Nomenclature of [60]Fullerene Derivatives by Edge Labeling

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A new nomenclature of [60]fullerene derivatives or adducts is proposed. It can express most derivatives to image their stereochemical properties. Moreover, it can name racemates rather concisely.

Since a large quantity of [60]fullerene became available, its chemistry has been developed extensively. Many reactions have been applied to it, often to obtain simple products derived from an addition at a double bond, and its interesting reactivity has been disclosed. As far as we searched in chemical literature, the recent trend of the derivatization seems to direct to the multiple addition to one sphere.[1-7] At this moment, however, researchers in this field have now suffered a severe difficulty on the nomenclature, because of the complicated long IUPAC name even for [60]fullerene itself.[8]

Cahill and his coworkers for the first time labeled each carbon in the fullerene and classified isomers of dihydro[60]fullerene.[9] Despite of their pioneering work, the labeling resulted in rather confusion instead of finding some regularity. Hirsch and his coworkers designated reactive [6,6]-junctions by *cis*-1, *e*, *trans*-1, etc., relative to the first addition site.[5] This designation can give us only a certain stereochemical image of di-adducts, and this is hardly applied to the precise nomenclature because of its over-simplification.

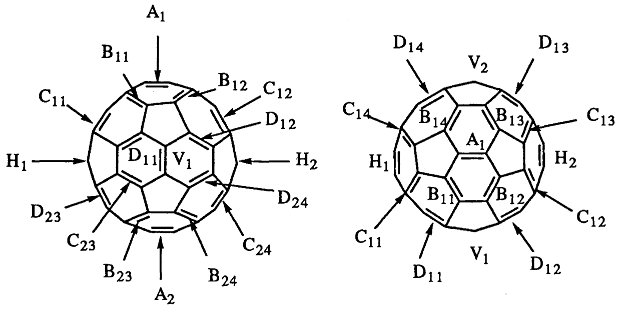
According to the graph theory,[10] Cahill's treatment is of the vertex labeling and Hirsch's one of the edge labeling. Since many addition reactions now are known to occur at the [6,6]-junction whose high reactivity is rationalized by the molecular orbital calculation,[9c,11] it is reasonable to label each [6,6]-junction relative to the first (or base) addition site. Hence, taking advantage of the edge labeling or [6,6]-junction labeling, we reached a nomenclature of [60]fullerene derivatives, which is applicable to almost all derivatives, not only [6,6]-addition products but also [5,6]-ones and others.

The new nomenclature is as follows: (1) By the following three criteria, the base [6,6]-junction A_1 is selected among those having substituent(s); i.e., firstly by making those locating on the upper hemisphere, as many as possible (the first condition), secondly by making them as near as possible to the selected A_1 (the second condition), and finally by bringing them to a position as high as possible (the third condition): The site hierarchy is in the order of A>H>V>B>C>D. If these are not consistent with each other, the first one should be taken. The base C-C junction A_1 is placed at the top of the sphere; at this moment, its higher class substituent based on the sequence rule is arranged at the left carbon and its lower one at the right. Sites A_2, H_1, H_2, V_1, and V_2 are self-explainable in Figure 1. Other sites B_1, C_1, and D_1 are defined as ones in a naphthalene skeleton including A_1 successively from upper to lower (see Figure 1-side view), and each group of sites is classified by the second subscript, counted from left to right such as B_{11}, B_{12}, B_{13}, and B_{14}. The lower hemisphere sites (around A_2) are named with the first subscript letter of 2 and second ones as the same as those of the centrosymmetric upper sites, in order to inspect easily their superscript (vide infra) and subscript letters around the base A_1.

(2) The regiochemically higher carbon of each C-C bond site is defined as the left carbon at site H, the upper one at V, the D-side at B, the B-side at C, and the C-side at D. If the higher class substituent (based also on the sequence rule) is attached to the higher carbon at a site and the lower to the lower, the site is written with the superscript letter e (equal), and when the case is reverse, with the letter u (unequal).

(3) Using a set of substituents and the multiplicative prefix such as mono, bis, tris, etc, the substituted sites are expressed as follows; i.e., (A,B)-bis(the set)[60]fullerene. In the case of two monovalent substituents, they are written in the parenthesis by using a colon between them; i.e., (A,B)-bis-(ethyl:-methyl)[60]fullerene. If there is only one substituent at a [6,6]-junction (in other words, in the cases of [5,6]- and (1,4)-additions), the expression using the term "nil" such as in (nil:-phenyl) is used. When cycloaddition occurs at a site, the substituent is expressed as a bivalent one; e.g., (A,B)-bis(2,3-dimethylbut-2-ene-1,4-diyl)[60]fullerene.

Using this nomenclature, all T_h-symmetrical hexa-adducts can be named by the prefix (2A,2H,2V)-hexakis;[1,7] e.g., (2A,-2H,2V)-hexakis(2,3-dimethylbut-2-ene-1,4-diyl)[60]fullerene.[7] D_{2h} symmetrical di-adducts can be called as (2A)-bis-ones;[3,12] e.g., (2A)-bis(9,10-dihydroanthracene-9,10-diyl)[60]-fullerene.[3] Some complicated derivatives, obtained by the addition around a corannulene moiety[13,14] or a benzofluoranthene one,[14] have been named precisely; i.e., (A)-mono(chloro:phenyl)-($B^e{}_{11}$,$C^u{}_{11}$,-$B^e{}_{14}$,$C^u{}_{14}$)-tetrakis(nil:phenyl)[60]fullerene (Figure 2a)[13] or



side-view top-view

Figure 1. Designation of each [6,6]-junction relative to the base addition site, A_1.

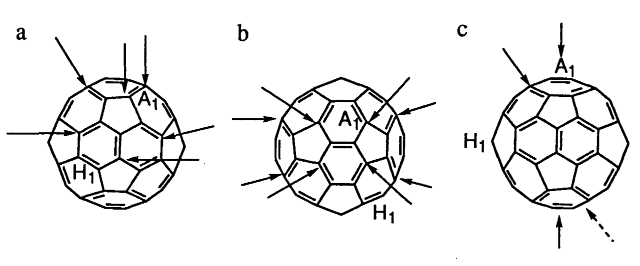


Figure 2. Some complicated addition or coordination products.

Table 1. Nomenclature of $C_{60}H_2$ Isomers

Isomer	Isomer		Enantiomer		Racemate[a]
No.	Edge Labeling	Vertex Labeling[b]	Edge Labeling	Vertex Labeling[b]	Edge Labeling
1	A_1	1a1b	-		-
2	A_1,A_2	1a3a'	-		-
3	A_1,A^u_2	1a3b'	-		-
4	A_1,H_1	1a5c,1a,3d	A_1,H^u_1	1a6c,1a8d	A_1,H^r_1
5	A_1,V^u_1	1a3d',1a,10c'	A_1,V^u_2	1a8d',1a1c'	A_1,V^u_r
6	A_1,B_{11}	1a2b,1a1c	A_1,B_{14}	1a10c,1a5b	A_1,B_{11r}
7	A_1,B_{12}	1a9c	A_1,B_{13}	1a2c	A_1,B_{12r}
8	A_1,B^u_{11}	1a5a	A_1,B^u_{14}	1a2a	A_1,B^u_{11r}
[c]	$A_1,B^u_{12}(=A_1,B_{11})$[d]		$A_1,B^u_{13}(=A_1,B_{14})$[d]		A_1,B^u_{12r}
[c]	$A_1,B_{21}(=A_1,B^u_{22})$[d]		$A_1,B_{24}(=A_1,B^u_{23})$[d]		A_1,B_{21r}
9	A_1,B_{22}	1a4c'	A_1,B_{23}	1a7c'	A_1,B_{22r}
10	A_1,B^u_{21}	1a2a'	A_1,B^u_{24}	1a4a'	A_1,B^u_{21r}
11	A_1,B^u_{22}	1a6c',1a2b'	A_1,B^u_{23}	1a5c',1a4b'	A_1,B^u_{22r}
12	A_1,C_{11}	1a4a	A_1,C_{14}	1a3a	A_1,C_{11r}
[c]	$A_1,C_{12}(=A_1,C^u_{11})$[d]		$A_1,C_{13}(=A_1,C^u_{14})$[d]		A_1,C_{12r}
13	A_1,C^u_{11}	1a3b,1a1d	A_1,C^u_{14}	1a4b,1a10d	A_1,C^u_{11r}
14	A_1,C^u_{12}	1a10d'	A_1,C^u_{13}	1a1d'	A_1,C^u_{12r}
15	A_1,C_{21}	1a1a'	A_1,C_{24}	1a5a'	A_1,C_{21r}
16	A_1,C_{22}	1a5d',1a5b'	A_1,C_{23}	1a1b',1a6d'	A_1,C_{22r}
[c]	$A_1,C^u_{21}(=A_1,C_{23})$[d]		$A_1,C^u_{24}(=A_1,C_{22})$[d]		A_1,C^u_{21r}
17	A_1,C^u_{22}	1a5d	A_1,C^u_{23}	1a6d	A_1,C^u_{22r}
18	A_1,D_{11}	1a4c,1a9d	A_1,D_{14}	1a7c,1a2d	A_1,D_{11r}
19	A_1,D_{12}	1a2d'	A_1,D_{13}	1a9d'	A_1,D_{12r}
20	A_1,D^u_{11}	1a8c	A_1,D^u_{14}	1a3c	A_1,D^u_{11r}
[c]	$A_1,D^u_{12}(=A_1,D_{14})$[d]		$A_1,D^u_{13}(=A_1,D_{11})$[d]		A_1,D^u_{12r}
[c]	$A_1,D_{21}(=A_1,D^u_{23})$[d]		$A_1,D_{24}(=A_1,D^u_{22})$[d]		A_1,D_{21r}
21	A_1,D_{22}	1a4d	A_1,D_{23}	1a7d	A_1,D_{22r}
22	A_1,D^u_{21}	1a3c'	A_1,D^u_{24}	1a8c'	A_1,D^u_{21r}
23	A_1,D^u_{22}	1a4d',1a2c'	A_1,D^u_{23}	1a7d',1a9c'	A_1,D^u_{22r}

[a] Superscript letter r and subscript letters r, 1r, and 2r mean e or u, 1 or 2, 1 or 4, and 2 or 3, respectively. [b] Reference 9. [c] It is valid, when each hydrogen atom is substituted by a different group. [d] For $C_{60}H_2$ or [60]fullerenes with two identical groups.

$(A,V^u_2,B^e_{11},C^u_{11},B^e_{13},D^e_{13},C^e_{14},D^u_{14})$-octakis(bromo:nil)[60]-fullerene (Figure 2b).[14] The famous Wudl's fulleroid[11] with a [5,6]-open structure can be named as (A,B^u_{12})-mono(methylene: nil)[60]fulleroid with a minor change of the fulleroid concept.

The present nomenclature is designed by taking the symmetry caused by the addition at a [6,6]-junction as the first priority, so that enantiomers can be rather easily expressed. Some enantiomers are named by changing the second subscript number 1 to 4 or 2 to 3, and vice versa (see Table 1). Therefore, a racemate needs not to have two names in the precise expression, such as "a racemic mixture of 1a2a and 1a5a," by Cahill's method,[9c] but it is simply written as "(A_1,B^u_{11r})" with its regiochemical prefix 1r, as shown in Table 1 (see Isomer No. 8 together with footnote a).

In the case of a multiple addition accompanied by some coordinations[15] or bridging tethers[6] between non-fullerene parts, we tentatively suggest the use of primes on the shoulders of the site labels, which mean the presence of bonding at the underlined atoms (or positions) across these sites; i.e., (A'_1,B'_{12})-bis((1,5-COD)$\underline{\mathrm{ClIr}}$)-$(A'_2,B'_{22})$-bis((1,5-COD)$\underline{\mathrm{ClIr}}$)[60]fullerene, whose schematic skeleton is depicted in Figure 2c.[15]

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