

Numbering and Naming of Fullerenes by Chemical Abstracts Service

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The development of fullerene nomenclature at Chemical Abstracts Service (CAS) is described. The numbering and naming rules successfully describe fullerenes of every point group symmetry indexed by CAS. Fullerene diagrams, with names and numbering, are being added to the CAS database and are being made available through *Chemical Abstracts* (CA) indexes, the *Ring Systems Handbook*, STN, and SciFinder.

INTRODUCTION

When the synthesis of fullerenes was first reported in 1985,¹ we recognized immediately that, apart from their inherent lack of hydrogen, they had the potential to be manipulated like organic compounds and that we needed to be prepared to name and index such derivatives in an orderly manner.

We attempted to name C₆₀ as a bridged fused ring system and quickly found, as anticipated, that the fullerene structure stretched the nomenclature beyond its capabilities.² Publication of four "correct" von Baeyer names demonstrated that this nomenclature was also being stretched beyond its capabilities.³ The names contained a large number of locants, implying a high probability of error, and the names were unwieldy even without any of the modifications anticipated above. It was therefore necessary for CAS to develop a simpler nomenclature system that could be used immediately.

We decided to adopt the term "fullerene", which was becoming accepted in the literature, as the short, simple class name. Initially, carbon counts were added to distinguish between the many fullerenes obtained during synthesis, e.g., fullerene-C₆₀. When ring (or face) sizes other than 5 and 6⁴ were reported and the names were no longer unique, we added ring sizes to all fullerene names (e.g., [3,10]fullerene-C₆₀, [4,6]fullerene-C₆₀, and [5,6]fullerene-C₆₀). When that also proved inadequate, we added point group symmetries, e.g., [5,6]fullerene-C₆₀-I_h, [5,6]fullerene-C₆₀-D_{2d}, and [5,6]-fullerene-C₆₀-C_{2v}. For further discussion on this topic, see the **Unmodified Fullerenes** section, below.

DEFINITIONS

We define fullerenes for CAS naming purposes as even-numbered, carbon clusters of 20 or more atoms, of connectivity three, that close upon themselves to form spherical or distorted spherical structures. Structures that do not conform to this definition but which have structures that resemble fullerenes are known by the class term "fulleroid" (fullerene-like).⁵ It is convenient for CAS nomenclature purposes to name such fulleroids as modified fullerenes. The numbering and naming rules developed at CAS are flexible enough to name the following:

1. partially and fully saturated fullerenes;

2. addended/substituted fullerenes, including functional groups;
3. carbon atom replacement by heteroatoms;
4. fullerenes fused to organic ring systems;
5. spiro derivatives;
6. polymers containing fullerenes;
7. fulleroids for which this nomenclature provides a convenient method of naming.

All ring systems that fit within the defined scope of the terms "fullerene" or "fulleroid" receive fullerene or modified fullerene CA index names.⁶

ASSUMPTIONS

So far, synthetic fullerenes contain only five- and six-sided faces. Such fullerenes contain 12, and only 12, pentagonal faces. Thus, the lower limit of fullerenes is universally assumed to be the dodecahedral C₂₀, which has 12 pentagonal faces. Theoretical carbon cages containing faces of other sizes have been reported in the literature.⁷ They are also considered by CAS to be fullerenes and subject to the C₂₀ lower limit.

UNMODIFIED FULLERENES

"Fullerene" was chosen as the class name for the unsaturated structures and "fullerane" for the fully hydrogenated ones. Fullerenes are distinguished from each other by including ring sizes, number of carbon atoms, and italicized point group symmetries in their names.⁸

[5,6]Fullerene-C₆₀-I_h

Incompletely described fullerenes (e.g., those identified only by carbon number) are named with only the number of carbons specified (see Table 1).

Fullerene-C₇₈

Among the larger synthetic fullerenes, beginning with C₄₀, point group symmetries may no longer be unique. For example, the common, ellipsoidal C₇₀ has a pentagonal face at each end that is surrounded by five hexagonal faces, while the cigar-shaped isomer has a pentagonal face at each end surrounded by five pentagonal faces. The point group symmetry symbols have been extended to include reference to these hexagonal and pentagonal faces.

[5,6]Fullerene-C₇₀-D_{5h(6)}

[5,6]Fullerene-C₇₀-D_{5h(5)}

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Table 1. Summary of Possible Specificity Implied by Components of the Parent Name

specificity	name	CA coverage
molecular formula	Fullerene-C ₇₈	single Registry Number
ring size	[5,6]Fullerene-C ₇₈	covered at Fullerene-C ₇₈
point group	[5,6]Fullerene-C ₈₀ -D _{5h}	unique Registry Number
degenerate point group	[5,6]Fullerene-C ₇₀ -D _{5h(5)}	unique Registry Number
degenerate point group	[5,6]Fullerene-C ₈₄ -D _{5h}	multiple Registry Numbers

Sometimes, even the addition of ring sizes 5 or 6 to the point group symmetries proves inadequate. When two or more fullerenes have identical names, they are handled as separate registrations, e.g., the four isomers of [5,6]fullerene-C₈₄-D₂ have CAS Registry Numbers 138015-77-7, 145226-11-5, 145809-18-3, and 145809-19-4, each with its own unique connection table.⁹

A summary of possible specificity implied by components of the parent name is given in Table 1.

NUMBERING OF FULLERENES

Functional groups, replacement atoms, substituents,¹⁰ etc., at known positions on fullerenes require the use of locants, as is common in other classes of compounds.¹¹ We have already assigned locants to a number of fullerenes and continue to do so as new ones are encountered.

Fullerenes cover a wide range from highly symmetrical to completely asymmetrical structures. Any system of assigning locant numbers must take this diversity into account to be of practical use. We decided to use the geometry of a fullerene as the basis for deriving its locant numbers.

There are two questions to address when determining a unique set of locant numbers for a fullerene. The first is where to begin numbering. The second is how to choose among multiple sets of locants from starting points of the same priority.

At the same time, it is important to minimize the number of trials necessary to obtain the correct set of locant numbers. The first priority is to obtain a contiguous spiral when possible. We looked at structures having symmetries at both extremes and then used the characteristics of each type to help in the numbering process.

The more symmetrical the fullerene, the greater the number of equivalent atoms. We chose to use rotation axes as reference points for numbering because they are easily derived from the point group in the name. The higher the order of the axis, the larger the set of equivalent atoms it passes through on the surface of the fullerene.¹² This set of atoms gives a starting point at which to begin numbering. Starting with the highest order axis minimizes the number of trials because it has the largest set of equivalent atoms. Because synthetic fullerenes tend to have high symmetry, this approach handles numbering for a large percentage of fullerenes.

The fullerenes of low to no symmetry, although mostly theoretical to date, must also be considered in any comprehensive numbering system. Such fullerenes are the opposite extreme. They have more unique atoms and may not have any axis other than C₁. We had to look at the environment of each atom as the basis for the numbering. Thus, we examine the environment of each atom in a manner similar to CIP ranking¹³ to determine seniority of atoms at chiral centers.

We use the sizes of the rings in which an atom or bond is common as the basis of comparison instead of atomic number. Thus, an atom common to three hexagons is labeled 666 and is senior to an atom common to two hexagons and one pentagon and labeled 665, etc. Similarly, a bond common to two hexagons is labeled 66 and is senior to a bond common to a hexagon and a pentagon and labeled 65. This gives a method of determining a preferred ring on the surface of the fullerene. We limit the number of trials by considering only the atoms in this ring as starting points. This limitation is a practical consideration because the number of unique atoms in low symmetry fullerenes makes an exhaustive examination too cumbersome to be practical.¹⁴

RULES USED FOR ASSIGNMENT OF NUMBERING

Rule 1: Axial, Linear and Special Group Fullerenes.

Examine rotation axes (C_n) in sequence from highest to lowest order until a contiguous spiral is found, always numbering an atom adjacent to one already numbered. An axis can pass through any of six combinations of ring, bond, or atom. Examine all paths, starting from each unique atom (which may be part of a ring or bond or may be an isolated atom). If no spiral can be found for any of the proper rotation axes, proceed to Rule 2.

Subrule A. When there is a choice for beginning of numbering, the priority order is ring > bond > atom.

Subrule B. When there is a choice of rings, a larger ring is preferred to a smaller one.

Subrule C. Each atom is a member of three rings. When there is a choice, the preferred atom is a component of the set of largest rings, e.g., 666 > 665 > 655 > 555.

Subrule D. When there is a choice, the preferred bond is a component of the set of largest rings, e.g., 66 > 65 > 55.

Subrule E. When there is a choice, the preferred bond is the one containing the preferred atom at the first point of difference.

Subrule F. When there is a choice, the preferred ring is the one containing the preferred atom at the first point of difference.

Subrule G. When there is a choice of spiral numberings, the preferred numbering terminates as close as possible to the axis of the spiral.

Subrule H. When there is a choice of spiral numberings, the numbering terminates at the preferred atom. If there is a tie, add locant numbering to the atom rankings. The highest locant at the first difference breaks the tie.

Subrule I. If there is a tie, then, starting again at the first atom, the preferred spiral is the one with the preferred bond at the first point of difference.

Subrule J. When there is a choice, a replacement atom of higher seniority is preferred to one of lower seniority.¹⁵

Rule 2: Axial Fullerenes with No Spiral and Nonaxial Fullerenes of Point Group C_s.

If, from Rule 1, no spiral is found for any C_n axis, slice the fullerene into planes of atoms perpendicular to the principal axis, starting from the preferred end of the axis and then, *when necessary*, combine two or more planes to form contiguous rings throughout the fullerene. From the set of contiguous rings, begin numbering from the plane at the preferred end of the fullerene. If none of the remaining unnumbered atoms are directly bonded to the atom just numbered, a new starting point is needed. Examine the remaining unnumbered atoms and continue

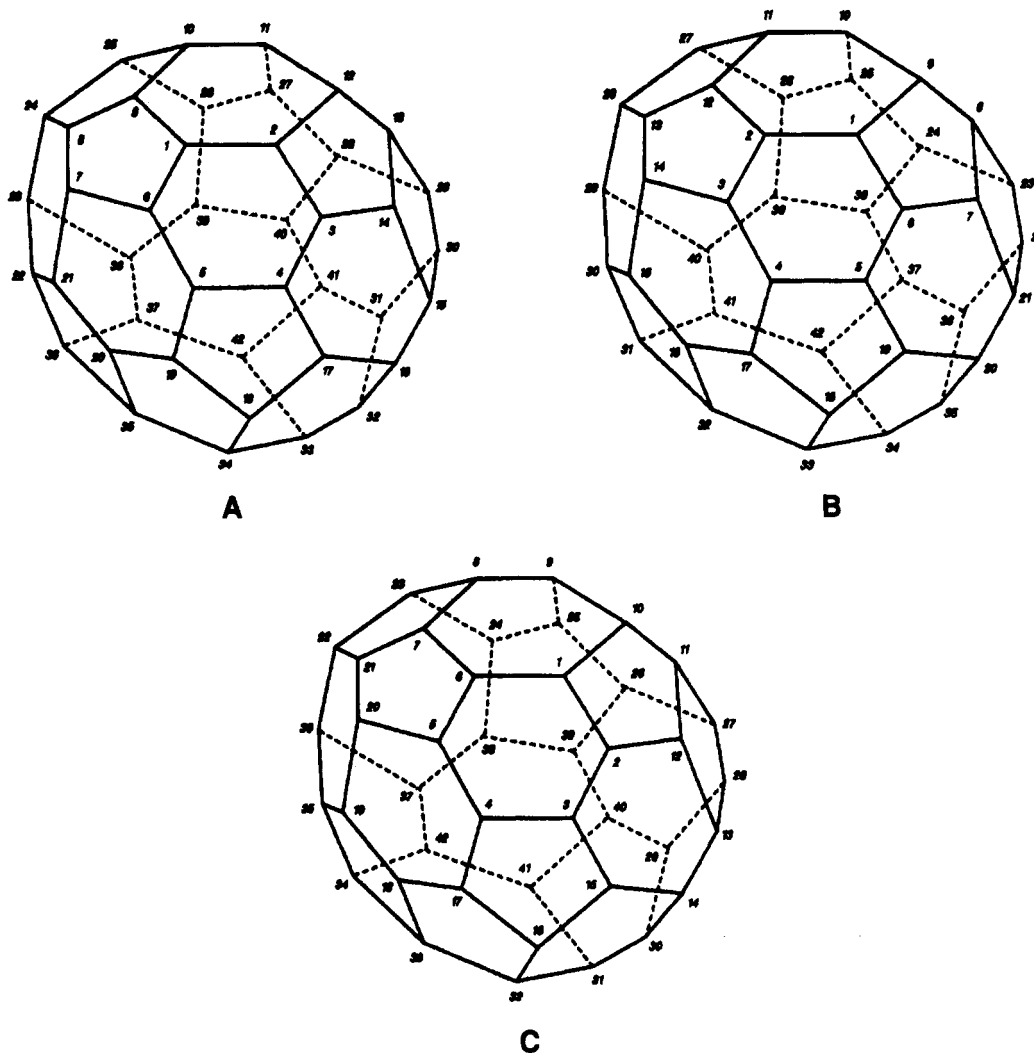


Figure 1. Three candidate spiral numberings of [5,6]Fullerene- $C_{42}-D_3$.

numbering from the atom directly bonded to the highest-numbered atom. Proceed in the same direction as the original spiral. Repeat as necessary until all atoms are numbered.

If the point group is C_s , there is no primary axis. Slice the fullerene into planes of atoms parallel to the σ_h plane in the middle of the fullerene. Start from the plane at the preferred end of the fullerene and then, *when necessary*, combine two or more planes to form contiguous rings throughout the fullerene. From the set of contiguous rings, begin numbering from the plane at the preferred end of the fullerene. If none of the remaining unnumbered atoms are directly bonded to the atom just numbered, a new starting point is needed. Examine the remaining unnumbered atoms and continue numbering from the atom that is directly bonded to the highest-numbered atom. Proceed in the same direction as the original spiral. Repeat as necessary until all atoms are numbered.

Subrule A. When there is a choice for beginning of numbering, the priority order is ring > bond > atom.

Subrule B. When there is a choice of rings, a larger ring is preferred to a smaller one.

Subrule C. Each atom is a member of three rings. When there is a choice, the preferred atom is a component of the set of largest rings, e.g., 666 > 665 > 655 > 555.

Subrule D. The preferred bond is a component of the set of largest rings, e.g., 66 > 65 > 55.

Subrule E. When there is a choice, the preferred bond is the one containing the preferred atom at the first point of difference.

Subrule F. When there is a choice, the preferred ring is the one containing the preferred atom at the first point of difference.

Subrule G. When there is a choice of numberings, or sets of planes for numbering, the preferred numbering terminates in each ring so that numbering can continue via a bond to the next ring. If contiguous, spiral numbering is not possible, the set of planes is chosen in which the discontinuity starts at the highest-numbered atom.

Subrule H. When there is a choice of spiral numberings, the numbering terminates as close as possible to the principal axis. If the point group is C_s , then the numbering terminates as close as possible to the last plane.

Subrule I. When there is a choice of spiral numberings, the numbering terminates at the preferred atom. If there is a tie, add locant numbering to the atom rankings. The highest locant at the first difference breaks the tie.

Subrule J. If there is a tie, then, starting again at the first atom, the preferred spiral is the one with the preferred bond at the first difference.

Subrule K. When there is a choice, a replacement atom of higher seniority is preferred to one of lower seniority.¹⁵

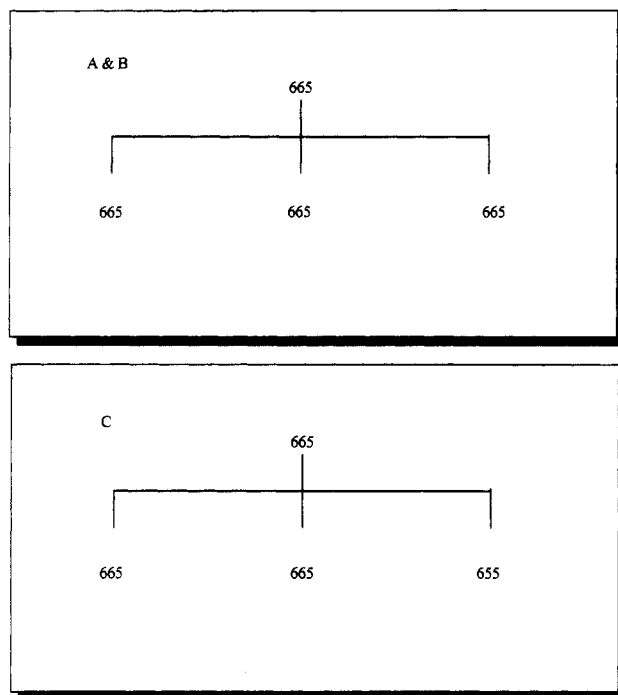


Figure 2. Comparing the rankings of the three locant sets.

Rule 3: C_1 and C_i Fullerenes. Examine all paths from each unique atom in the preferred ring until a contiguous spiral is found. If no contiguous spiral is found, start at the preferred atom and proceed to its most preferred neighbor. If none of the remaining unnumbered atoms are directly bonded to the atom just numbered, a new starting point is needed. Examine the remaining unnumbered atoms and continue numbering from the atom directly bonded to the highest-numbered atom. Proceed in the same direction as the original spiral. Repeat as necessary until all atoms are numbered.

Subrule A. When there is a choice for beginning of numbering, the priority order is ring > bond > atom.

Subrule B. When there is a choice of rings, a larger ring is preferred to a smaller one.

Subrule C. Each atom is a member of three rings. When there is a choice, the preferred atom is a component of the set of largest rings, e.g., 666 > 665 > 655 > 555.

Subrule D. The preferred bond is a component of the set of largest rings, e.g., 66 > 65 > 55.

Subrule E. When there is a choice, the preferred bond is the one containing the preferred atom at the first point of difference.

Subrule F. When there is a choice, the preferred ring is the one containing the preferred atom at the first point of difference.

Subrule G. When there is a choice of spiral numberings, the numbering terminates at the preferred atom. If there is a tie, add locant numbering to the atom rankings. The highest locant at the first difference breaks the tie.

Subrule H. If there is a tie, then, starting again at the first atom, the preferred spiral is the one with the preferred bond at the first difference.

Subrule I. When there is a choice, a replacement atom of higher seniority is preferred to one of lower seniority.¹⁵

Use of these rules to determine the preferred numbering of a fullerene is illustrated with [5,6]fullerene- C_{42} - D_3 , which has two C_3 and three C_2 axes. The preferred axis (Rule 1) passes through a pair of six-membered rings. Because of symmetry, there are four spiral paths possible from either of the rings on the principal axis, from which numbering can begin (Rule 1A). One of the paths is an incomplete spiral, leaving three complete spirals, which are illustrated in Figure 1.

Two of the spirals form a pair (A and B) and end at the same atom (i.e., 42), while spiral C ends at a different atom. The tie between numberings A and B vs C is broken (see Figure 2) by application of the first sentence of Rule 1H, where 665 is preferred to 655 (Rule 1C).

To break the tie between numberings A and B, locant numbers are added to the atom rankings (second sentence of Rule 1H) and, beginning again at the preferred atom, the highest locant at the first difference (see Figure 3) separates the third branch from the other two, but the tie between the first and second branches cannot be broken. (Had the tie been broken, the preferred numbering would have been decided here.) Atoms 41 and 37 of both A and B are equivalent because they are interchanged by rotation about the C_3 axis. The atom rankings for both of the branches are therefore identical so the locants 41 and 37 cannot be unambiguously assigned to a specific branch.

To break the tie between numberings A and B, starting again at the first atom of each spiral, the bond priorities are compared (Rule 1I). The tie is broken at bond 7–8 which,

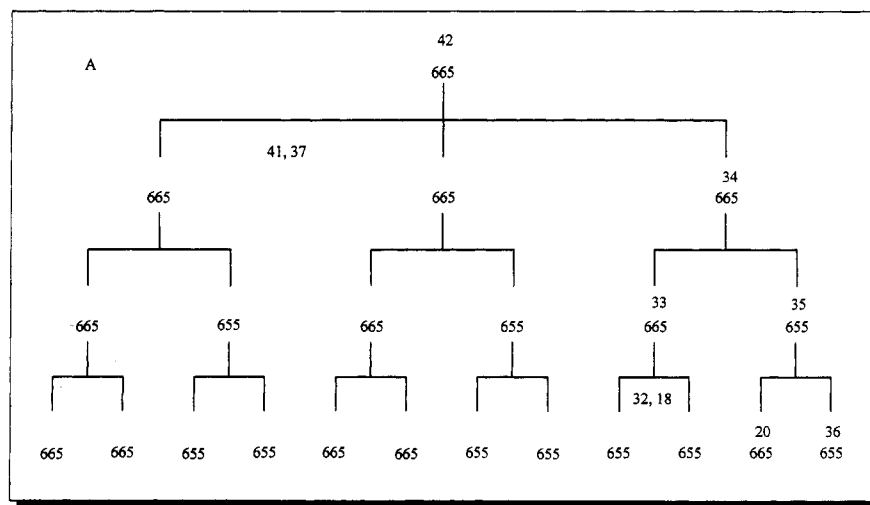


Figure 3. Attempting to add the locant numbers to the ranking of atom 42 of spiral A.

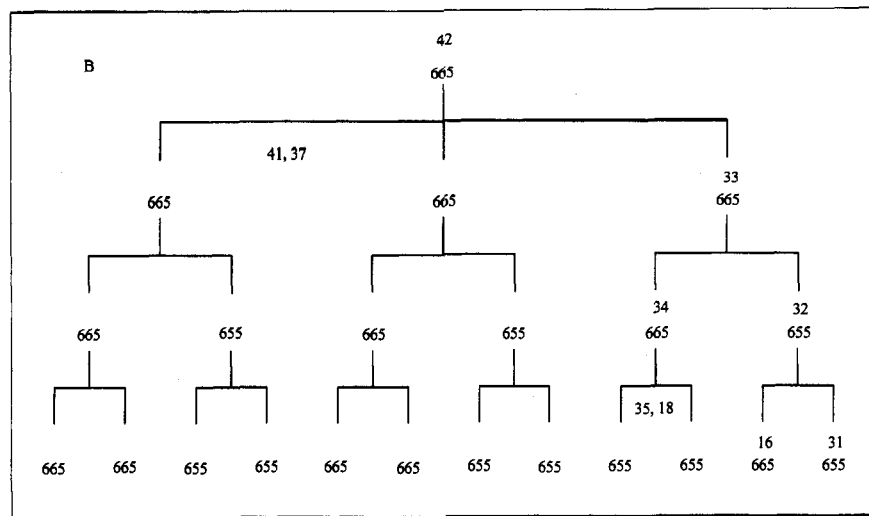


Figure 4. Attempting to add the locant numbers to the ranking of atom 42 of spiral B.

in spiral A, has seniority 65 compared with 55 in B (Figure 1). The final numbering of [5,6]fullerene- $C_{42}-D_3$ is illustrated in Figure 1A.

The numbering of 12 other fullerenes, derived with these rules, are illustrated in Figure 5.

The direction of numbering is not important for achiral fullerenes of high symmetry, e.g., [5,6]fullerene- $C_{60}-I_h$. Numbering in either direction around any five-membered ring gives two equivalent sets of numbers, differing only in the direction of the spiral.

For chiral fullerenes, the direction of the spiral depends on which enantiomer is numbered, e.g., [5,6]fullerene- $C_{76}-D_2$ and [5,6]fullerene- $C_{28}-D_2$ (see Figure 5). In both examples, the preferred locant set can be determined by use of the appropriate rules. When the process is repeated for the other enantiomer, the same locant set is obtained in each case, but the direction of the spiral is reversed. The direction of the spiral defined by the locant set can be used to describe the absolute configuration of a chiral fullerene.

CARBON CLUSTERS CONTAINING AN ODD NUMBER OF CARBON ATOMS

When articles on fullerenes report carbon clusters of unknown structure and containing an odd number of carbon atoms, the clusters are named as such. For example, C_{51} has been named as Carbon, mol. (C_{51}).

MODIFIED FULLERENES

A. Ions and Free Radicals. All ionic unsubstituted (i.e., carbon only) fullerenes are structured as neutral species. This policy is applied for both records that have connection tables and those that are manually registered. The parent name is "fulleride($n-$)" for anions and "fullerene, ion($n+$)" for cations and does not include the term "radical".

[5,6]Fullerene- $C_{80}-C_{2v}$,
ion(2+)

[5,6]Fulleride(2-)- $C_{80}-C_{2v}$

Metal fullerides are named using the "compd. with" nomenclature.

[5,6]Fullerene- $C_{60}-I_h$,
compd. with potassium (1:1)

Radical ions of substituted or fused fullerenes are treated analogously to organic radical ions.¹⁶

[5,6]Fullerene- $C_{60}-I_h$,
1,9-dihydro-1-methyl-,
radical ion(1+)

[5,6]Fullerene- $C_{60}-I_h$,
1,9-dihydro-,
radical ion(4-)

Because fullerenes lack hydrogen, a free radical implies the addition of added hydrogen. For naming purposes, addition of hydrogen is assumed, and any other atom or group is named as a substituent.¹⁰ Unless otherwise specified, the free radical is assumed to be in the lowest locant position.

[5,6]Fulleren- $C_{60}-I_h-1(2H)-yl$

[5,6]Fulleren- $C_{70}-D_{5h(6)}-1(21H)-yl$,
21-(1,1-dimethylethyl)-

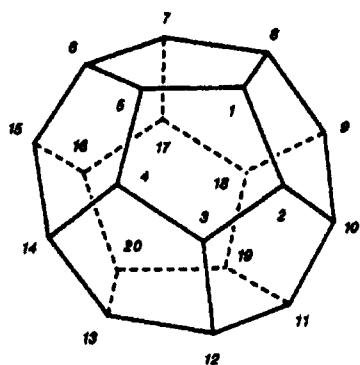
For fullerenes with multiple free radicals, added hydrogen is usually unnecessary because double bonds can be drawn between pairs of carbon atoms not carrying the odd electrons. However, added hydrogen is necessary if, for example, a carbon atom is surrounded by three others, each with an odd electron.

[5,6]Fullerene- $C_{60}-I_h-1,6,8,16,28,30,35,37,41,43$,
48,56-dodecayl, 2,3,5,7,9,12,13,14,15,17,19,20,21,
24,25,26,27,29,31,34,36,38,39,40,42,44,45,47,
49,50,51,52,55,57,59,60-hexatriacontahydro-

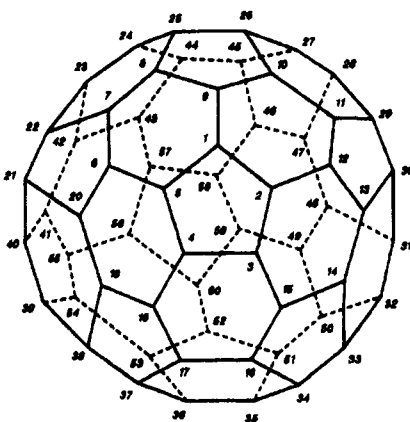
[5,6]Fullerene- $C_{60}-I_h-1,3,6,8,12,14,16,19,21,24,26$,
28,30,35,37,39,41,43,45,48,50,52,56,59(2H,13H,
15H,20H,25H,27H,38H,40H,44H,49H,51H,60H)-
tetracosayl, 4,5,7,9,10,11,17,18,22,23,29,31,32,33,
34,36,42,46,47,53,54,55,57,58-tetracosahydro-

This reasoning does not apply to fullerenes because they are saturated with hydrogen:

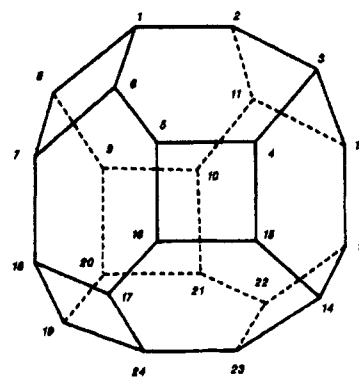
[5,6]Fulleran- $C_{60}-I_h-yl$,
pentatetracontafluoro-



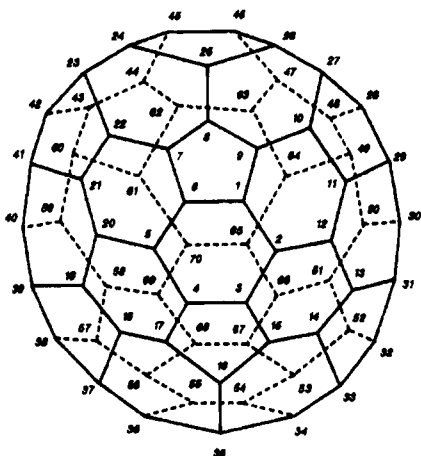
[5,6]Fullerene- $C_{20}-I_h$
Rule 1



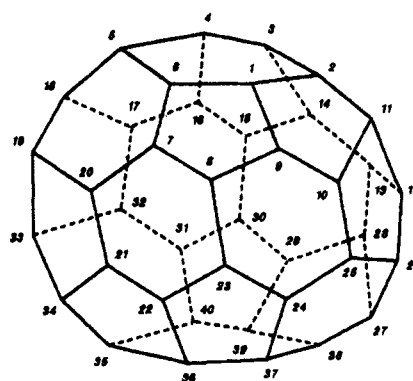
[5,6]Fullerene- $C_{60}-I_h$
Rule 1



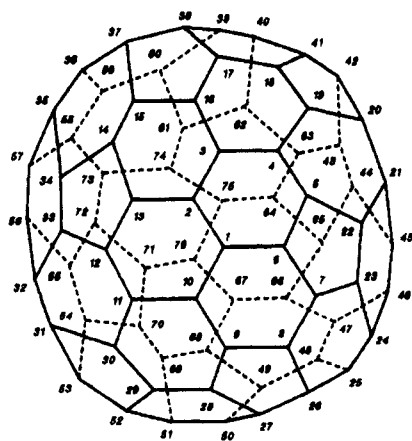
[4,6]Fullerene- $C_{24}-O_h$
Rule 1



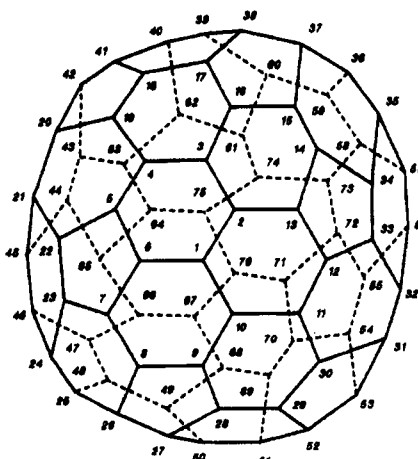
[5,6]Fullerene- $C_{70}-D_{5h(6)}$
Rules 1, 1A, 1G



[5,6]Fullerene- $C_{40}-D_2$
Rules 1, 1A, 1H



[5,6]Fullerene- $C_{76}-D_2$
Rules 1, 1D, 1G, 1H



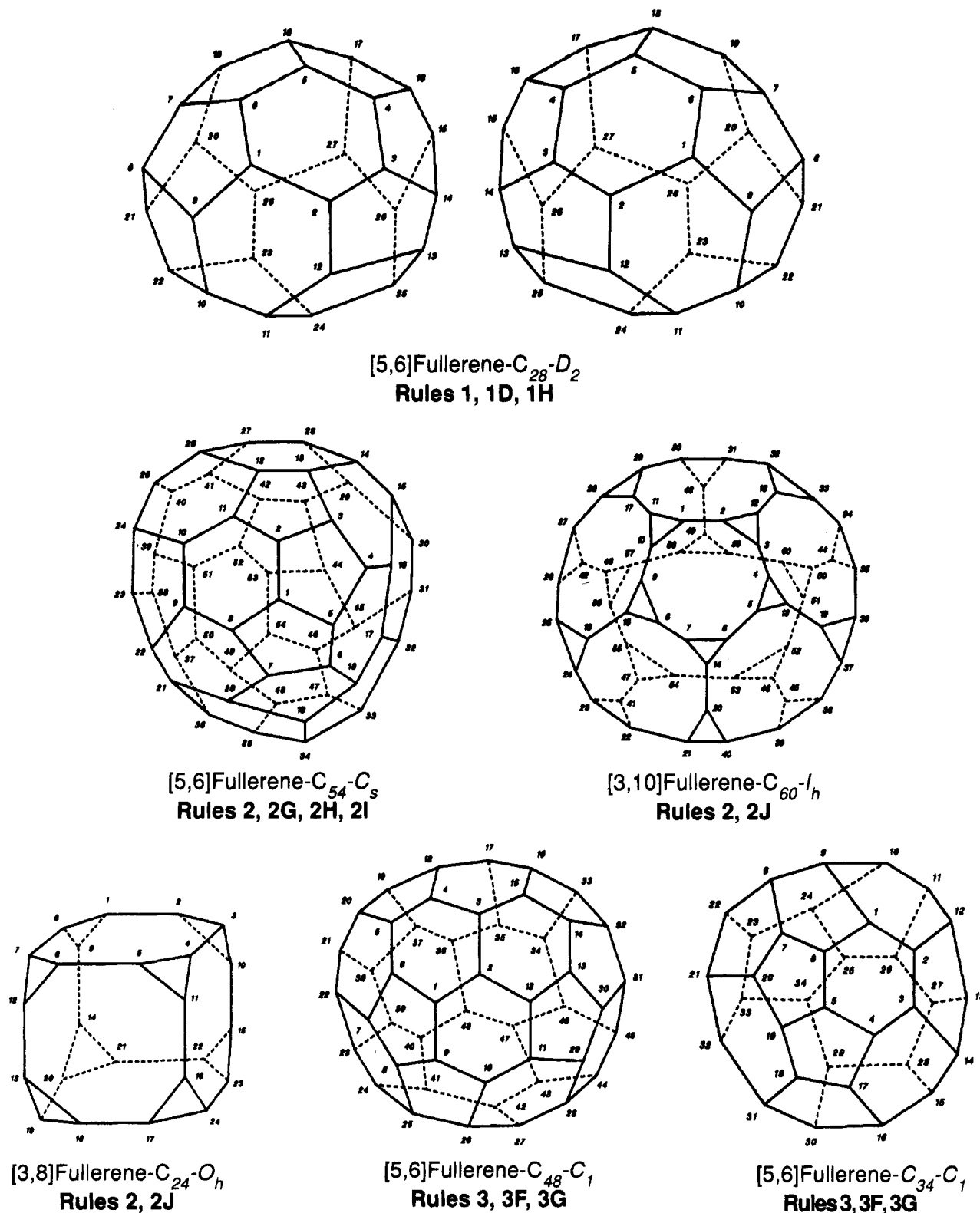


Figure 5. Examples of the use of CAS numbering rules.

[5,6]Fullerene- C_{80} - I_h -6,9,12,15,18,22,26,30,34,38,
41,45,49,53,57,62,65,68,71,74-eicosayl

FULLERENE ASSEMBLIES

Fullerene assemblies are named similarly to ring assemblies, e.g., 2,2'-bi-2*H*-1,2,3-triazole:

1,1'-(2*H*,2'*H*)-Bi[5,6]fullerene- C_{60} - I_h ,
2,2'-bis(trichloromethyl)-

REPLACEMENT FULLERENES

Replacement nomenclature is used for naming fullerenes with one to every carbon atom replaced by Hantzsch-Widman heteroatoms.

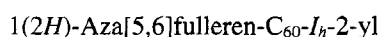
1,9-Diaza[5,6]fullerene- C_{60} - I_h

Azonia[5,6]fullerene- C_{60} - I_h

1-Aza-60-bora[5,6]fullerene- C_{60} - I_h

λ^4 -Thia[5,6]fullerene- C_{60} - I_h

Single, 3-valent replacement atoms result in free radicals:

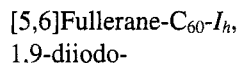


SUBSTITUTED FULLERENES

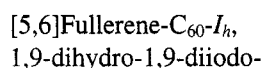
Fulleranes (i.e., fully saturated fullerenes) are named analogously to the unsaturated forms (cf. above):



Their substitution derivatives are also named analogously to those of other hydrogen-containing substances:



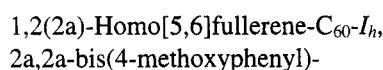
However, for similar derivatives of fullerenes, hydrogen must be added before substitution can occur:¹⁰



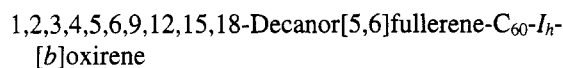
MODIFIED FULLERENE CAGES

Fullerene cages are modified by the addition or deletion of atoms or by the breaking of bonds. These modifications are denoted by the use of "homo", "nor", and "seco" in the name.

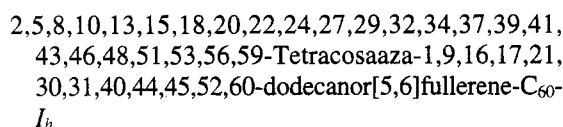
Use of "homo". When a fullerene bond is replaced by a methylene bridge, the original numbering is retained and the locant for the added atom is included in the homofullerene name:



Use of "nor". Deletion of an atom from a fullerene implies that the connectivity of three atoms is reduced from 3 to 2. The connectivity is assumed to be satisfied by addition of hydrogen:



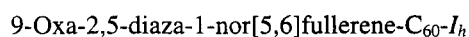
Limitation on the Use of "nor". Use of "nor" is limited to deletion of (a) no more than 20% of the atoms and (b) no more than six 5-membered rings:



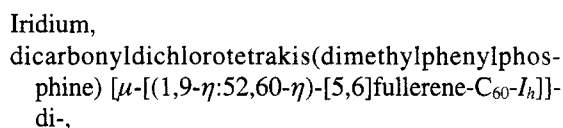
Use of "seco". Scission of a fullerene bond is indicated by the prefix "seco". The original fullerene numbering is retained, with lowest possible locants assigned where there is a choice:



Use of "homo", "nor", and "seco" with Replacement Terms. When "homo", "nor", or "seco" co-occur with replacement terms such as "aza" and "oxa", the replacement prefixes are named in atom seniority order,¹⁵ and the ring modification prefixes are then named alphabetically. Seniority for numbering is in the order homo, nor, seco and then replacement terms in atom seniority order:¹⁵



Coordination Derivatives. Existing policies are followed for naming coordination derivatives of fullerenes:

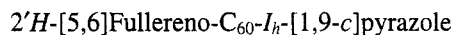
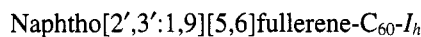
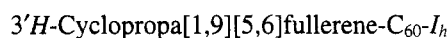
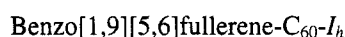


FUSED FULLERENES

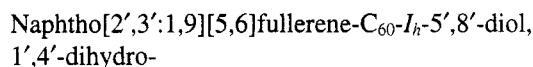
As in other fusions, a pair of atoms are shared by two rings so, when a fused fullerene is named, the fusion pair is regarded as part of both components. Unlike other fusions, the fusion pair are connected by a single bond instead of a double bond because of the nature of fullerenes.

The following rules are applied in forming fullerene fusion names:

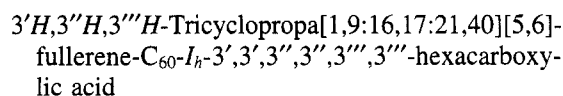
1. The fullerene component of the fusion name appears last when the nonfullerene component is a carbocycle, e.g., benzofullerene. With heterocycles, the reverse order is used with the prefix "fullereno", e.g., fullerenopyrazole. The "o" of fullereno is never elided.



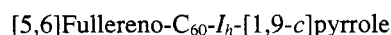
2. Each system retains its own numbering for both addition or substitution and for fusion. The fullerene addition/substitution locants are always unprimed, while primes are added to the carbocycle or heterocycle numbering.



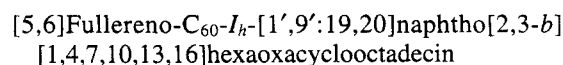
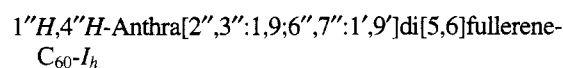
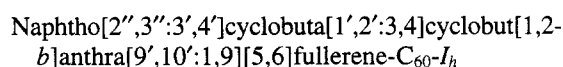
When more than one ring system is fused to a fullerene, primes are assigned to the locants of the systems in sequence from left to right in the name. The position of fusion is indicated in brackets, as in the examples above, by means of primed locants for the carbocycle component (except for single rings, when the carbocycle locants are omitted) and unprimed locants for the fullerene component.



The position of fusion between a fullerene and a heterocycle is indicated in brackets by unprimed locants for the fullerene and letter locants for the heterocycle.



3. When fused ring systems are fused to fullerenes, the ring systems are first named and numbered independently of the fullerene. They are then fused to the fullerene, retaining their locants.



4. When von Baeyer ring systems are fused to fullerenes, they are also first named and numbered independently of the fullerene, including any double bonds, and then fused to it.

Bicyclo[4.2.0]octano[7',8':1,9][5,6]fullerene-C₆₀-I_h

Tricyclo[4.2.1.0^{2,5}]non[7]eno[3',4':1,9][5,6]fullerene-C₆₀-I_h

[5,6]Fullereno-C₆₀-I_h-[1',9':6,7][1,5]diazabicyclo[3.2.2]-nonane

5. Bridges can be part of a ring system or part of a fullerene. They can also span a fullerene and a ring system fused to it or span two ring systems fused to a fullerene. They are given lower priority than fusions.

[1,4]Epoxynaphtho[2',3':1,9][5,6]fullerene-C₆₀-I_h

[1,4]Epoxynaphtho[6',7':1,9][5,6]fullerene-C₆₀-I_h

[9,10]Ethenoanthra[11',12':1,9]fullerene-C₆₀-I_h

[7,12]Ethano[5,14:6,13]dimethanonaphtho[2'',3'':3',4']-cyclobuta[1',2':3,4]cyclobut[1,2-*b*]anthra[9',10':1,9][5,6]fullerene-C₆₀-I_h

[7,12]Ethano[5,14:6,13]dimethanonaphtho[2'',3'':3',4']-cyclobuta[1',2':3,4]cyclobut[1,2-*b*]anthra[9',10':1,9][5,6]fullerene-C₆₀-I_h

[5,6]Fullereno-C₆₀-I_h-[1',9':20,21][18,23]etheno[4,7:14,17]diimino[2,24]metheno[9,12]nitrido[27*H*,29*H*]-benzo[4,5]cyclohept[1,2-*b*]azacyclononadecine

6*H*-4',5-Epoxybicyclo[3.2.2]nonano[6',7':1,9][5,6]fullerene-C₆₀-I_h

5',3''-(Ethano[1,4]benzenomethanoxymethano)-3''*H*-benzo[1,9]cyclopropa[16,17][5,6]fullerene-C₆₀-I_h

POLYMERS

Polymers containing fullerenes are named in accordance with general naming principles:

Phenol, 4,4'-[1,2(2a)-homo[5,6]fulleren-C₆₀-I_h-2a-ylidene]bis-, polymer with 1,6-diisocyanatohexane

Poly[oxy-1,4-phenylene-1,2(2a)homo[5,6]fulleren-C₆₀-I_h-2a-ylidene-1,4-phenyleneoxy(1,10-dioxo-1,10-decanediyl)]

CHARGE TRANSFER COMPLEXES

Some charge transfer complexes are named as neutral compounds.

1,3-Dithiolo[4,5-*b*][1,4]dithiin,
2-(5,6-dihydro-1,3-dithiolo[4,5-*b*][1,4]dithiin-2-ylidene)-5,6-dihydro-,
compd. with [5,6]fullerene-C₆₀-I_h (2:1)

SORTING OF AND SEARCHING FOR FULLERENES

Sorting of fullerenes in the printed indexes occurs in five steps, viz., (1) alphabetic string, (2) ring sizes, (3) number of atoms in the unmodified fullerene, (4) point group symmetries, and (5) any remaining characters. Step 1 is illustrated with the following five names:

1,17,23,29-Tetraaza-14,20,26,44-tetrabora[5,6]-fullerene-C₄₄-T_d

1-Aza-52-bora[5,6]fullerene-C₆₀-I_h

2'*H*-[5,6]Fullereno-C₇₀-D_{5h(6)}-[8,25-*c*]pyrrole

[4,6]Fulleride(1-)-C₂₄-O_h

[3,10]Fullerene-C₆₀-I_h

which sort as follows

Azaborafullerene

Fullerene

Fullerenopyrrole

Fulleride

Tetraazatetraborafullerene

The remaining steps are illustrated with the following names:

[3,10]Fullerene-C₆₀-I_h

[4,5,6]Fullerene-C₆₀-C_{2v}

[4,6]Fullerene-C₂₄-O_h

[5,6]Fullerene-C₄₀-C_{3v}

[5,6]Fullerene-C₄₀-D₂

[5,6]Fullerene-C₄₄-D₂

[5,6]Fullerene-C₄₄-D_{3h}

[5,6]Fullerene-C₆₀-I_h

This sorting sequence must be kept in mind when manually searching the printed indexes. For example, searching under "Azaborafullerene" would find all fullerenes with one nitrogen and one boron atom replacing carbon atoms. To find all fullerenes containing multiple nitrogen and boron atoms requires searching under every possible multiplier, e.g., "tetra" for "Tetraazatetraborafullerene". Searching under the term "Fullereno" would find all fullerenes fused to heterocyclic ring systems. Names of hydrocarbon ring systems fused to fullerenes appear at the front of the name. More specific searches are obtained by applying the subsequent sorting criteria, above.

Electronic searching of STN files provides greater flexibility. The most concise search strategy is using the molecular formula and the term fuller? (quotes are not necessary) to retrieve fullerenes of a specific molecular formula. These answer sets can then be refined by using name fragments for index names and synonyms. Homopolymers and structural repeating units can be retrieved by searching under "(molecular formula)x"/mf or "(molecular formula)n"/mf, respectively (the quotes are necessary). If a search provides too many answers, the answer set can be reduced by adding additional terms such as the number of specific atoms, ring sizes (e.g., 5,6) or point groups symmetries (e.g., ih or c2). Fullerenes can be retrieved with varying degrees of specificity by searching, for example, under ?fuller? (where the search term is truncated left and right), fuller? (where the search term is truncated right), fullerene (which also finds cations), or fulleride (which finds anions only). Because each geometric isomer that has been machine registered has a unique ring identifier (RID field),

RIDs can be used to match derivatives and ions of specific fullerenes when multiple isomers exist (e.g., [5,6]fullerene- $C_{84}-D_2$), even without diagrams.

Searches by chemical name, molecular formula, chemical structure, CAS Registry number, or research topic can also be conducted using the recently introduced SciFinder client-server tool. A structure search could find a name for a ring system or locant set for a substituent pattern, provided the queried structure is in the database. Chemical name and research topic searches can also find structures by specific name searches and query phrases such as "azafullerene", respectively. Clicking on the hypertext Registry numbers in the "Detail of Reference" allows viewing of a pop-up window containing the structure diagram with its corresponding name.

Further information can be obtained by contacting the CAS Help Desk at (phone) 800-848-6533 or (fax) 614-447-3798.

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- (2) This was confirmed when some C_{60} fragments were named. Below C_{50-55} , the ring systems could be named as fused and bridged fused ring systems; above that range, they could be named only as fullerenes. Similar results have been obtained for fragments of C_{70} . (a) Sastry, G. N.; Jemmis, E. D.; Mehta, G.; Shah, S. R. Synthetic Strategies towards C_{60} Fullerene. Molecular Mechanics and MNDO Study on Sumanene and Related Structures. *J. Chem. Soc., Perkin Trans. 2* **1993**, 10, 1867–1871. (b) Jemmis, E. D.; Sastry, G. N.; Mehta, G., *ibid.*, **1994**, 3, 437–441.
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- (4) The number of rings is often equated with the number of faces. In fact, the number of rings equals the number of faces – 1. Recently, a proposed structure for synthetic fullerene- C_{119} was reported in which the presence of a four-membered ring was noted. The CAS name for this fullerene is spiro[3'H-cyclopropa[1,9][5,6]fullerene- $C_{60}-I_h-3'$, 8''a-[1,8(8a)]homo[4,5,6,8]fullerene- $C_{58}-D_{2d}$]. Taylor, R. *J. Chem. Soc., Chem. Commun.* **1994**, 1629–30.
- (5) For a review of fullerenoids, see: Wudl, F. The Chemical Properties of Buckminsterfullerene (C_{60}) and the Birth and Infancy of Fullerenoids. *Acc. Chem. Res.* **1992**, 25(3), 157–161.
- (6) Another proposed C_{119} structure (cf. Note 4) is peanut shaped and is regarded as a fulleroid. Its bonding is satisfied by two atoms of connectivity 4. The only practical way to name this structure is as a fullerene. Adams, G. B.; Page, J. B.; O'Keeffe, M.; Sankey, O. F. *Chem. Phys. Lett.* **1994**, 228(4–5), 485–489. The definition of fullerene does not include carbon atom replacement by metal atoms. For example, $C_{12}Ti_8$ is treated as a cluster and is named Titanium, hexa- μ_4 -1,2-ethenediylideneocta-. An example of a fulleroid that is not named as a modified fullerene is $Si_{20}C_{20}$, where the C_{20} is [5]-fullerene- $C_{20}-I_h$ and the Si_{20} is its sila analog. Each silicon atom is covalently bonded to a carbon atom. This structure is named: Silicon carbide ($Si_{20}C_{20}$), fulleroid. Carbon clusters that are not fullerenes or fulleroids are named, for example, as Carbon, mol. (C_{32}), Carbon, ion (C_{32}^{1-}), or Carbon ion (C_{32}^{1+}).
- (7) Some do not regard carbon cages of other than five- or six-sided faces as being fullerenes. It is CAS policy to record fullerenes with faces of other sizes.
- (8) When a fullerene contains added hydrogen, substituents, functional groups, extra or fewer atoms, heteroatoms, etc., the point group in the name is **always** that of the idealized geometry of the unmodified fullerene. Minor differences in the conformation which reduce the symmetry of the point group (e.g., from D_{6h} to D_6) are not considered.
- (9) A. T. Balaban, X. Liu, and D. J. Klein are developing a system for eliminating this ambiguity. Private communication.
- (10) Because fullerenes contain no hydrogen, hydrogen must first be added before a fullerene can be substituted. See Rule C-32.1, *Nomenclature of Organic Chemistry, Sections A, B, C, D, E, F, and H*; 1979 ed.; IUPAC, Pergamon Press.
- (11) The long anticipated need for locants became reality in March 1991 when DuPont asked CAS for help with numbering their C_{60} platinum coordination compounds. See (a) Fagan, P. J.; Calabrese, J. C.; Malone, B. The Chemical Nature of Buckminsterfullerene (C_{60}) and the Characterization of a Platinum Derivative. *Science* **1991**, 252, 1160–1161. (b) Fagan, P. J.; Calabrese, J. C.; Malone, B. A Multiply-Substituted Buckminsterfullerene (C_{60}) with an Octahedral Array of Platinum Atoms. *J. Am. Chem. Soc.* **1991**, 113, 9408–9409.
- (12) Thus, a 360° rotation about a C_5 axis passes through five equivalent atoms, while rotation about a C_3 axis passes through three equivalent rings.
- (13) Cahn, R. S.; Ingold, C. K.; Prelog, V. *Angew. Chem., Int. Ed. Engl.* **1966**, 5, 385–415 (errata: **1966**, 5, 511). Prelog, V.; Helmchen, G. *Angew. Chem., Int. Ed. Engl.* **1982**, 21, 567–83.
- (14) A numbering system based on graph-theoretical principles has been proposed by Elk, S. B. A Canonical Assignment of Locant Numbers to Fusal Compounds—Especially Fullerenes—Based on Graph Theoretical Principles. *J. Chem. Inf. Comput. Sci.* **1995**, 35(1), 152–158. Another numbering system based on assignment of low locants to the most reactive sites has been proposed: Taylor, R. C_{60} , C_{70} , C_{76} , C_{78} , and C_{84} : Numbering, π -Bond Order Calculations and Addition Pattern Considerations. *J. Chem. Soc., Perkin Trans. 2* **1993**, 813–824.
- (15) For the order of precedence of replacement atoms, see: *Index Guide*, Appendix IV, Section 128, Chemical Abstracts Service, 1994, and Rule B-1.1, *Nomenclature of Organic Chemistry, Sections A, B, C, D, E, F, and H*, 1979 ed.; IUPAC, Pergamon Press.
- (16) For a discussion of inverted chemical names, see: *Index Guide*, Appendix IV, Section 104, Chemical Abstracts Service, 1994.

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