(q)$, in these graphs is equal to Vd^q. Note that the first vertex can be chosen in V ways and each its successor in the walk in d ways. We computed

Table 2
Complexity indices based on the augmented vertex-degree, ξ, and the total walk count, twc(q), the total path count, tpc(q), and the total trail count, ttc(q), of the Archimedean solids.

Archimedean solid	ξ	twc(q)	tpc(q)	ttc(q)
A	12.00	118092	1746	2850
B	14.16	236184	4788	6108
C	14.77	236184	6516	7788
D	18.498	590460	19650	21390
E	15.90	590460	12090	15270
F	18.500	1048572	18012	49620
G	16.61	472368	13752	15816
H	32.81	11718744	506052	984828
I	23.13	2097144	78408	121176
J	26.00	2621430	97350	147630
K	17.70	1180920	34500	39540
L	41.43	29296860	1460130	2524830
M	30.52	5242860	225120	315600

The numbers twc(q), ttc(q) and ttc(q) are given for $q = 8$.

the total walk count, twc(q), by summing up all walks up to the certain length q, $w(q)$:

$$\mathrm{twc}(q) = \sum_q w(q). \tag{10}$$

In our case, we computed tpc(q) up to $q = 8$. These numbers for Archimedean graphs are given in table 2.

3.2.2. The number of paths in the vertex-transitive graphs

The number of the paths in the vertex-transitive graph is calculated by the recursive algorithm. We present this algorithm in the pseudocode. We need the following variables:

- *Visited* – we assume that vertex is visited if the path passes through this vertex. At the beginning of the algorithm, we assume that all entries of this array are equal to false
- *NumOfPaths* – this is the array such that its i-th entry contains the number of paths of length i (at the end of algorithm). Of course, we assume that all its entries are equal to 0 to start.
- $b - Vd$ array such that $b[i][1], b[i][2], \ldots, b[i][d]$ are the neighbors of the vertex i (this is the input of the algorithm).
- *length* – represents the length of the observed path
- *last* – last represents the last vertex of the observed path

- *NumVertices* – number of vertices of the observed graph

Below we give the pseudocode of the recursive algorithm which enumerates all paths of length at most *MaxLength*:

RecEnumeratePaths(*length,last*)

1) $NumOfPathslength] = NumOfPaths[length] + 1$

2) If $x < MaxLength$

2.1) For $i = 1, \dots ,$deg

2.1.1) If *Visited* $[b[last][i]] = False$

2.1.1.1) *Visited* $[b[last][i]] = True$

2.1.1.2) $RecEnumeratePaths\ (length + 1, b\,[last]\,[i])$

2.1.1.3) *Visited* $[b\,[last]\,[i]] = False$

MainEnumeratePaths ( )

1) $RecEnumeratePaths(0, 1)$

2) For $i = 1, ..., MaxLength$

2.1) $NumOfPaths\,[length] = NumOfPaths\,[length] \cdot NumVertices/2$

The total path count, tpc(q), is obtained by summing up all paths up to the certain length q, $p(q)$:

$$\mathrm{tpc}(q) = \sum_p p(q). \tag{11}$$

In our case, we computed tpc(q) up to $q = 8$. The tpc(q) numbers for Archimedean graphs are given in table 2.

3.2.3. The number of trails in the vertex-transitive graphs

The number of the trails in the vertex-transitive graph is also calculated by the recursive algorithm. We present this algorithm in the pseudocode. The following variables are nedeed:

- *NumOfPaths* – this is the array such that its i-th entry contains the number of paths of length i (at the end of algorithm). Of course, we assume that all its entries are equal to 0 to start.
- $b - Vd$ array such that $b[i][1], b[i][2], \dots, b[i][d]$ are the neighbors of the vertex i (this is the input of the algorithm).
- *Visited* – Vd array such that $Visited\,[i]\,[j]$ is true only if the edge connecting vertices i and $b\,[i]\,[j]$ is contained in the observed trail.

- *length* – represents the length of the observed path
- *last* – last represents the last vertex of the observed path
- *NumVertices* – number of vertices of the observed graph

Below is given the pseudocode of the recursive algorithm which enumerates all paths of length at most $MaxLength$:

RecEnumerateTrails (*length,last*)

1) $NumOfTrails[length] = NumOfTrails[length] + 1$

2) If $x < MaxLength$

2.1) For $i = 1, \ldots, \deg$

2.1.1) If $Visited[last][i] = False$

2.1.1.1) $Visited[last][i] = True$

2.1.1.2) For j such that $b[b[last][i]][j] = last$ put $Visited[b[last][i]][j] = True$

2.1.1.3) $RecEnumeratePaths\,(length + 1, b[last][i])$

2.1.1.4) $Visited\,[last][i] = False$

2.1.1.5) For j such that $b[b[last][i]][j] = last$ put $Visited[b[last][i]][j] = False$

MainEnumeratePaths ( )

1) $RecEnumerateTrails\,(0, 1)$

2) For $i = 1, ..., MaxLength$

2.1) $NumOfTrails\,[length] = NumOfTrails\,[length] \cdot NumVertices/2$

The total trail count, ttc(q), is obtained by summing up all trails up to the certain length $q, t(q)$:

$$\mathrm{ttc}(q) = \sum_q t(q). \tag{12}$$

In our case, we computed ttc(q) up to $q = 8$. The ttc(q) numbers for Archimedean graphs are given in table 2.

4. Complexity ordering of Archimedean solids

In table 3 is given the complexity ordering, based on the four descriptors from table 2, from the least to the most complex Archimedean solid.

Table 3
Ordering of the Archimedean solids by the four complexity indices from Table 2.

Complexity index	Complexity ordering from the least to the most complex Archimedean solid
ξ	**A** < **B** < **C** < **E** < **G** < **K** < **D** < **F** < **I** < **J** < **M** < **H** < **L**
twc($q = 8$)	**A** < **B** = **C** < **G** < **D** = **E** < **F** < **K** < **I** < **J** < **M** < **H** < **L**
tpc($q = 8$)	**A** < **B** < **C** < **E** < **G** < **F** < **D** < **K** < **I** < **J** < **M** < **H** < **L**
ttc($q = 8$)	**A** < **B** < **C** < **E** < **G** < **D** < **K** < **F** < **I** < **J** < **M** < **H** < **L**

All four descriptors consider the truncated tetrahedron (**A**), the truncated cube (**B**) and the truncated octahedron as the least complex structures, and the rhombicuboctahedron (**I**), the icosidodecahedron (**J**), the rhombicosidodecahedron (**M**), the snub cuboctahedron (**H**) and the snub icosidodecahedron (**L**) the most complex structures among the Archimedean solids. The ordering of **D**, **E**, **F**, **G** and **K** differs from index to index. However, three indices: ξ , tpc(q) and ttc(q) placed the truncated dodecahedron (**E**) and the truncated cuboctahedron (**G**) immediately after structures **A**, **B** and **C**. The above can be visualized by the Hasse diagram based on the partial order of the four complexity indices (see figure 3). It should be noted that some authors consider the complexity as a partially-ordered quantity [31–35]. The Hasse diagram reflecting the partial order of indices appears to be a very useful device to be used for appraising the structural complexity of molecules and graphs.

The diagram in figure 3 is such that in following downward along a path from structure **X** to structure **Y**, all four indices have a smaller value for **X** than for **Y**. Furthermore, two structures **X** and **Y** are directly linked by an edge downward from **X** to **Y** if and only if no third structure is placed by this partial ordering between **X** and **Y**.

5. Conclusions

The complexity of Archimedean solids was investigated by four complexity indices: the index based on the concept of the augmented vertex-degree, and three indices based on the total numbers of walks, paths and trails. These indices agreed in predicting the truncated tetrahedron, the truncated cube and the truncated octahedron as the *least* complex structures, and the rhombicuboctahedron, the icosidodecahedron, the rhombicosidodecahedron, the snub cuboctahedron and the snub icosidodecahedron as the *most* complex structures among the Archimedean solids. This is graphically shown by the Hasse diagram representing the partial order for 13 Archimedean solids based on the four complexity indices (ξ, twc, tpc, ttc).

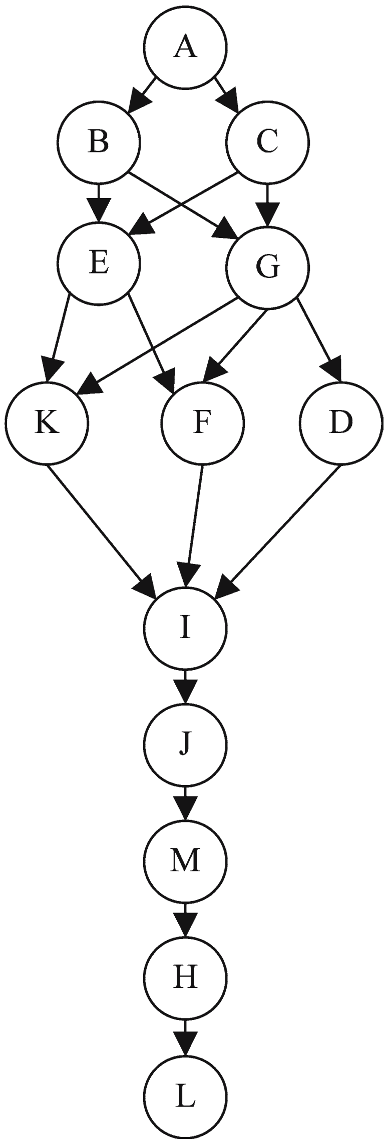

Figure 3. The partial order via the Hasse diagram for Archimedean solids based on the four considered complexity indices ξ, twc(q), tpc(q) and ttc(q).

There are also other approaches available to study the complexity of molecules and graphs [e.g., 20, 36]. For example, the number of spanning trees is a good indicator of the structural complexity [36–39], but in the present case it is impractical to use because this number is rather huge for Archimedean solids, e.g., the number of spanning trees for the truncated icosahedron that neatly models buckminsterfullerene is 375, 291, 866, 372, 898, 816, 000 [37,40].

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Noted added in proof

While our paper was refereed and revised, another paper on the complexity of Archimedean solids (and Platonic solids) appeared: A.T. Balaban and D. Bonchev, Complexity, sphericity, and ordering of regular and semiregular polyhedra, MATCH Commun. Math. Comput. Chem. 54 (2005) 137 (submitted October 20, 2004). The complexity criterion in this paper is the solid angle. However, the authors considered only 11 Archimedean solids, the snub octahedron and the snub icosadodecahedron were not included in their analysis.

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