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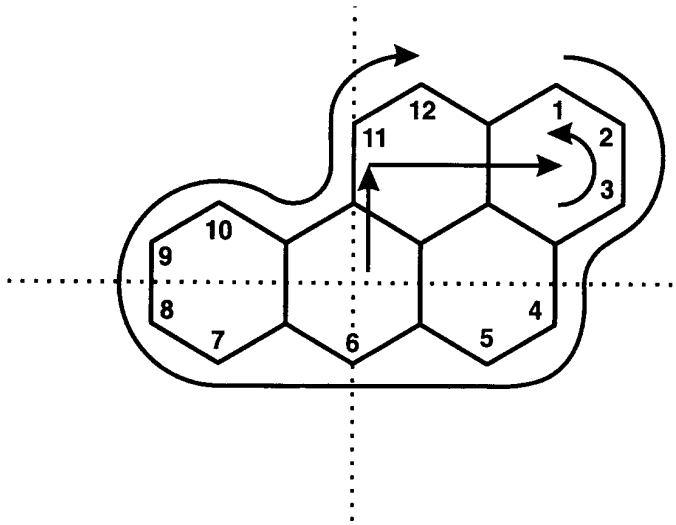
NIST Special Publication 922

Polycyclic Aromatic Hydrocarbon Structure Index

Lane C. Sander and Stephen A. Wise



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[1] At Boulder, CO 80303.
[2] Some elements at Boulder, CO.

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December 1997

U.S. Department of Commerce
William M. Daley, *Secretary*

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National Institute of Standards
and Technology
Special Publication 922
Natl. Inst. Stand. Technol.
Spec. Publ. 922
105 pages (Dec. 1997)
CODEN: NSPUE2

U.S. Government Printing Office
Washington: 1997

For sale by the Superintendent
of Documents
U.S. Government Printing Office
Washington, DC 20402

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This tabulation is presented as an aid in the identification of the chemical structures of polycyclic aromatic hydrocarbons (PAHs). The Structure Index consists of two parts: (1) a cross index of named PAHs listed in alphabetical order, and (2) chemical structures including ring numbering, name(s), Chemical Abstract Service (CAS) Registry numbers, chemical formulas, molecular weights, and length-to-breadth ratios (L/B) and shape descriptors of PAHs listed in order of increasing molecular weight. Where possible, synonyms (including those employing alternate and/or obsolete naming conventions) have been included. Synonyms used in the Structure Index were compiled from a variety of sources including "Polynuclear Aromatic Hydrocarbons Nomenclature Guide," by Loening, et al. [1], "Analytical Chemistry of Polycyclic Aromatic Compounds," by Lee et al. [2], "Calculated Molecular Properties of Polycyclic Aromatic Hydrocarbons," by Hites and Simonsick [3], "Handbook of Polycyclic Hydrocarbons," by J. R. Dias [4], "The Ring Index," by Patterson and Capell [5], "CAS 12th Collective Index," [6] and "Aldrich Structure Index" [7]. In this publication the IUPAC preferred name is shown in large or bold type.

The data supplied in this Structure Index comply with IUPAC rules for naming fused ring systems, detailed in "The Nomenclature of Organic Compounds" [8] and "A Guide to IUPAC Nomenclature of Organic Compounds" [9]. Names are based on the largest fragment with a trivial name. A list of recognized compounds specified by IUPAC convention is presented in Table 1. When a choice exists, the fragment lowest in the list (i.e., with the largest number) should be used. The simplest attachments are then selected for naming. Structures are typically oriented such that 1) the greatest number of rings in a row are aligned horizontally, 2) the maximum number of rings are positioned in the upper right quadrant, and 3) the least number of rings are positioned in the lower left quadrant. Numbering begins with the uppermost ring the furthest to the right, with the most counterclockwise carbon atom not involved with ring fusion. The numbering proceeds clockwise around the structure with hydrogenated carbon atoms. The numbering of Anthracene and Phenanthrene are "retained exceptions" to this rule. In this publication, double bonds are not explicitly indicated, but aliphatic carbons are designated by associated hydrogen atoms.

The L/B ratio is a shape-descriptive parameter that has been used in numerous studies of PAH retention in both liquid and gas chromatography [10-12]. This Structure Index represents the most comprehensive compilation of L/B values published. L/B values were calculated using algorithms based on the approach of Wise et al. [12]. A representation of this approach is illustrated in Figures 1 and 2. The molecular structure of each compound was generated using PC-Model and MMX molecular modeling programs (Serena Software, Bloomington, IN).[§] For planar PAHs, L/B can be

[§]Certain commercial equipment, instruments, or materials are identified in this report to specify adequately the experimental procedure. Such identification does not imply recommendation or endorsement by the National Institute of Standards and Technology, nor does it imply that the materials or equipment identified are necessarily the best available for the purpose.

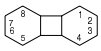
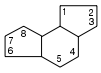
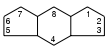
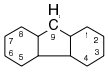
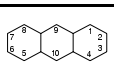
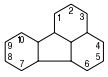
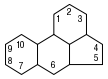
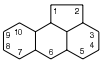
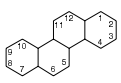
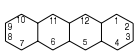
determined from a two dimensional representation of the molecule. The structure is rotated and various "trial" values for L/B are calculated until a maximum value for L/B is determined. Because different values for L/B will result for nonplanar molecules depending on the initial orientation, a procedure was developed to provide unambiguous orientation. The algorithm begins with an arbitrary molecular orientation. The molecule is sequentially rotated about x, y, and z axes and xy, yz, and xz projections are determined with each rotation. An orientation is set such that when a box is drawn about the molecule to enclose the van der Waals surface, the minimum dimension is aligned with the z axis and the maximum dimension, with the x axis. L/B is then calculated from the xy projection as if the molecule were planar. L/B values for planar PAHs determined using this algorithm are identical to L/B values generated using the more simplistic planar iterative program. The dimensions of the bounding box (Å) are listed in small type below the values for L/B (dimensions x, y, and z, respectively). A measure of solute thickness is provided by the "z" box dimension. For compounds that contain only aromatic carbons, values greater than ~3.9 Å are indicative of nonplanarity.

Isomers are listed in order of increasing L/B for groups of the same overall ring structure. Isomers containing five-membered rings are grouped separately from isomers containing only six-membered rings. When further distinction is possible, isomers are grouped based on the number of shared carbon atoms within the five-membered rings. For example, isomers of molecular weight (MW) 302 containing a five-membered ring with three shared carbon atoms are listed before isomers with five shared carbon atoms within the five-membered ring. MW 302 isomers containing only six-membered rings are grouped last.

The material presented is not intended to be all inclusive; however, an effort was made to include most common PAHs of environmental interest. Data was compiled from the sources provided in the reference list, and only compounds containing five- and six-membered rings are included. (Compounds were not arbitrarily drawn and named simply to enumerate all possible isomers.) Where possible, CAS numbers are supplied to facilitate literature searches. The absence of CAS numbers does not signify absence from the CAS Registry. Finally, a tabulation listing the theoretical number of possible *six-membered* ring configurations for various molecular weights is provided in Table 2. More detailed information on the synthesis and physical properties of many of these isomers is provided in reference [4]. The last column of this table lists the corresponding number of structures provided in this Index.

Considerable effort has been expended to make the Structure Index as accurate as possible. The authors welcome comments, corrections, and suggestions for improvements in the next revision.

Table 1. Parent Compounds (IUPAC Convention, listed in order of increasing priority) [9]

1	Pentalene	
2	Indene	
3	Naphthalene	
4	Azulene	
5	Heptalene	
6	Biiphenylene	
7	*as*-Indacene	
8	*s*-Indacene	
9	Acenaphthylene	
10	Fluorene	
11	Phenalene	
12	Phenanthrene	
13	Anthracene	
14	Fluoranthene	
15	Acephenanthrylene	
16	Aceanthrylene	
17	Triphenylene	
18	Pyrene	
19	Chrysene	
20	Naphthacene (Tetracene)	

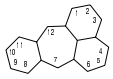
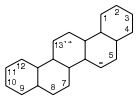
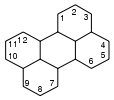
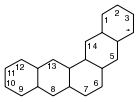
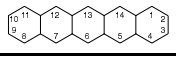
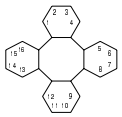
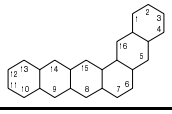
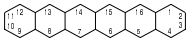
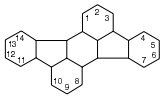
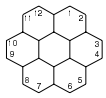
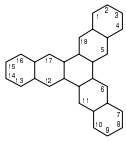
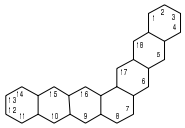
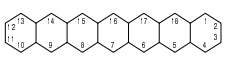
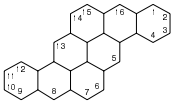
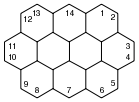
21	Pleiadene	
22	Picene	
23	Perylene	
24	Pentaphene	
25	Pentacene	
26	Tetraphenylene	
27	Hexaphene	
28	Hexacene	
29	Rubicene	
30	Coronene	
31	Trinaphthylene	
32	Heptaphene	
33	Heptacene	
34	Pyranthrene	
35	Ovalene	

Table 2. Possible Configurations for Six Membered Ring PAH Isomers[1]

MW	Chemical Formula	Number of Rings	Internal Carbons[2]	Isomers (theoretical)	Isomers (synthesized)	Isomers (listed)
78	C_6H_6	1	0	1	1	1
128	$C_{10}H_8$	2	0	1	1	1
178	$C_{14}H_{10}$	3	0	2	2	2
202	$C_{16}H_{10}$	4	2	1	1	1
228	$C_{18}H_{12}$	4	0	5	5	5
252	$C_{20}H_{12}$	5	2	3	3	3
276	$C_{22}H_{12}$	6	4	2	2	2
278	$C_{22}H_{14}$	5	0	12	12	12
300	$C_{24}H_{12}$	7	6	1	1	1
302	$C_{24}H_{14}$	6	2	13	13	13
326	$C_{26}H_{14}$	7	4	9	5	9
328	$C_{26}H_{16}$	6	0	37	27	37
350	$C_{28}H_{14}$	8	6	8	5	8
352	$C_{28}H_{16}$	7	2	62	24	45
374	$C_{30}H_{14}$	9	8	3	2	3
376	$C_{30}H_{16}$	8	4	58	11	50
378	$C_{30}H_{18}$	7	0	>123	23	93
398	$C_{32}H_{14}$	10	10	1	1	1
400	$C_{32}H_{16}$	9	6	46	7	40
402	$C_{32}H_{18}$	8	2	>289	16	8
424	$C_{34}H_{16}$	10	8	37	2	16
426	$C_{34}H_{18}$	9	4	very large	8	14
428	$C_{34}H_{20}$	8	0	>411	8	11
448	$C_{36}H_{16}$	11	10	20	2	20
450	$C_{36}H_{18}$	10	6	very large		9
452	$C_{36}H_{20}$	9	2	very large		13
478	$C_{38}H_{22}$	9	0	>1489	6	5

[1]Data adapted from Dias, “Handbook of Polycyclic Hydrocarbons” [4]
[2]Refers to carbon atoms not contained in the periphery of the ring structure

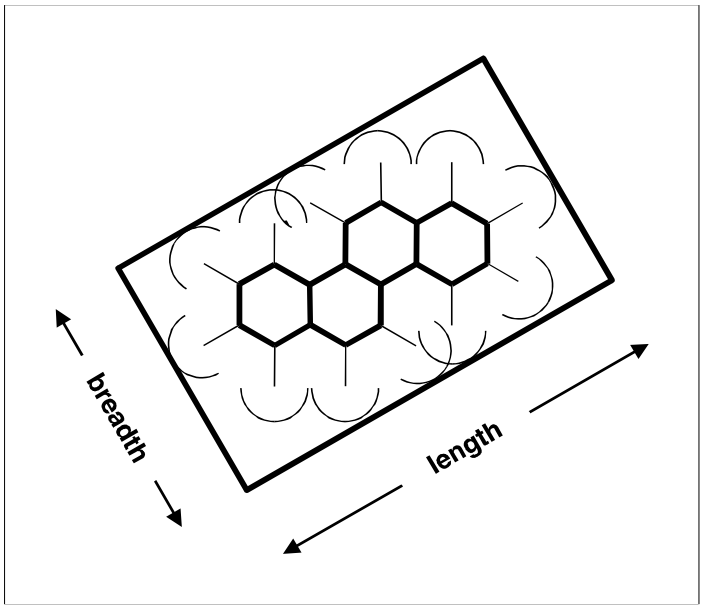


Figure 1. Depiction of Length-to-Breadth ratio for planar PAHs.

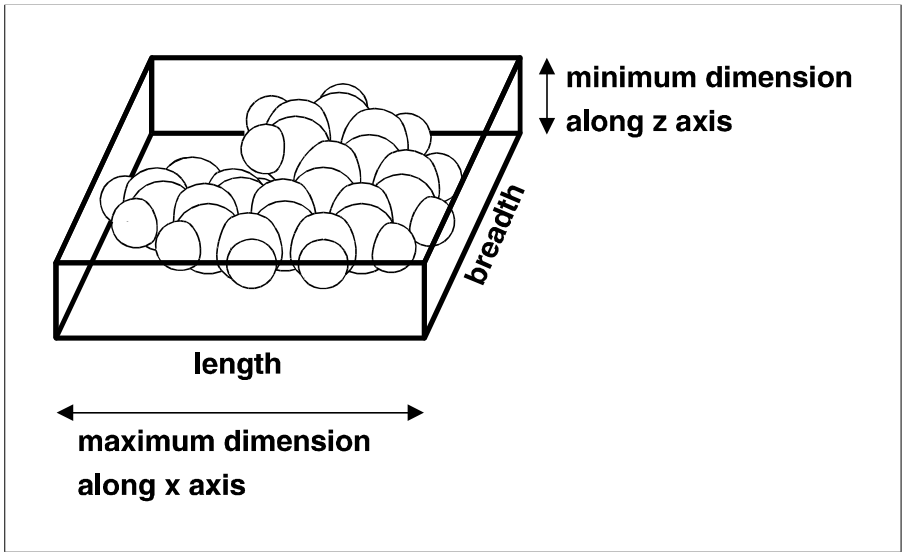


Figure 2. Depiction of Length-to-Breadth ratio algorithm for nonplanar molecules.

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