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Balaban, Alexandru T.; Rücker, Christoph

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How to specify the structure of substituted blade-like zigzag diamondoids

Invited Paper

Alexandru T. Balaban[1*], Christoph Rücker[2]

[1]*Texas A&M University at Galveston, Galveston, TX 77553, USA*

[2]*Leuphana University Lüneburg, D-21335 Lüneburg, Germany*

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Abstract: The dualist of an [*n*]diamondoid consists of vertices situated in the centers of each of the *n* adamantane units, and of edges connecting vertices corresponding to units sharing a chair-shaped hexagon of carbon atoms. Since the polycyclic structure of diamondoids is rather complex, so is their nomenclature. For specifying chemical constitution or isomerism of all diamondoids the Balaban-Schleyer graph-theoretical approach based on dualists has been generally adopted. However, when one needs to indicate the location of C and H atoms or of a substituent in a diamondoid or the stereochemical relationships between substituents, only the IUPAC polycycle nomenclature (von Baeyer nomenclature) provides the unique solution. This is so since each IUPAC name is associated with a unique atom numbering scheme. Diamondoids are classified into catamantanes (which can be regular or irregular), perimantanes, and coronamantanes. Regular catamantanes have molecular formulas $C_{4n+6}H_{4n+12}$. Among regular catamantanes, the rigid blade-shaped zigzag catamantanes (so called because their dualists consist of a zigzag line with a code of alternating digits 1 and 2) exhibit a simple pattern in their von Baeyer nomenclature. Their carbon atoms form a main ring with $4n + 4$ atoms, and the remaining atoms form two 1-carbon bridges. All zigzag [*n*]catamantanes with $n > 2$ have quaternary carbon atoms, and the first bridgehead in the main ring is such an atom. Their partitioned formula is $C_{n-2}(CH)_{2n+4}(CH_2)_{n+4}$. As a function of their parity, IUPAC names based on the von Baeyer approach have been devised for all zigzag catamantanes, allowing the unique location for every C and H atom. The dualist of such a zigzag catamantane defines a plane bisecting the molecule, and the stereochemical features of hydrogens attached to secondary carbon atoms can be specified relatively to that plane.

Keywords: *Diamondoids • Dualists • Catamantanes • IUPAC nomenclature*

1. Introduction

Diamondoids (or diamond hydrocarbons) have come recently into attention after they were found to be available from petroleum in fair amounts; their isolation and purification is based on their resistance to pyrolysis and oxidation due to their high thermodynamic stability (lowest steric strain among all isomeric aliphatic hydrocarbons) [1,2]. Synthetic methods cannot compete with the lower-cost natural products; moreover, Lewis-acid catalyzed isomerization can only produce [*n*] diamondoids with up to $n = 4$ [3-9]. Till now, the largest diamondoids isolated from natural sources have $n = 11$. Several reviews and recent books describe diamondoids and their potential applications [10-19].

Among all natural diamondoids, the long, straight, and rigid blade-like or rod-like molecules are believed to be the most promising for biomedical applications [20,21]. Whereas a rod-like shape suggests cylindrical symmetry, a blade-like shape involves two opposing faces of a slender long object. Regioselective functionalization at tertiary carbons situated at precise distances [22-25] may offer pathways to biologically active products by interaction with proteins, inhibiting or activating such biocatalysts. One has to take into account that blade-like or rod-like substances are not easily available. Unlike benzenoid nanotubes which are polydisperse mixtures of related but not identical molecules, diamondoids are pure substances. Among the numerous known, identified and isolated diamondoids, two classes seem to offer the highest promise: the achiral blade-like diamondoids which will be discussed in the present article, and the chiral diamondoids [25].

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* *E-mail: balabana@tamug.edu*

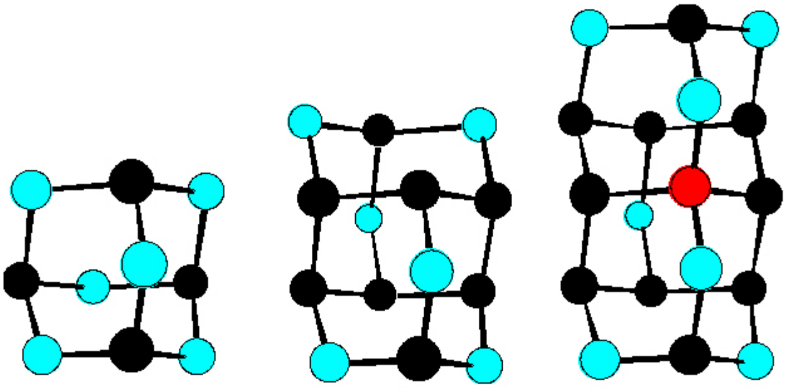

Figure 1. Carbon atoms of adamantane, diamantane, and triamantane; red, black, and blue denote quaternary, tertiary, and secondary carbon atoms. All figures show hydrogen-depleted structures.

Functionalized diamondoids by regioselective reactions have been investigated intensely by Schreiner and coworkers, in collaboration with Dahl and Carlson from Chevron USA, Inc. who provided the hydrocarbons [22-25]. It has long been known that hydrogens attached to tertiary carbon atoms can be substituted more readily than hydrogens attached to secondary carbon atoms. The partition of carbon and hydrogen atoms of diamondoids has been analyzed recently [26,27].

2. Classification and nomenclature of diamondoids

Whereas finding manually the correct IUPAC name of a polycyclic compound is often a hard task, the Balaban-Schleyer systematic approach based on dualists has been generally accepted for discriminating among constitutional isomers of diamondoids [28]. These codes use the four digits 1, 2, 3, and 4 for the tetrahedral directions of covalent bonds around an sp^3-hybridized carbon atom. As an example, the hydrogen-depleted structures of the first three diamondoids are shown in Fig. 1, and the corresponding IUPAC names as well as their 4-digit codes are indicated in the following.

Adamantane is tricyclo[3.3.1.1^{3,7}]decane. It has molecular formula $C_{10}H_{16}$ and partitioned formula $(CH)_4(CH_2)_6$.

Diamantane is pentacyclo[7.3.1.1^{4,12}.0^{2,7}.0^{6,11}]tetradecane and has code [1]. It has molecular formula $C_{14}H_{20}$ and partitioned formula $(CH)_8(CH_2)_6$.

Triamantane is heptacyclo[7.7.1.1^{3,15}.0^{1,12}.0^{2,7}.0^{4,13}.0^{6,11}]octadecane and has code [12]. It has molecular formula $C_{18}H_{24}$ and partitioned formula $C(CH)_{10}(CH_2)_7$.

One can view a diamondoid as a portion of the diamond lattice, with dangling bonds connected to hydrogen atoms. An [*n*]diamondoid with *n* adamantane units (cells) corresponds uniquely to a dualist consisting of vertices situated in the centers of each cell, and of edges connecting vertices of adjacent cells, *i.e.*, adamantane units sharing a chair-shaped hexagon of carbon atoms. Diamondoids and the diamond lattice are self-dual, *i.e.*, the centers of adamantane cells form another diamond lattice inside the original one, and the same is true for diamondoids, whose carbon atoms are cut-outs of the diamond lattice. As mentioned above, by using the digits 1 to 4 for representing the directions of tetrahedrally-situated edges around dualist vertices, a coding system was devised for the unique constitutional characterization of each diamondoid [28]. For diamondoids with $n > 3$, more than one isomer is possible.

A diamondoid with an acyclic dualist (identical to the carbon scaffold of a staggered rotamer of an alkane) is called a catamantane. Perimantanes have dualists that contain six-membered rings, and coronamantanes have dualists with larger rings that are not perimeters of six-membered ring aggregates. Catamantanes are regular when they have molecular formulas $C_{4n+6}H_{4n+12}$ and partitioned formula $C_{n-2}(CH)_{2n+4}(CH_2)_{n+4}$. According to a theorem in graph theory the number of odd-degree vertices in any graph must be even, which is why the number of tertiary carbon atoms or CH groups is an even number. Irregular catamantanes, perimantanes, and coronamantanes have molecular formulas with lower numbers of carbon and hydrogen atoms than the above molecular formula. Molecular descriptors of dualists (which, as mentioned earlier, are staggered alkane rotamers for catamantanes [29,30]) have been helpful for QSPR associations between the chemical structure of diamondoids and their GC-MS or HPLC characteristics [31].

We will discuss zigzag catamantanes which are narrow practically straight aggregates of adamantane units (Fig. 2).

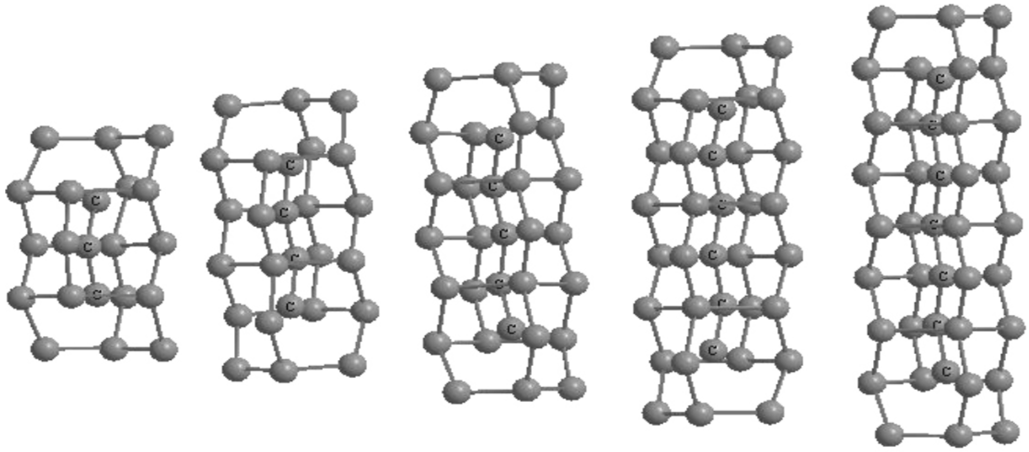

Figure 2. Carbon scaffolds of zigzag catamantanes with $n = 3, 4, 5, 6$, and 7. The four vertical carbon atom chains have n+2, n, n+2, n+2 carbon atoms for odd n, and $n + 2$, $n + 1$, $n + 1$, and $n + 2$ carbon atoms for even n. Dualists are indicated by a zigzag chain of adamantane Cell Centers denoted by letters C.

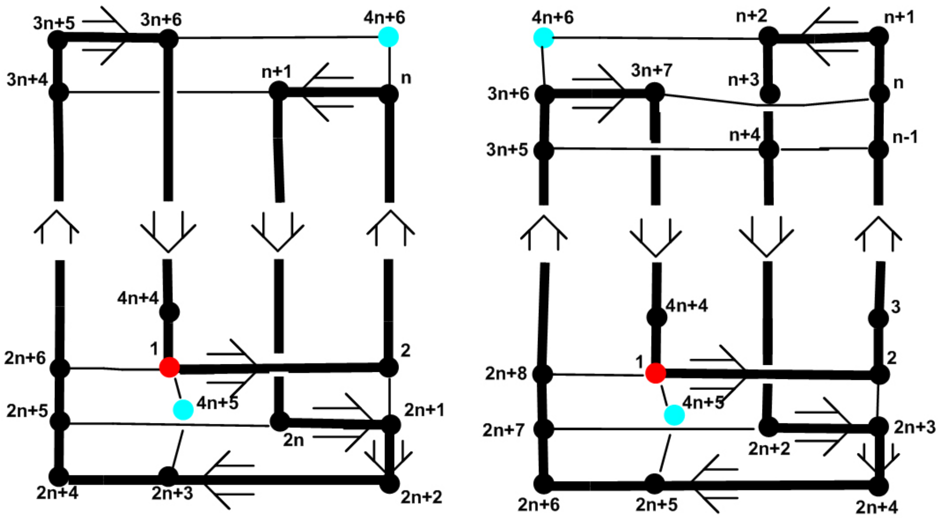

Figure 3. Numbering scheme for zigzag [n]diamondoids with $n > 2$ for odd n (left) and even n (right). One quaternary carbon atom (which is indicated here in red) closest to the end of the diamondoid as in Fig. 2 is numbered as 1; the numbering follows the arrows as shown covering all the other $4n + 3$ carbon atoms of the main ring (thick lines). The two blue carbon atoms connected by thinner lines form the 1-carbon bridges. The main bridge is the thin vertical line involving atom numbered $4n + 5$.

3. IUPAC names of regular zigzag catamantanes

The present article will deal only with rigid blade-like regular catamantanes whose dualists are non-branched and have a zigzag geometry expressed by a code with alternating digits 1 and 2. Although the dualist-based names are sufficient for distinguishing between constitutional isomers, they do not allow specifying the location of C and H atoms or substituents in the molecule, nor do they allow to indicate stereochemical relationships between substituents. Therefore we will discuss the Adolf von Baeyer naming and numbering system, adopted by the International Union of Pure and Applied Chemistry (IUPAC) Commission of Nomenclature for Organic Chemistry. For indicating locations of C and H atoms in diamondoids when reporting NMR or other spectroscopic data [32,33], numbering of carbon atoms according to the IUPAC rules is extremely helpful.

The 1999 IUPAC Recommendation on the von Baeyer system applies [34]: "***VB-1 Definitions and terminology***. … The main ring (selected so as to include as many skeletal atoms of the polycyclic compound as possible) includes the two bridgeheads. The main bridge is a bridge which connects the two main bridgeheads. A secondary bridge is any bridge not included in the main ring or the main bridge. An independent secondary bridge links bridgeheads which are part of the main ring or main bridge. A dependent secondary bridge links at least one bridgehead which is part of a secondary bridge.…

VB-5 Main bridge. … the main bridge is selected to include as many as possible of the atoms not in the main ring. …

VB-6 Naming hydrocarbon polycyclic system. Any rings not described by the bicyclic system are defined by citing the number of atoms making up each secondary bridge. The locants of the two attachment points of each secondary bridge are cited as a pair of superscript locants (lower first) separated by a comma. The numbers indicating independent secondary bridges are cited in decreasing order. The name of the polycyclic hydrocarbon is then constructed by:

- a prefix indicating the number of cycles (tricyclo, tetracyclo, *etc*.);
- numbers indicating the bridge lengths (with the appropriate superscript locants in the case of secondary bridges) separated by full stops and placed in square brackets;
- and the name of the parent hydrocarbon indicating the number of ring atoms.

Independent secondary bridges are cited before dependent secondary bridges. The numbers indicating dependent secondary bridges are cited in decreasing order.

VB-6-1 The main ring shall be divided as symmetrically as possible by the main bridge.

VB-6-2 If there is a choice of independent secondary bridges the first cited shall be as long as possible. Then if relevant the second cited independent secondary bridge shall be as long as possible, *etc*.

VB-6-3 The number of dependent secondary bridges is kept to a minimum.

VB-6-4 The superscript locants of the secondary bridges shall be as small as possible when considered as a set in ascending numerical order, a decision being made at the first point of difference.

VB-6-5 The superscript locants shall be as small as possible when considered in the order of citation in the name.

VB-7 Numbering of secondary bridges. After numbering the main ring and main bridge all independent secondary bridges are numbered before dependent secondary bridges. The numbering continues from the highest number of the main ring and bridge. Each secondary bridge is numbered in turn starting with the independent secondary bridge linked to the highest numbered bridgehead atom, then the independent secondary bridge linked to the next highest numbered bridgehead atom and so on. Each atom of a secondary bridge is numbered starting from the atom next to the higher numbered bridgehead.

VB-7.1 If there is still a choice lower locants are used for the atoms in the bridge linked to the higher numbered bridgehead.

VB-7.2 If there is still a choice longer bridges are numbered before shorter bridges."

The forthcoming IUPAC comments rephrase some details [35]: "***P-23.2.6.2** Selection of the main bridge and secondary bridges.* There is often a number of choices to be made in the selection of the main bridge and the secondary bridges. To make such choices, the following criteria are applied in order until a decision can be made. **P-23.2.6.2.1** The main ring must be divided as symmetrically as possible by the main bridge, which, as directed in P-23.2.4, includes as many of the atoms not included in the main ring as possible. **P-23.2.6.2.2** If there is a choice of independent secondary bridges, the first cited must be as long as possible. Then, if relevant, the second independent secondary bridge must be as long as possible, *etc*. **P-23.2.6.2.3** The number of dependent secondary bridges is to be kept to a minimum. **P-23.2.6.2.4** The superscript locants for the secondary bridges must be as low as possible when considered as a set in ascending numerical order, the decision being made at the first point of difference. **P-23.2.6.2.5** The superscript locants shall be as low as possible when considered in their order of citation in the name."

As a direct consequence of the above rules, whenever there is a quaternary carbon atom present in a regular catamantane (*i.e*., for all $n > 2$ values), the first bridgehead must be such an atom. Since the numbers of quaternary carbon atoms in a regular [n]catamantane is $n - 2$, triamantane is the first zigzag catamantane that will have the systematic numbering discussed in the present communication. The cyclomatic number of regular non-branched [n]catamantanes, specified in the IUPAC name as the conventional number of cycles, is denoted by μ. Yet another consequence is that the IUPAC name depends upon the parity of n, indicated by the parity function p which is zero for even n, and 1 for odd n. The zigzag catamantanes have all a simple structure involving $4n + 4$ carbon atoms in the main ring and two 1-atom bridges. For odd n values the two 1-atom bridges are of the form [$a.a.1.1^{x,y}.0$…], and for even n values the two 1-atom bridges are of the form [$a.b.1.1^{x,y}.0$…], where the following equations (found by induction) hold:

$$a = 2(n - p) + 3 \tag{1}$$

$$b = 2(n + p) - 1 \tag{2}$$

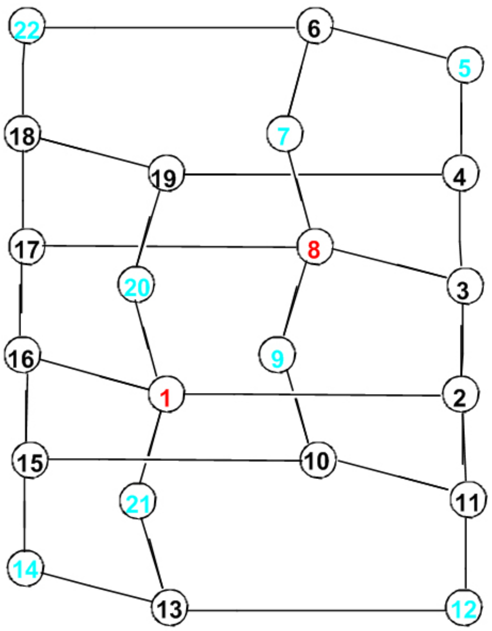

Figure 4. Numbering scheme for [121]tetramantane; red color applies for quaternary C, black for tertiary CH, and blue for secondary CH_2 groups.

$$p = [1 - (-1)^n] / 2 \tag{3}$$

$$\mu = 2n + 1 \tag{4}$$

It can be seen that the difference $a - b = 4 - 4p$ is constant, namely for any even n value, *i.e.*, when $p = 0$, $a - b = 4$, whereas for odd n values $a = b$. The general principle of choosing a pathway along the ring of $4n + 4$ carbon atoms of blade-like regular zigzag catamantanes may be seen in Fig. 3 for all (odd and even) $n > 2$ values. The horizontal cross-links in Figs. 3 and 4 involve three carbon atoms each, whereas the quasi-vertical chains involve n, $n + 1$, or $n + 2$ carbon atoms. The main ring consists of $4n + 4$ carbon atoms numbered from 1 to $4n + 4$. The first of the two one-atom bridges, namely the one that is not indicated by superscripts and contains the carbon atom numbered $4n$+5 (the main bridge), originates from the quaternary carbon atom numbered 1 (red dot in Fig. 3) and ends at the carbon atom numbered $2n$+3 for odd n, or $2n$+5 for even n. It consists of a secondary (CH_2) carbon atom and divides equally the main ring for odd n and unequally for even n. In other words, for odd n values, the main one-atom bridge connects carbons numbered 1 and $2n$+3 in a ring of $4n$+4 carbon atoms, dividing therefore this ring into two equal halves. The second one-atom bridge is also a secondary (CH_2) carbon atom numbered $4n$+6 and this bridge has endpoints x and y specified by the two superscripts [$a.b.1.1^{x,y}.0\ldots$.], where for odd n, we have $x = n$ and $y = 3n+6$, and for even n, we have $x = n+2$ and $y = 3n+6$. The reason for the difference $a - b = 4$ when n is even is the fact that the main bridge connects atoms 1 and $2n$+5 in the ring of $4n$+4 carbon atoms.

According to this principle, in addition to the well-known IUPAC names of diamondoids with n = 1, 2, and 3 indicated earlier, the full IUPAC names of higher zigzag catamantanes with n = 4, 5, 6, and 7 are as follows:

[121]tetramantane is nonacyclo[$11.7.1.1^{6,18}.0^{1,16}.0^{2,11}.0^{3,8}.0^{4,19}.0^{8,17}.0^{10,15}$]docosane and has molecular and partitioned formulas $C_{22}H_{28}$, and $C_2(CH)_{12}(CH_2)_8$, respectively (see Fig. 4);

[1212]pentamantane is undecacyclo[$11.11.1.1^{5,21}.0^{1,16}.0^{2,11}.0^{3,8}.0^{4,23}.0^{6,19}.0^{8,17}.0^{10,15}.0^{18,23}$]hexacosane and has molecular and partitioned formulas $C_{26}H_{32}$ and $C_3(CH)_{14}(CH_2)_9$, respectively;

[12121]hexamantane is tridecacyclo[$15.11.1.1^{8,24}.0^{1,20}.0^{2,15}.0^{3,12}.0^{4,27}.0^{5,10}.0^{6,25}.0^{10,23}.0^{12,21}.0^{14,19}.0^{22,27}$] triacontane, and has molecular and partitioned formulas $C_{30}H_{36}$ and $C_4(CH)_{16}(CH_2)_{10}$, respectively;

[121212]heptamantane is pentadecacyclo[$15.15.1.1^{7,27}.0^{1,20}.0^{2,15}.0^{3,12}.0^{4,31}.0^{5,10}.0^{6,29}.0^{8,25}.0^{10,23}.0^{12,21}.0^{14,19}.0^{22,31}.0^{24,29}$]tetratriacontane and has molecular and partitioned formulas $C_{34}H_{40}$ and $C_5(CH)_{18}(CH_2)_{11}$, respectively.

Although all bridges present regularities, we shall point out briefly only a few of the initial bridges for all zigzag catamantanes with $n > 2$. The first 1-atom bridge, which is the main bridge without explicitly specified endpoints, links atom 1 with atom $2n + 3$ (for odd n) or atom 1 with atom $2n + 5$ (for even n). The second 1-atom bridge (the first secondary bridge) links atoms n and $3n + 6$ (for odd n) or $n + 2$ and $3n + 6$ (for even n). The first zero-atom bridge (2nd secondary bridge) links atom 1 with atom $2n + 6$ (for odd n) or with atom $2n + 8$ (for even n). The 3rd secondary bridge links atoms 2 and $2n + 1$ (for odd n) or atoms 2 and $2n + 3$ (for even n).

The POLCYC computer program [36], which works quite independently of the considerations given here, correctly gives all the above names and numbers. Schreiner, Fokin and coworkers correctly numbered the atoms in several newly synthesized diamondoids with functional groups [22-24], after cyclohexamantane had been named incorrectly [32].

4. Locants and stereochemical specification of substituents for blade-like catamantanes with zigzag dualists

As indicated earlier, the IUPAC name provides an unambiguous numbering of all carbon atoms in a polycyclic molecule, allowing to specify the location

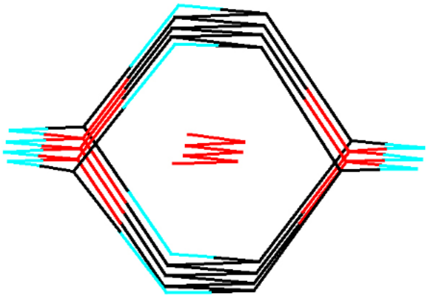

Figure 5. The carbon scaffold of [121212]heptamantane with the same color convention as in Fig. 1; in the center, the dualist is shown as a red zigzag line defining a plane that bisects the diamondoid and is a mirror plane.

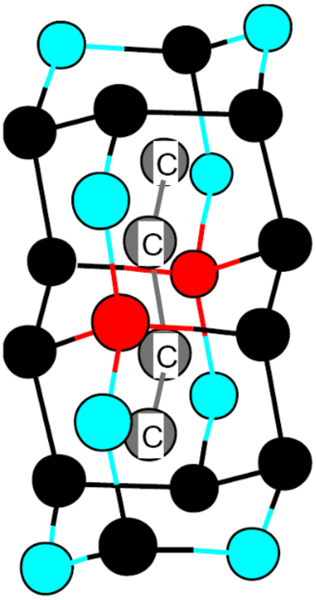

Figure 6. The carbon scaffold of [121]tetramantane (with the same color conventions as in Fig. 1) with its dualist, with centers of adamantane represented by grey circles with the letter C.

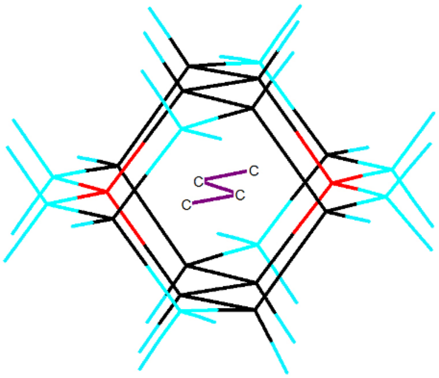

Figure 7. [121]Tetramantane (with the same color conventions for carbon atoms as in Figs. 1 to 6, except for hydrogen atoms which here also appear in blue color and are at the free end of each dangling bond). The dualist is in the middle, where the centers of adamantane cells are represented by the zigzag line with the letters C.

of any substituents. Unlike the more common *rod-like* molecules, the zigzag catamantanes are *blade-like* because their dualist defines a plane that divides the molecule into an upper and lower half. With reference to this plane, one can specify the geometrical and stereochemical features of substituents by Greek letters, just as in the steroid nomenclature that makes reference to cholestane. Fig. 5 shows the hydrogen-depleted zigzag [121212]heptamantane with its dualist defining a plane that bisects the diamondoid.

For illustrating how one may proceed with specifying the stereochemistry of substituents replacing hydrogen atoms, we shall use a shorter zigzag catamantane as example, namely [121]tetramantane. In Fig. 6 one can see [121]tetramantane in the same perspective as for Figs. 2 and 4, leading to the general principle of von Baeyer (IUPAC) nomenclature illustrated by Fig. 3. These figures show only the carbon skeleton of the zigzag catamantanes, and the *topological* information about connectivity results in the von Baeyer (IUPAC) numbering of all carbon atoms of the catamantane. For stereochemical features one needs to include *geometrical* information. Diastereo-isomerism can be specified relative to the plane defined by the dualist. We will not address problems of enantiomerism; although the carbon scaffold of each zigzag catamantane is achiral having mirror symmetry, any replacement of one hydrogen (attached to a secondary carbon atom) by a substituent destroys the mirror symmetry, thus creating chirality. As an exception, in the odd-*n* case such a replacement at the middle CH_2 group does not affect mirror symmetry, since these two H atoms are located on a second mirror plane (point group C_{2v}, see Fig. 5). Thus, these particular two H atoms cannot, and therefore need not be distinguished, they are homotopic.

Fig. 7 presents [121]tetramantane with all its hydrogen atoms. As one can see from this figure, the hydrogens attached to secondary carbon atoms have different geometries, which may be specified by letters α or β (adopting a convenient convention with reference to the plane defined by the dualist).

Whereas hydrogens attached to tertiary carbon atoms have a fixed position specified by the *topology*, *i.e.*, the numbering of the carbon atom to which they are attached, for hydrogens attached to secondary carbon atoms or their substituents such information needs to be supplemented by an indication of the *3-dimensional geometry*: the pairs of hydrogens attached to the medial plane defined by the dualist are either above or below this plane, and Greek letters α, β can define this geometry by analogy with steroid nomenclature; for the remaining pairs of hydrogens attached to secondary carbon atoms (or their substituents), one can again advocate "up-down" differences with respect to the plane defined by the dualist.

5. Conclusions

The connectivity scheme of zigzag regular catamantanes is simple, so that it is easy to find the general principles for the IUPAC numbering of carbon atoms in such diamondoids. Thus the location of carbon and hydrogen atoms can be uniquely specified. For hydrogens attached to secondary carbon atoms, whose geometry and stereochemistry need to be also precisely indicated, one can take advantage of the fact that the dualist of these diamondoids defines a plane bisecting the molecule, and differentiate these hydrogen atoms by Greek letters in relationship to that plane, following the example of steroids.

The present authors are aware that zigzag regular catamantanes are but a tiny fraction of diamondoids; however, this class of naturally-occurring polymantanes is connected to high expectations for applications, in which correctly naming functionalized derivatives is important.

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