

A CRITICAL EXAMINATION OF VARIOUS NOMENCLATURE SYSTEMS OF
CONDENSED BENZENOID HYDROCARBONS AND THEIR COMPARISON
WITH THE COMPACT NAMING

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Abstract : In order to assign a name to any polycyclic benzenoid hydrocarbon on the basis of its dualist's structure , the recently developed compact naming (CN) procedure is used. An extension of this algorithm to the non-planar systems (helicenes) is presented. A critical examination of various nomenclature systems applied to code BHs shows a considerable advantage of the CN system over other approaches. The examination was preceded by a compilation of all the known BH structures and then testing the resulting datafile.

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INTRODUCTION

Benzenoid hydrocarbons (BHs) are the compounds of an ultimate importance for such diverse branches of chemistry as the dyes and drugs technology on the one side and the theory of electronic structure and chemical topology on the other. The topological treatment of BHs is well documented¹ and is found to enable a lot of problems to be elucidated and a lot of questions concerning these species to be answered.

An enormous amount of the chemical data creates a need for effective algorithms to name organic compounds in such a way that is easily recognizable by both the digital computers and the human mind. In particular, a great effort has been made toward elaboration a nomenclature of BHs²⁻¹³. Surprisingly enough, the standard nomenclature, worked out in early 20's by Stelzner and Kuh¹⁴, and then (after some modifications) accepted by the IUPAC conventions¹⁵, still remains resistant to be removed from a wide use. The reason of this fact is probably a complex character of the novel approaches to the nomenclature, which prohibits a common application of these naming systems. The problem is, that some of them are too algorithmic for a human use, whereas others retain common names of BHs, which are hardly recognizable by digital machines. Thus, we are still looking for a naming procedure producing the shortest possible codes of BHs that can be easily interrelated to the respective structural formulae.

This situation, which is apparently undesirable because of the well known drawbacks of the traditional naming systems

2,3,10,12 encourages us to devise a new algorithm solving this problem. Recently we have developed the compact nomenclature (CN) system^{10,12}, which seems to be free of all shortcomings inherent in the known approaches to name BHs. A computer program facilitating the use of CN has been also worked out¹¹. The CN has been found to be a very convenient method for studying and storage of various data for BHs, especially when used in connection with the nodal increments method^{16,17,18}.

In the present paper we report results of a practical testing of the effectiveness of CN in naming BHs. As the base of our test we have selected the benzenoid compounds quoted in various widely used literature reference sources (Chemical Abstracts¹⁹ and Beilstein's Handbuch der Organischen Chemie²⁰). The results demonstrate clearly the far superiority of the CN over other methods of BH's nomenclature.

THE CN ALGORITHM

The rules of compact nomenclature were published elsewhere^{10,11,12} and therefore here we limit the description of them to a necessary minimum. The principles of CN are based on the superimposing the dualist corresponding to the considered BH on a parallelogram grid. The presence of a vertex of the dualist is read as 1 and the absence as 0, which results in a rectangular matrix. The rows of the matrix are then treated as binary numbers that, after translation into decimal ones, provide the code of the BH. There are (in general) 12 possible

codes for one BH structure which is a result of 12 possible different positions of the molecule on the grid , and among them one is chosen according to particular selection rules. This final numerical code is then inserted between slashes and followed by a core word (which defines the number of benzene rings) and the suffix -acene. It should be pointed out that the core word and the suffix contain redundant information and are added only for the sake of convenience.

The original selection rules from ref.10 were further simplified slightly¹² and in the present paper we have used the latest ones. The published CN algorithm has no capability of treating non-planar BHs , however , an extension to these structures is possible and straightforward. The goal is to replace a single parallelogram by a stack of grids. Thus , the main portion of BH is placed on the first grid , the remaining part on the second. If the remaining part still contains overlapping rings , then the division process is repeated. The detailed algorithm is as follows :

1. Project the dualist onto a parallelogram net. If some of nodes are multiply occupied , transfer the overlapping vertices into subsequent planes until every net is only singly occupied.
2. Apply the standard CN algorithm to the structure lying on the first plane. The nodes placed on the remaining nets should follow the inversions and rotations applied to the first one. Assign the digital code to every plane.
3. For planar BHs the positions of the dualist's vertices

determine uniquely its edges. In the case of the non-planar compounds we must be supplied with additional information about the redundant intraplanar edges and the additional interplanar connections. For this purpose we enumerate the occupied nodes in the order from the left to the right and from the top to the bottom. The final code consists of the digits corresponding to every plane separated by parentheses containing the numbers describing the aforementioned connections. For example , the structure depicted in Fig.1 has the redundant connections between the vertices 1 and 4 as well as between 3 and 4. In addition , the vertices 1 (first plane) and 11 (second plane) are connected , and this also applies to the pair 3 (1st plane) - 12 (second plane). Thus the code reads:

```
/6.13.11.6(1.4;3.4:1.11:3.12)0.4.0.0()0.4.0.0/
```

The following rules should be observed :

- a) the redundant connections are entered first , then followed by a colon and the interplanar connections between the first neighbor plane. This can be continued with next colon and the connections with the second neighbor plane , and so on;
- b) the semicolons separate the connected pairs within the same connectivity level (e.g. the same types of planes);
- c) if there is neither redundant nor interplanar connections then we put 'empty' parentheses between codes corresponding to two subsequent nets;
- d) if , for the same position of the vertices on the first

plane , different arrangements for other planes are possible , then the one producing a code with the smallest numbers is preferred ;

e) the absence of a colon in the code means that the whole structure is confined to only one plane. For example , for hexahelicene we get : /6.5.3(1.2)/

4. Finally a common core word and the suffix -acene is added to the digital code.

An example showed on Fig.1 should explain practical aspects of the algorithm:

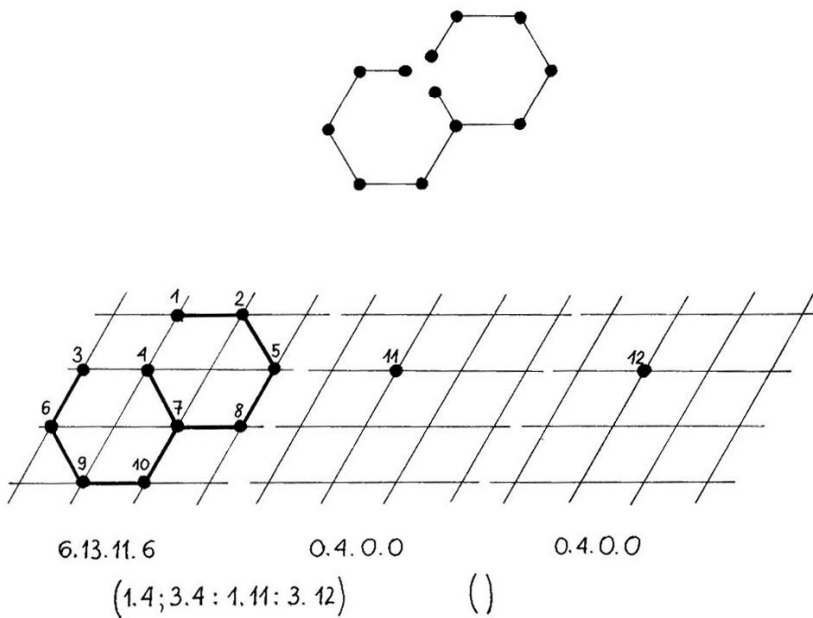


Fig.1

The aforementioned extension enables us to code any arbitrary benzenoid hydrocarbon. From the first glance it could seem that the codes would be extremely long and complicated, however it is found that for commonly encountered structures the complexity of the code is not too severe (see Conclusions for a further discussion).

CN VERSUS STANDARD NOMENCLATURE

The advantage of the CN system over the existing IUPAC¹⁵, Ring Index²¹ or Chemical Abstracts²² nomenclatures can be proven easily by examining the names of BHS quoted in these literature sources. This task should focus on two important factors. The first one, which is the average number of different names assigned to a particular hydrocarbon within one nomenclature system, shows the degree of ambiguity introduced by the use of a given naming algorithm. The second, the average number of letters and digits used to code the structure, should provide us with the information about simplicity (or complexity) of the names generated by considered nomenclature.

A detailed analysis of this kind has been performed for all entries corresponding to BHS in Chemical Abstracts Vols. 45 - 100 as well as in Beilstein Handbuch der Organischen Chemie (Vols. 3 and 4). Moreover, we have also analyzed this problem within Clar's monograph "Polycyclic Hydrocarbons" (Vols. 1 and 2)²³. The literature search resulted in the compilation of all the known BHS. The corresponding DATAFILE (Table 1) has been processed in order to obtain the information about

various names of the hydrocarbons and then to calculate 'the mean degeneracy' and 'the mean length' of the names. The results of this task are presented in Tables 2 , 4 and 5.

TABLE 1. THE /34.30.17/-OCTACENE ENTRY IN DATAFILE

/34.30.17/-octacene		C ₃₄ H ₂₀	CATA
CA/100	tetrabenzo[a,c,j,l]naphthacene		
E4/2935	tetrabenzo[a,c,j,l]naphthacen		
Cl/414	1.2,3.4,7.8,9.10-tetrabenzotetracene		

TABLE 2. AN ANALYSIS OF THE ENTRIES IN CA (VOLS. 45 - 100)^{a)}.

<u>The number of rings</u>	<u>The number of structures found</u>	<u><D></u>	<u><L></u>	<u>Lmin</u>	<u>Lmax</u>
1	1	1.00	7.0	7	7
2	1	1.00	11.0	11	11
3	3	1.33	11.2	9	14
4	7	1.00	13.1	6	20
5	22	1.23	17.6	6	26
6	80	1.17	21.6	8	34
7	90	1.11	24.8	8	38
8	69	1.10	28.4	5	52
9	51	1.10	31.6	8	61
10	45	1.04	35.0	7	63
11	32	1.06	38.7	10	70
12	15	1.00	39.5	10	75
13	14	1.00	48.5	11	78
14	6	1.00	47.3	13	75
15	7	1.00	52.9	13	105
16	2	1.00	44.0	12	76
19	2	1.00	102.5	102	103
37	1	1.00	199.0	199	199

- a) The total number of structures found is 448. Non-planar BHs (27 entries) are excluded. Description of symbols :
<D> - the average number of different names assigned to one structure ('the mean degeneracy' of the name)
<L> , Lmin and Lmax - the average , the minimal and the maximal number of figures and letters in the name ('the name length') , respectively.

It should be accentuated that all three literature sources suffer from a multiple naming of compounds. It is especially pronounced in Clar's book , but it arises from the use of some common names in the text. The situation is even worse in Chemical Abstracts , because different systematic names are assigned throughout different volumes (Table 3). This , of course , must produce several missings of data during scanning through CAs. The problem of 'name degeneracies' vanishes when CN is used because of the 1:1 name/structure correspondence inherent in this algorithm.

TABLE 3. AN EXAMPLE OF BH WITH A HIGH DEGENERACY OF NAMING IN CA.

/7.14.28/-nonacene		C ₃₄ H ₁₈	PERI
CA/100	benzo[<i>rst</i>]phenanthro[10,1,2- <i>cde</i>]pentaphene		
CA/97	dinaphtho[1,2,3- <i>cd</i> ;1',2',3'- <i>lm</i>]perylene		
CA/72	isoviolanthrene		
E4/2945	benzo[<i>rst</i>]phenanthro[10,1,2- <i>cde</i>]pentaphen		
	dinaphtho[1,2,3- <i>cd</i> :1',2',3'- <i>lm</i>]perylene		
C2/246	1.2,8.9-dibenzoperopyrene		
	isoviolanthrene		

Another point of our considerations should be devoted to 'the mean name length'. Again , we can see that CN is of superiority over any standard nomenclature. In almost all cases , the CN names are shorter than the traditional ones. The length of CA names appears to rise by about 3 letters (digits) per one ring added (Table 2) , when the corresponding increase in CN names is only about 1 letter (digit) (Table 6).

TABLE 4. AN ANALYSIS OF THE ENTRIES IN BEILSTEIN'S HANDBUCH (VOLS. 3 AND 4)^{a)}.

<u>The number of rings</u>	<u>The number of structures found</u>	<u><D></u>	<u><L></u>	<u>Lmin</u>	<u>Lmax</u>
1	1	1.00	6.0	6	6
2	1	1.00	10.0	10	10
3	3	1.00	9.3	8	11
4	7	1.43	11.6	5	19
5	20	1.30	16.3	5	25
6	32	1.09	19.6	7	33
7	32	1.16	21.9	7	36
8	19	1.32	26.3	8	40
9	15	1.33	28.9	13	49
10	9	1.22	40.3	6	59
11	5	1.40	41.7	11	62
12	2	1.00	34.0	33	35
13	2	1.50	29.0	15	35

a) The total number of structures found is 148. Non-planar BHs (1 entry) are excluded. The meaning of symbols as in Table 2.

TABLE 5. AN ANALYSIS OF THE ENTRIES IN CLAR'S MONOGRAPH (VOLS. 1 AND 2)^{a)}.

<u>The number of rings</u>	<u>The number of structures found</u>	<u><D></u>	<u><L></u>	<u>Lmin</u>	<u>Lmax</u>
1	1	1.00	7.0	7	7
2	1	1.00	11.0	11	11
3	3	1.00	11.7	10	13
4	7	2.43	15.1	6	26
5	22	1.82	22.2	6	33
6	36	1.17	23.3	8	42
7	43	1.12	26.4	8	44
8	29	1.17	28.0	8	41
9	25	1.20	29.1	8	51
10	17	1.00	33.5	7	48
11	15	1.00	38.9	10	46
12	2	1.00	39.0	38	40
13	3	1.00	30.0	16	44

a) The total number of structures found is 214. Non-planar BHs (1 entry) are excluded. The meaning of symbols as in Table 2.

TABLE 6. AN ANALYSIS OF THE CN CODING OF THE BHs APPEARING IN CHEMICAL LITERATURE a).

<u>The number of rings</u>	<u>The number of structures found</u>	<u>Full name</u>			<u>Digital code</u>		
		<u><L></u>	<u>Lmin</u>	<u>Lmax</u>	<u><L></u>	<u>Lmin</u>	<u>Lmax</u>
1	1	13.0	13	13	1.0	1	1
2	1	11.0	11	11	1.0	1	1
3	3	13.3	12	14	2.3	1	3
4	7	15.1	14	17	3.1	2	5
5	22	16.3	14	18	4.3	2	6
6	80	16.4	13	19	5.4	2	8
7	91	18.4	15	22	6.4	3	10
8	70	17.7	14	21	6.8	3	10
9	52	19.0	14	23	8.0	3	12
10	48	19.6	15	26	8.6	4	15
11	34	22.7	17	28	9.7	4	15
12	15	23.6	17	30	10.6	4	17
13	14	26.0	18	37	12.0	4	23
14	6	28.2	21	35	12.2	5	19
15	7	28.6	21	43	12.6	5	27
16	2	25.0	20	30	10.0	5	15
19	2	26.5	25	28	11.5	10	13
37	1	45.0	45	45	24.0	24	24

a) The total number of entries is 456. The planar BHs taken from Chemical Abstracts , Beilstein's Handbuch and Clar's monograph. The meaning of symbols as in Table 2. A digital code is the first part of the CN name (without slashes). For example , the digital code corresponding to the name /7.14.28/-nonacene is 7.14.28 .

A closer inspection of the DATAFILE reveals the fact that , especially for large BH structures , the application of CN retrenches significantly the effort needed to visualize the structural formula while name of compound is provided. Usually , when the standard names involve a complicated combination of commas , semicolons , colons as well as sub- and superscripted letters and digits , CN produces simple and short codes which are easily liable to automatic self-correcting procedures. The name/structure relationships are clear and straightforward and , moreover , similar structures tend to have similar

codes , which is (unfortunately) not common in the IUPAC naming.

On balance , it seems to be no reasons to prefer the usage of the standards , while novel approach offers an improvement in every aspect.

CN VERSUS OTHER TOPOLOGICALLY BASED NOMENCLATURE SYSTEMS

Introduction of the graph theory into organic chemistry enables us to develop diverse nomenclature systems for BHS which are free from the ambiguities inherent in standard naming approaches. At the present moment the following systems based on topological concepts have been reported in the literature :

- a) 2D and 3D codes worked out by Balaban^{3,4} and by Gutman as so called LA sequence⁵;
- b) graph-center based approach by Bonchev and Balaban⁸ (B/B) ;
- c) the boundary code method by Trinajstić et al.^{6,7} (DZG) ;
- d) the compact name system by Cioslowski and Turek^{10,11,12} (CN) ;
- e) the method of Elk⁹ ;
- f) the method of Wenchen and Wenjle¹³ .

Among these methods the 2DC and 3DC descriptions are only suitable for cata-condensed BHS , whereas the method of Elk uses some common names , thus not being based purely on chemical topology. The very recently published approach of Wenchen and Wenjle seems to offer no advantage over the CN system , although utilizing similar concepts. Therefore we

will confine our comparison of the convenience in use and efficiency in naming to the approaches b), c) and d).

The application of chemical topology in nomenclature systems removes the difficulties connected with name ambiguities, however there are still some points in which these methods differ. Especially, two points are worthwhile to discuss. One of them (purely practical) is their simplicity considered from the point of view of potential users (mainly organic chemists). Another one is the amount of a redundant information comprised in the code. Expecting this redundancy to be minimal, we should try to optimize the length of the name.

Taking into account this matter we can see easily that CN again competes favorably with DZG and B/B methods. As far as the redundancy is considered, one can compare the corresponding figures in Table 7.

TABLE 7. AN AVERAGE CODE LENGTH OF DIFFERENT TOPOLOGICALLY BASED NAMING SYSTEMS OF BHs

<u>The number of rings</u>	<u>The number of structures^{a)}</u>	<u>BZG</u>	<u>B/B</u>	<u>CN</u>
1	1	6.0	1.0	1.0
2	1	10.0	1.0	1.0
3	3	13.3	3.0	2.3
4	7	17.1	5.0	3.1
5	22	20.6	7.0	4.3
6	81	24.1	9.2	5.3

a) All planar polyhexes with a given number of rings were generated.

In this case , the DZG coding is the worst one , while B/B and CN codes have comparable lengths for small systems. However , situation is changed when one goes to larger BHs. For these molecules , the CN method is by no discussion the best one , that assures us of its real 'compact' character.

Some practical aspects of application of the aforementioned methods are presented in Table 8. We comment briefly some weak points of every approach. The DZG suffers from limitation to only non-circulene structures. This serious shortcoming is not present in the B/B approach , however practice shows that localization of the graph focal point becomes very tedious procedure even for medium-sized hydrocarbons. Also , in case of complex molecules , the B/B nomenclature rules become very complicated (cf. original paper⁸). The CN method seems not to be afflicted by these drawbacks , albeit for non-planar structures it becomes more difficult to use. Finally , it should be also pointed out that the similarity among BH's structures is often concealed in DZG and B/B codes but not in CN ones.

CONCLUSIONS

A detailed comparison of the CN approach with other traditional as well as topological naming algorithms allows us to draw a conclusion that the CN method is in fact the best one , offering the simplest and shortest codes with minimal effort in coding procedure.

TABLE 8. SOME PRACTICAL ASPECTS OF THE APPLICATION OF DIFFERENT NOMENCLATURE SYSTEMS TO CODE BHs

<u>Naming System</u>	<u>DZG</u>	<u>B/B</u>	<u>CN</u>

Capability to name			
helicenes:	yes	yes	yes
circulenes:	no	yes	yes

Stages of the coding: (degree of complexity ^{a)})	1.Construction of the trial boundary code (1)	1.Construction of the dualist (0)	1.Construction of the dualist (0)
	2.Permutation of the code (1)	2.Looking for the focal point of a graph (3)	2.Transformation of the dualist into the matrix (0)
	3.Rotations and inversions of the code (2)	3.Assignment of the code (1)	3.Translation of the matrix into the code (1)
		4.Rotations and inversions of the molecule(1)	4.Rotations and inversions of the molecule(1)

Translation of name into structural formula	easy	easy	easy

Translation of structural formula into name	easy	difficult	easy

a) 0 - easily performed by a slightly experienced person			
1 - as above , but the use of a computer can result in some saving in the time of operation			
2 - computer assistance strongly recommended			
3 - very difficult to perform without access to a computer			

The extension of the CN algorithm to non-planar BHs is found to work quite nicely as far as the problem of lengthy standard names is concerned. In most cases the CN names are shorter and not much more complicated than the ones of planar

compounds. The great advantage is that now all BHs can be coded within one system , which excludes any possibility of ambiguities. The comparison of the IUPAC with the CN names is given for all non-planar BHs found in Chemical Abstracts (Table 9).

Benzenoid hydrocarbons establish a relatively small (about 500 compounds) class of organic molecules. One should remember, however , that CN , providing enumeration of carbon atoms of a particular BH , enables us also to name all the heterocyclic species consisting of six-membered rings. The number of these compounds which , as we can easily realize , is rather huge , seems to make it worthwhile to replace the old standard systems with the CN. This should result in a dramatic reduction of human effort as well as a great improvement in the storage of chemical data.

Table 9. THE IUPAC AND THE CN NAMES OF THE NON-PLANAR BENZENOID HYDROCARBONS QUOTED IN CA

1. /6.5.3(1.2)/-HEXACENE
phenanthro[3,4-c]phenanthrene
2. /6.5.3(1.2:1.7)2.0.0/-HEPTACENE
dinaphtho[2,1-c;1'.2'-g]phenanthrene
3. /6.5.7(3.5;3.6)/-HEPTACENE
benzo[5,6]phenanthro[4,3-a]anthracene
4. /6.13.3(1.2)/-HEPTACENE
benzo[g]naphtho[2,1-c]chrysene
5. /6.13.3(1.4)/-HEPTACENE
phenanthro[3,4-c]chrysene
6. /6.13.3(2.5)/-HEPTACENE
benzo[c]naphtho[1,2-g]chrysene
7. /6.5.3(1.2:1.7)2.1.0/-OCTACENE
naphtho[2,1-c]phenanthro[4,3-g]phenanthrene
8. /6.13.3(2.5:2.8)0.1.0/-OCTACENE
benzo[c]phenanthro[4,3-g]chrysene

9. /6.13.7(1.4)/-OCTACENE
benzo[mno]phenanthro[3,4-c]chrysene
10. /6.13.11(1.4)/-OCTACENE
benzo[c]phenanthro[3,4-l]chrysene
11. /2.6.13.3(2.3:3.9)0.4.0.0/-NONACENE
benzo[g]triphenyleno[2,1-c]chrysene
12. /2.6.13.3(6.8:6.9)0.0.0.1/-NONACENE
benzo[2,1-g;3,4-g']dichrysene
13. /6.5.3(1.2:1.7)2.1.1/-NONACENE
diphenanthro[3,4-c;4',3'-g]phenanthrene
14. /6.5.3(1.2:2.7)4.4.4/-NONACENE
phenanthro[4',3';5,6]phenanthro[4,3-a]anthracene
15. /14.9.7(1.2:1.9)4.0.0/-NONACENE
diphenanthro[4,3-a;3',4'-j]anthracene
16. /3.26.22.12(7.10)/-DECACENE
diphenanthro[3,2-c;3',4'-l]chrysene
17. /4.12.26.6.1(2.3:3.10)0.8.0.0.0/-DECACENE
benzo[f]triphenyleno[1,2-j]picene
18. /6.5.3(1.2:1.7)2.1.3/-DECACENE
benzo[g]phenanthro[3,4-c;6,5-c']diphenanthrene
19. /6.13.11.6(1.4;7.10)/-DECACENE
diphenanthro[3,4-c;3',4'-l]chrysene
20. /6.5.3(1.2:1.7)2.5.3/-UNDECACENE
bisbenzo[5,6]phenanthro[3,4-c;4',3'-g]phenanthrene
21. /6.13.11.6(1.4;4.7:1.11)0.4.0.0/-UNDREACENE
dinaphtho[1,2-g;1',2'-g']benzo[2,1-c;3,4-c']diphenanthrene
22. /6.5.3(1.2:1.8)6.5.3(7.8)/-DODECACENE
dinaphtho[1,2-g;1',2'-g']naphtho[2,1-c;7,8-c']
~diphenanthrene
23. /6.13.11.6(1.4;4.7:1.11)0.4.2.0/-DODECACENE
dinaphtho[1,2-g;1',2'-g']naphtho[1,2-c;6,5-c']
~diphenanthrene
24. /6.13.11.6(1.4;3.4:1.11:3.12)0.4.0.0()0.4.0.0/-DODECACENE
dinaphtho[1,2-g;1',2'-g']naphtho[2,1-c;3,4-c']
~diphenanthrene
25. /54.45.27(2.6;3.7)/-DODECACENE
naphtho[1',2';5,6]phenanthro[4,3-c]phenanthro[3,4-l]
~chrysene
26. /6.5.3(1.2:1.8)6.5.3(7.8:7.13)2.0.0/-TRIDECACENE
bisnaphtho[1',2';5,6]phenanthro[3,4-c;4',3'-g]phenanthrene
27. /6.5.3(1.2:1.8)6.5.3(7.8:7.13)2.1.0/-TETRADECACENE
diphenanthro[4,3-g,4',3'-g']naphtho[2,1-c;7.8-c']
~diphenanthrene

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