Fig. 22. Systematic numbering for (C_{82}-C_{3v})[5,6]fullerene

3.2.9 Systematic numbering for (C_{84}-D_{2d})[5,6]fullerene (Fig. 23) (Atlas Ref. No. 84:23; CAS Reg. No. 145809-03-6).

This fullerene contains three C_2 axes, each intersecting midpoints of opposite bonds as shown in Fig. 23a. Since the axes have the same order, the numbering can start at any of the bonds bisected by the axes. Only three pathways must be evaluated: **a** to **a'** to **d**; **b** to **b'** to **e**; **c** to **c'** to **f**. None of these leads to a contiguous numbering: all of them are discontiguous at position 81 (Figs. 23b, 23c, and 23d). Exploration of the numberings according to **Fu-3.2.3** shows that the numberings reported in Fig. 23b and 23d are preferred because they contain a 6,6,6 atom at position 15. Further exploration shows that the numbering of Fig. 23b is preferred since it contains a 6,6,6 atom at position 19, whereas that of Fig. 23d contains a 6,6,5 atom at the same position. According to **Fu-3.2.4**, the completion of the numbering requires a discontiguous step to reach position 82 connected to the higher locant 80 (**Fu-3.2.4a**), a contiguous step to position 83 (**Fu-3.2.4b**), and a final discontiguous step to reach position 84.

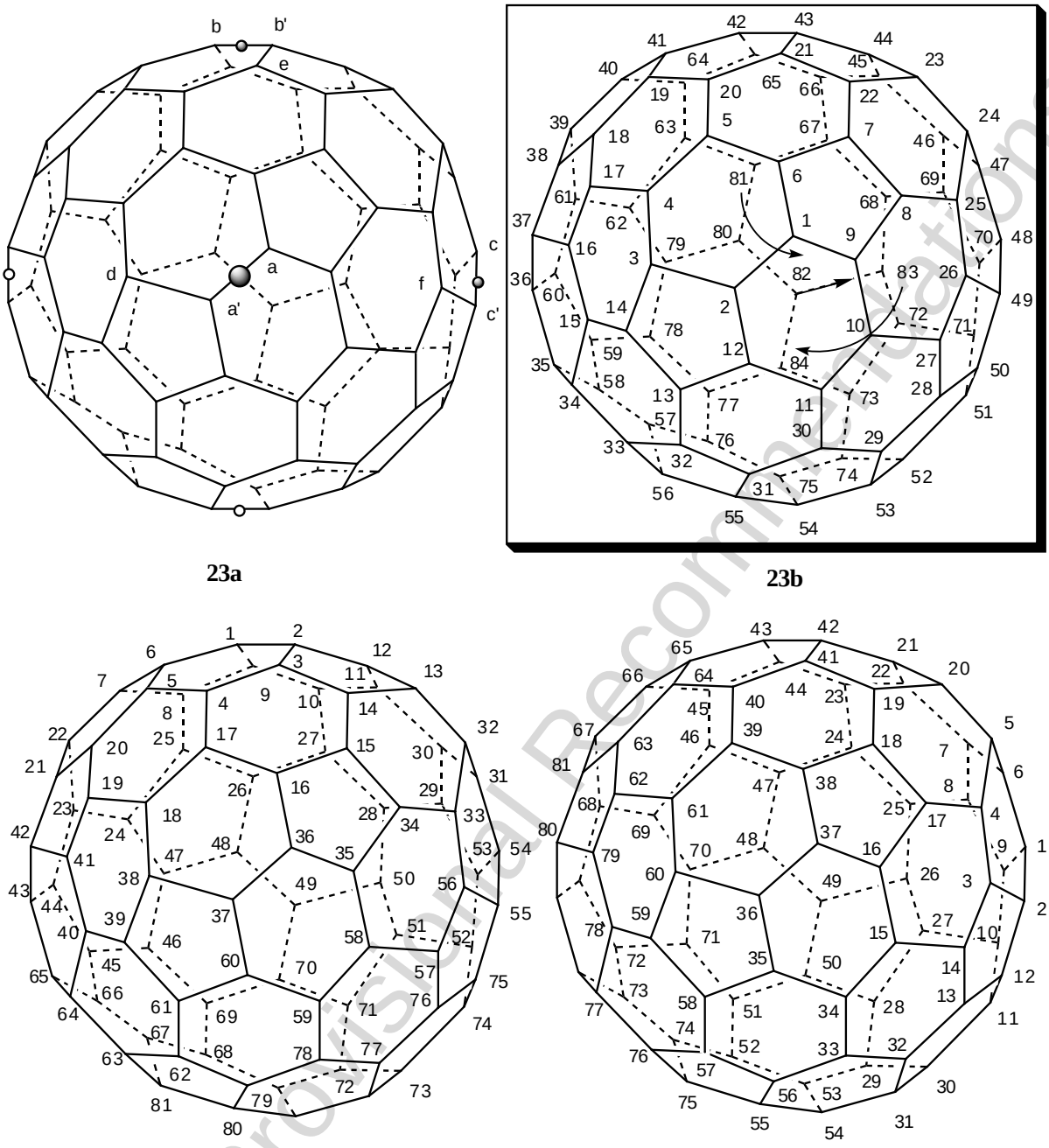
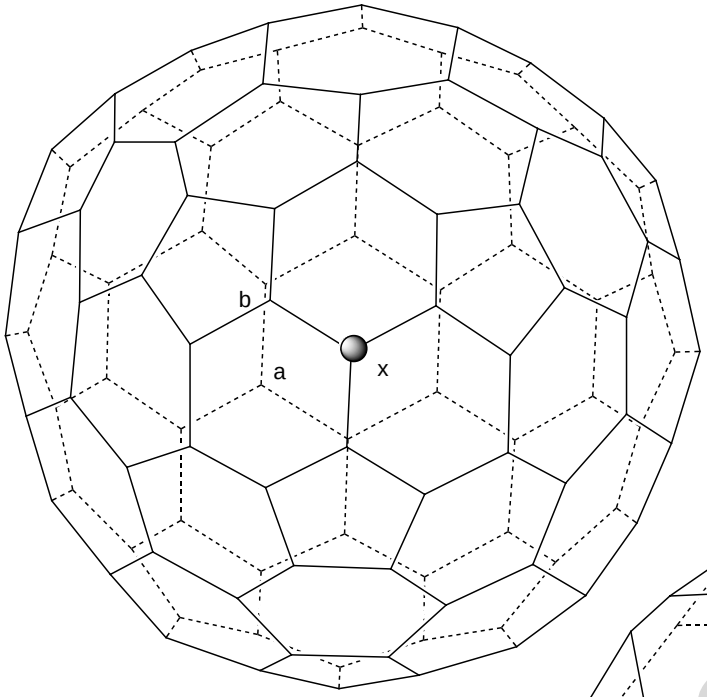


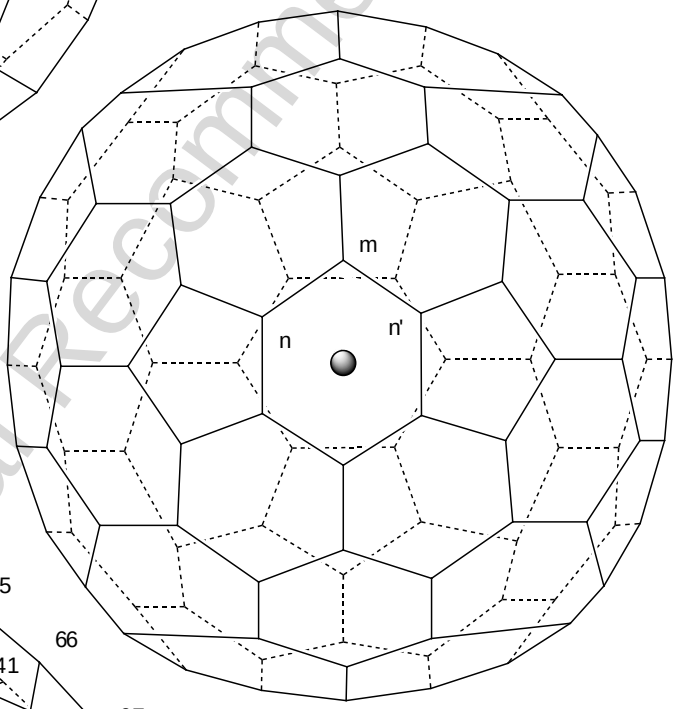
Fig. 23. Systematic numbering for (C_{84}-D_{2d})[5,6]fullerene

3.2.10 Systematic numbering for (C_{112}-T_d)[5,6]fullerene (Fig. 24) (CAS Reg. No. 160763-20-2).

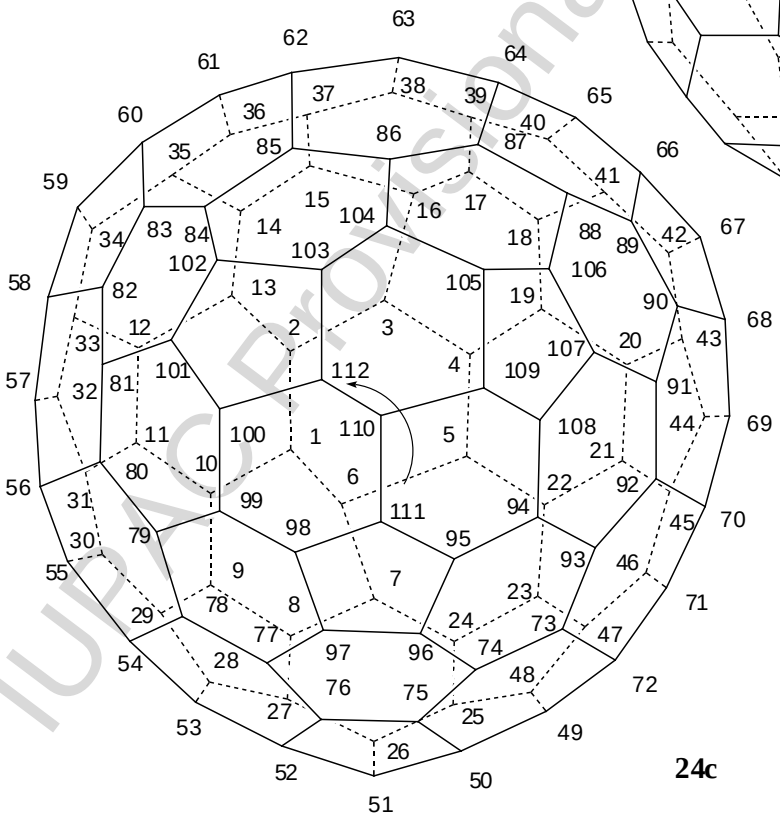
This fullerene features four equivalent C_3 axes connecting the midpoint of a six- membered ring on one side and an atom at the intersection of three six-membered rings on the other side (Fig. 24a); and three equivalent C_2 axes connecting the midpoints of opposite six-membered rings (Fig. 24b). For symmetry reasons, there are two clockwise pathways to be considered starting from the hexagon bisected by the C_3 axis: from **a** and from **b**. The former (shown in Fig. 24c) becomes discontiguous at position 111; the latter at position 93. The only pathway starting from the atom **x** (Fig. 24a) lying on the C_3 axis becomes discontiguous at position 72. Using one of the C_2 axes as the reference axis, three clockwise pathways must be considered: from **m**, from **n'**, and from **n** (Fig. 24b). They lead to numberings becoming discontiguous at positions 74, 104, and 107, respectively. Therefore, the numbering in Fig. 24c is preferred according to **Fu-3.2.1**.



24a



24b

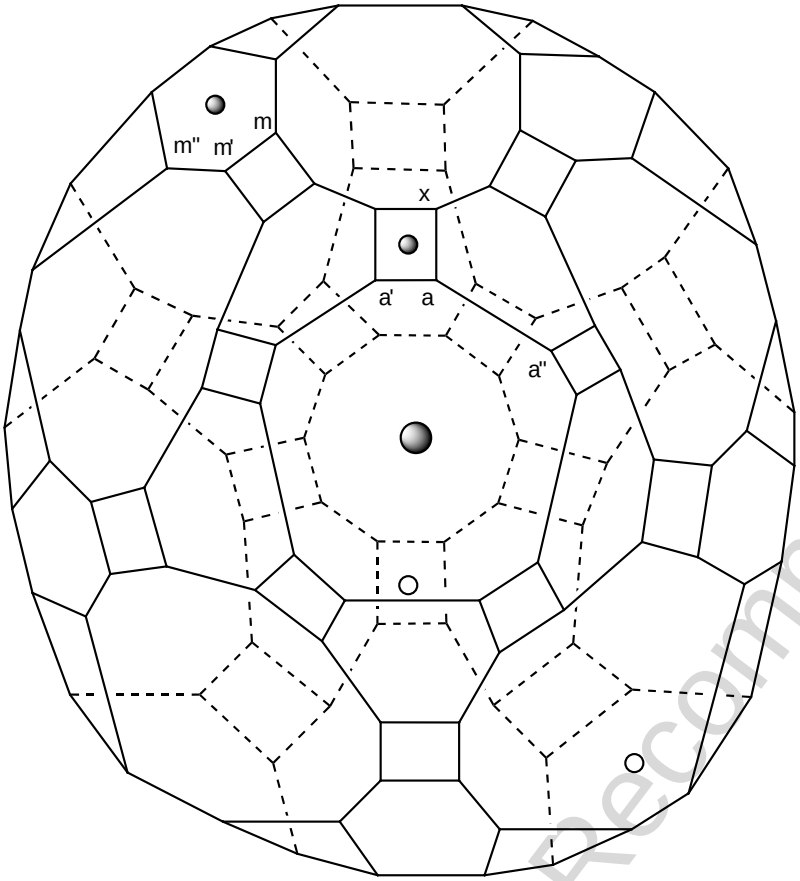


24c

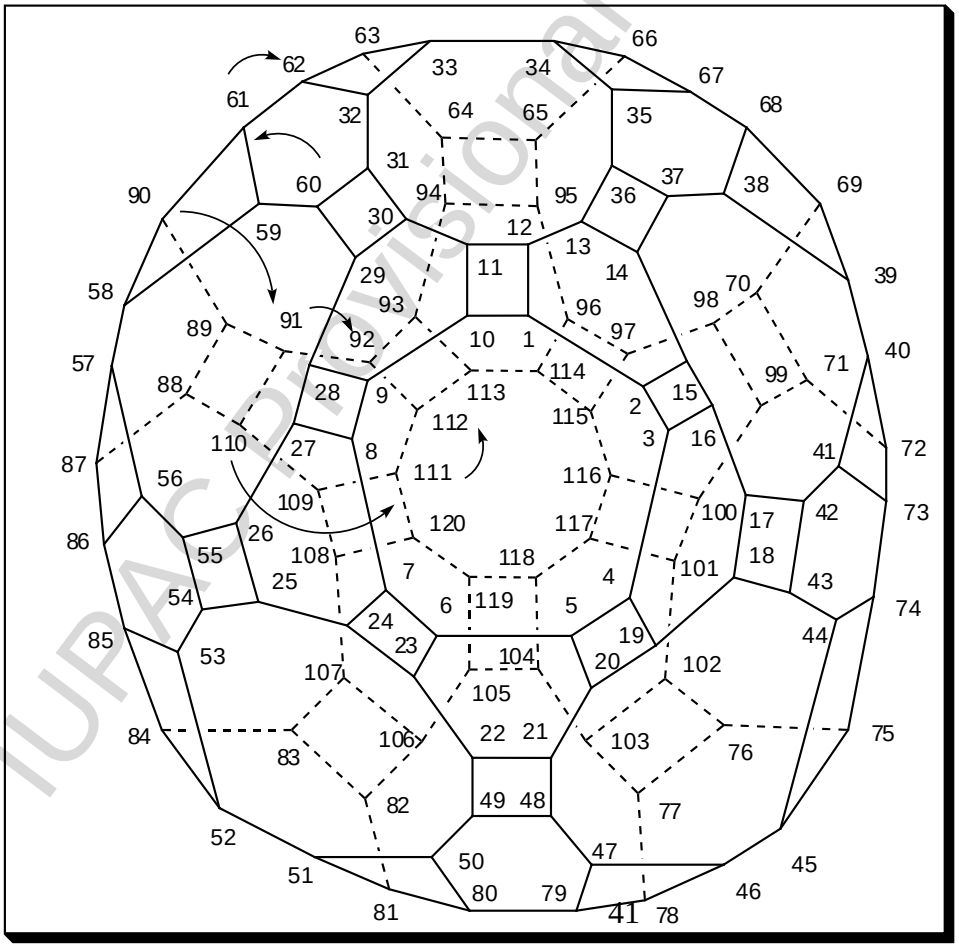
Fig. 24. Systematic numbering for (C_{112}-T_d)[5,6]fullerene

3.2.11 Systematic numbering for (C_{120}-I_h)[4,6,10]fullerene (Fig. 25) (CAS Reg. No. 103598-39-6).

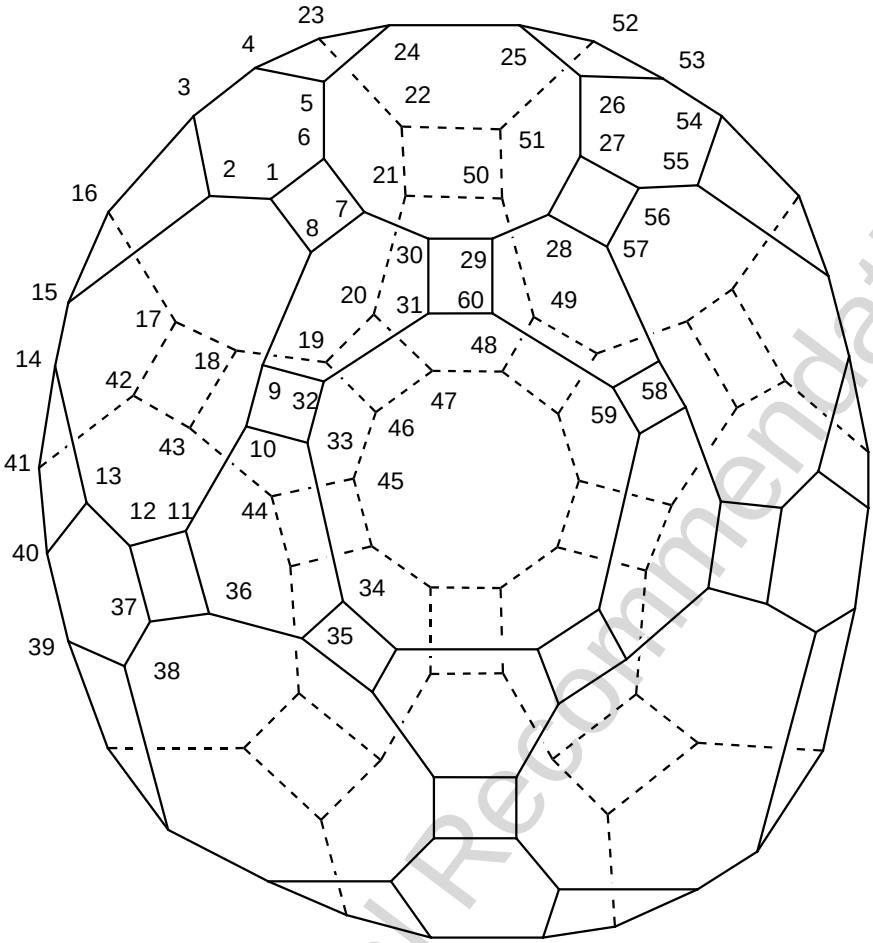
This fullerene features six equivalent C_5 axes, ten equivalent C_3 axes, and fifteen equivalent C_2 axes. The C_5 axes connect midpoints of opposite ten-membered rings; the C_3 axes connect midpoints of opposite six-membered rings; the C_2 axes connect midpoints of opposite four-membered rings (Fig. 25a). Even if all the atoms in this fullerene are equivalent, different lettering is maintained for clarity. For symmetry reasons there are two pathways to be considered in the ten-membered ring: **a** to **a"** and **a'** to **a**. Of these, the **a** to **a"** one leads to a numbering that becomes discontiguous at position 60 (Fig. 25b); the **a'** to **a** one leads to a numbering discontiguity at position 30. For symmetry reasons, there are two pathways to be considered in the six-membered ring: **m** to **m'** and **m'** to **m"**. Of these, the **m** to **m'** pathway leads to a numbering that becomes discontiguous at position 30; the **m'** to **m"** pathway leads to a numbering discontiguous at position 60 (Fig. 25c). For symmetry reasons, there are two pathways to be considered in the four-membered ring: **a'** to **a** and **a** to **x**. Of these, the **a'** to **a** pathway leads to a numbering that becomes discontiguous at position 32; the **a** to **x** pathway leads to a numbering discontiguity at position 36. Selection between the numberings of Figs. 25b and 25c, that have the first discontiguity at the same position (60), can be made considering that the numbering of Fig. 25b is built around an axis of higher order (**Fu-3.2.1b**) and is therefore preferred. The completion of the preferred discontiguous numbering is made according to **Fu-3.2.4**.



25a



25b



25c

Fig. 25. Systematic numbering for (C_{120}-I_h)[4,6,10]fullerene

3.3. Fullerenes having only a symmetry plane (σ) and a contiguous helical numbering pathway.

The lack of proper rotation axes C_n (n > 1) in these fullerenes requires an approach to spiral pathway identification that is different from the one employed in the cases of fullerenes with axial symmetry. Conceptually, however, the new approach should follow the previous one as much as possible. Accordingly, the following rules are adopted for C_s-symmetric fullerenes.

Fu-3.3.1. Since there are no proper rotation axes, the plane of symmetry is used as the reference element. A search is made for a contiguous numbering helix that starts in a ring bisected by the plane of symmetry or along a bond lying in the plane.

Fu-3.3.2. If there is a choice for the beginning of the numbering, rings bisected by the plane are preferred over bonds lying in the plane.

Fu-3.3.2.1. If there is a choice among rings, a larger ring is preferred to a smaller one and, among rings of the same size, the preferred ring contains the higher number of higher-ranking atoms at the first point of difference.

Fu-3.3.2.2. If there is a choice among bonds lying in the plane, the preferred bond contains the higher number of higher-ranking atoms.

Fu-3.3.3. If there is still a choice among contiguous numberings, the preferred pathway should

(a) begin and

(b) terminate as close as possible to the reference plane in terms of number of bonds.

Fu-3.3.4. If there is still a choice among contiguous numberings, they are evaluated by sequential comparison of their atom rankings. The preferred pathway contains the highest-ranking atom at the first point of difference.

It must be noted that in the approach used by CAS [3] the plane of symmetry is used as a pivot plane. The spheroidal structure is then sliced into planes parallel to the pivot plane, constructed using specific rules. Either one of the two outer planes can be the reference plane. It should also be mentioned that the assignment of atoms to a given plane in the CAS procedure may depend on the geometry of the structure rather than the connectivity of atoms and can lead to ambiguities.

As a consequence, the numberings produced by CAS are always different from those described here. The following examples illustrate the use of the rules as recommended in this document.

3.3.1 Systematic numbering for (C_{54}-C_s)[5,6]fullerene (Fig. 26) (CAS Reg. No. 136201-95-1).

In this fullerene the plane of symmetry, orthogonal to the plane of the paper in Fig. 26, bisects five six-membered rings and two five-membered rings. The six-membered rings are preferred for beginning the numbering (**Fu-3.3.2.1**); they are indicated as A, B, C, D, and E in Fig. 26a (smaller-font letters denote rings away from the viewer; larger, bold letters denote rings closer to the viewer). Ring A contains only 6,6,5 atoms; rings B, C, and D contain two 6,6,6 and four 6,6,5 atoms, each; ring E contains four 6,6,6 and two 6,6,5 atoms. Therefore, ring E is preferred (**Fu-3.3.2.1**). The six atoms of ring E form three pairs of symmetry-equivalent atoms indicated as **a/a'**, **b/b'**, and **c/c'** in Fig. 26b. Because of symmetry only the six anticlockwise (or clockwise) pathways from each atom must be considered. They all lead to contiguous numbering. However, those starting from atoms **b**, **b'**, **c**, and **c'** are preferred because they begin closer (0.5 bond) to the reference plane (**Fu-3.3.3a**). Two of these numberings (Figs. 26c and 26d) are preferred because they terminate at an atom 1.5 bonds removed from the reference plane (indicated by a bold dot), whereas the other terminates at an atom 2.5 bonds away from the plane (**Fu-3.3.3b**). Inspection of the atom ranking in the two preferred sequences reveals that the numbering in Fig. 26c is the correct numbering pathway because it begins with a 6,6,6 atom, whereas that in Fig. 26d begins with a 6,6,5 atom.

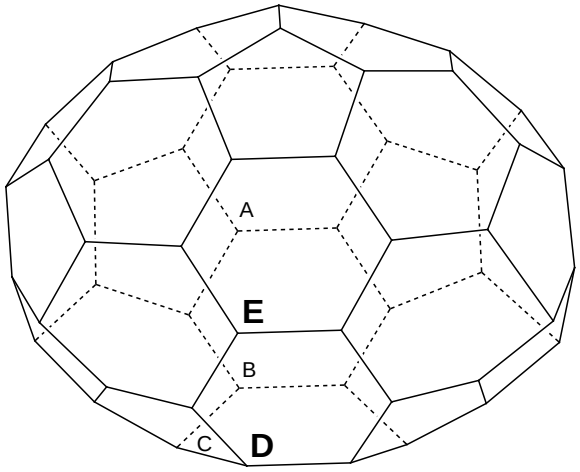


Fig. 26a

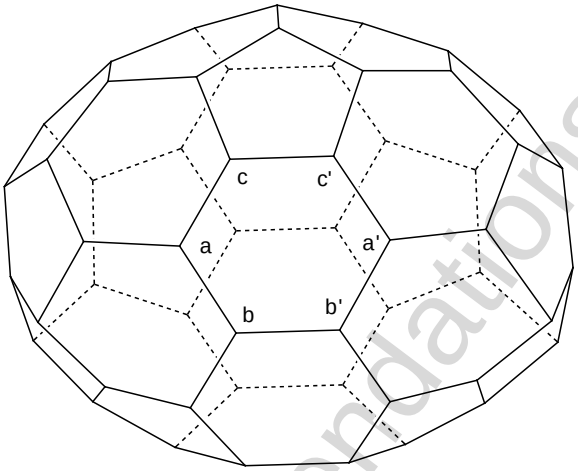


Fig. 26b

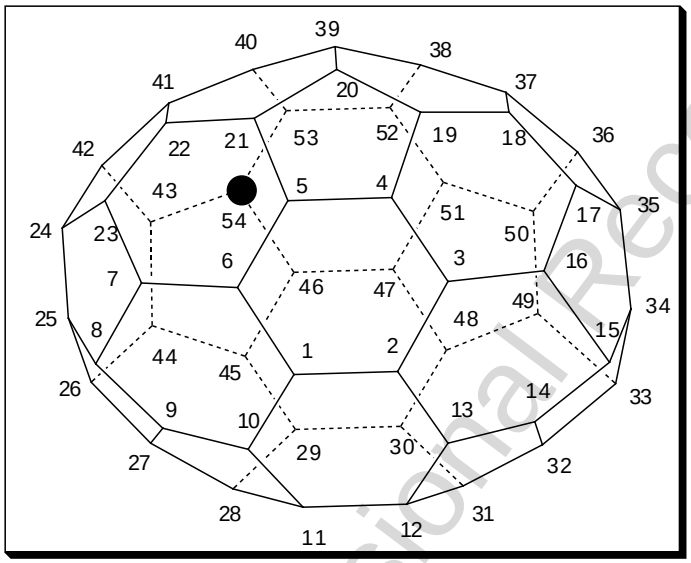


Fig. 26c

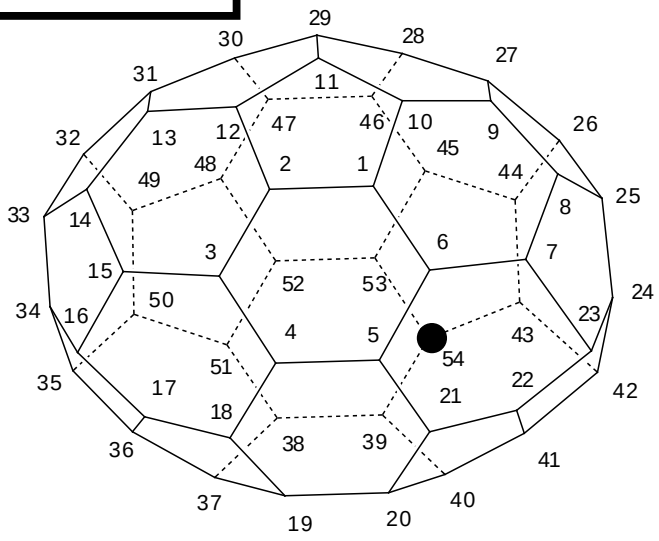


Fig. 26d

Fig. 26. Systematic numbering for (C_{54}-C_s)[5,6]fullerene3.3.2

3.3.2 Systematic numbering for (C_{36}-C_s)[5,6]fullerene (Fig. 27) (Atlas Ref. No. 36:4; CAS Reg. No. 165552-43-2).

In this fullerene the plane of symmetry corresponds to the plane of the paper in Fig. 27 and bisects only two six-membered rings which are preferred according to **Fu-3.3.2.1** indicated as A and B in Fig. 27a. Ring A contains the higher number of higher ranking atoms at the first point of difference (namely, four 6,6,5 atoms in a row), whereas ring B contains two pairs of 6,6,5 atoms intercalated by single 6,5,5 atoms. According to **Fu-3.3.2.1**, ring A is preferred for beginning the numbering. There are six pathways to be considered: clockwise and anticlockwise from **a**, from **b**, and from **c** (Fig. 27b). Of these, only the two starting from **c** lead to contiguous numberings, shown in Figs. 27c and 27d, respectively. Since both start from an atom 0.5 bond removed from the plane of symmetry and terminate at an atom lying on the plane of symmetry, they cannot be distinguished on the basis of **Fu-3.3.3**. However, application of **Fu-3.3.4** shows that the numbering reported in Fig. 27c must be preferred because it features a 6,6,5 atom at position 2 instead of the 6,5,5 atom of the numbering of Fig. 27d.

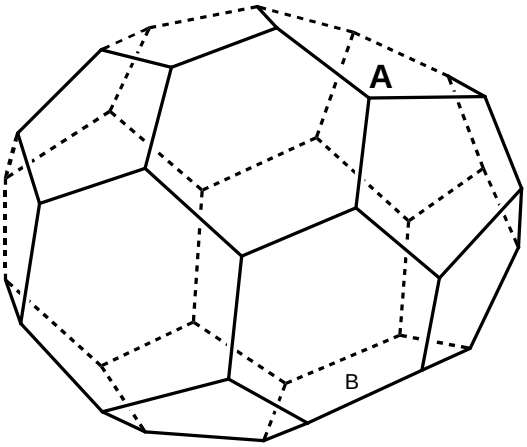


Fig. 27a

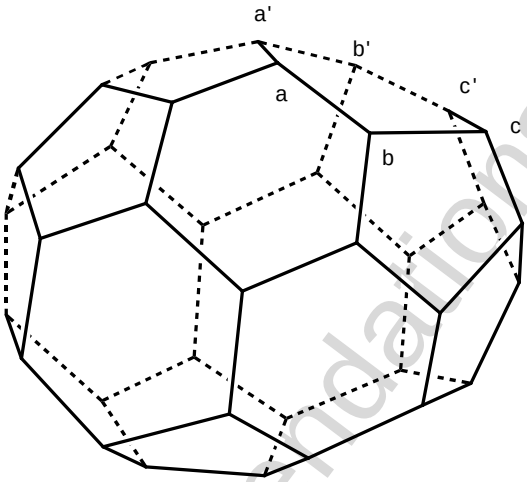


Fig. 27b

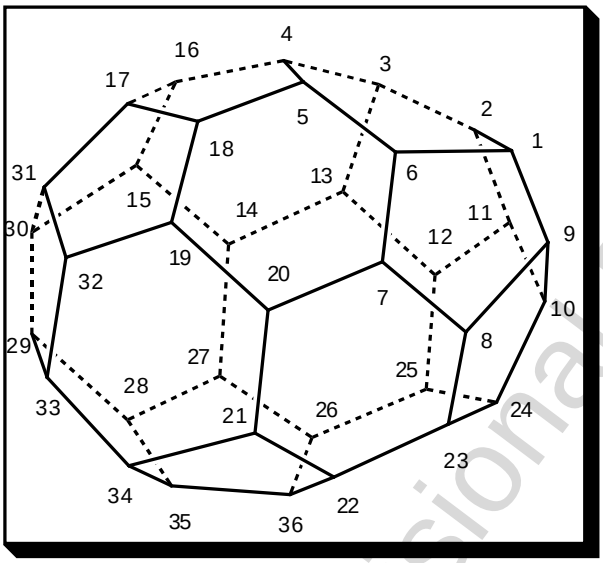


Fig. 27c

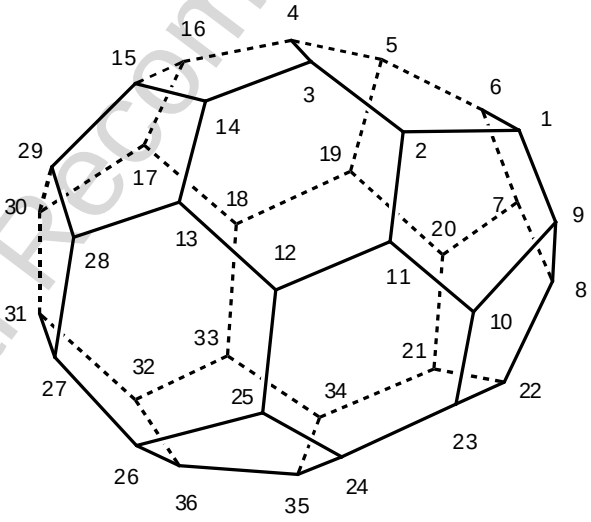


Fig. 27d

Fig. 27. Systematic numbering for (C_{36}-C_s)[5,6]fullerene

3.3.3 Systematic numbering for (C_{50}-C_s)[5,6]fullerene (Fig. 28) (Atlas Ref. No. 50:126).

In this fullerene the plane of symmetry (the plane of the paper in Fig. 28) bisects three six-membered rings indicated as A, B, and C in Fig. 28a. Ring A contains a greater number of higher-ranking atoms at the first point of difference than both rings B or C (ring A: four contiguous 6,6,5 atoms; rings B and C: two pairs of 6,6,5 atoms intercalated by single 6,5,5 atoms), and is therefore preferred to begin the numbering (**Fu-3.3.2.1**). However, none of the six possible pathways from A (clockwise and anticlockwise from **a**, **b**, and **c**) is contiguous. There are six pathways to be examined from ring B: from **d** and **g** (because these atoms are lying in the plane of symmetry it

does not matter whether the numbering proceeds clockwise or anticlockwise), and clockwise and anticlockwise from **e** and **f**; and six from ring C: from **h** and **k** (because these atoms are lying in the plane of symmetry it does not matter whether the numbering proceeds clockwise or anticlockwise), and clockwise and anticlockwise from **i** and **j**. Of these only those from **d**, **g**, and the clockwise numbering from **j** are contiguous. They are shown in Figs. 28b, 28c, and 28d, respectively. Among these numberings, the one from **j** (Fig. 28d) is discarded because it begins out of the plane, whereas the others begin in the plane (**Fu-3.3.3a**). Application of rule **Fu-3.3.3b** does not help, since both numberings terminate at an atom 0.5 bond away from the plane. Eventually, a selection is made in favor of the numbering reported in Fig. 28c, because it features a 6,6,5 atom instead of a 6,5,5 atom at position 8 (**Fu-3.3.4**).

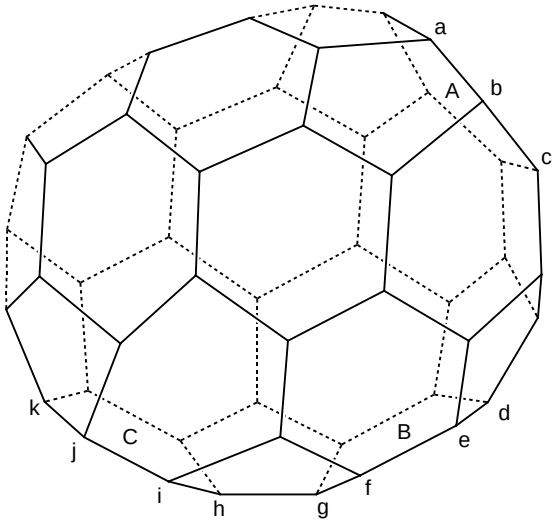


Fig. 28a

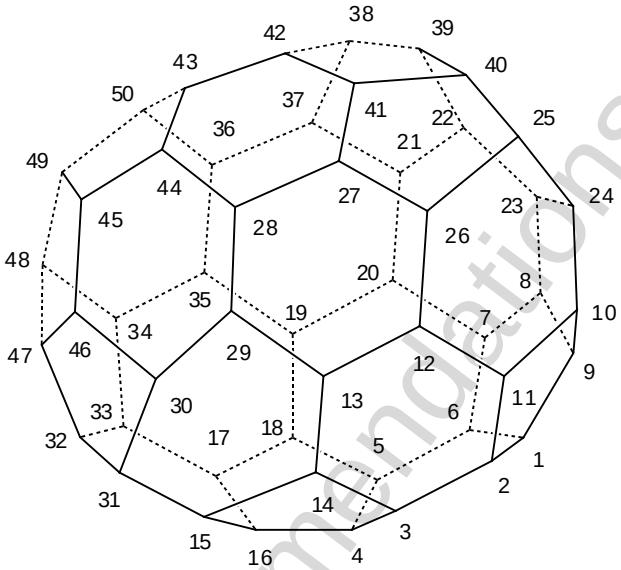


Fig. 28b

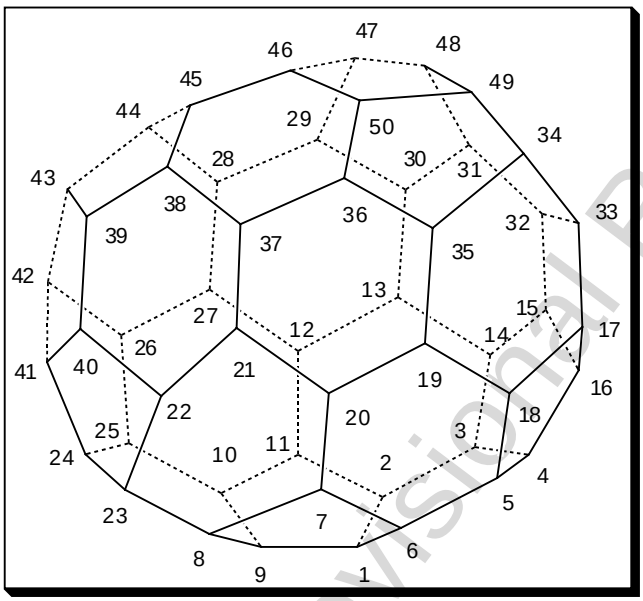


Fig. 28c

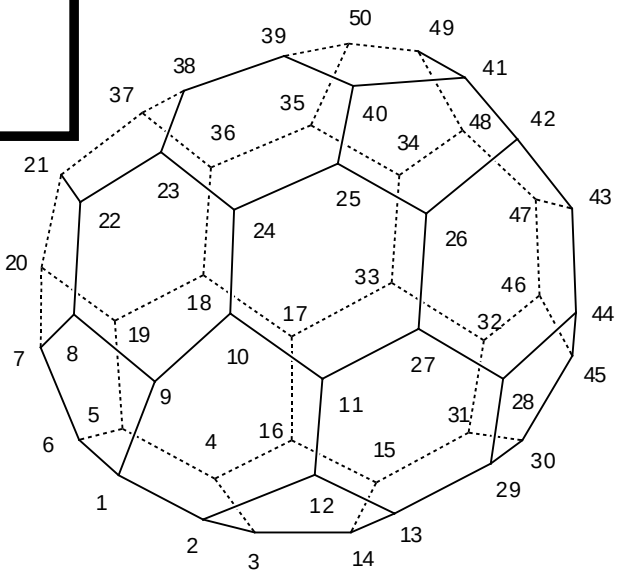


Fig. 28d

Fig. 28. Systematic numbering for (C_{50}-C_s)[5,6]fullerene

3.3.4 Systematic numbering for (C_{70}-C_s)[5,6]fullerene (Fig. 29) CAS Reg. No. 184642-88-4).

In this fullerene the plane of symmetry (the plane of the paper in Fig. 29) bisects three six-membered rings indicated as A, B, and C in Fig. 29a. Ring A contains two 6,6,6 atoms, and is therefore preferred to begin the numbering over the other six-membered rings that contain only 6,6,5 atoms (**Fu-3.3.2.1**). Of the six pathways to be considered from ring A (clockwise and anticlockwise from **a**, **b**, and **c**), only those proceeding anticlockwise from **a** and anticlockwise from **b** lead to contiguous numberings. The former, shown in Fig. 29b, begins at an atom 0.5 bond away from the reference plane; the latter (Fig. 29c) begins at an atom 1.5 bonds away from the plane. According to **Fu-3.3.3a**, the former (Fig. 29b) is correct.

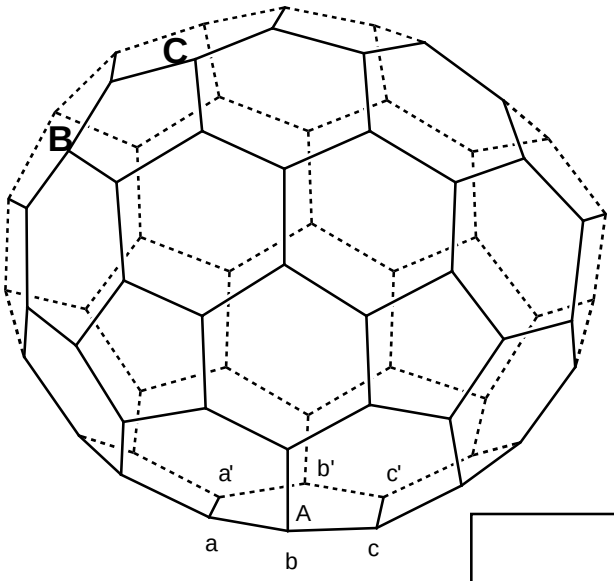


Fig. 29a

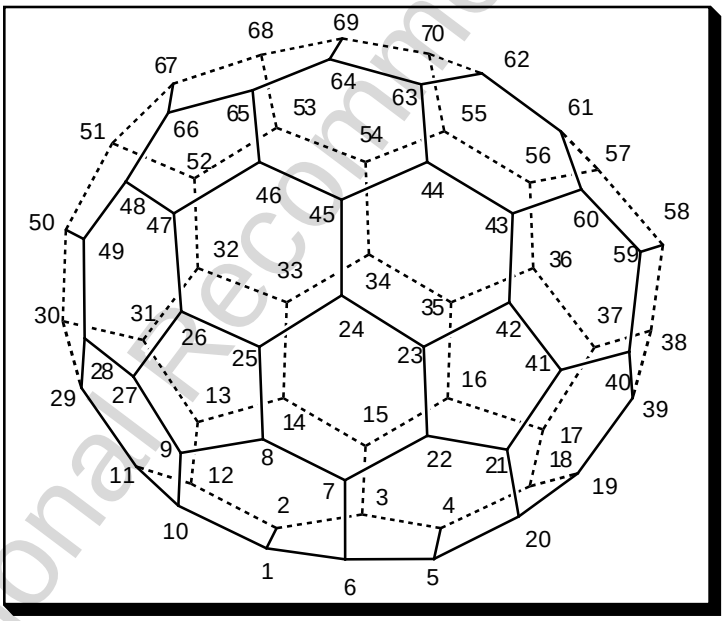


Fig. 29b

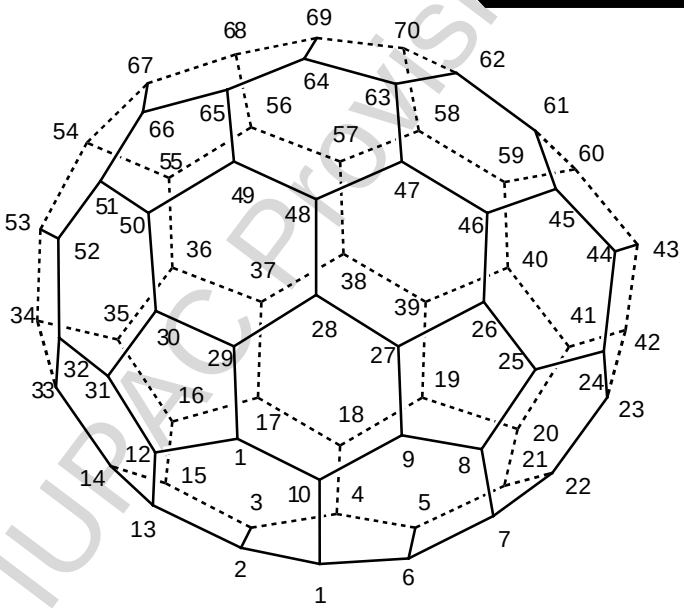


Fig. 29c

Fig. 29. Systematic numbering for (C_{70}-C_s)[5,6]fullerene

3.3.5 Systematic numbering for (C_{82}-C_s)[5,6]fullerene (Fig. 30) (Atlas Ref. No. 82:2; CAS Reg. No. 145954-07-0).

In this fullerene the plane of symmetry (orthogonal to the plane of the paper in Fig. 30) bisects five six-membered rings indicated as A, B, C, D, and E in Fig. 30a. Ring C contains only 6,6,5 atoms; rings B and E contain two 6,6,6 and four 6,6,5 atoms, each; ring A contains four 6,6,6 and two 6,6,5 atoms; ring D contains only 6,6,6 atoms, and thus is preferred to begin the numbering (**Fu-3.3.2.1**). However, none of the pathways from this ring is contiguous, and the pathways from ring A, which contains a sequence of four 6,6,6 atoms must be examined. The atoms of this ring are indicated as **a**/**a'**, **b**/**b'**, and **c**/**c'** in Fig. 30a. There are six clockwise pathways to be examined, one from each atom. Only those from **a** (Fig. 30b) and from **b'** (Fig. 30c) are contiguous. The latter is preferred because it starts closer to the reference plane (**Fu-3.3.3a**).

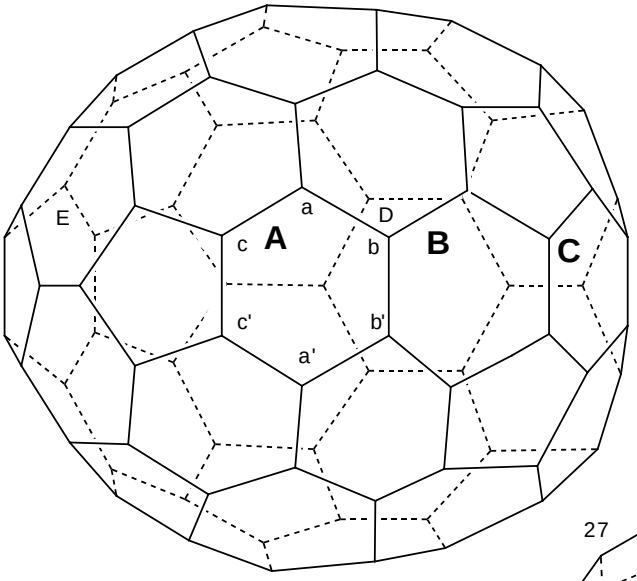


Fig. 30a

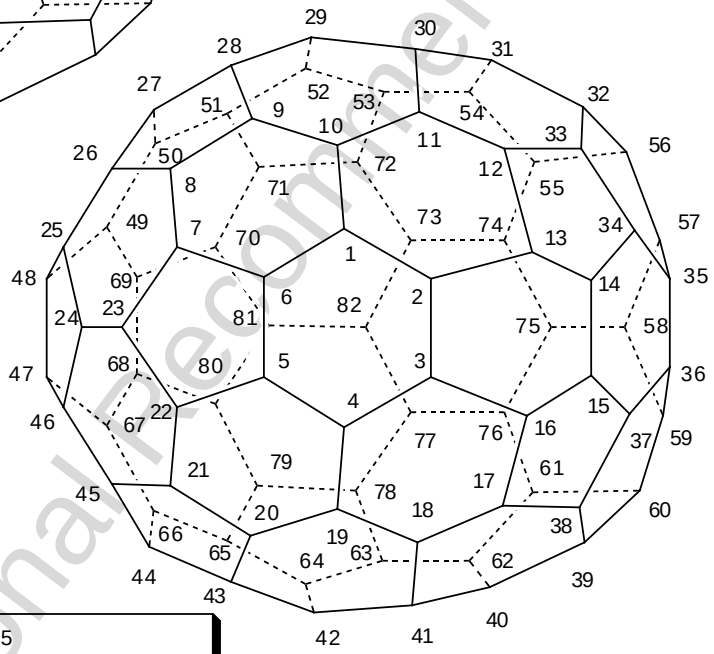


Fig. 30b

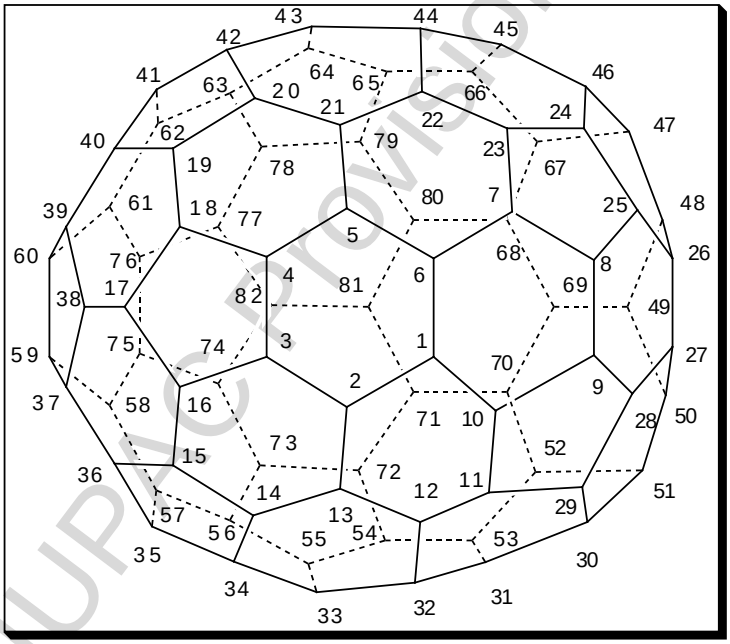


Fig. 30c

Fig. 30. Systematic numbering for (C_{82}-C_s)[5,6]fullerene

3.4. Fullerenes having as their sole symmetry elements a center of inversion (*i*) or a C_1 axis (point groups C_i and C_1) and a contiguous helical numbering pathway determined unambiguously as described below.

In the achiral C_i fullerenes the center of inversion *i* is the only symmetry element. Different from the fullerenes examined so far, there are neither axes nor planes of symmetry passing through or lying upon a ring, a bond, or an atom, and the symmetry element, being inside the spheroid, cannot be used as a reference to begin the numbering. The chiral C_1 fullerenes possess exclusively a C_1 axis: this means that they can be made identical to themselves only by a 360° rotation around any axis passing anywhere through the fullerene. Therefore, no axis can be used as a reference to begin the numbering since it does not have an unambiguously determined location.

For both C_i and C_1 fullerenes, the absence of reference elements could lead to an undesirable increase of the number of possible numbering pathways. Therefore, the primary requirement of any numbering system should be the reduction of the allowed numbering options. Much in line with the procedure employed for the numbering of other fullerenes and in particular of C_s fullerenes, the following rules are adopted in order to decide where to begin the numbering.

Fu-3.4.1. A larger ring is preferred to a smaller one to begin the numbering; among rings of the same size, the preferred ring contains the highest-ranking atom at the first point of difference.

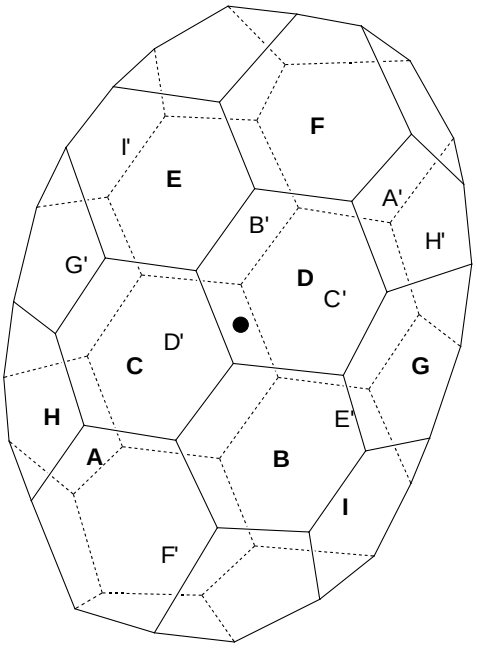
Fu-3.4.2. If there is still a choice among contiguous numberings, they are compared according to their atom ranking sequence. The preferred pathway contains the highest-ranking atom at the first point of difference.

The numbering of C_i and C_1 fullerenes proposed by CAS [3] is also based on the identification of a preferred ring to begin the numbering. Incidentally, no example of numbering of C_i fullerenes has been reported by CAS.

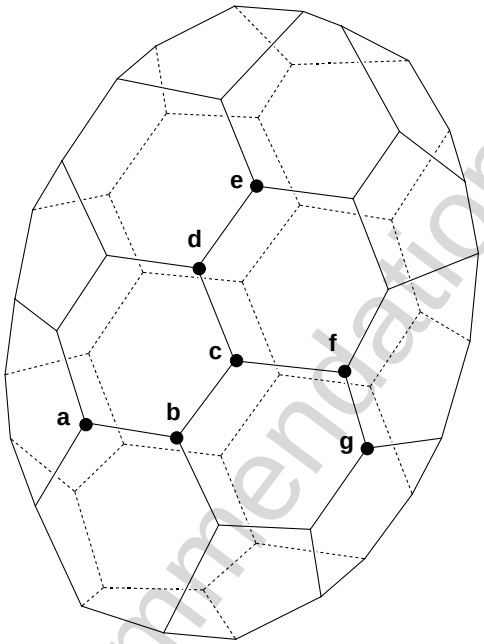
3.4.1. Systematic numbering for (C_{56}-C_i)[5,6]fullerene (Fig. 31) (see ref. 5, p. 100).

This fullerene contains nine pairs of symmetry-equivalent six-membered rings preferred for the beginning of the numbering according to rule **Fu-3.4.1**. They are related by the center of inversion (shown by a bold dot in Fig. 31a). Symmetry-equivalent rings are identified by the same letter, unprimed and primed (in Fig. 31a primed letters indicate rings away from the viewer and bold letters rings closer to the viewer). Because of symmetry only one set of nine nonequivalent six-membered rings are considered (those denoted by unprimed letters). Each of these rings is *a priori* eligible to begin the numbering, and they are ranked on the basis of their atoms (**Fu-3.4.1**).

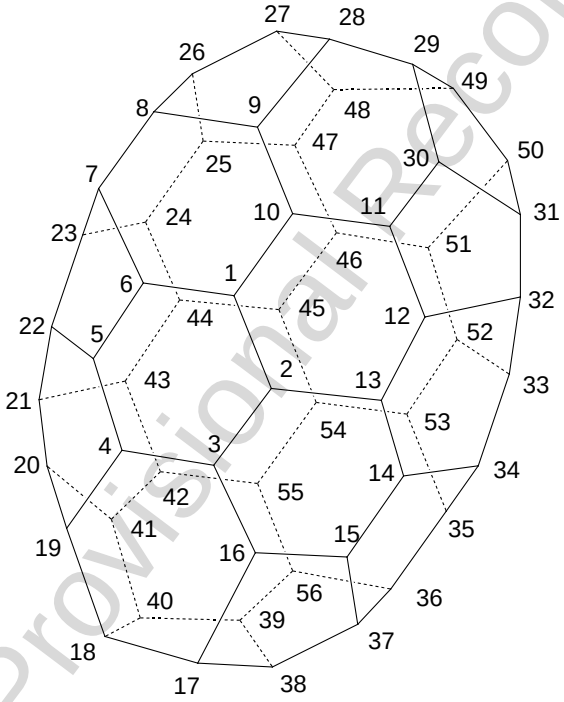
Rings B, C, and D contain four contiguous 6,6,6 atoms and two 6,6,5 atoms, and are preferred for beginning the numbering. Please note that some of the other rings also contain four 6,6,6 and two 6,6,5 atoms, but the 6,6,6 atoms are not contiguous. Since the numberings having four contiguous 6,6,6 atoms at position 1-4 would be preferred according to **Fu-3.4.2**, they are examined first for contiguous numberings to reduce the number of necessary inspections. The 6,6,6 atoms are indicated by the letters **a** to **g** in Fig. 31b. There are six pathways to be considered: **a** to **b** to **c** to **d** and **d** to **c** to **b** to **a**, from ring C; **b** to **c** to **f** to **g** and **g** to **f** to **c** to **b**, from ring B; **f** to **c** to **d** to **e** and **e** to **d** to **c** to **f**, from ring D. Only one of these pathways (**d** to **c** to **b** to **a**, from ring C) leads to a contiguous numbering, that is shown in Fig. 31c.



31a



31b



31c

Fig. 31. Systematic numbering for (C_{56}-C_i)[5,6]fullerene

3.4.2. Systematic numbering for (C_{36}-C_1)[5,6]fullerene (Fig. 32) (Atlas Ref. No. 36:7).

This fullerene contains eight six-membered rings indicated by the letters A to H in Fig. 32a (smaller-font letters denote rings away from the viewer; larger-font, bold letters denote rings closer to the viewer). According to **Fu-3.4.1**, ring H is preferred to begin the numbering since it contains the highest-ranking atom at the first point of difference. There are twelve pathways to be considered in ring H, clockwise and anticlockwise from each atom **a** - **f**. In order to reduce the number of pathways to be actually examined, those beginning from the 6,6,6 atom (clockwise and anticlockwise) are studied first since, if contiguous, these pathways will be preferred to any other pathway starting in this ring according to **Fu-3.4.2**. Unfortunately, they are both discontiguous. The two pathways having the 6,6,6 atom **a** at position 2 are then examined for contiguous numbering: again these would be preferred at this point, since no other pathway can have a 6,6,6 atom at position 2. The two pathways are clockwise from atom **f**, and anticlockwise from atom **b**. They lead to the contiguous numberings shown in Figs. 32b and 32c, respectively. These contiguous sequences are then compared using **Fu-3.4.2** to discover that there is a 6,6,5 atom at position 4 in the pathway from atom **f** (Fig. 32b) and a 6,5,5 atom at the same position in the pathway from atom **b** (Fig. 32c). Therefore the numbering sequence shown in Fig. 32b, is correct. The enantiomer shown here has the ($^{f,s}C$) configuration [4].

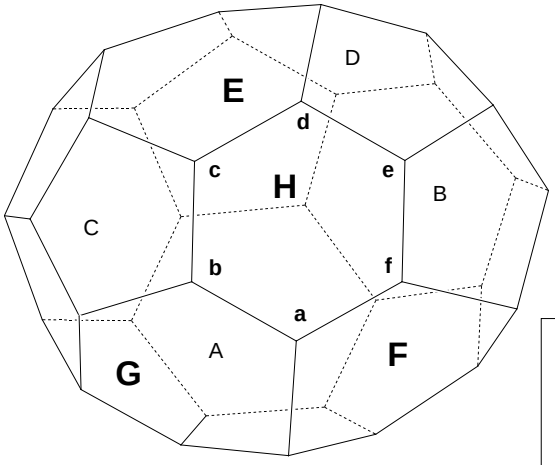


Fig. 32a

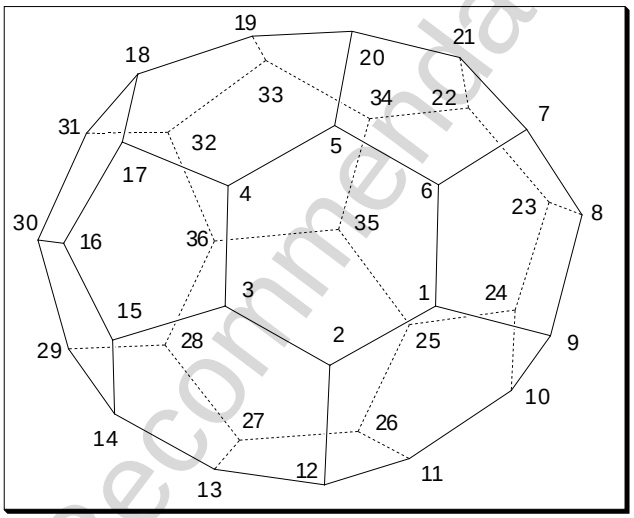


Fig. 32b

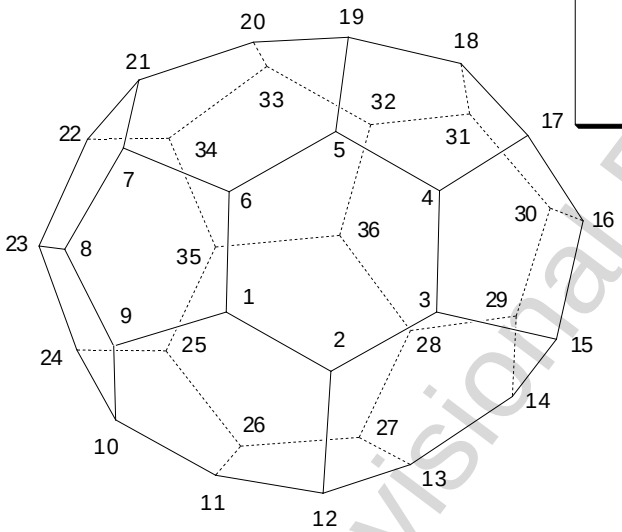


Fig. 32c

Fig. 32. Systematic numbering for ($^{f,s}C$)(C_{36}-C_1)[5,6]fullerene

3.4.3. Systematic numbering for (C_{44}-C_1)[5,6]fullerene (Fig. 33) (Atlas Ref. No. 44:10)

This fullerene contains twelve six-membered rings shown as A to L in Fig. 33a (smaller-font letters denote rings away from the viewer; larger, bold letters denote rings closer to the viewer). Among these, rings C, I, and K are preferred according to **Fu-3.4.1** to begin the numbering, since they contain the higher ranking atoms at the first point of difference. From these rings there are in principle thirty-six pathways to be examined. To reduce the number of pathways to be actually examined, the six pathways featuring the three 6,6,6 atoms at the first three positions are examined first, since, if contiguous, they will be preferred to all other possible pathways

according to **Fu-3.4.2**. Only the two pathways beginning in ring I (clockwise from atom **a**, and anticlockwise from atom **c** in Fig. 33b, which shows a different view of (C_{44}-C_1)[5,6]fullerene) lead to contiguous spiral numberings. These are shown in Figs. 33c and 33d. These numbering sequences are compared using **Fu-3.4.2** to discover that there is a 6,6,5 atom at position 23 in the sequence of Fig. 33c and a 6,5,5 atom at the same position in the sequence of Fig. 33d. The former is therefore preferred. The configuration of the shown enantiomer is ($^{f,s}A$) [4].

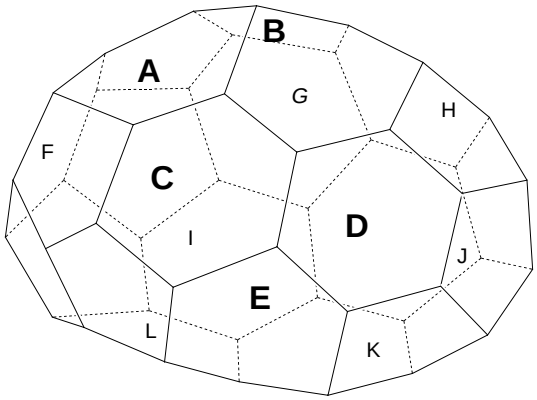


Fig. 33a

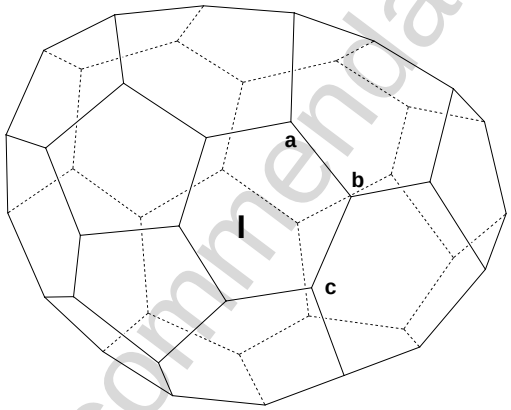


Fig. 33b

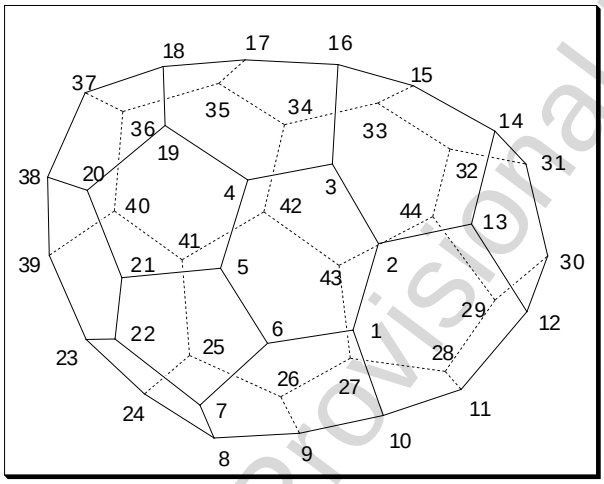


Fig. 33c

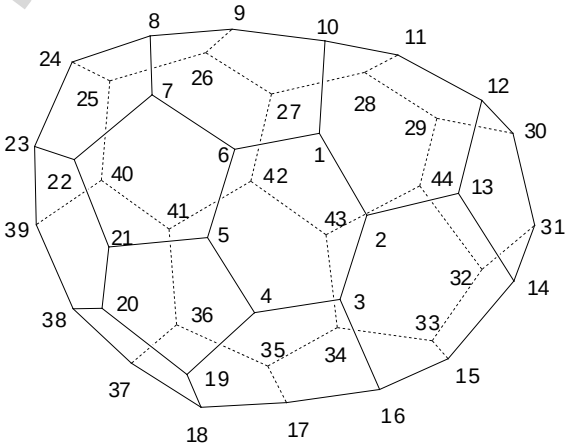


Fig. 33d

Fig. 33. Systematic numbering for ($^{f,s}A$)(C_{44}-C_1)[5,6]fullerene

3.4.4. Systematic numbering for (C_{94}-C_1)[5,6]fullerene (Fig. 34)

This fullerene contains only 6,6,6 or 6,6,5 atoms and thirty-six six-membered rings. Seventeen rings contain a sequence of four 6,6,6 and two 6,6,5 atoms and the numbering should begin from these rings according to **Fu-3.4.1**. Of all the possible numberings, the seventeen

clockwise and the seventeen anticlockwise pathways featuring the four 6,6,6 atoms in a row at the beginning of the numbering are considered first, since, if contiguous, they will be preferred according to rule **Fu-3.4.2**. Eleven of these pathways lead to contiguous numberings: clockwise from rings A, B, C, E, and F; anticlockwise from rings D, E, G, H, I, and J (Fig. 34a; smaller-font letters denote rings away from the viewer; larger, bold letters denote rings closer to the viewer). Comparison of the atom sequences by application of **Fu-3.4.2** eliminates five numberings because of the ranking of the atoms at position 8, two of the six remaining numberings at position 9, and two of the four remaining numberings at position 11. This leaves only the two numberings reported in Figs. 34b (clockwise from ring C) and 34c (anticlockwise from ring J). Selection between these can be made by inspection of the atoms up to position 15, that is a 6,6,6 atom in the numbering of Fig. 34b and a 6,6,5 atom in the numbering of Fig. 34c. The former is therefore preferred based on **Fu-3.4.2**. The configuration of the shown enantiomer is ($^{f,s}C$) [4].

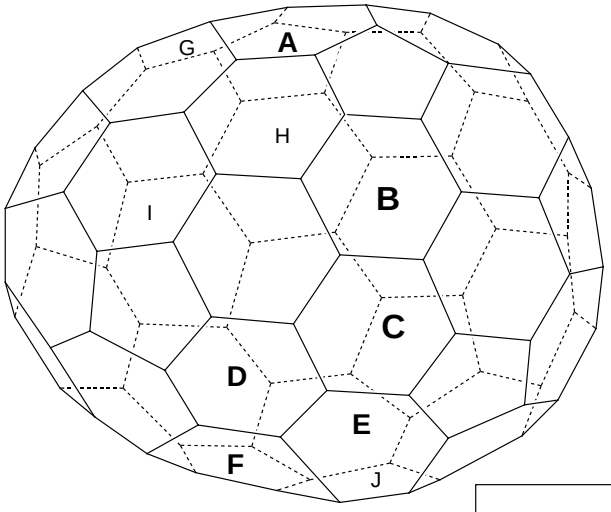


Fig. 34a

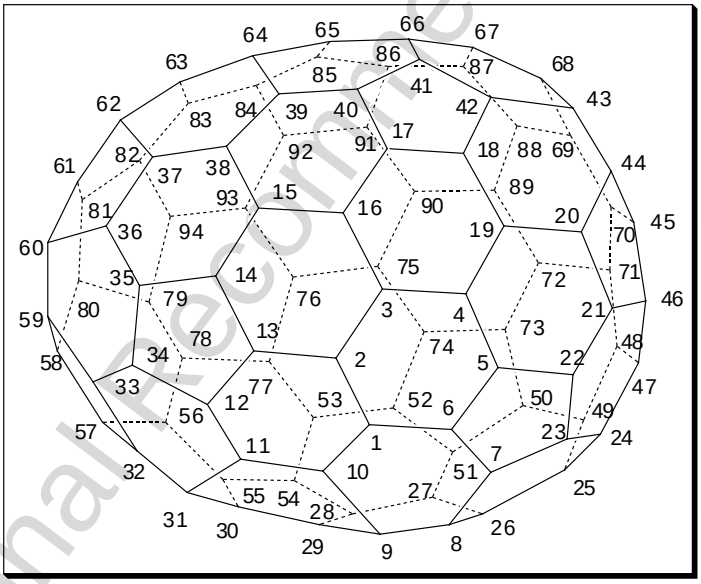


Fig. 34b

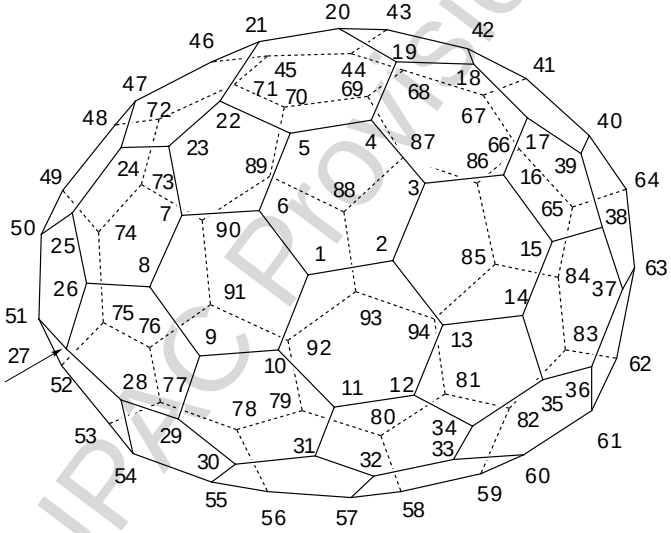


Fig. 34c

Fig. 34. Systematic numbering for ($^{f,s}C$) (C_{94}-C_1)[5,6]fullerene

Finally, it must be noted that this document does not deal with C_s, C_i, and C_1 fullerenes without contiguous numbering, of which no examples are known so far. Since these fullerenes have a large number of possible numbering pathways, it seems very unlikely that a contiguous numbering cannot be found for these structures. In any case, application of **Rules Fu-3.2.1.a**, **Fu-3.2.3**, and **Fu-3.2.4** should allow to identify a preferred discontiguous numbering.

References

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2. R. Taylor, *J. Chem. Soc., Perkin Trans. 2*, **1993**, 813-824.
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4. International Union of Pure and Applied Chemistry, Division of Organic Chemistry, Commission on Nomenclature of Organic Chemistry. "Nomenclature for the (C_{60}-I_h) and fullerene (C_{70}-$D_{5h(6)}$) *Pure Appl. Chem.* **2002**, *74*, 629-695.
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Numbering of Fullerenes
Appendix 1 to Draft 9
Rules

Fullerenes having at least one symmetry axis (C_n, n>1) *and* a contiguous helical pathway.

Rule 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 helical 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 helical pathway, and the corresponding axis is called the "reference axis".

Rule Fu-3.1.2: If there is a choice for the selection of a reference axis or for the end of the reference axis to begin the numbering, a ring is preferred to a bond which, in turn, is preferred to an atom.

Rule Fu-3.1.2.1: When there is a choice between rings for the beginning of numbering, a larger ring is preferred to a smaller one. When there is still a choice, the preferred ring contains the highest-ranking atom at the first point of difference. The highest-ranking atom is defined as the common atom of the set of three largest rings. For example, in a [5,6]fullerene, an atom at the intersection of three six-membered rings (in short, a 6,6,6 atom) ranks higher than an atom at the intersection of two six-membered rings and a five-membered ring (a 6,6,5 atom).

Rule Fu-3.1.2.2: When there is a choice between bonds bisected by an axis for the beginning of numbering, the preferred bond contains the higher number of higher-ranking atoms.

Rule Fu-3.1.2.3: When there is a choice between atoms lying on an axis for the beginning of numbering, the numbering must start at the higher-ranking atom.

Rule Fu-3.1.3: When there is a choice among helical numbering pathways, the preferred pathway terminates as close as possible, in terms of the number of bonds, to the reference axis.

Rule Fu-3.1.4: When there is still a choice among helical pathways for numbering, they are evaluated by sequential comparison of the ranking of their atoms. The preferred pathway contains the highest-ranking atom at the first point of difference.

Fullerenes having at least one symmetry axis (C_n, n>1) but no contiguous helical numbering pathway determined on the basis of rules Fu-3.1.1 to Fu-3.1.4.

Rule Fu-3.2.1 (cf. **Fu-3.1.1**):
a. The n^{th} discontiguity must occur as late as possible in the numbering.
b. Among different pathways having the n^{th} discontiguity at the same highest locant, the preferred numbering pathway is built around the proper rotation axis of higher order.

Rule Fu-3.2.2 (cf. **Fu-3.1.2**): If there is a choice among reference axes of the same order or between the end of a reference axis to begin the numbering, **Fu-3.1.2** is applied.

Rule Fu-3.2.3 (cf. **Fu-3.1.4**; for practical reasons, no rules analogous to **Fu-3.1.3** is applied to segments of discontiguous numberings): When there is still a choice, the n^{th} segments are compared according to rule **Fu-3.1.4**.

Once a preferred segment is identified based on rules **Fu-3.2.1** to **Fu-3.2.3**, the numbering of the fullerene is completed by construction of the subsequent segment(s). The starting point of a new segment is defined according to rule **Fu-3.2.4a** (see below), and numbering within a segment is continued according to rule **Fu-3.2.4b**.

Rule Fu-3.2.4: After a discontiguity,

a) the next atom to be numbered must be directly connected to one of the previously numbered atoms; among the latter, the atom with the highest locant is preferred.

b) numbering continues by the shortest path, in terms of number of bonds, to reach an unnumbered atom that is directly connected to a numbered atom with the lowest locant within reach. In this way, the sense of the dicontiguous numbering helix should be maintained and its pitch kept as small as possible.

Fullerenes having only a symmetry plane (σ) *and* a contiguous helical pathway.

Fu-3.3.1. Since there are no proper rotation axes, the plane of symmetry is used as the reference element. A search is made for a contiguous numbering helix that starts in a ring bisected by the plane of symmetry or along a bond lying in the plane.

Fu-3.3.2. If there is a choice for the beginning of the numbering, rings bisected by the plane are preferred over bonds lying in the plane.

Fu-3.3.2.1. If there is a choice among rings, a larger ring is preferred to a smaller one and, among rings of the same size, the preferred ring contains the higher number of higher-ranking atoms at the first point of difference.

Fu-3.3.2.2. If there is a choice among bonds lying in the plane, the preferred bond contains the higher number of higher-ranking atoms.

Fu-3.3.3. If there is still a choice among contiguous numberings, the preferred pathway should

(a) begin and

(b) terminate as close as possible to the reference plane in terms of number of bonds.

Fu-3.3.4. If there is still a choice among contiguous numberings, they are evaluated by sequential comparison of their atom rankings. The preferred pathway contains the highest-ranking atom at the first point of difference.

Fullerenes having as their sole symmetry elements a center of inversion (*i*) or a C_1 axis and a contiguous helical numbering pathway.

Fu-3.4.1. A larger ring is preferred to a smaller one to begin the numbering; among rings of the same size, the preferred ring contains the highest-ranking atoms at the first point of difference

Fu-3.4.2. If there is still a choice among contiguous numberings, they are compared according to their atom ranking sequence. The preferred pathway contains the highest-ranking atom at the first point of difference.