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**NOMENCLATURE AND TERMINOLOGY OF  
FULLERENES: A PRELIMINARY SURVEY**

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# Nomenclature and terminology of fullerenes: A preliminary survey

A Fullerene Working Party [composed of workers active in the field: Dr. F. Wudl (Chairman), Dr. R.E. Smalley, Prof. A.B. Smith III, Dr. R. Taylor, Dr. E. Wasserman - Mr. E.W. Godly (Observer)] met in Boston in February, 1993, and a set of recommendations was taken forward to the IUPAC Meeting held in Lisbon, August 1993, for consideration by Commission II.3 (High Temperature and Solid State Chemistry). Meetings held there between Mr. E. W. Godly, Dr. R. Taylor, Prof. G.M. Rosenblatt, Prof. J. Corish, and Prof. A. J. Bard, resulted in an updated set of recommendations, which were sent to all members of the working party, and to fifteen expert referees. There was common feedback that existing nomenclature should be used wherever possible. Mr. E.W. Godly and Dr. R. Taylor then produced a further set of recommendations for consideration by a working group which included members and former members of the IUPAC Commission on Nomenclature of Organic Chemistry, and Chemical Abstracts Service representatives (P.M. Giles, E.W. Godly, A.D. McNaught, G.P. Moss, W.H. Powell, and R. Taylor), at Balatonfüred, Hungary in September, 1994. Further meetings under IUPAC auspices took place at Guildford, Surrey, UK in August, 1995, and at Prague, Czech Republic in August 1996.

Some difficult problems are encountered with these molecules, in particular with regard to numbering, the description of isomers having the same symmetry, the question of describing ring systems attached to the fullerene structure, and indeed how to define a fullerene adequately in the first place.

The preparative chemistry of fullerenes is growing rapidly and this document cannot claim to be a 'state-of-the-art' report. What follows has resulted from the various meetings, *viz.* a set of proposals for naming the principal fullerene structures and some of their derivatives, using IUPAC nomenclature principles and practices insofar as they can be taken to apply, together with usages developed by the Chemical Abstracts Service (CAS), cited wherever such comparison has been considered useful.

## 1. DEFINITION

A definition in terms of all closed-cage structures consisting of tri-coordinated carbon atoms would include nanotube-like structures, spheres with bumps and tunnels (these would have regions of negative curvature arising from the presence of ring sizes greater than six), toroidal structures, and also all trivalent polyhedra such as tetrahedral C<sub>4</sub> and cubic C<sub>8</sub>. These are thus all polyhedrenes of which fullerenes are a well-defined sub-class. It was decided to maintain the relatively narrow definition of fullerenes, and to refer to analogues with ring sizes of other than 5 and 6, as *quasi*-fullerenes. It is accordingly proposed that:

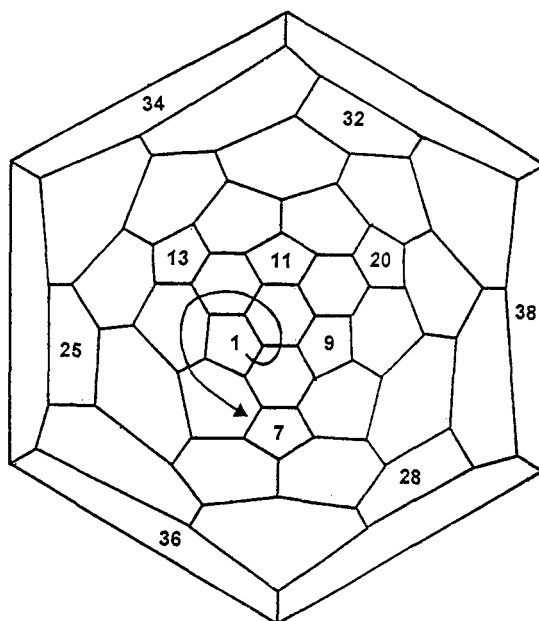
**Fullerenes are defined as polyhedral closed cages made up entirely of  $n$  three-coordinate carbon atoms and having 12 pentagonal and  $(n/2-10)$  hexagonal faces, where  $n \geq 20$ .**

**Other polyhedral closed cages made up entirely of  $n$  three-coordinate carbon atoms shall be known as *quasi*-fullerenes.**

The CAS has developed a broad-based systematic nomenclature and numbering for fullerenes,<sup>1</sup> not restricted to polyhedra of 5- and 6-membered faces only. Their definition and their heirarchical set of rules for numbering are reproduced in Appendix II. This covers theoretical structures as well as those known to occur.

## 2. NAMING OF FULLERENES

The above definition renders unnecessary any description of the number of constituent polygonal faces, since it automatically follows from the fullerene size.



**Fig. 1** Example of the ring spiral sequence, applied to  $[78-D_3]$  fullerene

Fullerenes may be named as for annulenes, for which the number of carbon atoms is indicated in square brackets in front of the word annulene. A problem arises with regard to fullerenes  $C_n$  which have the same point-group symmetry *i.e.* are degenerate. It is necessary to subdivide these (using capital Roman numbers), the subgrouping being defined by the contiguous ring spiral which orders the polygonal faces. An example of a numerical spiral is shown in Figure 1 for  $[78-D_3]$  fullerene, which has only two distinct pentagon environments and thus only ten clockwise, and ten anticlockwise possibilities; the lowest locant spiral is indicated. There are  $6n$  positions for commencement of the spiral, and the position chosen is such that the pentagonal faces have the lowest locants in the series. Use of the nomenclature is shown together with the corresponding fullerene structures (in the form of Schlegel diagrams) in Figures 4-14.

It is therefore proposed that:

**Fullerenes shall be named as such, the number of carbons in the molecule being indicated in square brackets before the word "fullerene", followed by the point group symmetry and, where necessary due to degeneracy, subdivision by means of capital Roman numerals (in parentheses). Thus for 'Buckminsterfullerene' (this name can now be discarded), a full description is:**



The point group symmetry symbols may be omitted if they can be dispensed with without ambiguity.

The priority for subdividing those fullerenes with the same symmetry shall be by Roman numerals assigned on the basis of the lowest numeral sequence at the first point of difference, when the incidence of the twelve pentagonal faces in a ring spiral is stated as a list of numbers in the range 1 to  $n/2 + 2$  in ascending order, using the sequence given in the 'Atlas of Fullerenes';<sup>2</sup> for the principles involved see ref. 3.

**Examples:**

<b>Fullerene</b>	<b>Spiral (location of pentagonal faces)</b>	<b>Figure</b>
[78- $D_3$ ]fullerene	1 7 9 11 13 20 25 28 32 34 36 38	5
[78- $C_{2v}(I)$ ]fullerene	1 7 9 11 13 24 27 30 32 36 38 40	6
[78- $C_{2v}(II)$ ]fullerene	1 7 9 11 14 22 26 28 30 34 39 41	7
[78- $D_{3h}(I)$ ]fullerene	1 7 9 11 15 18 22 25 33 37 39 41	8
[78- $D_{3h}(II)$ ]fullerene	1 7 9 12 14 21 26 28 30 34 39 41	9
[82- $C_{3v}(I)$ ]fullerene	1 7 9 12 14 20 27 32 34 36 38 40	10
[82- $C_{3v}(II)$ ]fullerene	1 7 9 13 20 22 26 28 30 35 41 43	11
[84- $D_2(I)$ ]fullerene	1 7 9 11 13 18 24 35 38 40 42 44	--
[84- $D_2(II)$ ]fullerene	1 7 9 11 14 23 28 30 36 40 42 44	--
[84- $D_2(III)$ ]fullerene	1 7 10 12 14 18 26 31 33 37 39 42	--
[84- $D_2(IV)$ ]fullerene	1 7 10 13 18 22 25 27 31 34 38 44	12
[84- $D_{2d}(I)$ ]fullerene	1 7 9 11 14 22 27 30 35 39 41 43	--
[84- $D_{2d}(II)$ ]fullerene	1 7 10 13 18 22 25 27 31 38 41 43	13
[84- $D_{3d}$ ]fullerene	1 7 9 13 20 22 26 28 30 34 36 44	14
[84- $D_{6h}$ ]fullerene	1 7 10 13 19 22 25 28 30 34 37 44	15

CAS names are distinguished by the inclusion of ring size designators in square brackets at the beginning, and carbon numbers and symmetry designators at the end, *e.g.* [5,6]fullerene- $C_{60}-I_h$  rather than [60- $I_h$ ]fullerene.

**3. NAMING OF QUASI-FULLERENES**

For polyhedral closed cages made up entirely of  $n$  three-coordinate carbon atoms and having faces other than, or in addition to, pentagons and hexagons, the types of constituent rings present shall be indicated by numbers in parentheses. Thus the structure shown by the Schlegel diagram in Figure 16 is (4,6,8)[48- $O_h$ ]quasi-fullerene.

In the nomenclature system developed by CAS (see below) this compound would be described as [4,6,8]fullerene- $C_{48}-O_h$ .

**4. NUMBERING**

The object of numbering is to facilitate communication between chemists. They may reasonably be expected to recall and use an agreed *simple* numbering scheme, as realistically this is likely to concern only a dozen or so parent molecules. It may thus prove unwieldy to apply to practical cases a set of rules to cover every conceivable eventuality, when the number of fullerenes stable enough to be isolated and distinguishable from isomers is likely to be relatively few. (These alternative numberings may be compared to the IUPAC codification of "trivial numbering" for certain important structures (*e.g.* purines, steroids) as exceptions to systematic general principles for numbering polycyclic structures, maintained for practical convenience.)

With some fullerenes, contiguous spiral numbering may not be achievable. A further problem is that the majority of fullerenes do not have a principal symmetry axis *e.g.*, of the 104 (isolated pentagon) isomers of [94]fullerene, 89 of them do not have such an axis, which renders difficult the task of defining a point of numbering commencement. One method that may be satisfactory in such a case is to commence numbering from the polygon that comprises one of the pair that provides the longest face-to-face distance in the molecule. Where a structure has several axes of highest order, one connecting two polygons is chosen. Criteria 4.2 to 4.11 (Appendix I) should be applied in order until a decision is reached.

For some fullerenes, (*e.g.* [70]fullerene) contiguous numbering cannot be achieved from the polygon at the end of the principal axis, though it can be achieved from an adjacent polygon and also from others further removed from this axis. Since the chemistry of [70]fullerene has many similarities to that of [60]fullerene, it is advantageous if the numbering scheme for [70]fullerene parallels that of [60]fullerene (Fig. 2). This is possible (see Fig. 3), and one of the bonds of highest reactivity can be numbered 1,2 as in

[60]fullerene. The close structural similarity (and probable chemistry) of the five main isomers for [78]fullerene makes it advantageous to use the longest axis for each (Figs. 5-9), although this is not the axis of highest order for the  $C_{2v}(I)$  and  $C_{2v}(II)$  isomers. Likewise the two main isomers of [84]fullerene [ $D_{2d}(II)$  and  $D_2(IV)$ ] have almost identical structures (differing only by interchange of two pentagon-hexagon pairs). Allowed number choice for the  $D_2(IV)$  isomer permits closely similar numbering for each (Figs. 12 and 13).

The widely used numbering system shown in Figs. 2-9, 12,13, is based on the article in ref. 4; it differs only in the updated numbering (Fig. 3) for [70]fullerene.

For *quasi*-fullerenes which contain 4-membered rings, contiguous *spiral* numbering cannot be achieved in some (perhaps all) examples. Contiguous numbering may be possible in some cases such as that shown in Figure 16, though necessarily the procedure does not follow the general rules proposed for fullerenes, and the numbering is not truly spiral (see C26 → C27 etc.).

## 5. ENANTIOMERS

A problem with chiral fullerenes is that *R* and *S* cannot apply as these relate to tetrahedral atoms. The experimental observables + and - are inapplicable since addition of a functional group may alter the sign of rotation thereby causing confusion. Accordingly the following procedure may be followed:

**5.1 The point of reference shall be the appropriate Schlegel diagram, drawn perpendicular to the reference axis. It shall be understood that the central polygon, bond or atom of the diagram shall refer to the feature in the three-dimensional structure that is nearest the viewer.**

**5.2 The polygon at the far end of the principal or reference axis, is observed from the three-dimensional model to be rotated with respect to the corresponding nearest polygon [the one containing the sequence C1 → C5(C6)], when viewed along this axis.**

**5.3 Determine the minimum rotation of the far polygon, and its immediate neighbours required to bring them into an eclipsing arrangement relative to the nearest corresponding feature (usually depicted centrally on the Schlegel diagrams in this document) and its immediate neighbours. If this is a clockwise rotation then the molecule shall be defined as *C* and if it is an anticlockwise rotation the molecule shall be defined as *A*.**

The directions of spiral numbering for enantiomer pairs are in opposite senses.

The enantiomers shown in the Schlegel diagrams of Fig. 4 ([76- $D_2$ ]fullerene) and Fig. 12 ([84- $D_2(IV)$ ]fullerene) are both *A* forms; the enantiomer of [78- $D_3$ ]fullerene shown in Fig. 5 is a *C* form.

A proposal for designating stereoisomers of derivatives<sup>5</sup> is currently under consideration.

In the CAS system the point of reference is the symmetry axis used for numbering. If the *numbering* spirals clockwise it is *C*, and if anticlockwise it is *A*.

## 6. ADDITION PRODUCTS

Unless hydrogenated, a fullerene can be modified only by addition and not by substitution, so in the first instance there can only be *addends* on fullerenes and not *substituents*. Thus the use of the term 'substituent' in the context of fullerenes is normally inappropriate, except where one *addend* is being replaced by another. It is accordingly proposed that:

**6.1 The lowest locant numbering is to be used.<sup>6a</sup>**

**6.2 Groups attached to non-hydrogenated fullerenes shall be described as addends and not substituents. The term substituent may only be applied to a reagent entity that is replacing an addend.**

Since the term 'hydro' is an additive prefix, it is proposed that:

**6.3.1 Compounds such as [60]fullerene with hydrogens attached to the 1- and 2-positions may be described as 1,2-dihydro[60]fullerene.**

**The CAS name for this compound is 1,9-dihydro[5,6]fullerene-C<sub>60</sub>-I<sub>h</sub>.**

*Fully reduced fullerenes are to be known as fulleranes.*

Although fullerene derivatives are formed by additive processes, individual species are conveniently named by substitutive nomenclature in order to comply with the most generally accepted established method of systematic organic chemical nomenclature. In such situations, names are formed by supplying H-atoms by notional addition (a pair for each double bond so saturated) and these are then substituted as appropriate, e.g. 1,2-dibromo-1,2-dihydro[60]fullerene for addition of bromine across the 1,2-bond (cf. 4a,8a-dibromo-4a,8a-dihydronaphthalene). For HBr-addition across the same bond the product would be named 1-bromo-1,2-dihydro[60]fullerene. For two HBr-additions a name such as 1,3-dibromo-1,2,3,4-tetrahydro[60]fullerene could be required.

Although the full name will be required for indexing and abstracting purposes, abbreviation by H-atom deletion may become the norm in many instances since the structure of fullerenes means that complex derivatives (with very lengthy names) are possible; for example a [60]fullerene derivative with 48 addends has already been characterised.

It is therefore proposed that:

**6.3.2 The product of addition of two atoms e.g. bromine atoms to a fullerene e.g. across the 1,2-bond of [60]fullerene shall preferably be described in terms of substitutive nomenclature i.e. as 1,2-dibromo-1,2-dihydro[60]fullerene.**

**The CAS name for this compound is 1,9-dibromo-1,9-dihydro-[5,6]fullerene-C<sub>60</sub>-I<sub>h</sub>.**

(Where there is no possibility of ambiguity in relation to other unsaturated addends in the molecule, and where the number of addends is large, the polyhydro prefix is often omitted, but such names are not IUPAC approved.)

The product of addition of ammonia across the 1,2-bond gives 1-amino-1,2-dihydro[60]fullerene; the addition of water across the 1,2-bond of [70]fullerene gives 1-hydroxy-1,2-dihydro[70]fullerene or 2-hydroxy-1,2-dihydro[70]fullerene depending upon the direction of addition.\*\* However, such use of the amino and hydroxy prefixes is reserved for cases where the name-ending is determined by the presence of a more senior suffix-group, e.g. carboxamide. These three structures are named correctly in section 6.4.

The term *fullerols* has been widely, but incorrectly, used to describe fullerenes possessing hydroxy addends. For naming individual species using the 'ol' suffix the term *fullerenol* should be used. The 'en' suffix is to be used since compounds such as C<sub>60</sub>H<sub>59</sub>OH could eventually be made. Clearly it would be easier to describe such compounds as (say) [60]fulleran-1-ol rather than using the term fullerene with a multiple hydro prefix. Similarly, amino derivatives should be described as fullerenamines. It is therefore recommended that:

**6.4 Hydroxy and amino derivatives of fullerenes can also be named as fullerlenols and fullerenamines, respectively. Thus the three example compounds given in Sect. 6.3.2 are named as 1,2-dihydro[60]fulleren-1-amine, 1,2-dihydro[70]fulleren-1-ol, and 1,2-dihydro[70]fulleren-2-ol, respectively.**

**The corresponding CAS names are [5,6]fulleren-C<sub>60</sub>-I<sub>h</sub>-1(9H)-amine, [5,6]fulleren-C<sub>70</sub>-D<sub>5h</sub>(6)-8(25H)-ol, and [5,6]fulleren-C<sub>70</sub>-D<sub>5h</sub>(6)-25(8H)-ol, respectively.**

**6.5 Bridged fullerenes shall be named by the bridging methods used for fused systems, but with the fullerene retaining its own numbering system, and primed locants for the bridge. Thus the example in Fig. 17 is named 2',3'-dihydro-1'H-1,2-**

**([1,3]epicyclopenta)[60]fullerene. The derivative with the double bond in the addend reduced, would then be 2',3',4',5',-tetrahydro-1'H-1,2-([1,3]epicyclopenta)= [60]fullerene or 1,2-**

\* The order of preference of hydro prefixes is under consideration by IUPAC (see ref. 6b). This document treats them as non-detachable from the name of the fullerene parent-structure, whether or not fused or bridged.

(tetrahydro[1,3]epicyclopenta)[60]fullerene. The derivative with six such reduced addends at the octahedral sites would be 1,2:18,36:22,23:27,45:31,32:55,60-hexakis(tetrahydro[1,3]epicyclopenta)=[60]fullerene.

CAS treats 1,2-bridges as fusions. Whether or not the use of 'fullerene' as a fusion-component name is compatible with existing practice, it is clear that IUPAC ("Blue Book")<sup>7</sup> fusion rules A-21 and B-3 will not as they stand provide convenient fusion-names for bridged fullerene derivatives. Accordingly, special provisions are necessary for the 'fullerene' stem to be maintained in such names. The approach has some points in common with that used for fusion to steroid structures.<sup>8</sup> Use of unprimed and primed numerals respectively for the fullerene and non-fullerene components avoids the problems of repeated exhaustion of the alphabet and of choice (for assignment of fusion letter) at certain of the fullerene Y-junctions. In accordance with CAS rules, the non-fullerene component is treated as a single coherent unit, even if it is itself named by fusion procedures (as Fig. 21b).

Thus convenience is to be a prime consideration here and it remains only to draw up the details for delineation between use of bridging and fusion.

**6.6 Addition of a methylene group across a carbon-carbon double bond gives a methanofullerene. The compound in Fig. 18 (X = CH<sub>2</sub>) is thus**

1,2-methano[60]fullerene (bridging) or 3'*H*-cyclopropa[1,2][60]fullerene (fusion).  
The CAS name is 3'*H*-cyclopropa[1,9][5,6]fullerene-C<sub>60</sub>-*I<sub>h</sub>*.

**6.7 Addition of oxygen across a carbon-carbon double bond gives an epoxyfullerene. The compound in Fig. 18 (X = O) is thus 1,2-epoxy[60]fullerene (bridging) or oxireno[2',3':1,2][60]fullerene (fusion).**

The CAS name is [5,6]fullereno-C<sub>60</sub>-*I<sub>h</sub>*-[1,9-*b*]oxirene.

**6.8 Addition of nitrogen across a carbon-carbon double bond gives an epiminofullerene. The compound in Fig. 18 (X = NH) is thus 1,2-epimino[60]fullerene (bridging) or 1'*H*-azireno[2',3':1,2][60]fullerene (fusion).**

The CAS name is 1'*H*-[5,6]fullereno-C<sub>60</sub>-*I<sub>h</sub>*-[1,9-*b*]azirene.

In the bridging names for these examples, the locant of X is 1'. Thus the compound in Fig 19 is 1'-bromo-1,2-methano[60]fullerene.

**6.9 If a fusion name is used, the fullerene has priority for choice as the component to which all other rings are fused. Unprimed numeral locants shall be used for the fullerene and primed for the other component(s), even if heterocyclic. Thus the compound in Fig. 20 may be named phenazino[2',3':1,2][60]fullerene.**

The CAS name is [5,6]fullereno-C<sub>60</sub>-*I<sub>h</sub>*-[1,9-*b*]phenazine. If the non-fullerene component itself is a fused system, it is named (and numbered) independently before formal fusion to the fullerene.

(Here, as under 6.7 and 6.8, the CAS maintains the IUPAC-preference for the heterocyclic over the carbocyclic component. This is reversed in the special case of fusion to a steroid<sup>8</sup> and the non-CAS fusion names cited illustrate the results of such an approach for fullerenes.)

The following example demonstrates naming according to the 'bridging' and 'fusion' alternatives. Here, 'bridging' yields the simpler name, but this might not be the case with more complex molecules now being synthesized, and it may be that practicality will determine which system shall be used in a particular case.

**6.10 The molecule in Fig. 21 shall be named either as:**

1,2-([2,3]naphthaleno)[60]fullerene (bridging nomenclature), OR  
(cyclobuta[*b*]naphthaleno)[1',2':1,2][60]fullerene (fusion nomenclature).

The CAS name is (cyclobuta[*b*]naphthaleno)[1',2':1,9][5,6]fullerene-C<sub>60</sub>-*I<sub>h</sub>*.

**Numbering:** In the bridging name, the composite bridge [bounded by (...)] retains its own (primed) numbering (Fig. 21a). Use of fusion nomenclature here is governed by the proviso that **the fullerene-**

component numbering is fully retained before considering the other attached component(s) (Fig. 21b). Any attached component (even if itself named by fusion procedures) is then treated as a single coherent unit and assigned primed locants.

**6.11 The molecule in Fig. 22 shall be named as:**

**4',9'-dihydro-1,2-([4',9']epicyclobuta[b]anthraceno)[60]fullerene**  
(bridging nomenclature).

The CAS name is 4',9'-dihydro[4,9]ethanocyclobuta[b]anthraceno[11',12':1,9][5,6]-fullerene-C<sub>60</sub>-I<sub>h</sub> (fusion).

**Note:** The above-described methods for the construction of fusion names and for numbering are intended for use only with fullerenes and *quasi*-fullerenes, and **not** for general use.

Fullerenes with methylene groups inserted into carbon-carbon single bonds should be described by use of the prefix 'homo' having precisely the same significance as in Steroid Nomenclature.<sup>8</sup> Compounds of this type have hitherto been provisionally described as fulleroids. It is therefore proposed that:

**6.12 Fullerenes with carbon-carbon single bonds replaced by methylene groups shall be described as homofullerenes.** The compounds in Fig. 23 (X = CH<sub>2</sub>, O, NH) are named as 1(6)a-homo[60]fullerene, 1a-oxa-1(6)a-homo[60]fullerene, and 1a-aza-1(6)a-homo[60]fullerene, respectively. The compound in Fig. 23 (X = CPh<sub>2</sub>) is named as 1a,1a-diphenyl-1(6)a-homo[60]fullerene.

The CAS names are 1,2(2a)-homo[5,6]fullerene-C<sub>60</sub>-I<sub>h</sub>, 2a-oxa-1,2(2a)-homo[5,6]fullerene-C<sub>60</sub>-I<sub>h</sub>, 2a-aza-1,2(2a)-homo[5,6]fullerene-C<sub>60</sub>-I<sub>h</sub>, and 2a,2a-diphenyl-1,2(2a)-homo[5,6]fullerene-C<sub>60</sub>-I<sub>h</sub>, respectively.

## 7. INCARCERANES

Hitherto the prefix *endo* has been used to describe fullerenes containing an enclosed component. This should be discontinued in recognition of the fact that fullerenes with *endo* and/or *exo*-substituted Diels-Alder adducts are already being described in the literature; in due course we may expect to see such derivatives of fullerenes that contain an enclosed component.

The symbol @ has been widely used to describe fullerenes that contain an enclosed component, is liked by many and is on every keyboard. However the term *incarcerane* already exists to describe such compounds. It is therefore proposed that:

**7.1 The prefix *incar* is to be used in naming a fullerene containing an enclosed element. In formulae the symbol *i* shall be used to denote encapsulation, the symbol being placed to the left of the incarcerated atom. Thus for [82-C<sub>3v</sub>(II)]fullerene-*incar*-lanthanum the formula shall be written *i*LaC<sub>82</sub>{C<sub>3v</sub>(II)}.**

The use of a square bracket to denote metal atoms located outside the fullerene cage (already in use) is considered unsatisfactory, because of potential confusion with coordination nomenclature. If potassium (say) is part of some ionic lattice, then a formula such as K<sub>3</sub>C<sub>60</sub> is necessary. It is therefore recommended that:

**7.2 Fullerenes with metals incorporated in the lattice (i.e. outside the cage) shall be given names of the form tripotassium [60]fulleride(3-) and the formula written as K<sub>3</sub>C<sub>60</sub>.**

**7.3 The formula for *incar*-fullerenes with metals also incorporated in the lattice shall be written as e.g. K<sub>3</sub>{*i*LaC<sub>82</sub>{C<sub>3v</sub>(II)}}.**

## 8. CATIONS, ANIONS, AND RADICALS

Distinction needs to be made between cations formed by electron loss and those produced by protonation. Conversely those anions formed by electron gain (the term fullerides is already gaining wide acceptance) must be differentiated from those arising from hydride addition. This matter is still under



general discussion by IUPAC, and the outcome is awaited. Nevertheless, some guidance is needed for those who are already producing these species, and the following appear to be satisfactory; in the case of radicals, this takes account of the fact that the term 'uide'<sup>6c</sup> indicates addition of H<sup>-</sup>, and that the term 'yl' means loss of a hydrogen atom:

8.1 Cations formed by proton addition shall be named as fullerenium.

8.2 Anions formed by proton loss from a hydrogenated fullerene shall be named as *e.g.* 1,2-dihydro[60]fulleren-1-ide.

8.3 Radical anions formed by electron addition shall be described as fullerene radical anions and given names of the form fulleren-1-elide.

8.4 Radicals shall be named as fullerenyl. If for example, addition of a hydrogen atom to the 2-carbon of [60]fullerene produced a radical localised largely at the 1-position, the radical would be 1,2-dihydro[60]fulleren-1-yl.

The CAS name is [5,6]fullerene-C<sub>60</sub>-I<sub>h</sub>-1(9H)-yl.

## 9. FULLERENES WITH CARBONS REPLACED BY HETEROATOMS

The usual atomic prefixes<sup>6d</sup> (whether for metal or non-metal atoms) are used with appropriate locants:

Thus if, for example, the 1- and 2-carbons in [60]fullerene are replaced by nitrogen and boron respectively, the compound shall be described as 1-aza-2-bora[60]fullerene.

The CAS name is 1-aza-9-bora-[5,6]fullerene-C<sub>60</sub>-I<sub>h</sub>.

Replacement terms shall be ordered as in ref. 6d followed by any homo, nor, and seco terms (having their usual meaning as for steroids<sup>8</sup>) in front of the fullerene name.

## 10. COORDINATION COMPOUNDS

A fullerene directly attached to a metal atom named as a coordination centre is named as a ligand in the normal way. Where more than one such metal atom centre is directly attached, the fullerene is treated as a bridging ligand. Thus a compound such as  $\{[Pd(PEt_3)_2]_6(C_{60})\}$  in which the palladium ligand is bonded at the octahedrally disposed sites of [60]fullerene shall be named as  $\{\mu_6-(1,2\eta:18,36-\eta:22,23-\eta:27,45-\eta:31,32-\eta:55,60-\eta)[60]fullerene\}$ -hexakis[bis(triethylphosphine)palladium].

The CAS name is  $[\mu_6-(1,9-\eta:16,17-\eta:21,40-\eta:30:31-\eta,44,45-\eta:52,60-\eta)] = [5,6]fullerene-C_{60}-I_h$ -dodecakis(triethylphosphine)hexapalladium.

## REFERENCES

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2. P.W. Fowler and D.E. Manolopoulos, 'Atlas of Fullerenes' Clarendon Press, Oxford, 1995 (ISBN 019 855787).
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6. Guide to IUPAC Nomenclature of Organic Compounds, Blackwell Scientific Publications, Oxford, 1993 (a) Section R-0.2.4.2; (b) p. 69, footnote 49; (c) p. 64, sect. R-3.2.1.2; (d) p. 182, Table 33.
7. "Nomenclature of Organic Chemistry, Sections A, B, C, D, E, F, and H", Pergamon, Oxford, 1979, Rules A-21 and B-3.
8. IUPAC-IUB 1989-Recommendations: *European J. Biochem.* 1989, **186**, 429-458; *Pure and Applied Chem.*, 1989, **61**, 1793-1822, (Rule 3S-10.2).

## APPENDIX I

4.1. Site locations are to be designated by numbers.

4.2. The rotation axis is, where possible, to be located. This can pass through any of the six combinations of atom, bond, or ring. As far as is possible, numbering shall proceed as a contiguous spiral from one end of the axis through to the other.

4.3 Where there is a choice for beginning of numbering, the priority order shall be: ring > bond > atom.

4.4 Where there is a choice, a larger ring shall take preference over a smaller one. The numbering for [60]fullerene that results from this rule is shown in Fig. 2.

4.5 Where contiguous sequential numbering cannot be achieved from the polygon at the end of the principal or chosen axis, then numbering shall be attempted from the adjacent polygons, or from the polygons adjacent to them and so on, until contiguous sequential numbering is achieved. The numbering for [70]fullerene that results from this rule is shown in Fig. 3.

4.6 Where there is a choice, the numbering shall terminate as close as possible to the principal axis.

4.7 Where there is a choice, and there are polygons at the opposite ends of a principal axis, then the commencement position for numbering in one polygon shall be chosen so as to produce maximum contiguity in the other.

4.8 Where there is a choice once the above conditions have been met, numbering across interpentagonal bonds shall take precedence over all other combinations. The numbering for [60]fullerene in Fig. 2 is consistent with this condition.

4.9 For fullerenes with either no symmetry axis or no principal axis, the polygon chosen for numbering commencement shall be one of the pair comprising the longest face-face distance in the molecule.

4.10 For consistency in representation on Schlegel diagrams, numbering shall commence in a clockwise direction, and be so maintained as far as is possible. (However, see under Enantiomers, section 5.)

4.11 Where *no contiguous sequential numbering* is possible, the numbering shall proceed as in 4.3, with the priority sequence for the beginning of numbering being across a bond connecting two pentagons > across a bond connecting a pentagon and a hexagon > across a bond connecting two hexagons.

[82- $C_{3v}$ (II)]Fullerene is believed to be such an example and is numbered according to this procedure in Fig. 11.

4.12 In accordance with the above rules, for all molecules in Figs. 2-15, the numbering is as shown in these figures.

The following features apply regarding the consequences for contiguous numbering for each molecule as a result of the commencement position.

- |                                       |   |
|---------------------------------------|---|
| Fig. 4 [76- $D_2$ ]fullerene.         | Position 1 is unique in the hexagon containing C1 → C6, adjacent to the longest $C_2$ axis which bisects the C1-C6 and C71-C76 bonds.   |
| Fig. 5 [78- $D_3$ ]fullerene.         | Position 1 = 3 = 5. Contiguous numbering cannot be achieved from positions 2,4,6.   |
| Fig. 6 [78- $C_{2v}$ (I)]fullerene.   | Position 1 is unique.   |
| Fig. 7 [78- $C_{2v}$ (II)]fullerene.  | Position 1 is better than 3 (no deviation from the 70-78C-perimeter). Position 5 requires a reversal of direction. Contiguous numbering cannot be achieved from positions 2,4,6.                      |
| Fig. 8 [78- $D_{3h}$ (I)]fullerene.   | Position 1 = 3 = 5. Contiguous numbering cannot be achieved from positions 2,4,6.   |
| Fig. 9 [78- $D_{3h}$ (II)]fullerene.  | Position 1 = 3 = 5. Contiguous numbering cannot be achieved from positions 2,4,6.   |
| Fig. 10 [82- $C_{3v}$ (I)]fullerene.  | Commences at an atom in a hexagon.  |
| Fig. 11 [82- $C_{3v}$ (II)]fullerene. | No position gives contiguous numbering. Rule 4.11 is followed.  |
| Fig. 12 [84- $D_2$ (IV)]fullerene.    | The longest hexagon-hexagon $C_2$ axis is used. Numbers commencing at any position in the hexagon are satisfactory, but chosen position gives maximum consistency with the related isomer in Fig. 13. |
| Fig. 13 [84- $D_{2d}$ (II)]fullerene  | Position 1 is unique.   |
| Fig. 14 [84- $D_{3d}$ ]fullerene.     | Contiguous numbering can also be achieved by commencing across the 2,3-bond, but rule 4.8 applies.  |
| Fig. 15 [84- $D_{6h}$ ]fullerene.     | The polygon chosen follows from rule 4.5.   |

## APPENDIX II. CAS PROCEDURE

## (a) Definition of fullerenes

CAS define fullerenes as even-numbered carbon clusters of twenty or more atoms, of connectivity three, that close upon themselves to form spherical or distorted spherical structures.

## (b) Rules for assignment of numbering

Where these numberings differ from those in Figs 2-15, they are given in Figs. 24-29 of Appendix III.

**Rule 1: Axial, Linear and Special Group Fullerenes.** Examine rotation axes ( $C_n$ ) in sequence from highest to lowest order until a contiguous spiral is found; always numbering an atom adjacent to one already numbered. An axis can pass through any of six combinations of ring, bond, or atom. Examine all paths, starting from each unique atom (which may be part of a ring or bond or may be an isolated atom). If no spiral can be found for any of the proper rotation axes, proceed to Rule 2.

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

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

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

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

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

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

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

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

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

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

**Rule 2: Axial Fullerenes with No Spiral and Nonaxial Fullerenes of Point Group  $C_n$ .** If, from Rule 1, no spiral is found for any  $C_n$  axis, slice the fullerene into planes of atoms perpendicular to the principal axis, starting from the preferred end of the axis and then, *when necessary*, combine two or more planes to form contiguous rings throughout the fullerene. From the set of contiguous rings, begin numbering from the plane at the preferred end of the fullerene. If none of the remaining unnumbered atoms are directly bonded to the atom just numbered, a new starting point is needed. Examine the remaining unnumbered atoms and continue numbering from the atom directly bonded to the highest-numbered atom. Proceed in the same direction as the original spiral. Repeat as necessary until all atoms are numbered.

If the point group is  $C_n$ , there is no primary axis. Slice the fullerene into planes of atoms parallel to the  $\sigma_h$  plane in the middle of the fullerene. Start from the plane at the preferred end of the fullerene and then, *when necessary*, combine two or more planes to form contiguous rings throughout the fullerene. From the set of contiguous rings, begin numbering from the plane at the preferred end of the

fullerene. If none of the remaining unnumbered atoms are directly bonded to the atom just numbered, a new starting point is needed. Examine the remaining unnumbered atoms and continue numbering from the atom that is directly bonded to the highest-numbered atom. Proceed in the same direction as the original spiral. Repeat as necessary until all atoms are numbered.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

### APPENDIX III

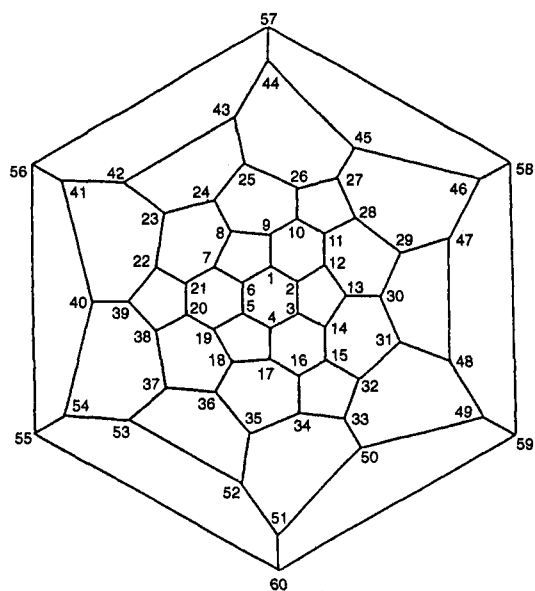


Fig. 2 Numbering for  $[60-I_h]$ fullerene; in this the most reactive bond is the 1,2- bond. See also Appendix IV.

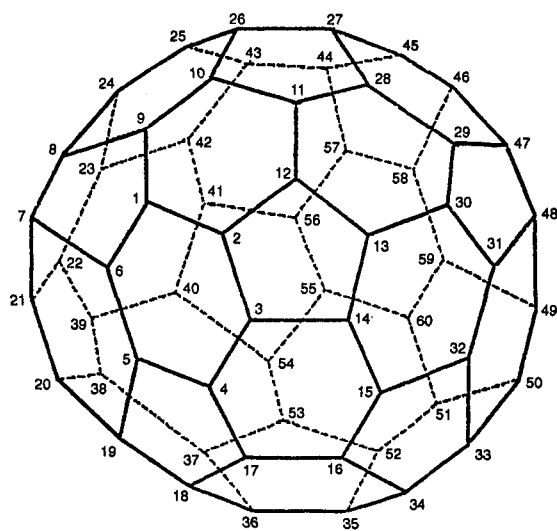


Fig. 2a The numbering in Fig. 2 displayed in 3D format.

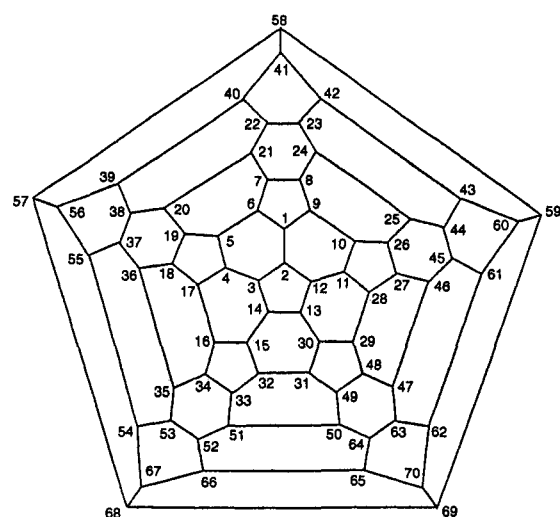


Fig. 3 Numbering for  $[70-D_{5h}]$ fullerene; in this the most reactive bond is the 1,2- bond (see also Appendix IV). The 5,6-bond is the next most reactive one.

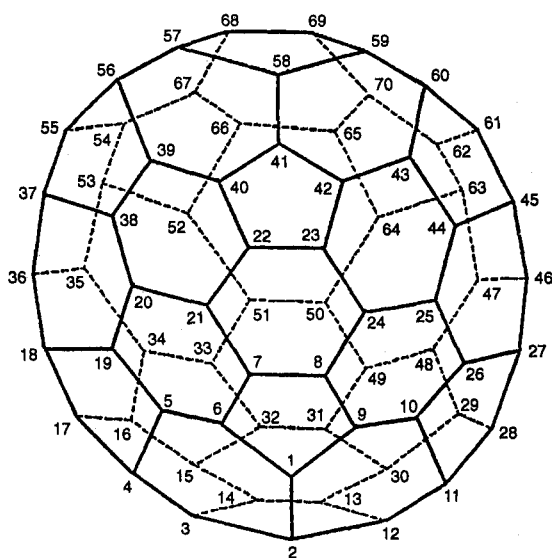


Fig. 3a The numbering in Fig. 3 displayed in 3D format.

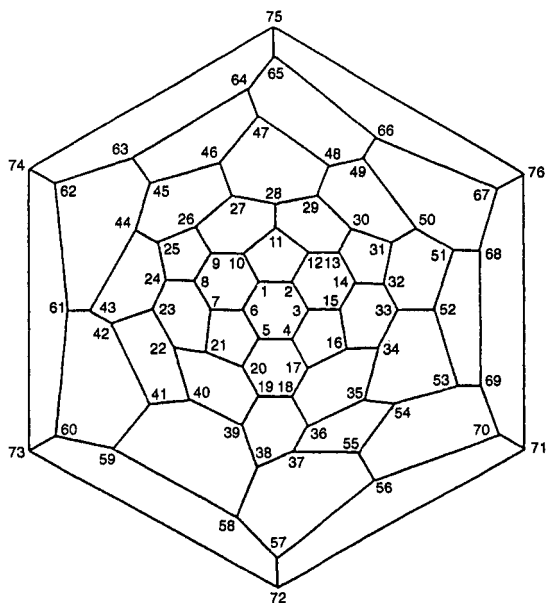


Fig. 4 Numbering for  $[76-D_2]$  fullerene (*A* form shown).

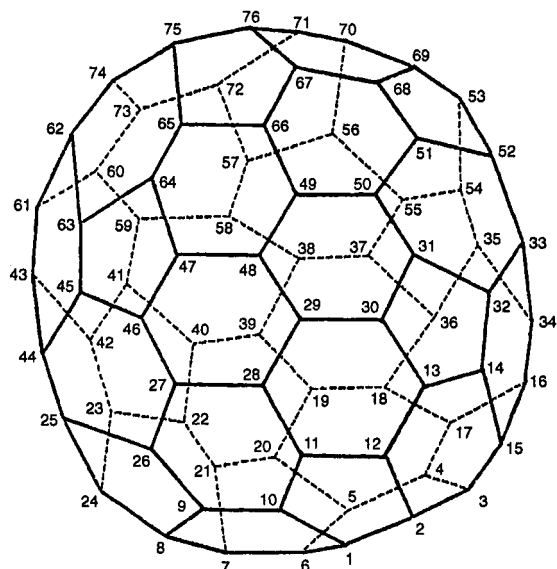


Fig. 4a The numbering in Fig. 4 displayed in 3D format.

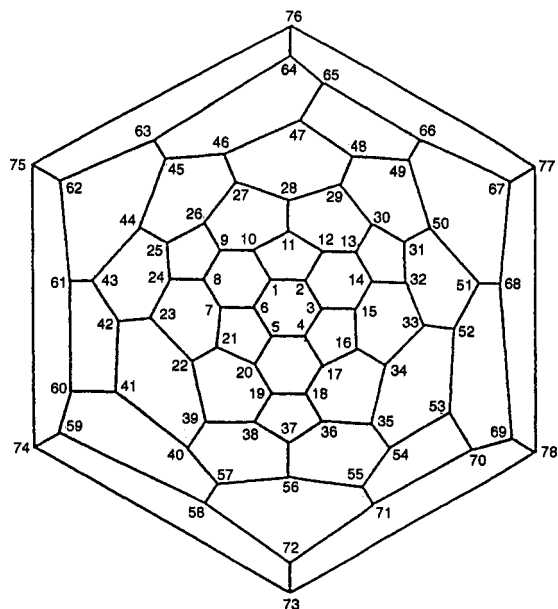


Fig. 5 Numbering for  $[78-D_3]$  fullerene (*C* form shown).

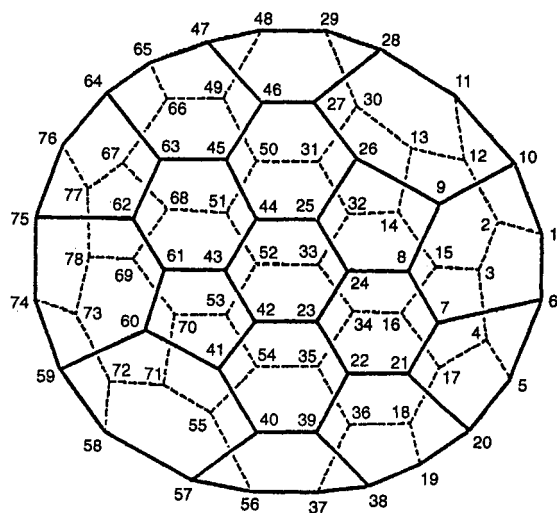


Fig. 5a The numbering in Fig. 5 displayed in 3D format.

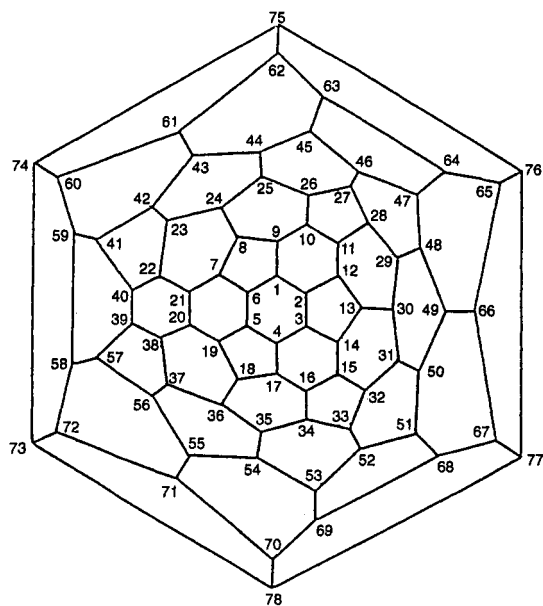


Fig. 6 Numbering for  $[78-C_{2v}(I)]$  fullerene.

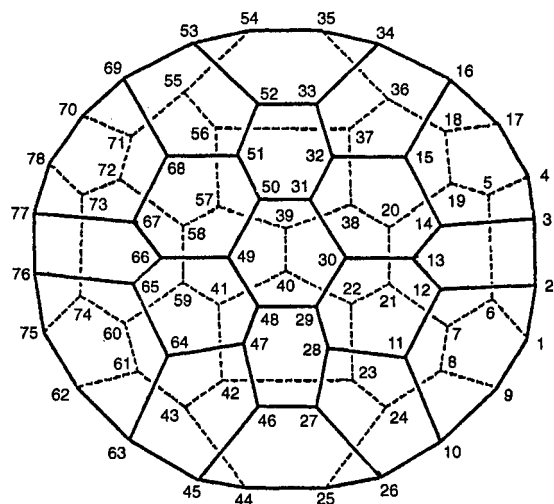


Fig. 6a The numbering for Fig. 6 displayed in 3D format.

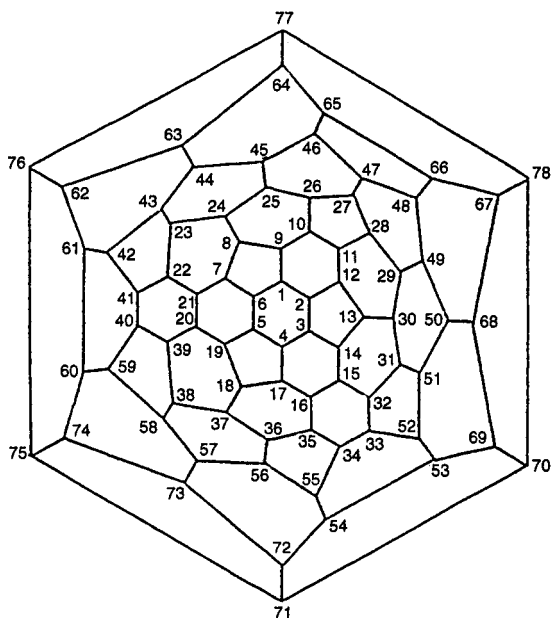


Fig. 7 Numbering for  $[78-C_{2v}(II)]$  fullerene.

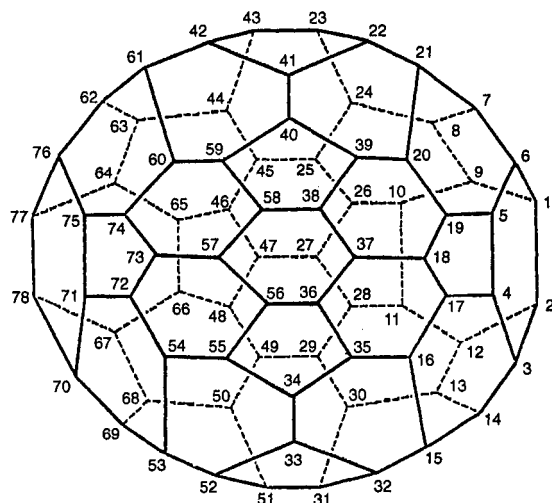
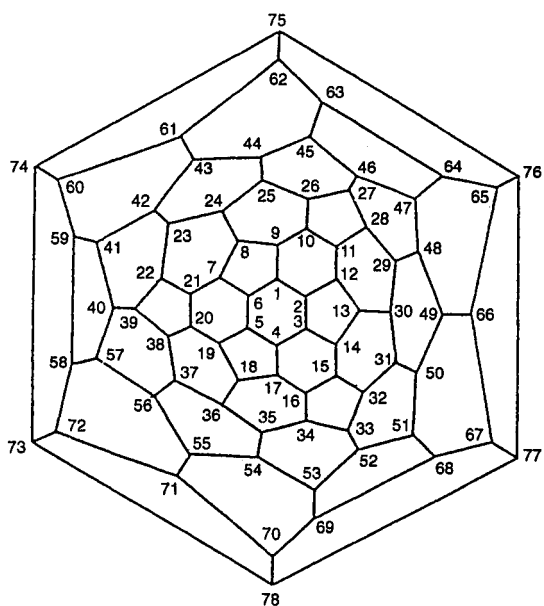
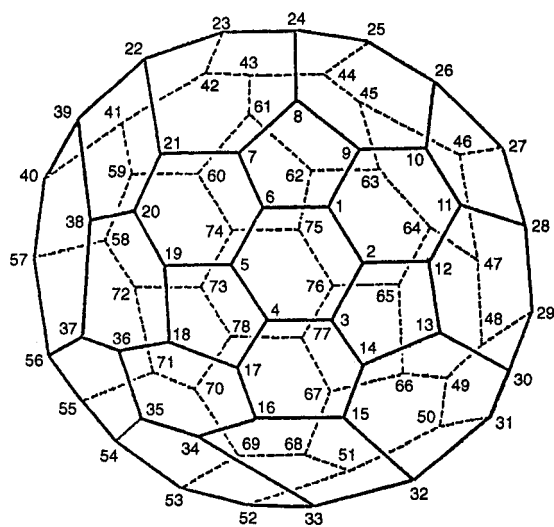


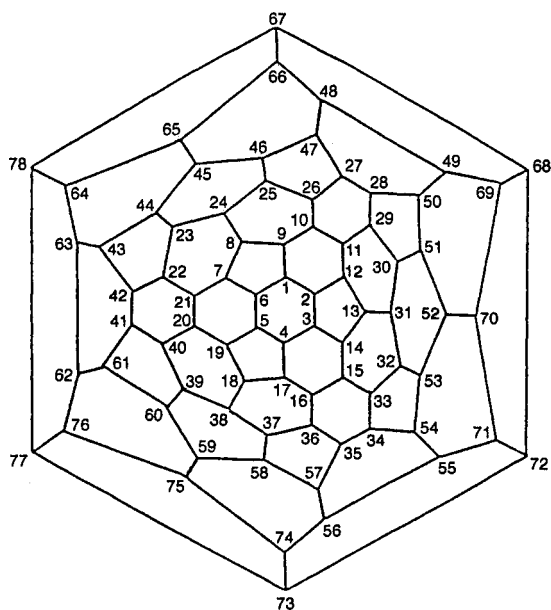
Fig. 7a The numbering in Fig. 7 displayed in 3D format.



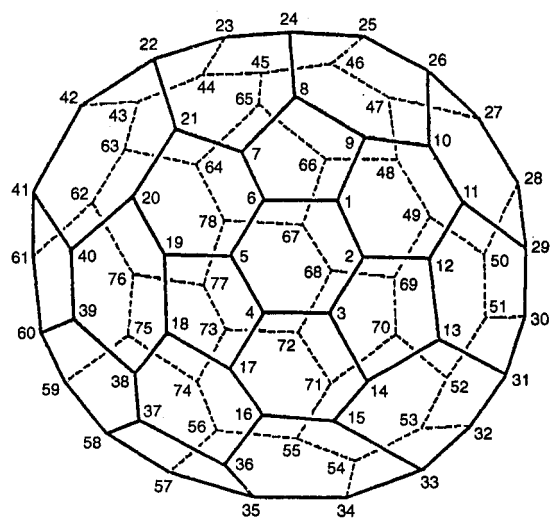
**Fig. 8** Numbering for  $[78-D_{3h}(I)]$  fullerene.



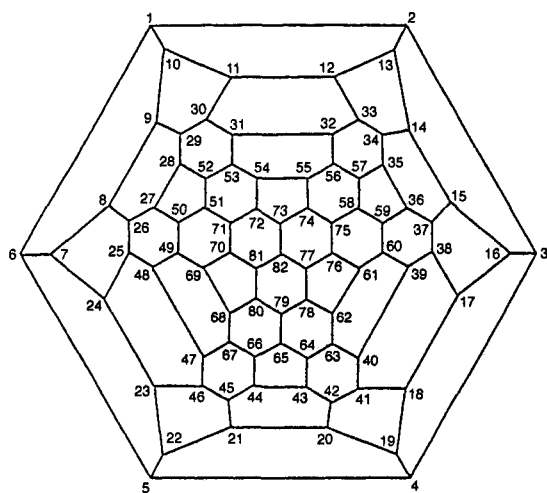
**Fig. 8a** The numbering in Fig. 8 displayed in 3D format.



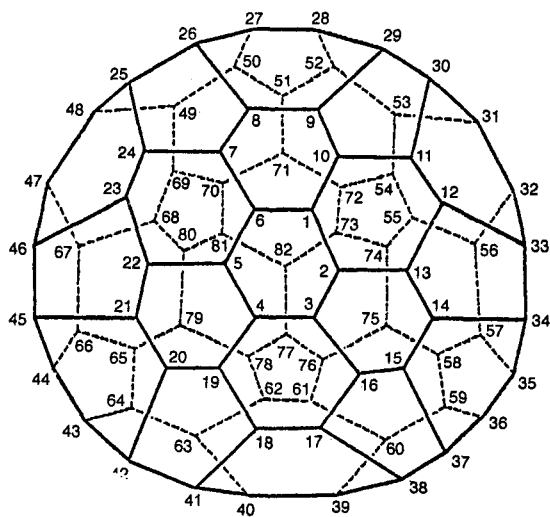
**Fig. 9** Numbering for  $[78-D_{3h}(II)]$  fullerene.



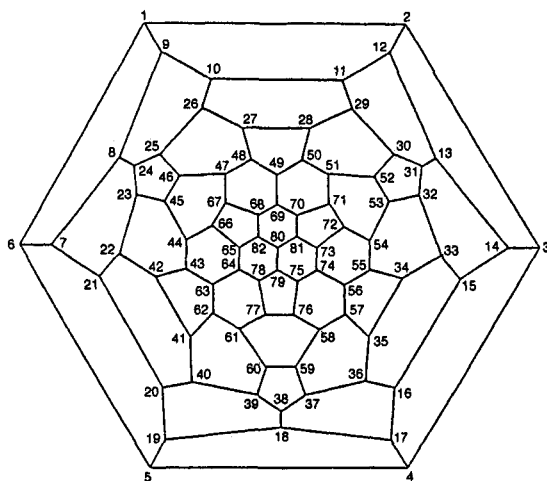
**Fig. 9a** The numbering in Fig. 9 displayed in 3D format.



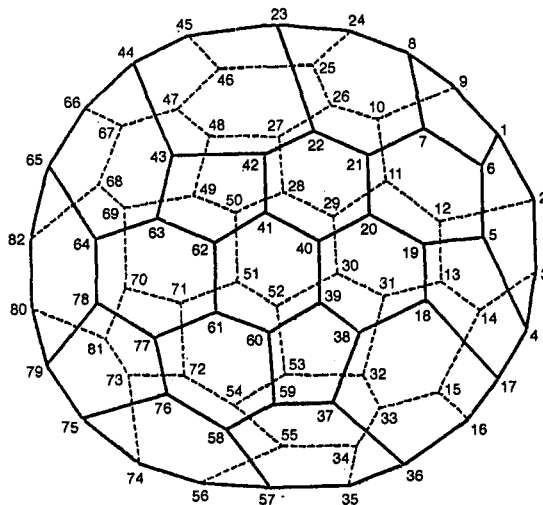
**Fig. 10** Numbering for  $[82-C_{3v}(I)]$ fullerene.



**Fig. 10a** The numbering in Fig. 10 displayed in 3D format.

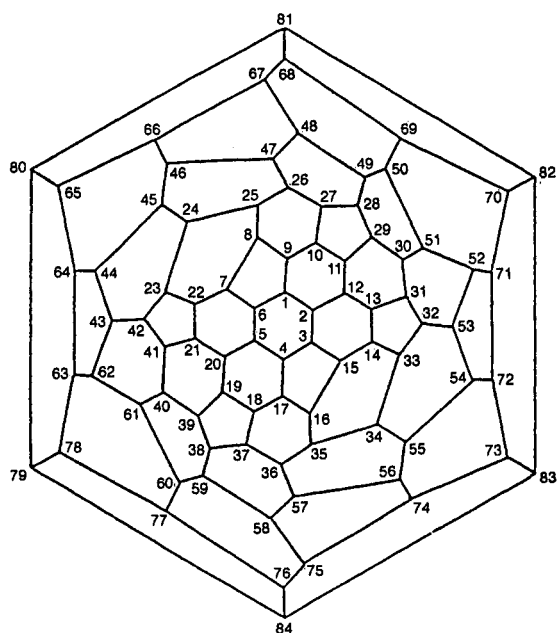


**Fig. 11** Numbering for  $[82-C_{3v}(II)]$ fullerene.

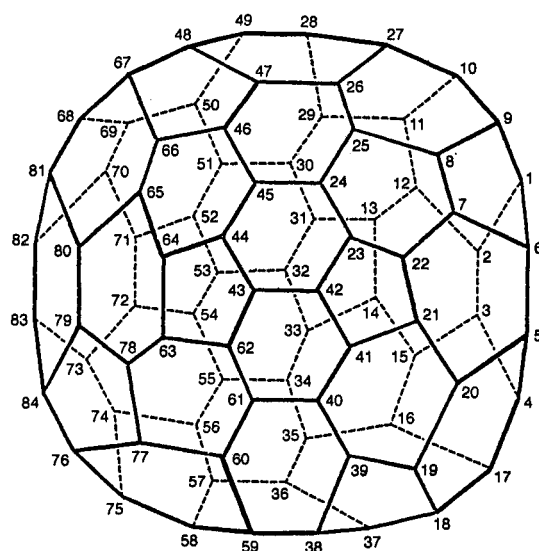


**Fig. 11a** The numbering in Fig. 11 displayed in 3D format.

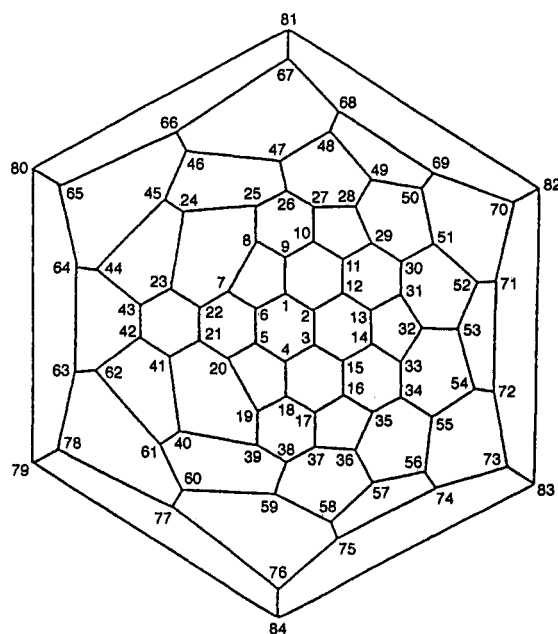




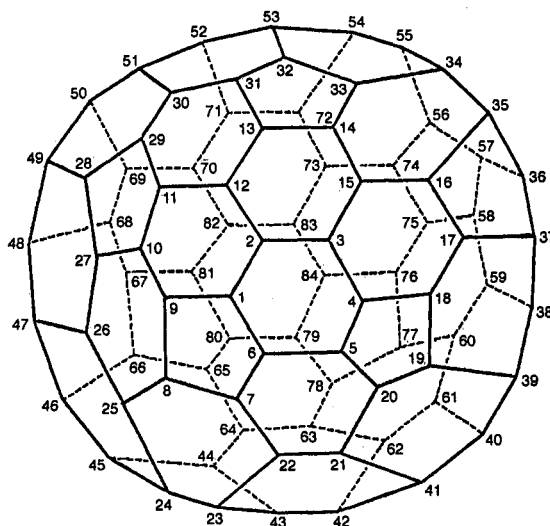
**Fig. 12** Numbering for  $[84-D_2(IV)]$  fullerene (A form shown).



**Fig. 12a** The numbering in Fig. 12 displayed in 3D format.



**Fig. 13** Numbering for  $[84-D_{2d}(II)]$  fullerene.



**Fig. 13a** The numbering in Fig. 13 displayed in 3D format.

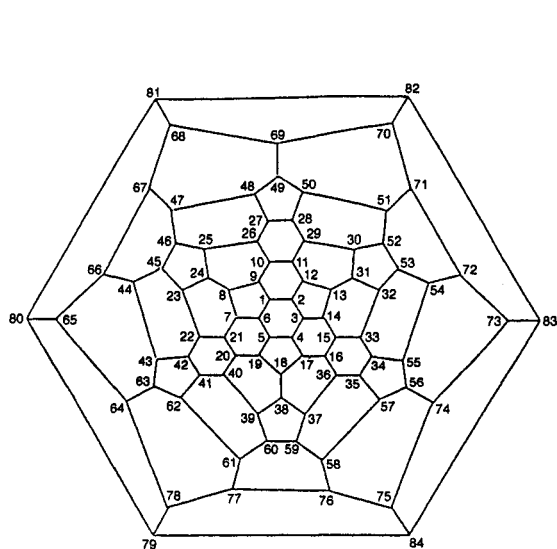


Fig. 14 Numbering for  $[84-D_{3d}]$  fullerene.

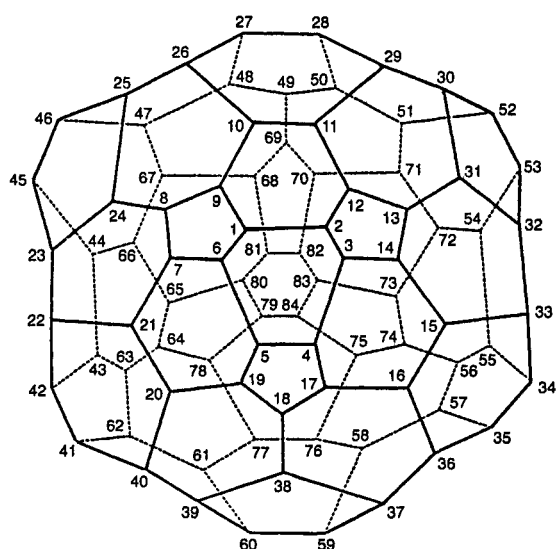


Fig. 14a The numbering in Fig. 14 displayed in 3D format.

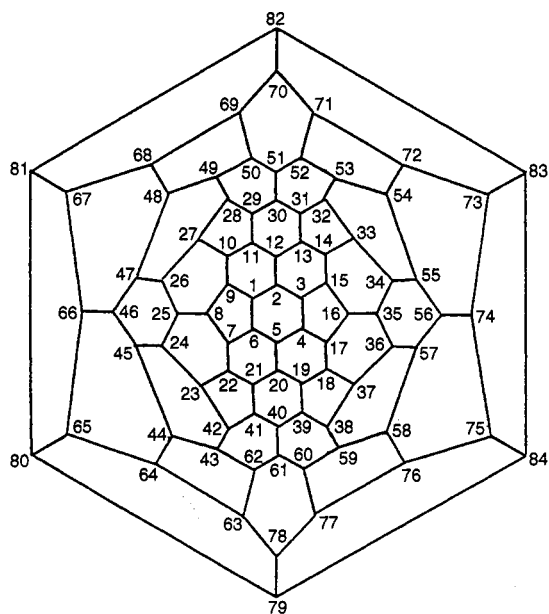


Fig. 15 Numbering for  $[84-D_{6h}]$  fullerene.

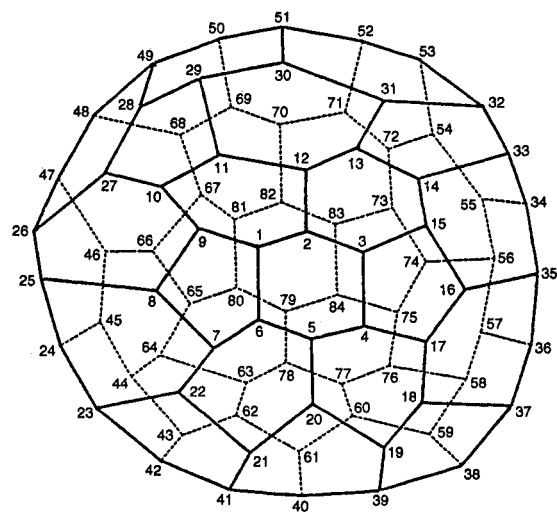


Fig. 15a The numbering in Fig. 15 displayed in 3D format.

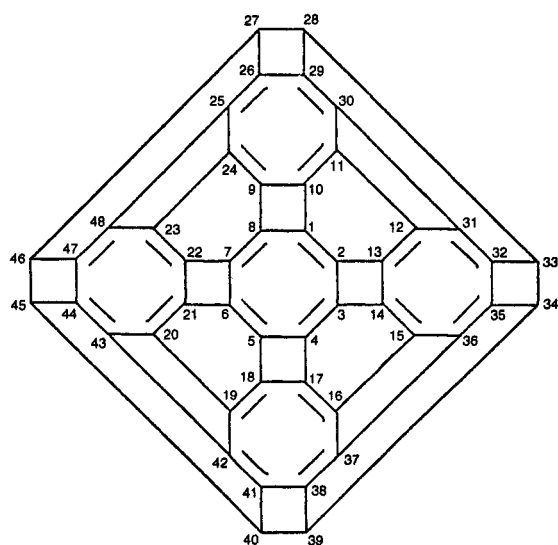


Fig. 16 (4,6,8)[48- $O_h$ ]quasi-fullerene.

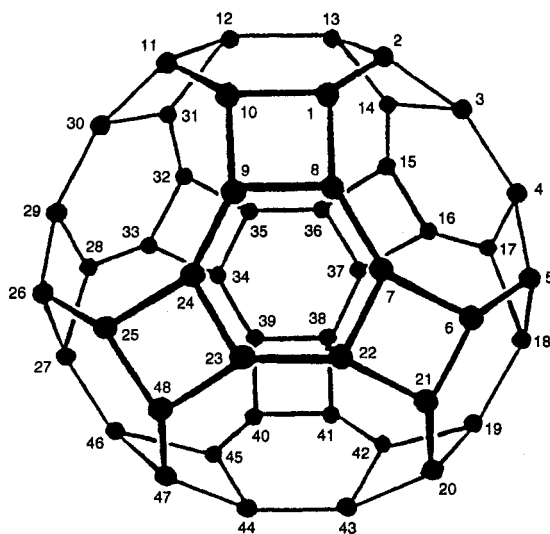


Fig. 16a The numbering in Fig. 16 displayed in 3D format.

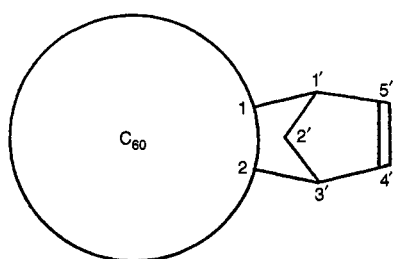


Fig. 17 2,3'-Dihydro-1'H-1,2-([1,3]epicyclopenta)[60]fullerene.

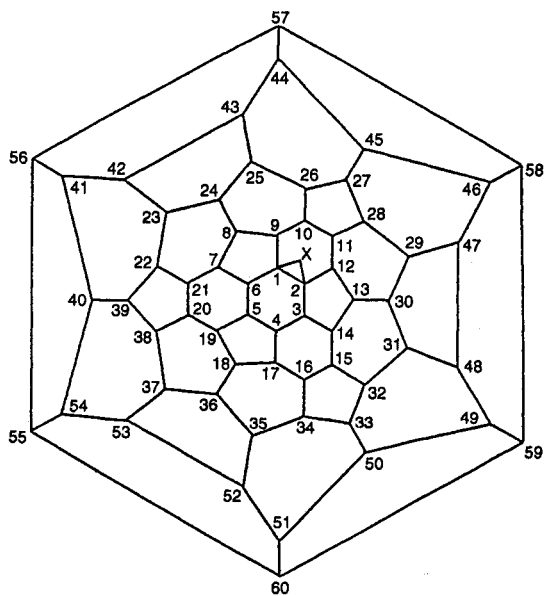


Fig. 18 1,2-Methano[60]fullerene ( $X = CH_2$ ) 1,2-Epoxy[60]fullerene ( $X = O$ ) 1,2-Epimino[60]fullerene ( $X = NH$ ).

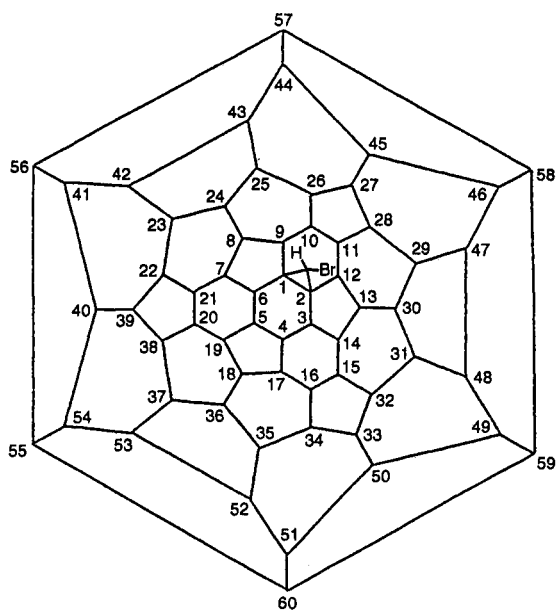


Fig. 19 1'-Bromo-1,2-methano[60]fullerene.

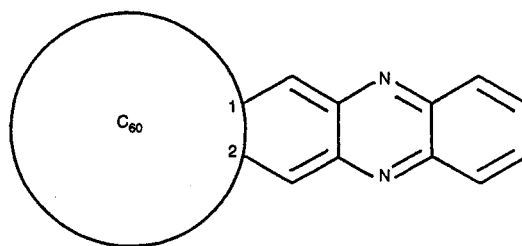


Fig. 20 Phenazino[2',3':1,2][60]fullerene.

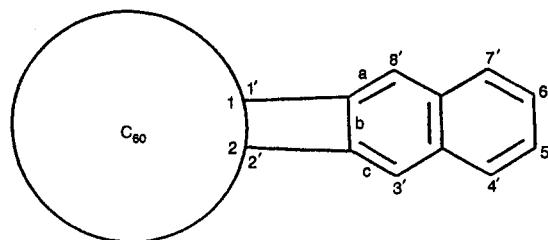


Fig. 21b (Cyclobuta[*b*]naphthaleno)[1',2':1,2][60]fullerene (fusion nomenclature).

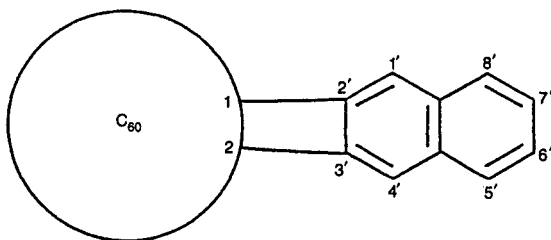


Fig. 21a 1,2-([2,3]Naphthaleno)[60]fullerene (bridging nomenclature).

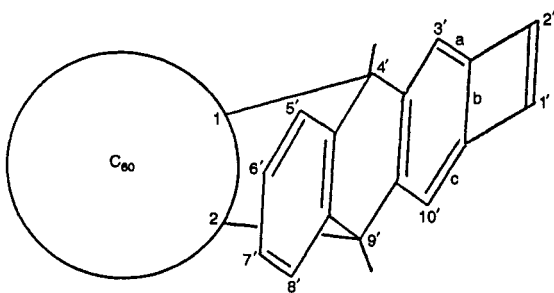


Fig. 22 4',9'-Dihydro-1,2-([4',9']epicyclobuta[*b*]anthraceno)[60]fullerene (bridging nomenclature).

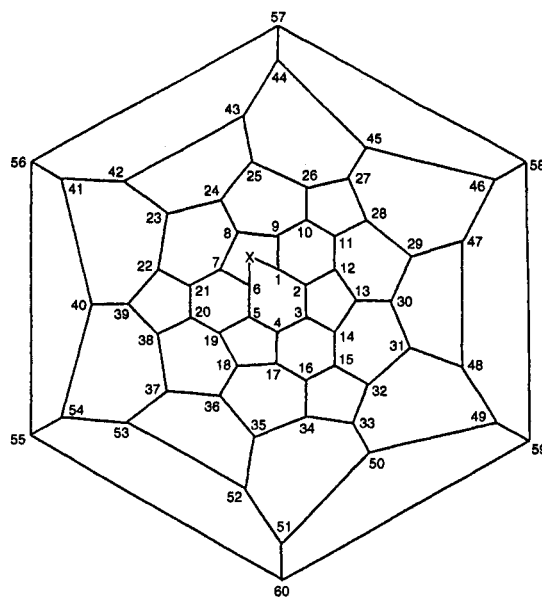
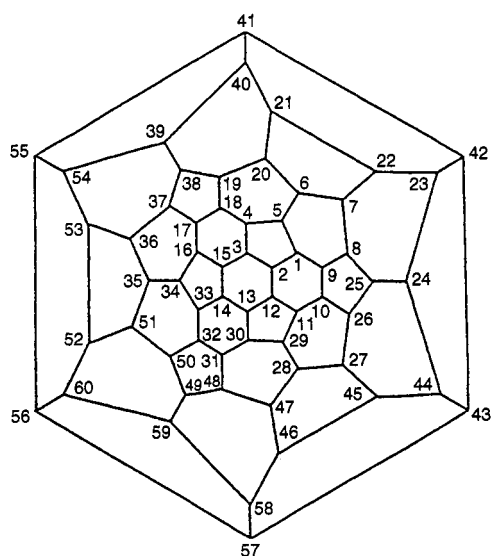
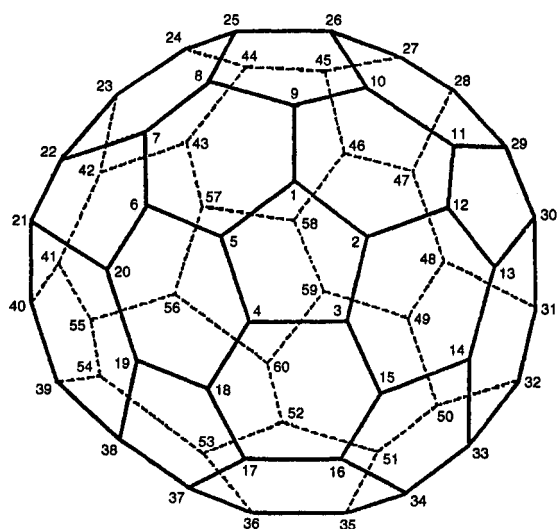


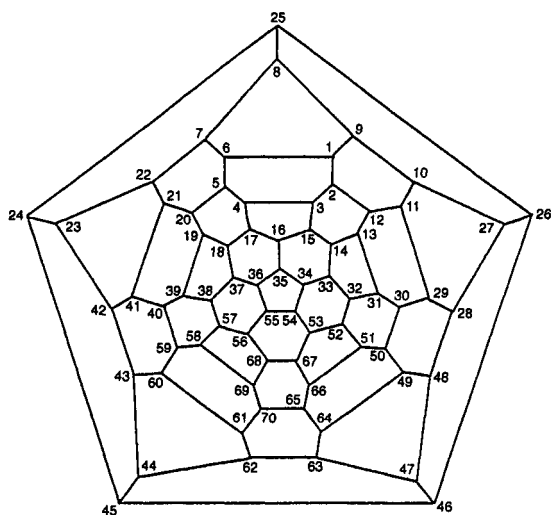
Fig. 23 1(6)a-Homo[60]fullerene ( $X = \text{CH}_2$ ) 1a-Oxa-1(6)a-homo[60]fullerene ( $X = \text{O}$ ) 1a-Aza-1(6)a-homo[60]fullerene ( $X = \text{NH}$ ) 1a,1a-Diphenyl-1(6)a-homo[60]fullerene ( $X = \text{CPh}_2$ ).



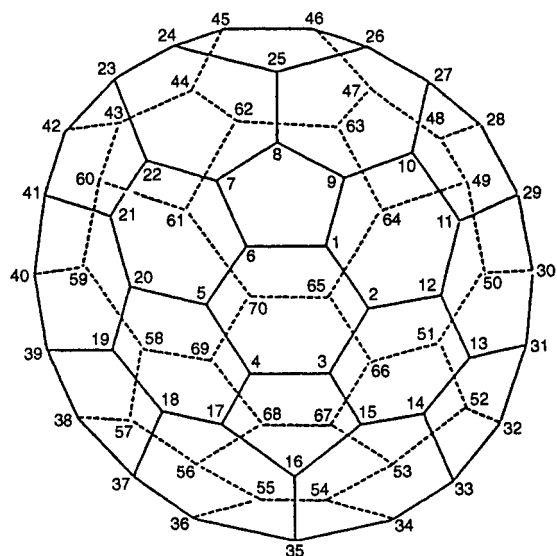
**Fig. 24** CAS numbering of  $C_{60}$  (denoted [5,6]fullerene- $C_{60}-I_h$ ). Here the 1,9-bond is the most reactive one.



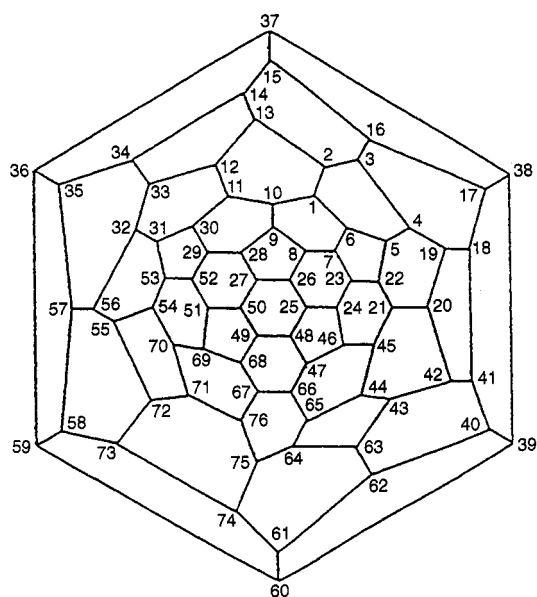
**Fig. 24a** The numbering in Fig. 24 displayed in 3D format.



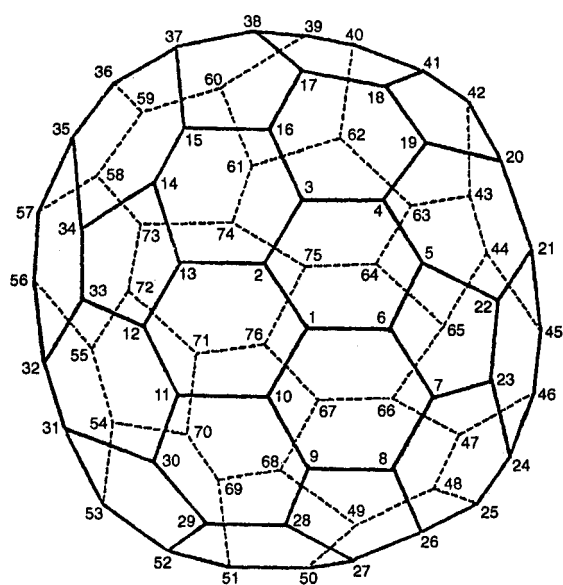
**Fig. 25** CAS numbering of  $C_{70}$  (denoted [5,6]fullerene- $C_{70}-D_{5h}$ ). Here the 8,25 bond is the most reactive one, the next most reactive being the 7,22-bond.



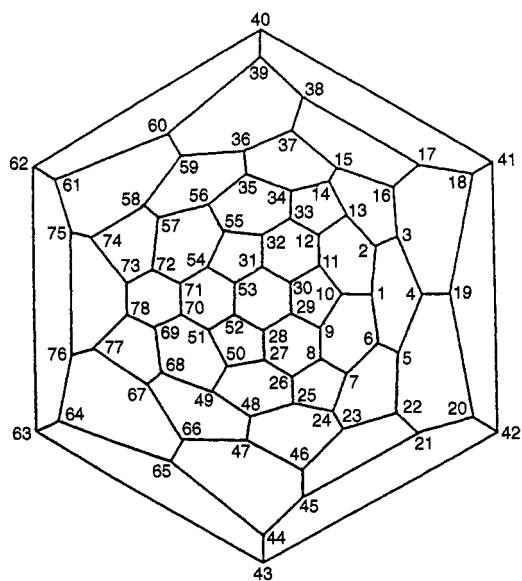
**Fig. 25a** The numbering in Fig. 25 displayed in 3D format.



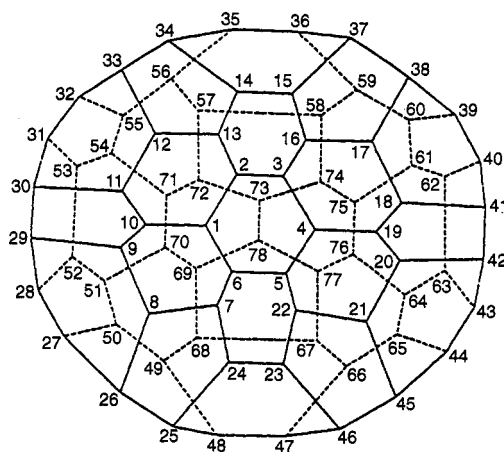
**Fig. 26** CAS numbering for Fig. 4, denoted [5,6]fullerene-C<sub>76</sub>-D<sub>2</sub>.



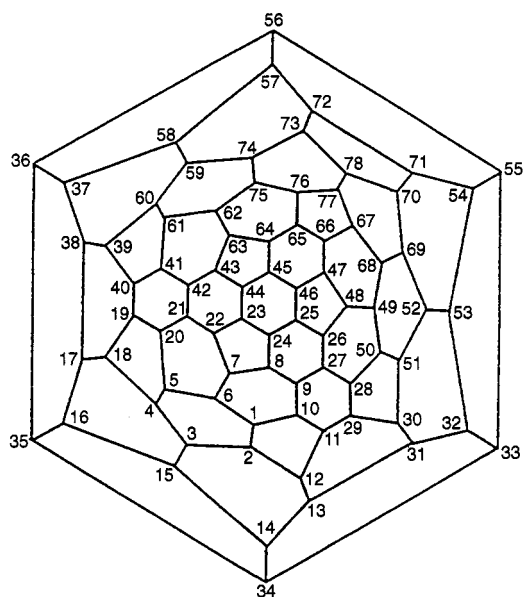
**Fig. 26a** The numbering in Fig. 26 displayed in 3D form.



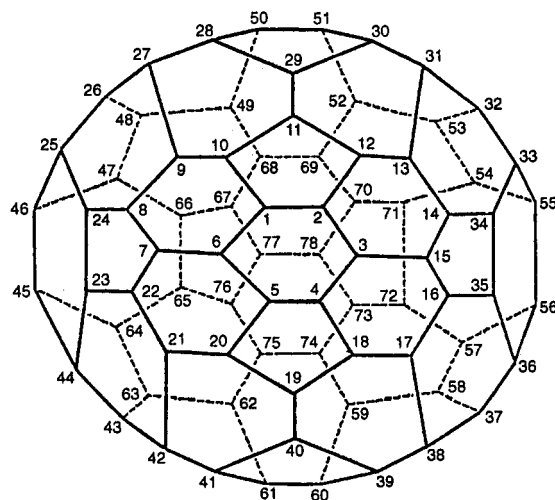
**Fig. 27** CAS numbering for Fig. 6, denoted [5,6]fullerene-C<sub>78</sub>-C<sub>2v</sub>.



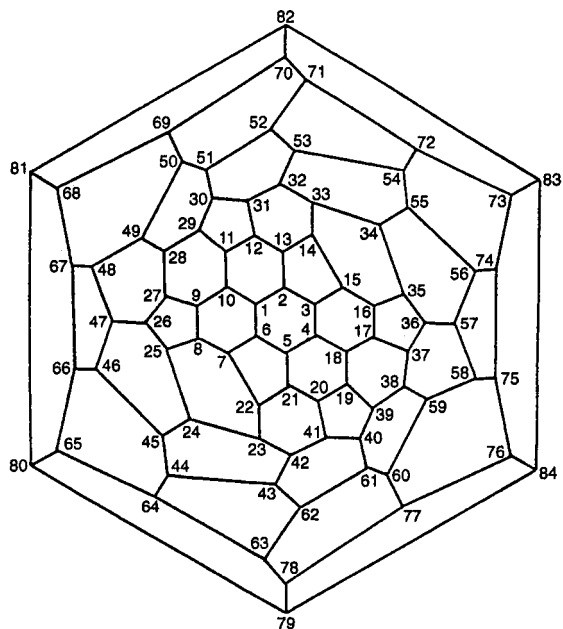
**Fig. 27a** The numbering in Fig. 27 displayed in 3D format.



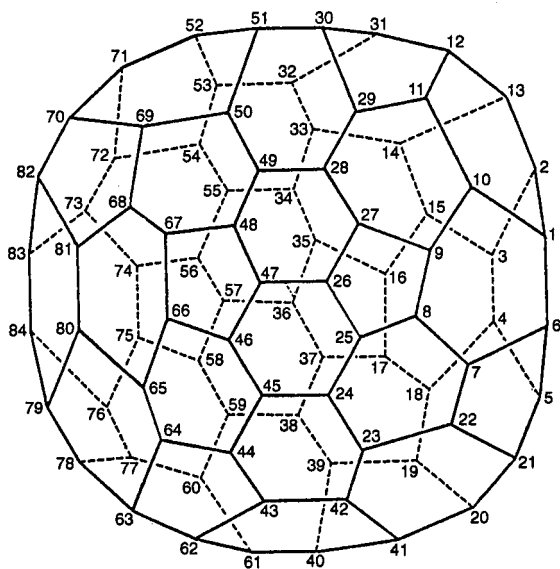
**Fig. 28** CAS numbering for Fig. 7, denoted [5,6]fullerene-C<sub>78</sub>-C<sub>2v</sub>.



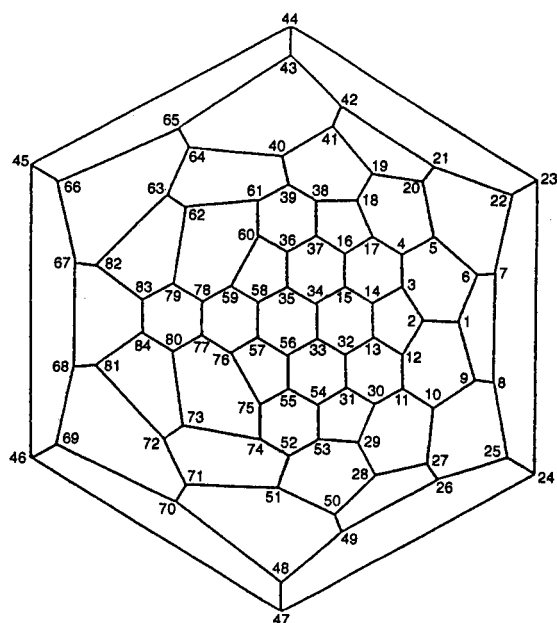
**Fig. 28a** The numbering in Fig. 28 displayed in 3D format.



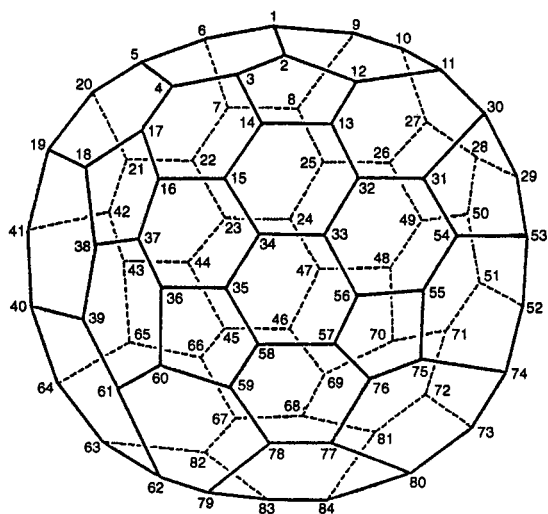
**Fig. 29** CAS numbering for enantiomer of structure in Fig. 12, denoted [5,6]fullerene-C<sub>84</sub>-D<sub>2</sub>.



**Fig. 29a** The numbering in Fig. 29 displayed in 3D format.



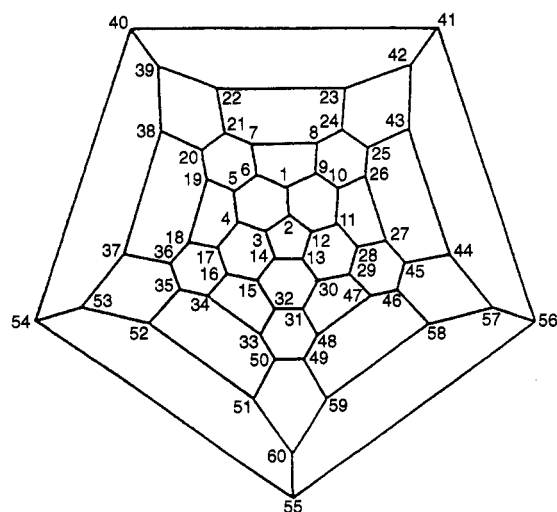
**Fig. 30** CAS numbering for Fig. 13, denoted [5,6]fullerene-C<sub>84</sub>-D<sub>2d</sub>. There are numbering discontinuities here between (C79-C82).



**Fig 30a** The numbering in Fig 30 displayed in 3D format.

#### APPENDIX IV.

Figure 31 shows the same numbering for [60]fullerene as shown in Figure 2, but in a pentagonal format. This demonstrates the similarity to the contiguous numbering scheme for [70]fullerene shown in Figure 3. The numbering in relation to the occurrence of pentagons and hexagons is identical for both fullerenes up to carbon atom no. 38.



**Fig. 31** Numbering for [60]fullerene in pentagonal format; the numbering scheme is the same as that shown in Figure 2.