HAL open science

# [6.6]Chiralane: A Remarkably Symmetric Chiral Molecule

Alan Schwartz, Michel Petitjean

## To cite this version:

Alan Schwartz, Michel Petitjean. [6.6]Chiralane: A Remarkably Symmetric Chiral Molecule. Symmetry: Culture and Science, 2008, 19 (4), pp.307-316. hal-01941526

**HAL Id: hal-01941526**

**https://hal.science/hal-01941526v1**

Submitted on 1 Dec 2018

**HAL** is a multi-disciplinary open access archive for the deposit and dissemination of scientific research documents, whether they are published or not. The documents may come from teaching and research institutions in France or abroad, or from public or private research centers.

L'archive ouverte pluridisciplinaire **HAL**, est destinée au dépôt et à la diffusion de documents scientifiques de niveau recherche, publiés ou non, émanant des établissements d'enseignement et de recherche français ou étrangers, des laboratoires publics ou privés.

Copyright

*Symmetry: Culture and Science*
*Vol. 19, No. 4, 307-316, 2008*

# [6.6]CHIRALANE: A REMARKABLY SYMMETRIC CHIRAL MOLECULE

Alan M. Schwartz [1] and Michel Petitjean *,[2]

[1] 49 Fabriano, Irvine, CA 92620, USA. E-mail: schwartz.alan@gmail.com
[2] CEA Saclay/DSV/iBiTec-S/SB2SM (CNRS URA 2096), 91191 Gif-sur-Yvette Cedex, France. E-mail: michel.petitjean@cea.frhttp://petitjeanmichel.free.fr/itoweb.petitjean.html
* Corresponding author.

*Received*: 30 December 2008; *Accepted*: 23 March 2009

**Abstract:** *We present [6.6]chiralane, a rotationally symmetric, rigid, extremal chiral molecule with some remarkable properties.*

## 1. INTRODUCTION

[6.6]Chiralane is a point group **T** highly condensed polycycloalkane $C_{27}H_{28}$ (Figure 1) containing 68 single bonds. There are five quaternary carbons, 16 tertiary carbons and six secondary carbons (methylenes). The connection table of the full molecular graph with atomic coordinates is given in the appendix.

[6.6]Chiralane (central atom), several [m.n] homologs (*m, n* = 5 or greater), and [m]chirolanes (no central atom) were designed by Schwartz to explore maximally chiral nanostructures (Schwartz, 2004).

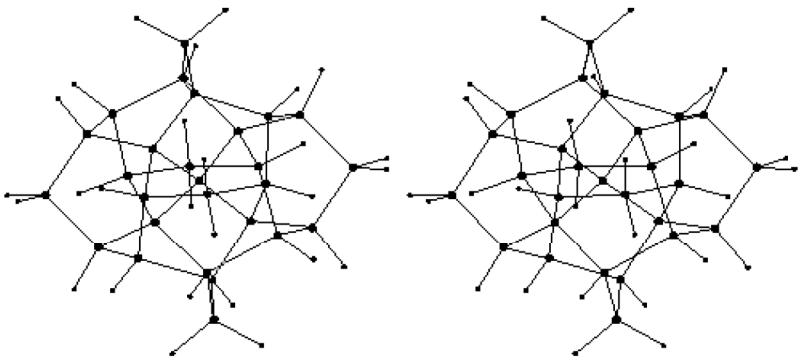

**Figure 1**: Stereogram of Hartree Fock/6-31G(d)-modeled [6.6]chiralane.

## 2. GRAPH SYMMETRIES AND NOMENCLATURE

The molecular graph of the chiralane has 55 nodes, 68 edges, and 1 component. Thus, the Euler formula requires the associated molecular graph to have 68+1-55=14 independant cycles. The difference between dependant cycles and independant cycles may be illustrated by naphthalene: it has three cycles (containing respectively 6, 6, and 10 carbons), but only two of them are independant because the third one (a bicyclic ring) is deduced from the other two. The chiralane has only one cyclic system, containing all carbon atoms. An example compound with two cyclic systems is diphenylmethane, in which the two cyclic systems are joined by bonds not included in a cycle. The smallest chiralane rings are homochiral twist-boat conformation six-membered rings. All larger rings are polycyclic, and are composed from six-membered rings. The structural formula is usefully described in terms of concentric layers around a central atom called the focus (Petitjean 1992). The first layer of atoms contains the neighbours of the focus (i.e. the atoms bonded to the focus), the second layer contains the next neighbours, and so on. The focus is usually set at the center of the graph, the center being a node bearing the largest number of concentric layers. For clarity, we further consider the hydrogen-suppressed graph.

[6.6]Chiralane possesses a unique center with three concentric layers around it. The carbons of each layer are noted according to their layer number and to their number of hydrogens, as indicated in the first column of Table 1.

| Carbon type | Layer | Hydrogens | Total carbons per layer | Atom numbers range |
|---|---|---|---|---|
| Focus | 0 | 0 | 1 | 1 |
| C(1) | 1 | 0 | 4 | 2-5 |
| CH(2) | 2 | 1 | 12 | 6-17 |
| CH(3) | 3 | 1 | 4 | 18-21 |
| $CH_2$(3) | 3 | 2 | 6 | 22-27 |

**Table 1**: Carbon types classified by their distance from the focus.

The full molecular graph of [6.6]chiralane has 768 automorphisms, but its hydrogen-suppressed graph has only twelve automorphisms. The difference arises from the six methylene groups that multiply the number of automorphisms by $2^6$. The twelve automorphisms define five classes of equivalent atoms. Remarkably, these classes correspond exactly to the 5 carbon types defined in Table 1. According to Petitjean (2007), a graph having more than one automorphism is symmetric.

All monocycles found in [6.6]chiralane are cyclohexane rings, and all bicyclic systems based upon two cyclohexane rings exist in [6.6]chiralane: bicyclo[2.2.2]octane, bicyclo[3.3.1]nonane, bicyclo[4.4.0]decane (decalin), and spiro[5.5]undecane. There are 30 cyclohexane rings. The full list is given in the appendix. These 30 rings are partitioned into three classes:

Class 1: 12 rings Focus-C(1)-CH(2)-CH(3)-CH(2)-C(1)-Focus
Class 2: 6 rings Focus-C(1)-CH(2)-$CH_2$(3)-CH(2)-C(1)-Focus
Class 3: 12 rings C(1)-CH(2)-CH(3)-CH(2)-$CH_2$(3)-CH(2)-C(1)

Kuratowski's theorem (Berge 1973) requires the [6.6]chiralane molecular graph to be non-planar. It contains as minor the complete graph $K_5$, the five nodes being the focus and its four neighbours C(1).

Given its highly condensed cyclic but non-planar graph structure, [6.6]chiralane resisted assignment of a systematic name following nomenclature rules such as the IUPAC Blue Book, Section A (1979), and its electronic version (ACD/labs, 1997). Fullerenes' planar graphs readily yield to nomenclature rules (Fowler et al. 2007).

Nomenclator software (ChemInnovation Software 2006) assigned (3*S*,5*S*,6*S*,7*S*,9*S*,10*S*,11*S*,13*S*,14*S*,15*S*,17*S*,19*S*,21*S*,22*S*,23*S*,25*S*,2*R*,18*R*,26*R*,27*R*)tetra-cyclo[13.11.1.$0^{1,18}$.$0^{2,7}$.$0^{2,11}$.$0^{3,14}$.$0^{5,27}$.$0^{6,25}$.$0^{9,26}$.$0^{10,19}$.$0^{13,18}$.$0^{17,22}$.$0^{21,26}$.$0^{23,27}$]heptacosane. All carbon atoms are members of homochiral twist-boat cyclohexane rings. The assignment of *R*-configuration atoms is then curious. HyperChem detected twelve *S*-

configuration atoms only. The central atom is an undistorted tetrahedral $sp^3$-hybridized carbon bearing four rigorously identical homochiral substituents. It possesses no improper (rotation-reflection, alternating) axes of symmetry and is therefore chiral - but appears not to be labeled by existing nomenclature rules.

## 3. GEOMETRIC DATA

All bond lengths and valence angles have been computed. The bond lengths depend only on the bond type. Their values are reported in Table 2. They are unremarkable compared to *trans*-decalin values. The longer twelve surface bonds between tertiary carbons are typical of their class. The molecule as a whole is in slight compression compared to diamond with 1.54456 Å C-C bonds (Hom et al. 1975).

| Bond type | Bond length | Total bonds |
|---|---|---|
| Focus-C(1) | 1.536 | 4 |
| C(1)-CH(2) | 1.540 | 12 |
| CH(2)-CH(3) | 1.564 | 12 |
| CH(2)-$CH_2$(3) | 1.539 | 12 |
| C-H bond | 1.086 | 28 |

**Table 2**: Bonds lengths, Å.

Except around the focus, bond angles are progressively twisted from the unstrained $sp^3$-hybridized carbon value expected to be arccos(-1/3) or 109.5°. The values are reported in Table 3.

| Carbon type | types of neighbours | Valence angle | Total bonds |
|---|---|---|---|
| Focus | C(1), C(1) | 109.5 | 6 |
| C(1) | Focus, CH(2) | 103.5 | 12 |
| C(1) | CH(2), CH(2) | 114.8 | 12 |
| CH(2) | C(1), CH(3) | 104.2 | 12 |
| CH(2) | C(1), CH(3) | 106.2 | 12 |
| CH(2) | C(1), H | 112.3 | 12 |
| CH(2) | CH(3), CH(3) | 111.7 | 12 |
| CH(2) | CH(3), H | 111.2 | 12 |
| CH(2) | CH(3), H | 110.9 | 12 |
| CH(3) | CH(2), CH(2) | 107.7 | 12 |
| CH(3) | CH(2), H | 111.1 | 12 |
| CH(3) | CH(2), CH(2) | 105.9 | 6 |
| CH(3) | CH(2), H | 111.1 | 12 |
| CH(3) | CH(2), H | 111.2 | 12 |
| CH(3) | H, H | 106.4 | 6 |

**Table 3**: Valence angles, degrees.

All 30 spatial cyclohexane skeletons have been pairwise compared with the CSR freeware (Petitjean 1998), which optimally superposes two molecules and returns their

largest common spatial motif together with their RMS (Root Mean Square) distance, i.e. the quadratic mean distance of the atom-pairs defined by the common motif in each molecule. Here, the two molecules are always two cyclohexane rings. Among the 435 pairs of cyclohexane rings, the computed common spatial motif is always the full six-membered ring. All RMS distances within any of the three classes of cyclohexane rings mentioned in section 2 are null: a privileged conformation is associated with each class of ring. The RMS distances values between rings of each three classes are: 0.050 Å (class 1 - class 2), 0.069 Å (class 1 - class 3), and 0.079 Å (class 2 - class 3). The respective largest distances among all carbon-pairs are 0.078 Å, 0.105 Å, and 0.093 Å. So, the three privileged conformations are very similar. All rings are chiral. The rings involving a secondary carbon (class 2) offer a $C_2$ rotational symmetry and the other ones offer a slightly distorted $C_2$ rotational symmetry. The three classes of rings have a twist-boat conformation. The deviation from perfect direct rotational symmetry is measured with the direct symmetry index (DSI) and the deviation from achirality is measured with the chiral index (CHI), these two indices being computed with the QCM freeware (Petitjean 1999). The definition of the chiral index is based on the normalized minimized root mean square distance between the set and its rotated and translated mirror image, and take a more general form in the case of continuous and/or infinite sets, which are beyond the scope of this paper (Petitjean 2002). The DSI and CHI values are reported in Table 4. A null value indicates a perfect symmetry or achirality. The maximal theoretical value for DSI and CHI is equal to 1.

| Ring class | DSI | CHI |
|---|---|---|
| 1 | 0.00014 | 0.07280 |
| 2 | 0.00000 | 0.07258 |
| 3 | 0.00019 | 0.05087 |

**Table 4**: The direct symmetry index and the chiral index for each class of rings.

## 4. SYMMETRY AND CHIRALITY

[6.6]Chiralane has the following rotational symmetries: three orthogonal axes of order 2, each one being the bisector of two of the six C(1)-focus-C(1) valence angles; and four axes of order 3, each of them passing through one of the four focus-C(1) bond. [6.6]Chiralane has all the direct rotational symmetries of the regular tetrahedron, but none of its mirror symmetries or higher order improper symmetries!

The focus is the center of the following regular polyhedra:

| Atome type | Number of vertices | Geometric figure |
|---|---|---|
| C(1) | 4 | regular tetrahedron |
| CH(3) | 4 | regular tetrahedron |
| CH(3) | 6 | regular octahedron |
| H bonded to CH(3) | 4 | regular tetrahedron |

**Table 5**: Some geometrical figures defined by the [6.6]chiralane atoms.

Given [6.6]chiralane as a set of 55 points in the 3D space together with the equivalence classes induced by the associated graph automorphisms, the chiral index takes the value CHI=0.9824. Similarly, the chiral index of its skeleton takes the value CHI=1.0000. The chiral index being a continuous function of the coordinates and of the weights, attributing weights proportional to the atomic masses of the 55 atoms would not substantially change the value of the chiral index.

CHI=1 is the largest value permitted for the chiral index. This maximal value can be reached only when the variance matrix is proportional to the identity matrix (Petitjean 2002). Both [6.6]chiralane and its skeleton satisfy to this condition. For the skeleton, the corresponding standard deviation is 1.768 Å on each axis. For the full set of the 55 points, the standard deviation is 1.399 Å on each axis, the calculation being done on a geometric basis, i.e. all 55 punctual atoms have the same weight.

[6.6]Chiralane is a quantitatively maximally chiral molecule. There are other chirality measures (Petitjean 2003) that may be interesting to apply. Thus, a set which maximizes some chirality measure is not, in general, of maximal chirality for the other chirality measures. Rassat and Fowler (2004) have shown that any chiral tetrahedron is the most chiral for some legitimate choice of degree of chirality. However, a CIP-like scheme based on edge length allows classification of chiral tetrahedra, free of labels and considered as geometric objects, into left- and right-handed forms, despite the chiral connection between enantiomers (Fowler and Rassat 2006). An isolated formula unit does not predict the quantitative chirality of its aggregated bulk. Crystallographic space groups such as enantiomorphic $P3_121$ and $P3_221$ can be predictive. Optical rotation arises from electronic effects. It does not measure mass distribution chirality. 2-Norborn<u>a</u>none with $[\alpha]_D$ = 29.8° and 2-norborn<u>e</u>none with $[\alpha]_D$ = 1146.° (both in homogeneous solution) are nearly superposable chiral mass distributions (Wiberg et al. 2006, Crawford et al. 2007). Resolved chiral alkanes with no additional chromophores typically exhibit small optical rotations, $[\alpha]_D$ of a few degrees. Resolved chiral globular cycloalkanes can do much better. Twistane, $C_{10}H_{16}$ as fused twist-boat cyclohexanes,

has $[\alpha]_D$ = 446° or a molar rotation of 60,800° (Nakazaki et al. 1982). [6.6]Chiralane has calculated $[\alpha]_D$ = 692° or a molar rotation of 244,000° (Autschbach et al. 2002).

Each of the twelve CH(2) tertiary carbons is asymmetric, because its four neighbours are always a quaternary carbon C(1), a tertiary carbon CH(3), a secondary carbon $CH_2$ (3), and a hydrogen. Owing to the data in appendix, the twelve CH(2) configurations are *S*. They would be *R* for the other [6.6]chiralane enantiomer. Then, none of the other carbons is asymmetric, due to the molecular graph automorphisms structure of [6.6]chiralane: the four neighbours of the focus are equivalent, three of the four neighbours of the C(1) carbons are equivalent, the three non hydrogen neighbours of the CH(3) are equivalent, and the $CH_2$(3) methylene groups are of course non-asymmetric. Even the subrule of preference *R*>*S* cannot help to order the equivalent carbons. Attributing a flag to the enantiomers such as left/right, d/l, *R*/*S*, P/M, Δ/Λ, etc. is a challenging problem given its graph automorphisms structure. We propose to conventionally assign [6.6]chiralane CH(2) atom configuration.

## 5. CONCLUSION

[6.6]Chiralane is a calculated structure. Though no synthesis is evident, it could be shelved in an air-filled bottle. Consider a central quaternized boron anion or nitrogen cation. Lord Kelvin's frugal definition of chirality (Thomson 1904) goes back to 1893 (Bentley 2009): "I call any geometrical figure, or group of points, chiral, and say that it has chirality if its image in a plane mirror, ideally realized, cannot be brought to coincide with itself ". There are no equations, symmetry arguments, or mentions of composition (color). If a set and its mirror image cannot be superposed (by translation and rotation), they are chiral - e.g., a scalene triangle in 2D. [6.6]Chiralane exemplifies this definition while possessing a center carbon atom whose chiral configuration remains outside nomenclature. Any student would be heartened to learn of its audacity.

## ACKNOWLEDGEMENTS

We are grateful to François Maurel and Lionel Perrin for help with ab initio calculations. We thank Henry Li for help and access to Nomenclator software and Jochen Autschbach for optical rotations calculations. We thank also the first reviewer for helpful suggestions to enhance the clarity of the paper and the second reviewer for pointing useful references about chiral tetrahedra.

# APPENDIX

The connection table of the [6.6]chiralane is given below. It is split into two parts: the first part contains the carbons (Table 6), from which is derived the list of the six-membered rings (Table 7), and the second part contains the hydrogens (Table 8). The internal atomic numbering has been set in order to have a clear view of the spatial arrangement of the atoms. The cartesian coordinates are issued from a Hartree-Fock/6-31G(d) ab initio computation using Gaussian 98. It is let to the reader to see whether or not some other internal numbering would help in understanding both the graph structure and the spatial structure of the [6.6]chiralane.

| Carbon | Layer | x | y | z | neighbours | H atoms |
|---|---|---|---|---|---|---|
| 1 | 0 | 0.0000 | 0.0000 | 0.0000 | 2 3 4 5 | |
| 2 | 1 | 0.8868 | 0.8868 | 0.8868 | 1 7 11 15 | |
| 3 | 1 | 0.8868 | -0.8868 | -0.8868 | 1 6 12 17 | |
| 4 | 1 | -0.8868 | 0.8868 | -0.8868 | 1 9 10 16 | |
| 5 | 1 | -0.8868 | -0.8868 | 0.8868 | 1 8 13 14 | |
| 6 | 2 | 2.0795 | -1.2281 | 0.0261 | 3 20 22 | 28 |
| 7 | 2 | 2.0795 | 1.2281 | -0.0261 | 2 21 22 | 29 |
| 8 | 2 | -2.0795 | -1.2281 | -0.0261 | 5 18 23 | 30 |
| 9 | 2 | -2.0795 | 1.2281 | 0.0261 | 4 19 23 | 31 |
| 10 | 2 | 0.0261 | 2.0795 | -1.2281 | 4 21 24 | 32 |
| 11 | 2 | -0.0261 | 2.0795 | 1.2281 | 2 19 24 | 33 |
| 12 | 2 | -0.0261 | -2.0795 | -1.2281 | 3 18 25 | 34 |
| 13 | 2 | 0.0261 | -2.0795 | 1.2281 | 5 20 25 | 35 |
| 14 | 2 | -1.2281 | 0.0261 | 2.0795 | 5 19 26 | 36 |
| 15 | 2 | 1.2281 | -0.0261 | 2.0795 | 2 20 26 | 37 |
| 16 | 2 | -1.2281 | -0.0261 | -2.0795 | 4 18 27 | 38 |
| 17 | 2 | 1.2281 | 0.0261 | -2.0795 | 3 21 27 | 39 |
| 18 | 3 | -1.4370 | -1.4370 | -1.4370 | 8 12 16 | 40 |
| 19 | 3 | -1.4370 | 1.4370 | 1.4370 | 9 11 14 | 41 |
| 20 | 3 | 1.4370 | -1.4370 | 1.4370 | 6 13 15 | 42 |
| 21 | 3 | 1.4370 | 1.4370 | -1.4370 | 7 10 17 | 43 |
| 22 | 3 | 3.0063 | 0.0000 | 0.0000 | 6 7 | 44 45 |
| 23 | 3 | -3.0063 | 0.0000 | 0.0000 | 8 9 | 46 47 |
| 24 | 3 | 0.0000 | 3.0063 | 0.0000 | 10 11 | 48 49 |
| 25 | 3 | 0.0000 | -3.0063 | 0.0000 | 12 13 | 50 51 |
| 26 | 3 | 0.0000 | 0.0000 | 3.0063 | 14 15 | 52 53 |
| 27 | 3 | 0.0000 | 0.0000 | -3.0063 | 16 17 | 54 55 |

**Table 6**: Connection table and cartesian coordinates (Å) of the [6.6]chiralane skeleton.

| Class 1 | Class 2 | Class 3 |
|---|---|---|
| 1-2-7-21-10-4-1 | 1-2-7-22-6-3-1 | 2-7-21-10-24-11-2 |
| 1-2-7-21-17-3-1 | 1-2-11-24-10-4-1 | 2-7-22-6-20-15-2 |
| 1-2-11-19-14-5-1 | 1-2-15-26-14-5-1 | 2-11-19-14-26-15-2 |
| 1-2-11-19-9-4-1 | 1-3-12-25-13-5-1 | 3-6-20-13-25-12-3 |
| 1-2-15-20-13-5-1 | 1-3-17-27-16-4-1 | 3-6-22-7-21-17-3 |
| 1-2-15-20-6-3-1 | 1-4-9-23-8-5-1 | 3-12-18-16-27-17-3 |
| 1-3-6-20-13-5-1 | | 4-9-19-11-24-10-4 |
| 1-3-12-18-16-4-1 | | 4-9-23-8-18-16-4 |
| 1-3-12-18-8-5-1 | | 4-10-21-17-27-16-4 |
| 1-3-17-21-10-4-1 | | 5-8-18-12-25-13-5 |
| 1-4-9-19-14-5-1 | | 5-8-23-9-19-14-5 |
| 1-4-16-18-8-5-1 | | 5-13-20-15-26-14-5 |

**Table 7**: The 30 six-membered rings of the [6.6]chiralane (each first member appears twice).

| H atom | x | y | z | neighbour |
|---|---|---|---|---|
| 28 | 2.6076 | -2.1192 | -0.3001 | 6 |
| 29 | 2.6076 | 2.1192 | 0.3001 | 7 |
| 30 | -2.6076 | -2.1192 | 0.3001 | 8 |
| 31 | -2.6076 | 2.1192 | -0.3001 | 9 |
| 32 | -0.3001 | 2.6076 | -2.1192 | 10 |
| 33 | 0.3001 | 2.6076 | 2.1192 | 11 |
| 34 | 0.3001 | -2.6076 | -2.1192 | 12 |
| 35 | -0.3001 | -2.6076 | 2.1192 | 13 |
| 36 | -2.1192 | -0.3001 | 2.6076 | 14 |
| 37 | 2.1192 | 0.3001 | 2.6076 | 15 |
| 38 | -2.1192 | 0.3001 | -2.6076 | 16 |
| 39 | 2.1192 | -0.3001 | -2.6076 | 17 |
| 40 | -2.0643 | -2.0643 | -2.0643 | 18 |
| 41 | -2.0643 | 2.0643 | 2.0643 | 19 |
| 42 | 2.0643 | -2.0643 | 2.0643 | 20 |
| 43 | 2.0643 | 2.0643 | -2.0643 | 21 |
| 44 | 3.6565 | -0.0192 | -0.8693 | 22 |
| 45 | 3.6565 | 0.0192 | 0.8693 | 22 |
| 46 | -3.6565 | -0.0192 | 0.8693 | 23 |
| 47 | -3.6565 | 0.0192 | -0.8693 | 23 |
| 48 | 0.8693 | 3.6565 | 0.0192 | 24 |
| 49 | -0.8693 | 3.6565 | -0.0192 | 24 |
| 50 | -0.8693 | -3.6565 | 0.0192 | 25 |
| 51 | 0.8693 | -3.6565 | -0.0192 | 25 |
| 52 | -0.0192 | -0.8693 | 3.6565 | 26 |
| 53 | 0.0192 | 0.8693 | 3.6565 | 26 |
| 54 | -0.0192 | 0.8693 | -3.6565 | 27 |
| 55 | 0.0192 | -0.8693 | -3.6565 | 27 |

**Table 8**: Cartesian coordinates (Å) of the hydrogens atoms of the [6.6]chiralane.

# REFERENCES


ACD/Labs (1997) *Nomenclature of Organic Chemistry*, Sections A, B, C, D, E, F, and H. Oxford: Pergamon, http://www.acdlabs.com/iupac/nomenclature/

Autschbach J., Ziegler T., Patchkovskii S., van Gisbergen S.J.A., Baerends, E.J. (2002) Chiroptical properties from time-dependent density functional theory. II. Optical rotations of small to medium sized organic molecules. *J. Chem. Phys.*, 117[2], 581-592.

Bentley R. (2009) Chiral: A confusing etymology, *Chirality*, DOI 10.1002/chir.20699.

Berge C. (1973) *Graphs and Hypergraphs*, New-York: Elsevier.

ChemInnovation Software Inc. (2006) C*hemistry 4-D Draw*, Nomenclator version 8.0, http://www.cheminnovation.com/products/nomenclature.asp.

Crawford T.D., Tam M.C., Abrams M.L. (2007) The Current State of Ab Initio Calculations of Optical Rotation and Electronic Circular Dichroism Spectra, *J. Phys. Chem. A*, 111[48], 12057-12068.

Fowler P.W., Horspool D., Myrvold W. (2007) Vertex Spirals in Fullerenes and Their Implications for Nomenclature of Fullerene Derivatives, *Chemistry. A European Journal*, 13[8], 2208-2217.

Fowler P.W., Rassat A. (2006) A Classification Scheme for Chiral Tetrahedra, *Compt. Rend. Chimie*, 9[9], 1203-1208.

Hom T., Kiszenick W., Post B. (1975) Accurate Lattice Constants from Multiple Reflection Measurements II. Lattice Constants of Germanium, Silicon, and Diamond, *J. Appl. Cryst.*, 8[4], 457-458.

IUPAC (1979) *Nomenclature of Organic Chemistry*, Sections A, B, C, D, E, F, and H, Oxford: Pergamon.

Nakazaki M., Chikamatsu H., Taniguchi M. (1982) Horse Liver Alcohol Dehydrogenase (HLADH) Mediated Chemicoenzymatic Asymmetric Synthesis of (+)-Twistane from cis-Decalin-2,7-dione, *Chemistry Letters*, 11[11], 1761-1764.

Petitjean M. (1992) Applications of the Rdius-Diameter Diagram to the Classification of Topological and Geometrical Shapes of Chemical Compounds, *J. Chem. Inf. Comput. Sci.*, 32[4], 331-337.

Petitjean M. (1998) Interactive Maximal Common 3D Substructure Searching with the Combined SDM/RMS Algorithm, *Comp. Chem.* 22[6], 463-465.

Petitjean M. (1999) On the Root Mean Square Quantitative Chirality and Quantitative Symmetry Measures, *J. Math. Phys.*, 40[9], 4587-4595.

Petitjean M. (2002) Chiral mixtures, *J. Math. Phys.*, 43[8], 4147-4157.

Petitjean M. (2003) Chirality and Symmetry Measures: A Transdisciplinary Review, *Entropy*, 5[3], 271-312, http://www.mdpi.org/entropy/papers/e5030271.pdf

Petitjean M. (2007) A Definition of Symmetry, *Symmetry: Culture and Science*, 18, 2-3, 99-119. http://petitjeanmichel.free.fr/itoweb.paper.SCS.2007.petitjean.pdf

Rassat A., Fowler P. (2004) Is There a "Most Chiral Tetrahedron"? *Chemistry, A European Journal*, 10[24], 6575-6580.

Schwartz A. (2004) Affine vs. Metric Gravitation Parity Test, *Bull. Am. Phys. Soc.*, 49[2], 54, APS Meeting, Denver, Colorado, abstract D9.006, http://flux.aps.org/meetings/YR04/APR04/baps/abs/S690006.html

Thomson W. (1904) Baltimore Lectures on Molecular Dynamics and the Wave Theory of Light, Appendix H., sect. 22, footnote p. 619, London: Cambridge University Press Warehouse.

Wiberg K.W., Wang Y.-G., Wilson S.M., Vaccaro P.H., Cheeseman J.R. (2006) Sum-over-States Calculation of the Specific Rotations of Some Substituted Oxiranes, Chloropropionitrile, Ethane, and Norbornenone, *J. Phys. Chem. A*, 110[51], 13995-14002.