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NOMENCLATURE FOR THE C_{60}-I_h AND C_{70}-$D_{5h(6)}$ FULLERENES

(IUPAC Recommendations 2002)

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Nomenclature for the C_{60}-I_h and C_{70}-$D_{5h(6)}$ fullerenes

(IUPAC Recommendations 2002)

Abstract: Fullerenes are a new allotrope of carbon characterized by a closed-cage structure consisting of an even number of three-coordinate carbon atoms devoid of hydrogen atoms. This class was originally limited to closed-cage structures with 12 isolated five-membered rings, the rest being six-membered rings.

Although it was recognized that existing organic ring nomenclature could be used for these structures, the resulting names would be extremely unwieldy and inconvient for use. At the same time it was also recognized that established organic nomenclature principles could be used, or adapted, to provide a consistent nomenclature for this unique class of compounds based on the class name fullerene. However, it was necessary to develop an entirely new method for uniquely numbering closed-cage systems.

This paper describes IUPAC recommendations for naming and uniquely numbering the two most common fullerenes with isolated pentagons, the icosahedral C_{60} fullerene and a D_{5h}-C_{70} fullerene. It also describes recommendations for adapting organic nomenclature principles for naming fullerenes with nonclosed-cage structures, heterofullerenes, derivatives formed by substitution of hydrofullerenes, and the fusion of organic rings or ring systems to the fullerene cage. Finally, this paper suggests methods for describing structures consisting of two or more fullerene units and for denoting configurations of chiral fullerenes and their derivatives.

CONTENTS

FU-0. INTRODUCTION

In 1997, a preliminary survey of numbering and nomenclature for fullerenes prepared by a working group appointed by the President of IUPAC, Alan Bard, was published [1]. It described two types of names for fullerenes, one proposed by some workers in the field and the one used by Chemical Abstracts Service (CAS); and two systems for numbering fullerene skeletons, one proposed in a publication by R. Taylor [2] and one published by CAS [3]. In addition, alternative methods for naming derivatives of fullerenes were discussed. However, no approved IUPAC recommendations were contained in the IUPAC preliminary survey [1]. The present report contains approved IUPAC recommendations for naming and numbering the C_{60}-I_h and C_{70}-$D_{5h(6)}$ fullerenes and their derivatives. It is limited to these fullerenes because there are only a very small number of known derivatives of only a few other fullerenes. Apart from the numbering and identification of other fullerenes with degenerate point group symbols, which will require complex rules, the nomenclature for all fullerenes can be amply illustrated by the derivatives of these two fullerenes.

FU-1. DEFINITIONS

Fu-1.1 Fullerenes

The classical definition of a fullerene is a compound composed solely of an even number of carbon atoms which form a cage-like fused-ring polycyclic system with 12 five-membered rings and the rest six-membered rings; the archetypal example is the 60-atom structure, where the atoms and bonds delineate a truncated icosahedron [4,5]. However, the term has been broadened to include any closed-cage structure having 20 or more carbon atoms consisting entirely of 3 coordinate carbon atoms [3].

Fu-1.2 Fulleranes

Fulleranes are fully saturated fullerenes, for example, the hydrocarbon $C_{60}H_{60}$.

Fu-1.3 Fulleroids

Heterofullerenes, norfullerenes, homofullerenes, and secofullerenes have been called fulleroids (fullerene-like) because they resemble fullerenes in structure but do not conform to the definition of a fullerene as given above. It is convenient to refer to them as fulleroids and name them as modified fullerenes.

FU-2. NAMES

Fu-2.1 Systematic names

The recommended systematic names for the icosahedral C_{60} and the $D_{5h(6)}$-C_{70} fullerenes are (C_{60}-I_h)[5,6]fullerene and (C_{70}-$D_{5h(6)}$)[5,6]fullerene. The parenthetical prefix gives the carbon content and the point group symbol; and the bracketed numbers indicate the ring sizes in the fullerene. The latter is important in fullerenes with rings other than five- and six-membered. The subscript parenthetical (6) following the point group symbol D_{5h} in the latter name indicates that the five-membered ring on the five-fold symmetry axis is surrounded by six-membered rings. This differentiates this fullerene from an isomeric (C_{70}-D_{5h})[5,6]fullerene, which has five-membered rings surrounding the five-membered ring on the five-fold symmetry axis, which would have the name (C_{70}-$D_{5h(5)}$)[5,6]fullerene. This technique is being further evaluated to determine its value for differentiating among other fullerenes with degenerate point group symbols. The recommended names have the same information as the corresponding CAS names, but in a different format.

Fu-2.2 Trivial names

The names [60-I_h]fullerene and [70-D_{5h}]fullerene given in the IUPAC Preliminary Survey [1] are names first introduced into the literature for the C_{60}-I_h and C_{70}-$D_{5h(6)}$ fullerenes. Since important structural information is omitted from these names, they are to be considered as trivial names to be used only for these specific compounds.

FU-3. NUMBERING

Fu-3.1 Systematic numbering

Systematic numbering for (C_{60}-I_h)[5,6]fullerene and (C_{70}-$D_{5h(6)}$)[5,6]fullerene is based on the following rules adapted from the CAS publication [3]. These rules are sufficient to systematically number (C_{60}-I_h)[5,6]fullerene and (C_{70}-$D_{5h(6)}$)[5,6]fullerene. More rules are needed for other fullerenes. The CAS rules [3] are being evaluated and, if found appropriate, will be included in a subsequent report.

Fu-3.1.1

Proper rotation axes, (C_n), are examined in sequence, from the highest-order to the lowest-order axis, until at least one contiguous spiral pathway is found that begins in a ring through which a proper rotation axis passes, at the end of a bond bisected by a proper rotation axis, or at an atom through which a proper rotation axis passes. Numbering begins at the end of such a contiguous spiral pathway.

Fu-3.1.2

If there is a choice for the selection of a reference axis or for the end of a reference axis to begin the numbering, a ring is preferred to a bond, which, in turn is preferred to an atom.

Fu-3.1.2.1

When there is a choice between rings, a larger ring is preferred to a smaller one. Where there is still a choice, the preferred ring contains the preferred atom (see Fu-3.1.2.3) at the first point of difference.

Fu-3.1.2.2

When there is a choice between bonds, the preferred bond is the common bond between the set of largest rings, for example, 66 > 65 > 55. Where there is still a choice, the preferred bond contains the preferred atom (see Fu-3.1.2.3) at the first point of difference.

Fu-3.1.2.3

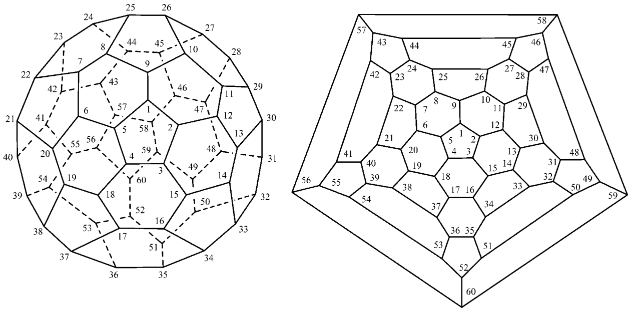
When there is a choice among atoms, the preferred atom is the common atom in the set of largest rings, for example, 666 > 665 > 655 > 555.

Fu-3.1.3

Where there is a choice of spiral pathways for numbering, the preferred pathway terminates as close as possible, in terms of the number of bonds, to the axis of the spiral.

Fu-3.2 Systematic numbering for (C_{60}-I_h)[5,6]fullerene

This fullerene (see Fig. 1) has six equivalent C_5 axes passing through opposite pentagons, each of which gives identical contiguous spiral pathways in either direction from any atom of any pentagon. Thus, each of these C_5 axes can be the reference axis. According to Fu-3.1.1, it is not necessary to investigate any of the ten equivalent C_3 axes passing through opposite hexagons nor the 15 equivalent C_2 axes passing through opposite bonds, all of which give contiguous spiral pathways. The systematic numbering is given in Fig. 1 in both 3-D and Schlegel format.[a]



3-D Representation Schlegel Representation[a]

Fig. 1 Systematic numbering for (C_{60}-I_h)[5,6]fullerene[b].

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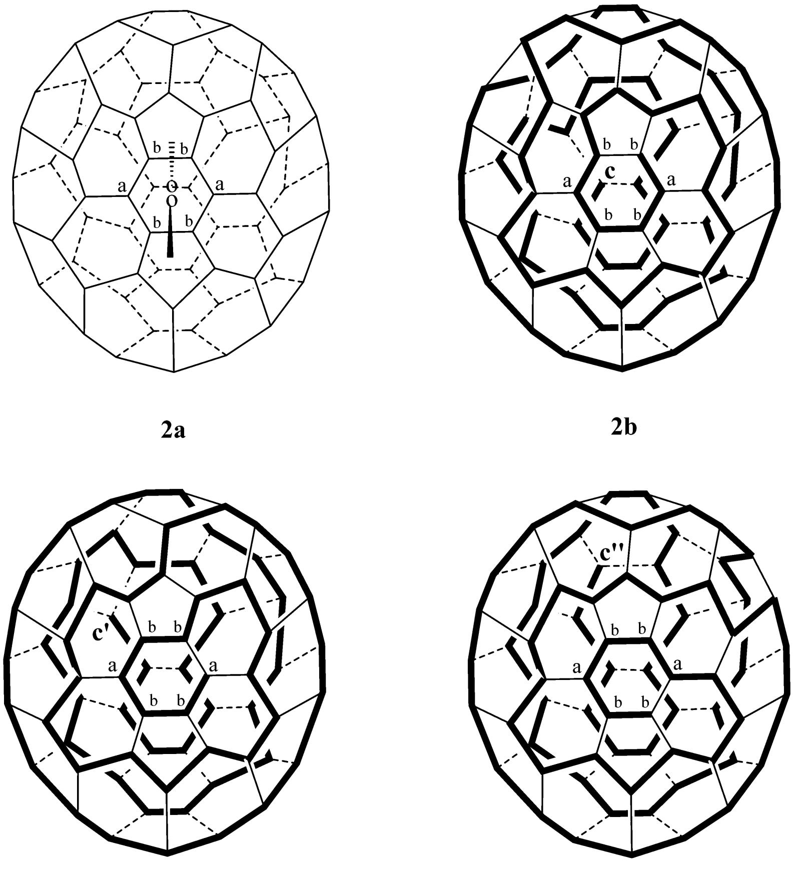
[a] In this document, the convention for Schlegel diagrams is that the central polygon is considered to be closer to the viewer.

[b] For clarity, double bonds are not shown in fullerene structures throughout this report.

Fu-3.3 Systematic numbering for (C_{70}-$D_{5h(6)}$)[5,6]fullerene

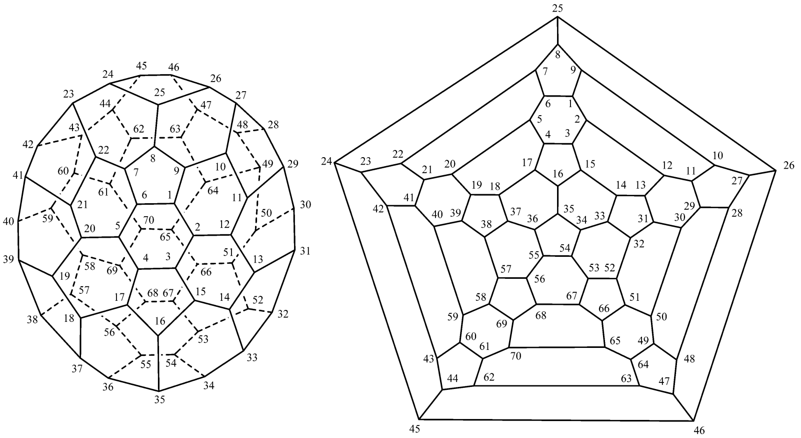
The principal axis for this fullerene (see Fig. 3) is the C_5 axis through opposite pentagons. There are no contiguous spiral pathways from any atom in either pentagon and thus the C_5 axis cannot be a reference axis. Therefore, possible contiguous spiral pathways must be investigated from any of the five equivalent C_2 axes that pass through the center of a six-membered ring at one end and bisect the bond between the two six-membered rings at the other end (see Fig. 2a). Since, according to Fu-3.1.2, a ring is preferred to a bond, the search for a contiguous spiral pathway must start in the six-membered ring. There are twelve possible pathways, one in each direction, clockwise and anticlockwise from each atom of the six-membered ring. However, because of symmetry, atoms marked 'a' in Fig. 2a are equivalent, as are atoms marked 'b' Therefore, there are only three possible pathways to explore, i.e., 'bab', clockwise (Fig. 2b); 'abb', clockwise (Fig. 2c); and 'bba', clockwise (Fig. 2d). The clockwise 'bab' pathway (Fig. 2b) terminates at atom 'c' at the end of the bond bisected by the reference axis. The clockwise 'abb' pathway (Fig. 2c) and the clockwise 'bba' pathway (Fig. 2d) terminate at 'c′', an atom at the end of a bond one removed from the bond bisected by the reference axis, and 'c″', an atom at the end of a bond two removed from the bond bisected by the reference axis, respectively. Thus, according to Fu-3.1.3, the preferred contiguous spiral pathway for numbering is the clockwise 'bab' pathway (Fig. 2b) and thus the systematic numbering for (C_{70}-$D_{5h(6)}$)[5,6]fullerene is that shown in Fig. 3.



2a **2b**

2c **2d**

Fig. 2 Procedural drawings for numbering (C_{70}-$D_{5h(6)}$)[5,6]fullerene.



3-D Representation

Schlegel Representation[c]
(viewed along the C_5 axis)

Fig. 3 Systematic numbering for (C_{70}-$D_{5h(6)}$)[5,6]fullerene[d].

Fu-3.4 Trivial numbering

This numbering, shown in Figs. 4 and 5, is to be used when the trivial names [60-I_h]fullerene and [70-D_{5h}]fullerene given in Fu-2.2 are used; they are based on the reported 'most reactive bond' [2].

> *Note*: Such a criterion does not lend itself to the establishment of a systematic method for numbering other fullerenes, especially ones that haven't yet been characterized.

FU-4. STRUCTURALLY MODIFIED FULLERENES

Modification of fullerene structures by the addition or deletion of atoms, or by the breaking or formation of bonds is described by the prefixes 'homo', 'nor', 'seco', and 'cyclo' in a manner similar to their use in organic stereoparent nomenclature, including their combinations [6].

Fu-4.1 Homofullerenes

The replacement of a carbon–carbon bond of a fullerene by a methylene group is described by attaching the nondetachable prefix 'homo' to the name of the parent fullerene. The original numbering of the parent fullerene is retained. The location of the homo operation is described by a complex locant formed according to the method devised for insertion of a methylene group into a bond sector of a stereoparent [6]. The complex locant is formed by adding the letters 'a', 'b', etc. to the pair of locants for the replaced bond which are the lowest locants consistent with the numbering of the fullerene, and enclosing the higher number in parentheses, for example, '1(9)a'; such complex locants must be used in parent names, but where there is no ambiguity, simple locants formed by adding the letter 'a' to the lower locant, such as '1a' for the case above, may be used in structural formulas and for citation of substituents, etc.

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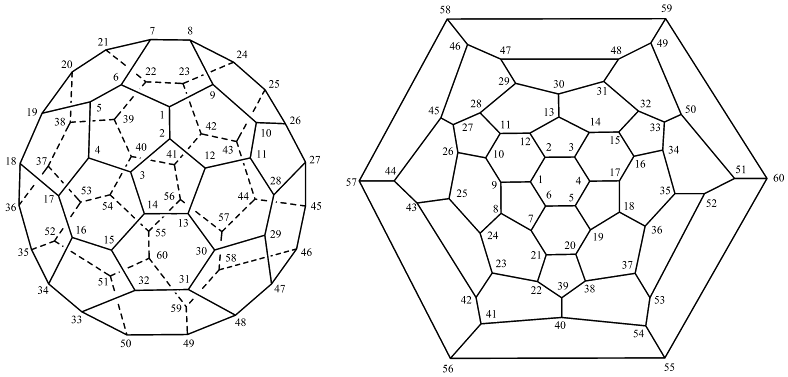
[c] In this document, the convention for Schlegel diagrams is that the central polygon is considered to be closer to the viewer.

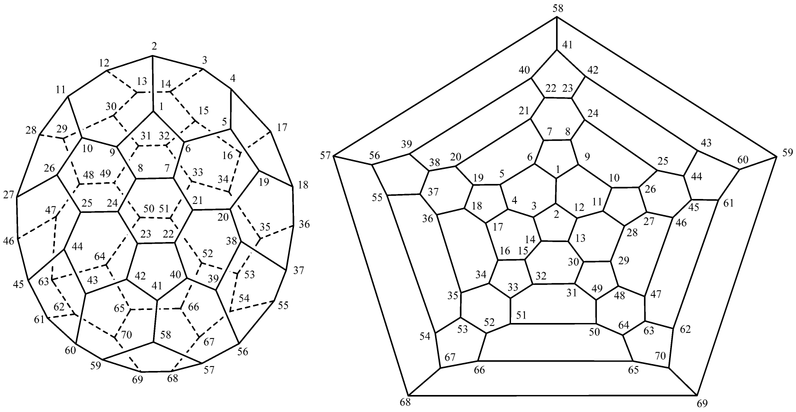
[d] For clarity, double bonds are not shown in fullerene structures throughout this report.



3-D Representation

Schlegel Representation[e]

Fig. 4 Trivial numbering for [60-I_h]fullerene[f].



3-D Representation

Schlegel Representation[e]

Fig. 5 Trivial numbering for [70-D_5h]fullerene[f].

Because of the possibility of rearrangement of the double bonds in homofullerene structures, indicated hydrogen is used to designate the 'extra' hydrogen on the homo atom, even for di-, tri-, tetra-, etc. homofullerenes that could be considered to be hydro derivatives of fully unsaturated structures (see Examples II and III, below).

> *Note*: A complex locant format is used by CAS [3] in which the higher-numbered locant and the letter 'a' are enclosed in parentheses following the locants of the replaced bond, as 1,2(2a); the corresponding simple locant for the added methylene group would be 2a. This was done in an attempt to remove the ambiguity in dihomofullerenes where two of the homo bonds originate from the same atom (see Example III, below), where, according to the preliminary fullerene report [1], both homo atoms would be assigned the same locant. Although this would remove ambiguity in a large number of cases, it would not do so in cases like the following (CA index name): 3,15(15a):14,15(15a)-dihomo-1,9-dinor[5,6]fullerene-C_{60}-I_h [g], where the simple locants for the added methylene groups would both be 15a; the IUPAC name recommended herein for

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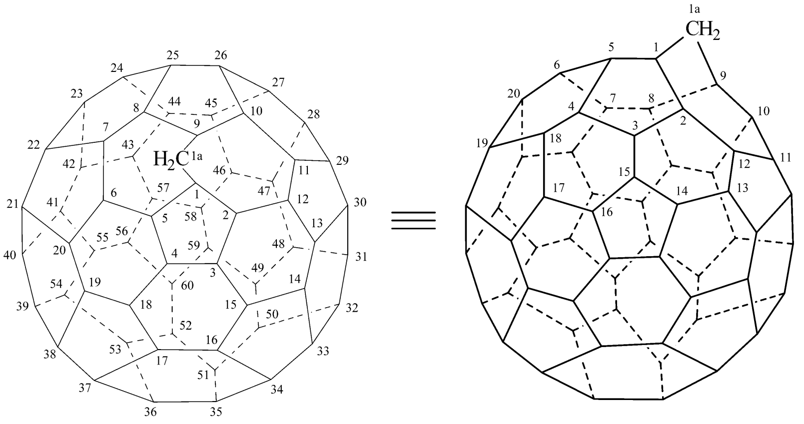
[e] In this document, the convention for Schlegel diagrams is that the central polygon is considered to be closer to the viewer.

[f] For clarity, double bonds are not shown in fullerene structures throughout this report.

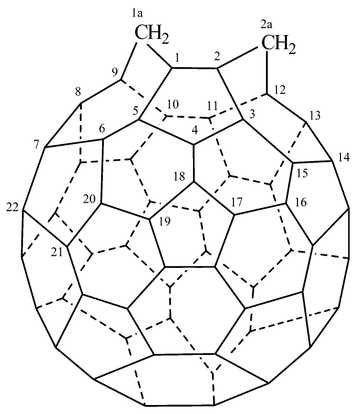
[g] In CAS index names, the complete point group symbol is in italic type in contrast to IUPAC names in which only the on-line capital letter is in italic type, the subscript letters or numbers being given in normal type.

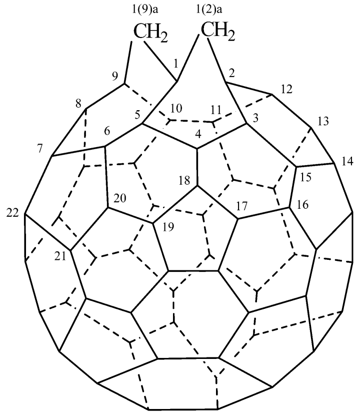
this modified fullerene would be 3(15)a,14(15)a-dihomo-1,9-dinor(C_{60}-I_h)[5,6]fullerene with the corresponding simple locants 3a and 14a, respectively.

Examples:



I 1a*H*-1(9)a-Homo(C_{60}-I_h)[5,6]fullerene
(locant for structure, 1a)





II **III**

II 1a*H*,2a*H*-1(9)a,2(12)a-Dihomo(C_{60}-I_h)[5,6]fullerene
[not la,2a-Dihydro-1(9)a,2(12)a-dihomo(C_{60}-I_h)[5,6]fullerene; locants for the structure, 1a and 2a]

III 1(2)a*H*,1(9)a*H*-1(2)a,1(9)a-Dihomo(C_{60}-I_h)[5,6]fullerene
[not l(2)a,1(9)a-Dihydro-1(9)a,2(12)a-dihomo(C_{60}-I_h)[5,6]fullerene; locants for the structure must be 1(2)a and 1(9)a, because both simple locants would be 1a]

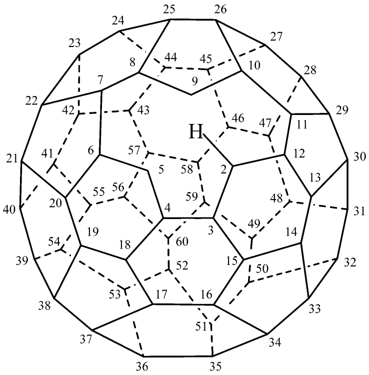
Fu-4.2 Norfullerenes

The nondetachable prefix 'nor' describes the deletion of carbon atoms from a fullerene structure; however, bonds attached to the atom removed are not reconnected as is the case in stereoparent nomenclature [6]. As a result, the connectivity of remaining atoms may be reduced from three to two, which requires the presence of hydrogen atoms. An even number of hydrogen atoms is implied by the name; if there is an odd number, one is expressed as indicated hydrogen because one carbon atom has changed from sp^2 to sp^3 hybridization. A connectivity of three may also be satisfied by a heteroatom, such as nitrogen or boron and a connectivity of two by a heteroatom such as oxygen or sulfur. Where there is a choice, locants for the atoms removed and indicated hydrogen are as low as possible.

Note 1: In organic stereoparent nomenclature atoms removed by the 'nor' operation are those having the highest possible number of the ring or chain segment [6].

Note 2: The main problem with the 'nor' operation is the limit to the number of carbon atoms that can be removed from a particular fullerene structure. Eventually, systematic ring nomenclature will provide a name that may be easier to understand than a polynorfullerene name. It would not be helpful to set a precise number of carbon atoms that can be removed by the nor operation; a realistic figure would depend a lot on whether blocks of carbon atoms or isolated carbon atoms are being removed. For CAS, more than 20 % of the carbon atoms of a fullerene cannot be removed by the nor operation unless it can be shown to be a special situation. For (C_{60}-I_h)[5,6]-fullerene and (C_{70}-$D_{5h(6)}$)[5,6]fullerene it is recommended that at least two 'belts' of rings or at least one-half of the atoms of the parent fullerene must remain intact after the 'nor' operation.

Examples:



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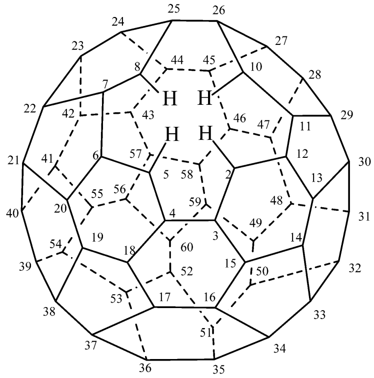
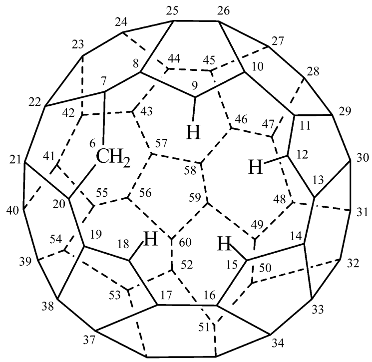
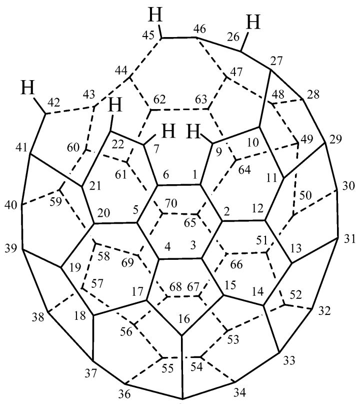


II

I $2H$-1-Nor(C_{60}-I_h)[5,6]fullerene
II 1,9-Dinor(C_{60}-I_h)[5,6]fullerene

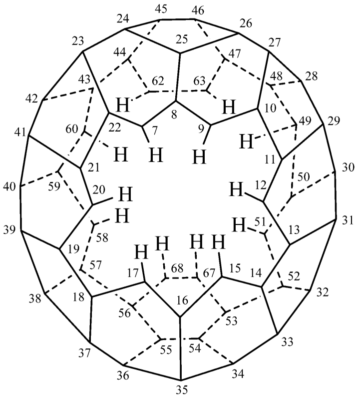


III



IV

III $6H$-1,2,3,4,5-Pentanor(C_{60}-I_h)[5,6]fullerene
IV 8,23,24,25-Tetranor(C_{70}-$D_{5h(6)}$)[5,6]fullerene



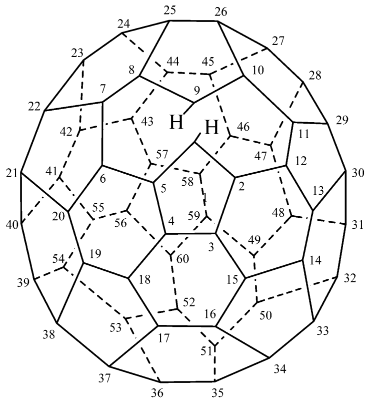
V 1,2,3,4,5,6,61,64,65,66,69,70-Dodecanor(C_{70}-$D_{5h(6)}$)[5,6]fullerene

Fu-4.3 Secofullerenes

The nondetachable prefix 'seco' indicates the removal of fullerene bonds. Numbering of the parent fullerene is retained; where there is a choice, lowest possible locants are used to describe seco positions. The reduced connectivity of the resulting carbon atoms is satisfied by hydrogen atoms following appropriate rearrangement of the double bonds. These hydrogen atoms are implied in the name.

> *Note*: As for the 'nor' operation, the main problem with the 'seco' operation is the limit to the number of fullerene bonds that can be removed from a particular fullerene structure. Eventually, systematic ring nomenclature will provide a name that is easier to understand than a polysecofullerene name. It would not be helpful to set a precise number of fullerene bonds that can be removed by the 'seco' operation; a realistic figure would depend a lot on which fullerene bonds are removed. Obviously, a parent fullerene should not be split into separate fragments.

Examples:



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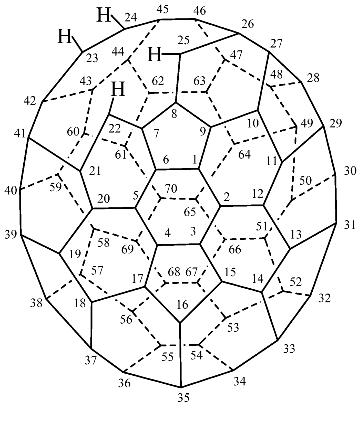
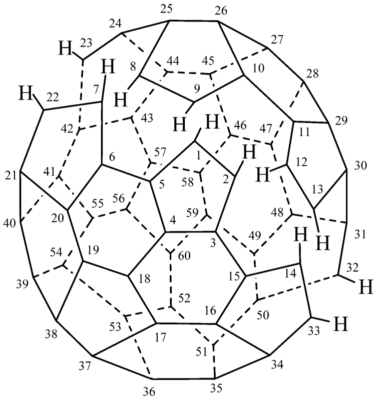


II

I 1,9-Seco(C_{60}-I_h)[5,6]fullerene
II 22,23:24,25-Diseco(C_{70}-$D_{5h(6)}$)[5,6]fullerene



III

III 1,9:2,12:7,8:13,14:22,23:32,33-Hexaseco(C_{60}-I_h)[5,6]fullerene

Fu-4.4 Cyclofullerenes

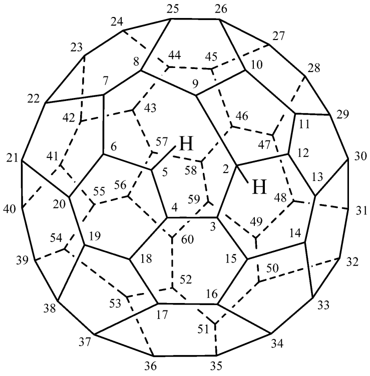
The nondetachable prefix ‘cyclo’ indicates the formation of a bond between two atoms of a modified fullerene or a multicomponent fullerene (see Fu-11). In single component fullerenes, it almost always occurs in combination with one or more of the structure-modifying prefixes described above.

Fu-4.5 Combinations of structure-modifying prefixes

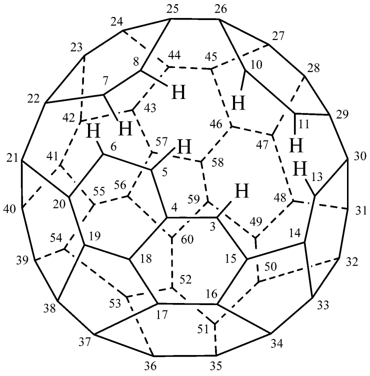
Combinations of structure-modifying prefixes described above may be used and are cited in the order nor, homo, seco, cyclo ‘advancing backwards’ from the parent fullerene name, i.e., proceeding from right to left away from the parent fullerene name. This is also the order that the operation indicated by each prefix takes for assignment of lowest locants. Nor prefixes are preferred for lowest locants, and homo prefixes are preferred to seco or cyclo for lowest locants since homo locants may be needed for the latter operations. Locants for cyclo and seco prefixes are determined by the lowest set of locants, then by the order of citation of the locants in the name.

> *Note*: This order of citation is not the same as given in the Revised Section F: Natural Products and Related Compounds [6] where alphabetical order is preferred reading left to right unless such an order would not be possible given the construction of the structure by ‘advancing backwards’ from the parent structure. CAS uses alphabetical order reading from left to right.

Examples:

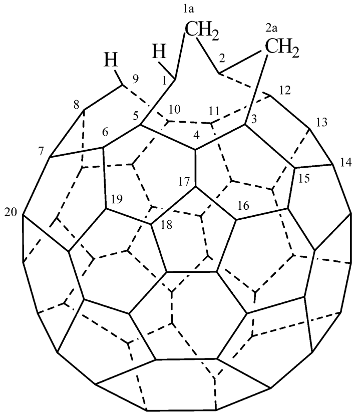


I

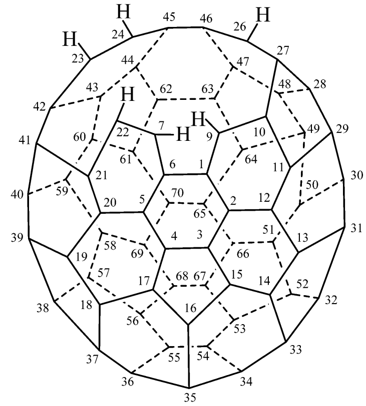


II

I 2*H*-2,9-Cyclo-1-nor(C_{60}-I_h)[5,6]fullerene
II 6,7-Seco-1,2,9,12-tetranor(C_{60}-I_h)[5,6]fullerene



III



IV

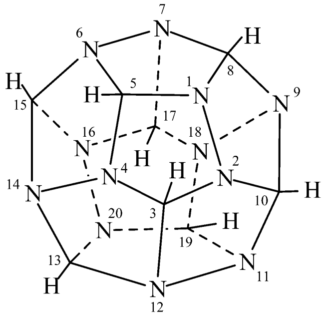
III 1a*H*,2a*H*-1,9-Seco-1(2)a,2(3)a-dihomo(C_{60}-I_h)[5,6]fullerene
IV 22,23-Seco-8,25-dinor(C_{70}-$D_{5h(6)}$)[5,6]fullerene

FU-5. HETEROFULLERENES

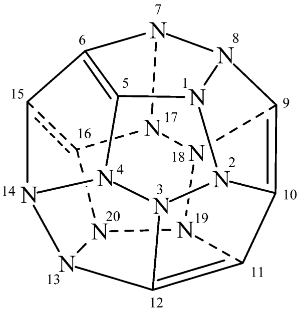
Fu-5.1 Skeletal replacement ('a') nomenclature for fullerenes

Fullerenes in which carbon atoms have been replaced by heteroatoms having standard bonding numbers or by bonding numbers indicated by the λ-convention [7] are named by citing the 'a' prefixes of skeletal replacement nomenclature [8a] in front of the name of the fullerene.

The parent name is fullerene if double bonds are present or are possible in the fullerene; if double bonds are not possible, the parent name is fullerane. This is illustrated by the dodecaaza-(C_{20}-I_h)[5]fullerane and dodecaaza(C_{20}-I_h)[5]fullerene structures shown below.



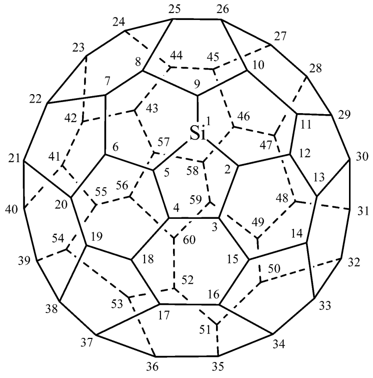
1,2,4,6,7,9,11,12,14,16,18,20-Dodeca-aza(C_{20}-I_h)[5]fullerane



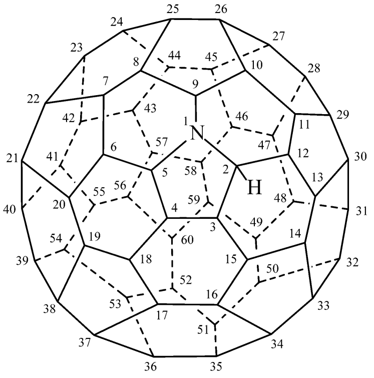
1,2,3,4,7,8,13,14,17,18,19,20-Dodeca-aza(C_{20}-I_h)[5]fullerene[h]

The heteroatoms include all elements capable of being tricoordinate, including metals and semimetals; no heteroatoms have attached hydrogen atoms. All carbons atoms of a fullerene may be replaced by the same or by different heteroatoms. Replacement of carbon atoms by trivalent heteroatoms may result in the need for indicated hydrogen.

Examples:



I

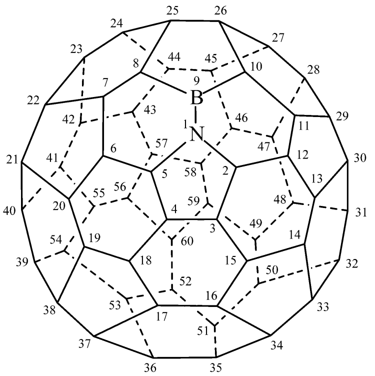


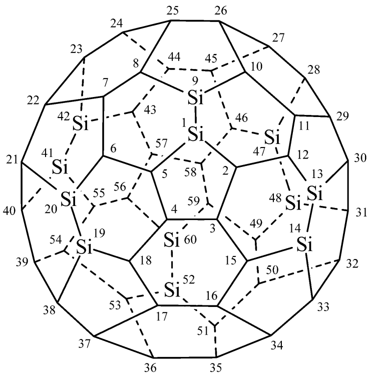
II

I Sila(C_{60}-I_h)[5,6]fullerene
II 2*H*-1-Aza(C_{60}-I_h)[5,6]fullerene

---

[h] The double bonds in this structure are for illustrative purposes only. Double bonds are not shown in fullerenes, fulleroids, or fullerene component structures elsewhere in these recommendations.



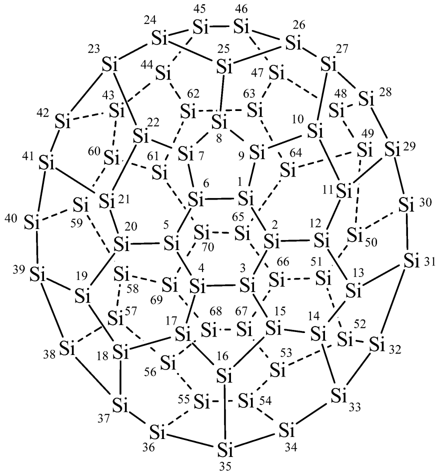


III

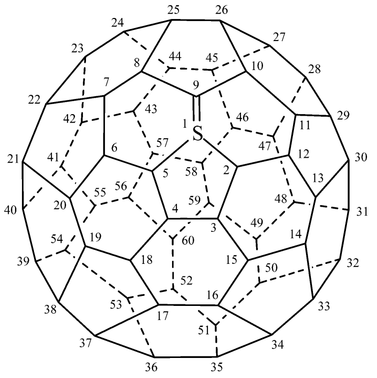
IV

III 1-Aza-9-bora(C_{60}-I_h)[5,6]fullerene

IV 1,9,13,14,19,20,41,42,47,48,52,60-Dodecasila(C_{60}-I_h)[5,6]fullerene



V



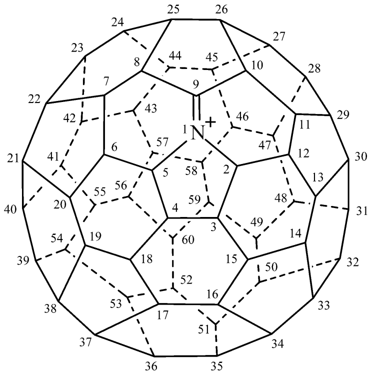
VI [i]

V Heptacontasila(C_{70}-$D_{5h(6)}$)[5,6]fullerene

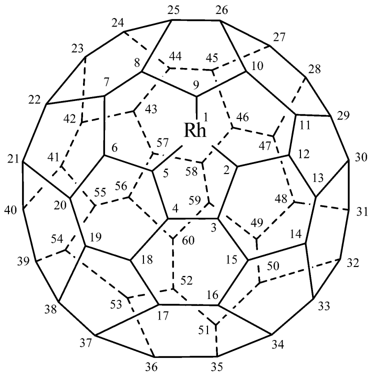
VI $1\lambda^4$-Thia(C_{60}-I_h)[5,6]fullerene

---

[i] The double bonds in this structure are for illustrative purposes only. Double bonds are not shown in fullerenes, fulleroids, or fullerene component structures elsewhere in these recommendations.



VII[j]



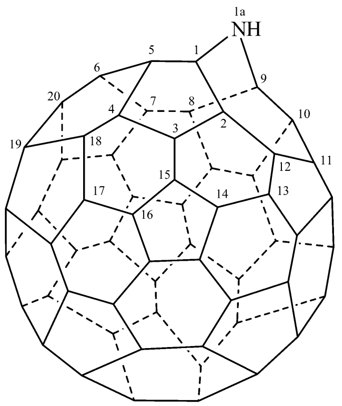
VIII

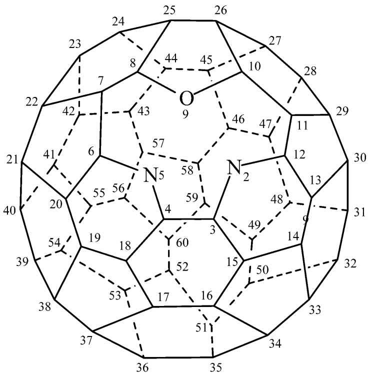
VII Azonia(C_{60}-I_h)[5,6]fullerene
VIII Rhoda(C_{60}-I_h)[5,6]fullerene

Fu-5.2 Skeletal replacement ('a') nomenclature for structurally modified fullerenes

When 'homo', 'nor', 'cyclo', or 'seco' co-occur with replacement terms, such as 'aza' and 'oxa', the replacement prefixes are cited in order of their seniority in front of any structure-modifying prefixes. Structure-modifying prefixes have preference over replacement prefixes for low locants.

Examples:





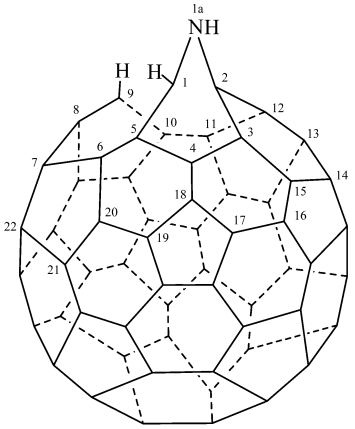
I

II

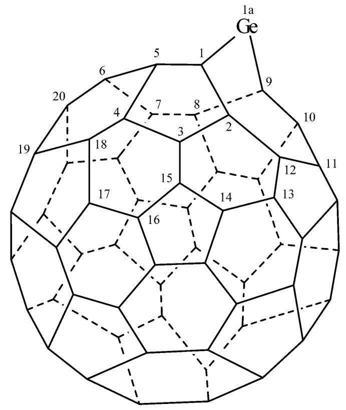
I 1a*H*-1a-Aza-1(9)a-homo(C_{60}-I_h)[5,6]fullerene
II 9-Oxa-2,5-diaza-1-nor(C_{60}-I_h)[5,6]fullerene

---

[j] The double bond in this structure is for illustrative purposes only. Double bonds are not shown in fullerenes, fulleroids, or fullerene component structures elsewhere in these recommendations.

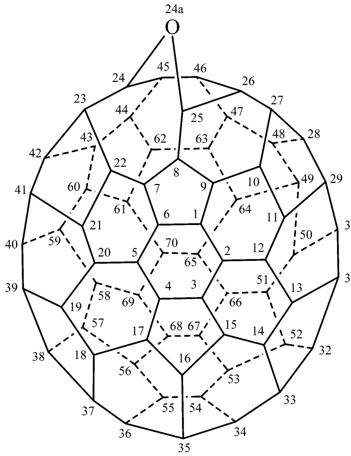


III

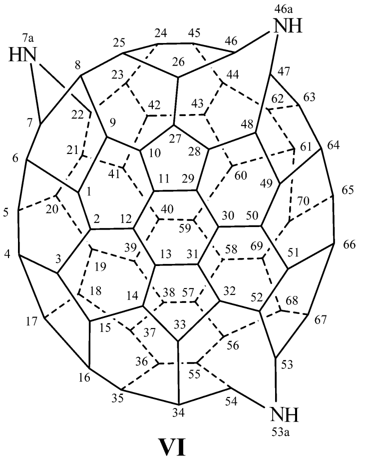


IV

III 1a*H*-1a-Aza-1,9-seco-1(2)a-homo(C_{60}-I_h)[5,6]fullerene
IV 1aλ^2-Germa-1(9)a-homo(C_{60}-I_h)[5,6]fullerene

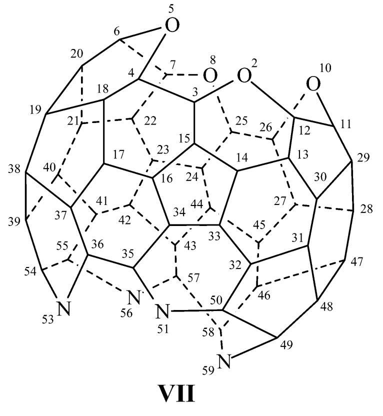


V



VI

V 24a-Oxa-24(25)a-homo(C_{70}-$D_{5h(6)}$)[5,6]fullerene
VI 7a*H*,46a*H*,53a*H*-7a,46a,53a-Triaza-7(22)a,46(47)a,53(54)a-trihomo(C_{70}-$D_{5h(6)}$)[5,6]-fullerene



VII

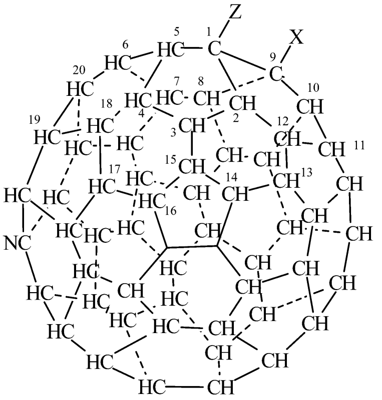
VII 2,5,8,10-Tetraoxa-51,53,56,59-tetraaza-1,9,52,60-tetranor(C_{60}-I_h)[5,6]fullerene

FU-6. FULLERENE DERIVATIVES

Fu-6.1 Fulleranes

Fulleranes are fully saturated fullerenes, i.e., C_nH_n, and their derivatives, radicals, and ions, can be named by application of the principles of substitutive nomenclature normal to saturated hydrocarbons.

Examples:



I Z = • ; X = H
II Z = + ; X = H
III Z = • ; X = +
IV Z = − ; X = H
V Z = • ; X = −
VI Z = OH; X = H

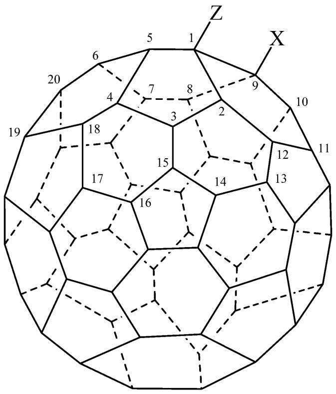
I (C$_{60}$-I_h)[5,6]Fulleran-1-yl
II (C$_{60}$-I_h)[5,6]Fulleran-1-ylium
III (C$_{60}$-I_h)[5,6]Fulleran-9-ylium-1-yl
IV (C$_{60}$-I_h)[5,6]Fulleran-1-ide
V (C$_{60}$-I_h)[5,6]Fulleran-9-id-1-yl
VI (C$_{60}$-I_h)[5,6]Fulleran-1-ol

Fu-6.2 Fullerenes

Fullerenes however, do not have hydrogen atoms for direct substitution and thus their derivatives, radicals, and ions, are named by application of the principles of substitutive nomenclature applicable to fusion atoms of fused ring systems, for example, the 4a and 8a positions of naphthalene. The characteristic group names and substituent prefix names normal to substitutive nomenclature are used.

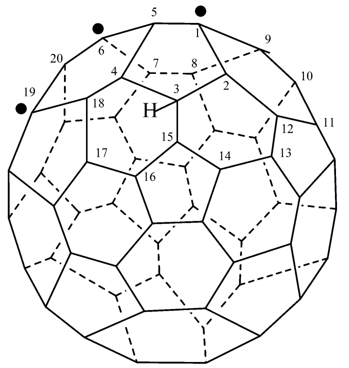
> *Note*: The lack of hydrogen atoms for substitution in fullerenes led to the conclusion in the preliminary survey [1] that atoms and groups attached to fullerenes should be designated as addends and not substituents. This would imply that principles of additive nomenclature should be used which might lead to names such as dibromo[60-I_h]fullerene. However, this leads to difficulties since such names are, in fact, formed by coordination nomenclature (bromo is the current ligand name for Br), a nomenclature method not approved for use with carbon compounds; the additive operation in the nomenclature of organic compounds would produce names such as [60-I_h]fullerene dibromide, for $C_{60}Br_2$. Since such additive names have been discarded in the nomenclature of organic compounds, where substitutive names are preferred, the only acceptable method is to use substitutive nomenclature, in which atoms and groups cited as prefixes substitute hydrogen atoms previously added by means of the additive prefix ‘hydro’; or groups cited as suffixes require the concomitant addition of hydrogen atoms cited as ‘added hydrogen’. Thus, names such as 1,9-dibromo-1,9-dihydro(C$_{60}$-I_h)[5,6]fullerene and (C$_{60}$-I_h)[5,6]fulleren-1(9*H*)-ol result, names that are fully in accordance with the principles, rules, and conventions of substitutive nomenclature. This approach provides a completely consistent method for naming fullerenes with atoms or groups attached to skeletal carbon atoms and all compounds derived from them.

Examples (radicals, ions, and radical ions):



I Z = • ; X = H
II Z = + ; X = H
III Z = • ; X = +
IV Z = – ; X = H
V Z = • ; X = –
VI Z = • ; X = •

I (C_{60}-I_h)[5,6]Fulleren-1(9H)-yl
II (C_{60}-I_h)[5,6]Fulleren-1(9H)-ylium
III (C_{60}-I_h)[5,6]Fulleren-9-ylium-1(9*H*)-yl[k]
IV (C_{60}-I_h)[5,6]Fulleren-1(9H)-ide
V (C_{60}-I_h)[5,6]Fulleren-9-id-1(9H)-yl[k]
VI (C_{60}-I_h)[5,6]Fullerene-1,9-diyl[l]



VII

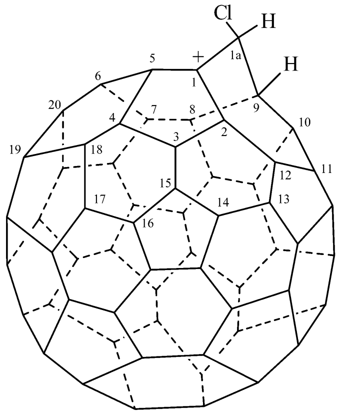
VII (C_{60}-I_h)[5,6]Fullerene-1,6,19(3*H*)-triyl

---

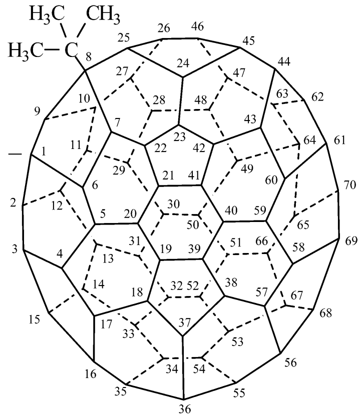
[k] The hydrogen needed for the -ide or -ylium suffix is provided by the added hydrogen required by the -yl suffix.

[l] Added hydrogen is not used since the multiple suffixes simply remove a double bond, as in naphthalene-4a,8a-diol.

Examples (substituted derivatives):

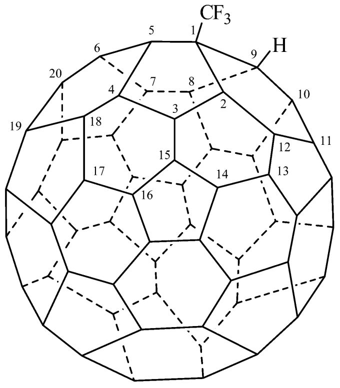


I

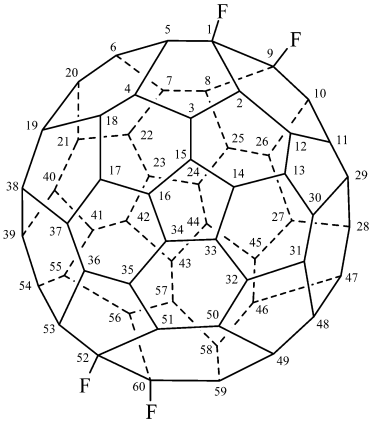


II

I 1a-Chloro-1a*H*-1(9)a-homo(C_{60}-I_h)[5,6]fulleren-1(9*H*)-ylium
II 8-*tert*-Butyl(C_{70}-$D_{5h(6)}$)[5,6]fulleren-1(8*H*)-ide[m]



III



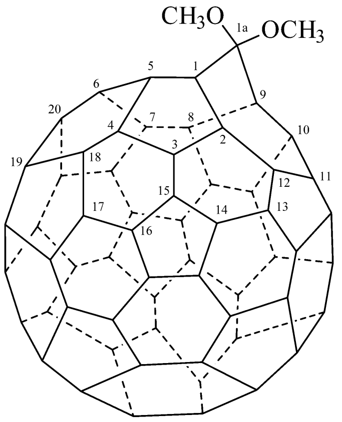
IV

III 1-(Trifluoromethyl)-1,9-dihydro(C_{60}-I_h)[5,6]fullerene[n]
IV 1,9,52,60-Tetrafluoro-1,9,52,60-tetrahydro(C_{60}-I_h)[5,6]fullerene

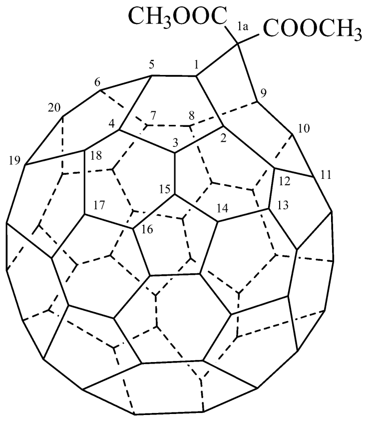
---

[m] The uninverted CA index name is 8-(1,1-dimethylethyl)-1,8-dihydro[5,6]fullerene-C_{70}-$D_{5h(6)}$ ion(1–).

[n] Hydro prefixes are treated as nondetachable in these recommendations.



V



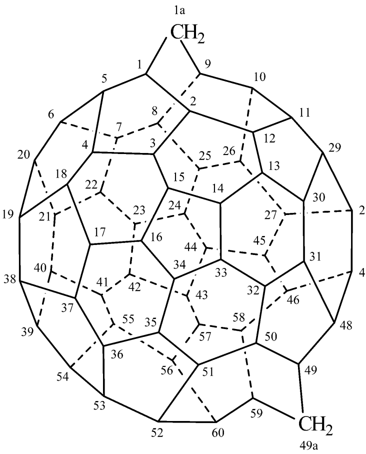
VI

V 1a,1a-Dimethoxy-1a*H*-1(9)a-homo(C_{60}-I_h)[5,6]fullerene
VI Dimethyl 1a*H*-1(9)a-homo(C_{60}-I_h)[5,6]fullerene-1a,1a-dicarboxylate

Fu-6.3 Lowest locants

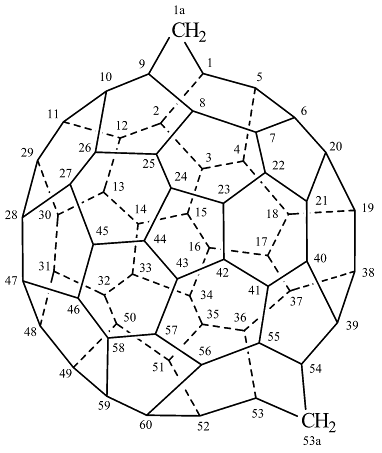
For the C_{60}-I_h and C_{70}-$D_{5h(6)}$ fullerenes and fulleranes the high symmetry can result in difficulty in determining the lowest set of locants for derivatives. Numbering in (C_{60}-I_h)[5,6]fullerene can begin at any atom of any one of the 12 five-membered rings and proceed around the chosen five-membered ring in either direction.

Example:



Ia

not

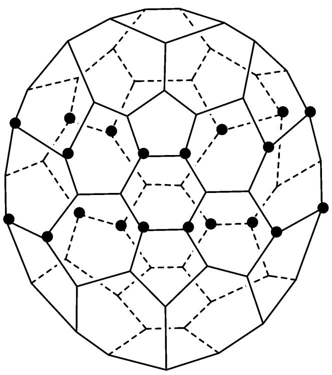


Ib

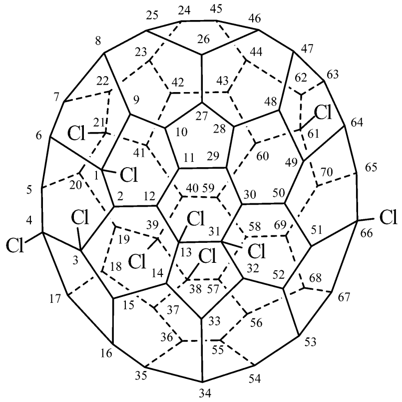
1a*H*,49a*H*-1(9)a,49(59)a-Dihomo(C_{60}-I_h)[5,6]fullerene (**Ia**)
[*not* 1a*H*,53a*H*-1(9)a,53(54)a-Dihomo(C_{60}-I_h)[5,6]fullerene (**Ib**); the locant set 1,9,49,59 is lower than 1,9,53,54]

In (C_{70}-$D_{5h(6)}$)[5,6]fullerene numbering can begin at four positions of each of the five six-membered rings in the middle of the fullerene structure perpendicular to the C_2 axis, as shown by the enlarged dots in **Ia,** below, but may proceed in only one direction from each position. The correct numbering is shown in **Ia** and incorrect numberings in **Ib** and **Ic**.

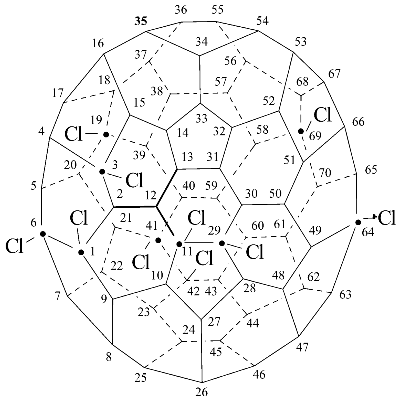
Example:



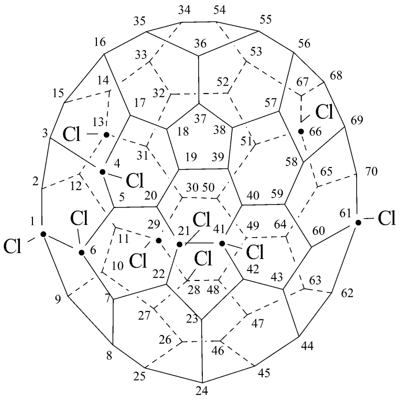
Ia



Ib
(correct numbering)



Ic
(incorrect numbering)



Id
(incorrect numbering)

1,3,4,13,21,31,38,39,61,66-Decachloro-1,3,4,13,21,31,38,39,61,66-decahydro(C_{70}-$D_{5h(6)}$)-[5,6]fullerene (**Ib**)

[*not* 1,3,6,11,19,29,41,42,64,69-Decachloro-1,3,6,11,19,29,41,42,64,69-decahydro(C_{70}-$D_{5h(6)}$)-[5,6]fullerene (Ic); the locant set 1,3,4… is lower than 1,3,6…]

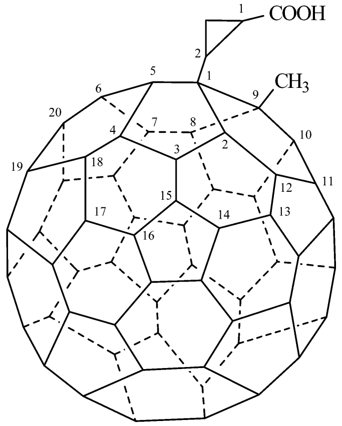
[*not* 1,4,6,13,21,28,29,41,61,66-Decachloro-1,4,6,13,21,28,29,41,61,66-decahydro(C_{70}-$D_{5h(6)}$)-[5,6]fullerene (Id); the locant set 1,3,4… is lower than 1,4,6…]

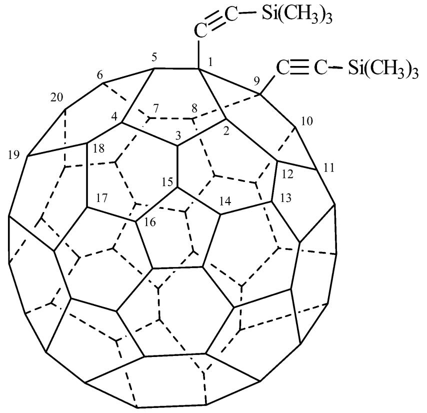
Explanation: All but one of the chlorine substituents fall at one of the possible starting points for numbering the (C_{70}-$D_{5h(6)}$)[5,6]fullerene (see **Ia**). However, one of the candidate benzene rings has three chlorine atoms and thus would obviously provide the lowest initial locants of the locant set. Of the three possible numberings starting in this benzene ring, 1,3,4… is lower than 1,3,6…., or 1,4,6…]

Fu-6.4 Fullerenes and fulleranes as substituents

When a fullerene is a substituent to a more preferred parent compound, the name of the appropriate fullerene (free) radical (see above) is used as its substituent prefix name.

Examples:





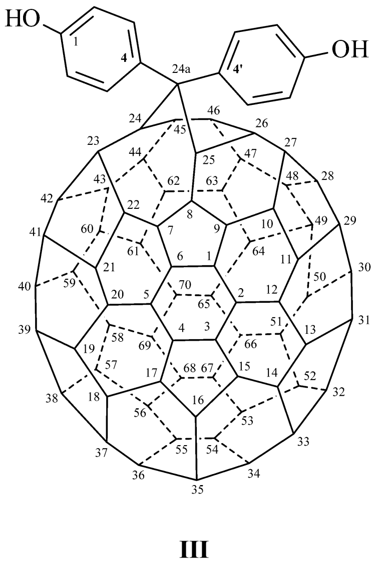
I **II**

I 2-[9-Methyl(C_{60}-I_h)[5,6]fulleren-1(9*H*)-yl]cyclopropane-1-carboxylic acid

II [(C_{60}-I_h)[5,6]Fullerene-1,9-diyldiethyne-2,1-diyl]bis[trimethylsilane][o]

or

Hexamethyl[(C_{60}-I_h)[5,6]fullerene-1,9-diyldiethyne-2,1-diyl]bis[silane][p]



III

III 4,4′-[24a*H*-24(25)a-Homo(C_{70}-$D_{5h(6)}$)[5,6]fullerene-24a,24a-diyl]diphenol

---

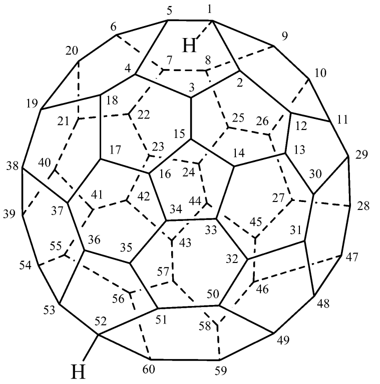
[o] A multiplicative name following the method used in CA index nomenclature.

[p] A multiplicative name following the method currently recommended by IUPAC.

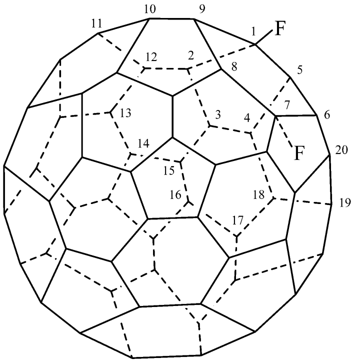
Fu-6.5 *endo*-Substituted fullerenes and fulleranes

All substituents are assumed to project away from the fullerene cage. However, some fullerene substituents are small enough so that they can project into the fullerene cage. To describe such substituents, the term *endo,* enclosed in parentheses, is cited after the appropriate locant.

Examples:



I



II

I 1(*endo*),52-Dihydro(C_{60}-I_h)[5,6]fullerene

II 1,7(*endo*)-Difluoro-1,7-dihydro(C_{60}-I_h)[5,6]fullerene

FU-7. FULLERENES AND MODIFIED FULLERENES FUSED TO ORGANIC RINGS OR RING SYSTEMS

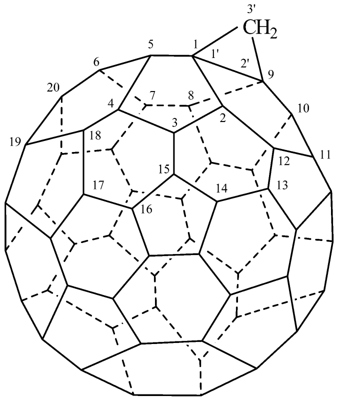
Fullerenes that share an adjacent pair of atoms with an organic ring or ring system are named by **adapting** and **extending** the principles of fusion nomenclature [9]. As in normal organic fused ring systems, the pair of atoms shared by the fullerene and the organic ring or ring system is regarded as part of both components. However, unlike organic fused ring systems, each component retains its own bonding pattern and numbering. Because of the nature of bonding in fullerenes, the fusion bond is always a single bond and the fusion atoms cannot accept an 'exo' double bond. After fusion, nonfullerene components other than alicyclic bi- and polycyclic ring systems have the maximum number of double bonds and indicated hydrogen is cited as needed.

> *Note*: Although when the nonfullerene component is a simple ring, such as cyclopropane or oxirene, the additional atoms could be cited by means of bridge prefixes, such as methano and epoxy, for consistency it is recommended that all be named as fused systems. Both methods were included in the preliminary survey [1]. It is clear that as the attached organic system becomes more complex, the formation of bridge names becomes more difficult. For example, the CAS Ring Systems Handbook [10] contains many examples of a fullerene fused to two organic rings which themselves are connected by a bridge. For bridged fullerenes, see Fu-8.

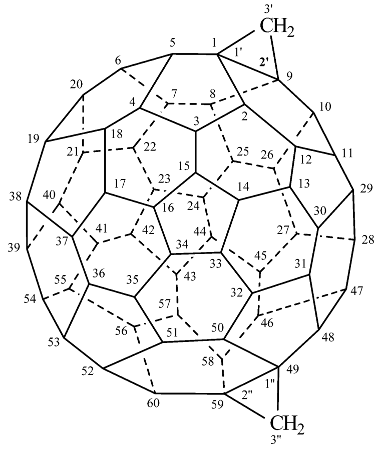
Organic rings and ring systems, including monocyclic rings and all polycyclic ring systems except spiro ring systems, are always cited as prefixes to the name of the fullerene or modified fullerene. Spiro systems that might be considered as fused to a fullerene are treated as spiro systems between modified fullerenes or fused fullerene systems and other components (see Fu-9). Each system retains its own name and numbering both for indicating fusion sites and for indicating positions of substitution. The fullerene locants are always unprimed and primes are added to the locants of the fused organic rings in the order described below. The fusion is described by citing the primed locants of the organic ring component and the unprimed locants of the fullerene in that order, enclosed in brackets and separated by a colon. Locants for monocyclic hydrocarbon components are usually omitted.

> *Note*: CAS prefixes the fullerene name to that of a heterocyclic ring system when the latter has a heteroatomic component preferred to the fullerene component [3]. For example, a fullerene component with no heteroatoms would be prefixed to any heterocyclic component, but a nitrogenous heterocyclic component would be prefixed to an nitrogenous fullerene component. This method was chosen for consistency with normal organic fusion nomenclature where heterocycles are preferred as base components. When the heterocycle is a monocycle, a fused ring system used as a base component in ordinary fusion nomenclature, or a heterocyclic ring system that is bridged, the fusion site is described by citing the **unprimed** locants of the fullerene component followed by the letter locant for the fusion side of the heterocycle. However, when the heterocycle is itself a fused ring system, a bridged fused system that is not a base component, or a bridged nonfused heterocycle, the fusion locants of the fullerene component are primed and those of the heterocycle are unprimed. As a result in the latter case, the fusion locants are not the same as the locants used for substitution, which are unprimed for the fullerene component and primed for the non-fullerene component, a situation that could be confusing. This situation is defended by the notion that locants within brackets in fusion names are those of the components, and are not the locants of the complete fused system. When the fullerene is always the base component, this confusion does not occur; in normal fusion nomenclature, the final fused ring system is renumbered, so the possibility of confusion does not exist.

Examples:

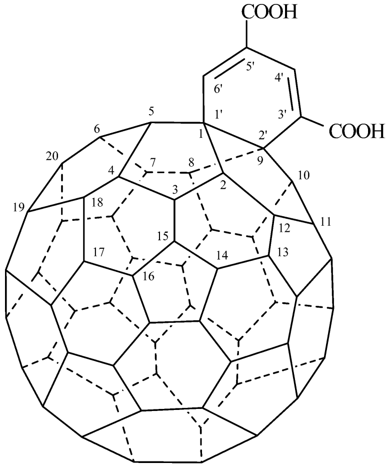


I



II

I *3′H*-Cyclopropa[1,9](C_{60}-I_h)[5,6]fullerene
II 3′*H*,3″*H*-Dicyclopropa[1,9:49,59](C_{60}-I_h)[5,6]fullerene



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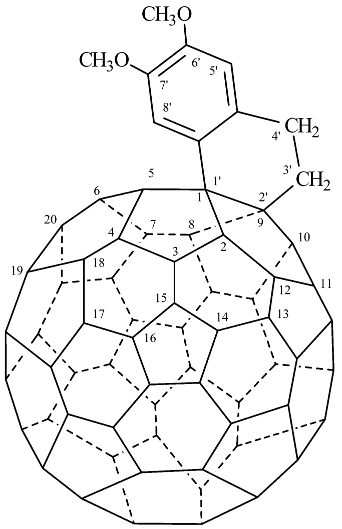
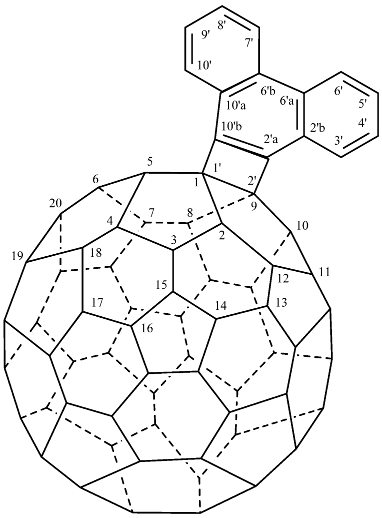


IV

III Benzo[1,9](C_{60}-I_h)[5,6]fullerene-3′,5′-dicarboxylic acid
IV 6′,7′-Dimethoxy-3′,4′-dihydronaphtho[1′,2′:1,9](C_{60}-I_h)[5,6]fullerene[q]



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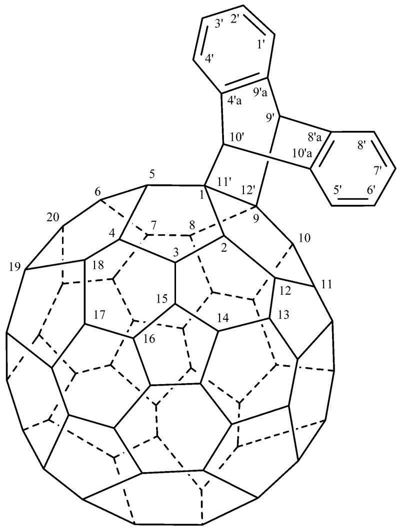

VI

V Cyclobuta[*l*]phenanthro[1′,2′:1,9](C_{60}-I_h)[5,6]fullerene
VI 9′,10′-Dihydro[9,10]ethanoanthra[11′,12′:1,9](C_{60}-I_h)[5,6]fullerene

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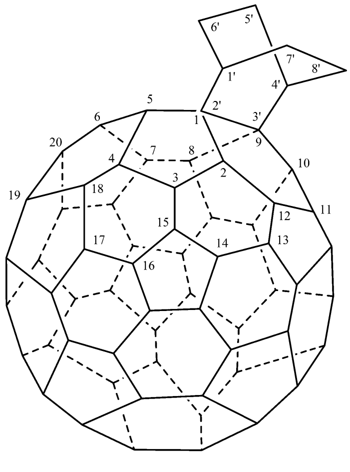
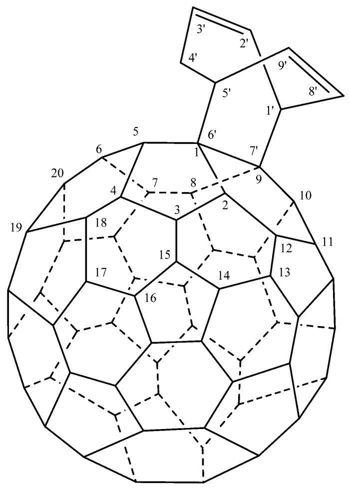
[q] Hydro prefixes are treated as nondetachable in these recommendations.



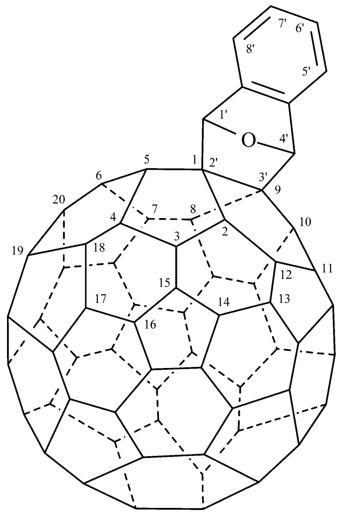
VII



VIII

VII Bicyclo[2.2.2]octano[2′,3′:1,9](C_{60}-I_{h})[5,6]fullerene (note that the double bond at the fusion site in the bicyclo component is not expressed)

VIII Bicyclo[3.2.2]nona[2,8]dieno[6′,7′:1,9](C_{60}-I_{h})[5,6]fullerene (not bicyclo[3.2.2]nona-[2,6]dieno[8′,9′:1,9](C_{60}-I_{h})[5,6]fullerene; there is a choice in numbering and the fusion site is preferred for lower locants)



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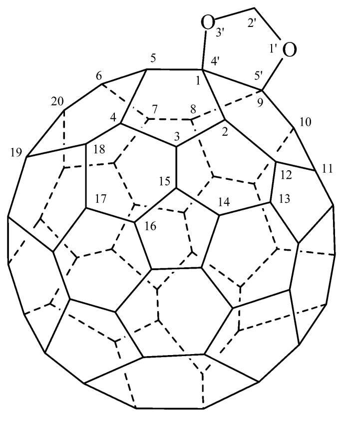

X

IX 1′,4′-Dihydro[1,4]epoxynaphtho[2′,3′:1,9](C_{60}-I_{h})[5,6]fullerene

X [1,3]Dioxolo[4′,5′:1,9](C_{60}-I_{h})][5,6]fullerene[r]

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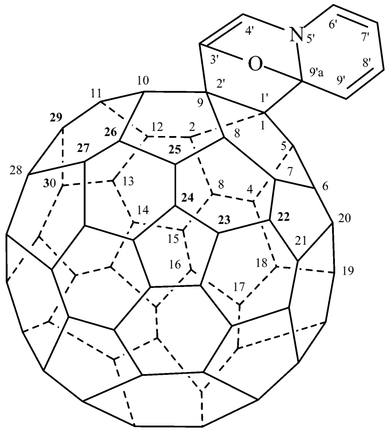
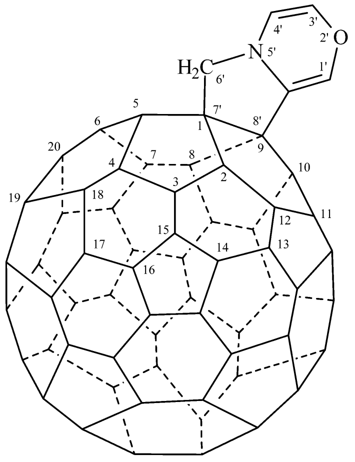
[r] The CA index name is [5,6]fullereno-C_{60}-I_h-[1,9-*d*][1,3]dioxole.

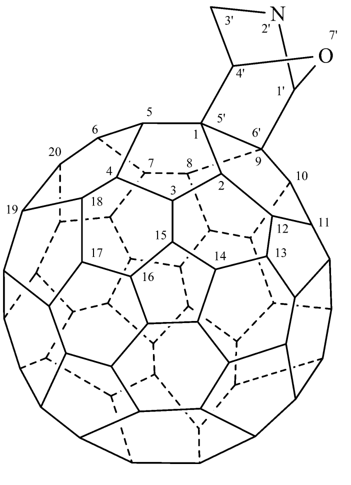


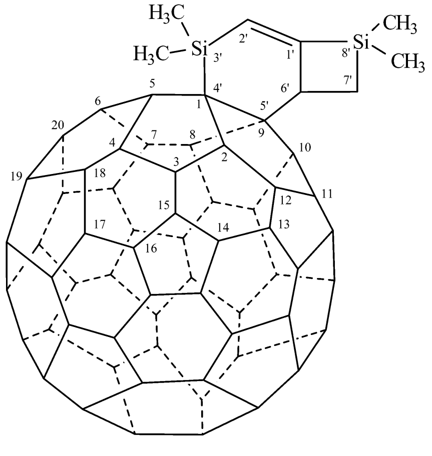
XI



XII

XI [3,9a]Epoxyquinolizino[1′,2′:1,9](C_{60}-I_h)[5,6]fullerene[s]
XII 6′*H*-Pyrrolo[2,1-*c*][1,4]oxazino[7′,8′:1,9](C_{60}-I_h)[5,6]fullerene[t]





XIII **XIV**

XIII [7]Oxa[2]azabicyclo[2.2.1]heptano[5′,6′:1,9](C_{60}-I_h)[5,6]fullerene[u]
XIV 3′,3′,8′,8′-Tetramethyl[3,8]disilabicyclo[4.2.0]oct[1]eno[4′,5′:1,9](C_{60}-I_h)[5,6]fullerene[v]

When two or more of the **same** nonfullerene component are fused to a fullerene, primes are assigned to the locants of the components according to the increasing value of the lower fullerene fusion locant. When **different** nonfullerene components are attached to a fullerene, primes are assigned in the

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[s] The CA index name is [5,6]fullereno-C_{60}-I_h-[1,9-*a*][3,9a]epoxy[9a*H*]quinolizine.

[t] The CA index name is [5,6]Fullereno-C_{60}-I_h-[1′,9′:7,8]pyrrolo[2,1-*c*][1,4]oxazine.

[u] The CA index name is [5,6]Fullereno-C_{60}-I_h-[1′,9′:5,6][7]oxa[2]azabicyclo[2.2.1]heptane.

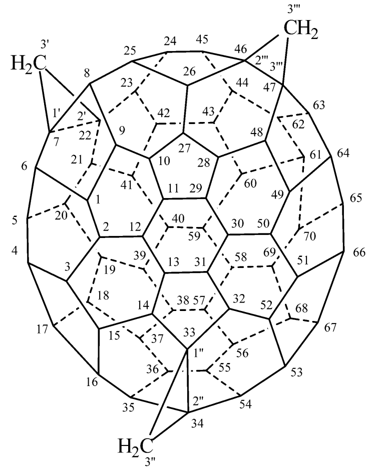
[v] The uninverted CA index name is 3′,3′,8′,8′-Tetramethyl[5,6]fullereno-C_{60}-I_h-[1′,9′:4,5][3,8]disilabicyclo[4.2.0]oct-1-ene.

alphabetical order of citation of the fusion prefix in the name reading from left to right, respecting the criterion for multiples of the same nonfullerene component given above.

Note 1: As shown by examples V and VI, below, the fullerene fusion locants are assigned based on the lowest set of locants for all fusion sites at the first point of difference when compared term by term in ascending numerical order. Primes for the nonfullerene fusion components are assigned in order of the appearance of the component in the name.

Note 2: Fullerene fusion locants are not assigned on the basis of the lowest locants for nonfullerene fusion components first cited in the name.

Examples:



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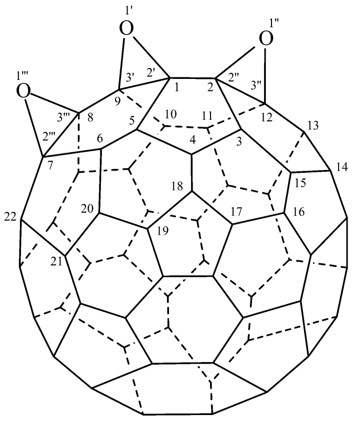
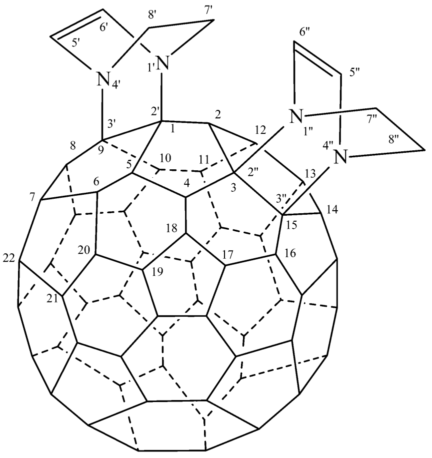


II

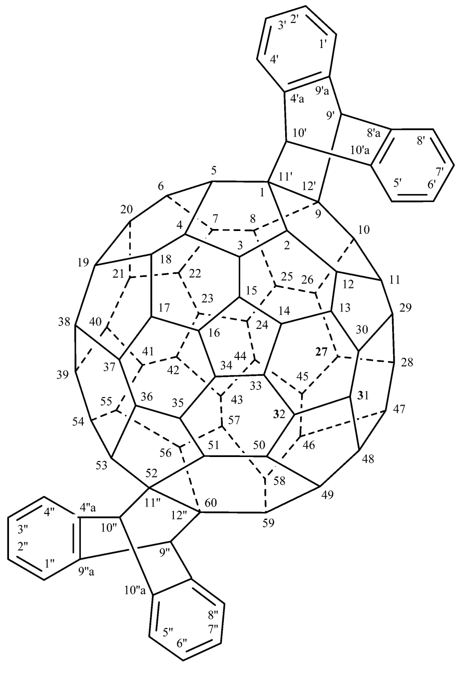
I 3′*H*,3″*H*,3‴*H*-Tricyclopropa[7,22:33,34:46,47](C_{70}-$D_{5h(6)}$)[5,6]fullerene

II Trisoxireno[2′,3′:1,9; 2″,3″:2,12; 2‴,3‴:7,8](C_{60}-I_h)[5,6]fullerene[W]

[W] The CA index name is [5,6]fullereno-C_{60}-I_h-[1,9-*b*:2,12-*b*′:3,15-*b*″]trisoxirene.



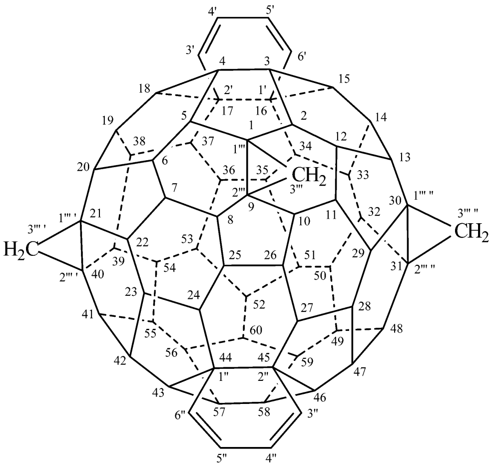
III



IV

III Bis[1,4]diazabicyclo[2.2.2]oct[5]eno[2′,3′:1,9;2″,3″:3,15](C$_{60}$-*I*$_h$)[5,6]fullerene[x]

IV 9′,9″,10′,10″-Tetrahydrobis[9,10]ethanoanthra[11′,12′:1,9;11″,12″:52,60](C$_{60}$-*I*$_h$)-[5,6]fullerene



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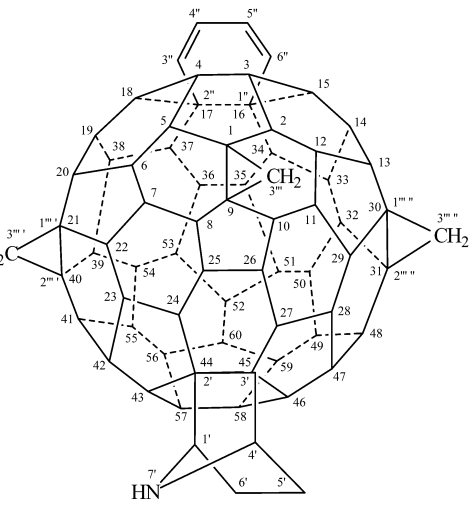

VI

V 3‴*H*,3‴′*H*,3‴″*H*-Dibenzo[16,17:44,45]tricyclopropa[1,9:21,40:30,31](C$_{60}$-*I*$_h$)[5,6]fullerene

VI 3‴*H*,3‴′*H*,3‴″*H*-[7]Azabicyclo[2.2.1]heptano[2′,3′:44,45]benzo[16,17]tricyclopropa-[1,9:21,40:30,31](C$_{60}$-*I*$_h$)[5,6]fullerene[y]

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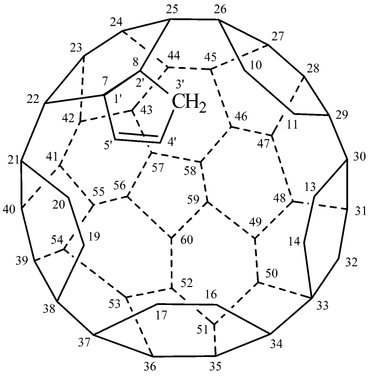
[x] The CA index name is [5,6]fullereno-C$_{60}$-*I*$_h$-[1″,9″:2,3;3″,15″:2′,3′]bis[1,4]diazabicyclo[2.2.2]oct[5]ene.

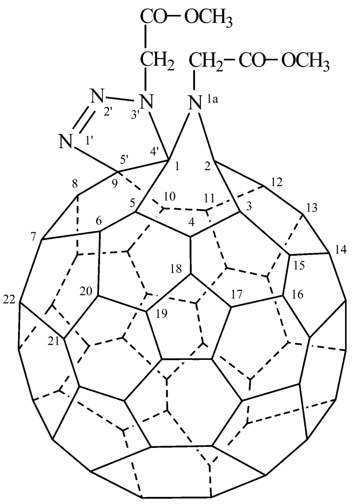
[y] The CA index name is 3′*H*,3″*H*,3‴*H*,3⁗*H*,3‴″*H*-Pentacyclopropa[1′,9′:16′,17′:21′,40′:30′,31′:44′,45′][5,6]fullereno-C$_{60}$-*I*$_h$-[52′,60′:2,4][1,4]diazabicyclo[2.2.2]octane.

The fusion principles described above for fullerenes are fully applicable to modified fullerenes.

Examples:



I



II

I 3′*H*-Cyclopenta[7,8]-1,2,3,4,5,6,9,12,15,18-decanor(C_{60}-I_h)[5,6]fullerene

II Dimethyl 2,2′-[1a*H*,3′*H*-[1,2,3]triazolo[4′,5′:1,9]-1a-aza-1(2)a-homo(C_{60}-I_h)[5,6]fullerene-1a,3′-diyl]diacetate

or

Dimethyl 1a*H*,3′*H*-[1,2,3]triazolo[4′,5′:1,9]-1a-aza-1(2)a-homo(C_{60}-I_h)[5,6]fullerene-1a,3′-diacetate (a conjunctive name)[z]

FU-8. BRIDGED FULLERENES

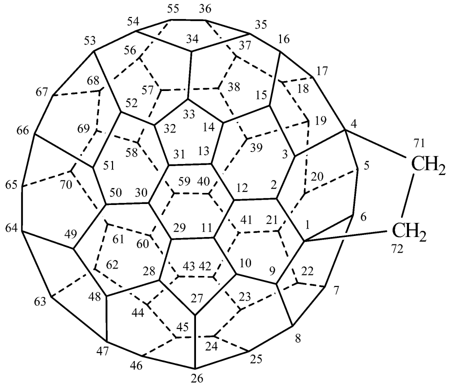
Bridges between nonadjacent atoms of a fullerene or modified fullerene are named and numbered according to established principles for bridged fused ring systems [9]. Numbering of bridge atoms begins with the number following the highest number of the fullerene and starts with the atom adjacent to the fullerene atom with the higher locant number.

Bridges between rings fused to a fullerene and a parent fullerene or between two different rings fused to the same fullerene are named using established bridge prefix names. In the latter case, citation of bridge components and numbering begins with the bridge atom adjacent to the fused component with the least primed numbers (the lower number) and continues with the next primed number following the highest primed number of the fused component.

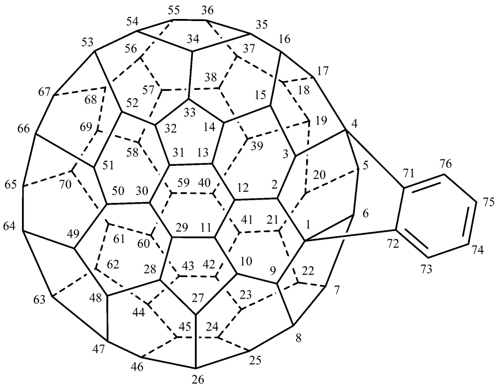
---

[z] The uninverted CA index name is Dimethyl 3′*H*-[1,2,3]triazolo[4′,5′:1,9]-2a-aza-1,2(2a)-homo[5,6][5,6]-fullerene-C_{60}-I_h-2a,3′-diacetate.

Examples:

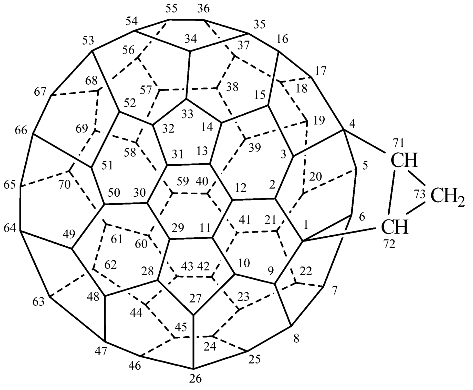


I

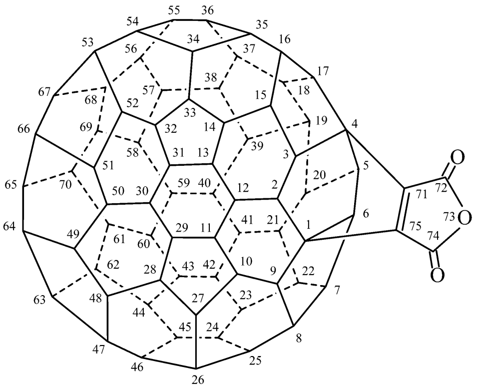


II

I 1,4-Ethano(C_{70}-$D_{5h(6)}$)[5,6]fullerene
II 1,4-[1,2]Benzeno(C_{70}-$D_{5h(6)}$)[5,6]fullerene[aa]



III



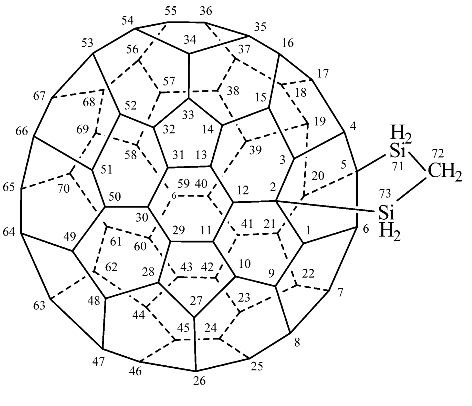
IV

III 72,73-Dihydro-71*H*-1,4-epicyclopropa(C_{70}-$D_{5h(6)}$)[5,6]fullerene[bb]
IV 1,4-[3,4]Furano(C_{70}-$D_{5h(6)}$)[5,6]fullerene-72,74-dione[cc]

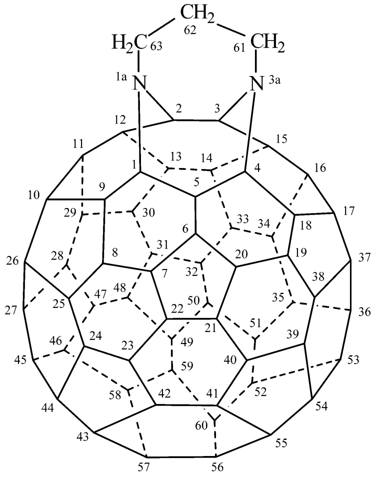
[aa] The CA index name is 1,4[1′,2′]-Benzeno[5,6]fullerene-C_{70}-$D_{5h(6)}$

[bb] The uninverted CA index name is 72,73-Dihydro-71*H*-1,4-*endo*-cyclopropa[5,6]fullerene-C_{70}-$D_{5h(6)}$.

[cc] The CA index name is 1,4[3′,4′]-Furano[5,6]fullerene-C_{70}-$D_{5h(6)}$-72,74-dione.

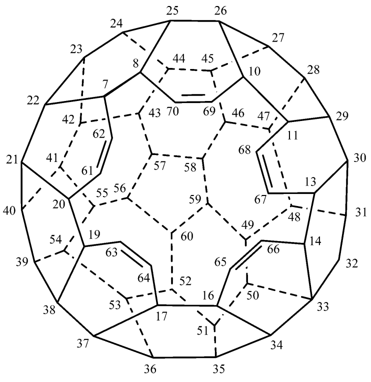


V

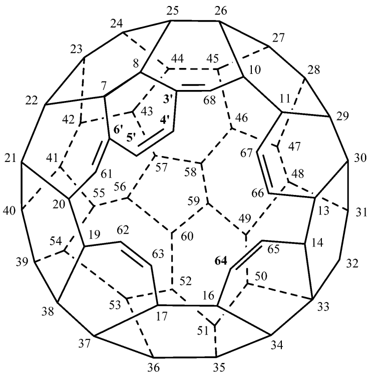


VI

V 2,5-(Silanomethanosilano)(C_{70}-$D_{5h(6)}$)[5,6]fullerene
VI 1a,3a-Propano-1a,3a-diaza-1(2)a:3(4)a-dihomo(C_{60}-I_h)[5,6]fullerene[dd]



VII[ee]



VIII[ee]

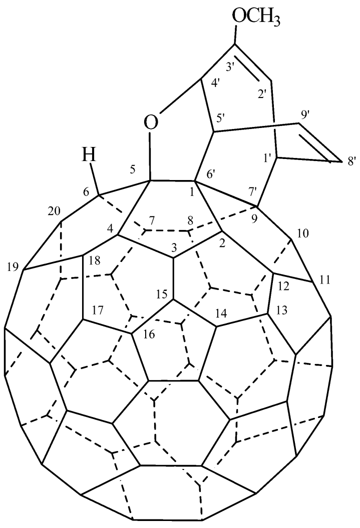
VII 7,20:8,10:11,13:14,16:17,19-Pentaetheno-1,2,3,4,5,6,9,12,15,18-decanor(C_{60}-I_h)-[5,6]fullerene

VIII 11,13:14,16:17,19-Trietheno-3′,10:6′,20-dimethenobenzo[7,8]-1,2,3,4,5,6,9,12,15,18-decanor(C_{60}-I_h)[5,6]fullerene[ff]

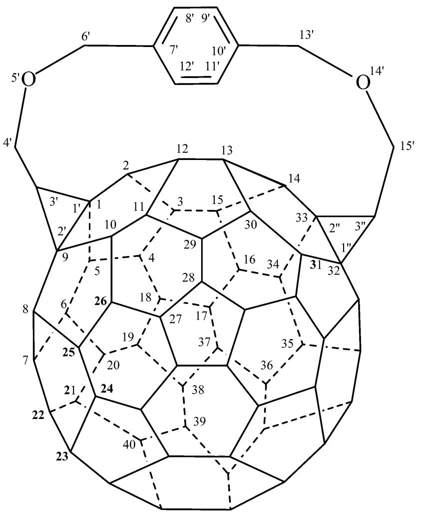
[dd] The CA index name is 3a,5a-Propano-3a,5a-diaza-1,5(5a):2,3(3a)-dihomo[5,6]fullerene-C_{60}-I_h.

[ee] Double bonds are shown here for illustrative purposes only. Double bonds are not normally shown in fullerene, fulleroid, or fullerene component structures in these recommendations.

[ff] The current CA index name is 6,7(7a):8,9(9a):11,12(12a):14,15(15a):17,18(18a)-Pentahomo-1,2,3-trinor[5,6]fullerene-C_{60}-I_h.



IX



X

IX 3′-Methoxy-6*H*-4′,5-epoxybicyclo[3.2.2]nona[2,8]dieno[6′,7′:1,9](C_{60}-I_h)[5,6]fullerene

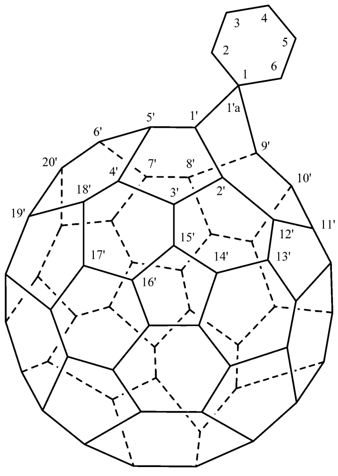
X 3′,3″-(Methanooxymethano[1,4]benzenomethanooxymethano)-3′*H*,3″*H*-dicyclopropa-[1,9:32,33](C_{60}-I_h)[5,6]fullerene

FU-9. SPIRO FULLERENES

Fullerenes cannot themselves form spiro compounds directly and, as mentioned earlier, spiro ring systems are **not** to be used as fusion components with fullerenes.

Spiro fullerenes formed from homofullerenes and fullerenes fused to organic rings follow the normal procedures for naming organic spiro systems that contain at least one polycyclic ring system [11]. Spiro fullerene parent hydrides will not necessarily have unprimed numbers as locants.

Examples:



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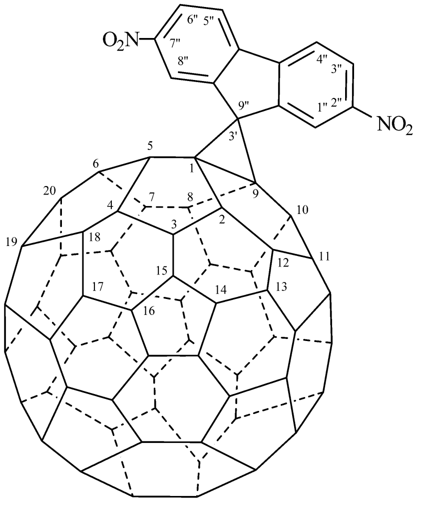
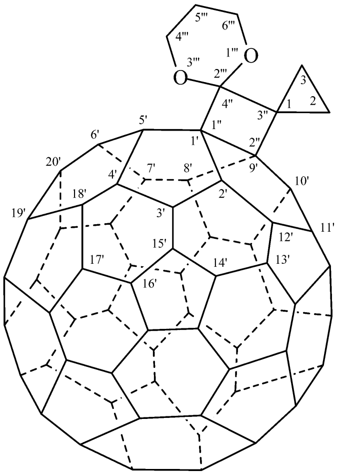


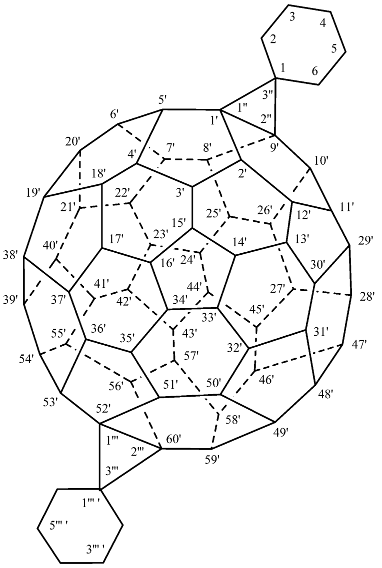
II

I Spiro[cyclohexane-1,1′a-[1(9)a]homo(C_{60}-I_h)[5,6]fullerene]

II 2″,7″-Dinitrospiro[cyclopropa[1,9](C_{60}-I_h)[5,6]fullerene-3′,9″-fluorene]



III



IV

III Dispiro[cyclopropane-1,3″-cyclobuta[1,9](C$_{60}$-I_h)[5,6]fullerene-4″,2‴-[1,3]dioxane]

IV Dispiro[cyclohexane-1,3″-]dicyclopropa[1,9:52,60](C$_{60}$-I_h)[5,6]fullerene-3‴,1‴ ′-cyclohexane]

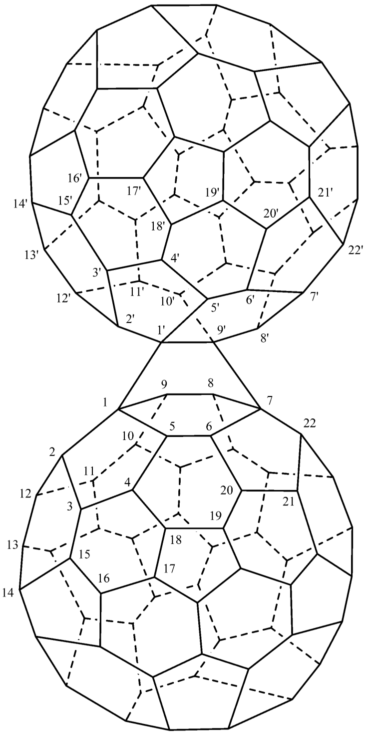
FU-10. FULLERENE STRUCTURES WITH TWO FULLERENE COMPONENTS

Fullerenes and/or fulleroids can be combined together in a variety of ways to form very large structures that can be described by extending, adapting, or modifying existing principles of organic nomenclature.

Fu-10.1 Bridged and fused two-component fullerenes

One fullerene can be considered as bridging another fullerene, or be connected to another by a non-fullerene fusion component, or be part of a fusion component.

Examples:



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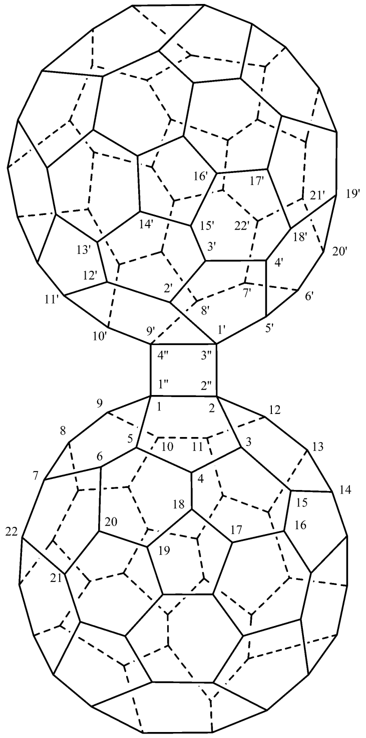
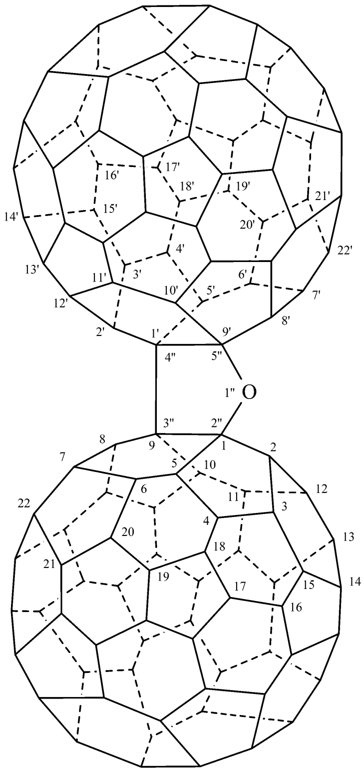


II

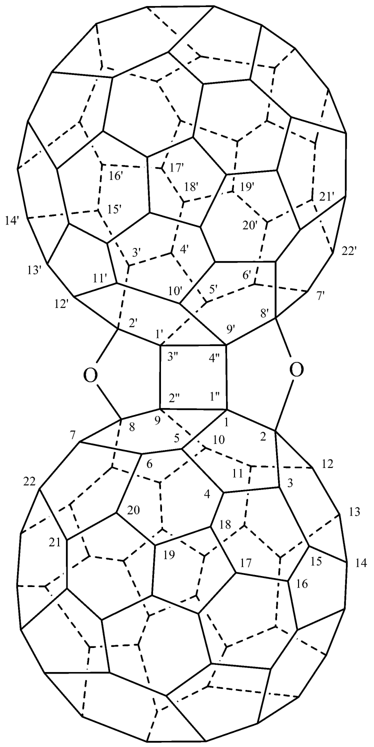
I 1,7-([1,9]Epi(C_{60}-I_h)[5,6]fullereno)(C_{60}-I_h)[5,6]fullerene[gg]
[a (C_{60}-I_h)[5,6]fullerene bridging another (C_{60}-I_h)[5,6]fullerene]

II Cyclobuta[1″,2″:1,2;3″,4″:1′,9′]di(C_{60}-I_h)[5,6]fullerene
[two (C_{60}-I_h)[5,6]fullerenes joined by a fused cyclobutane ring]

[gg] A bridging fullerene is not renumbered; therefore its locants are primed.



III

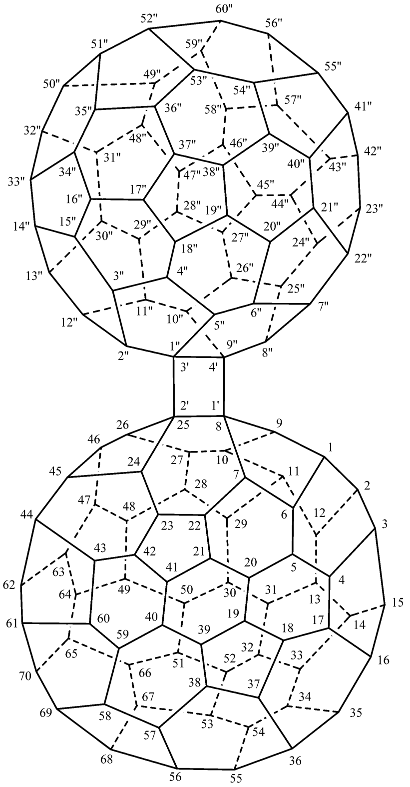


IV

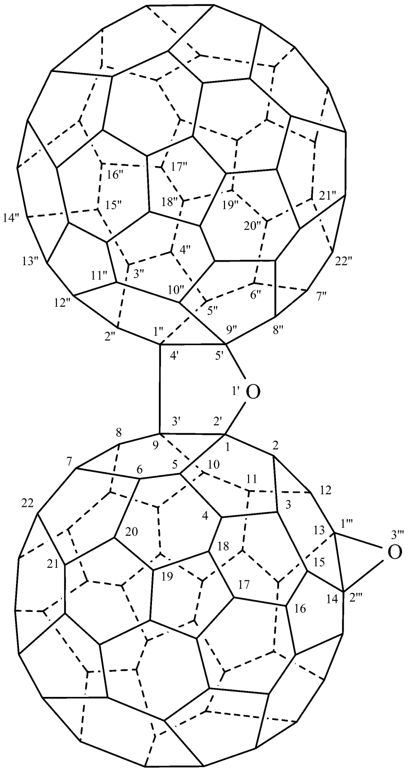
III Furano[2″,3″:1,9;4″,5″:1′,9′]di(C_{60}-I_h)[5,6]fullerene[hh]
[two (C_{60}-I_h)[5,6]fullerenes joined by a fused furan ring]

IV 2,8′:2′,8-Diepoxycyclobuta[1″,2″:1,9;3″,4″:1′,9′]di(C_{60}-I_h)[5,6]fullerene
[two bridges between two (C_{60}-I_h)[5,6]fullerenes joined by a fused cyclobutane ring]

[hh] The CA index name is Di[5,6]fullereno-C_{60}-I_h-[1,9-*b*:1′,9′-*d*]furan



V



VI

V $(C_{60}\text{-}I_h)$[5,6]Fullereno[1″,9″:3′,4′]cyclobuta[1′,2′:8,25]$(C_{70}\text{-}D_{5h(6)})$fullerene[ii]
[a $(C_{60}\text{-}I_h)$[5,6]fullerene joined to a $(C_{70}\text{-}D_{5h(6)})$fullerene by a fused cyclobutane ring]

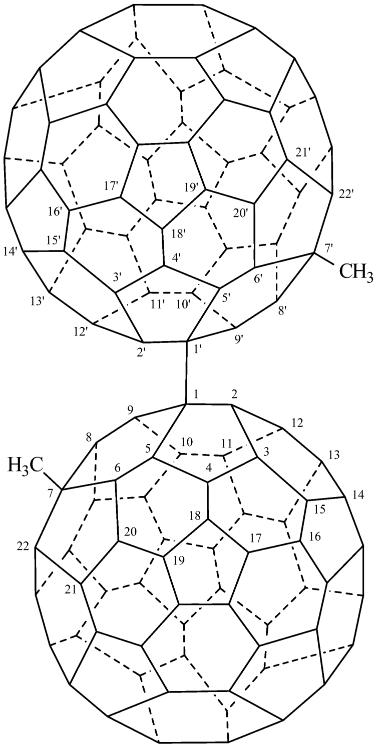
VI $(C_{60}\text{-}I_h)$[5,6]Fullereno[1″,9″:4′,5′]furano[2′,3′:1,9]oxireno[13,14]$(C_{60}\text{-}I_h)$[5,6]fullerene[ii]
[a $(C_{60}\text{-}I_h)$[5,6]fullerenofuran fused system and an oxireno ring fused to a $(C_{60}\text{-}I_h)$-[5,6]fullerene]

Fu-10.2 Fullerene ring assemblies

Two identical fullerenes or modified fullerenes joined by a single or double bond can be named by ring assembly nomenclature [8b]. Two different fullerenes are named by substituting one fullerene structure by the other.

[ii] Since a fused fullerene structure is not renumbered, each component must be identified by appropriate primed numbers.

Examples:



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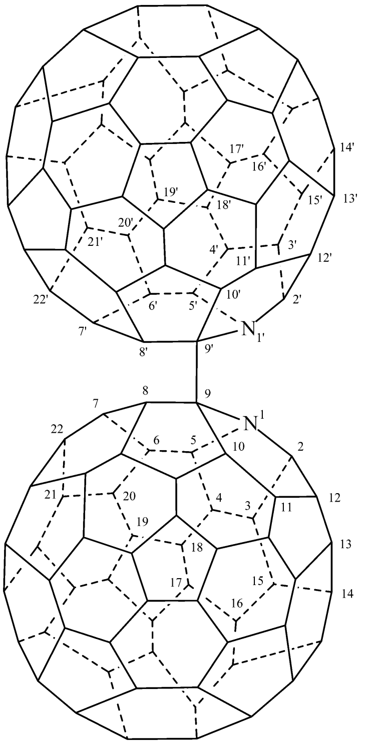
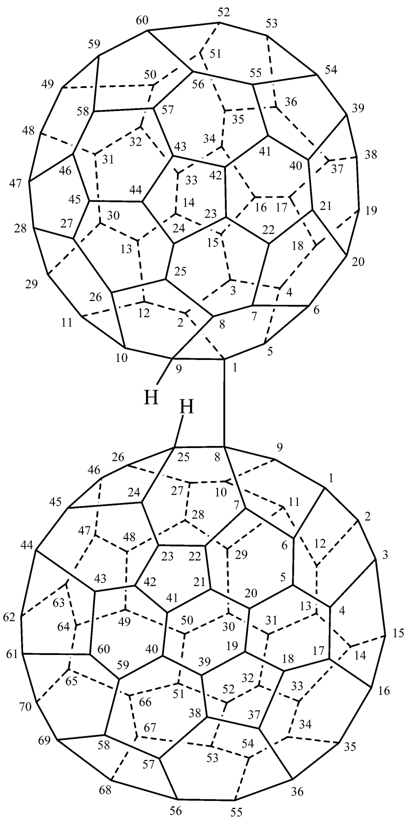


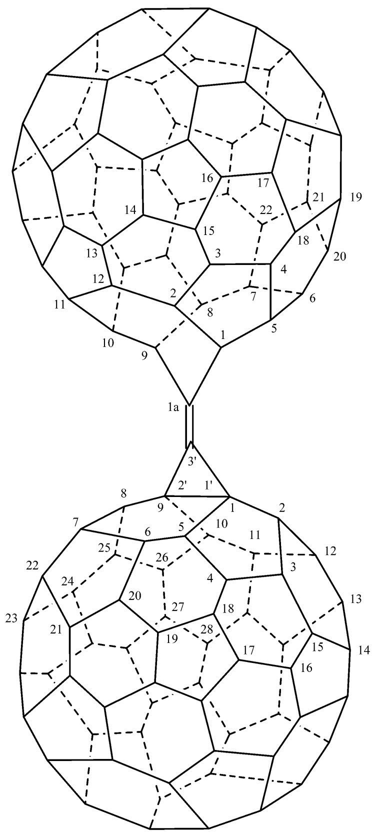
II

I 7,7′-Dimethyl-7*H*,7′*H*-1,1′-bi(C_{60}-I_h)[5,6]fullerene [a ring assembly name; two (C_{60}-I_h)[5,6]fullerenes linked by a single bond]

II 9,9′-Bi-1-aza(C_{60}-I_h)[5,6]fullerene [a ring assembly name; two 1-aza-(C_{60}-I_h)[5,6]-fullerenes linked by a single bond; although the name of the azafullerene is 9*H*-1-aza-(C_{60}-I_h)[5,6]fullerene, the ring assembly does not require citation of indicated hydrogen]



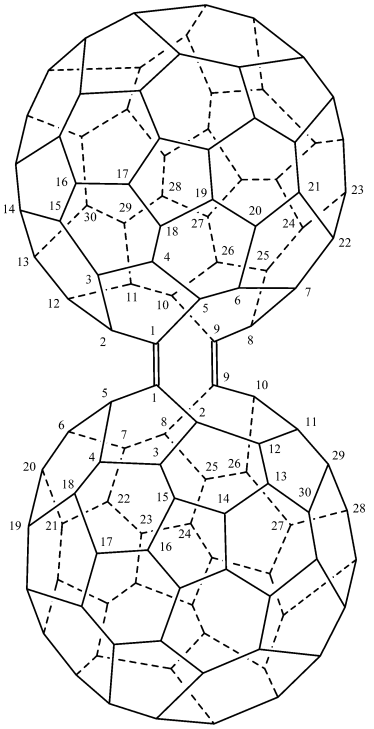
III



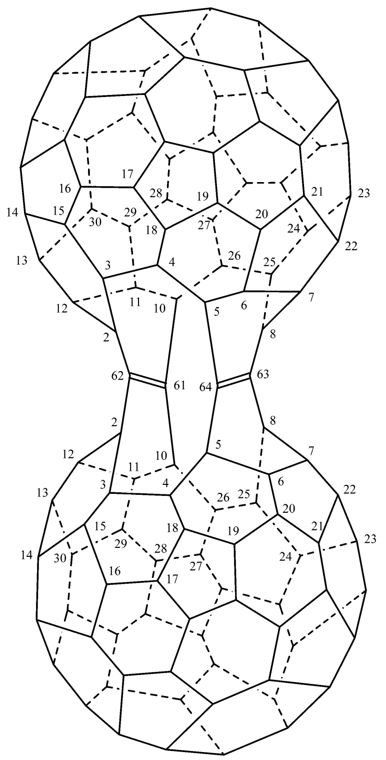
IV

III 8-[(C_{60}-I_h)[5,6]Fulleren-1(9*H*)-yl]-8,25-dihydro(C_{70}-$D_{5h(6)}$)[5,6]fullerene [a (C_{70}-$D_{5h(6)}$)fullerene substituted by a (C_{60}-I_h)[5,6]fullerene]

IV 3′-[1a*H*-1(9)a-Homo(C_{60}-I_h)[5,6]fulleren-1a-ylidene]-3′*H*-cyclopropa[1,9](C_{60}-I_h)[5,6]-fullerene [a cyclopropa(C_{60}-I_h)[5,6]fullerene substituted by a homo(C_{60}-I_h)[5,6]-fullerene; the cyclopropa(C_{60}-I_h)[5,6]fullerene is preferred on the basis of more rings]



V



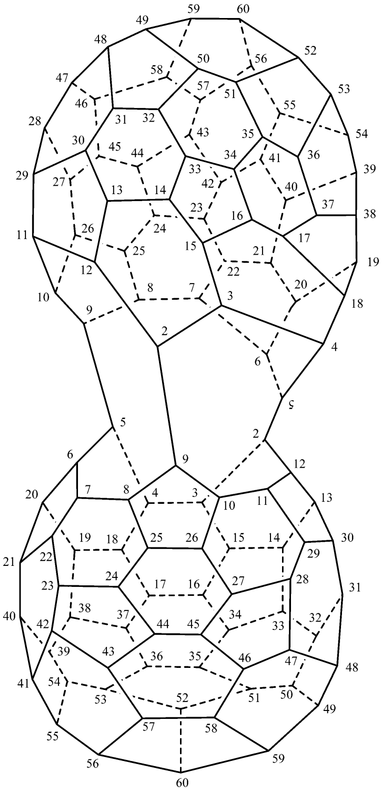
VI

V 1,9-[1,9-Seco(C_{60}-I_h)[5,6]fullerene-1,9-diylidene]-1,9-seco(C_{60}-I_h)[5,6]fullerene [a seco(C_{60}-I_h)[5,6]fullerene substituted by an identical seco(C_{60}-I_h)[5,6]fullerene or a seco(C_{60}-I_h)[5,6]fullerene bridged by an identical seco(C_{60}-I_h)[5,6]fullerene]

VI 61,63,64,62-(1,9-Dinor(C_{60}-I_h)[5,6]fullerene-2,5,8,10-tetrayl)-2,10:5,8-bis(ethene-1,2-diyl)-1,9-dinor(C_{60}-I_h)[5,6]fullerene [a bis(ethenediyl) bridged 1,9-dinor(C_{60}-I_h)[5,6]-fullerene substituted by a 1,9-dinor(C_{60}-I_h)[5,6]fullerene]

or

2,10:2′,10′;5,8:5′,8′-Bis(ethene-1,1:2,2-tetrayl)bis[1,9-dinor(C_{60}-I_h)[5,6]fullerene] [two dinor(C_{60}-I_h)[5,6]fullerenes bridged by two ethenetetrayl groups]



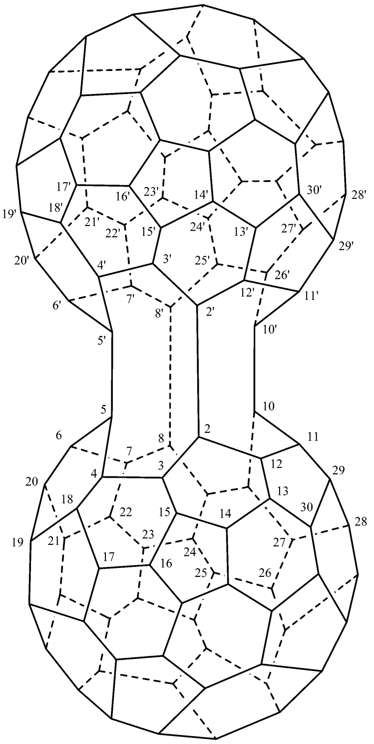
VII

VII 2,5,9-[1-Nor(C_{60}-I_h)[5,6]fullerene-2,5,9-triyl]-1-nor(C_{60}-I_h)[5,6]fullerene
[a 1-nor(C_{60}-I_h)[5,6]fullerene substituted by a 1-nor(C_{60}-I_h)[5,6]fullerene or a 1-nor-(C_{60}-I_h)[5,6]fullerene bridging a 1-nor(C_{60}-I_h)[5,6]fullerene]

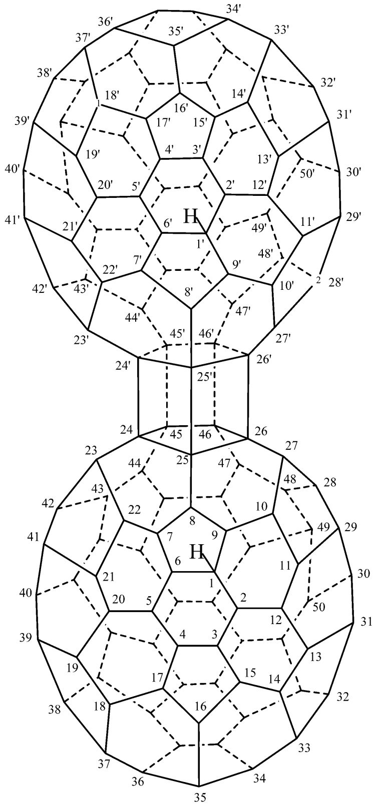
Fu-10.3 Fullerene ring assemblies plus the prefix 'cyclo'

Some two-component fullerenes with multiple connecting bonds can be named conveniently as ring assemblies with other connecting bonds denoted by the prefix 'cyclo'.

Examples:



I



II

I 5,5′:8,8′:10,10′-Tricyclo-2,2′-bi-1,9-dinor(C_{60}-I_h)[5,6]fullerene [a ring assembly name for two 1,9-dinor(C_{60}-I_h)[5,6]fullerenes plus three additional single bonds designated by the structure modifying prefix 'cyclo']

or

2,5,8,10-[1,9-Dinor(C_{60}-I_h)[5,6]fullerene-2,5,8,10-tetrayl]-1,9-dinor(C_{60}-I_h)[5,6]fullerene [a 1,9-dinor(C_{60}-I_h)[5,6]fullerene substituted or bridged by another 1,9-dinor(C_{60}-I_h)-[5,6]fullerene]

II 1*H*,1′*H*-25,25′:26,26′:45,45′:46,46′-Tetracyclo-24,24′-bi(C_{70}-$D_{5h(6)}$)[5,6]fullerene [a ring assembly name between two (C_{70}-$D_{5h(6)}$)[5,6]fullerenes plus four additional single bonds designated by the structure modifying prefix 'cyclo']

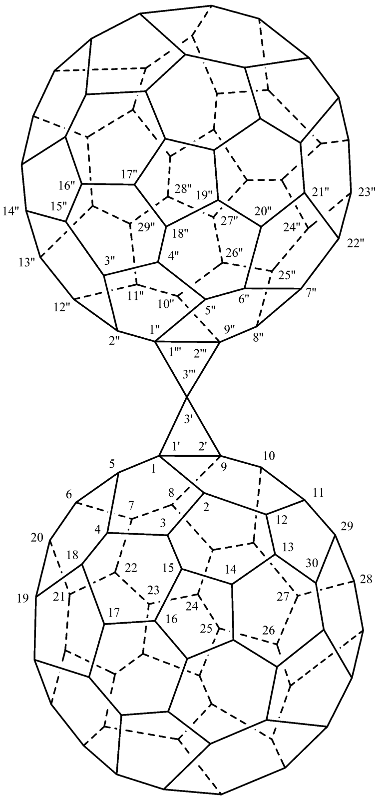
or

1*H*,1′*H*-Hexacyclo[4.4.0.$0^{2,5}$.$0^{3,9}$.$0^{4,8}$.$0^{7,10}$]decano[1″,2″,3″,9″,10″:24,25,26,46,45;-4″,5″,6″,7″,8″:24′,25′,26′,46′,45′]di(C_{70}-D_{5h})[5,6]fullerene [two (C_{70}-$D_{5h(6)}$)[5,6]fullerenes joined by the von Baeyer ring system hexacyclo[4.4.0.$0^{2,5}$.$0^{3,9}$.$0^{4,8}$.$0^{7,10}$]decane]

Fu-10.4 Spiro homo and fused ring fullerenes

Spiro homo and fused ring fullerenes are named by the established nomenclature for spiro ring systems containing at least one polycyclic ring system [11].

Examples:



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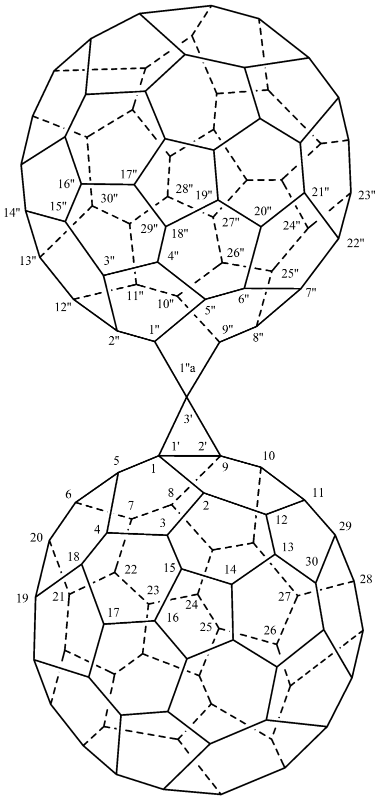


II

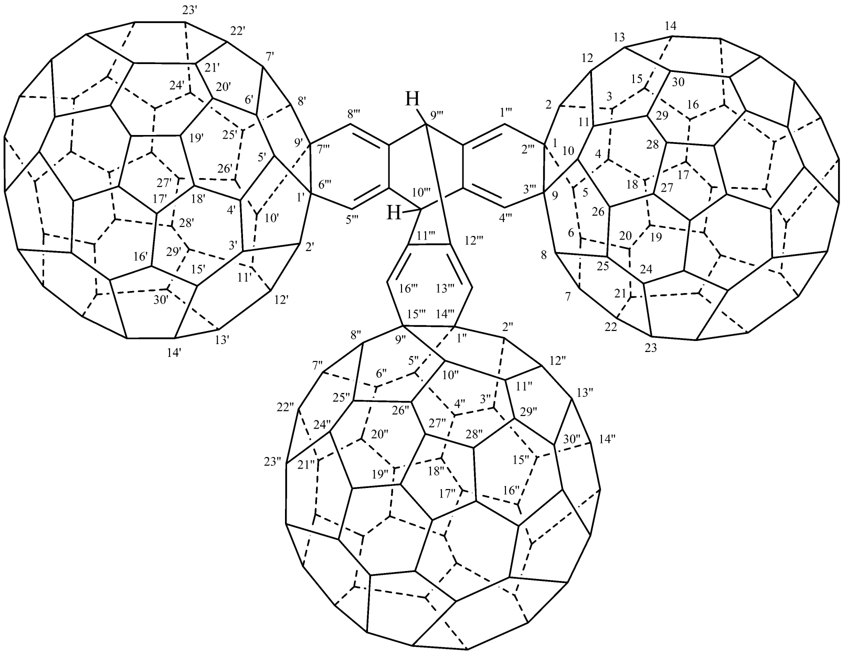
I 3′,3‴-Spirobi[cyclopropa[1,9](C_{60}-I_h)[5,6]fullerene] [two cyclopropa(C_{60}-I_h)[5,6]fullerenes linked by a spiro fusion]

II Spiro[3′*H*-cyclopropa[1,9](C_{60}-I_h)[5,6]fullerene-3′,1″a-[1(9)a]homo(C_{60}-I_h)[5,6]fullerene] [a cyclopropa(C_{60}-I_h)[5,6]fullerene spiro fused to a homo-(C_{60}-I_h)[5,6]fullerene]

FU-11. FULLERENE STRUCTURES WITH THREE OR MORE FULLERENE COMPONENTS

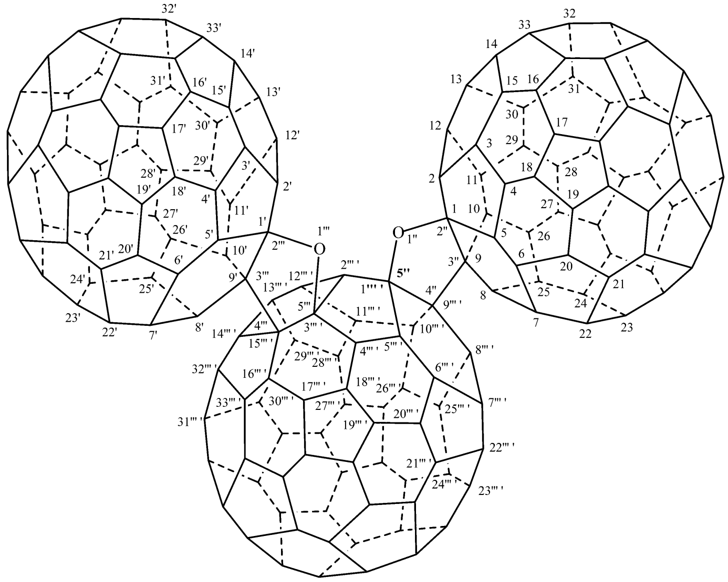
Fullerene structures with three or more components can be named by fusion principles, bridging principles, ring assembly nomenclature coupled with the structure modifying prefix ‘cyclo’, or by phane nomenclature [12].

Examples:

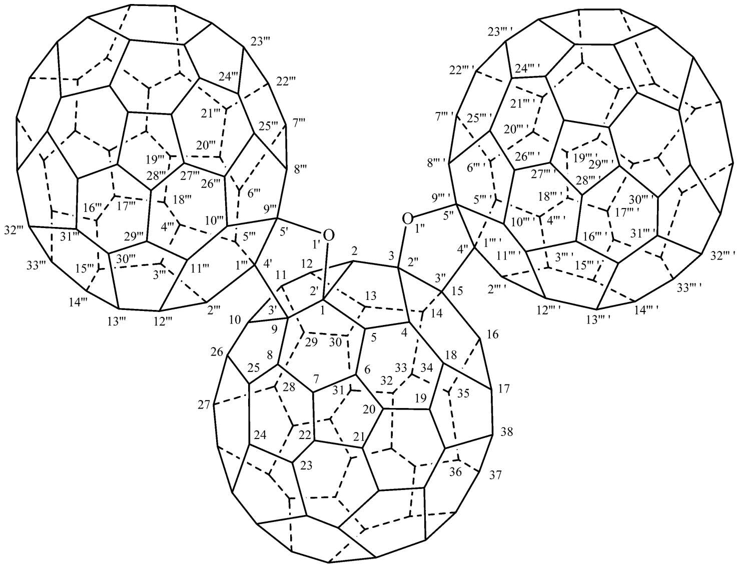


I

I 9‴*H*,10‴*H*-9,10-[1,2]Benzenoanthraceno[2‴,3‴:1,9;6‴,7‴:1′,9′;14‴,15‴:1″,9″]-tri(C_{60}-I_h)[5,6]fullerene [three (C_{60}-I_h)[5,6]fullerenes joined by the bridged fused ring system 9,10-[1,2]benzenoanthracene]



IIa

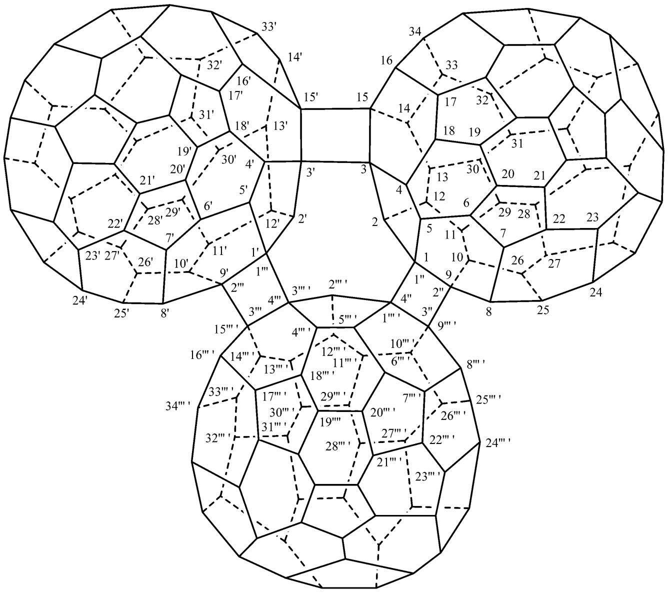


IIb

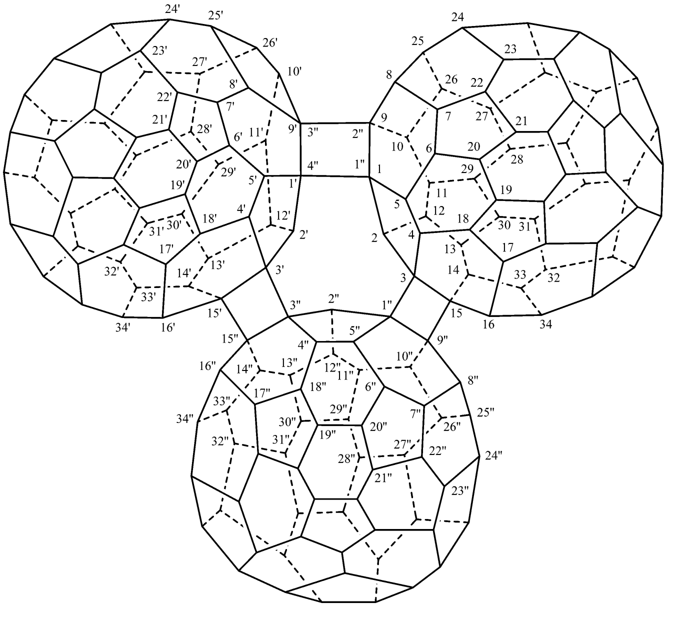
IIa (C$_{60}$-I_h)[5,6]Fullereno[9‴′,1‴′:4″,5″;15‴′,3‴′:4‴,5‴]difurano[2″,3″:1,9;2‴,3‴:1′,9′]di-(C$_{60}$-I_h)[5,6]fullerene[jj] [three (C$_{60}$-I_h)[5,6]fullerenes connected by two furan rings; a fusion name based on the terminal fullerenes]

IIb Bis[(C$_{60}$-I_h)[5,6]fullereno[1‴,9‴:4′,5′]furano[2′,3′:1,9;2″,3″:3,15]](C$_{60}$-I_h)[5,6]fullerene [three (C$_{60}$-I_h)[5,6]fullerenes connected by two furan rings; a fusion name based on the central fullerene)

[jj] The CA index name is based on furan, i.e., Di[5,6]fullereno-C$_{60}$-I_h-[1,9-*d*:1′,9′-*d*′]fullereno-C$_{60}$-I_h-[1,9-*b*:3,15-*b*′]difuran.



IIIa



IIIb

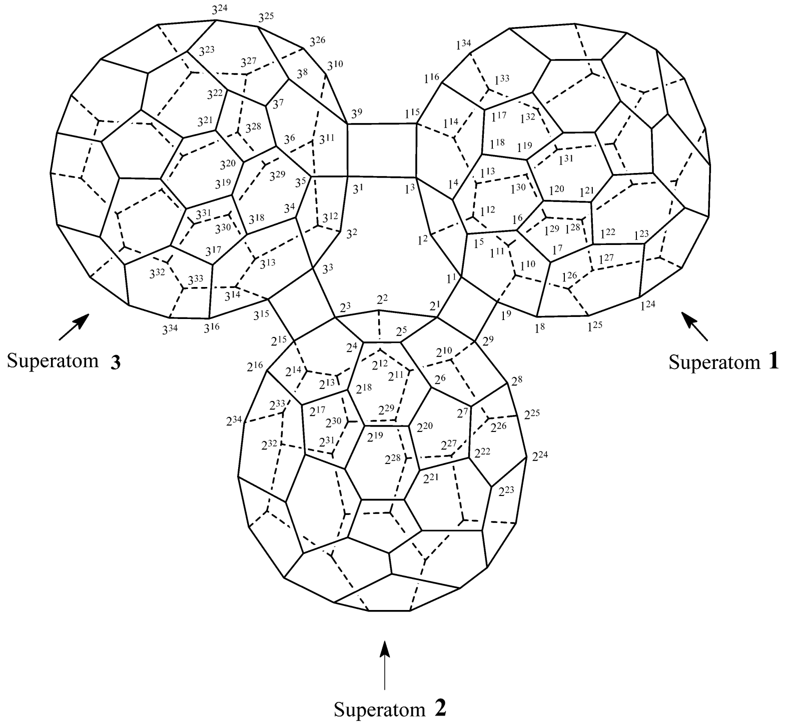
III This tricomponent fullerene structure cannot be named by fusion principles; nevertheless, there are three potential ways to name it.

1. Combine a fusion name for three (C_{60}-I_h)[5,6]fullerenes joined by two fused cyclobutane rings with the structure modifying prefix ‘cyclo’: 3,3′:15,15′-Dicyclo(C_{60}-I_h)[5,6]fullereno[9‴′,1‴′:3″,4″;15‴′,3‴′:3‴,4‴]dicyclobuta[1″,2″:1,9;1‴,2‴:1′,9′]di(C_{60}-I_h)[5,6]fullerene (**IIIa**) [three (C_{60}-I_h)[5,6]fullerenes connected by two cyclobutane rings; a fusion name based on

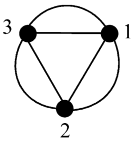
terminal fullerenes plus two additional single bonds denoted by the structure-modifying prefix 'cyclo']

2. Cite one fullerene as a bridge between the other two fullerenes fused together by a cyclobutane ring: 3,3′,15,15′-([1,3,9,15]Epi(C_{60}-I_h)[5,6]fullereno)cyclobuta[1″,2″:1,9;4″,3″:1′,9′]di(C_{60}-I_h)[5,6]fullerene (**IIIb**) [the bridging fullerene utilizes primed numbering, in this case double primes]

3. Adapt phane nomenclature [12] as follows (**IIIc**):

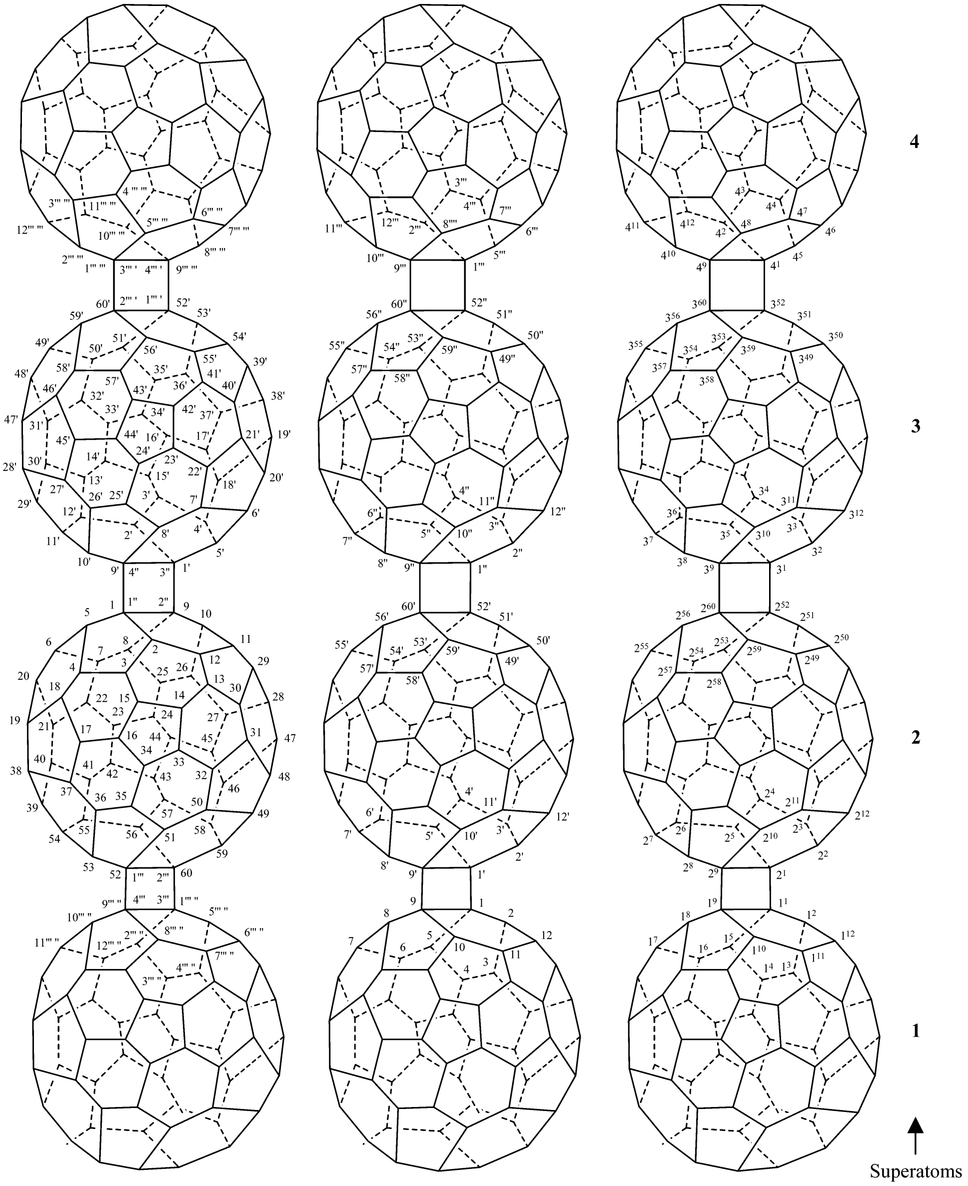


IIIc



Simplified Phane Parent
Hydride Skeleton
● = superatom

IIIc 1,2,3(1,9,3,15)-Tri(C_{60}-I_h)[5,6]fullerenatetracyclo[1.0.0.0^{1,2}.0^{2,3}]triphane



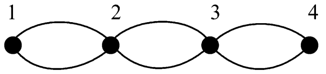
IVa **IVb** **IVc**

IV There are three ways to name this multicomponent fullerene consisting of four fullerenes interconnected by three cyclobutane rings.

1. Fused ring nomenclature: Bis[(C_{60}-I_h)[5,6]fullereno[1⁗,9⁗:3‴,4‴]cyclobuta[1‴,2‴:52,60]]cyclobuta[1″,2″:1,9;3″,4″:1′,9′]di(C_{60}-I_h)[5,6]fullerene **(IVa)** [two (C_{60}-I_h)[5,6]fullerenocyclobuta components fused to a cyclobutadi(C_{60}-I_h)[5,6]fullerene]

2. Ring assembly nomenclature plus ‘cyclo’: 9,9′:60′,9″:60″:9‴-Tricyclo-1,1′:52′,1″:52″,1‴-quater-(C_{60}-I_h)[5,6]fullerene **(IVb)** [a ring assembly name between four (C_{60}-I_h)[5,6]fullerenes plus three additional single bonds denoted by the structure-modifying prefix ‘cyclo’]

3. An adaptation of phane nomenclature [12]; see **IVc** above and the following:



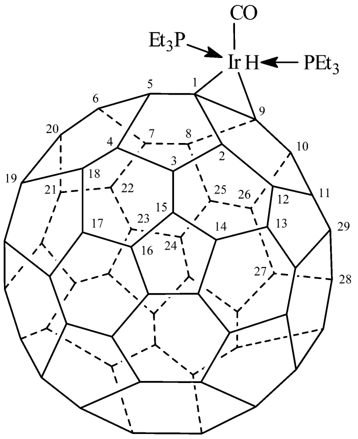
Simplified Phane Parent
Hydride Skeleton
● = superatom

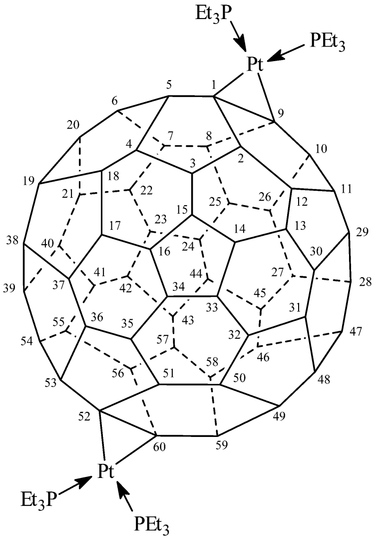
IVc 1,4(1,9),2,3(1,9,52,60)-Tetra(C_{60}-I_h)[5,6]fullerenadispiro[$1.0.1^3.0^2$]tetraphane

FU-12. FULLERENES IN COORDINATION COMPOUNDS

Principles of coordination nomenclature [13] are applied in naming fullerenes and fulleroids externally associated with metal atoms for which replacement nomenclature is not permitted.

Examples:

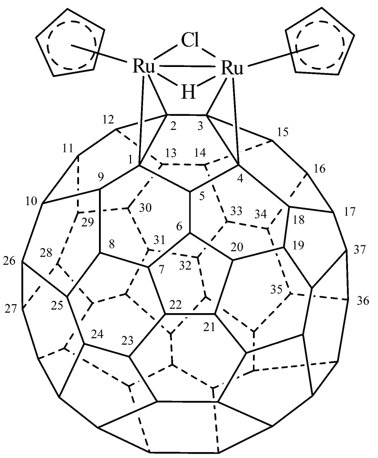




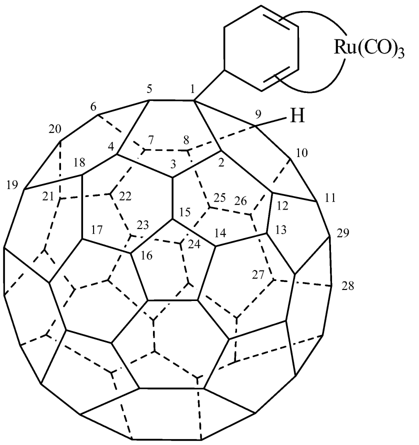
I **II**

I Carbonyl[(1,9-η)-(C_{60}-I_h)[5,6]fullerene]hydrobis(triethylphosphane)iridium

II {μ-[(1,9-η:52,60-η)-(C_{60}-I_h)[5,6]Fullerene]}-bis[bis(triethylphosphane)platinum]



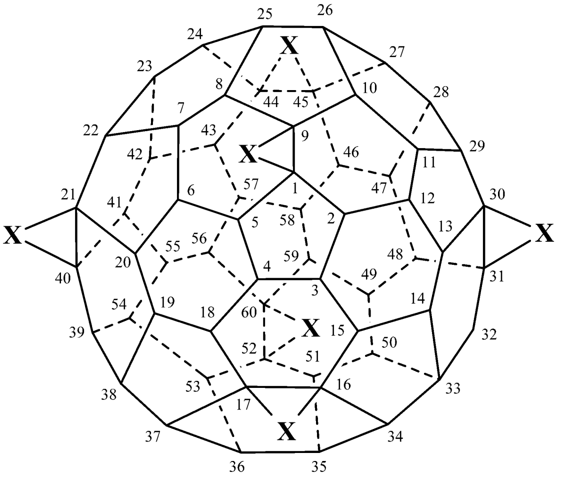
III



IV

III μ-Chloro-{μ-[(1,2-η:3,4-η)-(C_{60}-I_h)[5,6]fullerene]}-μ-hydro-bis(η^5-cyclopentadienyl-ruthenium)(*Ru–Ru*)

IV Tricarbonyl{1-[(2,3,4,5-η)-cyclohexa-2,4-dien-1-yl]-1,9-dihydro-(C_{60}-I_h)[5,6]fullerene}-ruthenium



V [**X** = Pd(PEt_3)]

V {[μ_6-(1,9-η:16,17-η:21,40-η:30,31-η:44,45-η:52,60-η)]-(C_{60}-I_h)[5,6]Fullerene}-hexakis[bis(triethylphosphane)palladium]

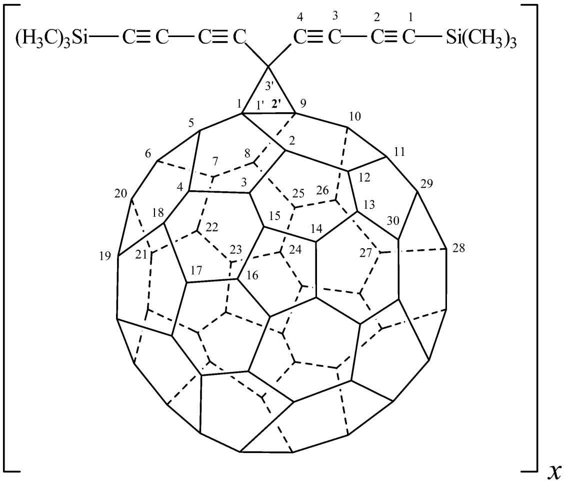
or

{[μ_6-(1,9-η:16,17-η:21,40-η:30,31-η:44,45-η:52,60-η)]-(C_{60}-I_h)[5,6]Fullerene}-dodecakis(triethylphosphane)hexapalladium

FU-13. FULLERENES IN POLYMERS

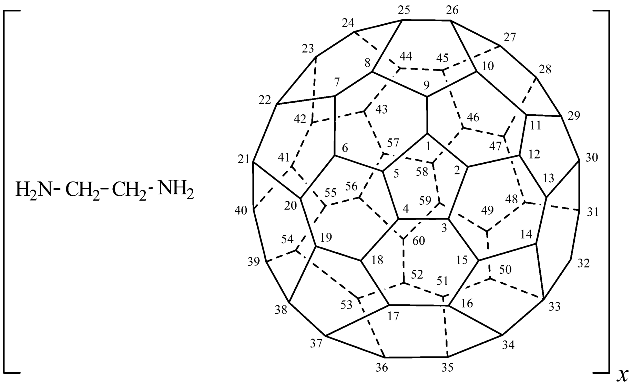
Polymers containing fullerenes are named in accordance with source-based [14] and structure-based [15] nomenclature principles for naming organic polymers.

Examples:[kk]



I A homopolymer

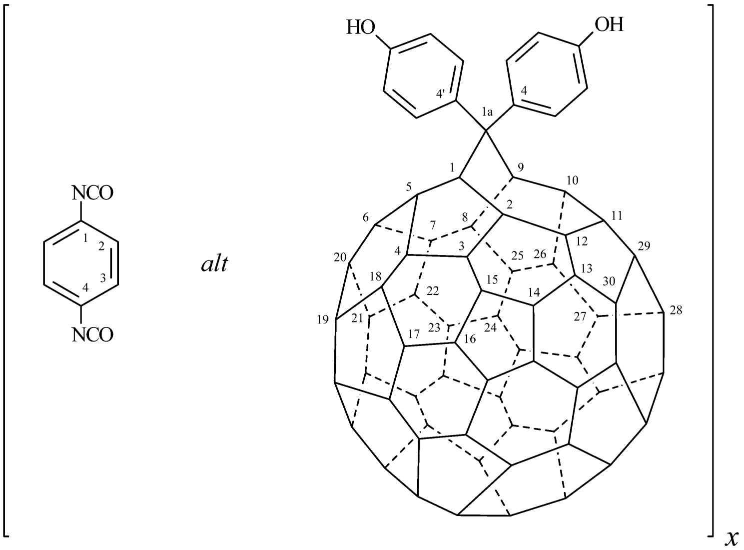
Poly{[3′*H*-cyclopropa[1,9](C_{60}-I_h)[5,6]fullerene-3′,3′-diyldibuta-1,3-diyne-4,1-diyl]-bis(trimethylsilane)} (a source-based name)



II A copolymer

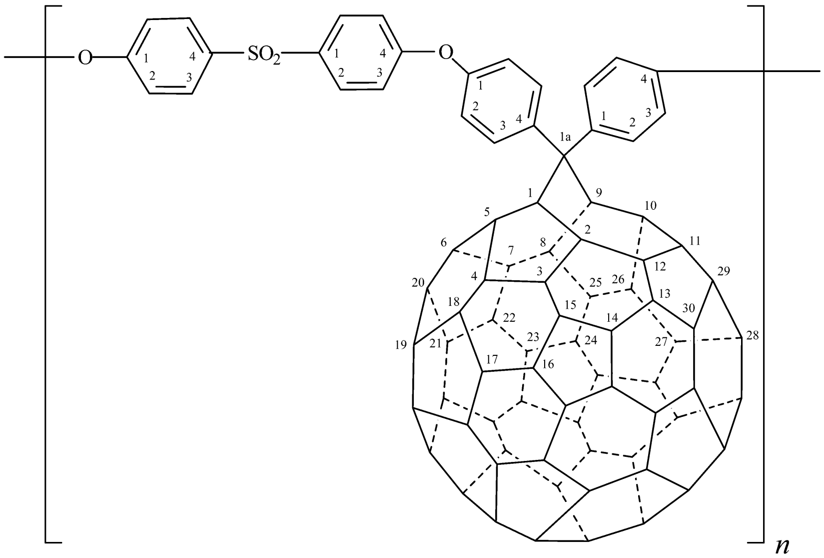
Poly[ethane-1,2-diamine-*co*-(C_{60}-I_h)[5,6]fullerene] (a source-based name)

[kk] There are no specific IUPAC recommendations for drawing source-based polymer structures. The structures in this section follow conventions adopted by CAS.



III An alternating copolymer

Poly[4,4′-1a*H*-1(9)a-homo(C_{60}-I_h)[5,6]fullerene-1a,1a-diyldiphenol-*alt*-1,6-diisocyanatohexane] (a source based name)

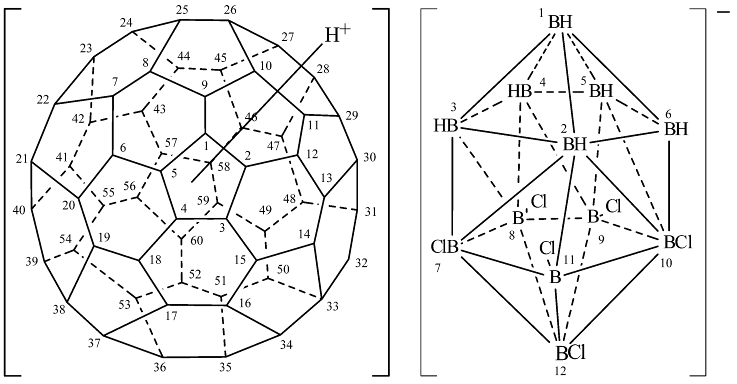


IV A polymer constitutional repeating unit (CRU)

Poly[oxy-1,4-phenylenesulfonyl-1,4-phenyleneoxy-1,4-phenylene-1a*H*-1(9)a-homo-(C_{60}-I_h)[5,6]fullerene-1a,1a-diyl-1,4-phenylene] (a structure-based name)

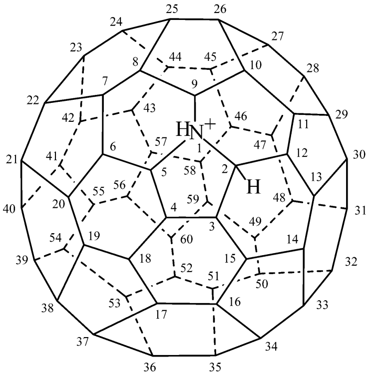
FU-14. FULLERENE CATIONS

Cations formed by the addition of a proton to a fullerene, a fullerene analog, or a fullerene derivative are named by replacing the final ‘e’ of the name of the fullerene with ‘-ium’ or by replacement nomenclature.

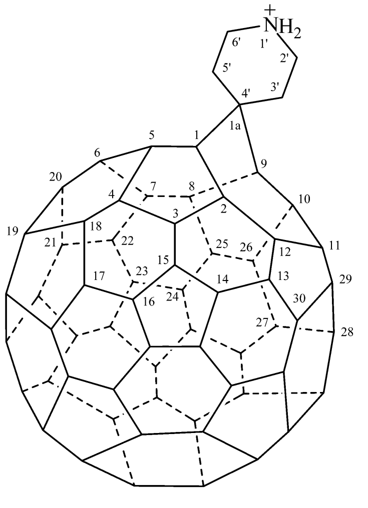


I

I (C_{60}-I_h)[5,6]Fullerenium hexachlorocarbadodecaborate(1−)



II



III

II 2*H*-1-Aza(C_{60}-I_h)[5,6]fulleren-1-ium *or* 1,2-Dihydro-1-azonia(C_{60}-I_h)[5,6]fullerene
III Spiro[1(9a)-homo(C_{60}-I_h)[5,6]fullerene-1a,4′-piperidin]-1′-ium

FU-15. FULLERENE RADICAL IONS

Radical ions formed by the addition of an electron to, or removal of an electron from, the fullerene cage are named by replacing the final ‘e’ of the fullerene name by ‘-elide’, ‘bis(elide)’, etc., or ‘-elium’, ‘bis(elium)’, etc.

Examples:

$[C_{60}]^{\bullet -}$	(C_{60}-I_h)[5,6]Fullerenelide
$[C_{60}]^{\bullet +}$	(C_{60}-I_h)[5,6]Fullerenelium

FU-16. METAL DERIVATIVES OF FULLERENES

The symbol @ and the term incarcerane have been widely used to describe fullerenes having an enclosed component, for example, La@C_{60}. The infix *incar* is used to name a fullerene containing an enclosed element. In the formula encapsulation is denoted by an italic *i* placed to the left of the incarcerated element.

Examples:

*i*La[C_{60}-I_h]	(C_{60}-I_h)[5,6]Fullerene-*incar*-lanthanum
	Lanthanum-*incar*-(C_{60}-I_h)[5,6]fullerene

The number of encapsulated metal atoms can be indicated in the formula, even fractional ones, but this must also be incorporated in the name. CAS treats these compositions as 'comp. (compound) with' at the name of the fullerene; the ratio of fullerene to the metal is given in parentheses. The charge distribution between the fullerene and the metal may be indicated by citing the oxidation state of the metal.

Examples:

iLa_2[C_{60}-I_h]	(C_{60}-I_h)[5,6]Fullerene-*incar*-dilanthanum[ll]
	Dilanthanum-*incar*-(C_{60}-I_h)[5,6]fullerene
*i*Ca(2+)$[C_{84}]^{2-}$	Calcium(2+)-*incar*-(C_{84})[5,6]fulleride(2–)
	(C_{84})[5,6]Fullerene-*incar*-calcium(2+)
*i*La(3+)$[C_{82}]^{3-}$	Lanthanum(3+)-*incar*-(C_{82})[5,6]fulleride(3–)
	(C_{82})[5,6]Fullerene-*incar*-lanthanum(3+)

When the metal is located outside the fullerene cage, the compound is named as a salt of the fullerene. The fullerene component name is fulleride and the charge corresponding to the number of metal cations is indicated by the appropriate negative charge enclosed in parentheses.

Example:

$K_3[C_{60}]$	Tripotassium (C_{60}-I_h)[5,6]fulleride(3–)

FU-17. CONFIGURATIONAL SPECIFICATION FOR THE C_{60}-I_h AND C_{70}-$D_{5h(6)}$ FULLERENES AND THEIR DERIVATIVES

The following recommendations deal only with configurational specification for the C_{60}-I_h and C_{70}-$D_{5h(6)}$ fullerenes and their derivatives. They are based on a publication by C. Thilgen, A. Herrmann, and F. Diederich [16].

Fu-17.1 Types of chiral fullerenes

Four types of chiral fullerenes and/or fullerene derivatives can be distinguished depending on the origin of their chirality. Although the discussion that follows concerns substituted fullerenes as described

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[ll] The CA index name is [5,6]fullerene-C_{60}-I_h compd. with lanthanum (1:2).

in Fu-6.2, it applies equally well to heterofullerenes and isotopically substituted fullerenes and their derivatives. Configurational specification for structurally modified fullerenes (fulleroids) is not discussed here; it will be considered in a later publication.

Type 1. **Inherently chiral** parent fullerenes. Since the C_{60}-I_h and C_{70}-$D_{5h(6)}$ parent fullerenes are not inherently chiral, they do not belong to this category. This type will only be illustrated here and more fully discussed in a later publication.

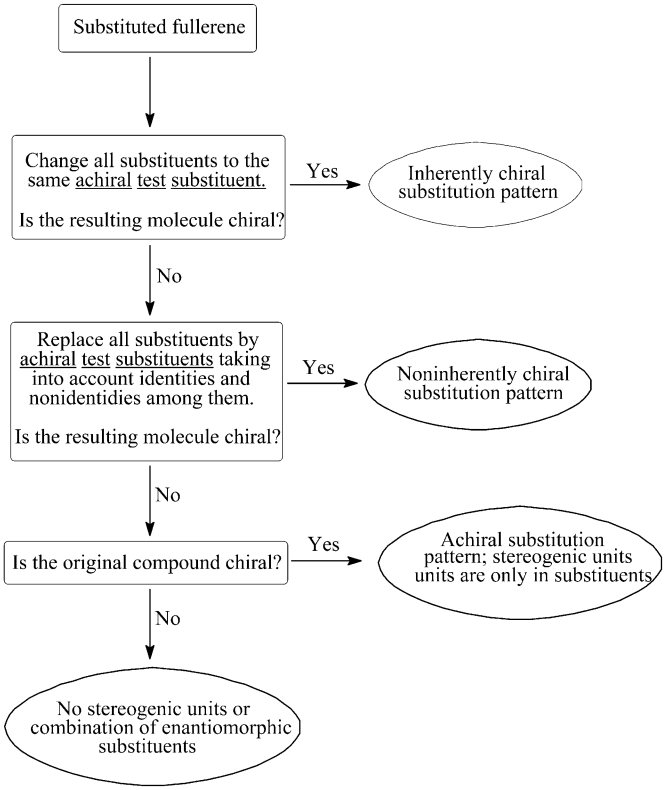
Type 2. Derivatives of achiral (and chiral) parent fullerenes in which the presence of substituents (see Fu-6.2), chiral or achiral, identical or different, on the fullerene skeleton, creates a chiral substitution pattern are said to have an **inherently chiral** substitution pattern.

Type 3. Derivatives of achiral parent fullerenes in which a chiral substitution (see Fu-6.2) pattern on the fullerene is due only to nonidentities among the substituents are said to have a **noninherently chiral** substitution pattern.

Type 4. Derivatives of achiral parent fullerenes in which the the presence of chiral substituents (see Fu-6.2) does not create a chiral substitution pattern have the stereogenic elements located exclusively in the substituents.

Fu-17.2 The substitution test

It must be recognized that a fullerene compound can belong to more than one of the above types when different stereogenic elements are superimposed in the same molecule. The above types of chirality can be classified by the simple substitution test shown in Scheme 1. To be precise, the scheme can be



Scheme 1 Classification of fullerene chirality by a stepwise substitution pattern.

applied only to a single fullerene unit. In cases where there are more than one unit and more than one are chiral, each unit gets its own descriptor.

The substitution test consists of (a) replacing *all* substituents (see Fu-6.2) by the *same achiral* test substituent; (b) replacing nonidentical substituents by *nonidentical achiral* test substituents; and (c) consideration of the original molecule. After each step, the resulting structure of increasing complexity is checked for chirality; as soon as it is found, the type of chirality can be identified.

Fu-17.3 Principles of the descriptor system

The descriptor system presented herein is based on the fact that the numbering schemes proposed for fullerenes in this document[mm] are chiral (helical) and thus constitute an ideal reference for differentiating between enantiomers of chiral carbon cages and of fullerene derivatives having a chiral substitution pattern. A single descriptor is sufficient to specify the configuration of a chiral fullerene or of a chiral fullerene substitution pattern, regardless of the degree of its substitution or skeletal replacement.

In a three-dimensional model, the pathway following the sequence of numbered carbon atoms consists of a helix, or of helical segments, and is therefore chiral. As a consequence, two isometric, mirror symmetric, numbering schemes can be applied to an achiral parent fullerene, as shown for (C_{60}-I_h)[5,6]fullerene in Fig. 6. The arrows indicate the direction of the numbering (see below); clockwise on the left and anticlockwise on the right looking from outside the cage.

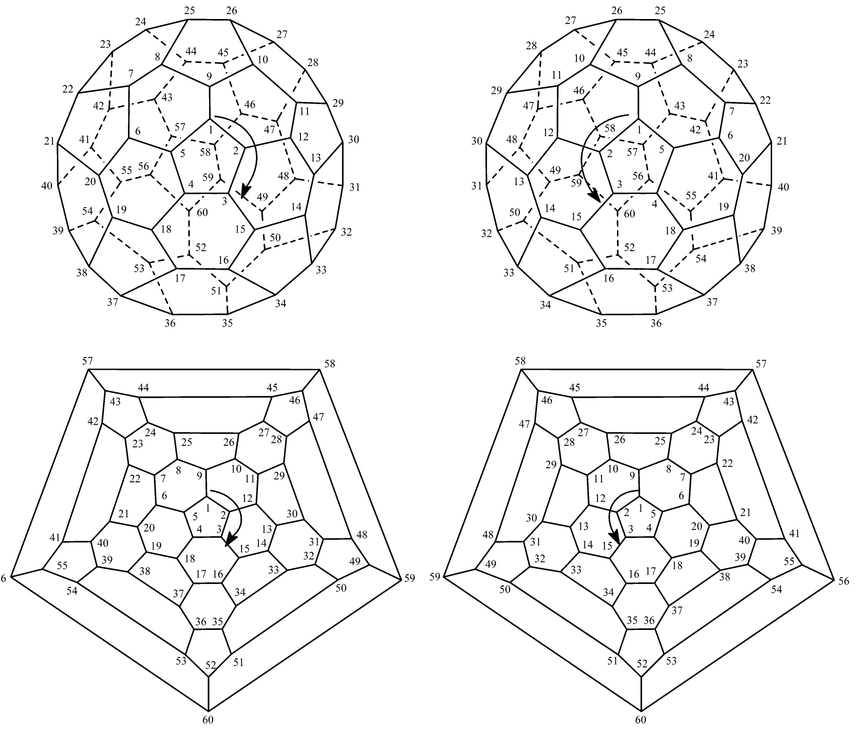


Fig. 6 Three-dimensional and Schlegel diagrams[nn] of (C_{60}-I_h)[5,6]fullerene with enantiomeric numberings.

[mm] Also applies to other numbering methods that are helical.

[nn] In this document, the convention for Schlegel diagrams is that the central polygon is considered to be closer to the viewer.

On the other hand, the numbering for a specific enantiomer of an inherently chiral fullerene is unique, and its mirror image must be applied to the other optical antipode. This is shown in Fig. 7 for the chiral (C_{76}-D_2)[5,6]fullerene[oo]. Again, the arrows indicate the direction of the numbering. The 3-D diagrams are viewed down the axis chosen as the basis for numbering; the Schlegel drawings are viewed down one of the C_2 axes.

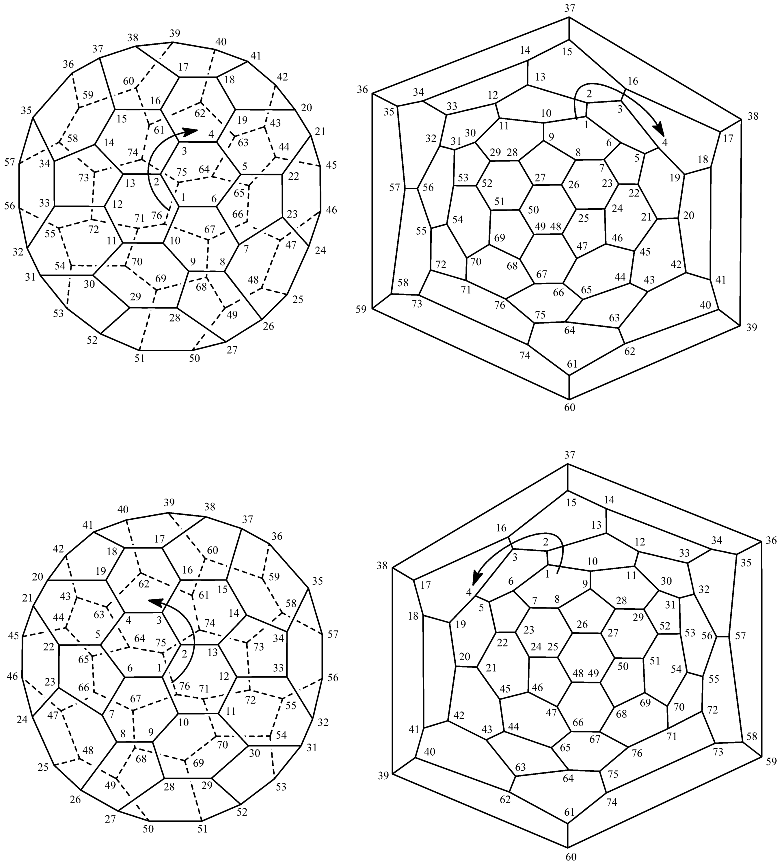


Fig. 7 Three-dimensional and Schlegel diagrams[pp] of the inherently chiral (C_{76}-D_2)[5,6]fullerene[oo] with enantiomeric numbering.

Because of the lack of mirror symmetry, each numbering fits only a single enantiomer. A description of the handedness of the numbering scheme used is sufficient to unambiguously characterize the absolute configuration of the fullerene. The viewer, looking at the polygon in which the numbering starts from outside the fullerene cage, traces a path from C-1 to C-2 to C-3, which are never aligned in a fullerene structure. If this path describes a clockwise direction, the configuration is indicated by the descriptor $({}^{f,x}C)$- [qq], where the superscript ‘f’ indicates that the descriptor refers to a fullerene, and the superscript ‘x’ is either ‘s’ for the systematic numbering described in Fu-3.2 or Fu-3.3 or ‘t’ for the triv-

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[oo] This fullerene is numbered by the system used in CA index nomenclature which has not been accepted by IUPAC; a future report will deal with numbering of fullerenes other than (C_{60}-I_h)[5,6]fullerene and (C_{70}-$D_{5h(6)}$)[5,6]fullerene.

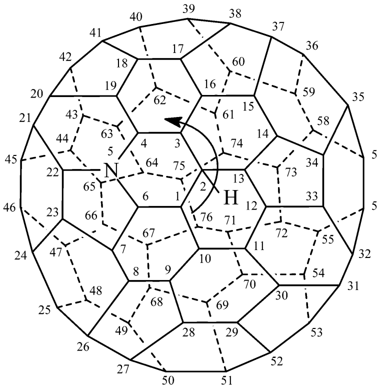
[pp] In this document, the convention for Schlegel diagrams is that the central polygon is considered to be closer to the viewer.

[qq] As is customary for stereodescriptors, parentheses are used as enclosing marks.

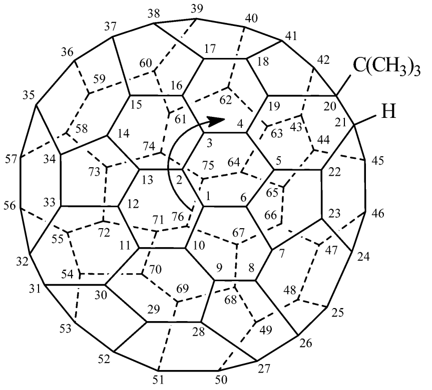
ial numbering described in Fu-3.4. If the path from C-1 to C-2 to C-3 describes an anticlockwise direction, the descriptor is $(^{\mathrm{f,x}}A)$- [rr]. Thus, the enantiomer of $(C_{76}$-$D_2)$[5,6]fullerene shown in the upper half of Fig. 7 is $(^{\mathrm{f,s}}C)$-$(C_{76}$-$D_2)$[5,6]fullerene and the enantiomer shown in the lower half of Fig. 7 is $(^{\mathrm{f,s}}A)$-$(C_{76}$-$D_2)$[5,6]fullerene.

This procedure is also valid for derivatives of inherently chiral fullerenes, because the numbering scheme applies to the parent fullerene as well as to the derivative.

Examples:



I [ss]



II [ss]

I $(^{\mathrm{f,s}}A)$-2*H*-5-Aza-$(C_{76}$-$D_2)$[5,6]fullerene
II $(^{\mathrm{f,s}}C)$-20-*tert*-Butyl-20,21-dihydro$(C_{76}$-$D_2)$[5,6]fullerene

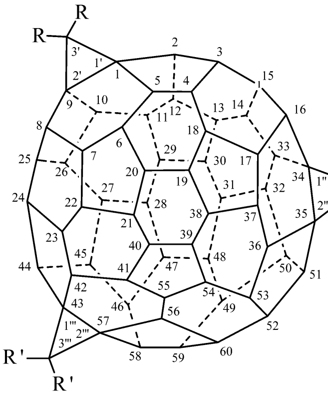
Fu-17.4 Achiral parent fullerenes with an inherently chiral substitution pattern

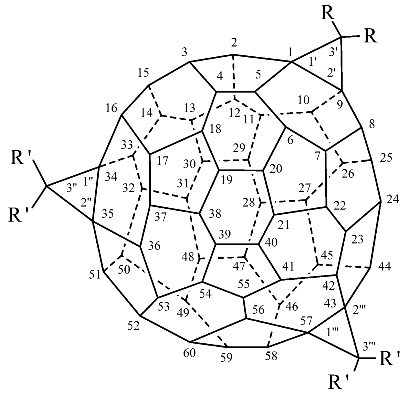
The fullerene compounds in this category are all substituted achiral fullerenes. They have an inherently chiral substitution pattern if the existence of enantiomeric species is inherent to the geometric arrangement of the substitution sites on the fullerene parent regardless of whether the substituents are identical or different. In these fullerene derivatives there is a unique numbering scheme that leads to the lowest set of locants for the substituents. As above, a description of the handedness of the numbering scheme that leads to the lowest set of locants is sufficient to unambiguously characterize the absolute configuration of the substituted fullerene as $^{\mathrm{f,x}}C$ or $^{\mathrm{f,x}}A$.

[rr] As is customary for stereodescriptors, parentheses are used as enclosing marks.

[ss] This fullerene is numbered by the system used in CA index nomenclature which has not been accepted by IUPAC; a future report will deal with numbering of fullerenes other than $(C_{60}$-$I_h)$[5,6]fullerene and $(C_{70}$-$D_{5h(6)})$[5,6]fullerene.

Example 1: 3′,3′-Diethyl 3″,3″,3‴,3‴-tetramethyl 3′*H*,3″*H*,3‴*H*-tricyclopropa[1,9:34,35:43,57]-(C_{60}-I_h)[5,6]fullerene-3′,3′,3″,3″,3‴,3‴-hexacarboxylate

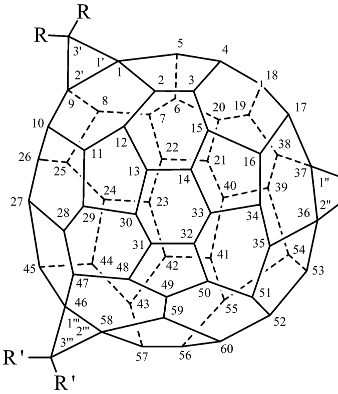


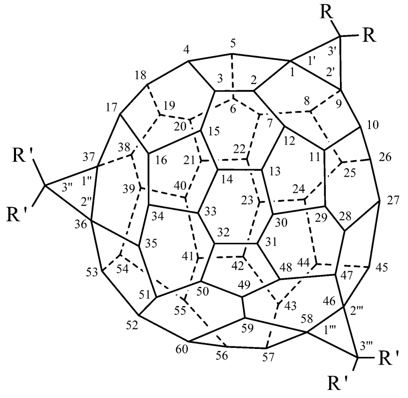


R = –CO–O–CH_2CH_3
R′ = –CO–O–CH_3

I ($^{\mathrm{f,s}}C$)-

II ($^{\mathrm{f,s}}A$)-





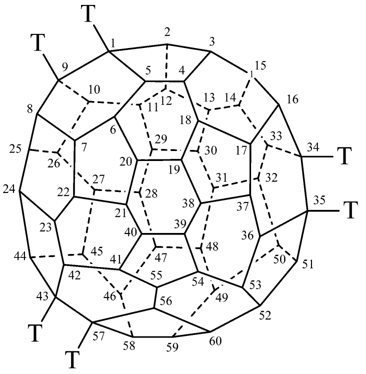
III
(enantiomeric numbering for **I**)

IV
(enantiomeric numbering for **II**)

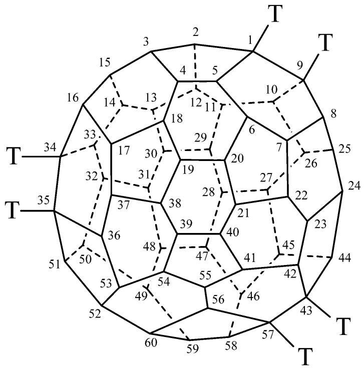
Explanations:

(a) In the enantiomers of the (C_{60}-I_h)[5,6]fullerene derivatives shown above, clockwise (**I**) and anticlockwise (**II**) numbering leads to the same lowest set of locants, namely, 1,9:34,35:43,57, respectively. Use of the enantiomeric numbering scheme for each, shown as **III** and **IV**, results in the locant set, 1,9:36,37:46,58, a higher locant set that is unacceptable according to the rule of lowest locants in organic nomenclature [8c].

(b) The parent fullerene, (C_{60}-I_h)[5,6]fullerene, is achiral but the compound is chiral by virtue of its substitution pattern. This compound is inherently chiral because replacement of all of its substituents by the same achiral test substituent, ‘T’, still results in a chiral structure as shown below.

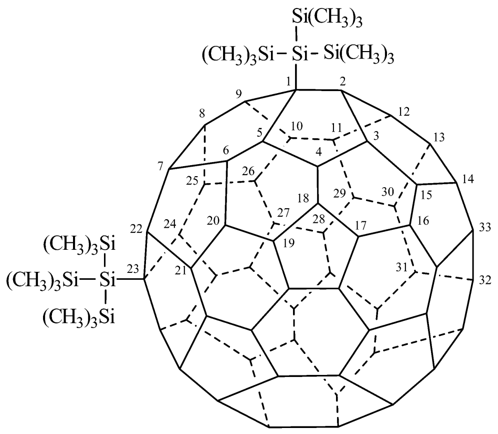


$({}^{\mathrm{f,s}}C)$-

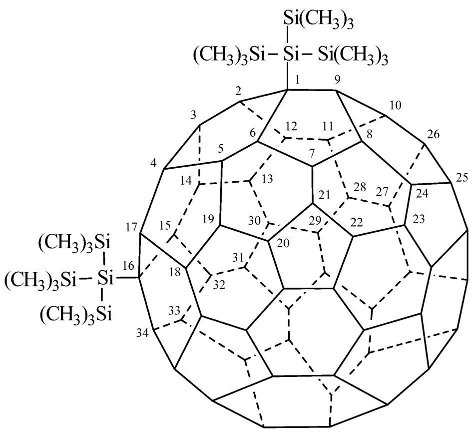


$({}^{\mathrm{f,s}}A)$-

Example 2



I (systematic numbering)



II (trivial numbering)

I $({}^{\mathrm{f,s}}C)$-1,23-Bis[1,1,1,3,3,3-hexamethyl-2-(trimethylsilyl)trisilan-2-yl]-1,23-dihydro-$(\mathrm{C}_{60}\text{-}I_\mathrm{h})$[5,6]fullerene

II $({}^{\mathrm{f,t}}A)$-1,16-Bis[1,1,1,3,3,3-hexamethyl-2-(trimethylsilyl)trisilan-2-yl]-1,16-dihydro-[60-I_h]fullerene

Note: This is a simple compound with an inherently chiral substitution pattern but it serves to illustrate that the configurational descriptor may be different when systematic numbering or trivial numbering is used.

Fu-17.5 Achiral parent fullerenes with a noninherently chiral substitution pattern

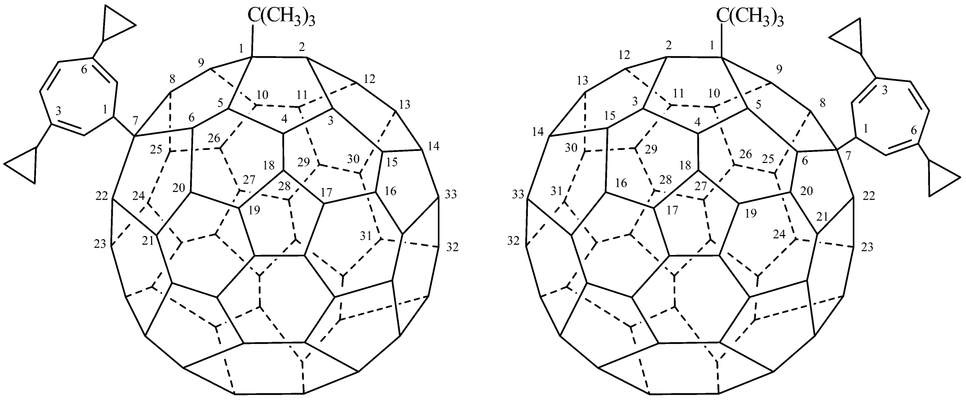
The fullerenes in this category are all substituted achiral parent fullerenes in which the chirality is neither inherent to the parent fullerene nor due to an inherently chiral substitution pattern, but is caused by the geometric arrangement of the substituents, all of which cannot be identical.

In all cases of fullerenes with a noninherently chiral substitution pattern, no distinction between enantiomers is possible on the basis of the criteria given above. The same set of lowest locants is obtained with both mirror-symmetric numberings. In order to make a distinction a classification of substituents is necessary. This can be achieved in the most convenient way by using the CIP (Cahn-Ingold-Prelog) method of ranking substituents by atom-by-atom exploration of each attached atom or group [17]. For fullerenes with a noninherently chiral substitution pattern, each substituent is compared by starting the exploration process at the atom located in the fullerene skeleton and moving outward progressively until a priority difference is identified[tt]. Of the two mirror-symmetric numbering schemes leading to the same lowest set of locants, the one assigning a lower locant to an atom or group of higher CIP priority at the first point of difference is preferred and confers its descriptor to the enantiomer in question.

A classification of substituents based on the principle of alphabetical order provides the same stereodescriptor assignment for fullerenes with noninherently chiral substitution patterns in some cases (see Example 1, below) but this is pure coincidence because the two methods are based on fundamentally different principles. Furthermore, alphabetical order cannot be applied in all cases (see Example 2, below) and therefore is not broadly applicable.

In considering fullerenes with noninherently chiral substitution patterns, their names must be based on nomenclature principles, such as alphabetical order and lowest locants, but their stereodescriptors are based on purely structural considerations for which the CIP method is clearly the method of choice.

Example 1: 1-*tert*-Butyl-7-(3,6-dicyclopropylcyclohepta-2,4,6-trien-1-yl)-1,7-dihydro-(C_{60}-I_h)[5,6]fullerene

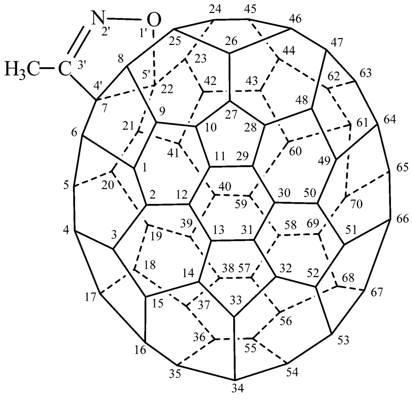


($^{\mathrm{f,s}}C$)- ($^{\mathrm{f,s}}A$)-

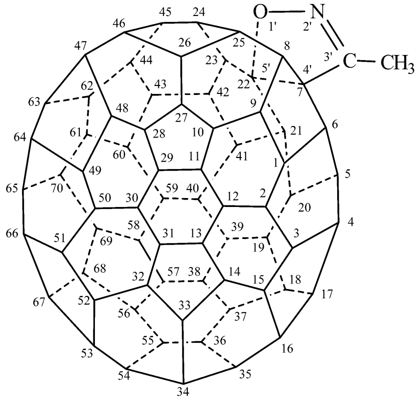
Explanation: This compound is chiral only because the substituents are constitutionally different. The parent fullerene is achiral and it does not have an inherently chiral substitution pattern because replacement of both substituents by the same achiral test substituent, 'T', results in an achiral compound. Therefore it has a noninherently chiral substitution pattern. The *tert*-butyl group is assigned the locant '1' because its CIP priority is higher than that of the 3,6-dicyclopropylcyclohepta-2,4,6-trien-1-yl group. For this example, using the nomenclature principle of alphabetic order of substituents would give the same result, but this is purely coincidental because the two procedures are based on fundamentally different principles (see Example 2, below, for which a different numbering is required in order to use the CIP priority method).

[tt] In case two enantiomorphic substituted fullerenes would need to be compared according to the CIP exploration procedure, it is suggested that, in addition to the priority of *R* over *S* and of *M* over *P* in subrule 5 (17), $^{\mathrm{f,,x}}C$ be given priority over $^{\mathrm{f,,x}}A$.

Example 2: 3′-Methylisoxazolo[4′,5′:7,22](C_{70}-$D_{5h(6)}$)[5,6]fullerene



($^{\mathrm{f,s}}$*C*)-



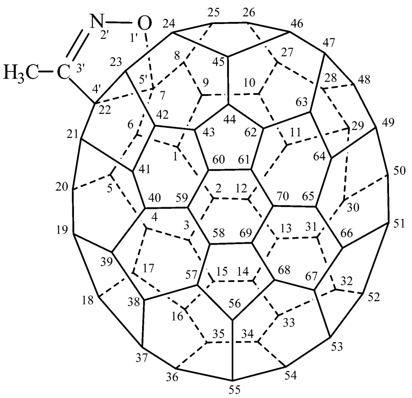
($^{\mathrm{f,s}}$*A*)-

Explanations:

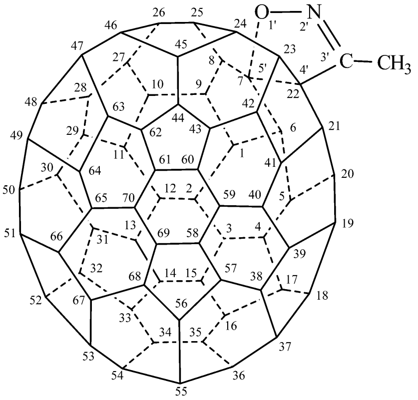
(a) This compound is chiral only because the fused ring is unsymmetrical. The parent fullerene is achiral and it does not have an inherently chiral substitution pattern because replacement of both substituents by the same achiral test substituent, ‘T’, results in an achiral compound. Therefore, it has a noninherently chiral substitution pattern.

(b) In this example, the numbering used to name the compound is based on the nomenclature principle of lowest set of locants [8c] for the fusion site and is not appropriate for assignment of the stereodescriptor. The numbering scheme to be used for assignment of the stereodescriptor is chosen so that the lower locant ‘7’ of the fullerene is associated with atom of highest priority in the isoxazole ring, i.e., the ‘O’ atom. This numbering is shown in the structures below which would lead to the incorrect name 3′-Methylisoxazolo[4′,5′:22,7](C_{70}-$D_{5h(6)}$)[5,6]fullerene because its locants are higher that those in the name above. Therefore, the stereodescriptors for the enantiomers shown above are ($^{\mathrm{f,s}}$*C*)- and ($^{\mathrm{f,s}}$*A*)-, respectively, as shown.

Note: It must be kept clearly in mind that the generation of the stereodescriptor is additional to name formation.

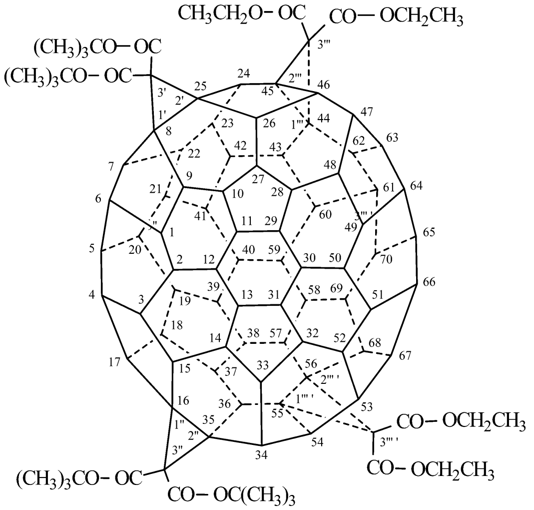


($^{\mathrm{f,s}}$*C*)-

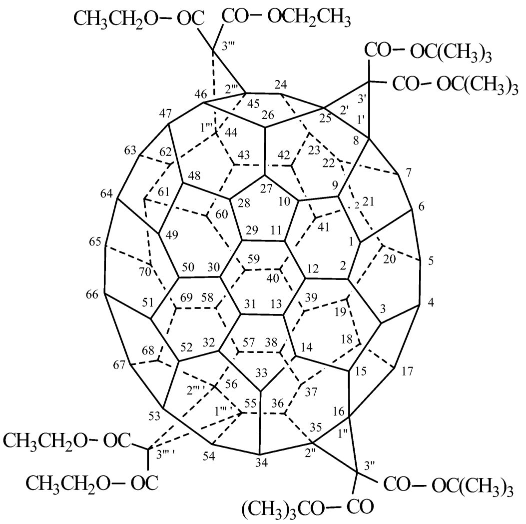


($^{\mathrm{f,s}}$*A*)-

Example 3: 3′,3′,3″,3″-Tetra-*tert*-butyl 3‴,3‴,3‴′,3‴′-tetraethyl 3′*H*,3″*H*,3‴*H*,3‴′-tetracyclopropa[8,25:16,35:44,45:55,56](C_{70}-$D_{5h(6)}$)[5,6]fullerene-3′,3′,3″,3″,3‴,3‴,3‴′,3‴′-octacarboxylate



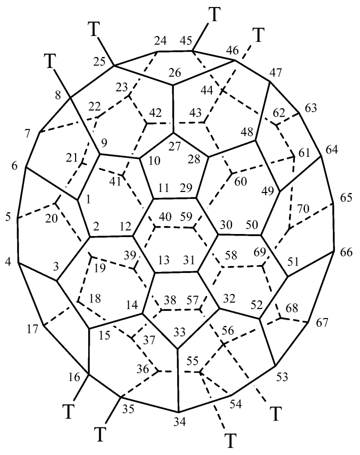
($^{f,s}C$)-



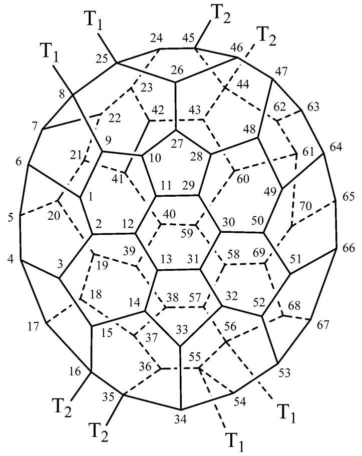
($^{f,s}A$)-

Explanations:

(a) The parent fullerene for this compound is achiral and replacement of all substituents by the achiral test substituent ‘T’ (see **I**, below) still results in an achiral compound.



I

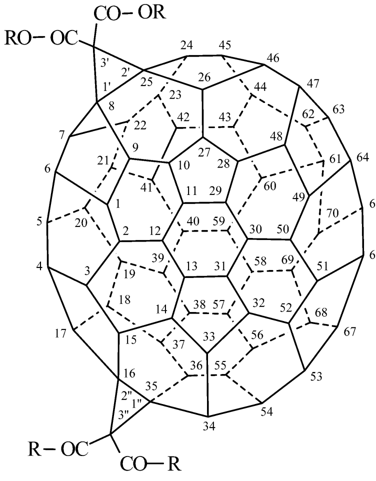


II

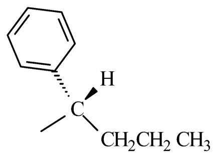
(b) Accordingly, the second step of the substitution test (see Scheme 1), i.e., replacement of the substituents by the achiral test substituents T_1 and T_2, which must respect the identities and nonidentities of the original substituents, is applied (see **II**, above), resulting in a chiral structure because T_1 is different from T_2. Hence, the compound has a noninherently chiral substitution pattern. The fused cyclopropane rings carying the *tert*-butyl ester groups have the highest CIP priority and are therefore assigned the lowest fusion locants.

Fu-17.6 Fullerene derivatives with achiral substitution patterns and chiral substituents

Example: Tetrakis[(1*S*)-1-phenylbutyl] 3′*H*,3″*H*-dicyclopropa[8,25:16,35](C_{70}-$D_{5h(6)}$)[5,6]fullerene-3′,3′,3″,3″-tetracarboxylate



R =



Configuration = *S*

Explanations:

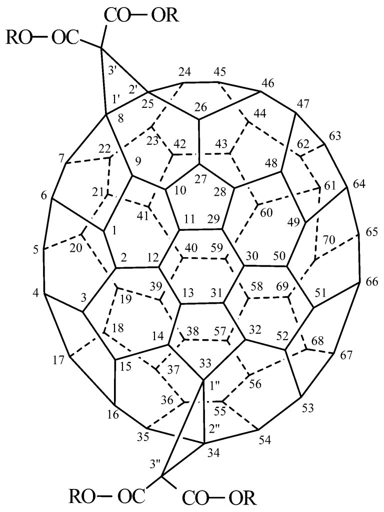
(a) This fullerene derivative is chiral. The parent fullerene is achiral and the derivative has an achiral substitution pattern. Replacement of all substituents by the achiral test group T (see Scheme 1) results in an achiral structure; and since the original substituents were already identical the second step of the substitution test is not necessary. Step 3 of the substitution test (see Scheme 1) asks if the original compound was chiral. The answer is yes, and thus the stereogenic units occur only in the groups attached to the fullerene core. The configuration of such stereogenic units can be described by the normal descriptors of organic nomenclature [18].

(b) If the esters of the acid in the above example were different, the structure resulting from step 2 of the substitution test would have the achiral substituents T_1 and T_2; but the parent fullerene and it substitution pattern would be achiral, and, therefore, any chirality of the original compound would be due to stereogenic centers located in the substituents.

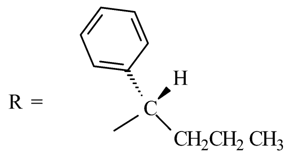
Fu-17. 7 Superimposition of stereogenic elements in a fullerene molecule

If a fullerene derivative with an inherently or noninherently chiral substitution pattern carries chiral substituents, the configuration of both types of stereogenic elements has to be indicated. The two types are independent of each other and the configuration of both must be specified for a full description of the compound.

Example:



Configuration = ($^{f,s}C$)-



Configuration = *S*

Tetrakis[(1*S*)-1-phenylbutyl] ($^{f,s}C$)-3′*H*,3″*H*-dicyclopropa[8,25:33,34](C_{70}-$D_{5h(6)}$)[5,6]fullerene-3′,3′,3″,3″-tetracarboxylate

Explanation: The chiralities of the stereogenic centers in the esters are superimposed on the descriptor for the fullerene with the inherently chiral substitution pattern. The enantiomer would be named tetrakis[(1*R*)-1-phenyl-butyl] ($^{f,s}A$)-3′*H*,3″*H*-dicyclopropa[8,25:33,34](C_{70}-$D_{5h(6)}$)[5,6]fullerene-3′,3′,3″,3″-tetracarboxylate and the same for the various diastereoisomers.

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