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NOMENCLATURE OF CYCLOPHANES

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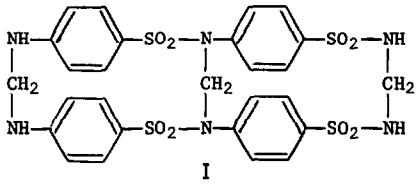
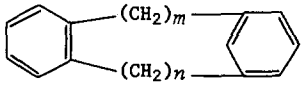
During the initial stage of the progress in studies on a new type of compounds, application of the existing nomenclature rules becomes difficult and the names of compounds often become confused. This is true in the case of cyclophanes, and their naming by the present IUPAC rules on organic nomenclature is rather complicated or difficult. The new nomenclature systems[1] are limited in its application, or, it is more of a nature of a chemical notation.

For example, the name of the rather simple compound (I) would be a long and tedious 2,8,12,18-tetrathia-3,9,11,17,23,25-hexaazahexacyclo[24.2.2.2^{4,7}.2^{13,16}.2^{19,22}.1^{3,17}]heptatriaconta-4,6,13,15,19,21,26,28(1),29,31,33,35-dodecaene 2,2,8,8,12,12,18,18-octaoxide, according to the nomenclature of *Chemical Abstracts* using the IUPAC rules[2], having to name the aromatic unsaturated bonds as aliphatic double bonds.

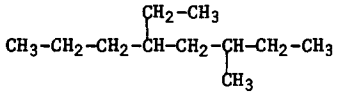


I



IIa: $m = 6$, $n = 4$

IIb: $m = 6$, $n = 6$



III

There is yet another nomenclature system in which the compound (IIa: $m = 6$, $n = 4$) would be [6.4]orthometacyclophane and (IIb: $m = 6$, $n = 6$) would be [6.6]orthometacyclophane, giving the same word, orthometacyclophane, irrespective of the number of m and n. If the compound (III) were named by such a method, it will be named 3-[1]alkyl-5[2]alkyl[8]alkane. Such an expression is not a nomenclature but should be termed a notation.

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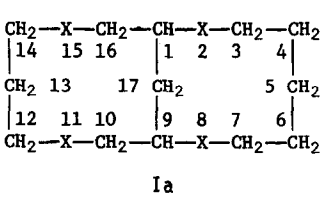
1) B.H.Smith, Bridged Aromatic Compounds, Academic Press Inc., New York (1964); F.Vögtle and P.Neumann, *Tetrahedron Letters*, No.60, 5329 (1969); *Tetrahedron*, **26**, 5847 (1970)

2) IUPAC, Nomenclature of Organic Chemistry, Butterworths Scientific Publication, London, 1971

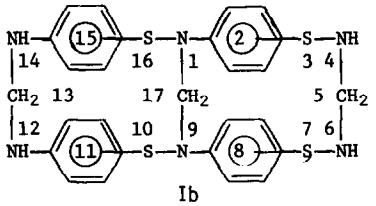
The nomenclature system proposed here uses the existing replacement nomenclature of IUPAC rules for organic chemistry with addition of a few rules. This nomenclature would be applicable to a wide variety of compounds, including the complicated cyclophanes. According to this nomenclature system, the compound (I) would be 2,8,11,15-tetra-*p*-benza-3,7,10,16-tetrathia 1,4,6,9,12,14-hexaazabicyclo[7.7.1]heptadecaphane 3,3,7,7,10,10,16,16-octaoxide, a very simple and concise name, and the structural formula would be easily reproduced from this name once the nomenclature rules are understood.

In this nomenclature, the aromatic ring system in the macroring is expressed by benza, indena, naphtha, pyrrola, thiena, *etc.*, which have "a" ending instead of "o" ending of the prefixes that represent the attached components in the nomenclature of fusion names of polycyclic system (IUPAC Rules 2-21.4, B-3.1, and B-3.3).

The hydrocarbon obtained by replacement of the aromatic ring systems and hetero atoms in the macroring of compound I with carbon atom group CH_2 (or CH, C) is bicyclo[7.7.1]heptadecane. The name of an imaginary compound Ia, bicyclo[7.7.1]heptadecaphane, formed by changing the ending "-ne" in the name of a hydrocarbon into "-phane", would be taken as the parent compound, to which the replacement nomenclature would be applied. Consequently, Ib would be 2,8,11,15-tetrabenza-3,7,10,16-tetrathia-1,4,6,9,12,14-hexaazabicyclo[7.7.1]heptadecaphane. The bonding position of the aromatic ring systems to the macroring would be indicated by the number of the substituted position of that ring in square brackets after the number of that ring in the macroring. Thus I would be 2-[1,4],8-[1,4],11-[1,4],15-[1,4]tetrabenza-3,7,10,16-tetrathia-1,4,6,9,12,15-hexaazabicyclo[7.7.1]heptadecaphane 3,3,7,7,10,10,16,16-octaoxide, but, since all the aromatic rings in I are bonded in *para*-positions, this can be abbreviated simply to 2,8,11,14-tetra-*p*-benza- and the compound is named as given above.

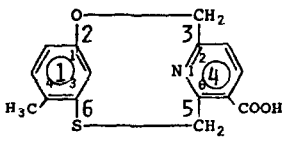


Ia

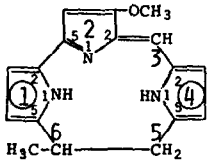


Ib

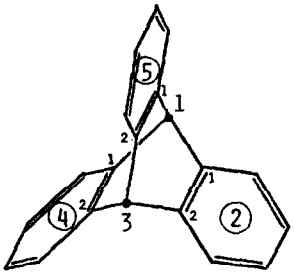
Similarly, IIa would be 1-*o*,6-*m*-dibenzacyclododecaphane and IIb, 1-*o*,8-*m*-dibenzacyclotetradecaphane. Some examples of cyclophanes of other types are shown below.



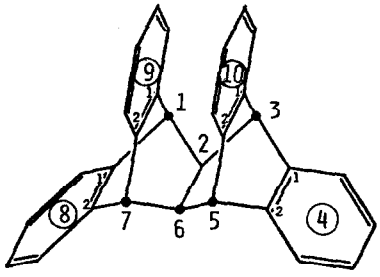
1^4-methyl-1-[1,3]benza-4-[2,6]pyrida-2-oxa-6-thiacyclohexaphane-4^5-carboxylic acid



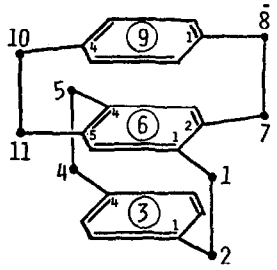
2^3-methoxy-6-methyl-1,4-di[2,5]pyrrola-2-[5,2]-2*H*-pyrrola-2-cyclohexaphene



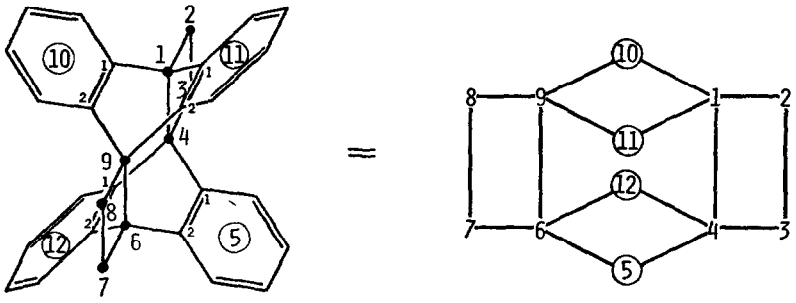
2,4,5-tri-*o*-benzabicyclo-[1.1.1]pentaphane
Trivial name: triptycene



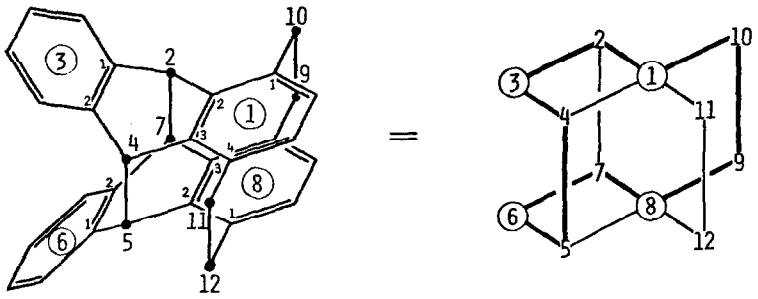
4,8,9,10-tetra-*o*-benzatetracyclo-[5.1.1.1^{3,5}.0^{2,6}]decaphane
Trivial name: janusene



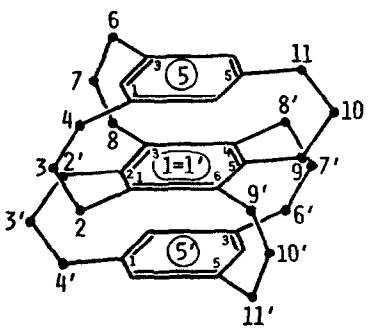
3-[1,4],6-[1,4,2,5],9-[1,4]-tribenzaspiro[5.5]undecaphane

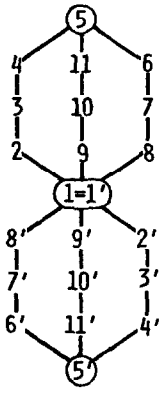


5,10,11,12-tetra-*o*-benzapentacyclo-[7.1.1.1^{4,6}.0^{1,4}.0^{6,9}]dodecaphane

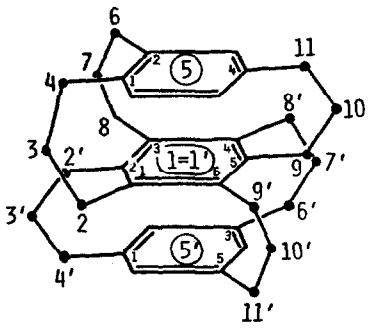


1-[2,3,1,4],3-[1,2],6-[1,2],8-[2,3,4,1]tetrabenza-pentacyclo[6.2.2.0^{1,4}.0^{2,7}.0^{5,8}]dodecaphane



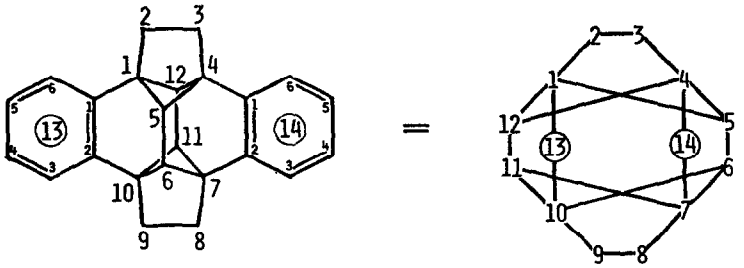


1-[1,2,3,4,5,6],5-[1,3,5],5'-[1,3,5]-tribenza-1,1'-spiro(bicyclo[3.3.3]-undecaphane)

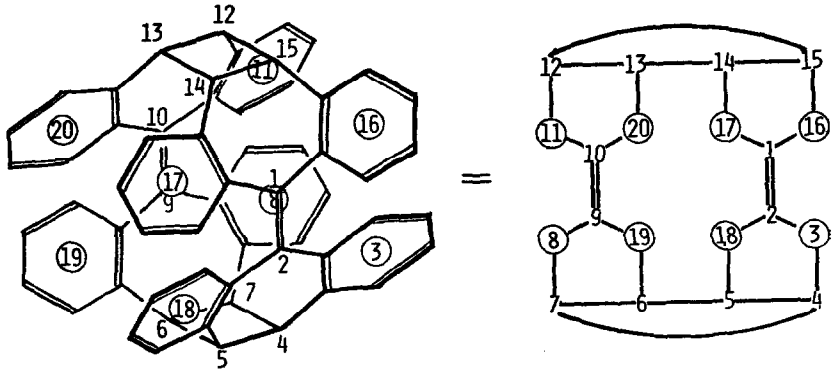


1-[1,2,3,4,5,6],5-[1,2,4],5'-[1,3,5]-tribenza-1,1'-spiro(bicyclo[3.3.3]-undecaphane)

This nomenclature system can conveniently be applied to the cage compound with fused aromatic rings as shown below.



13,14-di-*o*-benzaheptacyclo[8.2.1.1^{4,7}.0^{1,5}.0^{4,12}.0^{6,10}.0^{7,11}]tetradecaphane
Trivial name: dibenzoequinene



3,8,11,16,17,18,19,20-octa-*o*-benzaheptacyclo-[12.2.1.1^{2,5}.1^{6,9}.1^{10,13}.0^{4,7}.0^{12,15}]-eicosapha-1,9-diene