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Periodic system of fullerenes from the mathematical standpoint

A.I. Melker [1], M.A. Krupina [2]

[1] St. Petersburg Academy of Sciences on Strength Problems, St. Petersburg, Russia

[2] Peter the Great St. Petersburg Polytechnic University, St. Petersburg, Russia

ndtcs@inbox.ru

ABSTRACT
The types of classification for fullerenes' property are considered. It accumulates empirically found the horizontal and vertical symmetry of fullerenes which give a preliminary classification. Two different symmetries are united into a common symmetry producing the periodic system of fullerenes. This system may be considered as the topological lattice in the topological space of the points corresponding to the fullerenes. The system gives the general classification of fullerenes on the basis of symmetry.

KEYWORDS
carbon • fullerene • graph • growth • isomer • periodic system • topology

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Classification, Appearance and Development

Property

The term classification (*Lat* classis – class + facere – do, execute) is defined as the act or process of arranging people or things (such as plants, animals, books in libraries, etc.) into groups in the dependence on their common features [1–3]. Historically the term is originated from the sixth Roman tsar Servius Tullius, (578-534 B.C.) who divided the Roman people into six classes according with their property, the sixth class having nothing [4].

Libraries

The classification of books has appeared simultaneously with libraries. The world's first genuine library was arranged by the Assyrian tsar Ashshurbanipal (668 - 626 B.C.) who has carried on many campaigns [5–8]. After the victories, he driven a chariot harnessed by four captive tsars in his capital Ninevia (the north of the modern Iraq). Contrary to his ancestors, he was rather well educated; he wielded three languages, including dead language Sumerian, liked reading and history, and even wrote poetry. In his big palace there were special rooms for the library. The manuscripts were on astronomy, geography, history, literature, law, trades and myths. The huge library contained more than 30 thousand of clay plates, each plate being 40 cm in the high. They contained 400 lines of cuneiform (*Lat* cuneus – wedge) signs on both sides. In the end of text there were given the elements of bibliographical description: heading, plate's number, the first words of the next plate, and the name of owner or copyist. The plates were kept in boxes. It's

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interesting to note that the word *library* originated from the Latin word *librarium* what means a box for manuscripts or books.

Education

The book and knowledge classification was developing in parallel with education. The Roman system of education included seven fields of knowledge, so called seven crafts or "the seven liberal arts". Pupils studied trivium (1-st cycle: grammatics, dialectics, rhetoric) and quadrivium (2-d cycle: arithmetic, music, geometry, astronomy). The Latin both words mean crossing of three or four roads [4]. That standard education program was conserved in the middle-age schools of Europe, except of the principal addition – theology [9]. In due time, the schools had developed or were united into Universities [10]. However, the classified education has been carefully conserved [11].

In 1340 the professors of juridical faculty (Sorbonne) have adopted a resolution that any student should begin his education having a comprehensive knowledge of seven liberal arts. "We believe that if there is no base, it's no allowed to make a superstructure and that not by a breach of the sequence of degrees, but the rise to higher posts and sciences must be done gradually and timely. Since grammatics, logic, physics and other primary sciences are the way and base to other, more higher knowledge, we establish and prescribe that nobody is allowed to pretend to the degree of bachelor of cannon law at the juridical faculty in Paris, if he is not enough strong in primary knowledge".

To the end of the fifteen century the books were classified in accordance with the existing four faculties of the Universities, theological, philosophical, juridical and medical.

Real philosophy

The development of technique and natural sciences in West Europe in XVI-XVII centuries had led to the conclusion that the previous classification of knowledge is too narrow [12]. Some philosophers and writers, especially Michel Eyquem de Montaigne (1533-1592) and Francis Bacon (1561–1626), contradicted to speculative philosophy the knowledge based on experience which is connected with human nature [13–17]. In the beginning of the seventeenth century Sir Francis Bacon (1561–1626) had suggested classifying knowledge with respect to the ability of human spirit [15–17]. According to Bacon, memory originates history, imagination produces poetry and mind creates philosophy.

It should be mentioned that both philosophers were well educated; they knew foreign and ancient classical languages. Michel Montaigne studied law, at one time was a member of Bordeaux's parliament and later was elected the mayor of that city; he maintained friendly relations with Henri Bourbon, the future King Henri IV (1589-1610). Montaigne lived in the stormy period of Huguenot Wars (1562-1598). "In 1571 being 38 years old, tired by public duties, I decided to spend the rest of life devoting it to the Muses". In 1580, he traveled one year across Europe visiting Germany, Switzerland and Italy; in 1588 he was put for a short time into the Bastille. Montaige had exerted great influence on the intellectuals in many countries; in Russia he was highly appreciated by Pushkin, Herzen, Tolstoy and Gorky [14].

Francis Bacon succeeded to “practically philosophical outlook on things created by Montaigne” [14]. He studied at the Trinity College (Cambridge), then was incorporated in the English embassy in Paris, and due to his diplomatic work visited Germany, Spain, Poland, Denmark and Sweden [15]. Returning to England, Bacon had entered the Juridical Corporation where he studied jurisprudence and philosophy. As a jurist he took part in many trials concerning financial cases of the state. He was noticed and the new King Jacob I (1603-1625) at first knighted him and then he successively became Lord Keeper of the Great Seal, Lord Chancellor and Peer of England. In 1621, Bacon was accused of bribery; he had pleaded guilty, and although the penalty, heavy fine and Tower, was softened, his career had finished. Five years later he had died. According to his will, large sums were given to Oxford and Cambridge Universities for establishing the chairs of real philosophy.

It is interesting to note that Bacon is known especially because of the suggestion that he may have written some or all of Shakespeare’s plays [3]. Francis Bacon (1561–1626) and William Shakespeare (1564-1616) leaved in one and the same time.

Branches of knowledge

The first complete classification of sciences on the base of the sequence of human cognition was created by André Marie Ampère (1775–1836) [18–20]. “In 1829 I prepared the course in general and experimental physics at French college. Two questions were appeared [20]:

1. General physics, what does it mean? What is the exact feature that differ it from other sciences?

2. What are the different fields of physics which can be considered as separate sciences or the parts of a more common science? “

To answer these questions, André Marie Ampère had distinguished the four stages of the knowledge corresponding to the evolution of science development: direct observation (auto-optical point of view), studying what is hidden in an object (cryptoristic point of view, from κρυπτος – secret + οριζω – determine), studying the changing of an object (troponomic point of view, from τροπη – turn + νομος – custom, law) ,discovering the reasons and consequences (cryptologic point of view).

“Such is the natural sequence of human cognition”. The four standpoints can be united in two main ones. The first and second produce an elementary theory of an object; the third and fourth form a highest theory where the subjects are studied taking into account correlation and mutual connection.

Taking this principle as a base, Ampère had assumed that general physics can be divided into four groups: experimental physics (the first stage, auto-optical standpoint), chemistry (the second stage, cryptoristic standpoint), mathematical physics (the third stage, troponomic standpoint) and atomology (the forth stage, cryptologic standpoint).

On this concept, Ampère at first had considered physics and then other sciences. As a result, in 1832 he had created “The natural classification of sciences”. Ampère distinguished the orders of sciences. The science of the first order unites all the knowledge referring to one object. It can be divided into two sciences of the second order which correspond to the main points of view, elementary and high. In their turn, each of these sciences can be divided into two sciences of the third order referring to one of the four stages of human cognition. "Just a man has received some number of notions about any object; he tries to arrange them in a definite order for using them better. Such is the origin of classifications".

The existing sciences contained only a part of all the possible 128 sciences of the third order classified by Ampère, and he had predicted new sciences, giving them mostly Greek names. Thus he foresaw the appearance of medical physics but he is known especially because of predicting the science of the third order – cybernetics (from κυβερνητικη scilicet τεχνη). The ancient Greeks used that word as sea-craft, but Ampère accepted meaning of the word as management generally. It was done a hundred years before the appearance of cybernetics by Norbert Wiener (1894–1964).

"Thousands of people pronounce the word 'ampere' knowing nothing about that man. While his mortal remains had turned to dust, his name became the common property of mankind" (M. Berthelot, 1827–1907). André Marie Ampère (1775–1836) was born in Lion, in the family of a rich liberal merchant. When he learned to read, he began to eat up all the books being in the large library of his farther and in the Lion city library. At the age of twelve, he became proficient in differential calculus; at that he learned Latin, to read Euler and Bernoulli in the original, later he learned ancient Greek and Italian. At the age of fourteen, he studied all the twenty volumes of the Encyclopedia by Denis Diderot (1713–1783) and Jean le Rond d'Alembert (1717–1783). Having no teachers and not going to any school, he was well trained gaining wisdom by experience. In 1793 his farther was executed by Jacobeans, and for more than one year he was in mental disorder. After that Ampère successively indulged in botanic and poetry (since 1795, verses in French and Latin), mathematics (1802), chemistry (1816, he had done the first classification of chemical elements), physics (1820, he created new science - electrodynamics). Last years he engaged in systematization of flora and fauna, and all the knowledge.

Classification of fullerenes

Periodic system of fullerenes

In 2017, we created the periodic system of fullerenes, based on symmetry principles. It consists of horizontal series and vertical columns (groups) [21–28]. The horizontal series form the Δn periodicities, where the fullerene structure changes from threefold symmetry to sevenfold through four, five and sixfold ones. The vertical columns include the fullerenes of one and the same symmetry s, the mass difference of perfect fullerenes for each column being equal to a double degree of symmetry $\Delta m=2s$. The first version of the system contained the series beginning with Δn=6, later the series Δn=2, 4 were added. The full version is given below. We suppose the fullerenes of one and the same column have similar physical and chemical properties.

Two columns of three fold symmetry differ by the shape of their apices. The fullerenes of S-symmetry column have two sharp apices, the third order symmetry axis going through them; those of T-symmetry have two truncated apices, the third order axis going through the centers of equilateral apices triangles (Table 1).

Table 1. Periodic system of fullerenes

Series / Columns	Symmetry of fullerenes				
	3-fold S (Δm=6)	3-fold T (Δm=6)	4-fold (Δm=8)	5-fold (Δm=10)	6-fold (Δm=12)
Δn=2	$\mathbf{C_{2}}$	$\mathbf{C_{6}}$	$\mathbf{C_{8}}$	$\mathbf{C_{10}}$	$\mathbf{C_{12}}$
Δn=4	$\mathbf{C_{8}}$	$\mathbf{C_{12}}$	$\mathbf{C_{16}}$	$\mathbf{C_{20}}$	$\mathbf{C_{24}}$
Δn=6	$\mathbf{C_{14}}$ C_{16} C_{18}	$\mathbf{C_{18}}$ C_{20} C_{22}	$\mathbf{C_{24}}$ C_{26} C_{28} C_{30}	$\mathbf{C_{30}}$ C_{32} C_{34} C_{36} C_{38}	$\mathbf{C_{36}}$ C_{38} C_{40} C_{42} C_{44} C_{46}
Δn=8	$\mathbf{C_{20}}$ C_{22} C_{24}	$\mathbf{C_{24}}$ C_{26} C_{28}	$\mathbf{C_{32}}$ C_{34} C_{36} C_{38}	$\mathbf{C_{40}}$ C_{42} C_{44} C_{46} C_{48}	$\mathbf{C_{48}}$ C_{50} C_{52} C_{54} C_{56} C_{58}
Δn=10	$\mathbf{C_{26}}$ C_{28} C_{30}	$\mathbf{C_{30}}$ C_{32} C_{34}	$\mathbf{C_{40}}$ C_{42} C_{44} C_{46}	$\mathbf{C_{50}}$ C_{52} C_{54} C_{56} C_{58}	$\mathbf{C_{60}}$ C_{62} C_{64} C_{66} C_{68} C_{70}
Δn=12	$\mathbf{C_{32}}$ C_{34} C_{36}	$\mathbf{C_{36}}$ C_{38} C_{40}	$\mathbf{C_{48}}$ C_{50} C_{52} C_{54}	$\mathbf{C_{60}}$ C_{62} C_{64} C_{66} C_{68}	$\mathbf{C_{72}}$ C_{74} C_{76} C_{78} C_{80} C_{82}
Δn=14	$\mathbf{C_{38}}$ C_{40} C_{42}	$\mathbf{C_{42}}$ C_{44} C_{46}	$\mathbf{C_{56}}$ C_{58} C_{60} C_{62}	$\mathbf{C_{70}}$ C_{72} C_{74} C_{76} C_{78}	$\mathbf{C_{84}}$ C_{86} C_{88} C_{90} C_{92} C_{94}
Δn=16	$\mathbf{C_{44}}$ C_{46} C_{48}	$\mathbf{C_{48}}$ C_{50} C_{52}	$\mathbf{C_{64}}$ C_{66} C_{68} C_{70}	$\mathbf{C_{80}}$ C_{82} C_{84} C_{86} C_{88}	$\mathbf{C_{96}}$ C_{98} C_{100} C_{102} C_{104} C_{106}
Δn=18	$\mathbf{C_{50}}$	$\mathbf{C_{54}}$	$\mathbf{C_{72}}$	$\mathbf{C_{90}}$	$\mathbf{C_{108}}$

Theory of sets and fullerenes. Topological symmetry

From the standpoint of mathematics [27], the series and columns are sets. The notion 'set' or 'totality' is considered as one of the simplest mathematical notions. It is not defined and is explained by means of examples. For example, we may say 'a set of books' composing a library. At that the books are the elements of the set. To determine a set, it is necessary to point out such property of the set elements, what all the elements have and only they. In our case we may consider the fullerenes of one and the same column as the set $\Delta n=2m$.

For the sets it's possible to perform different operations. We need such operation as *crossing of two sets*, i.e. the set of elements being common to both sets. Joining the sets of series and columns into one set (the periodic systems of fullerenes) we have obtained the *crossing of those two sets*, i.e. the fullerenes being common to both sets. In our case they are regular (perfect) fullerenes; they are denoted by *bold symbols*. In doing so, we have obtained the possibility to mark out the regular part of the fullerene set, or the *ordered subset* which elements are the fullerenes of a regular shape. Other fullerenes compose the *subset of imperfect fullerenes*. However there is a curtain order in this subset, i.e. the imperfect fullerenes produce *partially ordered subset*.

By analogy with physics of crystals, consider what it means. In crystal physics there are such notions as a short-range and long-range order. In real crystals, the long-range order is impossible because defects violate a translational symmetry [28]. Nevertheless the long-range order is observed experimentally; however diffraction lines differ from theoretical δ–functions. The lines become broader and lower throughout the height, but they conserve a sequence, in other words they have a fixed place. Such real long-range order is known as a *topological* one (τοπος – place).

By analogy with physics of real crystals, we assume that imperfect fullerenes are originated in due to the appearance of extra carbon dimers which play the part of defects. In real crystals the number of defects is much less than the number of the atoms forming a crystal lattice. Likewise, in imperfect fullerenes the number of the extra dimers that distort the structure is many fewer than the number of regular atoms (It's clear from the periodic system). For this reason, the symmetry violation takes place only in a local region around the defect (extra dimer) but in the most part of a fullerene the symmetry is conserved. We have named such symmetry of imperfect fullerenes *topological symmetry* [22].

Topology and fullerenes

In the sentences above we used the adjectives (the part of speech being the indicator of a subject), *topological* long-rang order, *topological* symmetry. What does the noun, *topology*, mean? In mathematics, topology is defined as its part in which the idea of continuity of space and time is studied [27]. The formal definition of space and time is based on the notion of a set. The space is defined as the set of the elements (points) in which some relations between the points are fixed, these relation being similar to common space relations.

Historically the first mathematical space is the 3-dimensional Euclid space *(Ευκλειδης, IV–III Ages B.C.*), which corresponds with the real space approximately. The general notion of space is the result of generalization and modification of the Euclid geometry. The set of mathematical functions, the set of states of a physical system, the set of polyhedrons make up the spaces where the points are functions, states, polyhedrons. These sets are understood as spaces if there defined the *relations between the points*, e.g. the distances and properties which depend on them. For example, the distance between the states is defined as the difference of energies of the states. A *figure* is defined as an arbitrary set of points.

The *general relation* in any set is the *relation of belonging*: a point belongs to a set; a set is a part of another. If only these relations are taken into account, the set has no geometry and therefore it is not a space. However, if to separate some *special figures* (special sets of points), the laws of point connection with these figures create the geometry of space. The laws are named axioms. In particular, the Euclid geometry is created through the axioms of belonging, one of which looks like: through any two points it is possible to draw a line and only one. Here the special figure is the line.

As a special set, one can choose instead of points their neighborhood. At that, under the action of connection laws there appears a sort of space, so called *topological space*. All sorts of objects are studied in that space. This version of geometry is the most general geometry, and it is named *topology*.

Consider some examples. A special case of the more general topological space is a metric space which is generated by some metrics. A metrics (μετρον – measure) is the distance between two points of a set. The number scale, Euclid space of any dimensions, phase space of states of a physical system, all of them is an example of the metric spaces.

The topological spaces are classified into different types. These classes had appeared under the influence of different branches of mathematics and other sciences, which have different aims and they are unlike to each other, e.g. the sets of functions and polyhedrons. The latter is defined as the set built in a regular manner from elementary figures such as line segments, triangles, tetrahedrons, prisms etc.

The main problem of topology is considered to be revealing and studying topological properties of spaces or *topological invariants*, i.e. the properties of figures which are conserved during any continuous similar mapping one topological space into other. In particular, the number of measurements of a figure (dimensionality) is a topological invariant. We assume that topological long-rang order and topological symmetry are also topological invariants.

Coordinates, topology and periodic system of fullerenes

In 1637, René Descartes (*Cartesius, 1596 - 1650*) had published "Geometry", which incorporated into algebra all the classical geometry and later was named analytic geometry [27,29]. Nine years he studied at collège la Flèche, one of the best French educational institutions established by Jesuits by approbation of King Henri IV (1589-1610), who gave them his family castle 'château Nef'. Descartes studied at first Latin, ancient Greek, grammatics, dialectics, rhetoric, theology and scholasticism. The last three years were devoted to philosophy which embodied logics, ethics, physics, mathematics and Aristotle's metaphysics. Descartes highly appreciated the quality of education in Jesuit's college.

In 1615, he entered the Poitiers University for studying law and medicine. Having become a bachelor, he thirteen years traveled across Europe, visiting Italy, Poland, Denmark, Germany, Czechia and the Netherlands. It was the stormy period of Thirty Years' War (1618-1648). Descartes had served in three Armies: Dutch, Bavarian and Hungarian. Beginning with 1628, he had lived twenty years in the Netherlands devoting himself to science. In 1649, he arrived to Stockholm, having accepted the invitation of Queen Christina, who wanted to establish Sweden Academy of Sciences. The unusual severe climate led to pneumonia and some months later he had died.

Descartes was an adherent of real philosophy, but contrary to his forerunners, he was not only well educated in the humanities, but well educated in natural philosophy. He had searched a general method of reasoning. Whereas Montaigne and Bacon evolved the real philosophy on the base of inductive reasoning, Descartes developed deductive reasoning. "In those times the only science on nature, which had a systemized building, was mechanics [29]. A key to understanding mechanics could be given by mathematics." Thus the development of the real philosophy led to mathematics. "Taking in account that among the all seeking the truth only the mathematicians had managed to find precise and evident proofs, I did not doubt that it was necessary to begin with mathematics" [17].

Cartesian coordinates. Descartes' geometry contained the method of coordinates what lay in the following. We take two straight lines *Ox* and *Oy* intersecting at point *O* and perpendicular to each other. The indefinite straight line *Ox* is known as the *axis of the abscissas* or the *x-axis*; the indefinite straight line *Oy* is called the *axis of the ordinates* or the y-*axis*; point *O* is called the *origin of the coordinates* (abscisio – cut off, ordinatus – ordered, co – jointly). The lines *Ox* and *Oy* together with origin *O* make the Descartes' system of coordinates.

The position of any point *M* in this system is defined in the following manner. Let us assume M_x and M_y to be the projections of this point onto the axes of the coordinates, the values of segments OM_x and OM_y being numbers *x* and *y*; they are known as the Cartesian coordinates. The point *M* is denoted as *M* (*x, y*).

Topological lattice. It is a set of topological-space points having *whole coordinates* with respect to some system of coordinates [27]. In essence, the periodic system of fullerenes is the lattice of a definite plane of a topological space. Here the space points having whole coordinates are the knots of the lattice. A point *M* is the fullerene C_m of mass *m*, an abscissa *x* is the whole coordinate *s* (the order of symmetry) and an ordinate y is the whole even coordinate Δ*n*.

The abscissa *s* takes the value 3S, 3T, 4, 5, 6 and 7; the ordinate Δ*n* = 2, 4, 6, 8, 10, 12, 14, 16, 18. At that, the mass of the point *M* (the mass of fullerene C_m) can be calculated with the following formula: $m = s \times \Delta n$. The one exception is represented by the points having the abscissas *s*=3S; here the formula takes the form: $m = s \times \Delta n - 4$. The point *M* together with the coordinates can be written as C_m (*s*, Δ*n*). For the fullerenes of the third order symmetry, it is necessary to add argument S or T, for example, C_{32} (3S, 12) and C_{36} (3T, 12). In principle, one may include into the arguments of the point of topological space other values, e.g. energy. In such a form, the periodic system of perfect fullerenes was presented in [21] without evidence for its topological nature.

In the case of the complete periodic system of fullerenes, which embodies perfect and imperfect fullerenes, the situation becomes more complex. Here it is necessary to include into the topological lattice not only the knots but isolated points what correspond to imperfect fullerenes. These points are located on the coordinate lines parallel to the axis of the ordinates. For example, the coordinate line going through the abscissa *s=3S* has the following knots: $\mathbf{C_2}$**,** $\mathbf{C_8}$**,** $\mathbf{C_{14}}$**,** $\mathbf{C_{20}}$**,** $\mathbf{C_{26}}$**,** $\mathbf{C_{32}}$**,** $\mathbf{C_{38}}$**,** $\mathbf{C_{44}}$**,** $\mathbf{C_{50}}$.

Two points should be added in each interval between the knots (perfect fullerenes). As a result, the coordinate line takes additional points located between the knots: $\mathbf{C_2}$**,** $\mathbf{C_8}$**,** $\mathbf{C_{14}}$**,** C_{16}, C_{18}**,** $\mathbf{C_{20}}$**,** C_{22}, C_{24}, $\mathbf{C_{26}}$**,** C_{28}, C_{30}, $\mathbf{C_{32}}$**,** C_{34}, C_{36}, $\mathbf{C_{38}}$**,** C_{40}, C_{42}, $\mathbf{C_{44}}$**,** C_{46}, C_{48}, $\mathbf{C_{50}}$**.**

In a similar manner, it should be dealt with the fullerenes of other symmetry. In the general case, the number of added points in each interval between the knots is equal to *s-1*.

Graph representation. The periodic system of fullerenes can be also presented as a graph, if to connect some points of the topological lattice with arcs. If to specify direction to these arcs, we obtain an orientable graph. For example, let us connect the points of the number axis, such as $\mathbf{C_{26}} \rightarrow C_{28} \rightarrow C_{30} \rightarrow \mathbf{C_{32}}$. Then we obtain the finite-arc sequence which is called a route [30]. In our case, the route reflects the growth of the fullerene in the interval (**$\mathbf{C_{26}}$, $\mathbf{C_{32}}$**) through embedding carbon dimers. If to connect all the points corresponding to the fullerenes having one and the same mass, but different symmetry, we obtain the *route of isomers*. Inputting the routes into the periodic system of fullerenes allows lead well-directed investigations.

Conclusion

Empirically found horizontal and vertical symmetry allows give a preliminary classification of fullerenes. Two different symmetries are united into a common symmetry producing the periodic system of fullerenes. This system may be considered as the topological lattice in the topological space of the points corresponding to the fullerenes. The system gives the general classification of fullerenes on the basis of symmetry.

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About Authors

Alexander I. Melker Sc
Doctor of Physical and Mathematical Sciences
Professor (St. Petersburg Academy of Sciences on Strength Problems, St. Petersburg, Russia)

Maria A. Krupina iD Sc
Candidate of Physical and Mathematical Sciences
Associate Professor (Peter the Great St. Petersburg Polytechnic University, St. Petersburg, Russia)