

W. R. Hamilton

His Genius, His Circuits, and the IUPAC Nomenclature for Fulleranes

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Historical Information (1–9)

Genius has its pitfalls, and may not always be a blessing, as proved in music by Mozart and in mathematics by Galois. Another genius, William Rowan Hamilton (1805–1865, see Fig. 1), was born in Dublin where he lived all his life. He was, like Mozart, a child prodigy. At age three he was a superior reader of English and was considerably advanced in arithmetic. At four he was a good geographer. At five he read and translated Latin, Greek, and Hebrew. When he reached the age of 13 he spoke and read 13 foreign languages (including Italian, French, Persian, Arabic, and Sanskrit). He never attended school before going to the university, but he received his training privately, mainly from an uncle because both his parents had died when he was a child. He entered Trinity College, Dublin, and he carried off all the available prizes. His fame led to the unprecedented appointment of Hamilton as Royal Astronomer of Ireland, Director of the Dunsink Observatory, and Professor of Astronomy in an open competition in 1827 when he was still an undergraduate. His superabundant energy erupted in many directions including poetry. He befriended Coleridge and Wordsworth. Wordsworth persuaded Hamilton to concentrate on science. Wordsworth also said that the only two men who had ever given him a feeling of inferiority were Coleridge and Hamilton.

At the age of 23, Hamilton published "A Theory of Systems of Rays" that laid the mathematical structure of optics in the manner Lagrange had done for mechanics. Hamilton's treatment predicted surprising qualitatively new features of conical refraction that were subsequently found by Humphrey Lloyd in certain crystals. This triumph led to a knighthood for Hamilton when he was 30, and to his election in the Royal Irish Academy when he was 27; he served as its president between 1837 and 1845. In Ireland at that time, being knighted by the British Crown did not endear Sir William Rowan Hamilton to the general public and contributed to his increasing isolation.

In 1833 he married a sickly woman who soon became semi-invalid and neglected the household.

Hamilton introduced his ideas (which worked so well in optics) into mechanics by applying the principle of least action in two papers published in 1834 and 1835. For conservative systems (where the components of force are derivable from a potential that is a function of position only), Hamilton's principle reduces to Lagrange's, but unlike the latter principle, the former also holds for nonconservative systems. Jacobi described Hamilton's differential equations as "canonical".



Figure 1. W. R. Hamilton as portrayed by a contemporary artist with his mace of office as President of the royal Academy of Ireland.

After the formulation of quantum mechanics, Hamilton's function H has assumed a central role when Schrodinger formulated his stationary state equation expressible as

$$H \Psi = E \Psi$$

(here Ψ is the system's wave function and eigenvalues E correspond to allowed energies). Further, in another fundamental formulation of quantum mechanics via Feynman path integrals, the variable integrand in Hamilton's variational principle becomes the "phase" along each possible path. Indeed, this particular result might not be wholly unexpected because Hamilton was seeking to describe both optical and mechanical (i.e., wave and particle) phenomena within a unified variational principle.

Hamilton motivated the modern vectorial formulation of classical mechanics with his axiomatic introduction of the first non-commutative algebra, based on quaternions, which he believed to be his foremost contribution to science. In trying to approach algebra logically, he modeled complex numbers by pairs of ordered numbers, which can represent rotation in a two-dimensional space, and from here he went on trying to represent rotations in a three-dimensional space by triplets. For years his efforts remained unsuccessful. Frequently, at the breakfast table, his sons asked him: "Daddy, can you multiply triplets?" to which Hamilton replied ruefully: "I can add and subtract triplets, but I cannot multiply them". And then, one day in October 1843, as he was walking from the Observatory to Dublin for a meeting of the Academy, the basis for this quaternion

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algebra came to him in a flash: three “imaginary” units i, j, k , were needed for quaternions q :

$$q = ai + bj + ck + d$$

where a, b, c, d are ordinary real numbers. He was so impressed by his idea that he cut with a knife in the stone of Brougham Bridge the generative formulas:

$$i^2 = j^2 = k^2 = ijk = -1$$

Following Hamilton's publication, other types of “hypercomplex” algebras were announced (though Hamilton's quaternions remain a unique example of an associative algebra with no divisors of zero). Hamilton believed that quaternions were involved in a fundamental incorporation of time into theoretical science, and amusingly the four-dimensional quaternion algebra later turned out to be intimately related to the four-dimensional space-time frame of Maxwell's electromagnetism and of Einstein's special theory of relativity. Also hypercomplex algebras were the first forefront area of research focused on by the then fledgling American mathematical community.

In the last days of his life, Hamilton was elected as the first foreign member of the National Academy of Sciences of the United States (newly founded during the Civil War).

The chapter in Bell's classic “Men of Mathematics” (8) devoted to Hamilton starts: “William Rowan Hamilton is by long odds the greatest man of science that Ireland has produced”. But this chapter seems to be rather arguably entitled “An Irish Tragedy”. The tragedy is claimed to be due to Hamilton's nonideal marriage, his obsession with quaternions, and his indulgence with drinking (although as pointed out by Professor Lanczos (9), “his occasional drinking bouts are something that we would hardly call a ‘tragedy’ here in Ireland”). Perhaps some of these aspects are yet another parallel with Mozart.

Hamilton's scientific contributions (which he once described as his “real poetry”) are so fundamental that one might anticipate some of them to have importance not only in physics and mathematics, but also in chemistry and other fields.

Hamiltonian Circuits

By association with his noncommutative algebra, Hamilton invented and published in 1856 “the icosian calculus”, which involves paths on the graph of the regular dodecahedron. He then used the graphical interpretation as the basis of a puzzle which he called “The Icosian Game”, and exhibited it at the meeting of the British Association in Dublin in 1857. He sold the idea to a wholesale dealer in games for £25, but this game did not prove to be a commercial success; Rubik's cube seems more appealing.

The object of the game was to find paths and circuits on the dodecahedral graph, satisfying certain conditions. One version of Hamilton's game called “The Traveller's Dodecahedron” or “A Voyage Round the World” involved a solid regular dodecahedron whose vertices had pegs labelled with names of 20 world cities. The aim of the game was to loop a thread around these pegs to indicate a circuit passing once through each city (10).

Such circuits are now called “Hamiltonian circuits”, and occupy a prominent place in modern graph theory. These circuits lead to many interesting problems, some of which are not yet solved. For instance, to establish whether a given graph is Hamiltonian (i.e., whether it has a Hamiltonian circuit) is generally non-trivial.

Interestingly, it appears that the general problem of such circuits in graphs had been published independently in 1856 (before Hamilton's paper had appeared) by an amateur mathematician, Thomas Penyngton Kirkman, who for over 50 years (1840–1892) was rector of a small parish

in Lancashire but owing to his mathematical contributions was elected a Fellow of the Royal Society in 1857 (10). However, Hamilton's fame (and possibly his game) led to the general acceptance of the term “Hamiltonian circuit”.

Of course chemical structural formulas can be viewed as realizations of mathematical graphs, so that it should perhaps not be surprising that Hamiltonian circuits might also play an important role in chemistry.

IUPAC Names for Polycyclic Compounds

Adolf von Baeyer (1835–1917, Nobel Prize for Chemistry in 1905) was a PhD student of Kekulé, and taught organic chemistry at the University of Berlin and Munich (Germany). In the latter position he succeeded Liebig and remained there from 1875 till 1913. He devised syntheses for uric acid, isatin, indigo, and triarylmethane dyes. In addition to his experimental contributions to the founding and development of German dyestuff industry (from which he refused any profit), Baeyer developed theoretical views on steric strain in cyclic compounds and on aromaticity. From his investigations of cycloalkanes and polycyclic derivatives, he devised nomenclature rules that hold to this day (and, as we shall see, involve Hamiltonian circuits).

Adolf von Baeyer proposed a system for naming bicyclic compounds, which later had been generalized to polycyclic systems, and has been adopted by the IUPAC Committee for Nomenclature. Rule A-32.31 runs as follows (11).

IUPAC Rule A-32-31: The von Baeyer System

When there is a choice, the following criteria are considered in turn until a decision is made.

- The main ring shall contain as many carbon atoms as possible, two of which must serve as bridgeheads for the main bridge.
- The main bridge shall be as large as possible.
- The main ring shall be divided as symmetrically as possible by the main bridge.
- The superscripts locating the other bridges shall be as small as possible.

We shall apply this rule to naming polycyclic Hamiltonian graphs consisting of $v = 2n$ vertices, each of which is the meeting place for three edges (i.e., has degree 3). Such graphs are called cubic graphs. Molecular graphs of fullerenes $(CH)_{2n}$ and of all other valence isomers of annulenes (12) are represented by cubic graphs. In such graphs, there are $e = 3n$ edges, and the so-called cyclomatic number is $m = e - v + 1 = n + 1$. This number indicates how many edges one needs to remove in order to obtain an acyclic but still connected graph. The fullerene graphs studied here have the further feature that they can be embedded on the surface of a sphere showing only five- and six-membered rings.

Thus, according to (a), whenever possible, Hamiltonian circuits of the (hydrogen-depleted) molecular graph should be sought. When a Hamiltonian circuit is possible, as it is for all cases considered here, rule (b) is irrelevant, and according to rule (c), among all such circuits, one should look for those circuits that, whenever possible, are divided evenly by a bond (a line or an edge of the graph). One of the atoms (vertices or nodes of the graph) which is an endpoint of this edge is numbered 1, followed sequentially by the other vertices on the circuit. Thus, there are four possible numberings (and IUPAC names) for each edge that divides evenly the Hamiltonian circuit. According to (d), among all these numberings, one selects that one which leads to the smallest set of numbers (on first occurrence, in agreement with the *Chemical Abstracts* interpretation of this rule) corresponding to subsequent bridges; i.e., to the bridge starting from vertex 2, then from vertex 3, etc.; such bridges are described by a number specifying how many

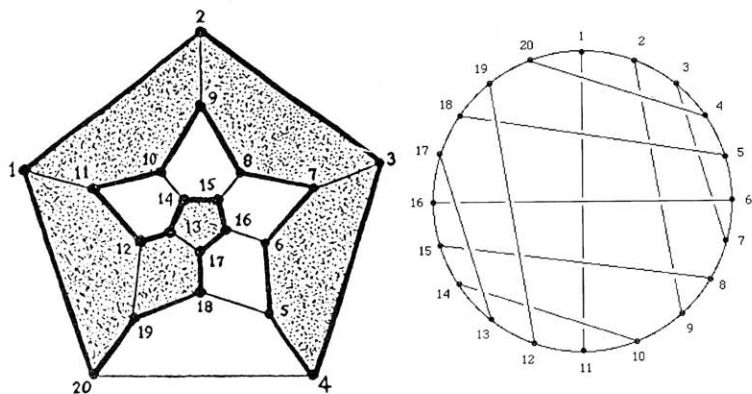


Figure 2. (a) Schlegel diagram for dodecahedrane or [20]fullerane **1**; the contour of the shaded area is the optimal Hamiltonian circuit for the IUPAC name. (b) The same with an external Hamiltonian circuit, highlighting the two bridges dividing it evenly.

vertices there are in the bridge (for Hamiltonian circuits all these bridges are bonds with zero atoms. Hence, all these numbers are zeroes) followed by locants as superscripts, separated by a comma, and indicating the numbers of the two endpoint vertices for the bridge.

The two halves of the Hamiltonian circuit involving all $2n$ vertices and the zero-atom bridge evenly dividing this circuit precede in square brackets the indication of subsequent bridges, thus: $[n-1, n-1, 0, 0^{2, \dots}, \dots]$. In the full name one places before this bracket the Greek prefix indicating the cyclomatic number m , and after the bracket the Greek phrase indicating the number $2n$ of vertices.

IUPAC Names for Fullerenes

We shall apply the above rules for finding the correct IUPAC names for polyhedral polycyclic compounds $(CH)_{2n}$.

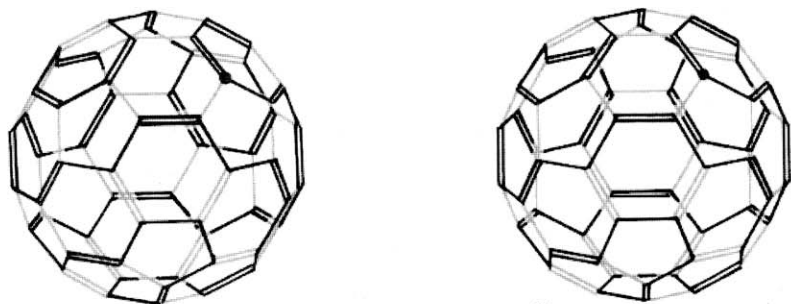
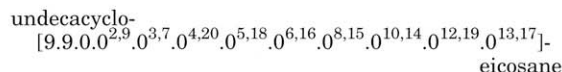


Figure 3. (a, above) Stereoview of the Hamiltonian circuit for Buckminsterfullerene. The black dot represents the carbon atom numbered 2 via a double bond. The hexagon represented with an asterisk in the Schlegel diagram is in the middle of the back side and is bordered by three double bonds of the Hamiltonian circuit. (b, right) Schlegel diagram for [60]fullerane **2**; the contour of the shaded area is the optimal Hamiltonian circuit for the IUPAC name. The asterisk marks the hexagon where the ribbon of condensed polygons is branched.

having 12 pentagonal faces and increasing numbers of hexagonal faces, starting with zero. These can be considered both as valence isomers of annulenes and as fully hydrogenated fullerenes; therefore, they will be called $[2n]$ fullerenes.

Thus, Hamilton's game, or more particularly Paquette's dodecahedrane (**1**), i.e. [20]fullerane $(CH)_{20}$, leads to the following IUPAC name (**13**):



where the sequence of nine superscripted zeroes in this full name is manifest in Figure 2a, where the dodecahedral graph is represented by a planar Schlegel diagram: imagining a face to be transparent and applying one's eye to it, one sees the Schlegel diagram for all remaining faces of the polyhedron. In Figure 2b, the Hamiltonian circuit is presented as a ring. Both parts of Figure 2 have the

same numbering of vertices corresponding to the requirements for IUPAC notation. For polycyclic cubic graphs consisting of few vertices ($2n$ up to 30), one can manually find Hamiltonian circuits, as indicated for the first time by Eckroth (**13**). One seeks a string of contiguous faces such that all vertices are included. In Figure 2a this string is indicated by shading. Then one finds the correct vertex numbering by assigning provisional numbers in an arbitrary direction along the contour of the shaded area, and one looks for bridges connecting vertex i to vertex $i+n$. If such a pair exists, then one of the endpoints of this bridge is numbered $i=1$ and all remaining vertices are renumbered sequentially. In Figure 2 there are two such bridges: 1-11 and 6-16. The symmetry of Figure 2b (with the axes indicated on it) is obvious. All four vertices (1, 6, 11, and 16) are equivalent. The direction of numbering is determined by the fact that the alternative possible numbering would lead to a bridge notation $0^{2,18}$ which does not comply with IUPAC rule (d), because the location 2,18 is larger than that of Figure 2, namely 2,9.

Several papers have been published (**14-16**) on the IUPAC nomenclature of buckminsterfullerene $(CH)_{60}$ with truncated icosahedral structure (**2**), represented in Figure 3. None of these, however, give the correct solution satisfying the four IUPAC rules reproduced above and in Eckroth's paper (**15**). Here we report the correct name for **2** and for a few other fullerenes.

The name indicated by Castells and Serratosa (**14**) in 1983 (before Kroto, Smalley, Curl, Kraetschmer, and Huffman (**17-25**)) had produced experimental evidence for **2** which has generated an unprecedented "epidemic" (**26**) of publications in the fullerene field) is based on a Hamiltonian circuit divided equally by a bridge between atoms numbered 1 and 31 and leading to an expression $[29.29.0 \dots]$. The next connection linked the atom numbered 2 with atom 47 (**14**). In 1986, the same authors revised this name and produced a somewhat improved circuit. Their (**15**) and Eckroth's (**16**) Hamiltonian circuit also leads to the expression $[29.29.0 \dots]$, but the next connections link atoms numbered 2 and 3 to atoms 14 and 29, respectively.

A correction is needed for Eckroth's paper (**16**) Castells and Serratosa did not propose a

name with the unsymmetrical system [30.28.0.0. . .]; on the contrary, their name in the 1986 paper is identical to the name proposed by Eckroth. However, this name is not optimal.

We have developed an algorithm for finding all possible Hamiltonian circuits in cubic graphs. The algorithm is based on the following procedure, carried out either on a Schlegel diagram, or on a three-dimensional representation of the cubic graph, such that at a chosen vertex one of the edges is parallel to a given direction (e. g., vertical for a Schlegel diagram).

Start a path at the chosen vertex by following the vertical edge, and turn alternatively left and right at each new vertex. If one reaches the starting vertex in the last step, the path closes to a Hamiltonian circuit. If not, one backtracks to the previous step and changes the left/right direction. To make the algorithm less time-consuming, one changes the "effective degrees" of vertices in the vicinity of the path: if the path goes from vertex $i - 1$ to vertex i , and then if one chooses a right-hand direction to vertex $i + 1$, then the "effective degree" of vertex j adjacent to vertex i must be decreased by 1, because the edge from i to j becomes forbidden for the Hamiltonian circuit; this edge is represented by a dotted line in Figure 4. The Hamiltonian circuit will include vertex j in a sequence: $j - 1 ; j ; j + 1$. If the effective degree reaches 1, it is certain that the path cannot result in a Hamiltonian circuit, and the last step is abandoned, going to the back-tracking procedure. Particular attention is paid to the vertices adjacent to the initial vertex, because one of them would become the last on the Hamiltonian circuit.

From all possible Hamiltonian circuits, one chooses those with a

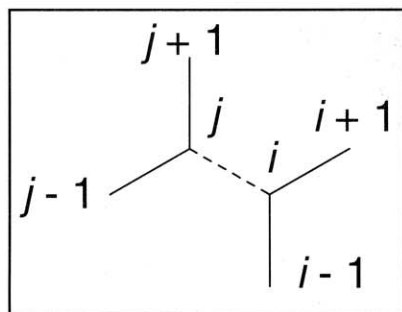


Figure 4. Six vertices in a cubic graph for which a Hamiltonian circuit is sought; on deciding to follow the path from $i - 1$ to i and $i + 1$, one reduces by 1 the effective degree of vertex j , adjacent to i . Thus, only path $j + 1$ to j and $j + 1$ is left for the Hamiltonian circuit.

Table 1. Pairs of Connected Bridge Endpoints (in Addition to the Bisecting Bridge, 1–31 in C_{60}).

Upper and lower numbers indicate zero-atom bridge connections in fullerenes **2–12**; parameter p denotes the number of pairs of pentagons sharing one edge, and q is the number of pentagon triplets sharing a common vertex.

No.	p	q	Bridge endpoints																													
2^a	0	0	2	3	4	5	6	7	8	9	11	13	15	16	17	19	14	12	59	10	58	55	53	21	20	18	30	28	25	24		
			22	23	26	27	29	32	33	34	35	36	37	38	39	40	42	52	50	49	47	45	44	60	57	43	56	41	54	51	48	46
3	2	0	2	3	4	5	7	8	10	11	13	14	16	17	19	20	6	15	12	9	30	27	25	23	21	18	60	46	45	42		
			22	24	26	28	29	32	34	35	38	40	43	44	47	48	50	41	39	37	36	33	58	56	54	53	52	51	49	59	57	55
4	3	0	2	3	4	5	7	8	10	11	13	14	16	17	19	20	6	15	12	9	30	27	25	22	21	18	60	57	55	53		
			23	24	26	28	29	32	33	35	36	40	42	43	46	47	49	52	39	38	37	34	59	45	44	41	51	50	48	58	56	54
5	3	0	2	3	4	5	7	8	10	11	13	14	16	17	19	20	6	15	12	9	30	27	25	22	21	18	60	46	45	42		
			23	24	26	28	29	32	34	35	38	40	43	44	47	48	50	41	39	37	36	33	58	56	54	53	52	51	49	59	57	55
6	3	0	2	3	4	5	7	8	10	11	13	14	16	17	19	20	6	15	12	9	30	27	25	22	21	18	60	46	44	42		
			23	24	26	28	29	32	34	35	38	40	43	45	47	48	50	41	39	37	36	33	58	56	54	53	52	51	49	59	57	55
7	6	0	2	3	4	5	7	8	9	10	11	14	16	17	19	20	6	29	26	13	60	12	58	18	15	25	23	21	57	54		
			22	24	27	28	30	32	33	34	35	36	40	42	44	45	46	52	50	49	39	38	37	59	56	43	41	48	47	55	53	51
8	12	0	2	3	4	5	7	8	9	10	13	14	16	17	18	20	6	30	15	12	11	60	58	55	54	19	29	26	23	53		
			21	22	24	25	27	28	32	34	35	37	39	42	44	45	51	43	41	40	38	36	33	59	57	50	48	47	46	52	49	56
9	11	1	2	3	4	5	7	8	10	12	13	15	16	17	19	22	6	14	11	9	30	23	21	20	18	60	47	44	43	42		
			24	25	26	27	28	32	34	35	37	39	40	46	48	49	50	29	41	38	36	33	58	57	55	53	52	45	51	59	56	54
10	16	6	2	3	4	5	7	8	10	12	13	16	17	19	22	23	6	21	11	9	30	15	14	20	18	29	26	24	60	40		
			25	27	28	32	34	35	37	39	41	42	43	44	45	46	47	38	36	33	58	56	54	52	50	59	49	57	48	55	53	51
11	18	8	2	3	4	5	7	8	10	12	14	15	18	20	21	22	6	13	11	9	30	19	17	16	60	46	45	29	44	27		
			23	24	25	26	28	32	34	36	38	40	41	43	47	49	51	42	39	37	35	33	58	56	54	53	52	50	48	59	57	55
12	20	10	2	3	4	5	7	8	10	12	14	15	16	20	22	23	6	13	11	9	30	19	18	17	60	57	21	29	56	28		
			24	25	26	27	33	34	36	37	39	40	42	44	46	47	48	54	38	35	32	59	45	43	41	53	51	50	49	58	55	52

^aFor **2** there are 1090 Hamiltonian circuits (16 different), and 14 possible names, from which only one was selected.

Table 2. Pairs of Connected Bridge Endpoints (in Addition to the Bisecting Bridge, 1–36 in C₇₀)

Upper and lower numbers indicate zero-atom bridge connections in fullerenes 13–14.

No.	<i>p</i>	<i>q</i>	Bridge endpoints																	
13 ^a	0	0	2	3	4	5	7	8	9	11	12	13	14	15	16	17	18	19	20	
			6	34	31	10	69	63	61	30	60	58	29	56	27	54	26	23	53	
			21	22	24	25	28	38	39	41	42	43	44	45	46	47	49	50	64	
14	1	0	2	3	4	5	7	8	9	11	12	14	15	17	18	21	23	24	25	
			6	34	13	10	69	67	20	19	16	33	30	28	22	66	27	65	55	
			26	29	31	32	35	37	38	41	43	46	48	51	53	56	58	61	63	
			45	44	42	40	39	60	50	49	47	54	52	59	57	64	62	70	68	

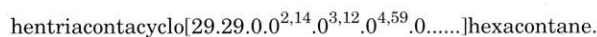
^a For 13 there are 2790 Hamiltonian circuits (144 different) and 198 possible names, from which only one was selected.

Table 3. Numbers of the 1812 C₆₀-cage isomers, as Function of Parameters *p* and *q*.

<i>p</i>	<i>q</i>	0	1	2	3	4	5	6	7	8	9	10
0		1										
1												
2		1										
3		3										
4		17										
5		81	5									
6		215	39									
7		210	147	6								
8		145	214	54								
9		23	132	31	11							
10		7	28	16	42	4						
11			1	31	54	11						
12		1		6	16	25	2					
13				2	10	7						
14					3	5	2					
15								2				
16									1			
17												
18										1		
19												
20												1

bridge that divides equally the circuit, and then one examines the connections of vertices adjacent to the two vertices that form the bridge dividing equally the circuit (one of these two atoms receives number 1): the smallest numbers should appear as bridges for the atom numbered 2, then for atom numbered 3, etc.

The complete correct IUPAC name for 2 using the A. von Baeyer nomenclature system adapted to polycyclic graphs is:



Tables 1 and 2 present in full in a different form the same information, by providing on two successive lines the connections (bridges) between atoms starting with atom numbered 2; the connections appear as superscripts for the zero-atom bridges in the IUPAC name. In the same tables and with the same format one sees IUPAC names for sev-

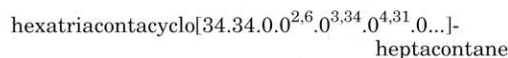
eral other (CH)₆₀ and (CH)₇₀ isomers: for obtaining IUPAC names, in all cases the information of Tables 1 and 2 is converted into superscripts following zero-atom bridges in the square brackets after the expression [29.29.0. . . .] for (CH)₆₀, and [34.34.0. . . .] for (CH)₇₀.

Our result for (CH)₆₀ confirms the IUPAC name for buckminsterfullerene cited in reference 19 as unpublished work being due to P. Roesse, and the name first published by G. Ruecker and C. Ruecker using their computer program POLYCYC which is applicable also to systems without Hamiltonian circuits (27).

In Table 1 the 11 particular 60-atom fullerenes described are but a small fraction of the 1812 possible ones (not distinguishing mirror im-

ages). The fullerenes of Tables 1 and 2 are identified there by what usually are incomplete labels (28–31) namely: *p*, the number of abutments between pairs of pentagons; and *q*, the number of vertices where three pentagons abutt. All possible 60-atom fullerenes with the given *p*, *q*-values appear in Table 1 with one exception, namely 7 with *p* = 6, *q* = 0 (among all such isomers, 7 is the unique one with six pairs of condensed pentagons arranged octahedrally). Stabilities of (CH)₆₀ cage isomers are expected to decrease in the order: 2 > 3 > 4 > 5 > 6. . . and for (CH)₇₀ cage isomers in the order: 13 > 14. The numbers of (CH)₆₀ isomers for other *p*, *q* values are given in Table 3, which in fact corrects (30) a table earlier given in reference (29).

The IUPAC name for the (experimentally relevant) unique (CH)₇₀ cage with no abutting (condensed) pentagons is (see Table 2):



One can also see in Tables 1 and 2 the numbers of all Hamiltonian circuits, and of possible names from which the optimal one (the only one included in these tables) was selected in agreement with IUPAC rules.

It should be noted that the Hamiltonian circuits leading to the correct IUPAC names define on the surface of all fullerene cages with 2*n* ≥ 60 (or on their Schlegel diagrams) arrays of condensed polygons which form branched (catacondensed) ribbons, unlike the linear ribbons on which the previously proposed names were based (14–16). Evidently, branching can only occur at a face which has at least six vertices. Therefore, we conjecture that this feature is a general one. Notably for every fullerene graph we have tried (out of hundreds), we have always found Hamiltonian circuits. Among the two dozens examined in more detail we have always found one with a circuit which is equally divided by a bridge bond. Further, the occurrence of Hamiltonian circuits extends to some fullerenes for which the “spiral labelling” of Manolopoulos and Fowler (32, 33) does not apply; this is indicated in Figure 5 where a Hamiltonian circuit (not optimized for IUPAC notation) is shown for their example of a “spirallness” C₃₈₀ fullerene.

Hamiltonian circuits differ markedly for Platonic solids (regular polyhedra, namely tetrahedrane, cubane, dodecahedrane) and Archimedean solids (semiregular polyhedra such as fullerenes (16), among others), in that these circuits are perimeters of linearly condensed polygons only for Platonic solids. For Archimedean solids, Hamiltonian circuits can be perimeters of branched “ribbons” of condensed polygons. This difference arises because such

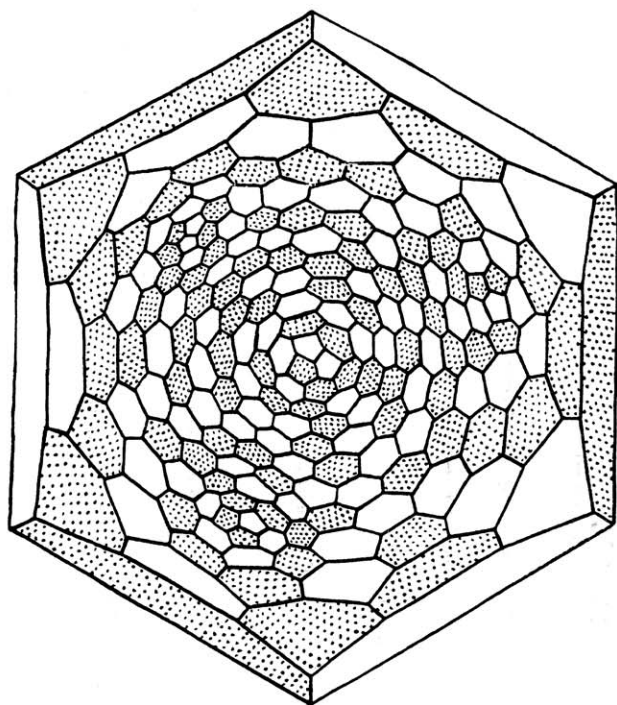
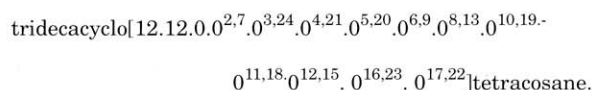


Figure 5. Schlegel diagram with a Hamiltonian circuit (contour of shaded area) for the "spiralless" C_{380} fullerene.

branching can occur only in the presence of hexagons, which do not exist in the three Platonic solids corresponding to valence isomers of annulenes. In a cage containing at least one hexagon and no triangles, a large number of Hamiltonian circuits arises from such "branched" perimeters. Strict adherence to IUPAC rule A-32.31 allows for selection of the correct IUPAC name. Thus, the truncated octahedron (another Archimedean solid, corresponding to $(CH)_{24}$), has the IUPAC name:



A further remark concerns the usefulness of IUPAC names for fulleranes. While we consider them to be too cumbersome and to include some redundancies, namely the numbers of vertices and rings (34), they do provide a unique numbering for all carbon atoms. In particular, for classroom instruction, manually generating the IUPAC names seems to be feasible for systems such as cubane or adamantane, and a complexity no larger than that of dodecahedrane. We have explored (35) several graph-theoretical and quantum-chemical invariants that will be presented separately, and which may provide a better basis for naming fullerenes.

In addition to being useful for IUPAC nomenclature, Hamiltonian circuits have been proposed (36, 37) as a basis for coding graphs with vertices of degree three (cubic graphs). Any graph can be converted into a cubic graph by an appropriate algorithm. Furthermore, whenever a graph with an even number of vertices possesses a Hamiltonian circuit, it also has at least two Kekulé structures derived from alternating single and double bonds along that circuit.

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