

INTERNATIONAL UNION OF PURE AND APPLIED CHEMISTRY  
ORGANIC AND BIOMOLECULAR CHEMISTRY DIVISION  
COMMISSION ON NOMENCLATURE OF ORGANIC CHEMISTRY

**NOMENCLATURE FOR THE C<sub>60</sub>-I<sub>h</sub> AND C<sub>70</sub>-D<sub>5h(6)</sub> FULLERENES**  
(IUPAC Recommendations 2001)

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## Summary

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 twelve isolated five-membered rings, the rest being six-membered rings.

Although it was recognized that organic ring nomenclature could be used for these structures, the resulting names would be extremely unwieldy and inconvenient for use. At the same time, it was also recognized that established organic 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 the  $D_{5h}$ - $C_{70}$  fullerene. It also describes adaptations of organic nomenclature principles for naming derivatives of 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.

**NOMENCLATURE FOR THE C<sub>60</sub>-I<sub>h</sub> AND C<sub>70</sub>-D<sub>5h(6)</sub> FULLERENES**  
**(IUPAC RECOMMENDATIONS 2001)**

**CONTENTS**

Fu-0. Introduction.....	1
Fu-1. Definitions.....	1
Fu-2. Names.....	1
Fu-3. Numbering.....	2
Fu-3.1. Systematic numbering.....	2
Fu-3.2. Systematic numbering of (C <sub>60</sub> -I <sub>h</sub> )[5,6]fullerene.....	2
Fu-3.3. Systematic numbering for (C <sub>70</sub> -D <sub>5h(6)</sub> )[5,6]fullerene.....	3
Fu-3.4. Trivial numbering.....	5
Fu-4. Structurally modified fullerenes.....	5
Fu-5. Heterofullerenes.....	13
Fu-6. Fullerene derivatives.....	18
Fu-6.1. Fulleranes.....	18
Fu-6.2. Fullerenes.....	18
Fu-6.3. Lowest locants.....	22
Fu-6.4. Fullerenes and fulleranes as substituents.....	24
Fu-6.5. <i>endo</i> -Substituted fullerenes and fulleranes.....	25
Fu-7. Fullerenes Fused to Organic Rings or Ring Systems.....	26
Fu-8. Bridged Fullerenes.....	34
Fu-9. Spiro Fullerenes.....	38
Fu-10. Compounds with two Fullerene Components.....	40
Fu-11. Compounds with three or more Fullerene Components.....	50
Fu-12. Fullerenes in Coordination Compounds.....	56
Fu-13. Fullerenes in Polymers.....	58
Fu-14. Fullerenes cations.....	61
Fu-15. Ionic Fullerenes.....	62
Fu-16. Metal Derivatives of Fullerenes.....	62
Fu-17. Configurational Specification for (C <sub>60</sub> -I <sub>h</sub> ) and (C <sub>70</sub> -D <sub>5h(6)</sub> ) Fullerenes and their Derivatives.....	63

# NOMENCLATURE FOR THE $C_{60}$ - $I_h$ AND $C_{70}$ - $D_{5h(6)}$ FULLERENES (IUPAC RECOMMENDATIONS 2001)

## 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 (ref. 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 (ref. 2) and one published by CAS (ref. 3). In addition, alternative methods for naming derivatives of fullerenes were discussed. However, no approved IUPAC recommendations were contained in this publication. The present report contains approved IUPAC recommendations for the  $C_{60}$ - $I_h$  and  $C_{70}$ - $D_{5h(6)}$  fullerenes and their derivatives. It is limited to these fullerenes because there is 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** 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 twelve five-membered rings and the rest six-membered rings; the archetypal example is the sixty atom structure, where the atoms and bonds delineate a truncated icosahedron (refs. 4, 5). However, the term has been broadened to include any closed-cage structure having more than twenty carbon atoms consisting entirely of three coordinate carbon atoms (ref 3).

**Fu-1.2. Fullerenes** 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.** The recommended systematic names for the common C-60 and 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 italic subscript parenthetical (6) following the italic 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 (ref. 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 only for these specific compounds.

### Fu-3. Numbering

**Fu-3.1. 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 rules (ref. 3). These rules are sufficient to systematically number  $(C_{60}-I_h)[5,6]$ fullerene and  $(C_{70}-D_{5h(6)})[5,6]$ fullerene. Other rules are needed for other fullerenes. The CAS rules (ref. 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.

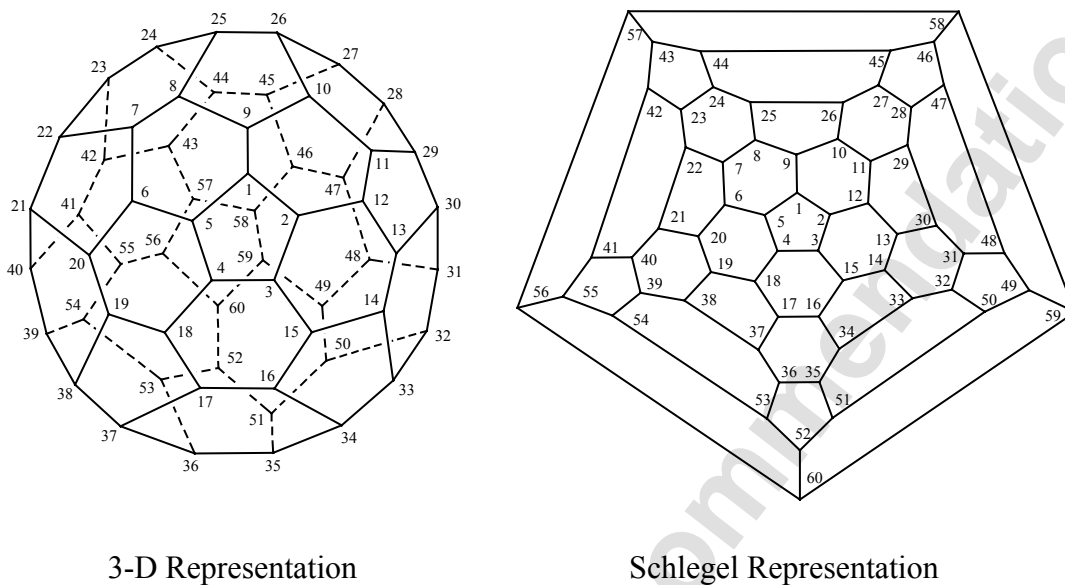
**Fu-3.1.2.1.** When there is a choice between rings, a larger ring is preferred to a smaller one. Where there is still a choice, the preferred ring contains the preferred atom (see Fu-3.1.2.3) at the first point of difference.

**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, e.g.,  $66 > 65 > 55$ . 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, e.g.,  $666 > 665 > 655 > 555$ .

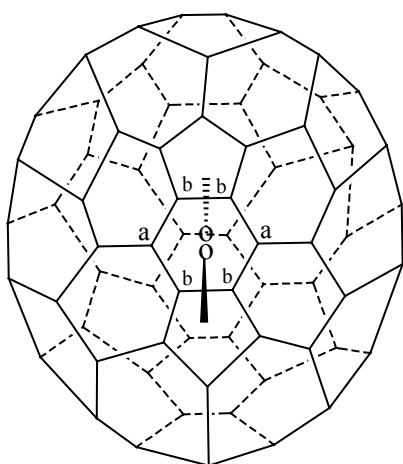
**Fu-3.1.3.** Where there is a choice of spiral pathways for numbering, the preferred pathway terminates as close as possible to the axis of the spiral in terms of the number of bonds.

**Fu-3.2 Systematic numbering of  $(C_{60}-I_h)[5,6]$ fullerene** (see Fig. 1). This fullerene 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 fifteen 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.

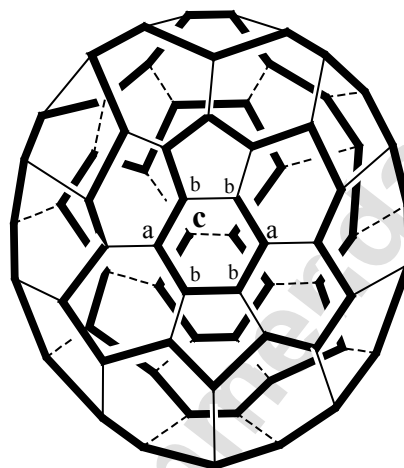


**Fig. 1 Systematic Numbering for  $(C_{60}-I_h)[5,6]$ Fullerene**

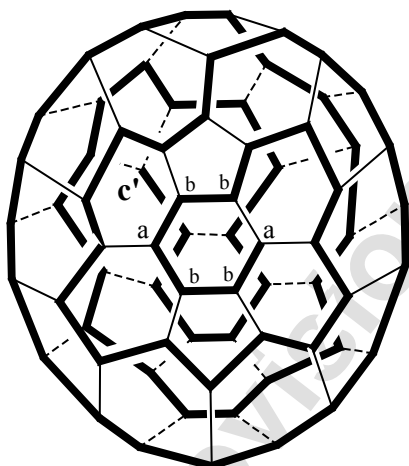
**Fu-3.3 Systematic numbering for  $(C_{70}-D_{5h(6)})[5,6]$ fullerene** (see Fig. 3); The principal axis for this fullerene is the  $C_5$  axis through opposite pentagons. There are no contiguous spiral pathways from any atom in either pentagon and therefore the  $C_5$  axis cannot be a reference axis. 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 equatorial 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 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.



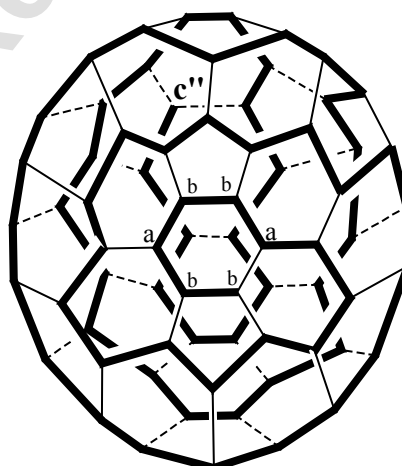
2a



2b

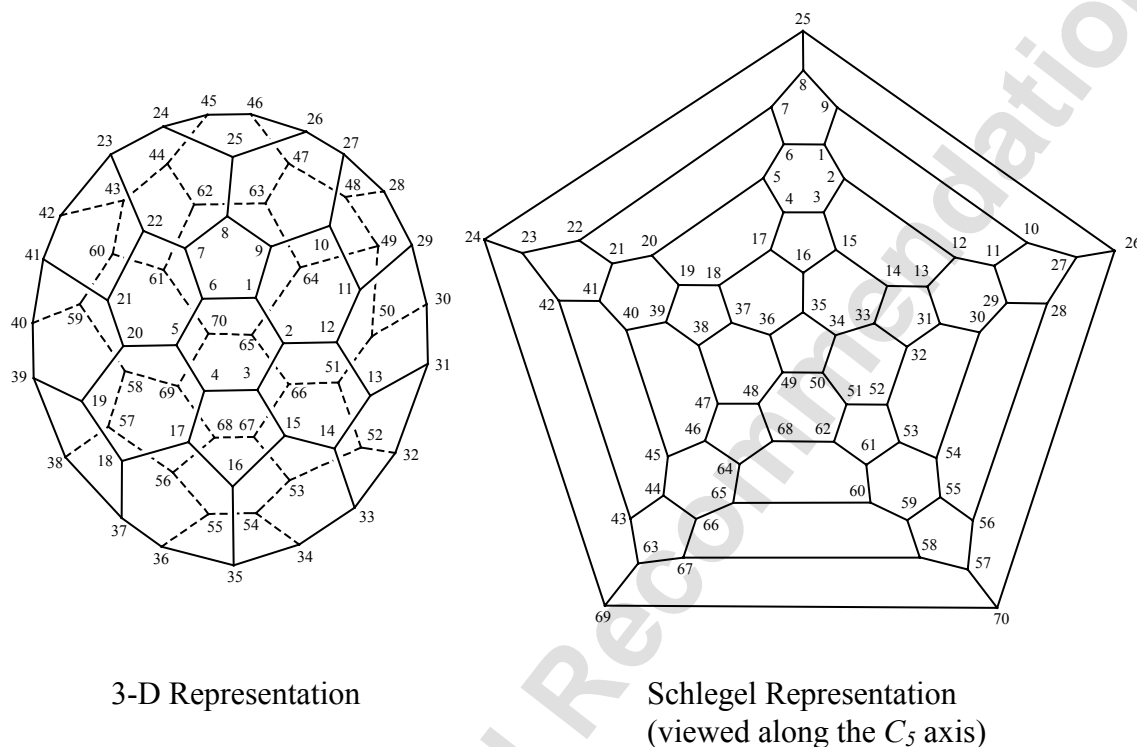


2c



2d

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



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

**Fu-3.4.** The **trivial numbering** to be used when the trivial names  $[60-I_h]$ fullerene and  $[70-D_{5h}]$ fullerene are used is based on the reported "most reactive bond" (ref. 2). These numberings are shown in Figs. 4 and 5.

**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.

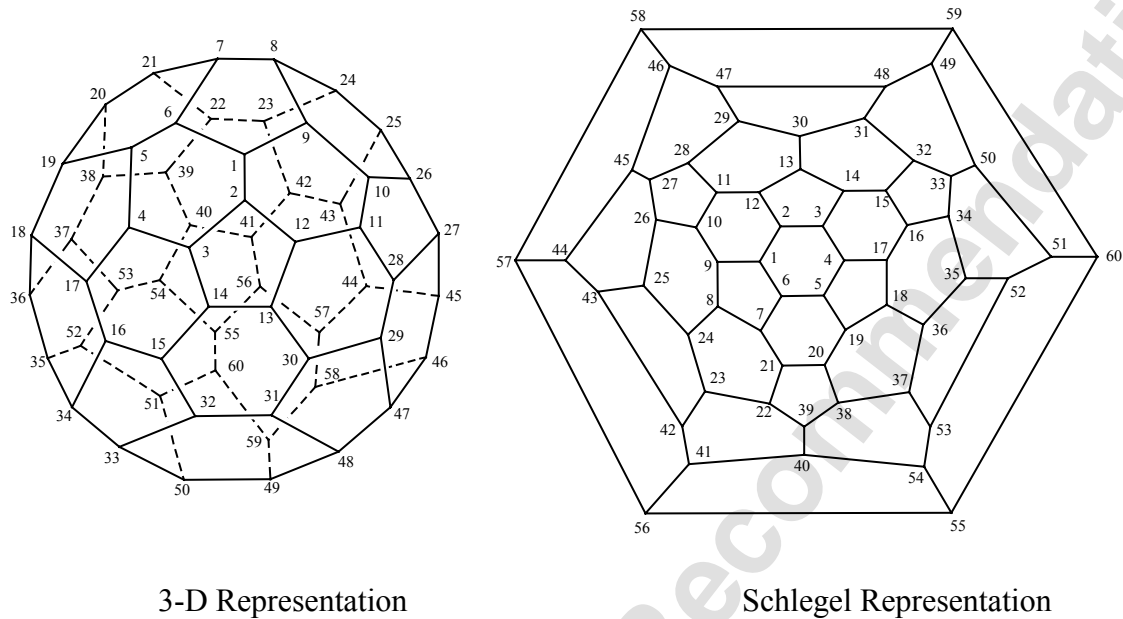
#### **Fu-4. Structurally Modified Fullerenes**

Modification of fullerene structures by the addition or deletion of atoms, or by the breaking of bonds is described by the prefixes "homo", "nor", "seco", and "cyclo" in a way that is similar to their use in organic stereoparent nomenclature, including combinations (ref. 6).

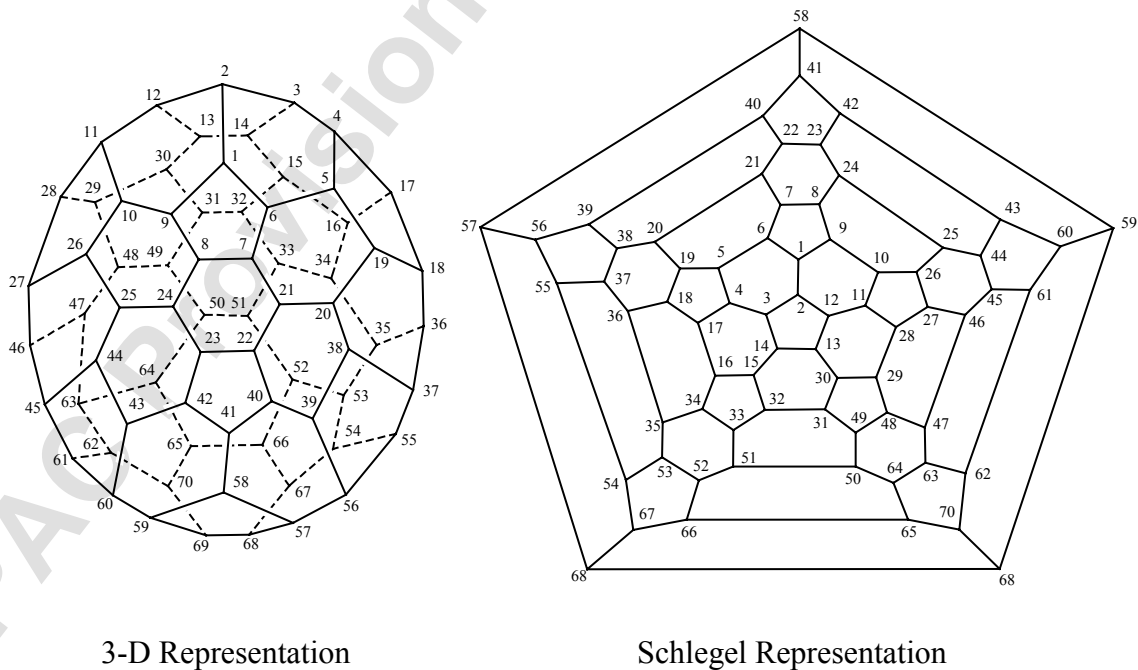
**Fu-4.1. Homofullerenes.** The replacement of a carbon-carbon bond of a fullerene by a methylene group is described by attaching the nondetachable prefix "homo" to the name of the parent fullerene. The original numbering of the parent fullerene is retained. The location of the homo operation is described by a complex locant formed according to the method devised for insertion of a methylene group into a bond sector of a stereoparent (ref. 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.



**Fig. 4. Trivial Numbering for  $[60-I_h]$ fullerene**

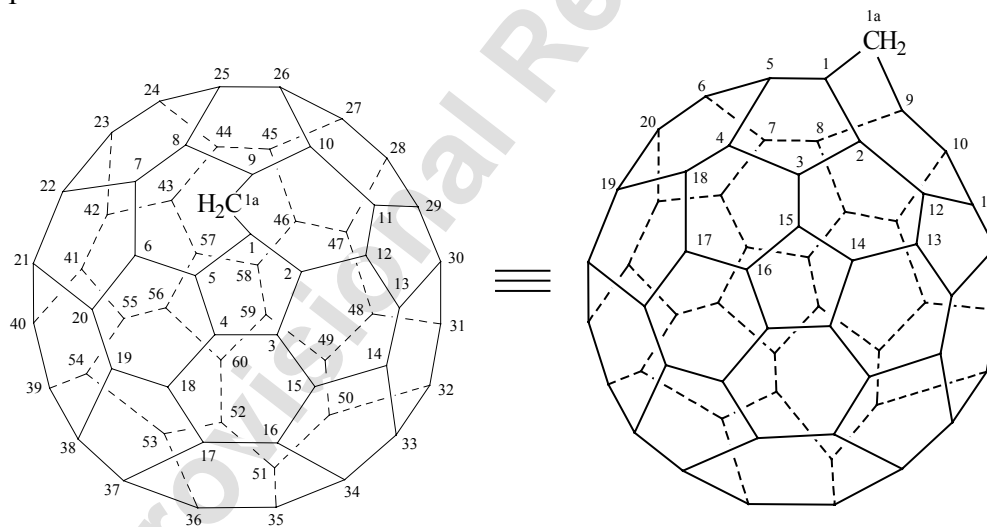


**Fig. 5 Trivial Numbering for [70- $D_{5h}$ ]fullerene**

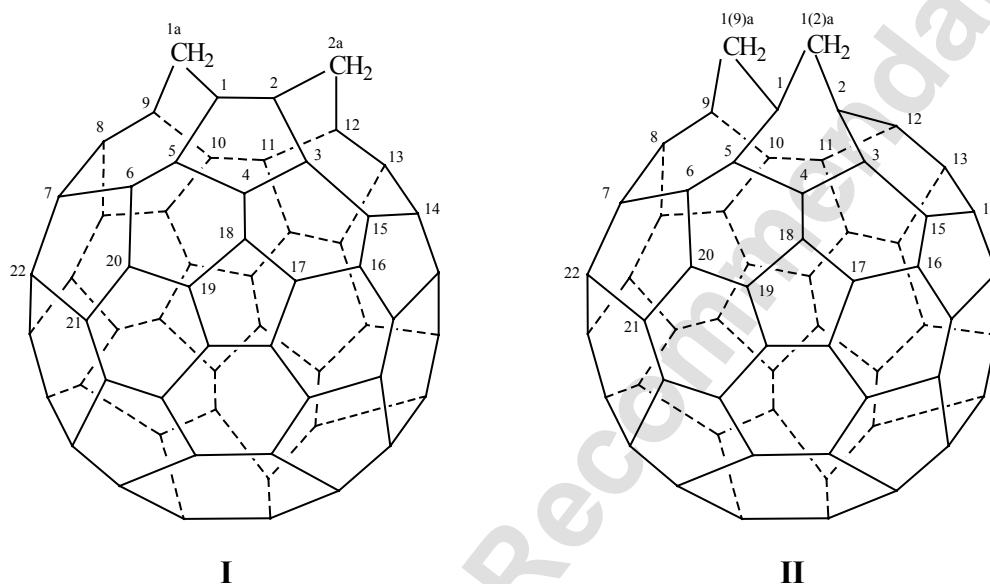
Because of the possibility of rearrangement of the double bonds in the fullerene structure with the homo atom, indicated hydrogen is used to designate the “extra” hydrogen of the homo atom.

**Note:** CAS (ref. 3) uses a complex locant format 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 illustrated by the third example above. Although this would remove ambiguity in a large number of cases, it would not do so in cases like the following: 3,15(15a):14,15(15a)-dihomo-1,9-dinor-[5,6]fullerene- $C_{60}$ - $I_h$  (CAS name), where the simple locants for the added methylene groups would both be 15a. The IUPAC name recommended herein for the latter 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:



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



- I** 1aH,2aH-1(9)a,2(12)a-Dihomo( $C_{60}$ - $I_h$ )[5,6]fullerene  
(locants for structure, 1a and 2a)
- II** 1(9)aH,1(2)aH-1(2)a,1(9)a-Dihomo( $C_{60}$ - $I_h$ )[5,6]fullerene  
(locants for structure must be 1(2)a and 1(9)a, because both simple locants would be 1a)

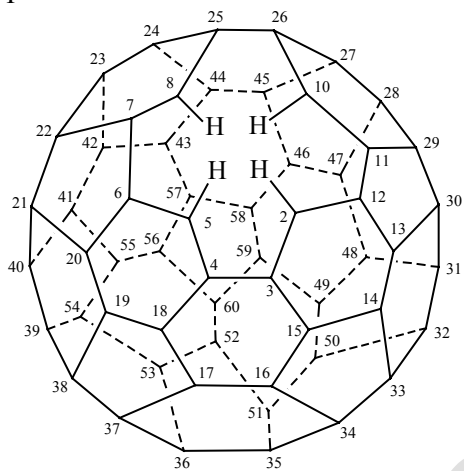
**Fu-4.2 Norfullerenes.** The nondetachable prefix "nor" describes the deletion of carbon atoms from a fullerene structure; however, bonds attached to the atom removed are not reconnected as is the case in stereoparent nomenclature (ref. 6). As a result, the connectivity of remaining atoms may be reduced 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. Locants for the atoms removed from a ring or chain segment 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 (ref. 6).

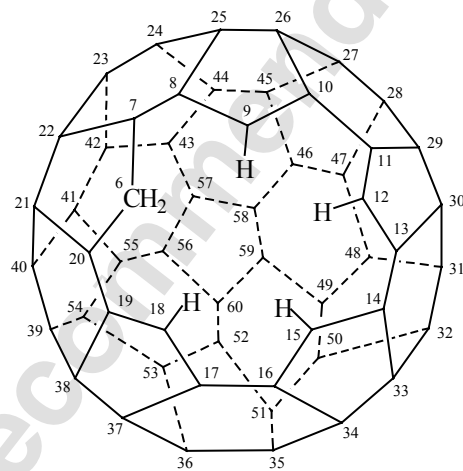
**Note 2:** The main problem with the nor operation is the limit to the number of carbon atoms that can be removed from a particular fullerene structure. Eventually, systematic ring nomenclature will provide a name that may be easier to understand than a

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 twenty percent 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 the  $(C_{60}-I_h)[5,6]$ - and  $(C_{70}-D_{5h(6)})[5,6]$ fullerenes 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.

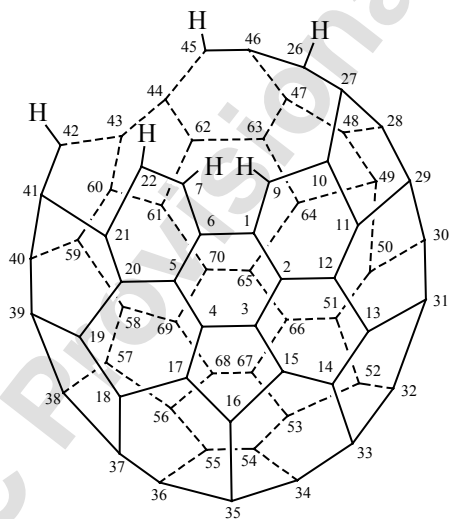
Examples:



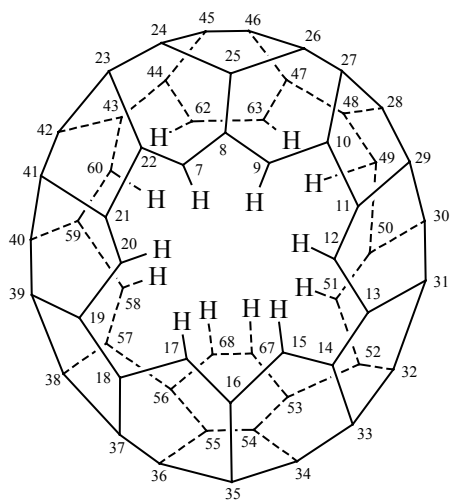
**I**



**II**



**III**



**IV**

**I** 1,9-Dinor $(C_{60}-I_h)[5,6]$ fullerene

**II** 6H-1,2,3,4,5-Pentanor $(C_{60}-I_h)[5,6]$ fullerene (citation of the indicated hydrogen

is not really necessary because of the symmetry of the compound)

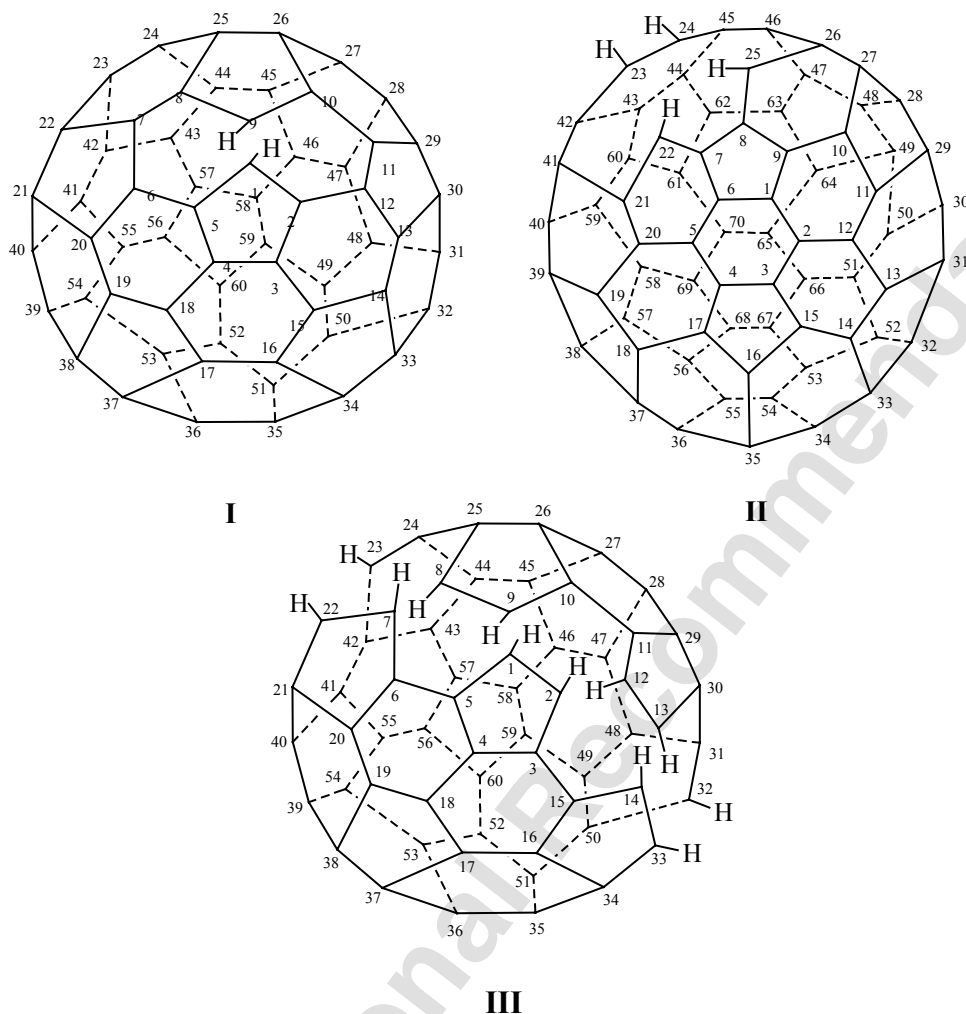
III 8,23,24,25-Tetranor( $C_{70}$ - $D_{5h(6)}$ )[5,6]fullerene

IV 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 the 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:



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

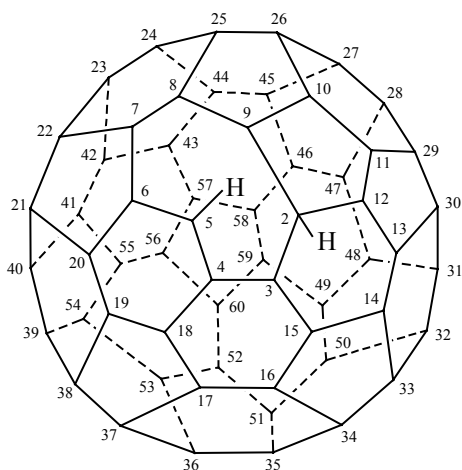
**Fu-4.4 Cyclofullerenes.** The nondetachable prefix "cyclo" indicates the formation of a bond between two atoms of a modified fullerene or a multicomponent fullerene (see Fu-11). In single component fullerenes, it almost always occurs in combination with one or more of the structure-modifying prefixes described above.

**Fu-4.5 Combinations of the 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 from the parent fullerene. This is the order that the operation indicated by each prefix has for assignment of lowest locants. Nor prefixes are preferred for lowest locants and homo prefixes are preferred to seco or cyclo for lowest locants

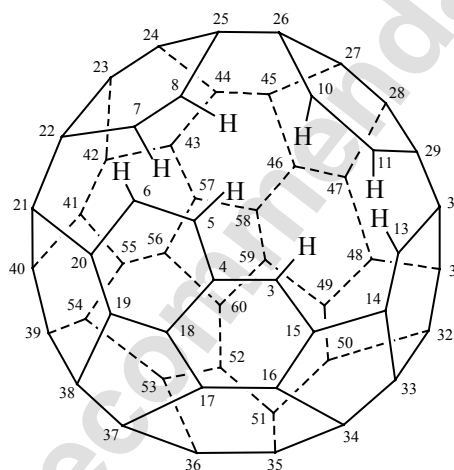
since homo locants may be needed for the latter operations. Locants for cyclo and seco prefixes are determined by the lowest set of locants, then by the order of citation of the locants in the name.

**Note:** This order of citation is the same as given in the Revised Section F: Natural Products and Related Compounds (ref. 6). CAS uses alphabetical order reading from left to right.

Examples:



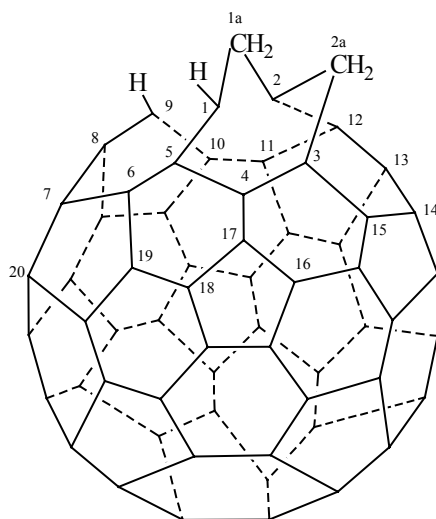
**I**



**II**

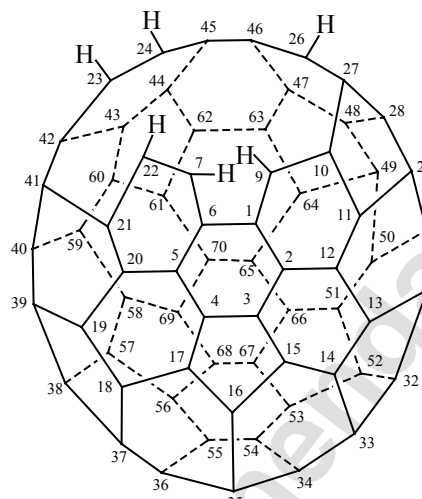
**I** 2*H*-2,9-Cyclo-1-nor( $C_{60}$ - $I_h$ )[5,6]fullerene

**II** 6,7-Seco-1,2,9,12-tetranor( $C_{60}$ - $I_h$ )[5,6]fullerene



III

III 1aH,2aH-1,9-Seco-1(2)a,2(3)a-dihomo(C<sub>60</sub>-I<sub>h</sub>)[5,6]fullerene



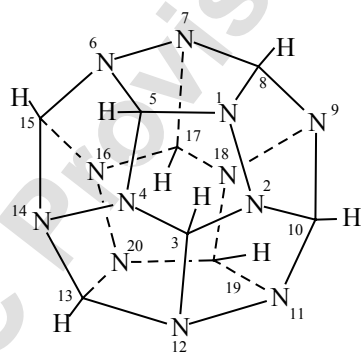
IV

IV 22,23-Seco-8,25-dinor(C<sub>70</sub>-D<sub>5h(6)</sub>)[5,6]fullerene

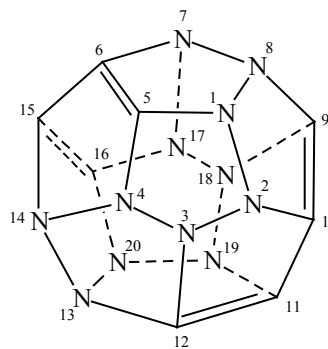
### Fu-5. Heterofullerenes.

**Fu-5.1** Skeletal replacement nomenclature is used to name fullerenes in which carbon atoms have been replaced by heteroatoms having standard bonding numbers as specified for the "a" prefixes of organic replacement nomenclature or bonding numbers indicated by the  $\lambda$ -convention (ref. 7).

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<sub>20</sub>-I<sub>h</sub>)[5]fullerane and dodecaaza(C<sub>20</sub>-I<sub>h</sub>)[5]fullerene structures shown below.



1,2,4,6,7,9,11,12,14,16,18,20-Dodecaaza(C<sub>20</sub>-I<sub>h</sub>)[5]fullerane



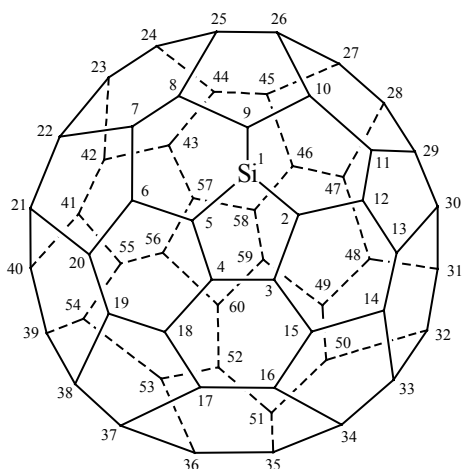
1,2,3,4,7,8,13,14,17,18,19,20-Dodecaaza(C<sub>20</sub>-I<sub>h</sub>)[5]fullerene<sup>1</sup>

<sup>1</sup> The double bonds in this structure are for illustrative purposes only. Double bonds are not shown in fullerene structures elsewhere in this report.

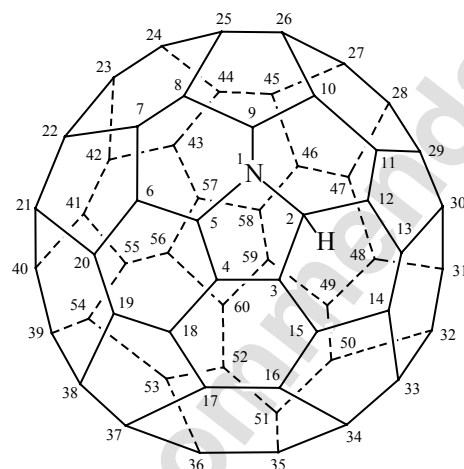


The heteroatoms include all elements capable of being tricoordinate, including metals and semimetals; no heteroatoms have attached hydrogen atoms. All carbon atoms of a fullerene may be replaced by the same or by different heteroatoms. Replacement of carbon atoms by trivalent heteroatoms may result in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

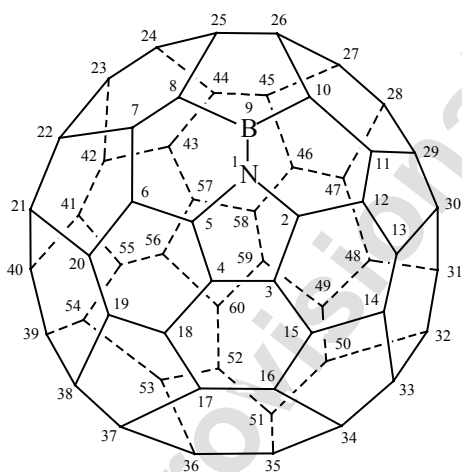
Examples:



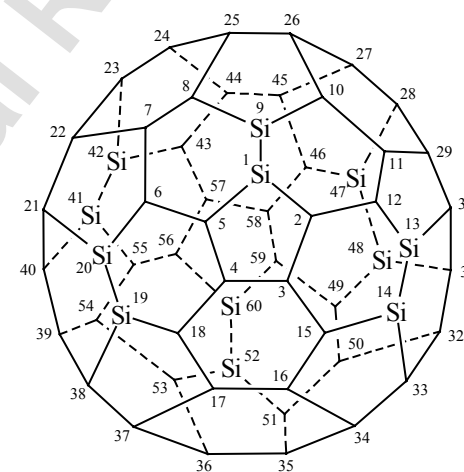
I



II



III



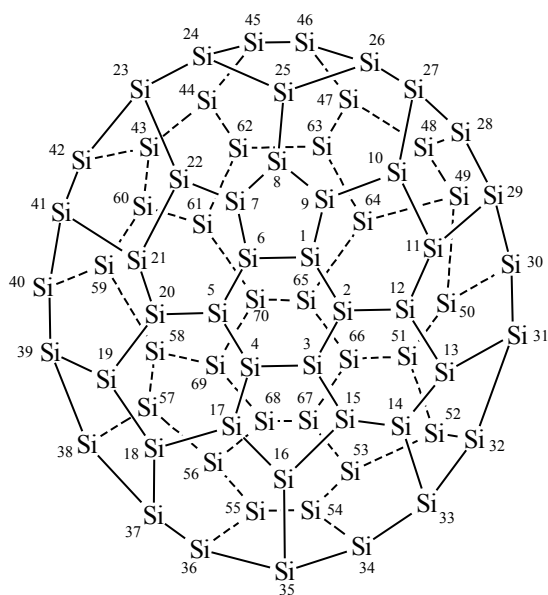
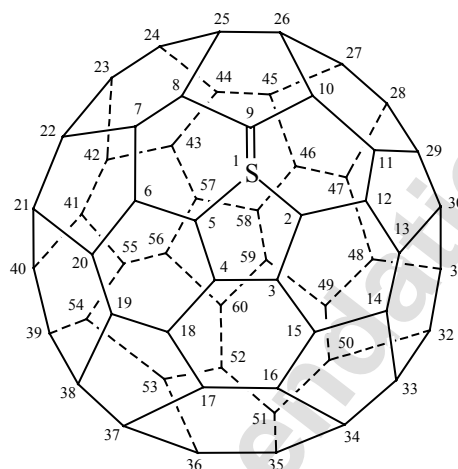
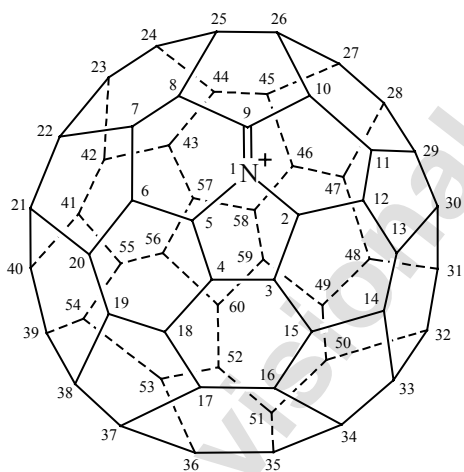
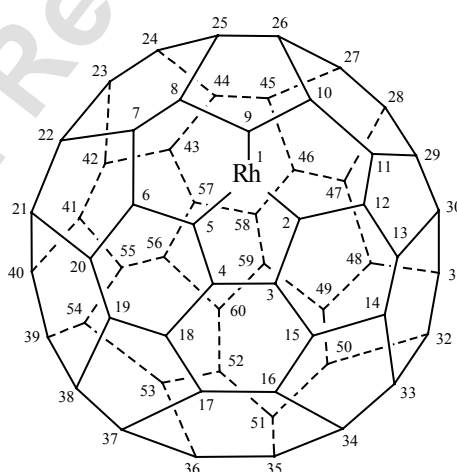
IV

I Sila(C<sub>60</sub>-I<sub>h</sub>)[5,6]fullerene

II 2H-1-Aza(C<sub>60</sub>-I<sub>h</sub>)[5,6]fullerene

III 1-Aza-9-bora(C<sub>60</sub>-I<sub>h</sub>)[5,6]fullerene

IV 1,9,13,14,19,20,41,42,47,48,52,60-Dodecasila(C<sub>60</sub>-I<sub>h</sub>)[5,6]fullerene

**V****VI****VII****VIII**

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

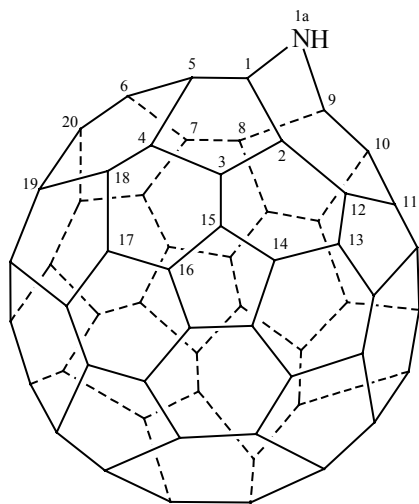
**VI**  $\lambda^4$ -Thia( $C_{60}-I_h$ )[5,6]fullerene

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

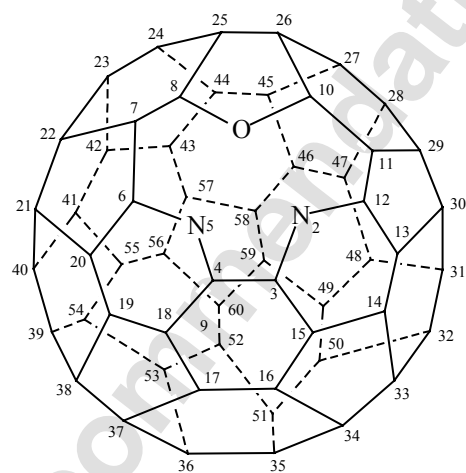
**VIII** Rhoda( $C_{60}-I_h$ )[5,6]fullerene

**Fu-5.2.** 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 before structure modifying prefixes. Structure modifying prefixes have preference for low locants over replacement prefixes.

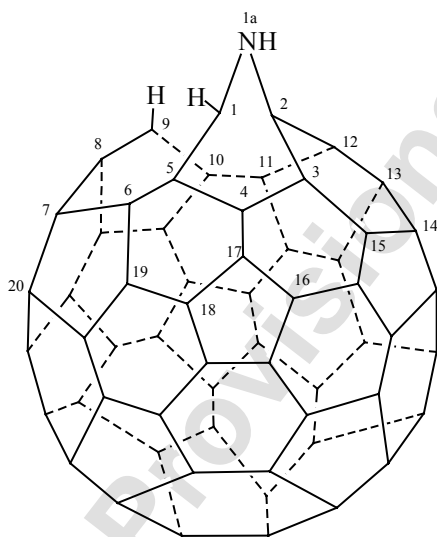
Examples:



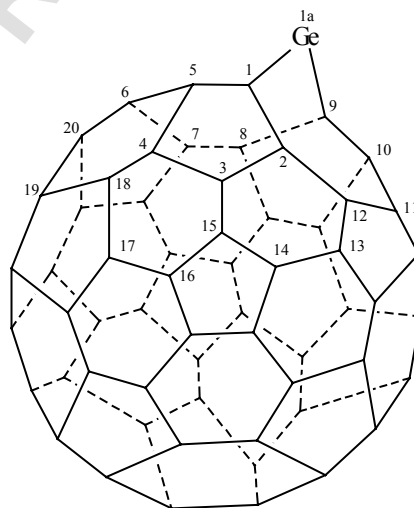
I



II



III



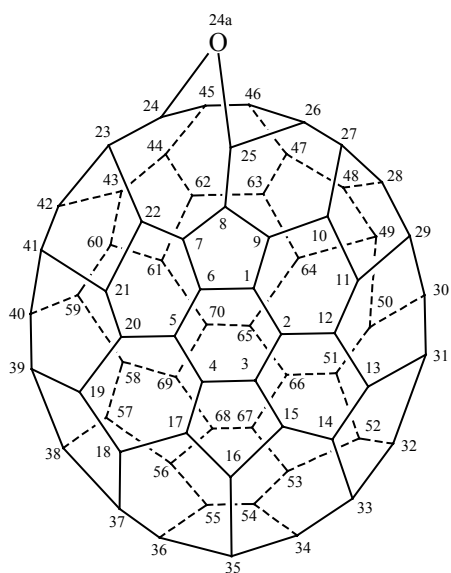
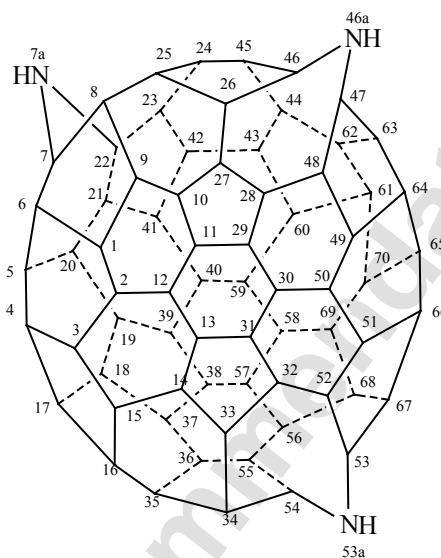
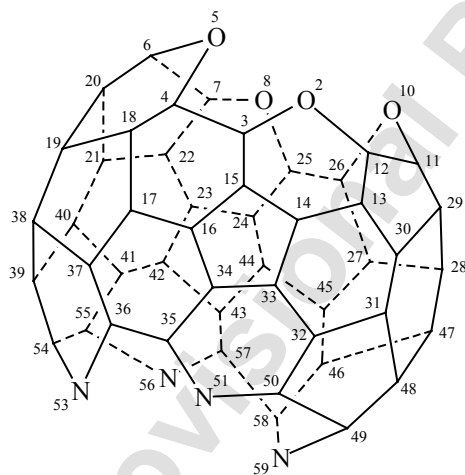
IV

I 1aH-1a-Aza-1(9)a-homo(C<sub>60</sub>-I<sub>h</sub>)[5,6]fullerene

II 9-Oxa-2,5-diaza-1-nor(C<sub>60</sub>-I<sub>h</sub>)fullerene

III 1aH-1a-Aza-1,9-seco-1(2)a-homo(C<sub>60</sub>-I<sub>h</sub>)[5,6]fullerene

IV 1aλ<sup>2</sup>-Germa-1(9)a-homo(C<sub>60</sub>-I<sub>h</sub>)[5,6]fullerene

**V****VI****VII**

**V** 24a-Oxa-24(25)a-homo( $C_{70}$ - $D_{5h(6)}$ )[5,6]fullerene

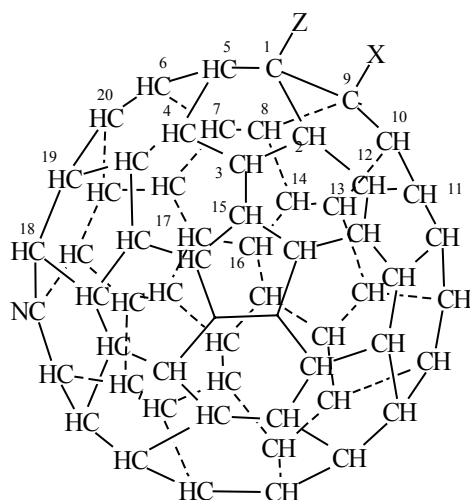
**VI** 7aH,46aH,53aH-7a,46a,53a-Triaza-7(8)a,46(47)a,53(54)a-trihomo-  
( $C_{70}$ - $D_{5h(6)}$ )[5,6]fullerene

**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** Fullerenes 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**  $Z = \bullet$ ;  $X = H$   
**II**  $Z = +$ ;  $X = H$   
**III**  $Z = \bullet$ ;  $X = -$   
**IV**  $Z = -$ ;  $X = H$   
**V**  $Z = \bullet$ ;  $X = -$   
**VI**  $Z = OH$ ;  $X = H$

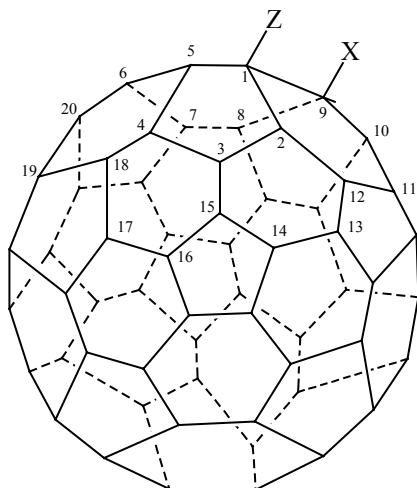
- I**  $(C_{60-I_h})[5,6]$ Fulleran-1-yl      **IV**  $(C_{60-I_h})[5,6]$ Fulleran-1-ide  
**II**  $(C_{60-I_h})[5,6]$ Fulleran-1-ylum      **V**  $(C_{60-I_h})[5,6]$ Fulleran-9-id-1-yl  
**III**  $(C_{60-I_h})[5,6]$ Fulleran-9-ylum-1-yl      **VI**  $(C_{60-I_h})[5,6]$ Fulleran-1-ol

**Fu-6.2** 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 IUPAC Preliminary Survey 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]fullerene. However, this leads to difficulties since such names are, in fact, formed by coordination nomenclature (bromo is the 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]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(9H)-ol will 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):

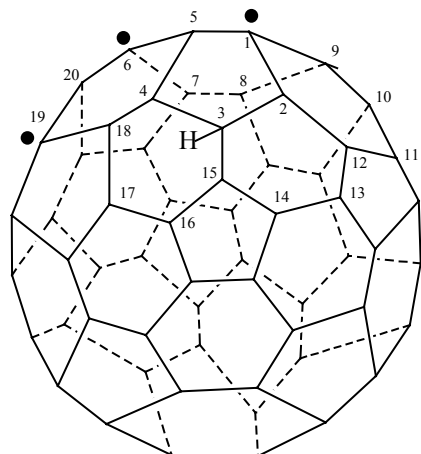


- I**  $Z = \bullet$  ;  $X = H$   
**II**  $Z = +$  ;  $X = H$   
**III**  $Z = \bullet$  ;  $X = +$   
**IV**  $Z = -$  ;  $X = H$   
**V**  $Z = \bullet$  ;  $X = -$   
**VI**  $Z = \bullet$  ;  $X = \bullet$

- I** ( $C_{60}$ - $I_h$ )[5,6]Fulleren-1(9H)-yl      **IV** ( $C_{60}$ - $I_h$ )[5,6]Fulleren-1(9H)-ide  
**II** ( $C_{60}$ - $I_h$ )[5,6]Fulleren-1(9H)-ylium      **V** ( $C_{60}$ - $I_h$ )[5,6]Fulleren-9-id-1(9H)-yl<sup>1</sup>  
**III** ( $C_{60}$ - $I_h$ )[5,6]Fulleren-9-ylium-1(9H)-yl<sup>1</sup>      **VI** ( $C_{60}$ - $I_h$ )[5,6]Fullerene-1,9-diyl<sup>2</sup>

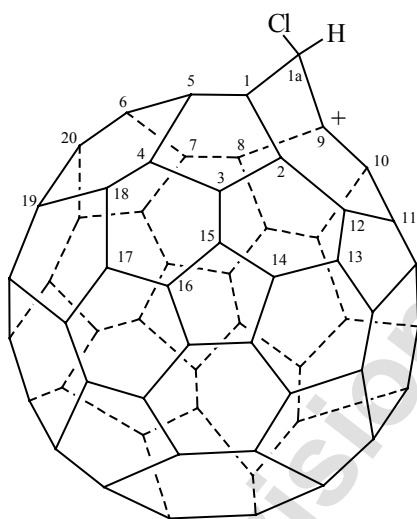
<sup>1</sup> The hydrogen atom needed for the -ide or -ylium suffix is provided by the added hydrogen required by the -yl suffix.

<sup>2</sup> Added hydrogen is not used since the multiple suffixes simply remove a double bond, as in naphthalene-4a,8a-diol

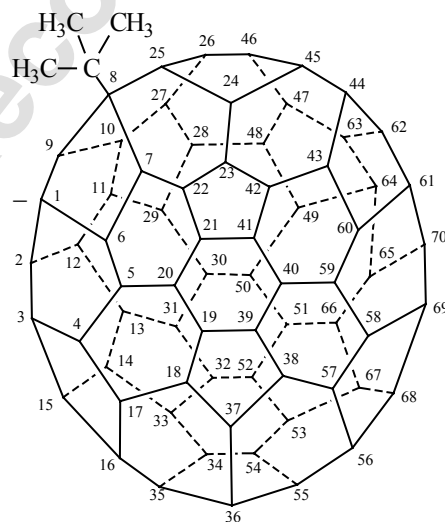


$(C_{60-I_h})[5,6]$ Fullerene-1,6,19(3H)-triyl<sup>2</sup>

Examples (substituted derivatives):

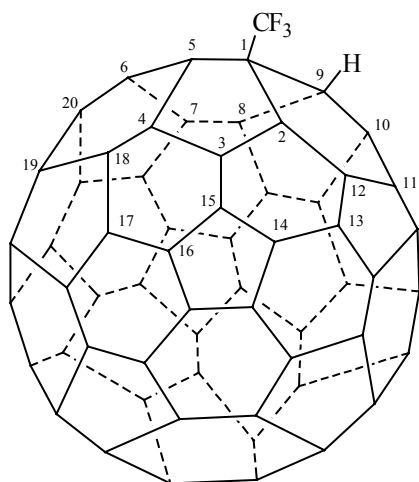


**I**

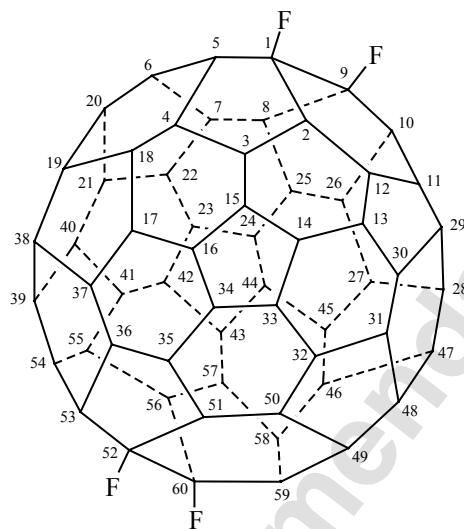


**II**

IUPAC Provisional Recommendation



III



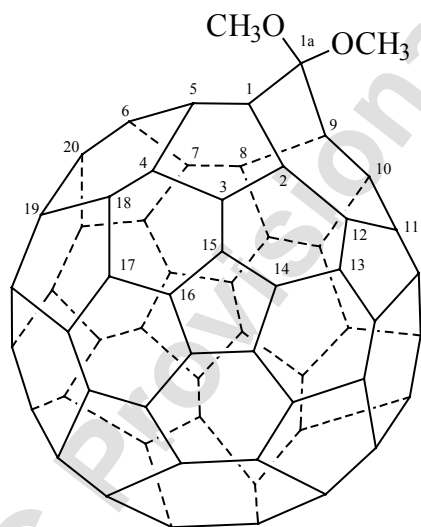
IV

**I** 1a-Chloro-1a*H*-1(9)a-homo( $C_{60}$ - $I_h$ )[5,6]fulleren-1(9*H*)-ylium

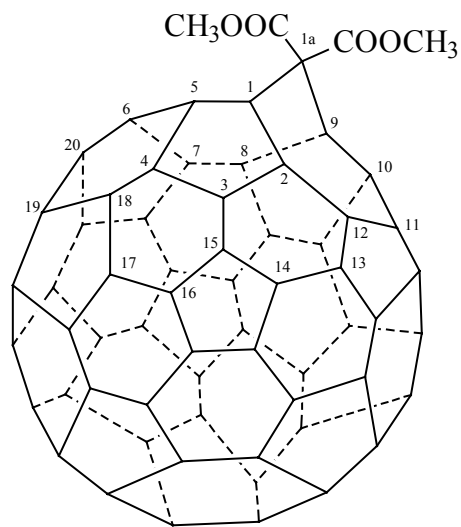
**II** 8-*tert*-Butyl( $C_{70}$ - $D_{5h(6)}$ )[5,6]fulleren-1(8*H*)-ide<sup>1</sup>

**III** 1-(Trifluoromethyl)-1,9-dihydro( $C_{60}$ - $I_h$ )[5,6]fullerene<sup>2</sup>

**IV** 1,9,52,60-Tetrafluoro-1,9,52,60-tetrahydro( $C_{60}$ - $I_h$ )[5,6]fullerene



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

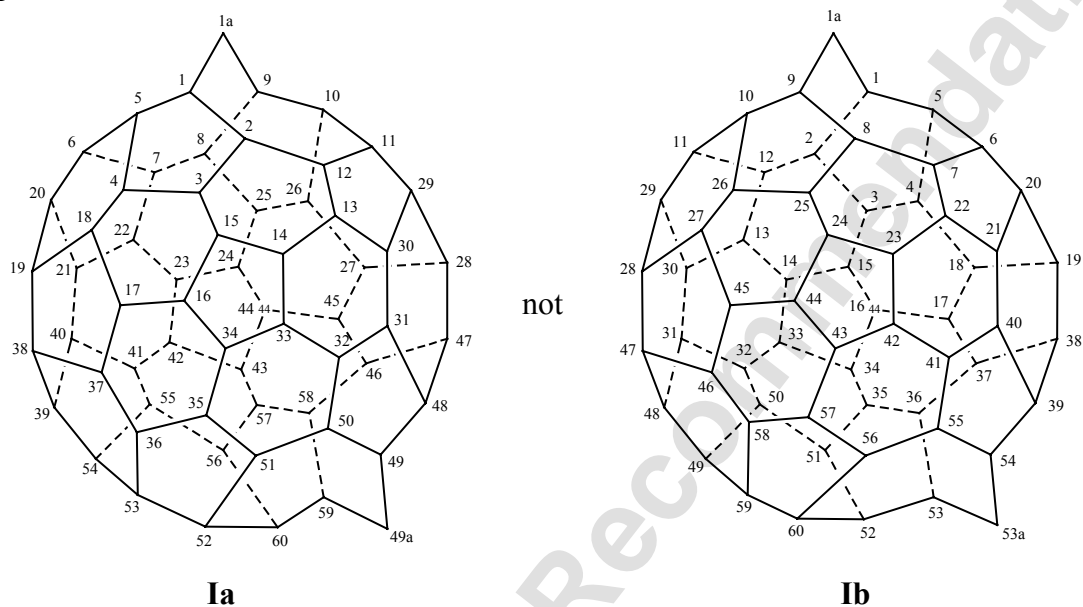
<sup>1</sup> CAS index name: [5,6]Fullerene- $C_{70}$ - $D_{5h(6)}$ , 8-(1,1-dimethylethyl)-1,8-dihydro-, ion(1-)

<sup>2</sup> Hydro prefixes are treated as nondetachable in this paper.



**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 twelve five-membered rings and proceed around the chosen five-membered ring in either direction

Example:

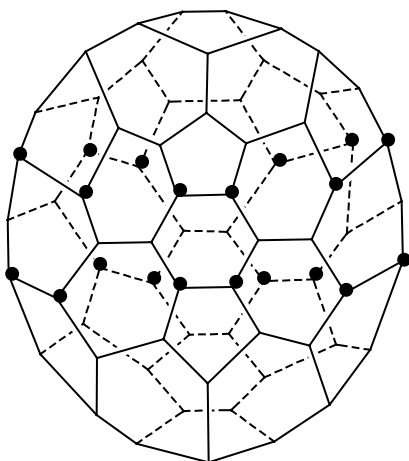
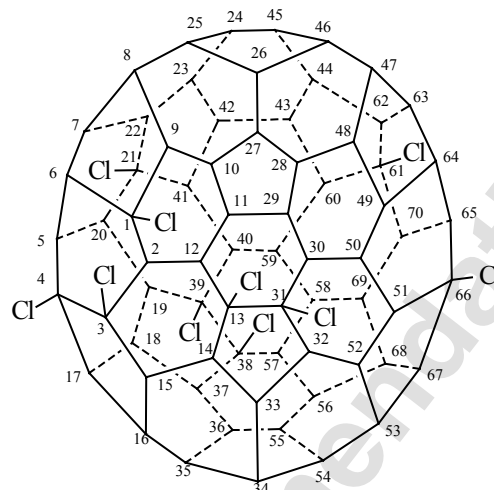


1aH,49aH-1(9)a,49(59)a-Dihomo( $C_{60}-I_h$ )[5,6]fullerene (**Ia**)

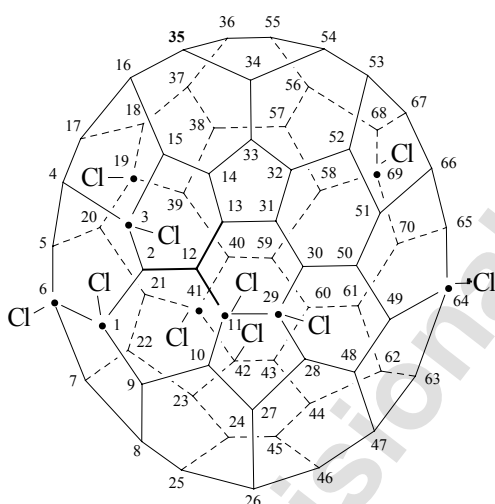
[not 1aH,53aH-1(9)a,53(54)a-Dihomo( $C_{60}-I_h$ )[5,6]fullerene (**Ib**);  
the locant set 1,9,49,59 is lower than 1,9,53,54]

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  $D_5$  axis, as shown by the enlarged dots in **Ia** of the example below, but may proceed in only one direction from each position.

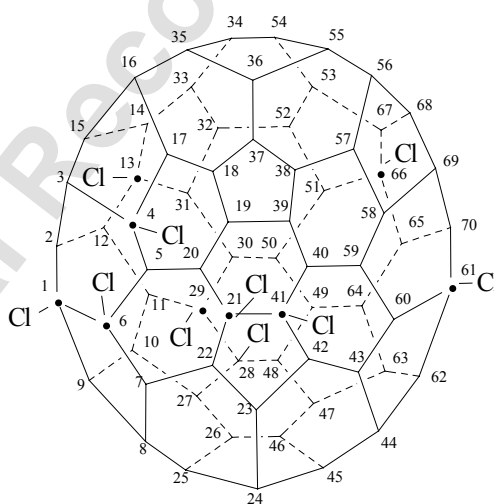
Example:

**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...]

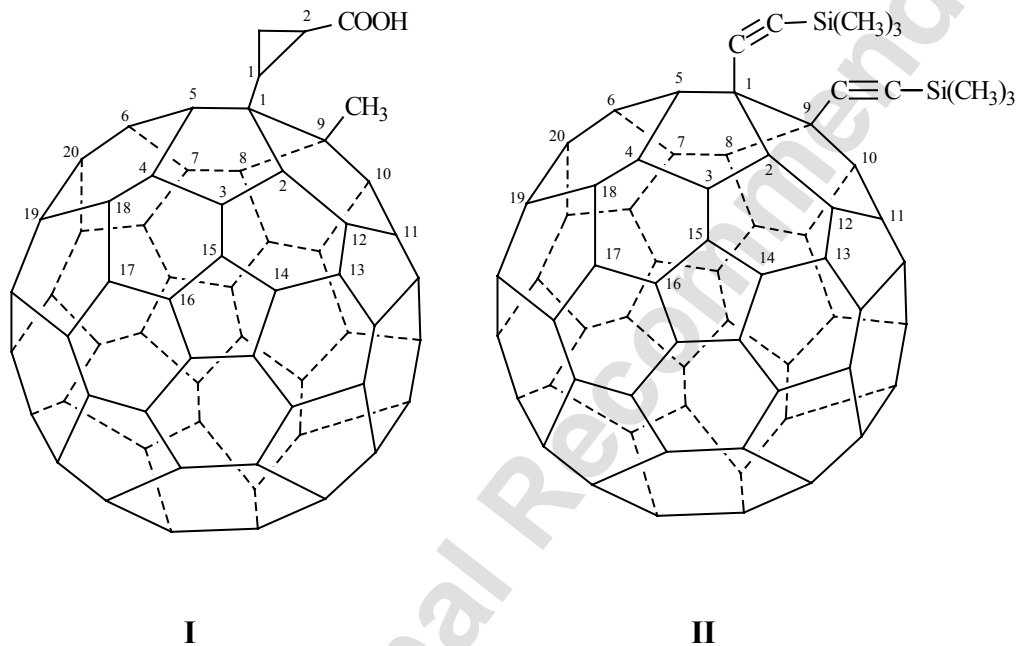
[not 1,4,6,13,21,28,29,41,61,66-Decachloro-1,4,6,13,21,28,29,41,61,66-decahydro( $C_{70}-D_{5h(6)}$ )[5,6]fullerene (**Id**); the locant set 1,3,4... is lower than 1,4,6...]

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:



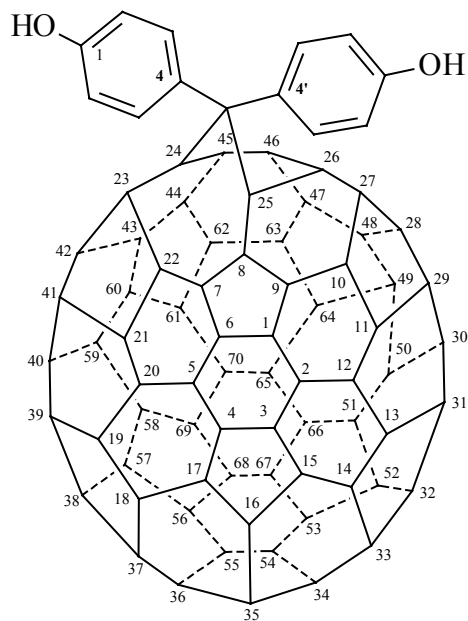
- I** 2-[9-Methyl( $C_{60}$ - $I_h$ )[5,6]fulleren-1(9*H*)-yl]cyclopropanecarboxylic acid  
**II** [( $C_{60}$ - $I_h$ )[5,6]Fullerene-1,9-diyldiethyne-2,1-diyl]bis[trimethylsilane]<sup>1</sup>

or

Hexamethyl[( $C_{60}$ - $I_h$ )[5,6]fullerene-1,9-diyldiethyne-2,1-diyl]bis[silane]<sup>2</sup>

<sup>1</sup> A CAS multiplicative name.

<sup>2</sup> An IUPAC multiplicative name.

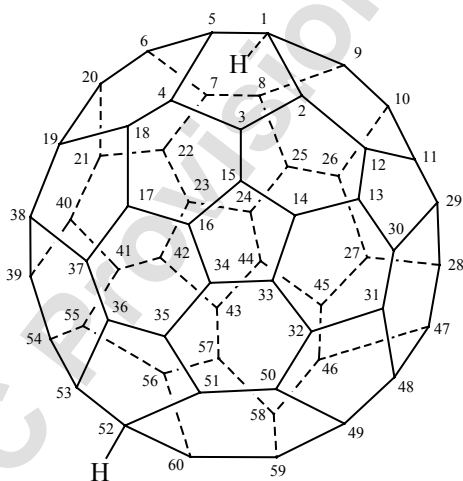


III

III 4,4'-[24a*H*-24(25)a-Homo(C<sub>70</sub>-D<sub>5h</sub>(6))][5,6]fullerene-24a,24a-diyl]diphenol

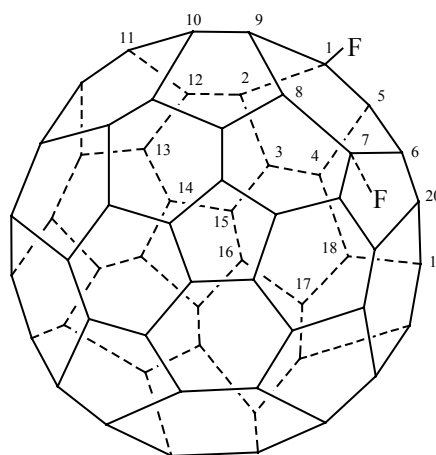
**Fu-6.5. *endo*-Substituted fullerenes and fullerenes.** Some fullerene substituents are small enough so they can project into the fullerene cage. All substituents are assumed to project away from the fullerene cage unless otherwise specified. To describe substituents that project into the cage, the term *endo*, enclosed in parentheses, is cited after the appropriate locant.

Examples:



I

I 1(*endo*),52-Dihydro(C<sub>60</sub>-I<sub>h</sub>)[5,6]fullerene



II

II 1,7(*endo*)-Difluoro-1,7-dihydro(C<sub>60</sub>-I<sub>h</sub>)[5,6]fullerene

### Fu-7. 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 (ref. 8). 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.

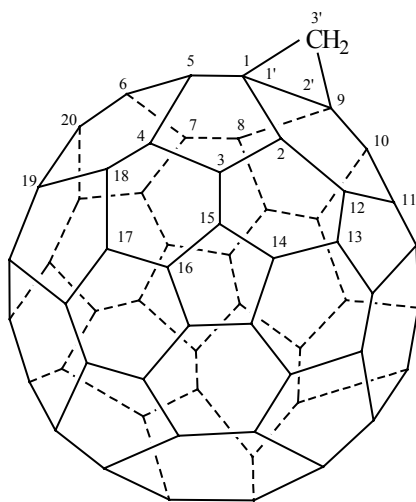
**Note:** Although when the nonfullerene component is a simple ring, such as cyclopropane or oxirene, the additional atoms could be cited by means of bridge prefixes, such as methano and epoxy, for consistency it is recommended that all be named as fused systems. Both methods were included in the IUPAC Preliminary Survey (ref. 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 (ref. 9) contains many examples of a fullerene fused to two organic rings which themselves are connected by a bridge. For bridged fullerenes, see below.

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 section on spiro fullerenes below). 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.

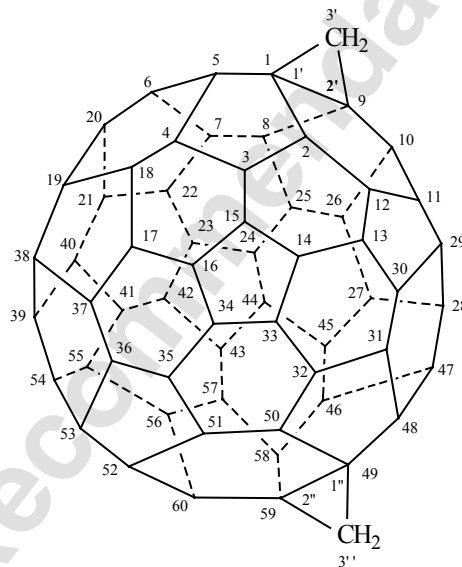
**Note:** CAS prefixes the fullerene name to that of a heterocyclic ring system when the latter has a heteroatomic component preferred to the fullerene component (ref. 3). For example, a fullerene component with no heteroatoms would be prefixed to any heterocyclic component, but a heterocyclic component would be prefixed to an azafullerene component. When the nonfullerene component is a heterocycle, CAS names are formed by prefixing the name of the fullerene to the name of the heterocycle. 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 base component 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

nonfullerene 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:



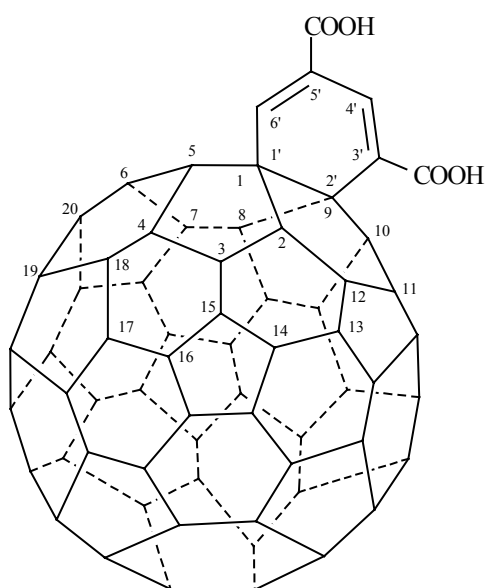
**I**



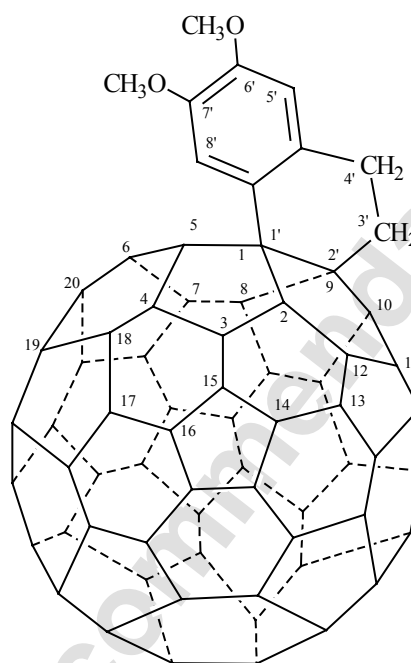
**II**

**I** 3'*H*-Cyclopropa[1,9](C<sub>60</sub>-I<sub>h</sub>)[5,6]fullerene

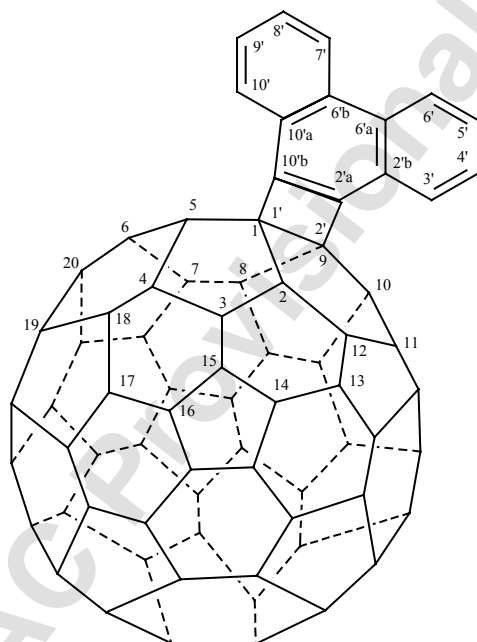
**II** 3'*H*,3''*H*-Dicyclopropa[1,9:49,59](C<sub>60</sub>-I<sub>h</sub>)[5,6]fullerene



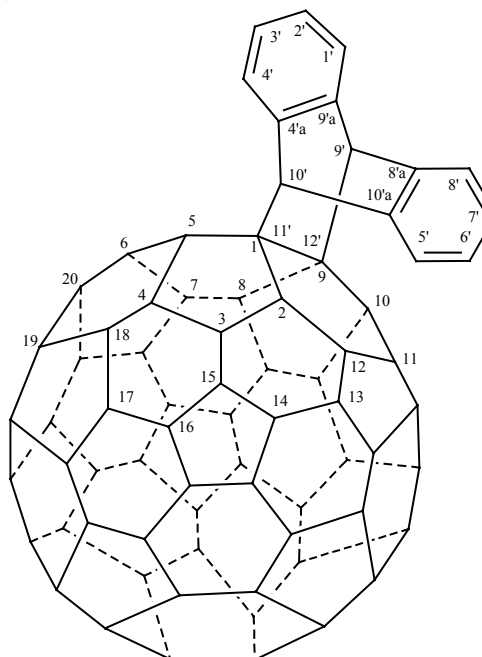
III



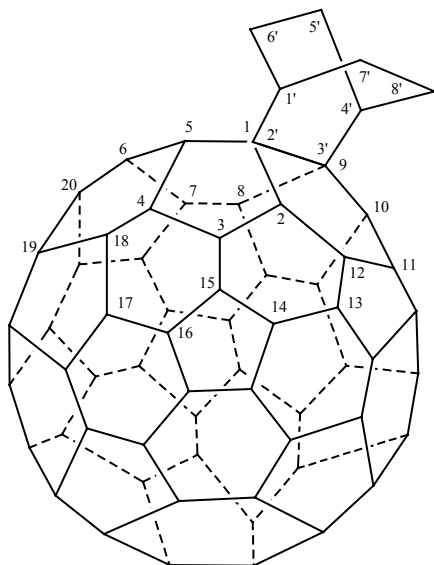
IV



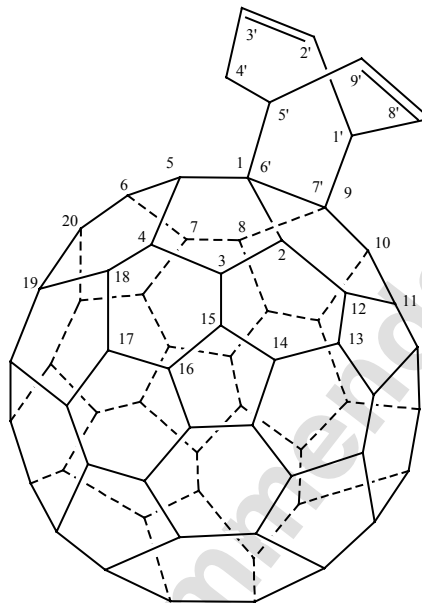
V



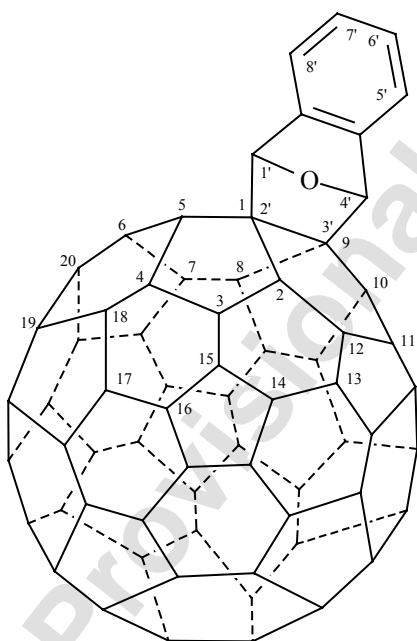
VI



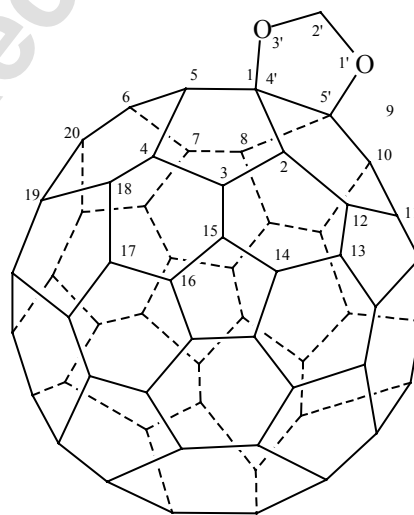
VII



VIII



IX



X

III Benzo[1,9](C<sub>60</sub>-I<sub>h</sub>)[5,6]fullerene-3',5'-dicarboxylic acid

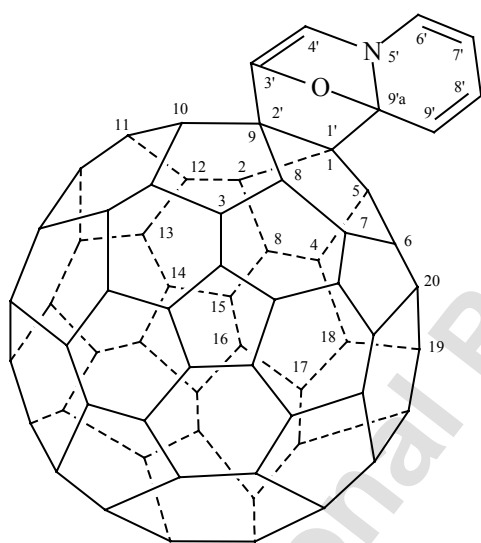
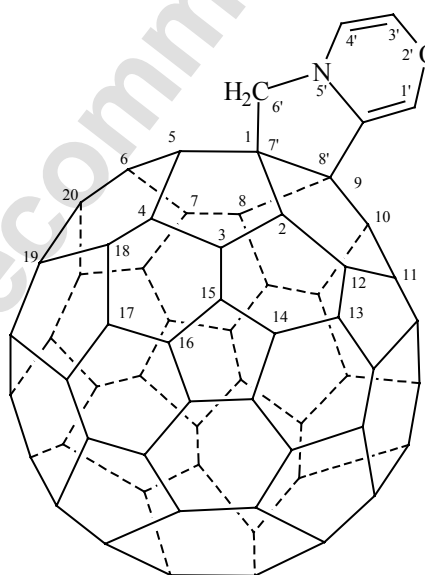
IV 6',7'-Dimethoxy-3',4'-dihydronaphtho[1',2':1,9](C<sub>60</sub>-I<sub>h</sub>)[5,6]fullerene<sup>1</sup>

V Cyclobuta[1]phenanthro[1',2':1,9](C<sub>60</sub>-I<sub>h</sub>)[5,6]fullerene

<sup>1</sup> Hydro prefixes are treated as nondetachable in this paper.



- VI** 9',10'-Dihydro[9,10]ethanoanthra[11',12':1,9](C<sub>60</sub>-I<sub>h</sub>)[5,6]fullerene
- VII** Bicyclo[2.2.2]octano[2',3':1,9](C<sub>60</sub>-I<sub>h</sub>)[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<sub>60</sub>-I<sub>h</sub>)[5,6]fullerene  
(not Bicyclo[3.2.2]nona[2,6]dieno[8',9':1,9](C<sub>60</sub>-I<sub>h</sub>)[5,6]fullerene; here there is a choice in numbering and the fusion sites are preferred for lower locants)
- IX** 1',4'-Dihydro[1,4]epoxynaphtho[2',3':1,9](C<sub>60</sub>-I<sub>h</sub>)[5,6]fullerene
- X** [1,3]Dioxolo[4',5':1,9](C<sub>60</sub>-I<sub>h</sub>)[5,6]fullerene<sup>1</sup>

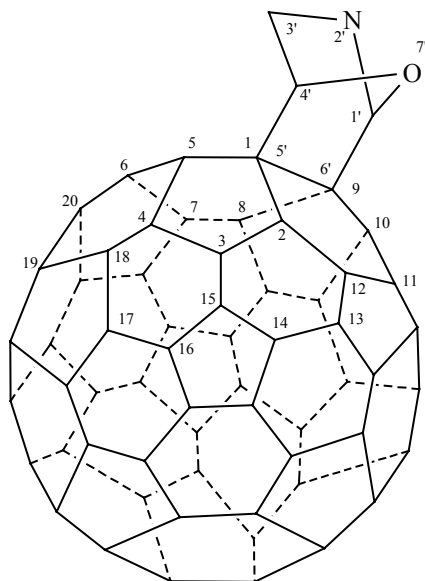
**XI****XII**

- XI** [3,9a]Epoxyquinolizino[1',2':1,9](C<sub>60</sub>-I<sub>h</sub>)[5,6]fullerene<sup>2</sup>
- XII** 6'*H*-Pyrrolo[2,1-*c*][1,4]oxazino[7',8':1,9](C<sub>60</sub>-I<sub>h</sub>)[5,6]fullerene<sup>3</sup>

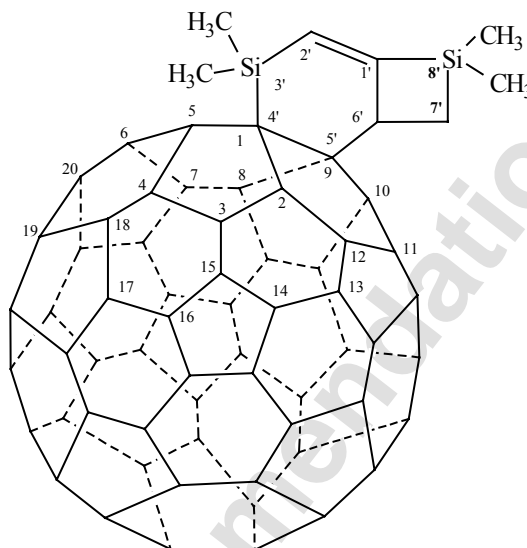
<sup>1</sup> The CAS name is [5,6]Fullereno-C<sub>60</sub>-I<sub>h</sub>-[1,9-*d*][1,3]dioxole

<sup>2</sup> The CAS name is [5,6]Fullereno-C<sub>60</sub>-I<sub>h</sub>-[1,9-*a*][3,9a]epoxy[9a*H*]quinolizine

<sup>3</sup> The CAS name 6'*H*-[5,6]Fullereno-C<sub>60</sub>-I<sub>h</sub>-[1',9':7,8]pyrrolo[2,1-*c*][1,4]oxazine



XIII



XIV

**XIII** [7]Oxa[2]azabicyclo[2.2.1]heptano[5',6':1,9](C<sub>60</sub>-I<sub>h</sub>) [5,6]fullerene<sup>1</sup>

**XIV** 3',3',8',8'-Tetramethyl[3,8]disilabicyclo[4.2.0]oct[1]eno[4',5':1,9]-(C<sub>60</sub>-I<sub>h</sub>)[5,6]fullerene<sup>2</sup>

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 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 just given.

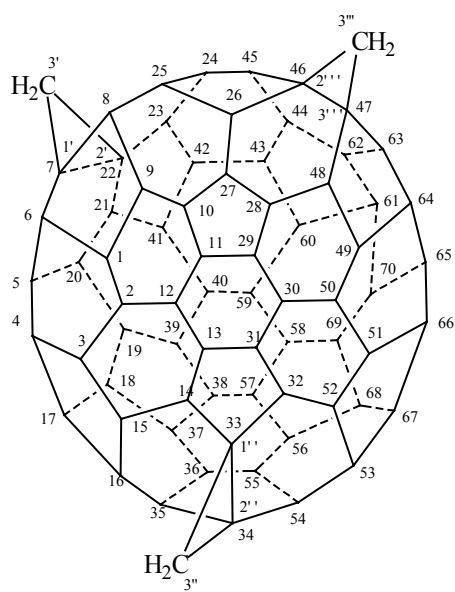
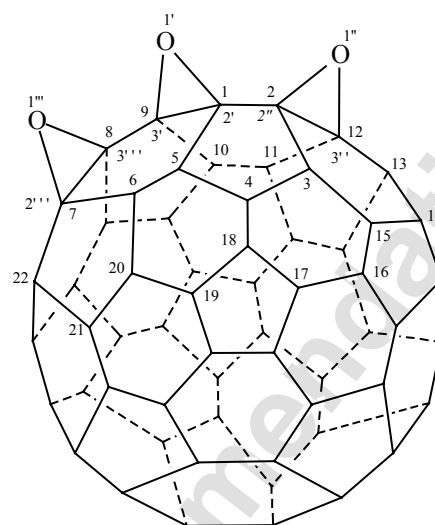
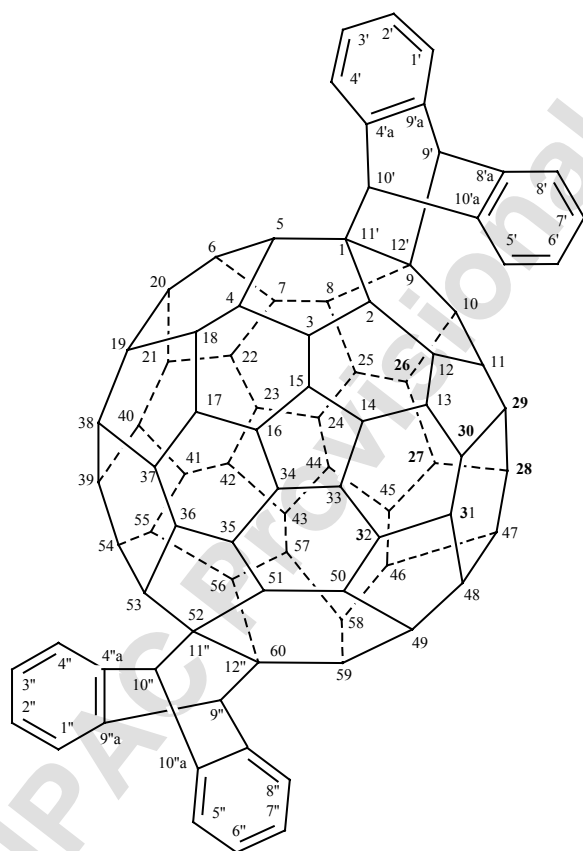
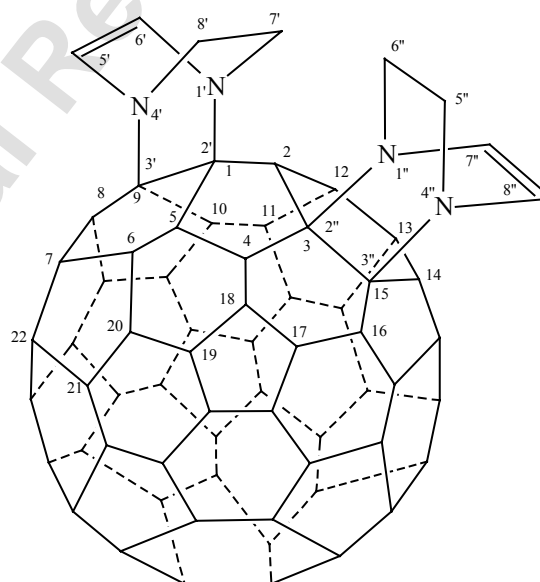
**Note 1:** As shown by examples V and VI, below, the fullerene fusion locants are assigned based on the lowest set of locants for all fusion sites at the first point of difference when compared term by term in ascending numerical order. Primes for the nonfullerene fusion components are assigned in order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

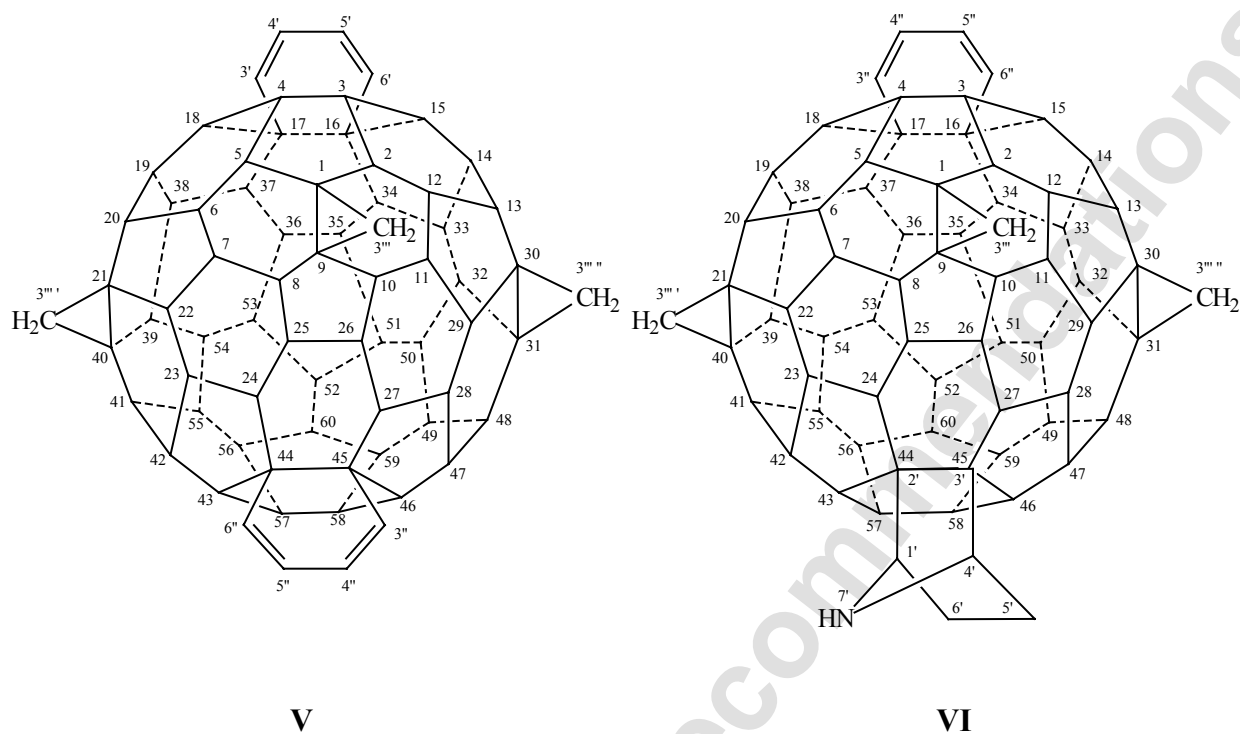
**Note 2:** Fullerene fusion locants are not assigned on the basis of the lowest locants for nonfullerene fusion components first cited in the name.

<sup>1</sup> The CAS name is [5,6]Fullereno-C<sub>60</sub>-I<sub>h</sub>-[1',9':5,6][7]oxa[2]azabicyclo[2.2.1]heptane

<sup>2</sup> The CAS name is 3',3',8',8'-tetramethyl[5,6]fullereno-C<sub>60</sub>-I<sub>h</sub>-[1',9':4,5][3,8]disilabicyclo[4.2.0]oct[1]ene

Examples:

**I****II****III****IV**



- I** 3'H,3''H,3'''H-Tricyclopropa[7,22:33,34:46,47](C<sub>70</sub>-D<sub>5h(6)</sub>)[5,6]fullerene
- II** Trisoxireno[2',3':1,9; 2'',3'':2,12; 2''',3''':7,8](C<sub>60</sub>-I<sub>h</sub>)[5,6]fullerene<sup>1</sup>
- III** 9',9'',10',10'''-Tetrahydrobis[9,10]ethanoanthra[11',12':1,9;11'',12'':52,60](C<sub>60</sub>-I<sub>h</sub>)-[5,6]fullerene
- IV** Bis[1,4]diazabicyclo[2.2.2]oct[5]eno[2',3':1,9;2'',3'':3,15](C<sub>60</sub>-I<sub>h</sub>)[5,6]fullerene<sup>2</sup>
- V** 3'''H,3''' 'H,3''' ''H-Dibenzo[16,17:44,45]tricyclopropa[1,9:21,40:30,31](C<sub>60</sub>-I<sub>h</sub>)-[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<sub>60</sub>-I<sub>h</sub>)[5,6]fullerene<sup>3</sup>

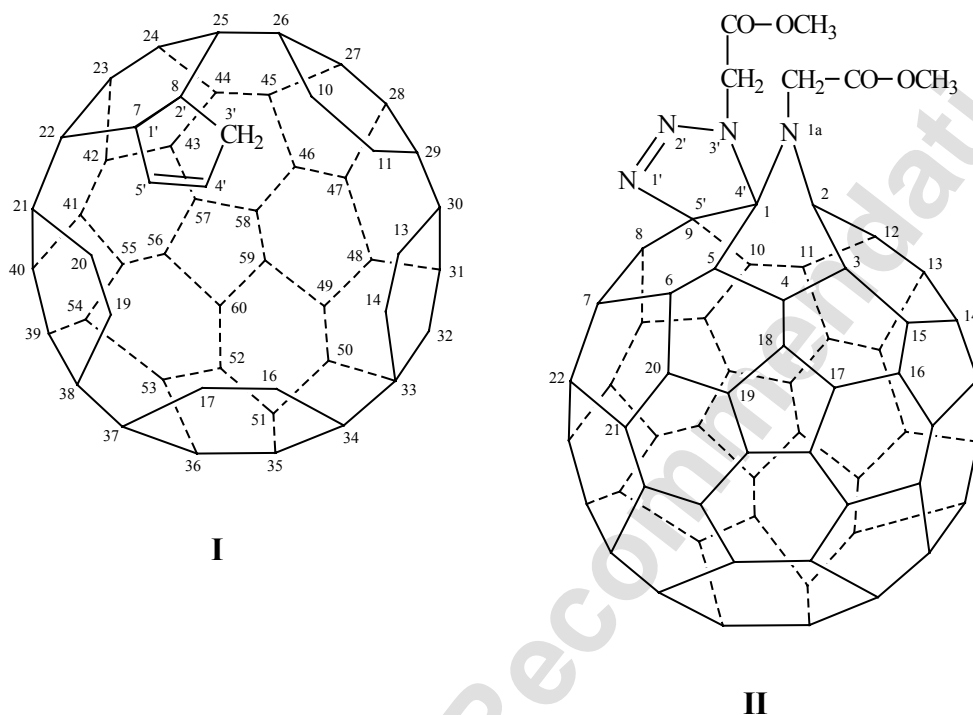
The fusion principles described above for fullerenes are fully applicable to modified fullerenes.

<sup>1</sup> The CAS name is [5,6]Fullereno-C<sub>60</sub>-I<sub>h</sub>-[1,9-b:2,12-b';3,15-b'']trisoxirene

<sup>2</sup> The CAS name is [5,6]Fullereno-C<sub>60</sub>-I<sub>h</sub>-[1'',9'':2,3;3'',15'':2',3']bis[1,4]diazabicyclo[2.2.2]oct[5]ene

<sup>3</sup> The CAS 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<sub>60</sub>-I<sub>h</sub>-52',60':2,3][1,4]diazabicyclo[2.2.2]octane

Examples:



- I** 3'*H*-Cyclopenta[7,8]-1,2,3,4,5,6,9,12,15,18-decanor(C<sub>60</sub>-I<sub>h</sub>)[5,6]fullerene  
**II** Dimethyl 2,2'-[1*aH*,3'*H*-[1,2,3]triazolo[4',5':1,9]-1*a*-aza-1(2)*a*-homo(C<sub>60</sub>-I<sub>h</sub>)-[5,6]fullerene-1*a*,3'-diyl]diacetate<sup>1</sup>

or

Dimethyl 1*aH*,3'*H*-[1,2,3]triazolo[4',5':1,9]-1*a*-aza-1(2)*a*-homo(C<sub>60</sub>-I<sub>h</sub>)[5,6]-fullerene-1*a*,3'-diacetate (a conjunctive name)

### 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. 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.

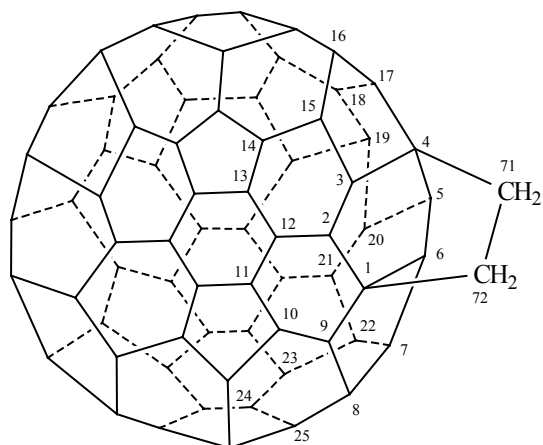
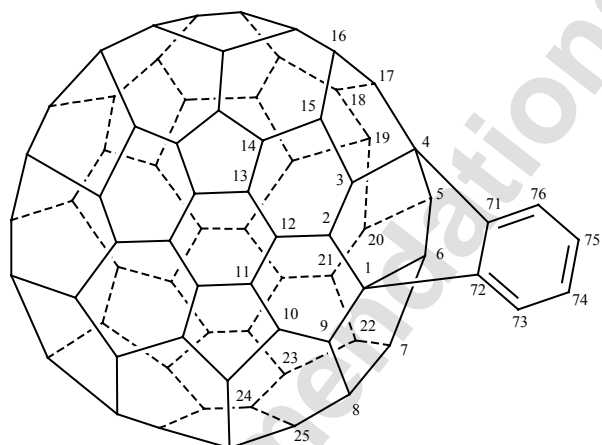
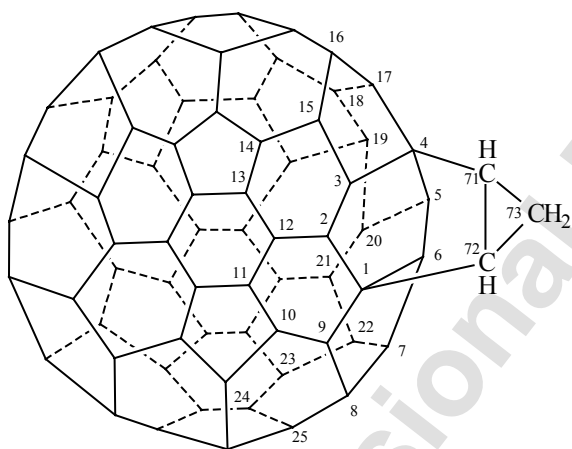
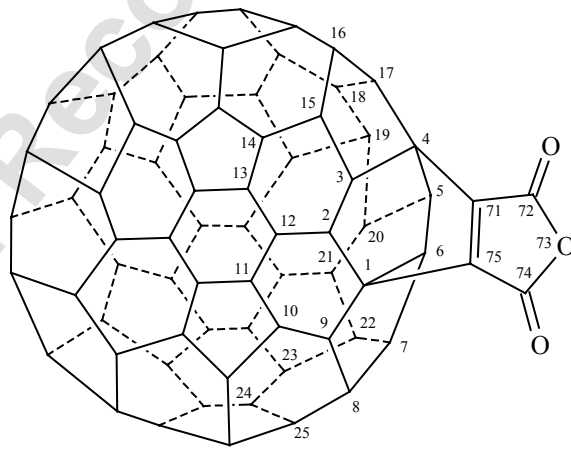
Bridges between rings fused to a fullerene and a parent fullerene or between two different rings fused to the same fullerene are named using established bridge prefix names. In the latter case, citation of bridge components and numbering begins with the bridge atom adjacent to the fused

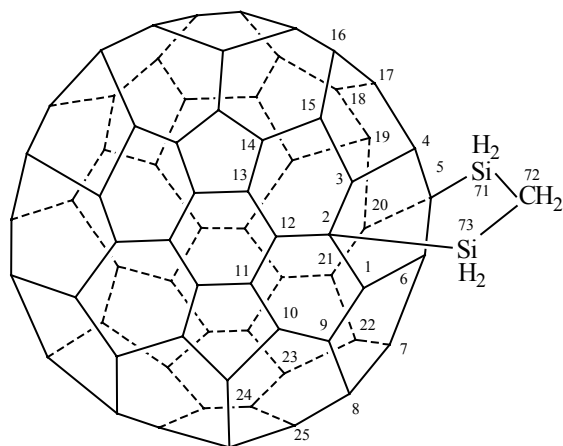
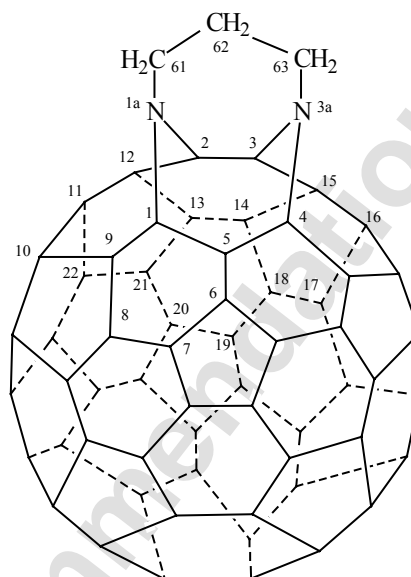
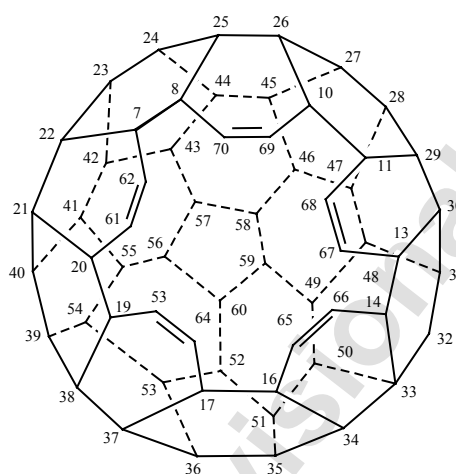
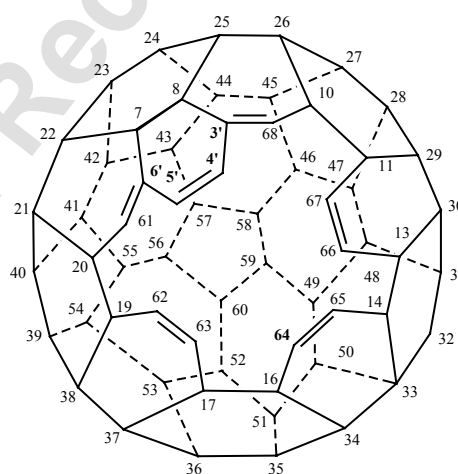
<sup>1</sup> The CAS name is 3'*H*-[1,2,3]Triazolo[4',5':1,9]-2*a*-aza-1,2(2*a*)-homo[5,6]fullereneC<sub>60</sub>-I<sub>h</sub>-2*a*,3'-diacetic acid, dimethyl ester

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.

IUPAC Provisional Recommendations

Examples:

**I****II****III****IV****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<sup>1</sup>**III** 72,73-Dihydro-71H-1,4-epicyclopropa( $C_{70}$ - $D_{5h(6)}$ )[5,6]fullerene<sup>2</sup>**IV** 1,4-[3,4]Furano( $C_{70}$ - $D_{5h(6)}$ )[5,6]fullerene-72,74-dione<sup>3</sup><sup>1</sup> The CAS name is 1,4[1',2']-Benzeno[5,6]fullerene- $C_{70}$ - $D_{5h(6)}$ <sup>2</sup> The CAS name is 72,73-Dihydro-71H-1,4-endo-cyclopropa[5,6]fullerene- $C_{70}$ - $D_{5h(6)}$ <sup>3</sup> The CAS name is 1,4[3',4']-Furano[5,6]fullerene- $C_{70}$ - $D_{5h(6)}$ -72,74-dione

**V****VI****VII****VIII**

**V** 2,5-(Silanomethanosilano)(C<sub>70</sub>-D<sub>5h(6)</sub>)[5,6]fullerene

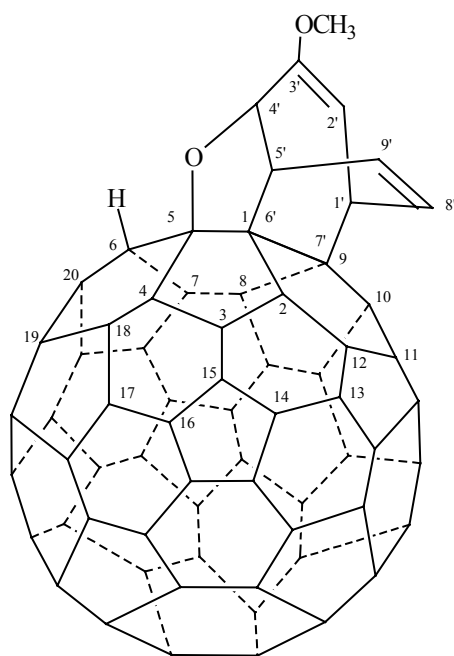
**VI** 1a,3a-Propano-1aH,3aH-1a,3a-diaza-1(2)a:3(4)a-dihomo(C<sub>60</sub>-I<sub>h</sub>)[5,6]fullerene

**VII** 7,20:8,10:11,13:14,16,17:19-Pentaetheno-1,2,3,4,5,6,9,12,15,18-decanor(C<sub>60</sub>-I<sub>h</sub>)-[5,6]fullerene

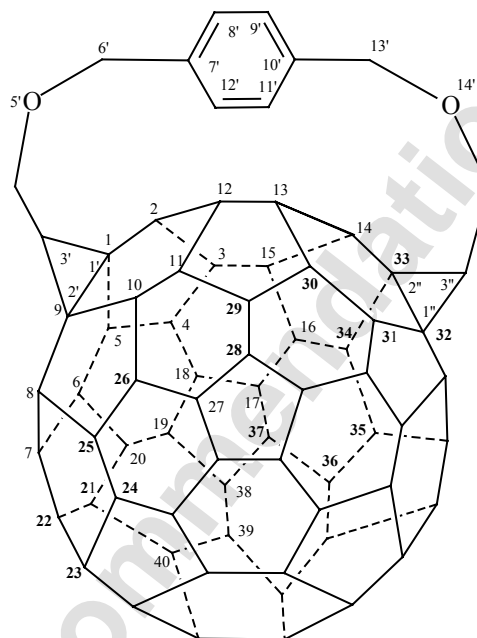
**VIII** 11,13:14,16:17,19-Trietheno-3',10:6',20-dimethenobenzo[7,8]-1,2,3,4,5,6,9,-12,15,18-decanor(C<sub>60</sub>-I<sub>h</sub>)[5,6]fullerene<sup>1</sup>

<sup>1</sup> The current CAS 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<sub>60</sub>-I<sub>h</sub>





IX



X

**IX** 3'-Methoxy-6*H*-4',5-epoxybicyclo[3.2.2]nona[2,8]dieno[6',7':1,9](C<sub>60</sub>-I<sub>h</sub>)[5,6]-fullerene

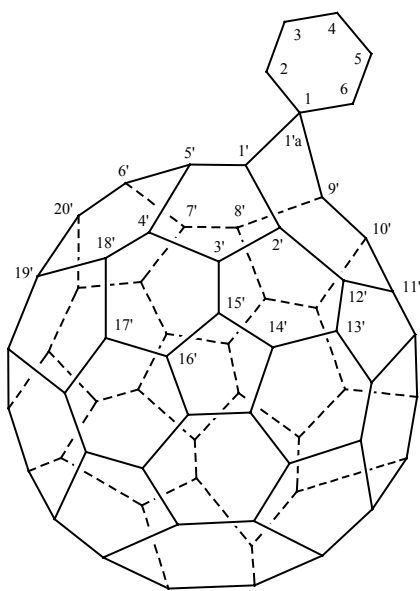
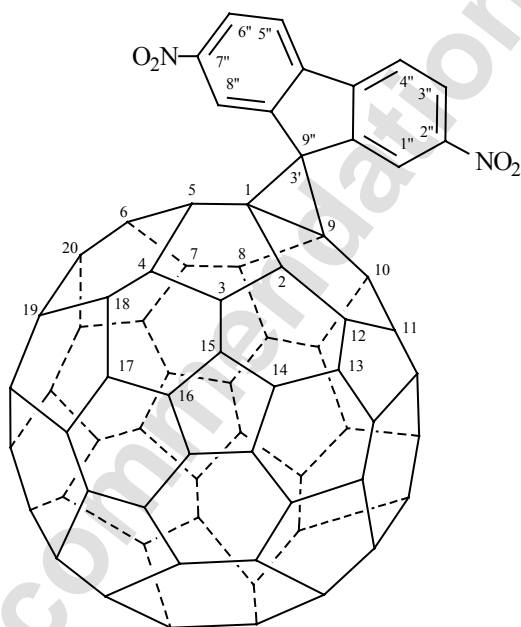
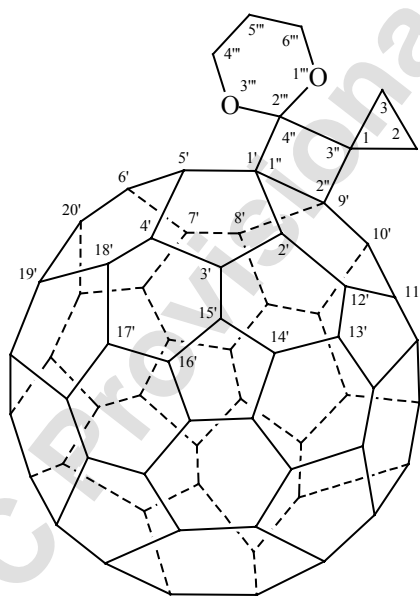
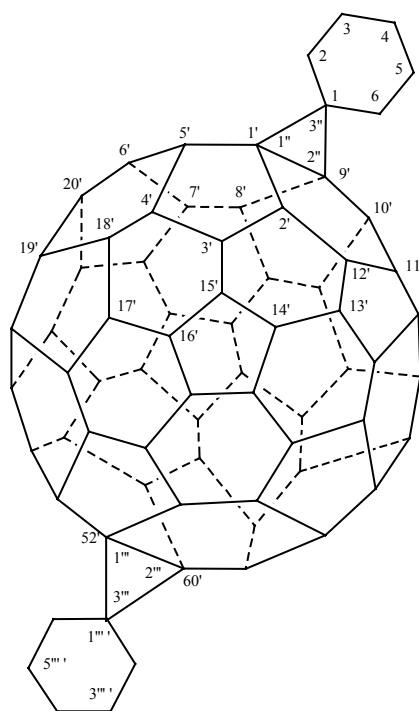
**X** 3',3''-(Methanoxymethano[1,4]benzenomethanoxymethano)-3'*H*,3''*H*-dicyclopropa-[1,9:32,33](C<sub>60</sub>-I<sub>h</sub>)[5,6]fullerene

### 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. Spiro fullerene parent hydrides will not necessarily have unprimed numbers as locants.

Examples:

**I****II****III****IV**

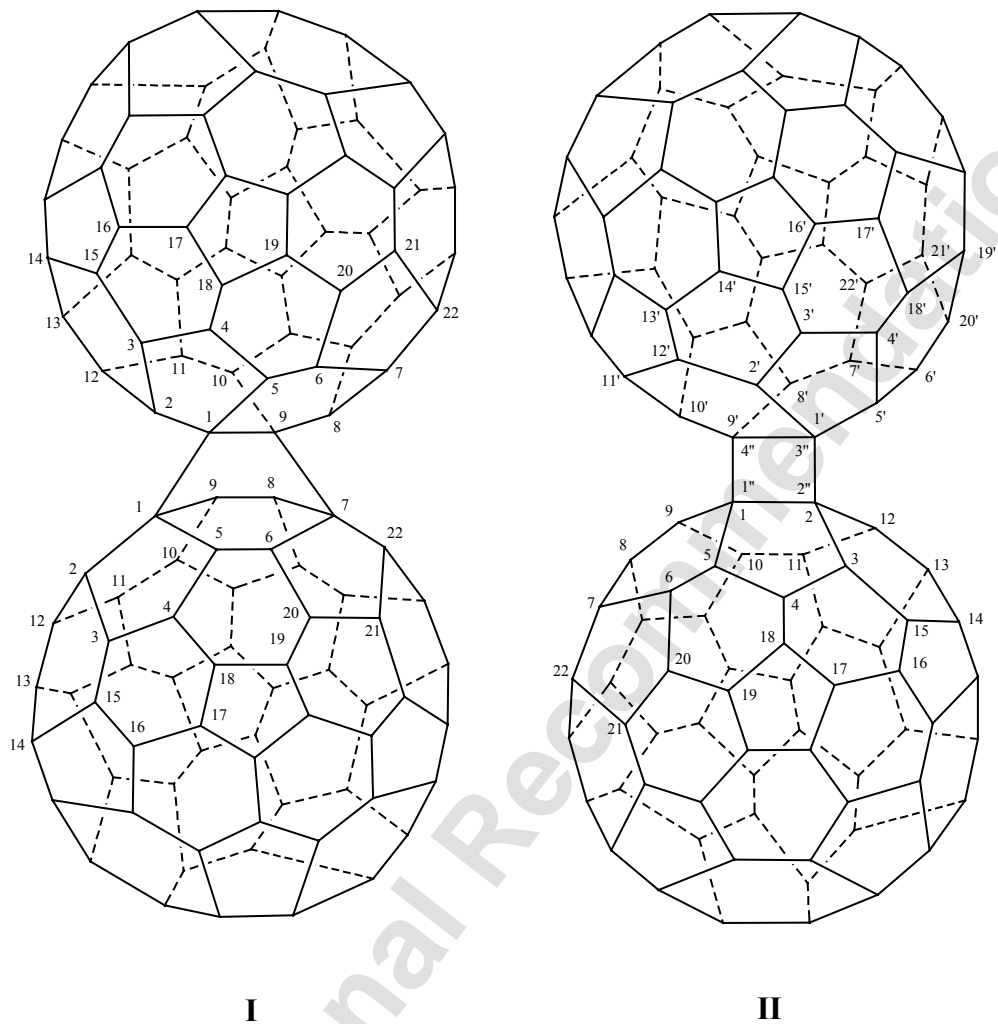
- I Spiro[cyclohexane-1,1'-[1a*H*-1(9)a]-homo(C<sub>60</sub>-I<sub>h</sub>)[5,6]fullerene]
- II 2'',7''-Dinitrospiro[3'*H*-cyclopropa[1,9](C<sub>60</sub>-I<sub>h</sub>)[5,6]fullerene-3',9''-fluorene]
- III Dispiro[cyclopropane-1,3''-cyclobuta[1,9](C<sub>60</sub>-I<sub>h</sub>)[5,6]fullerene-4'',2'''-[1,3]dioxane]
- IV Dispiro[cyclohexane-1,3''-]dicyclopropa[1,9:52,60](C<sub>60</sub>-I<sub>h</sub>)[5,6]fullerene-3''',1''''-cyclohexane]

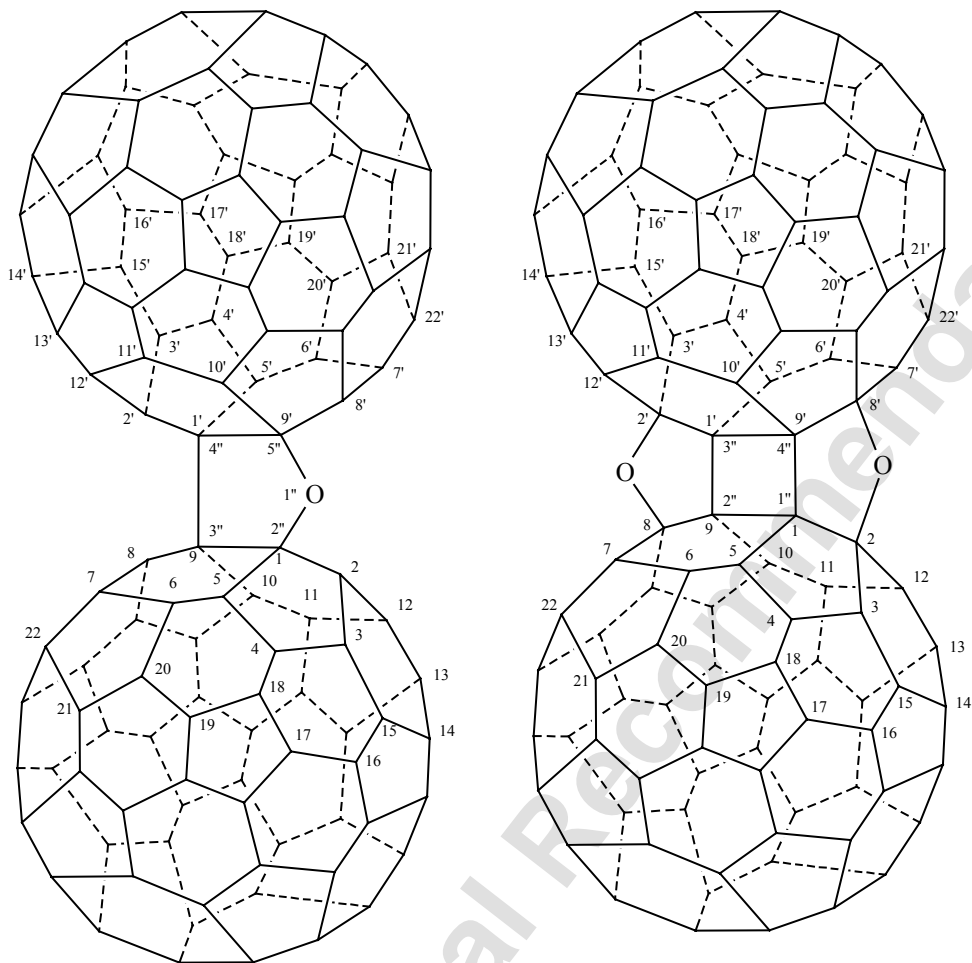
#### Fu-10. Compounds with two fullerene components

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.** One fullerene may bridge another fullerene, be connected to another fullerene by fusion components, be a part of a fusion component, or be a part of a ring assembly.

Examples:



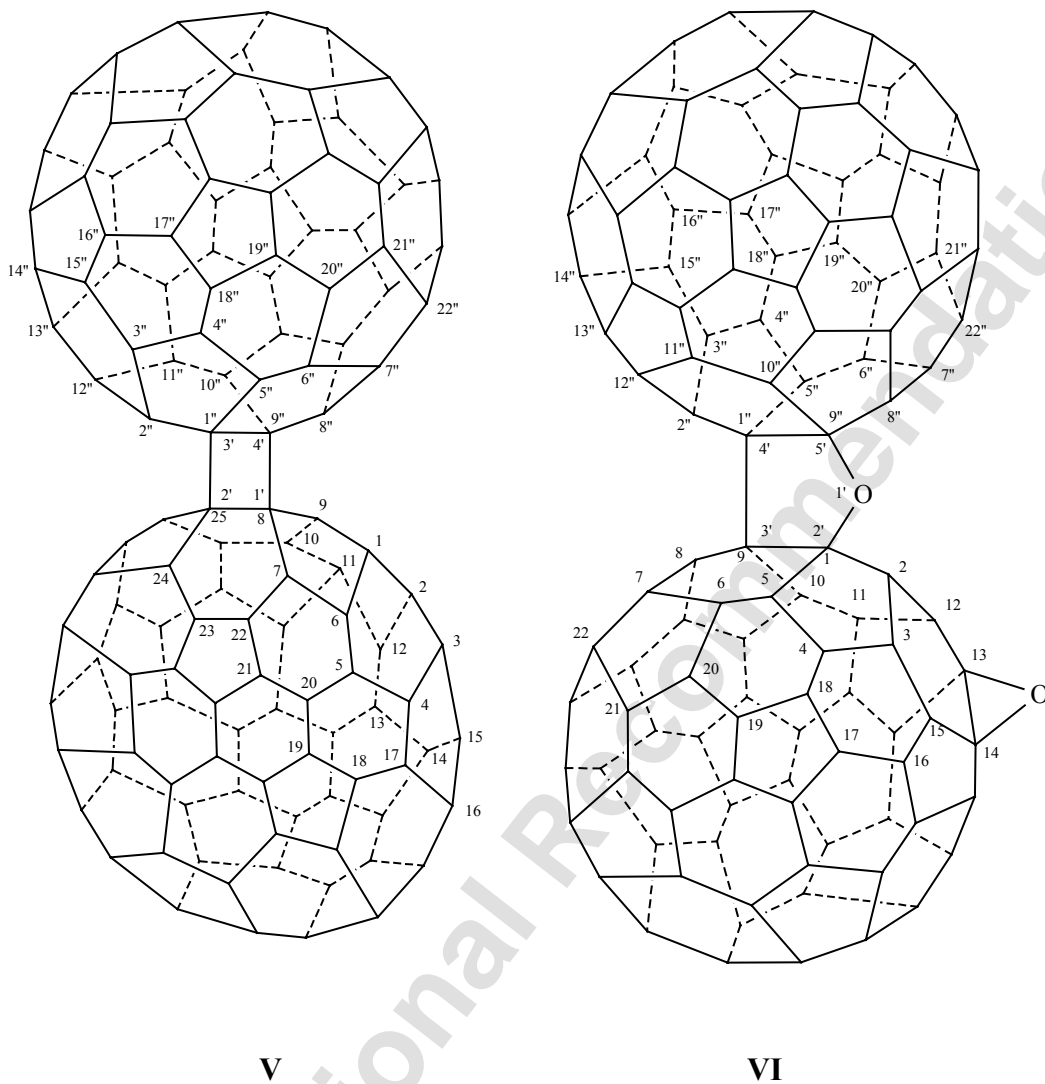


III

IV

- I** 1,7-(1',9'-Epi(C<sub>60</sub>-I<sub>h</sub>)[5,6]fullereno)(C<sub>60</sub>-I<sub>h</sub>)[5,6]fullerene  
[a (C<sub>60</sub>-I<sub>h</sub>)[5,6]fullerene bridging another (C<sub>60</sub>-I<sub>h</sub>)[5,6]fullerene]
- II** Cyclobuta[1'',2'':1,2;3'',4'':1',9']di(C<sub>60</sub>-I<sub>h</sub>)[5,6]fullerene  
[two (C<sub>60</sub>-I<sub>h</sub>)[5,6]fullerenes joined by a fused cyclobutane ring]
- III** Furano[2'',3'':1,9;4'',5'':1',9']di(C<sub>60</sub>-I<sub>h</sub>)[5,6]fullerene<sup>1</sup>  
[two (C<sub>60</sub>-I<sub>h</sub>)[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<sub>60</sub>-I<sub>h</sub>)[5,6]fullerene  
[two bridges between two (C<sub>60</sub>-I<sub>h</sub>)[5,6]fullerenes joined by a fused cyclobutane ring]

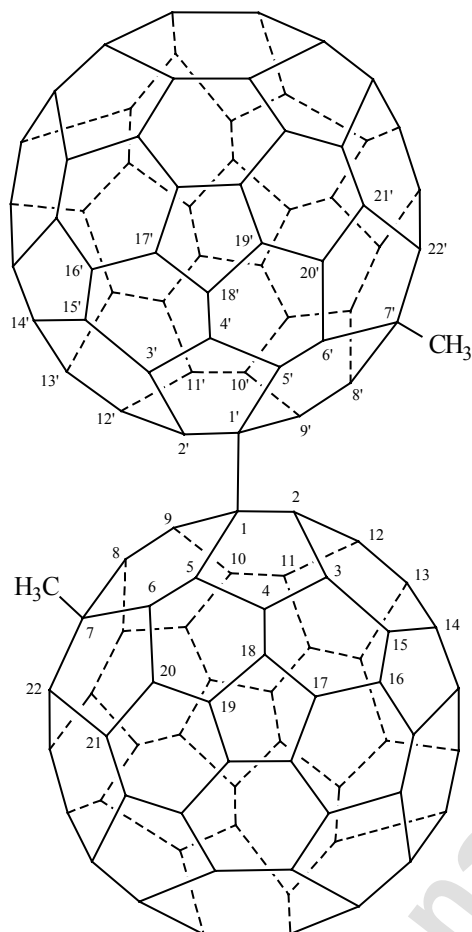
<sup>1</sup> The CAS name is Di[5.6]fullereno-C<sub>60</sub>-I<sub>h</sub>-[1,9-b:1',9'-d]furan



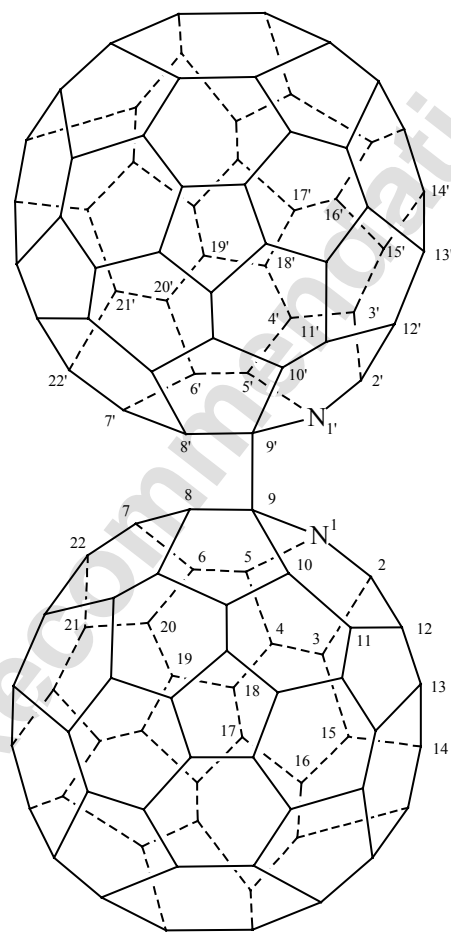
**V** (C<sub>60</sub>-I<sub>h</sub>)[5,6]Fullereno[1'',9'':3',4']cyclobuta[1',2':8,25](C<sub>70</sub>-D<sub>5h(6)</sub>)fullerene<sup>1</sup>  
[a (C<sub>60</sub>-I<sub>h</sub>)[5,6]fullerene joined to a (C<sub>70</sub>-D<sub>5h(6)</sub>)fullerene by a fused  
cyclobutane ring]

**VI** (C<sub>60</sub>-I<sub>h</sub>)[5,6]Fullereno[1'',9'':4',5']furano[2',3':1,9]oxireno[13,14](C<sub>60</sub>-I<sub>h</sub>)-  
[5,6]fullerene<sup>1</sup>  
[a (C<sub>60</sub>-I<sub>h</sub>)[5,6]fullerenofuran fused system and an oxireno ring fused  
to a (C<sub>60</sub>-I<sub>h</sub>)[5,6]fullerene]

<sup>1</sup> Since a fused fullerene structure is not renumbered, each component must be identified by appropriate primed numbers.



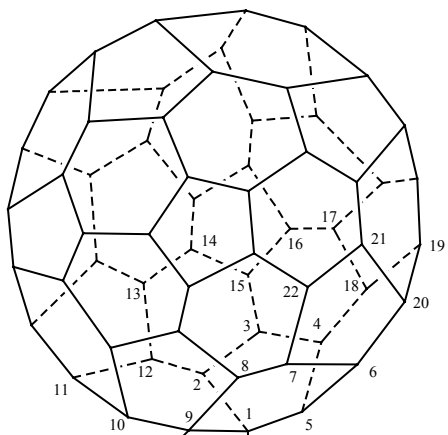
VII



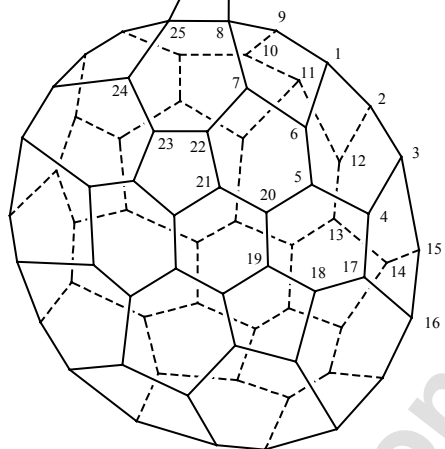
VIII

**VII** 7,7'-Dimethyl-1,1'-(7*H*,7'*H*)-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)

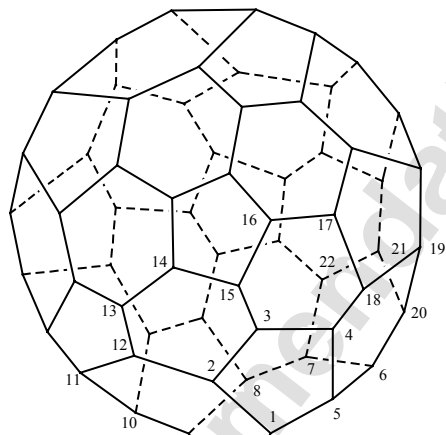
**VIII** 9,9'-Bi-1-aza( $C_{60}$ - $I_h$ )[5,6]fullerene  
(a ring assembly name; two 1-aza( $C_{60}$ - $I_h$ )[5,6]fullerenes linked by a single bond;  
although the name of the azafullerene is 9*H*-1-aza( $C_{60}$ - $I_h$ )[5,6]fullerene,  
the ring assembly does not require citation of indicated hydrogen)



H H



IX



X

**IX** 8-[(C<sub>60</sub>-I<sub>h</sub>)[5,6]Fulleren-1(9H)-yl]-8,25-dihydro(C<sub>70</sub>-D<sub>5h(6)</sub>)[5,6]fullerene  
[ a (C<sub>70</sub>-D<sub>5h(6)</sub>)fullerene substituted by a (C<sub>60</sub>-I<sub>h</sub>)[5,6]fullerene]

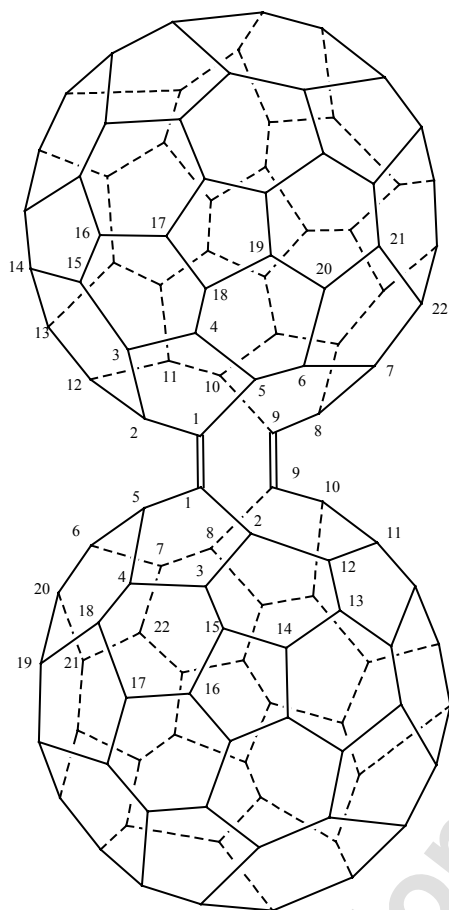
**X** 3'-[1aH-1(9)a-Homo(C<sub>60</sub>-I<sub>h</sub>)[5,6]fulleren-1a-ylidene]-3'H-cyclopropa[1,9]-  
(C<sub>60</sub>-I<sub>h</sub>)[5,6]fullerene  
[ a cyclopropa(C<sub>60</sub>-I<sub>h</sub>)[5,6]fullerene substituted by a homo(C<sub>60</sub>-I<sub>h</sub>)-  
[5,6]fullerene] (preferred on the basis of more rings)

or

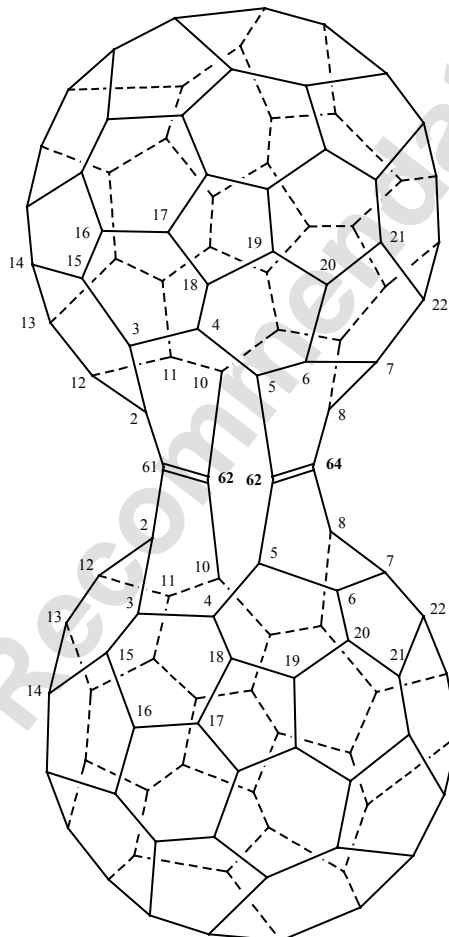
1a-[3'H-Cyclopropa[1,9](C<sub>60</sub>-I<sub>h</sub>)[5,6]fulleren-3-ylidene]-1aH-1(9)a-homo-  
(C<sub>60</sub>-I<sub>h</sub>)-[5,6]fullerene]



[a homo( $C_{60}-I_h$ )-[5,6]fullerene substituted by a cyclopropa( $C_{60}-I_h$ )-[5,6]fullerene]



**XI**



**XII**

**XI** 1,9-[1,9-Seco( $C_{60}-I_h$ )[5,6]fullerene-1,9-diyldene]-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 ( $C_{60}-I_h$ )-seco[5,6]fullerene]

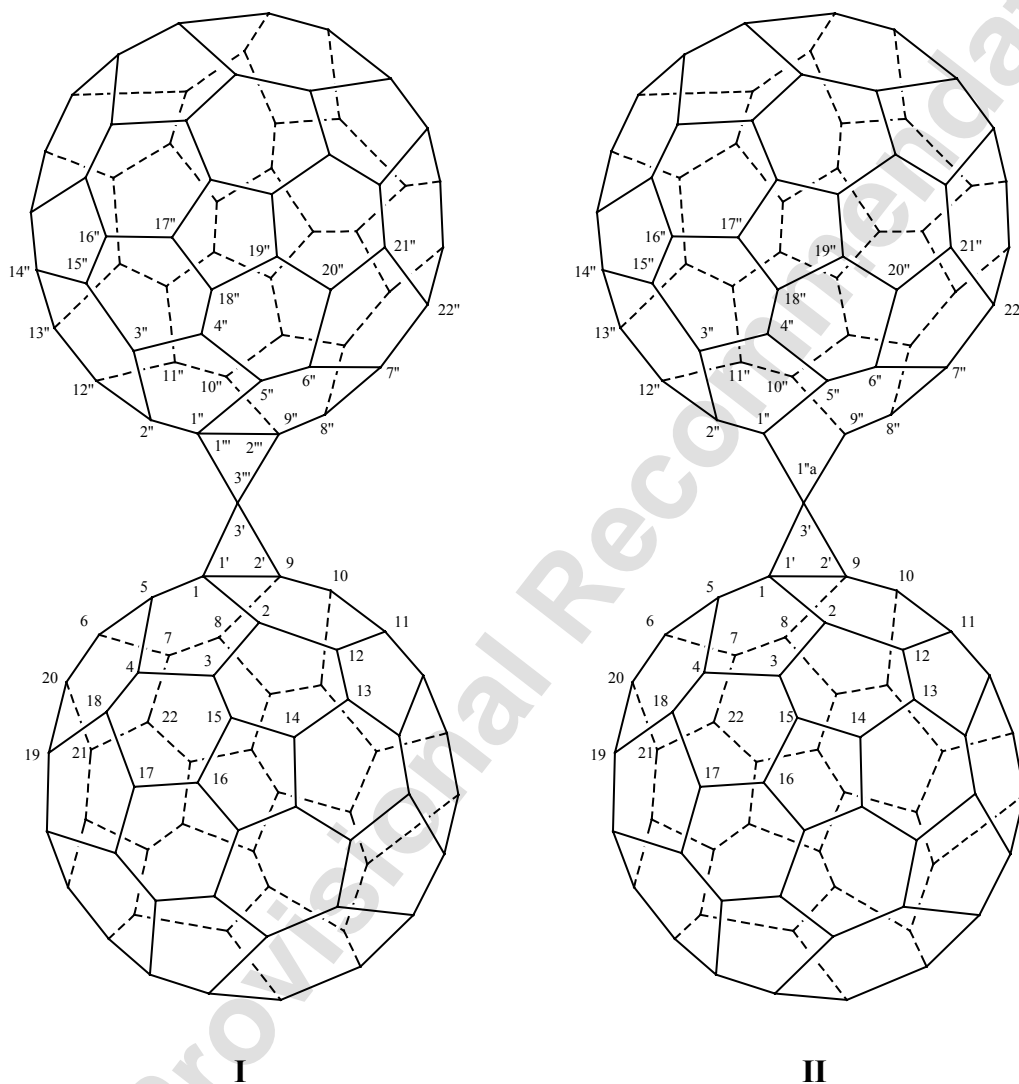
**XII** 61,63,64,62-(,9-Dinor( $C_{60}-I_h$ )[5,6]fullerene-2,5,8,10-tetrayl)-2,10:5,8-bis(ethene-1,2-diy1)-1,9-dinor( $C_{60}-I_h$ )[5,6]fullerene  
[a bis-bridged 1,9-dinor( $C_{60}-I_h$ )[5,6]fullerene substituted by a 1,9-dinor- ( $C_{60}-I_h$ )[5,6]fullerene

or

2,10:2',10';5,8:5',8'-Bis(ethene-1,1:2,2-tetrayl)b1s[1,9-dinor( $C_{60}-I_h$ )[5,6]fullerene]

[two dinor( $C_{60}$ - $I_h$ )[5,6]fullerenes bridged by two ethenetetrayl groups]

**Fu-10.2.** Homo and fused ring fullerenes can be linked by spiro fusions.

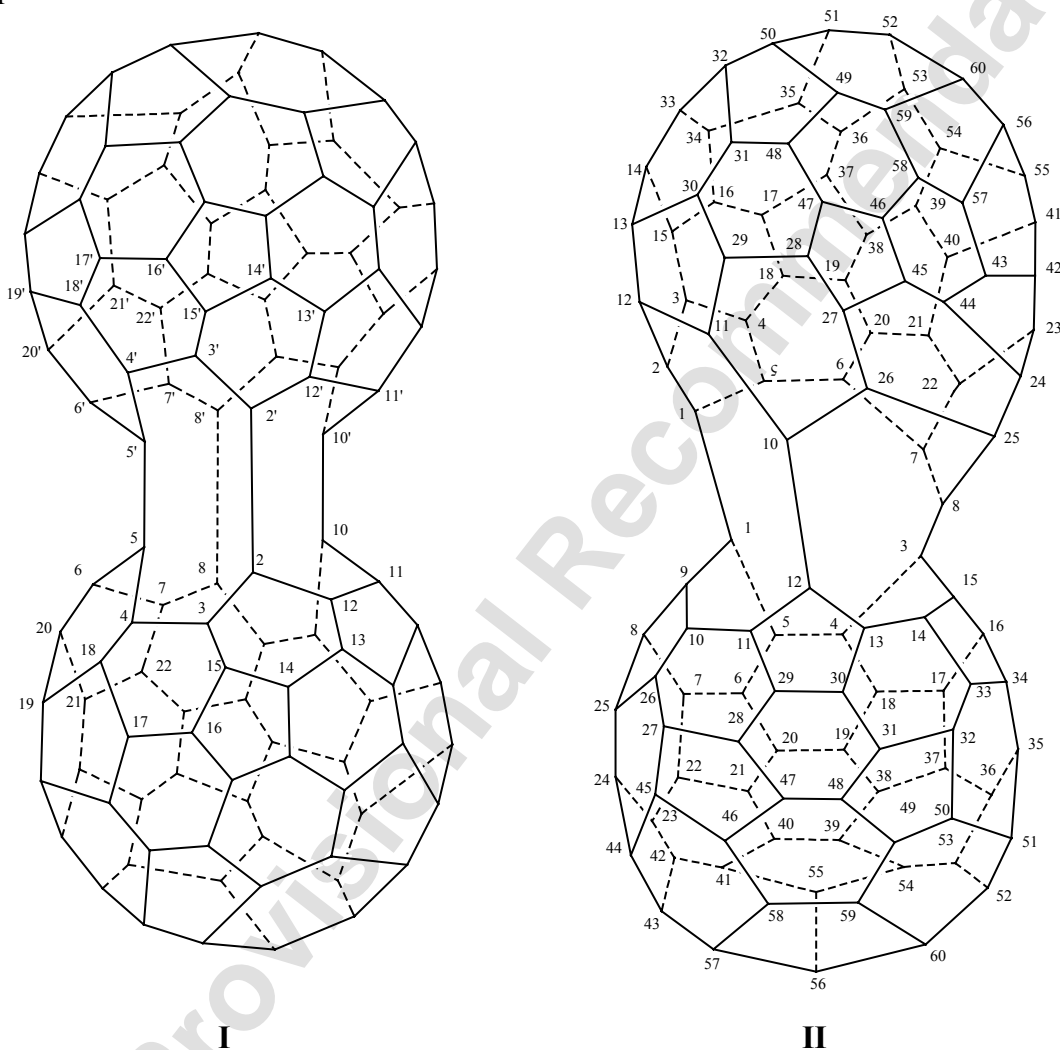


**I** 3',3'''-Spirobi[3'*H*-cyclopropa[1,9]( $C_{60}$ - $I_h$ )[5,6]fullerene]  
[two cyclopropa( $C_{60}$ - $I_h$ )[5,6]fullerenes linked by a spiro fusion]

**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-10.3.** Two fullerenes or modified fullerenes can be connected by substituting one fullerene into another, by treating one fullerene as a bridge to the other, or, if identical, by ring assembly nomenclature coupled with the prefix “cyclo”.

Examples:

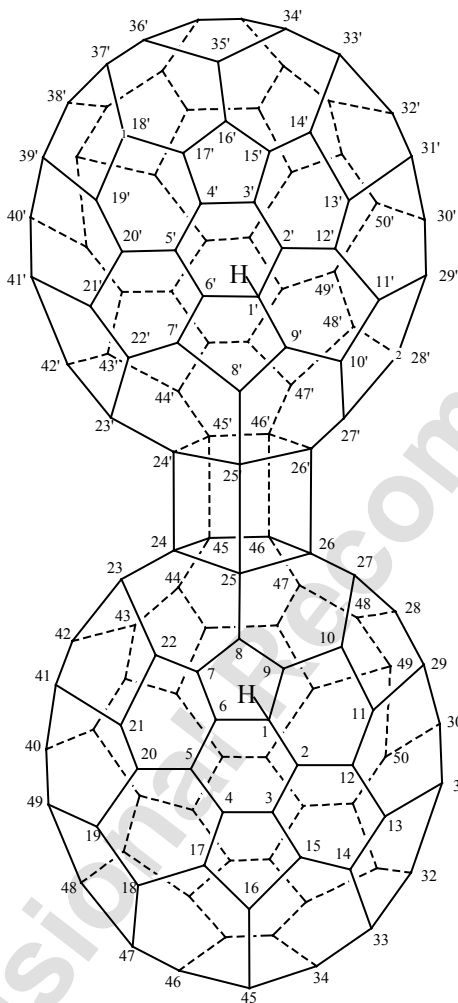


**I** 5,5':8,8':10,10'-Tricyclo-2,2'-bi-1,9-dinor( $C_{60}-I_h$ )[5,6]fullerene  
[a ring assembly name for two 1,9-dinor( $C_{60}-I_h$ )[5,6]fullerenes plus three additional single bonds designated by the structure modifying prefix “cyclo”]

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** 1,3,12-[9-Nor( $C_{60}$ - $I_h$ )[5,6]fullerene-1,8,10-triyl]-2-nor( $C_{60}$ - $I_h$ )[5,6]fullerene  
[a 2-nor( $C_{60}$ - $I_h$ )[5,6]fullerene substituted by a 9-nor( $C_{60}$ - $I_h$ )[5,6]fullerene,  
or a 9-nor( $C_{60}$ - $I_h$ )[5,6]fullerene bridging a 2-nor( $C_{60}$ - $I_h$ )[5,6]fullerene]



**III**

- III** 1*H*,1'*H*-25,25':26, 26':45, 45':46, 46'-Pentacyclo- 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"]

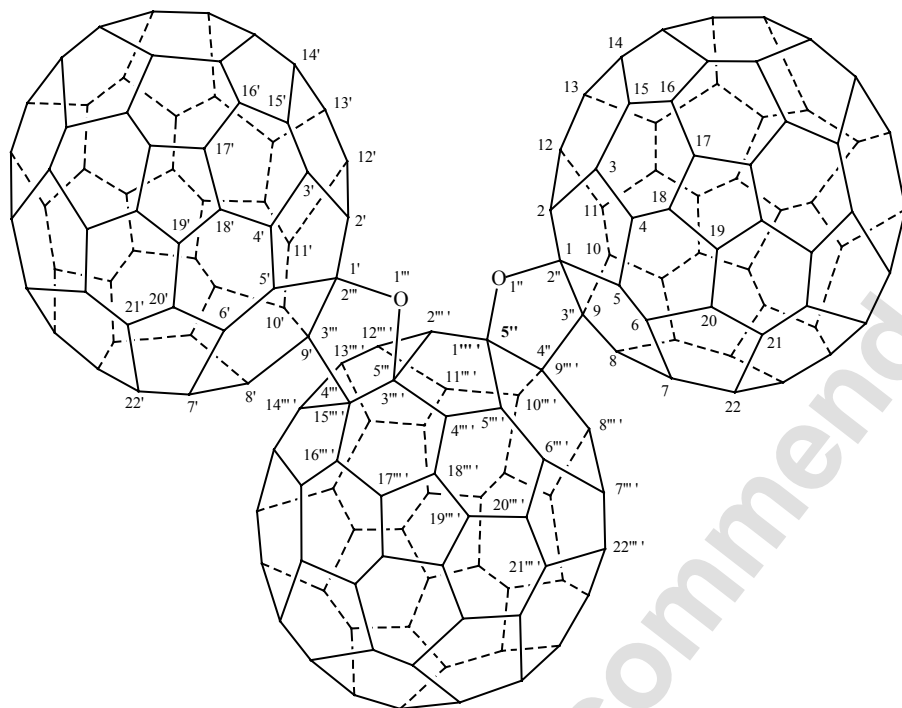
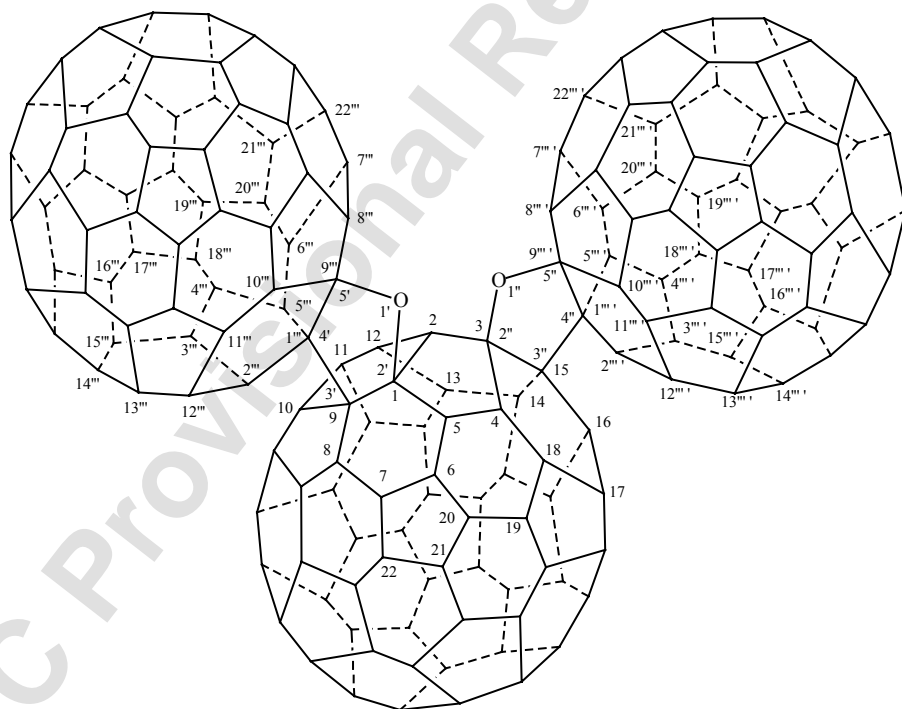
or

- 1*H*,1'*H*-Hexacyclo[4.4.0.0<sup>2,5</sup>.0<sup>3,9</sup>.0<sup>4,8</sup>.0<sup>7,10</sup>]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 fused von Baeyer ring system  
hexacyclo[4.4.0.0<sup>2,5</sup>.0<sup>3,9</sup>.0<sup>4,8</sup>.0<sup>7,10</sup>]decane

**Fu-11. Compounds with three or more fullerene components** can be named by fusion principles, bridging principles, ring assembly nomenclature coupled with the structure modifying prefix “cyclo”, or by phane nomenclature (ref. 10).

Examples:

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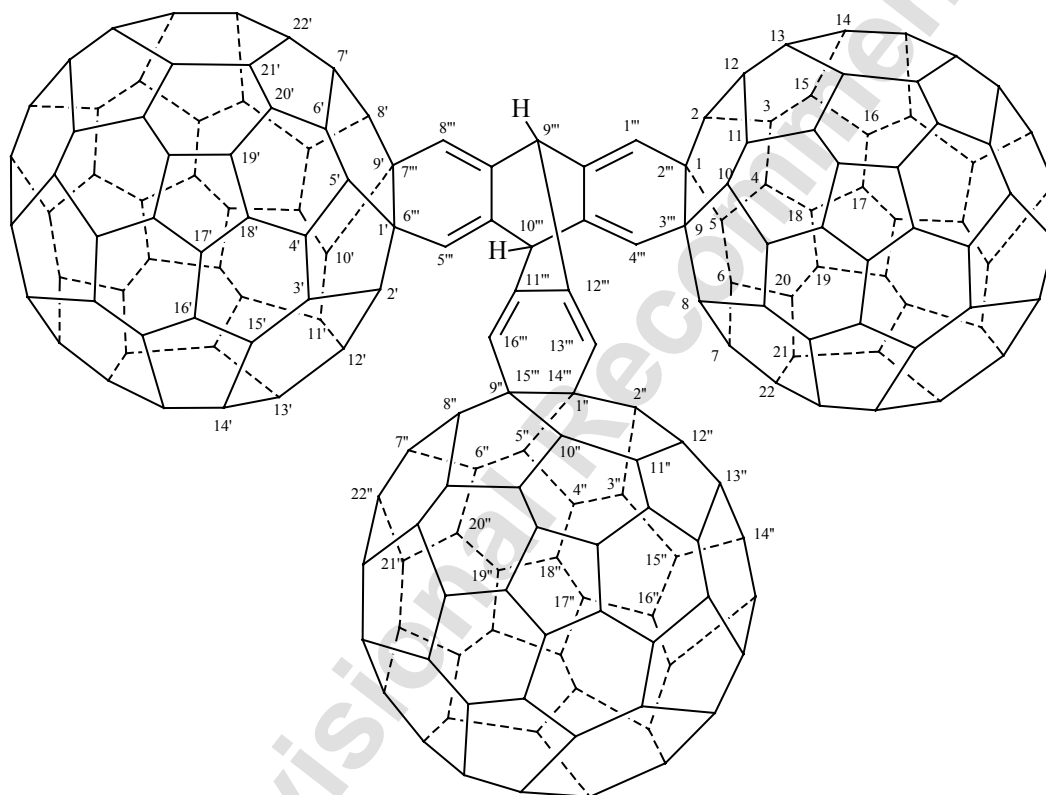
**Ia****Ib**

**1a**  $(C_{60}-I_h)[5,6]$ 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)

[three  $(C_{60}-I_h)[5,6]$ fullerenes connected by two furan rings; a fusion name based on the terminal fullerenes]

**1b** Bis $(C_{60}-I_h)[5,6]$ fullereno[1''',9''':4',5']furano[2''',3''':3,15;2',3':1,9] $(C_{60}-I_h)[5,6]$ fullerene<sup>1</sup>

[three  $(C_{60}-I_h)[5,6]$ fullerenes connected by two furan rings; a fusion name based on the central fullerene]

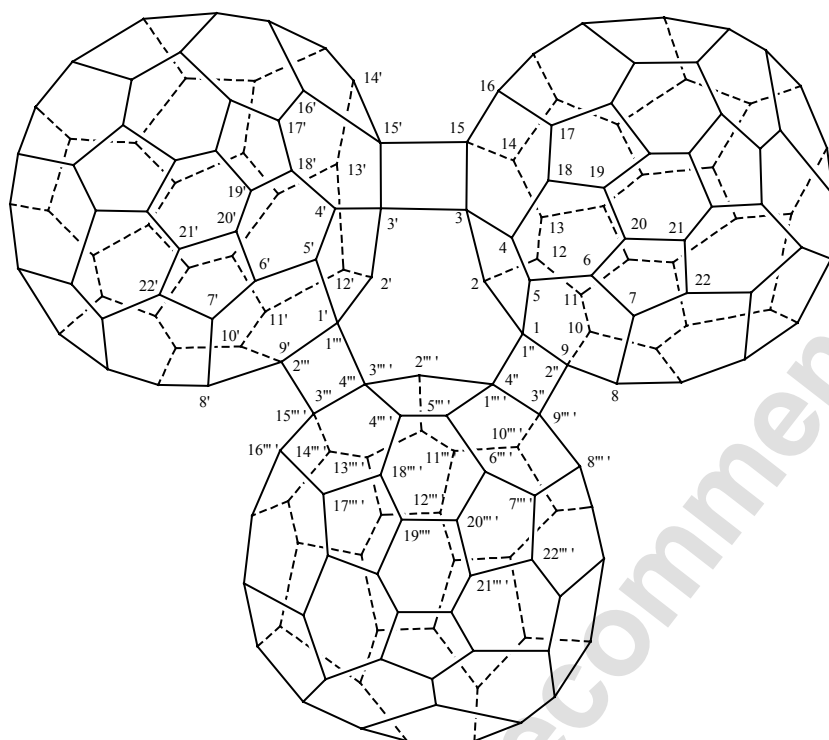
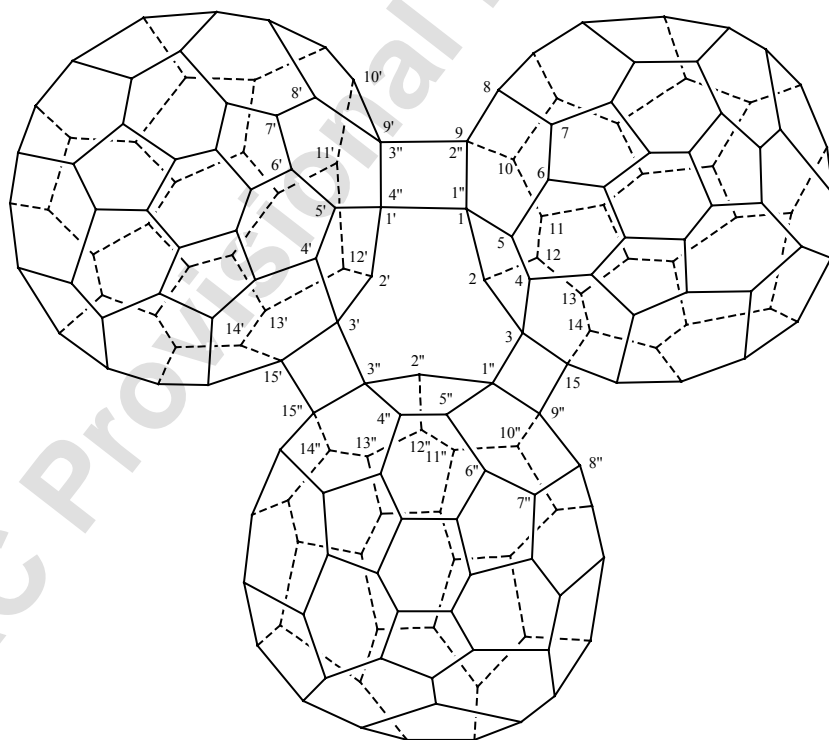


## II

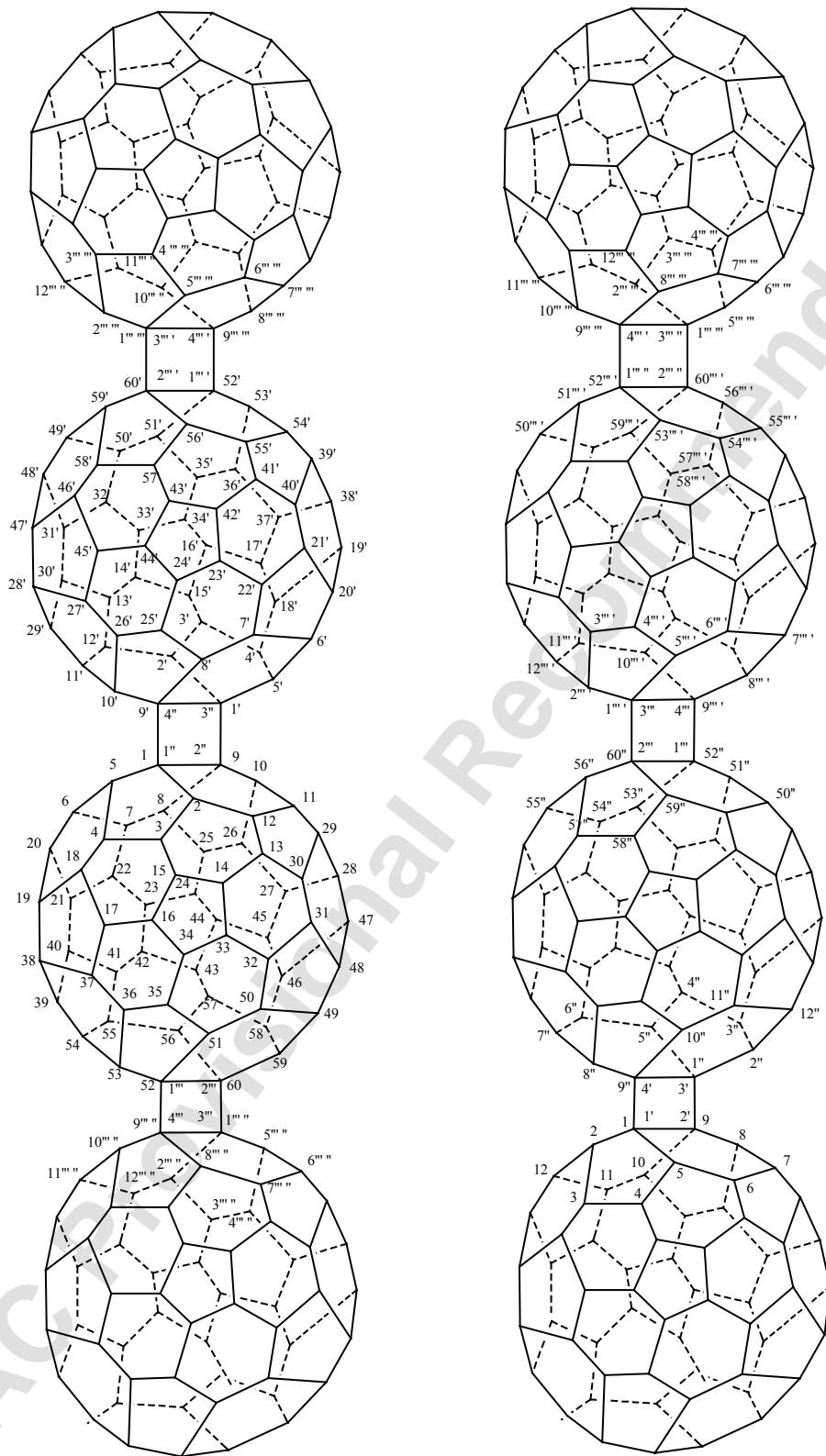
**II** 9'''H,10'''H-9,10-[1,2]Benzenoanthraceno[2''',3''':1,9;6''',7''':1',9':14''',15''':1'',9'']-  
tri $(C_{60}-I_h)[5,6]$ fullerene

[three  $(C_{60}-I_h)[5,6]$ fullerenes joined by a fused 9,10-[1,2]benzenoanthracene ring system]

<sup>1</sup> The CAS 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**



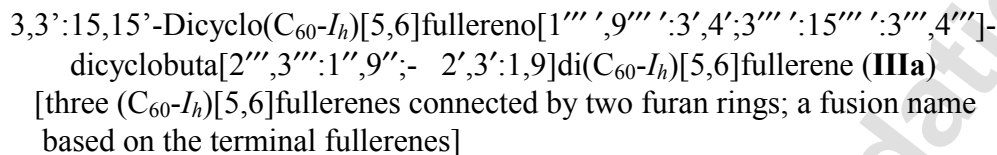


IVa

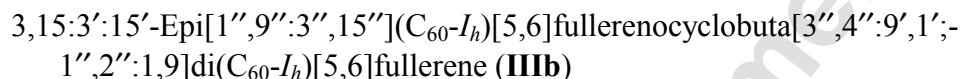
IVb

**III.** This multicomponent fullerene cannot be named by fusion principles. Nevertheless, there are three potential ways to name this multicomponent fullerene.

1. Combine a fusion name for three fullerenes ( $C_{60-I_h}$ )[5,6]fullerenes joined by two fused cyclobutane rings with the structure modifying prefix “cyclo”, for example:.

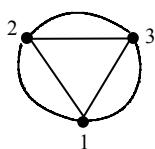


- 2.. A second method for naming this structure would be citing one fullerene as a bridge to the other two fullerenes fused together by a cyclobutane ring.



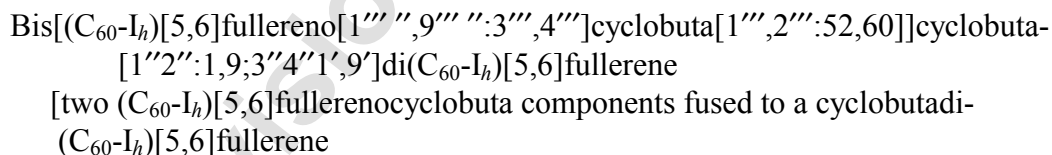
In such a name the bridging fullerene retains primed numbering, in this case, double primes.

3. A third method for naming this structure would be to adapt phane nomenclature (ref. 10)

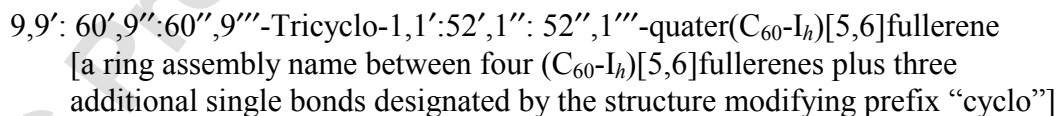


**IV.** There are three ways to name this multicomponent fullerene consisting of four fullerenes interconnected by three cyclobutane rings

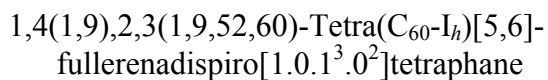
1. Fused ring nomenclature.



2. Ring assembly nomenclature plus cyclo.



3. An adaptation of phane nomenclature (ref. 10)

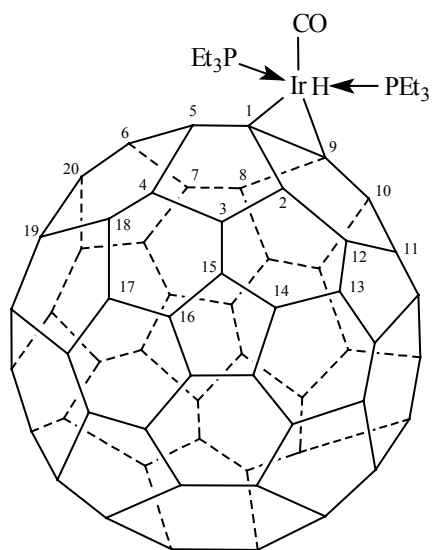


**Fu-12. Fullerenes in Coordination Compounds**

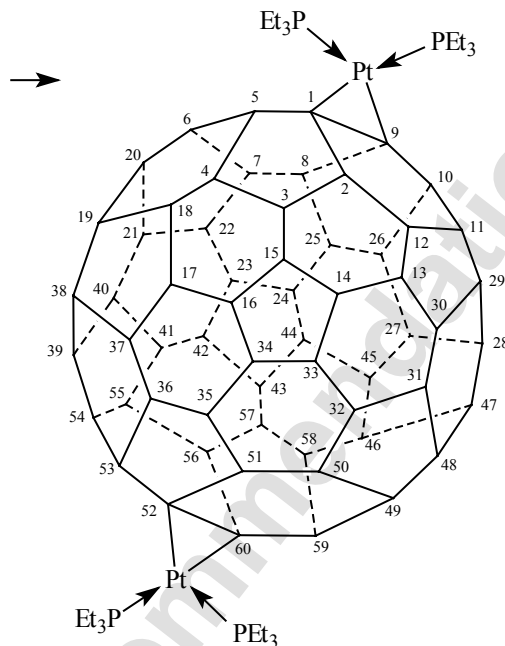
Principles of coordination nomenclature are applied in naming fullerenes and fulleroids externally associated with metal atoms for which replacement nomenclature is not permitted.

Examples:

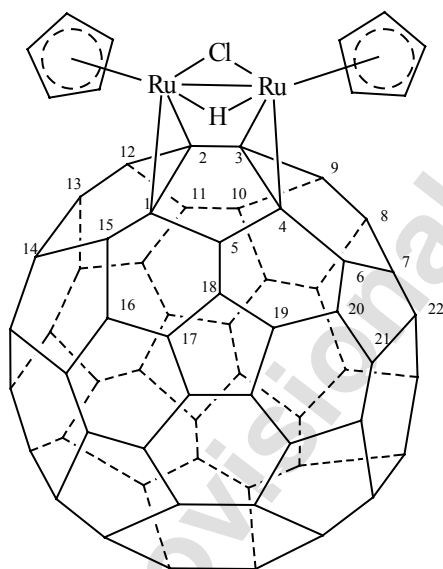
IUPAC Provisional Recommendations



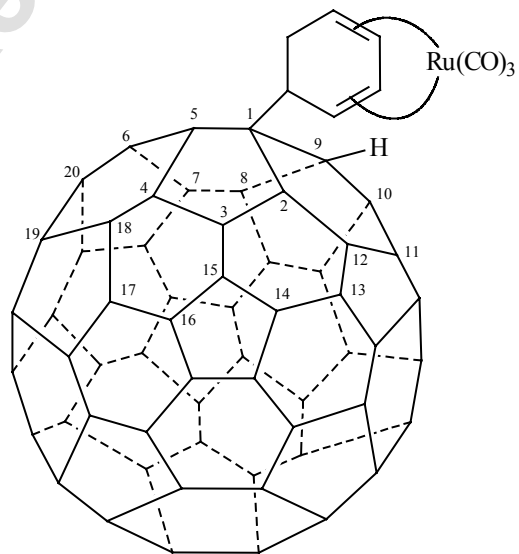
I



II

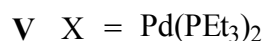
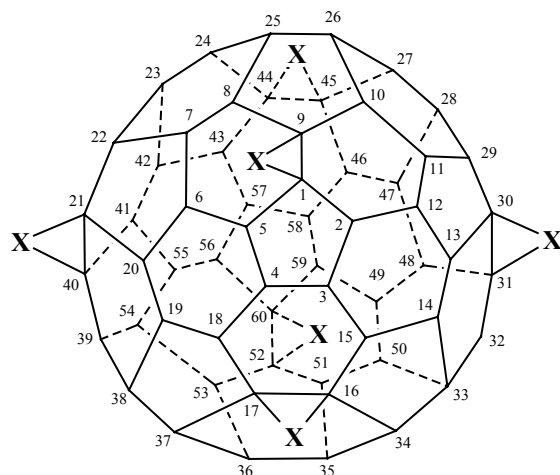


III



IV

IUPAC Pre-proof: Official Recommendations

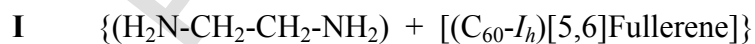


- I** Carbonyl[(1,9- $\eta$ )-(C<sub>60</sub>-I<sub>h</sub>)[5,6]fullerene]hydrobis(triphenylphosphine)iridium
- II** [ $\mu$ -[(1,9- $\eta$ :52,60- $\eta$ )-(C<sub>60</sub>-I<sub>h</sub>)[5,6]Fullerene]]-tetrakis(triethylphosphine)diplatinum
- III**  $\mu$ -Chloro[ $\mu$ -[(1,2- $\eta$ :3,4- $\eta$ )(C<sub>60</sub>-I<sub>h</sub>)[5,6]fullerene]]- $\mu$ -hydro-bis( $\eta^5$ -cyclopenta-2,4-dien-1-yl)diruthenium(*Ru-Ru*)
- IV** Tricarbonyl[1-[(2,3,4,5- $\eta$ )-cyclohexa-2,4-dien-1-yl]-1,9-dihydro-(C<sub>60</sub>-I<sub>h</sub>)-[5,6]fullerene]ruthenium
- V** [[ $\mu_6$ -(1,9- $\eta$ ):(16,17- $\eta$ ):(21,40- $\eta$ ):(30,31- $\eta$ ):(44,45- $\eta$ ):(52,60- $\eta$ )](C<sub>60</sub>-I<sub>h</sub>)[5,6]-Fullerene]-hexakis[bis(triethylphosphine)palladium]

### Fu-13. Fullerenes in Polymers.

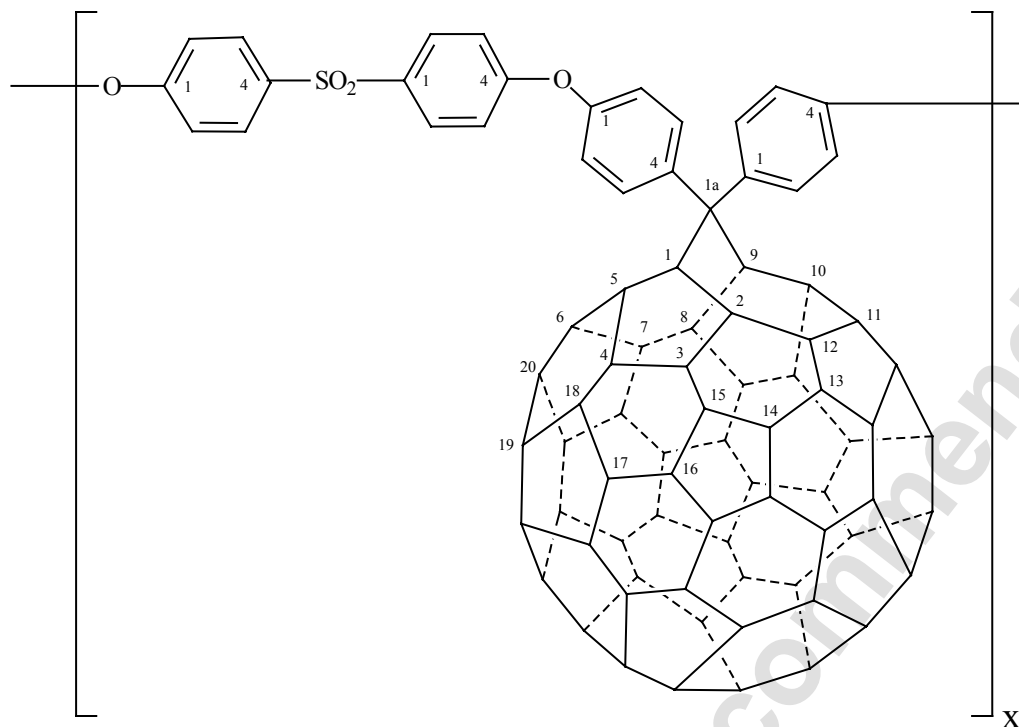
Polymers containing fullerenes are named in accordance with the general nomenclature principles for naming organic polymers.

Examples:



Poly(ethane-1,2-diamine-co-(C<sub>60</sub>-I<sub>h</sub>)[5,6]fullerene)



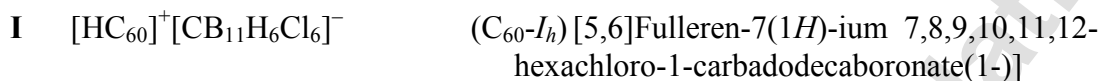


## IV

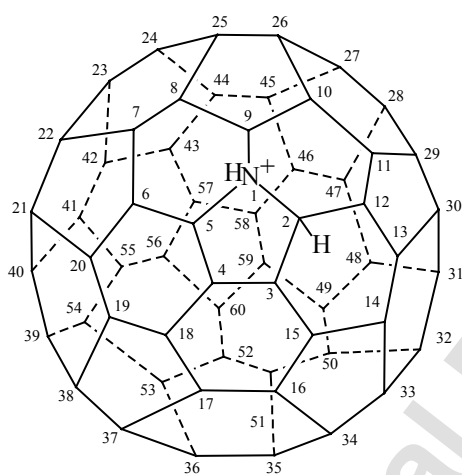
- II Poly[3'*H*-cyclopropa[1,9](C<sub>60</sub>-I<sub>h</sub>)[5,6]fullerene-3',3'-diyldibuta-1,3-diyne-4,1-diyl-bis(trimethylsilane)]
- III Poly[4,4'-1(9)a-homo(C<sub>60</sub>-I<sub>h</sub>)[5,6]fullerene-1a,1a-diyldiphenol-*alt*-1,6-diisocyanato-hexane]
- IV Poly[oxy-1,4-phenylenesulfonyl-1,4-phenyleneoxy-1,4-phenylene-1(9)a-homo-(C<sub>60</sub>-I<sub>h</sub>)[5,6]fullerene-1a,1a-diyl-1,4-phenylene]

**Fu-14. Fullerene 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.

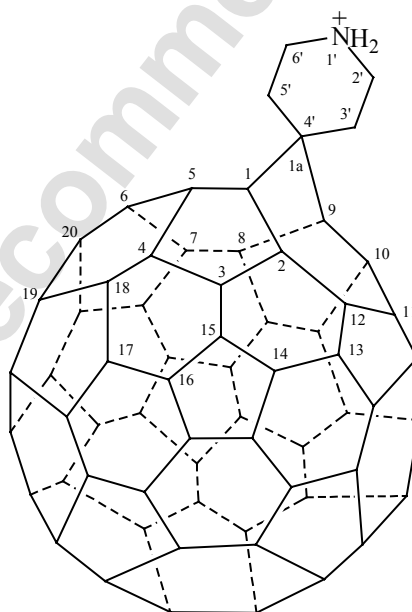
Examples:



[see Science, **289**, 101, 2000]



**II**



**III**

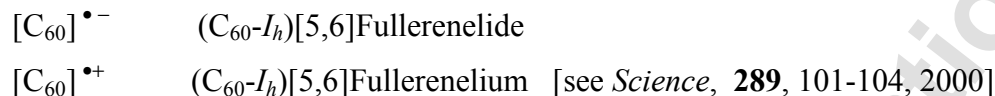
**II** 2*H*-1-Aza( $\text{C}_{60}\text{-}I_h$ )[5,6]fullerenium  
1,2-Dihydro-1-azonia( $\text{C}_{60}\text{-}I_h$ )[5,6]fullerene

**III** Spiro[1(9a)-homo( $\text{C}_{60}\text{-}I_h$ )[5,6]fullerene-1a,4'-piperidin]ium



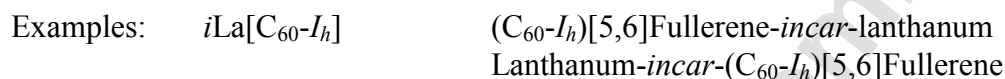
**Fu-15. Fullerene radical ions** formed by the addition of an electron to, or removal of an electron from, the fullerene cage are named by replacing the final "e" of the fullerene name by "-elide", "bis(elide)", etc., or "-elium", "bis(elium)", etc.

Examples:



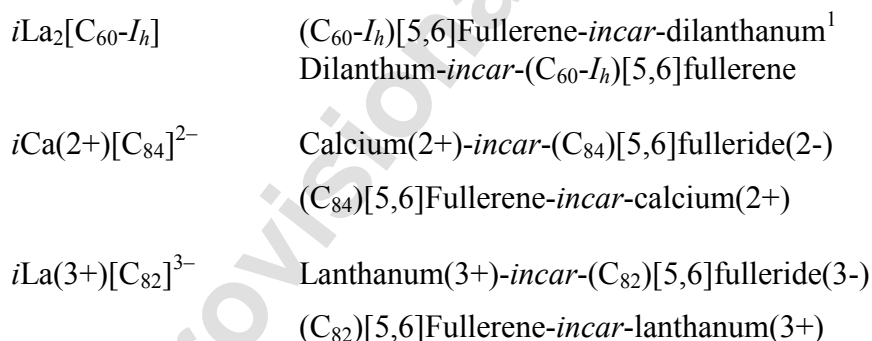
### Fu-16. Metal Derivatives of Fullerenes

The symbol @ and the term *incarcerane* have been widely used to describe fullerenes having an enclosed component. The prefix *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.

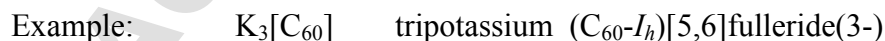


The number of encapsulated metal atoms can be indicated in the formula, even fractional ones, but this must also be incorporated in the name. CAS treats these compositions as 'comp. with' at the name of the fullerene; the ratio of fullerene to the metal is given in parentheses. The charge distribution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

Examples:



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.



<sup>1</sup> The CAS name is [5,6]Fullerene-C<sub>60-I<sub>h</sub></sub>, compd. with lanthanum (1:2)

## Fu-17. Configurational Specification for $C_{60}-I_h$ 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 the publication "Configurational Description of Chiral Fullerenes and Fullerene Derivatives with a Chiral Functionalization Pattern" by C. Thilgen, A. Herrmann, and F. Diederich, *Helv. Chim. Acta* **1997**, *80*, 183-199.

**Fu-17.1** 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 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.

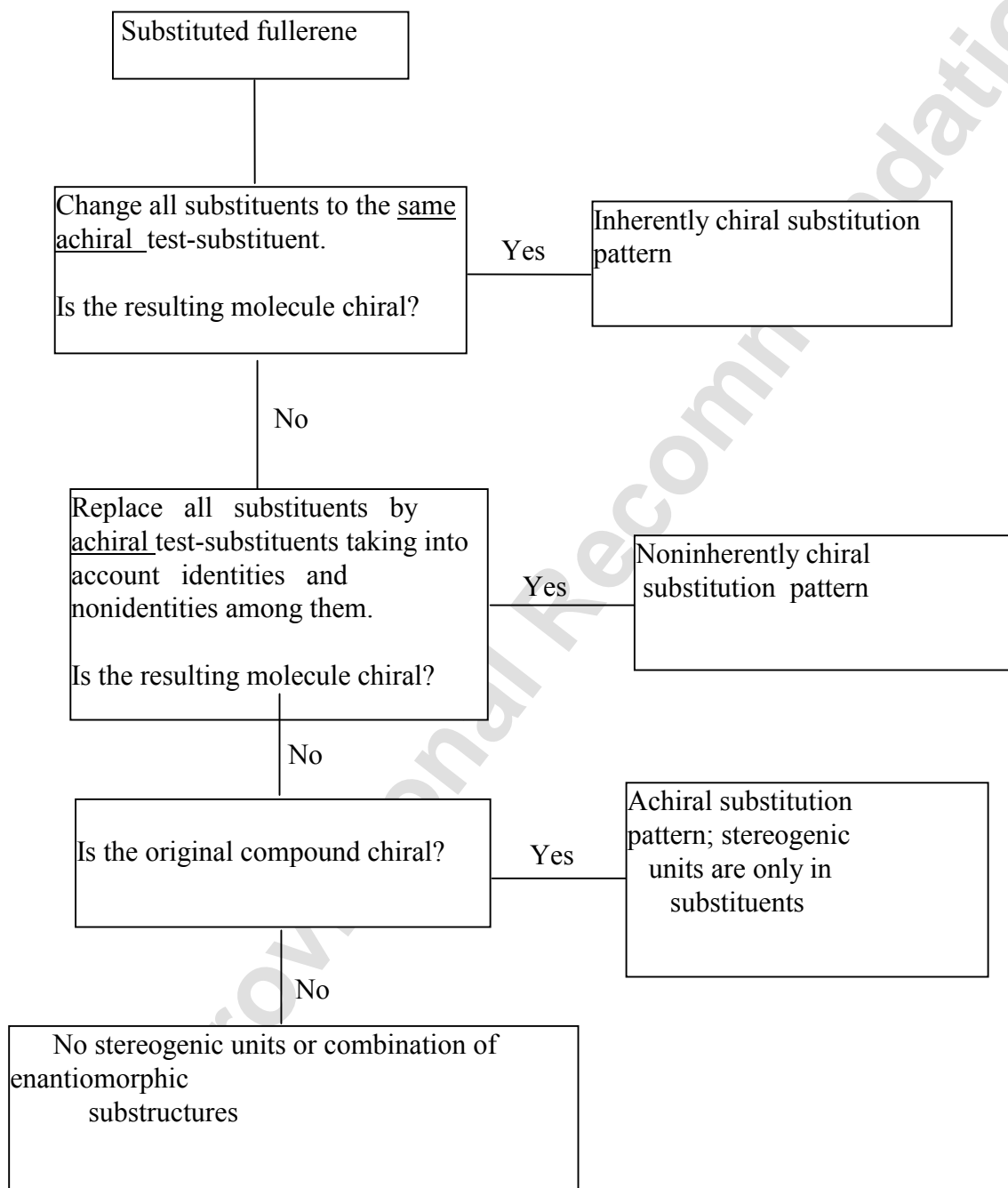
**Type 3.** Derivatives of achiral parent fullerenes in which a chiral substitution (see **Fu-6.2**) pattern on the fullerene is due only to nonidentities among the substituents are said to have a **noninherently chiral** substitution pattern.

**Type 4.** Derivatives of achiral parent fullerenes in which the 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 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.

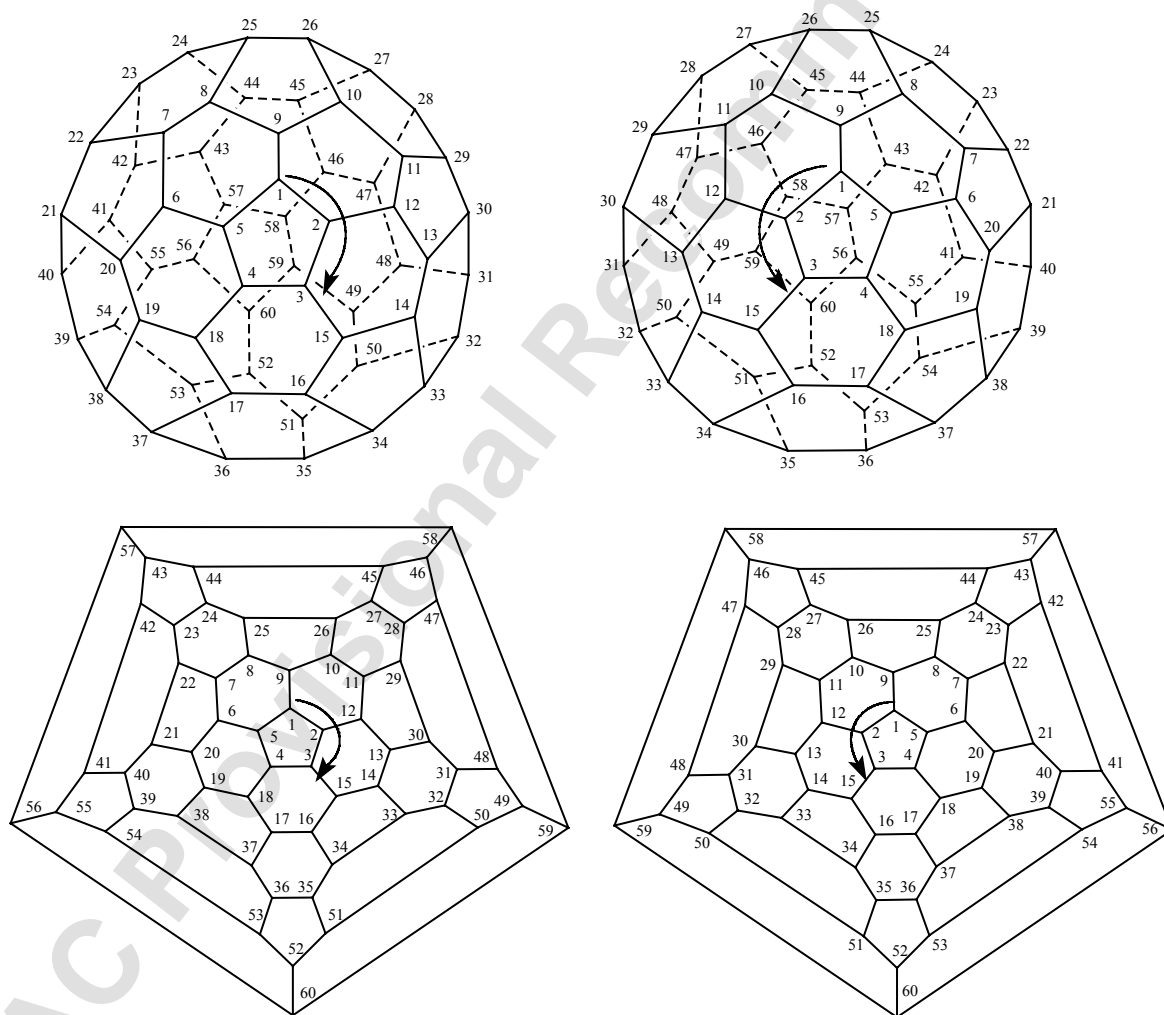
The substitution test consists of (a) replacing all substituents (see **Fu-6.2**) by the same achiral test substituent; (b) replacing nonidentical substituents by nonidentical achiral test substituents; and (c) consideration of the original molecule. After each step, the resulting structure of increasing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



**Scheme 1. Scheme for classifying fullerene chirality by a stepwise substitution test**

The descriptor system presented herein is based on the fact that the numbering schemes proposed for fullerenes in this document<sup>1</sup> 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.

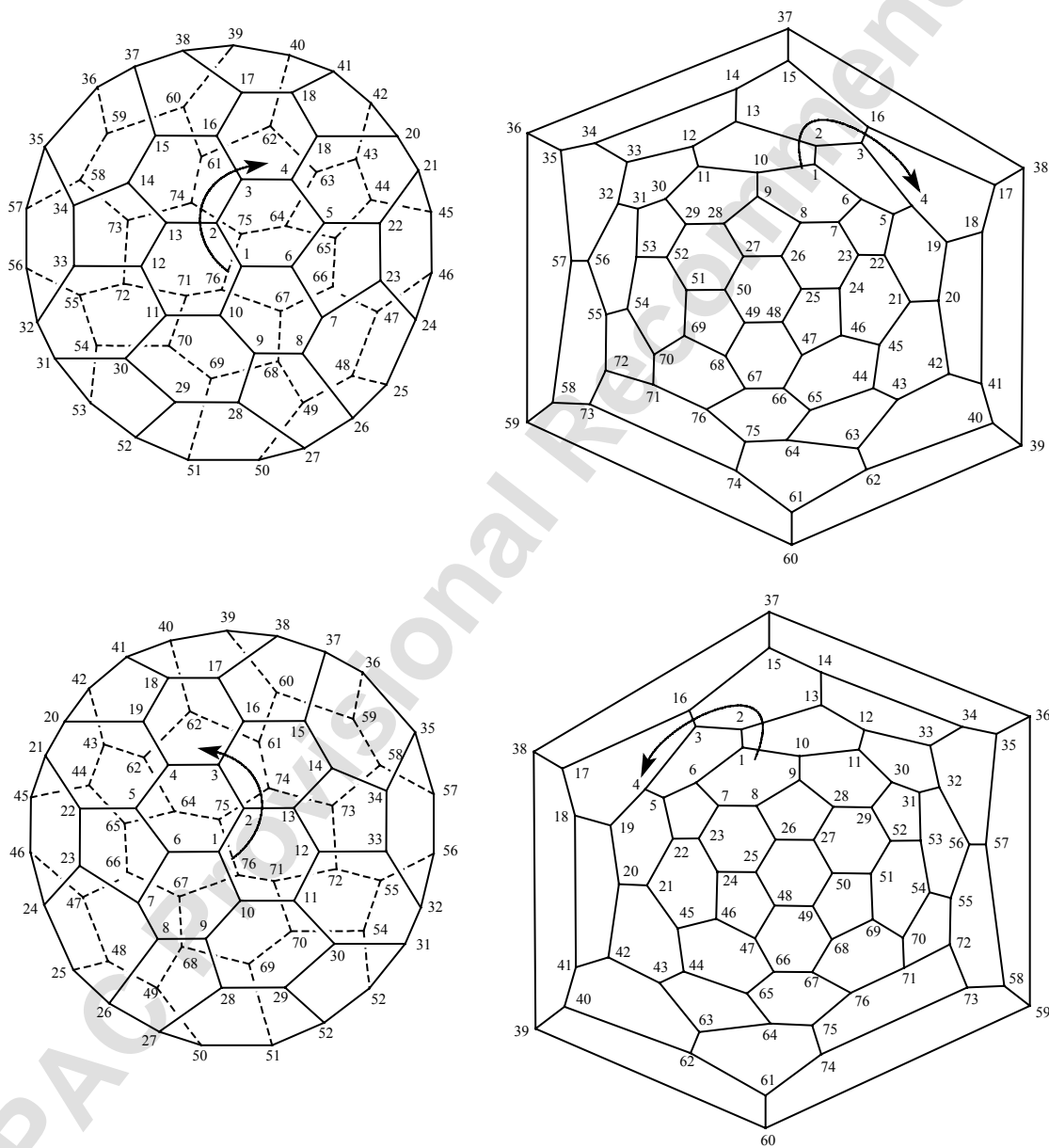
In a three dimensional model, the pathway following the sequence of numbered carbon atoms consists of a helix, or of helical segments, and is therefore chiral. As a consequence two isometric, mirror symmetric, numbering schemes can be applied to an achiral parent fullerene, as shown for  $(C_{60}-I_h)[5,6]$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



**Fig. 6. Three Dimensional and Schlegel Diagrams of  $(C_{60}-I_h)[5,6]$  Fullerene with Enantiomeric Numberings**

<sup>1</sup> Also applies to other numbering methods that are helical.

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<sup>1</sup>. Again, the arrows indicate the direction of commencement 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.



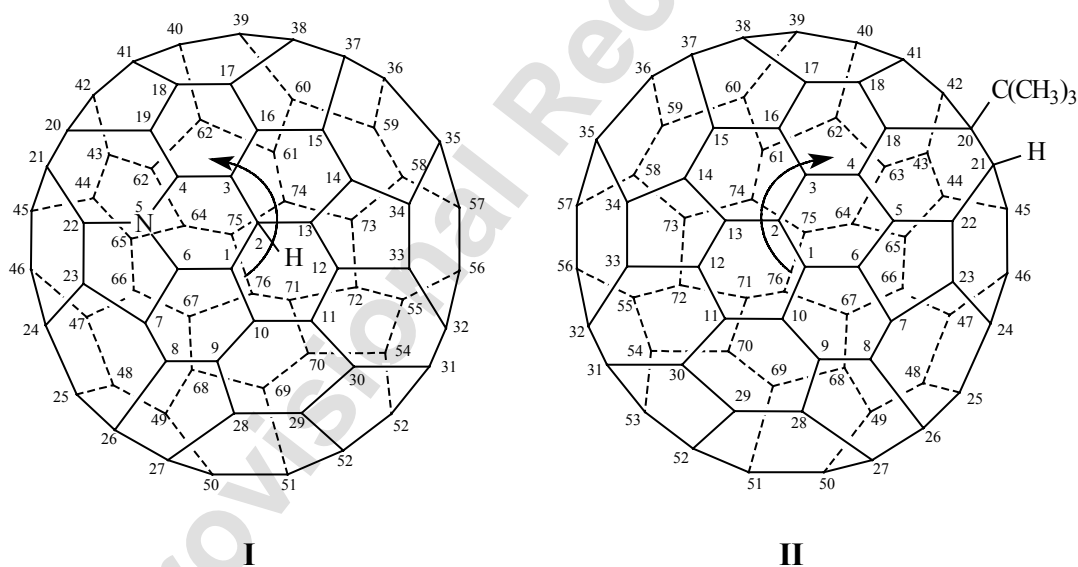
<sup>1</sup> This fullerene is numbered by the system used by CAS, which has not been accepted by IUPAC; a further report will deal with fullerenes other than  $(C_{60}-I_h)[5,6]$  fullerene and  $(C_{70}-D_{5h960})[5,6]$  fullerene.

**Fig. 7. Schlegel and 3-D diagrams of the enantiomers of the inherently chiral fullerene  $(C_{76}-D_2)[5,6]$ fullerene.**

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  $(^{f,x}C)^{-1}$ , 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 trivial 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  $(^{f,x}A)^{-1}$ . Thus, the enantiomer of  $(C_{76}-D_2)[5,6]$ fullerene shown in the upper half of Fig. 7 is  $(^{f,s}C)-(C_{76}-D_2)[5,6]$ -fullerene and the enantiomer shown in the lower half of Fig. 6 is  $(^{f,s}A)-(C_{76}-D_2)[5,6]$ 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**  $(^{f,s}A)-2H-5-Aza-(C_{76}-D_2)[5,6]$ fullerene

**II**  $(^{f,s}C)-20-tert-Butyl-20,21-dihydro-(C_{76}-D_2)[5,6]$ fullerene

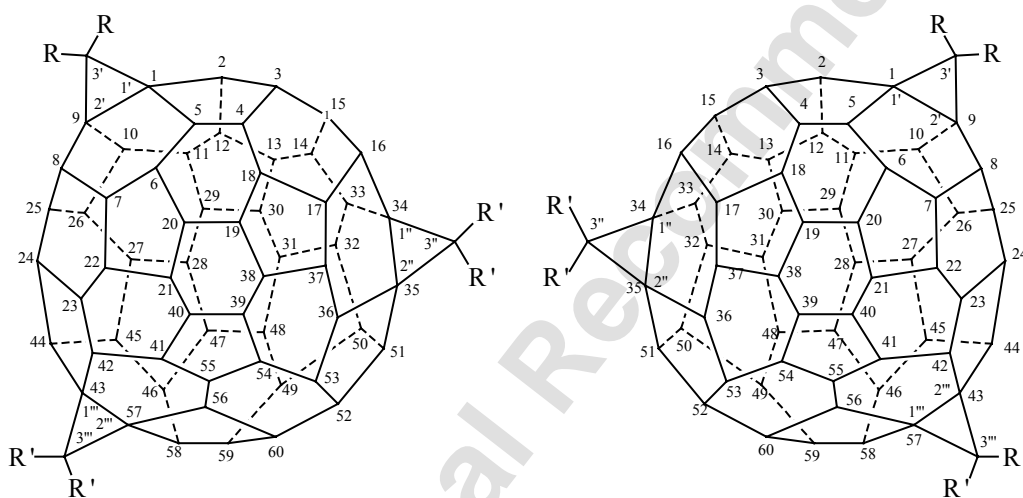
**Fu-17.4. Achiral parent fullerenes with an inherently chiral substitution pattern**

<sup>1</sup> As is customary for stereodescriptors, parentheses are used as enclosing marks.

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  $^{f,x}C$  or  $^{f,x}A$ .

**Example 1.**

3',3'-Diethyl 3'',3'',3''',3'''-tetramethyl 3'H,3''H,3'''H-tricyclopropa[1,9:34,35:43,57]-(C<sub>60</sub>-I<sub>h</sub>)[5,6]fullerene-3,3,3',3',3'',3''-hexacarboxylate



R = -CO-OCH<sub>2</sub>CH<sub>3</sub>

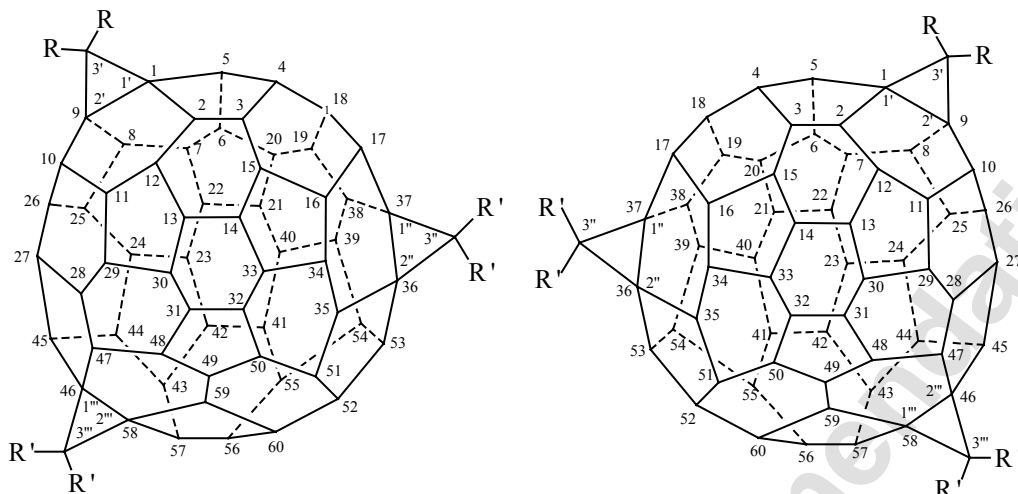
R' = -CO-OCH<sub>3</sub>

**I**

(<sup>f,s</sup>C)-

**II**

(<sup>f,s</sup>A)-

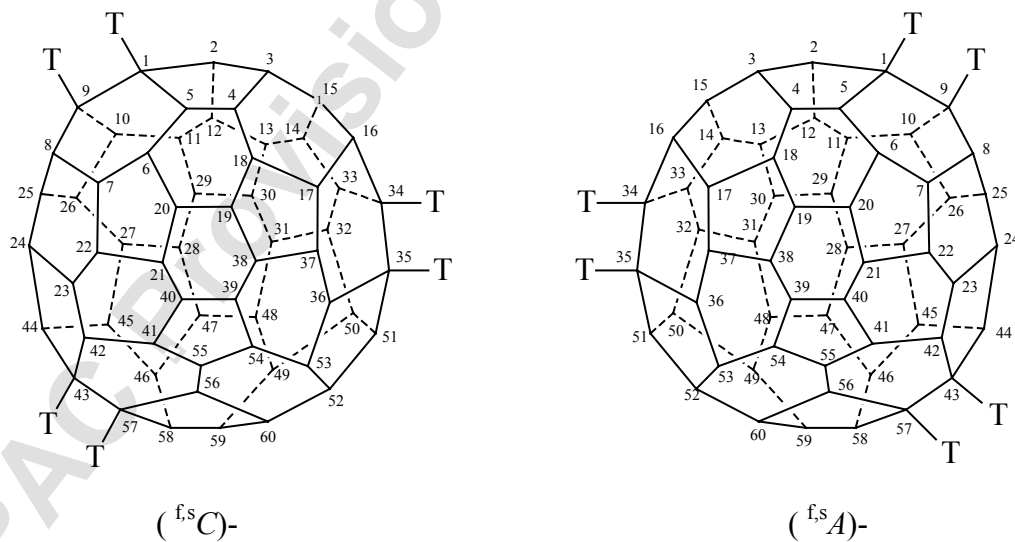


III (Enantiomeric numbering for I)

IV (Enantiomeric numbering for II)

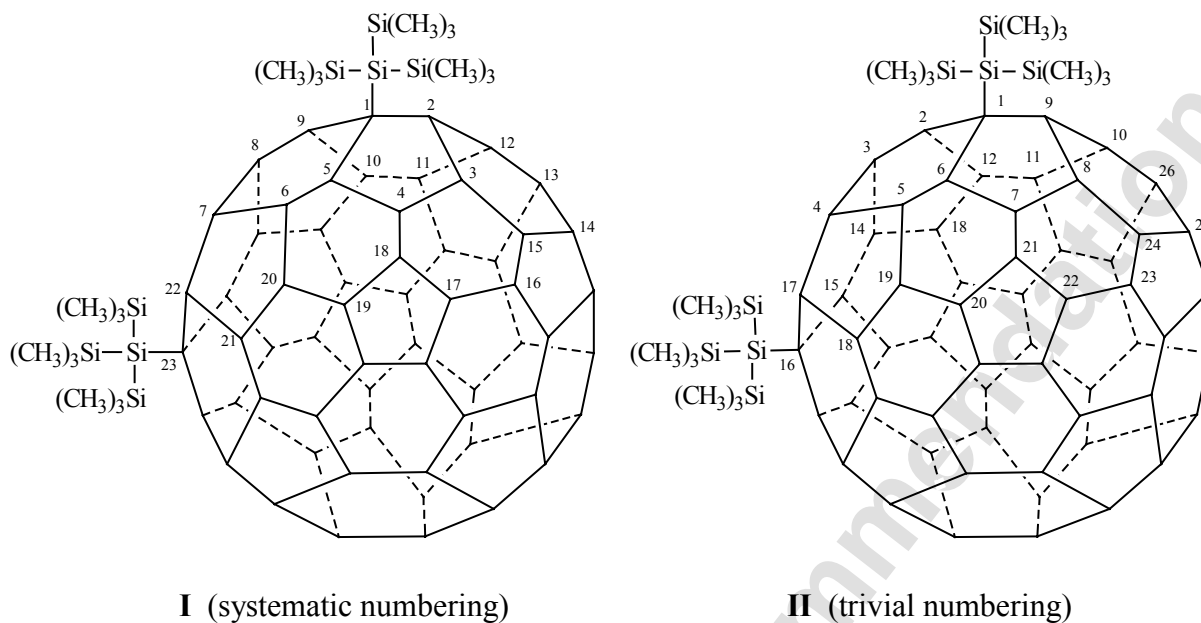
In the enantiomers of the  $(C_{60}-I_h)[5,6]$ fullerene derivatives shown above, clockwise (I) and anticlockwise (II) numbering leads to the same lowest set of locants, namely, 1,9:34,35:43,57, respectively. Use of the enantiomeric numbering scheme for each, shown as III and IV below, results in the 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.

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.



### Example 2.





**I** (<sup>f,s</sup>C)-1,23-Bis[1,1,1,3,3,3-hexamethyl-2-(trimethylsilyl)trisilan-2-yl]-1,23-dihydro-(C<sub>60</sub>-I<sub>h</sub>)[5,6]fullerene

**II** (<sup>f,t</sup>A)-1,16-Bis[1,1,1,3,3,3-hexamethyl-2-(trimethylsilyl)trisilan-2-yl]-1,16-dihydro-[60]fullerene

This is a simple compound with an inherently chiral substitution pattern but it illustrates that the configurational description may be different using systematic versus trivial numbering.

#### 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 due to the geometric arrangement of the substituents, all of which must not 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 (ref. 11). 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

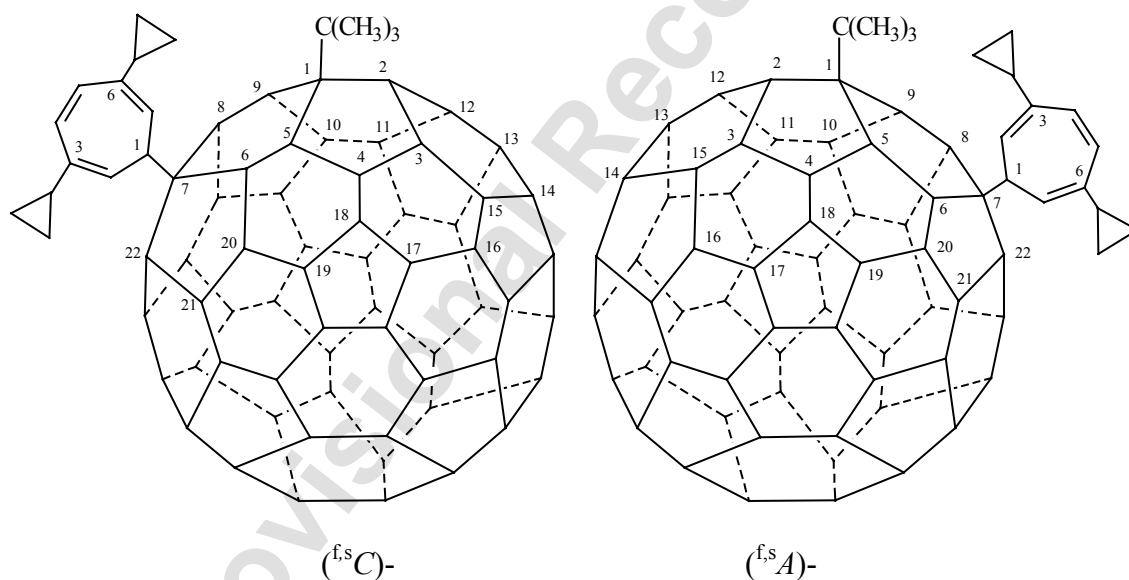
difference is identified<sup>1</sup>. Of the two mirror-symmetric numbering schemes leading to the same lowest set of locants, the one assigning a lower locant to an atom or group of higher CIP priority at the first point of difference is preferred and confers its descriptor to the enantiomer in question.

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



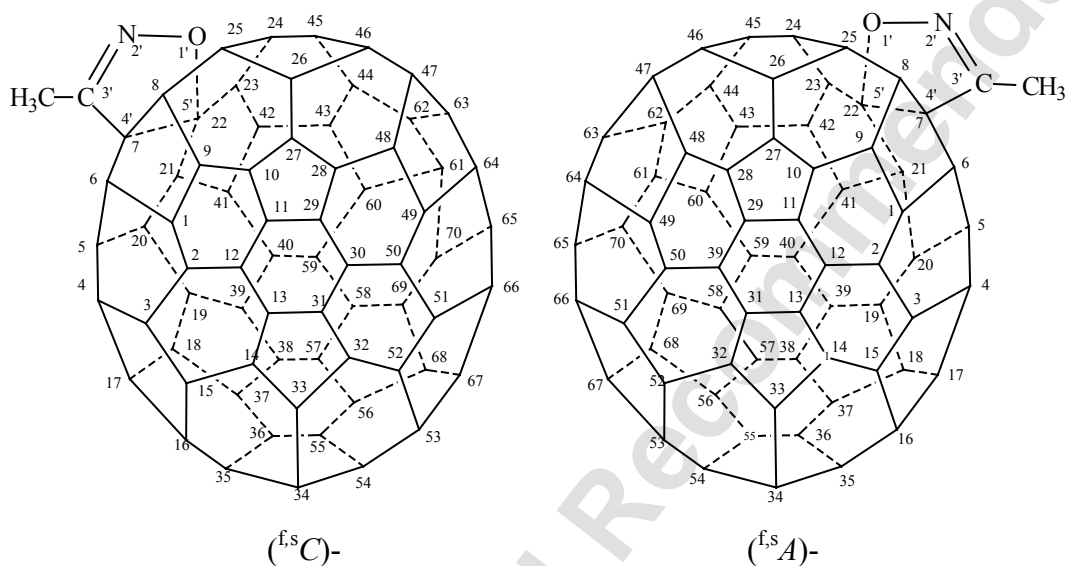
This compound is chiral only because the substituents are constitutionally different. The parent fullerene is achiral and it does not have an inherently chiral substitution pattern because replacement of both substituents by the same achiral test substituent, 'T', results in an achiral compound. Therefore 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-dicyclopropyl-

<sup>1</sup> In case two enantiomorphic substituted fullerenes would have 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 (ref. 11), <sup>f,x</sup>C be given priority over <sup>f,x</sup>A..

cyclohepta-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).

**Example 2:**

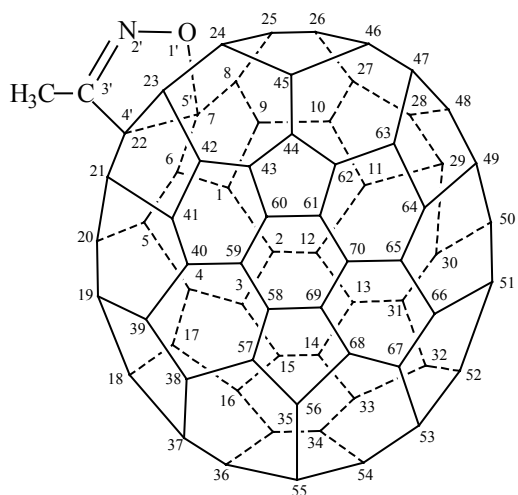
3'-Methylisoxazolo[4',5':7,22](C<sub>70</sub>-D<sub>5h(6)</sub>)[5,6]fullerene



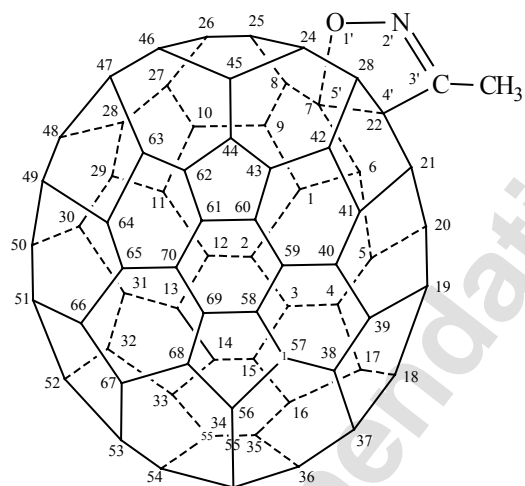
This compound is chiral only because the fused ring is unsymmetrical. The parent fullerene is achiral and it does not have an inherently chiral substitution pattern because replacement of both substituents by the same achiral test substituent, 'T', results in an achiral compound. Therefore it has a noninherently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

In this example, the numbering used to name the compound is based on the nomenclature principle of lowest set of locants for the fusion site and is not appropriate for assignment of the stereodescriptor. The numbering scheme to be used for assignment of the configurational descriptor 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<sub>70</sub>-D<sub>5h(6)</sub>)[5,6]fullerene because its locants are higher than those in the name above. Therefore, the stereodescriptors for the enantiomers shown above are  $(f,sC)-$  and  $(f,sA)-$ , respectively, as shown.

However, it must be kept clearly in mind that the generation of the stereodescriptor is additional to name formation.



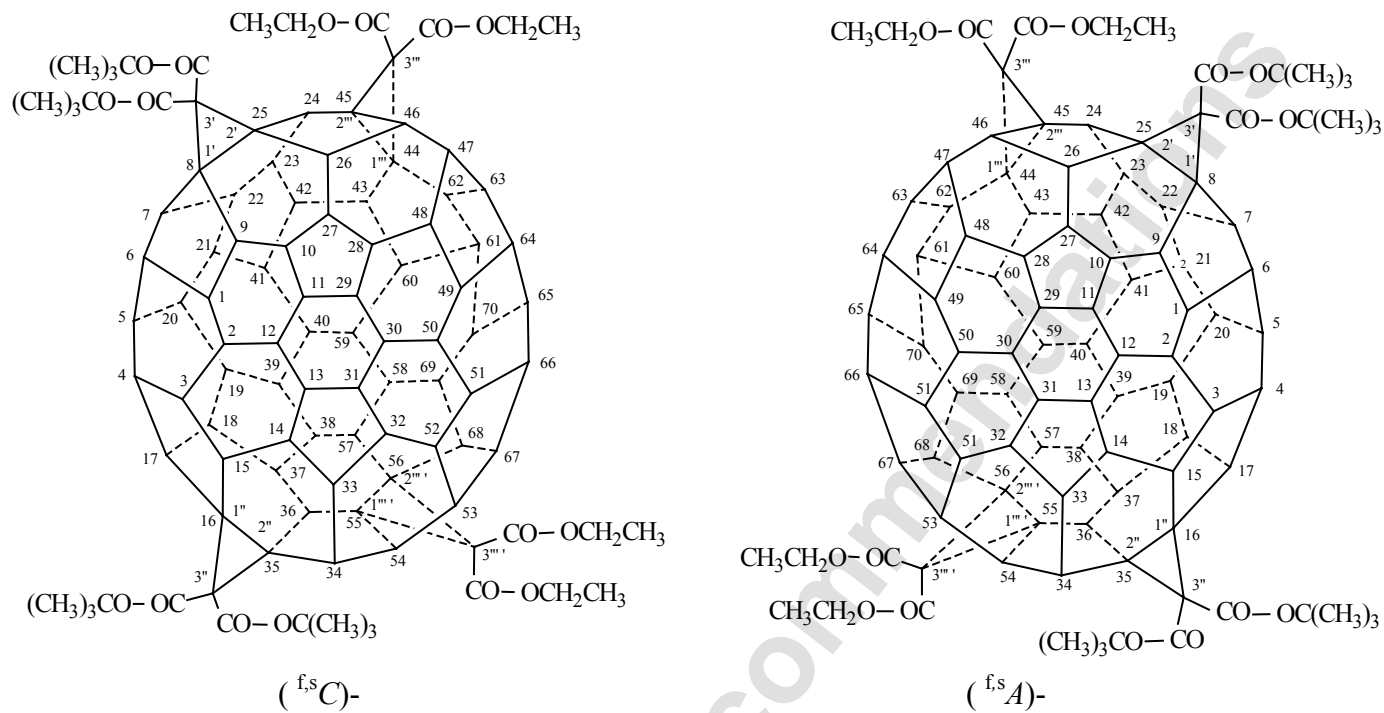
(<sup>f,s</sup>C)-



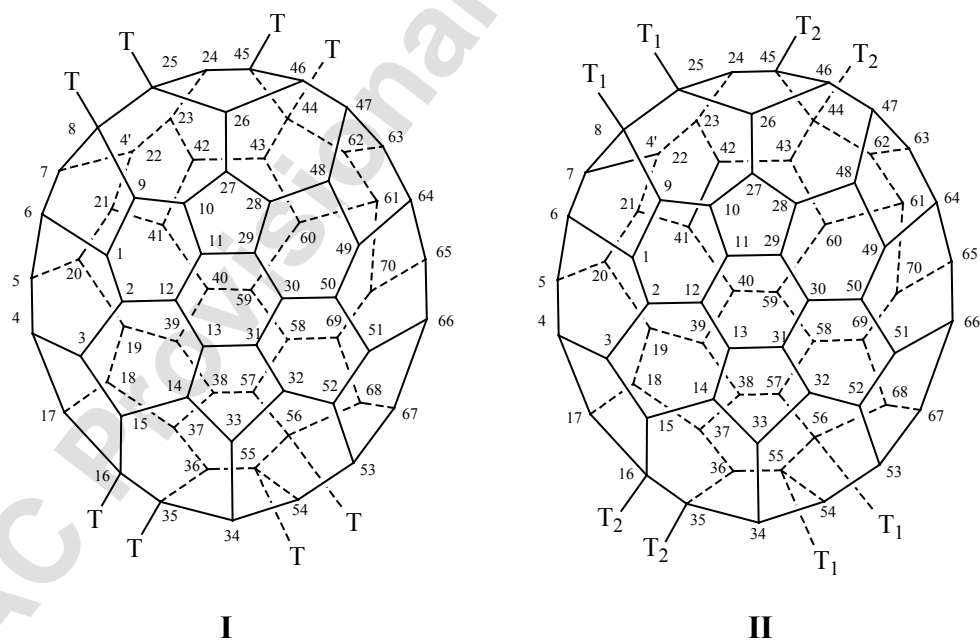
(<sup>f,s</sup>A)-

### Example 3.

3',3',3'''',3''''-Tetra-*tert*-butyl 3'',3'',3''',3''''-tetraethyl 3'H,3''H,3'''H,3''''H'-  
tetracyclopropa[8,25:16,35:44,45:55,56](C<sub>70</sub>-D<sub>5h(6)</sub>)[5,6]fullerene-  
3',3',3'',3''',3''',3''',3''''',3''''''-octacarboxylate



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.



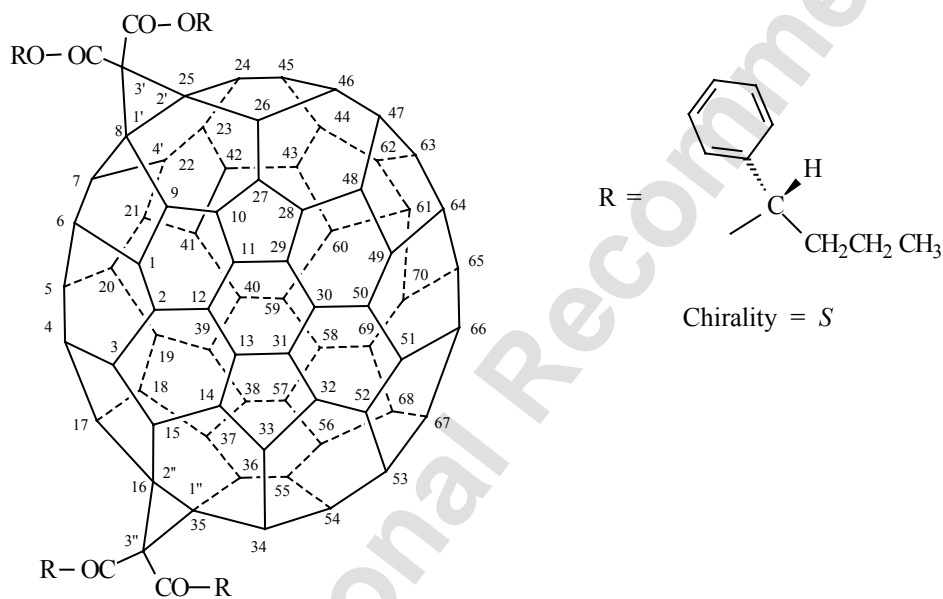
Accordingly, the second step of the substitution test (see Scheme 1), i.e., replacement of the substituents by achiral test substituents  $T_1$  and  $T_2$ , which respect the identities and nonidentities of the original substituents, is applied (see

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 carrying 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



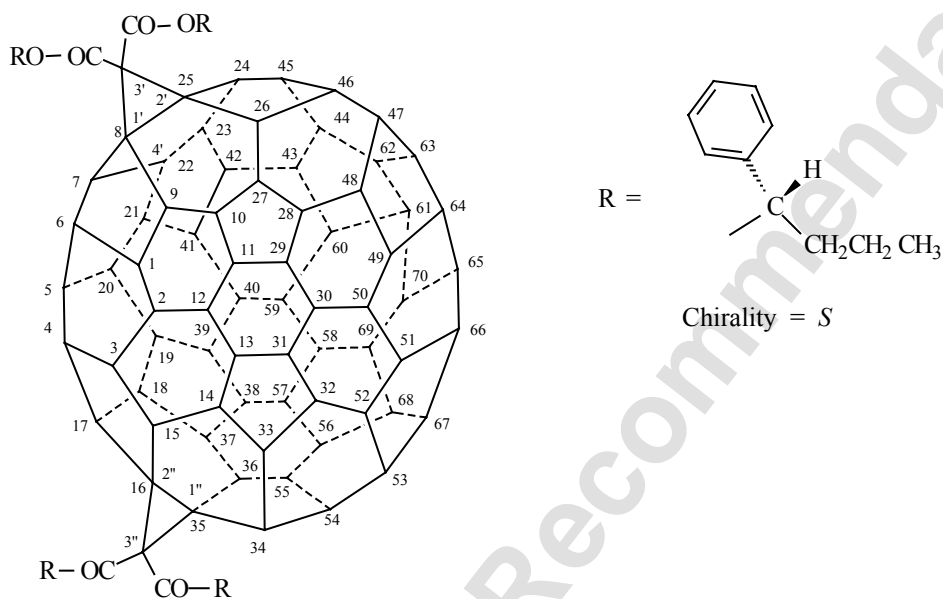
This fullerene derivative is chiral. The parent fullerene is achiral and the derivative has an achiral substitution pattern. Replacement of all substituents by the achiral test group T (see Scheme I) results in an achiral structure; and since the original substituents were already identical the second step of the substitution test is not necessary. Step 3 of the substitution test (see Scheme I) 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 (ref. 12).

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 its 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:**



Chirality = (<sup>f,s</sup>C)-

(<sup>f,s</sup>C)-Tetrakis[(1*S*)-1-phenylbutyl] 3'*H*,3''*H*-dicyclopropa[8,25:33,34]-  
(C<sub>70</sub>-D<sub>5h(6)</sub>)[5,6]fullerene-3',3',3'',3''-tetracarboxylate

or

(*S,S,S,S*, <sup>f,s</sup>C)-Tetrakis(1-phenylbutyl) 3'*H*,3''*H*-dicyclopropa[8,25:33,34]-  
(C<sub>70</sub>-D<sub>5h(6)</sub>)[5,6]fullerene-3',3',3'',3''-tetracarboxylate

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 (<sup>f,s</sup>*A*)-tetrakis[(1*R*)-1-phenylbutyl] 3'*H*,3''*H*-dicyclopropa[8,25:33,34](C<sub>70</sub>-D<sub>5h(6)</sub>)[5,6]fullerene-3',3',3'',3''-tetracarboxylate or (*R,R,R,R*, <sup>f,s</sup>*A*)-tetrakis(1-phenylbutyl) 3'*H*,3''*H*-dicyclopropa[8,25:33,34]- (C<sub>70</sub>-D<sub>5h(6)</sub>)[5,6]fullerene-3',3',3'',3''-tetracarboxylate, and similarly for the various diastereoisomers.

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