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JOINT COMMISSION ON BIOCHEMICAL NOMENCLATURE*

NOMENCLATURE OF TETRAPYRROLES

(Recommendations 1986)

(Supersedes provisional version published 1979)

Revision prepared for publication by
G. P. MOSS

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Nomenclature of tetrapyrroles (Recommendations 1986)

Synopsis - In the revised recommendations two new trivial names (isobacteriochlorin and sirohydrochlorin) are defined. Isobacteriochlorin is 2,3,7,8-tetrahydroporphyrin and is isomeric with bacteriochlorin. An example of an isobacteriochlorin is sirohydrochlorin, an intermediate in the biosynthesis of corrinoids. The names of linear tetrapyrroles are amended. The name bilin is now restricted to the fully oxidized parent, and less oxidized forms are named bilane, bilene, and biladiene. Names are now provided for the analogous dipyrrole system based on the parent dipyrrin. Tables are provided to show the structures of the more commonly encountered compounds using the Fischer system for denoting isomers (the fifteen isomers of mesoporphyrin defined by Fischer, and some isomers of biliverdin). Experience has shown that these names continue to be useful because of their brevity.

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PREFACE

In 1968 the IUPAC Commission on the Nomenclature of Organic Chemistry (CNOC) and the IUPAC-IUB Commission on Biochemical Nomenclature (CBN) set up a Joint Subcommission to examine, and to make recommendations on, the nomenclature of tetrapyrroles (excluding hemoproteins). This group consisted of Professor S. Aronoff, Professor R. Bonnett, Dr. L. C. Cross, Dr. K. L. Loening and Professor C. Rimington, with Professor M. R. Lemberg as Convenor. The convenorship passed to Professor R. Bonnett in 1971, and two new members, Professors A. Eschenmoser and H. H. Inhoffen, joined the group.

The IUPAC-IUB Commission on Biochemical Nomenclature was replaced by the IUPAC-IUB Joint Commission on Biochemical Nomenclature (JCBN) while the provisional recommendations were being prepared. During this process the Subcommission received and considered the views of many chemists and biochemists. Informal discussion sessions were held at a meeting on porphyrin chemistry in New York in 1972 [1] and at a meeting on bile pigment biochemistry at Hemsedal, Norway [2]. We appreciate the cooperation of the organisers of these meetings in making arrangements for these sessions.

The provisional recommendations on the nomenclature of tetrapyrroles were published in 1979.[a] They have since been widely adopted and the present revision is based on comments received on the provisional document. In the revised recommendations two new trivial names (isobacteriochlorin and sirohydrochlorin) are defined, the names of linear tetrapyrroles are amended, and the system is extended to dipyrrole systems. Tables are provided to show the structures of the more commonly encountered compounds using the Fischer system for denoting isomers (the fifteen isomers of mesoporphyrin defined by Fischer, and some isomers of biliverdin). Experience has shown that these names continue to be useful because of their brevity. The revision was formulated by Professor R. Bonnett in consultation with Professor S. Aronoff, Professor A. R. Battersby, Professor A. Eschenmoser, Professor H. Falk, Professor A. Gossauer, Professor H. H. Inhoffen, Professor A. H. Jackson, Professor D. A. Lightner, Professor S. Onishi, Dr J. M. Ribo, Professor C. Rimington, Dr M. S. Stoll and a subcommittee of the IUPAC-IUB Joint Commission on Biochemical Nomenclature composed of Professor P. Karlson, Dr K. L. Loening and Dr G. P. Moss.

INTRODUCTION

"Tetrapyrrole" is a term used widely, but loosely, to refer to a member of a class of compounds whose molecules have four rings of the pyrrole type, generally linked together by single-atom bridges between the alpha[b] positions of the five-membered pyrrole rings. The common arrangements of the four rings for which this name is used are macrocyclic (as in the porphyrins) and linear (as in the bile pigments).

Tetrapyrroles and their relatives are of importance in several disciplines. The international nomenclature commissions have not previously put forward specific recommendations for this field. The nomenclature most generally used has been that of Fischer [3,4] which is based on a very large number of trivial names which continue to appear (e.g. pemptoporphyrin [5], harderoporphyrin [6]) and a numeration scheme, shown in Fig. 1 for the unsubstituted porphyrin ring system, which is simple but incomplete.[c] The availability of a more systematic nomenclature would be expected to help interdisciplinary communication, and would considerably diminish the need for new trivial names.

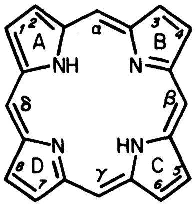

Fig. 1. Fischer numeration.

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[a] IUPAC-IUB Joint Commission on Biochemical Nomenclature, "Nomenclature of Tetrapyrroles, recommendations 1978", *Pure Appl. Chem.* 51, 2251-2304 (1979); *Eur. J. Biochem.* 108, 1-30 (1980).

[b] The alpha positions of the pyrrole ring are those adjacent to the nitrogen atom. This use of "alpha" should not be confused with its stereochemical meaning.

[c] See also Table 1.

These recommendations provide for naming porphyrins, hydroporphyrins, ring contracted or expanded porphyrins, porphyrins fused with other rings, skeletally replaced porphyrins and porphyrin-metal coordination complexes together with corresponding linear arrangements of three and four pyrrole rings. The application of these recommendations permits these substances to be named more systematically using fewer trivial names than are now currently used in the literature. Fundamental porphyrin and bilin nuclei form the basis of a systematic tetrapyrrole nomenclature in accord with the recommendations of the provisional rules for natural products.[a]

In parallel, a semisystematic tetrapyrrole nomenclature is developed based on a few trivial names[b], selected mainly from the Fischer system, that are so well established that is is desirable to retain them. The general rules for substitutive nomenclature, including operations of replacement, substitution and subtraction, are applied as appropriate. The application of these recommendations makes the use of a large number of trivial names no longer necessary. **Trivial names are not recommended[c] except for the select few retained as the basis of the systematic and semisystematic tetrapyrrole nomenclature systems.**

In addition, the incomplete Fischer numeration is abandoned for the porphyrin nucleus and the corresponding skeleton of the bile pigments. The 1-24 numbering scheme, already proven over an eighteen-year period with the closely related nucleus of the corrinoids[d], is adopted as shown in TP-1.1 Fig. 2. A comparison of the 1-24 numbering scheme with the Fischer numeration for the unsubstituted porphyrin nucleus is given in Table 1.

Table 1. Comparison of the 1-24 numbering scheme with the Fischer numeration for the unsubstituted porphyrin nucleus.

Recommended:	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24
Fischer:	-	1	2	-	α	-	3	4	-	β	-	5	6	-	γ	-	7	8	-	δ	-	-	-	-

Even though the 1-24 numbering scheme is used for the porphyrin and bilin nuclei, the numbering of the point of attachment of substituents on the nucleus may be different for systematic tetrapyrrole nomenclature than for semisystematic tetrapyrrole nomenclature. In systematic tetrapyrrole nomenclature the beginning and direction of numbering is determined by the rules for systematic substitutive nomenclature. Lowest locants are assigned according to the criteria of principal group named as suffix, substituents first cited, etc.[e] In contrast, in semisystematic tetrapyrrole nomenclature, the beginning and direction of numbering are the same as those established by Fischer for the trivially named porphyrins.[f] A comparison of the systematic and trivial numeration based on the 1-24 numbering scheme is presented in Appendix 2 for substituted porphyrins for which trivial names have been retained.

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a. **IUPAC, "Nomenclature of Organic Chemistry, Sections A, B, C, D, E, F and H, 1979 edition." Pergamon, 1979, Section F.**

b. See Appendix 1.

c. **Some of the Fischer trivial names (see Appendix 3) are likely to persist, for example, in the discussion section of a paper. This is regarded as permissible provided that the systematic or semisystematic name appears by way of definition at least once in each paper.**

d. IUPAC-IUB Commission on Biochemical Nomenclature, "Nomenclature of Corrinoids, Rules Approved 1975." *Pure Appl. Chem.* 48, 495-502 (1976) which supersedes IUPAC Commission on the Nomenclature of Biological Chemistry, "Definitive Rules for the Nomenclature of Vitamins." *J. Am. Chem. Soc.* 82, 5582 (1960), Rule V-15.

e. **IUPAC, "Nomenclature of Organic Chemistry, Sections A, B, C, D, E, F and H, 1979 edition." Pergamon, 1979, Rule C-15.1. See also TP-1.7.**

f. See Appendix 1.

RULE TETRAPYRROLES 0. GENERAL CONSIDERATIONS

TP-0.1. The established international rules for naming organic compounds and natural products[a] apply to tetrapyrroles, except where otherwise stated.

TP-0.2. Most of the structures considered here are based on delocalized π-electron systems: the double-bond distribution is represented in a formal way.

TP-0.3. Unless implied by a trivial name, the absolute configuration of a tetrahedral chiral center is designated by an *R* or *S* symbol assigned by the sequence-rule procedure. Similarly, the stereochemistry about a double bond is denoted by the prefixes *E* or *Z*. The symbols are assigned in accord with procedures given in the international recommendations for stereochemistry and are normally cited with their corresponding locants, when necessary, in front of the whole name.[b] Inversion of configuration or change in the configuration of a double bond from that implied by a name is expressed in front of the name in accord with IUPAC Rule F-6.3.

TP-0.4. The use of the diphthong (ae) or the single letter (e) in such words as haem, aetioporphyrin etc., is left to editorial discretion. (This vowel becomes (ä) in German). Here the single letter (e) is used throughout, heme additionally taking a terminal (e).

RULE TETRAPYRROLES 1. FUNDAMENTAL PORPHYRIN SYSTEMS

TP-1.1. The fundamental macrocyclic tetrapyrrolic ring system shown in Fig. 2 is named porphyrin.[c] It is tautomeric with respect to the location of the two hydrogen atoms not involved in the peripheral conjugated system. The two hydrogen atoms may be associated with any two of the four nitrogen atoms. Unless stated to the contrary the representation of one tautomeric form does not imply the absence of another tautomer. However, for nomenclature purposes, the name "porhyrin" implies that the saturated nitrogen atoms are at positions 21 and 23 unless specifically indicated otherwise.

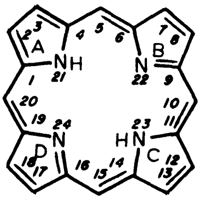

Fig. 2. Porphyrin 1-24 Numbering Scheme.

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a. IUPAC, "Nomenclature of Organic Chemistry, Sections A, B, C, D, E, F and H, 1979 edition." Pergamon, 1979.

b. IUPAC, "Nomenclature of Organic Chemistry, Sections A, B, C, D, E, F and H, 1979 edition." Pergamon, 1979, Rules E-2.2 and E-4.9.

c. The name "porphine" has also been used widely for the structure in Fig. 2. For further discussion see A. H. Corwin in "Organic Chemistry." (H. Gilman, ed.) Vol. 2. Wiley N. Y., 1943, p. 1272 and reference [1].

TP-1.2. Numbering. The 1-24 numbering system upon which the numbering system for corrinoids[a] is based is adopted for the porphyrin nucleus and is shown in Fig. 2. The 2,3,7,8,12,13,17 and 18 positions have commonly been referred to generically as "*beta*- positions" (i.e. of the pyrrole rings). Similarly, positions at 1,4,6,9,11,14,16 and 19 have been referred to generically as "*alpha*-positions," while those at 5,10,15 and 20 are referred to generically as "*meso*-positions." However, in order to avoid possible ambiguity with stereochemical designations the use of these generic terms is discouraged.

TP-1.3. Fused Systems.[b,c] Compounds with extra rings ortho-fused or ortho-perifused to the porphyrin nucleus are of some importance. Tetrabenzoporphyrin is defined and the extra positions numbered as shown in Fig. 3. The name may be used without fusion letters to refer to tetrabenzo[*b,g,l,q*]porphyrin. Systems in which the porphyrin nucleus is fused with other cyclic hydrocarbons[d] may be named by analogy to the IUPAC Rules B-3 and A-21 for naming fused-ring systems, but adopting the porphyrin nucleus with the implied hydrogen atoms at positions 21 and 23 as the basic component to which other rings are fused. Fusion locants are derived according to IUPAC Rule A-21.5. Indicated hydrogen is determined on the basis of the presence of implied hydrogen atoms at positions 21 and 23 of the porphyrin ring in contrast to the form containing the maximum number of noncumulative double bonds as in IUPAC Rule A-21.6.

The component rings fused to the porphyrin base are numbered as substituent groups of the lowest possible position of the porphyrin ring.[e] However, where the "extra" rings are formally derived, such as for lactones, from the reaction of noncyclic substituents implied by the trivial name the numbering of the noncyclized substituent is retained as illustrated by example 4 of Rule TP-3.1 and the examples of Rule TP-3.4.

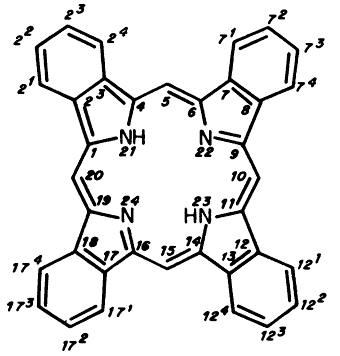
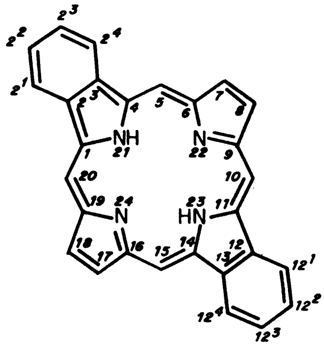


Fig. 3. Tetrabenzoporphyrin.

Examples:

1.



Dibenzo[*b,l*]porphyrin

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a. IUPAC-IUB Commission on Biochemical Nomenclature, "Nomenclature of Corrinoids, Rules Approved 1975." *Pure Appl. Chem.* 48, 495-502 (1976).

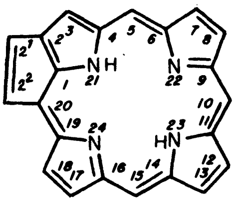
b. See also TP-3.4 for use of "cyclo".

c. See TP-1.6 for fused systems involving skeletally replaced porphyrins.

d. Fusion of the porphyrin ring system with heterocyclic rings, particularly one containing a bivalent atom may affect the tautomerism of the nitrogen atoms of the porphyrin ring system and needs further consideration.

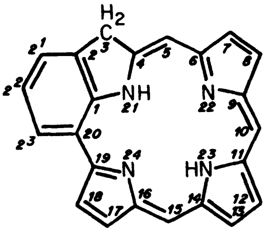
e. See TP-2.1 Fig. 6. This practice is in contrast to established procedures of systematic organic nomenclature for orienting and numbering fused rings according to IUPAC Rules A-22 and B-3.4.

2.



Cyclopenta[*at*]porphyrin[a]

3.

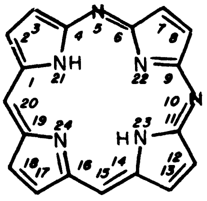


3*H*-Benzo[*at*]porphyrin

TP-1.4. Skeletal Replacement.[b,c] Replacement of a carbon atom of the porphyrin ring by an atom of another element may be denoted by adapting the IUPAC rules for systematic organic replacement nomenclature. The locants of replacement, followed by the appropriate multiplicative prefix (if any) and the replacement term of the element being introduced, are cited in front of the porphyrin name as directed in IUPAC Rules B-4, C-0.6 and D-1.6. When atoms of more than one kind of element are introduced, the replacement terms are cited in the order given in IUPAC Rule B-1.1, Table I. The porphyrin system is a "dihydro system" (i.e. contains one less than the maximum number of double bonds). "Indicated hydrogen," if needed, is assigned on the basis of implied hydrogen atoms at positions 21 and 23 of the porphyrin ring.

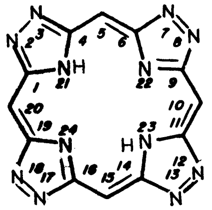
Examples:

1.



5,10-Diazaporphyrin

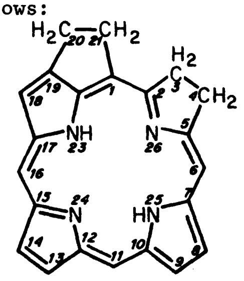
2.



2,3,7,8,12,13,17,18-Octaazaporphyrin

---

a. The name phorbine has been used for the tetrahydro derivative of this ring system, numbered and oriented as follows:

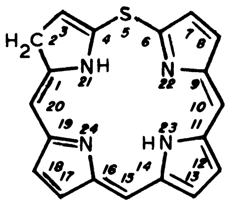


Phorbine

b. See TP-3.5 for skeletal replacement of substitued porphyrins.

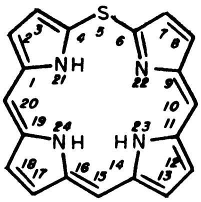
c. These rules have been developed in order to name the common replacement analogs. However further refinement is needed in order to name replacement analogs of other porphyrin types and for corrins and corroles.

3.



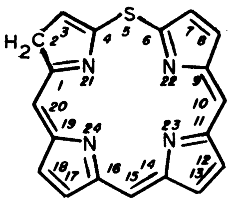
2*H*-5-Thiaporphyrin

4.



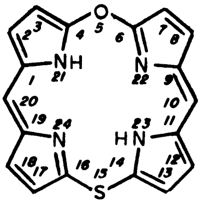
24*H*-5-Thiaporphyrin

5.



21,23-Didehydro-2*H*-5-thiaporphyrin

6.



5-Oxa-15-thiaporphyrin

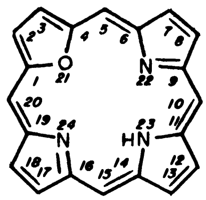
TP-1.5. Skeletal Replacement of Nitrogen Atoms. The replacement operation may be further extended *with caution* to denote the replacement of nitrogen atoms of the porphyrin ring.[a] The porphyrin system is a "dihydro system" containing one less double bond than the maximum possible. The two "extra" hydrogen atoms of the porphyrin system are tautomeric among the four nitrogen atoms. Thus in order to avoid ambiguity the convention that saturated nitrogen atoms are formally replaced before unsaturated nitrogen atoms is adopted, even if a tautomeric form other than the 21,23-dihydro form must be assumed as in example 3 below. Replacement of one -NH- group by a bivalent atom results in a structure with only one of the implied hydrogen atoms left. Hence this hydrogen atom is now denoted by indicated hydrogen in the usual way. The implied dihydro porphyrin structure is no longer assumed.

---

[a] Systematic organic nomenclature requires that the parent upon which replacement is performed be a hydrocarbon (see IUPAC Rules B-4, C-0.6 and D-1.6). Thus, the replacement operation is generally limited to replacement of carbon atoms by atoms of other elements. For natural products IUPAC provisional rules F-4.11 to F-4.13 permit replacement of carbon atoms of a heterocyclic parent, and also the replacement of noncarbon atoms by carbon atoms. The replacement of noncarbon atoms by other noncarbon elements is introduced for porphyrin nomenclature, but needs further consideration.

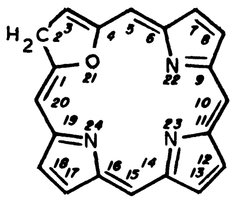
Examples:

1.



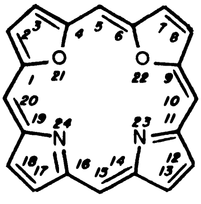
23*H*-21-Oxaporphyrin

2.



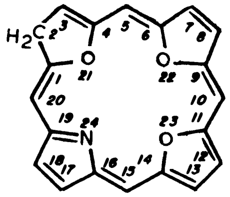
2*H*-21-Oxaporphyrin

3.



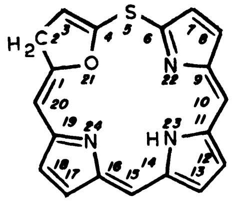
21,22-Dioxaporphyrin

4.



2*H*-21,22,23-Trioxaporphyrin

5.



2*H*,23*H*-21-Oxa-5-thiaporphyrin

TP-1.6. Fused Porphyrin Replacement Analogs. In denoting the fusion of a skeletally replaced porphyrin with cyclic hydrocarbons the procedures of TP-1.3 are followed using the skeletally replaced porphyrin as the base component.[a] As an exception, the name phthalocyanine is retained for the tetrabenzo[*b,g,l,q*]-5,10,15,20-tetraazaporphyrin system. The structure and numbering are as shown in Fig. 4.

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[a] This is in contrast to the procedures for systematic organic nomenclature in which the fusion operation is performed before skeletal replacement is carried out. See IUPAC Rule B-4.2.

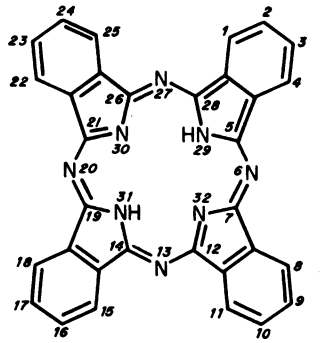
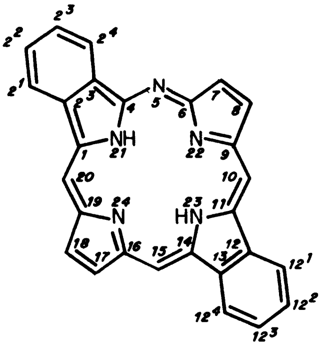


Fig. 4. Phthalocyanine.

Example:



Dibenz[*b*,*l*]-5-azaporphyrin

TP-1.7. Systematic Names for Substituted Porphyrins. Substituted fundamental porphyrins may be named systematically on the basis of the fundamental porphyrin ring nuclei given in TP-1.1 or that are formed as directed in TP-1.3 to TP-1.6. All substituents on the fundamental porphyrin ring are expressed by prefixes and/or suffixes as in organic nomenclature.[a] Hydrogenation of unsaturated positions may be indicated in the customary manner by the prefixes, dihydro-, tetrahydro-, etc.[b]

Substituted porphyrins named systematically are numbered by the rules for systematic organic nomenclature, IUPAC Rule C-15.1. When there is a choice the starting point and direction of numbering around the porphyrin nucleus are chosen so as to give lowest locants to the following structural factors (if present), considered successively in the order listed until a decision is reached:

(a) hydrogen atoms expressed as "indicated hydrogen"[c]

(b) principal groups named as suffix

(c) substituents named as prefixes and hydro prefixes all considered together in one series in ascending numerical order

(d) the substituent named as a prefix, which is cited first in a name.

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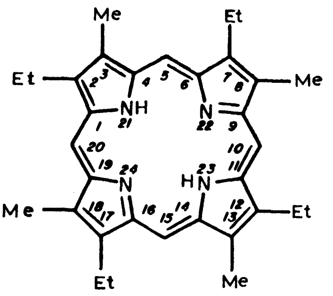
[a] IUPAC, "Nomenclature of Organic Chemistry, Sections A, B, C, D, E, F and H, 1979 edition." Pergamon, 1979.

[b] But see also TP-4 for nomenclature of reduced porphyrins including chlorins.

[c] Because the name "porphyrin" implies a "dihydro parent," which contains two more hydrogen atoms than the corresponding fully conjugated ring system, the notation of indicated hydrogen (a locant and a capital italic *H*), introduced in IUPAC Rule A-21.6, is adapted to denote one of several possible isomers of a particular parent porphyrin structure or a particular tautomer. See also TP-1.4.

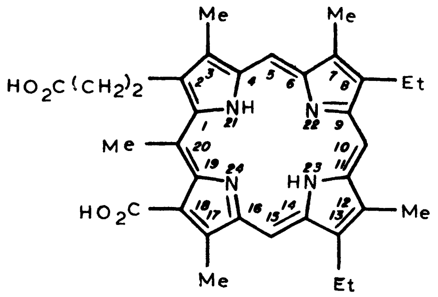
Examples:

1.



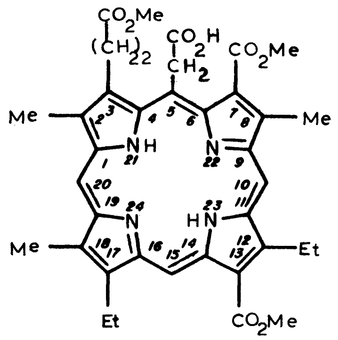
2,7,12,17-Tetraethyl-3,8,13,18-tetramethylporphyrin

2.



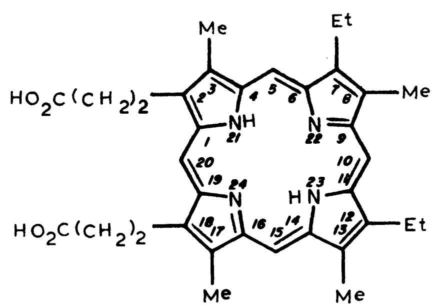
18-Carboxy-8,13-diethyl-3,7,-12,17,20-pentamethylporphyrin-2-propionic acid

3.



12,17-Diethyl-7,13-bis(methoxycarbonyl)-3-[2-(methoxycarbonyl)ethyl]-2,8,18-trimethylporphyrin-5-acetic acid[a]

4.

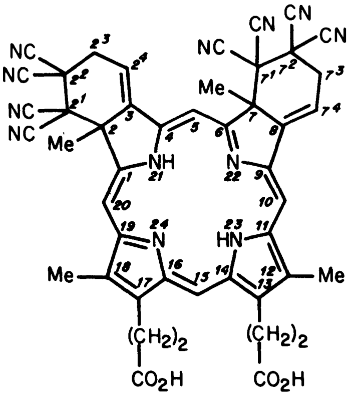


7,12-Diethyl-3,8,13,17-tetramethylporphyrin-2,-18-dipropionic acid

---

a. In line with IUPAC Rule C-10.3, a carboxylic acid is preferred to an ester. Thus the parent, porphyrin-5-acetic acid, is preferred to methyl porphyrin-3-propionate.

5.



$2^1,2^1,2^2,2^2,7^1,7^1,7^2,7^2$-Octacyano-2,$2^1$,$2^2$,$2^3$,7,$7^1$,$7^2$,$7^3$-octahydro-2,7,12,18-tetramethyldibenzo[*b,g*]porphyrin-13,17-dipropionic acid

RULE TETRAPYRROLES 2. TRIVIAL NAMES AND LOCANTS FOR CERTAIN SUBSTITUTED PORPHYRINS[a]

TP-2.1. Trivial Names and Locants. Eleven well-established trivial names and associated locants[b] are retained for naming certain substituted porphyrin structures containing the porphyrin nucleus.[c] They are listed in Tables 2 and 3. They are also explicitly shown in Appendix 1. In addition to these names the name phytoporphyrin is recommended for the hexacyclic structure numbered as shown in Fig. 5. Phylloerythrin, the name formerly used for this structure, is abandoned.

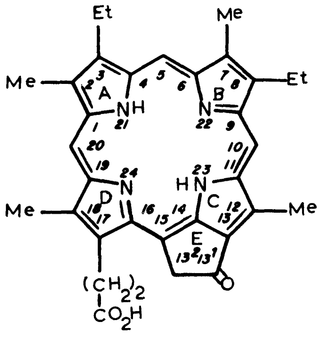


Fig. 5. Phytoporphyrin[d].

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a. See also TP-4.3 and TP-4.4 for trivial names of substituted reduced porphyrins including pheophorbides, pheophytins and chlorins.

b. The locants used with these trivial names are retained for semisystematic porphyrin names formed according to TP-3.1. However, they do not coincide with those used for systematic porphyrin names formed according to TP-1.7. A comparison of the locants of trivially named porphyrins with locants derived systematically is given in Appendix 2.

c. With the exception of the etioporphyrins, the structures denoted by these trivial names do not meet the criteria of IUPAC Rule F-2 regarding selection of parent structures for semisystematic names. However because of their firm establishment in the porphyrin field, these eleven names are carried over from the Fischer system. These names form the basis of a semisystematic nomenclature for naming other porphyrin derivatives.

d. A systematic porphyrin name of phytoporphyrin based on the fundamental ring named as in TP-1.3 would be: 7,12-Diethyl-2^1,2^2-dihydro-3,8,13,17-tetramethyl-2^1-oxocyclopenta[*at*]porphyrin-18-propionic acid.

Table 2. Trivial Names for Substituted Porphyrins[a]

Trivial Name[b]	Rank	Substituents[c] and locants								
		2	3	7	8	12	13	15	17	18
Coproporphyrin I	9	Me	Cet	Me	Cet	Me	Cet	H	Me	Cet
Cytoporphyrin[c]	11	Me	$-CH(OH)CH_2R'$	Me	Vn	Me	Cet	H	Cet	-CHO
Deuteroporphyrin[d,e]	1	Me	H	Me	H	Me	Cet	H	Cet	Me
Etioporphyrin I	3	Me	Et	Me	Et	Me	Et	H	Me	Et
Hematoporphyrin[e]	8	Me	$-CH(OH)CH_3$	Me	$-CH(OH)CH_3$	Me	Cet	H	Cet	Me
Mesoporphyrin[e]	7	Me	Et	Me	Et	Me	Cet	H	Cet	Me
Phylloporphyrin[f]	4	Me	Et	Me	Et	Me	H	Me	Cet	Me
Protoporphyrin[e]	6	Me	Vn	Me	Vn	Me	Cet	H	Cet	Me
Pyrroporphyrin[f]	2	Me	Et	Me	Et	Me	H	H	Cet	Me
Rhodoporphyrin[f]	5	Me	Et	Me	Et	Me	$-CO_2H$	H	Cet	Me
Uroporphyrin I.	10	Cm	Cet	Cm	Cet	Cm	Cet	H	Cm	Cet
Phytoporphyrin	12	Me	Et	Me	Et	Me	-C(O)—	CH_2-	Cet	Me

The side chains of trivially named porphyrins may be numbered using the number of the point of substitution in the porphyrin nucleus, with a following superscript numeral as shown in Fig. 6. The trivial names listed in Table 2 and TP-2.2., Table 3, may be used in deriving semisystematic names for other substituted porphyrins as directed in TP-3.1 and TP-3.2.

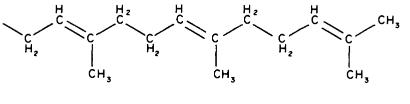
---

a. The porphyrins are arranged alphabetically. They are ranked according to (1) number of component rings (2) number of carbon atoms, (3) molecular weight. A porphyrin of higher rank number is preferred to one of lower rank for selection as parent for semisystematic names according to TP-3.1.

b. For explanation of Roman numerals associated with some of the trivial names see TP-2.2, and Table 3.

c. The following abbreviations are used; Cm for $-CH_2CO_2H$; Cet for $-CH_2CH_2CO_2H$; Me for $-CH_3$; Et for $-CH_2CH_3$; Vn for $-CH{=}CH_2$; see *Eur. J. Biochem.* 74, 1-6 (1977). The use of the symbols A and P, which is a parochial practice in the field of porphyrin chemistry for $-CH_2CO_2H$ and $-CH_2CH_2CO_2H$, respectively, is not recommended.

R' =



trans, *trans*-farnesyl which is (2*E*,6*E*)-3,7,11-trimethyl-2,6,10-dodecatrienyl. See *J. Chem. Soc. Chem. Commun.* 1977, 278.

d. Not to be confused with deuterioporphyrin, a possible name for an isotopically labeled compound.

e. Formerly type IX (see Appendix 3)

f. Formerly type XV.

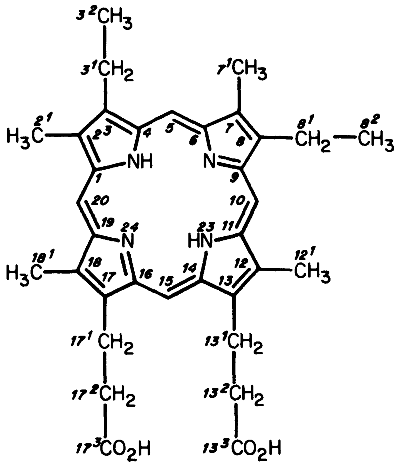
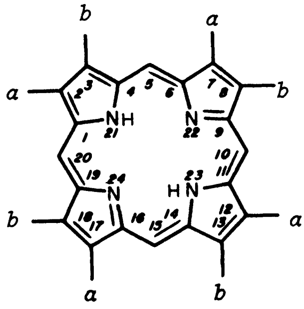
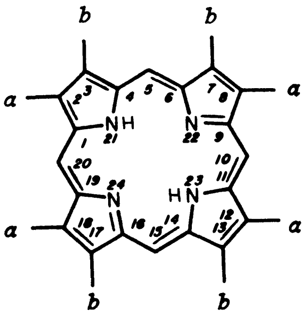


Fig. 6. Numbering of Mesoporphyrin.

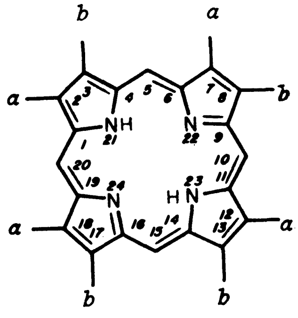
TP-2.2. Roman Numeral Type Notation. There are only four possible positional isomers for each of the 2,3,7,8,12,13,17,18-octasubstituted coproporphyrin, etioporphyrin and uroporphyrin structures in which (i) the substituents are of two sorts only, and (ii) one of each sort of substituent is present as a substituent in each of the component pyrrolic rings A,B,C and D.[a] The four positional isomers are distinguished by Roman numerals, I, II, III or IV applied to these substituted porphyrin rings, numbered and oriented[b] as shown below where substituent *a* is smaller than substituent *b*. The substituents and locants for these porphyrins are summarized in Table 3. The use of Roman numerals or "type nomenclature" is not recommended for more complex cases, or for porphyrins with more than four possible positional isomers.



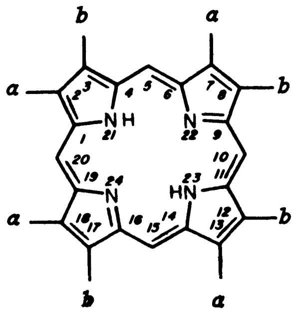
I



II



III



IV

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a. S. Aronoff, "The number of biologically possible porphyrin isomers," *Ann. N.Y. Acad. Sci.* 244, 327-333 (1975).

b. In orienting these trivially named structures the following guidlines were followed: (a) in ring A the sequence "smaller substituent-larger substituent" is clockwise; and (b) insofar as it is possible this order "smaller substituent-larger substituent" continues in turn for ring B, C, D, in that priority.

Table 3. Positional Isomers

Name	Substituents[a] and locants								
	2	3	7	8	12	13	15	17	18
Coproporphyrin I	Me	Cet	Me	Cet	Me	Cet	H	Me	Cet
Coproporphyrin II	Me	Cet	Cet	Me	Me	Cet	H	Cet	Me
Coproporphyrin III	Me	Cet	Me	Cet	Me	Cet	H	Cet	Me
Coproporphyrin IV	Me	Cet	Me	Cet	Cet	Me	H	Cet	Me
Etioporphyrin I	Me	Et	Me	Et	Me	Et	H	Me	Et
Etioporphyrin II	Me	Et	Et	Me	Me	Et	H	Et	Me
Etioporphyrin III	Me	Et	Me	Et	Me	Et	H	Et	Me
Etioporphyrin IV	Me	Et	Me	Et	Et	Me	H	Et	Me
Uroporphyrin I	Cm	Cet	Cm	Cet	Cm	Cet	H	Cm	Cet
Uroporphyrin II	Cm	Cet	Cet	Cm	Cm	Cet	H	Cet	Cm
Uroporphyrin III	Cm	Cet	Cm	Cet	Cm	Cet	H	Cet	Cm
Uroporphyrin IV	Cm	Cet	Cm	Cet	Cet	Cm	H	Cet	Cm

RULE TETRAPYRROLES 3. SEMISYSTEMATIC PORPHYRIN NAMES

TP-3.1. Semisystematic Names For Substituted Porphyrins. As an alternative to a systematic name based on the porphyrin ring nucleus,[b] compounds closely related to the trivially named porphyrins listed in Rule TP-2, Tables 2 and 3, but differing in that one or more hydrogen atoms[c] have been replaced (substituted) by one or more other atoms or groups, may be named semisystematically based on one of the trivially named parent porphyrins. Prefixes, and/or a suffix of the new substituents are combined with the trivial name of the parent porphyrin. The functional group of highest priority,[d] not implied in the trivial parent name, may be expressed as a suffix. The remaining substitutents not implied by the trivial name are expressed by prefixes. Locants and multiplying prefixes are added as appropiate, and the prefixes arranged in alphabetical order.

When there is a choice among trivially named parent porphyrins, the one with the highest possible rank number in Table 2 is preferred. However a porphyrin of lower rank may be selected where special emphasis is desired.

Functional derivatives such as esters and lactones are named similarly and in accord with the rules for organic nomenclature.[e]

---

[a] Abbreviations used are Me for "methyl;" Cet for "carboxyethyl;" Et for "ethyl;" Cm for "carboxymethyl;" see *Eur. J. Biochem.* 74, 1-6 (1977).

[b] See TP-1.7 for generation of systematic names.

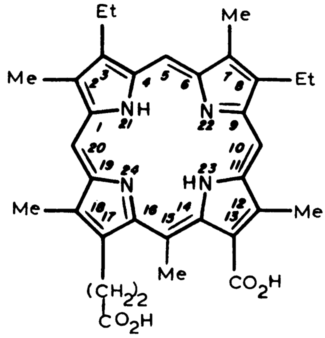
[c] Precise guidelines for naming modified or substituted side chains of trivially named natural products are needed. In general, chain lengthening of substituent groups by substitution of hydrogen atoms by alkyl groups is less preferred than removal of the entire side group and the addition of the new group. See TP-3.2 for subtractive nomenclature.

[d] See IUPAC Rule C-10.3.

[e] See Rule C-4.6 and C-4.7. See also TP-3.4

Examples:

1.

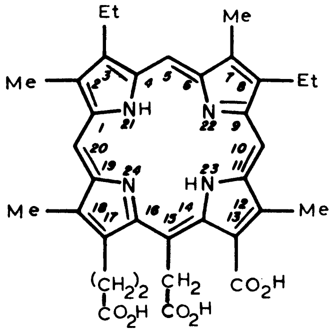


Semisystematic:[a] 15-Methylrhodoporphyrin

Systematic:[b] 18-Carboxy-8,13-diethyl-3,7,12,-17,20-pentamethylporphyrin-2-propionic acid.

Fischer: Chloroporphyrin e_4

2.

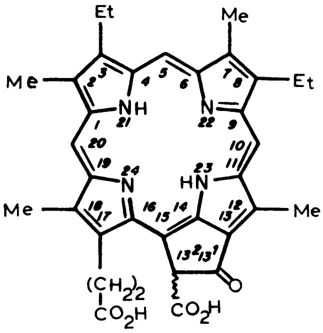


Semisystematic:[c] Rhodoporphyrin-15-acetic acid

Systematic:[e] 18-Carboxy-20-(carboxymethyl)-8,-13-diethyl-3,7,12,17-tetramethylporphyrin-2-propionic acid

Fischer: Chloroporphyrin e_6

3.



Semisystematic:[c,d] Phytoporphyrin-13^2-carboxylic acid

Systematic:[d,e] 2^2-Carboxy-7,12-diethyl-2^1,2^2-dihydro-3,8,13,17-tetramethyl-2^1-oxocyclopenta [*at*] porphyrin-18-propionic acid

Fischer: Pheoporphyrin a_5

---

a. Not phylloporphyrin-13-carboxylic acid. Rhodoporphyrin has a higher rank number than phylloporphyrin.

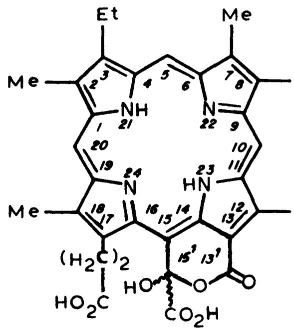
b. See TP-1.7 for generation of systematic names.

c. Note that in contrast to regular practices of substitutive nomenclature that the propionic principal group is unexpressed. In these rules a subordinate group may be cited as a suffix. Compare IUPAC Rule C-10.3.

d. If it is necessary to specify the absolute stereochemistry of this molecule, it should be indicated by *R* or *S* in accord with TP-0.3.

e. For systematic numbering see TP-1.1 and TP-1.7

4.

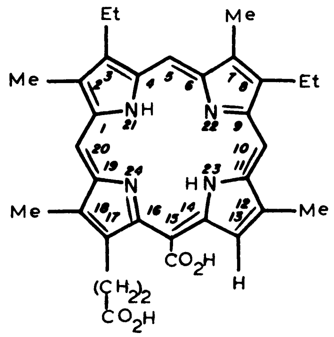


Semisystematic:[a,b] 15^1,15^1-Dihydroxyrhodoporphyrin-15-acetic acid δ-lactone

Systematic:[b,c,d] 18-Carboxy-20-(carboxydihydroxymethyl)-8,13-diethyl-3,7,12,17-tetramethylporphyrin-2-propionic acid δ-lactone

Fischer: Pheoporphyrin a_7

5.

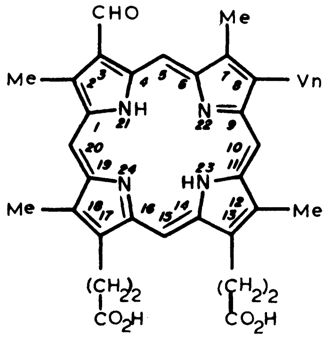


Semisystematic:[e] Phylloporphyrin-15^1-oic acid

Systematic: 20-Carboxy-8,13-diethyl-3,7,12,-17-tetramethylporphyrin-2-propionic acid

Fischer: γ-Carboxypyrroporphyrin

6.



Semisystematic: 3-Formyl-8-vinyldeuteroporphyrin

Systematic: 8-Formyl-3,7,12,17-tetramethyl-13-vinylporphyrin-2,18-dipropionic acid

Fischer: Chlorocruoroporphyrin

or

Spirographisporphyrin

---

[a] Note that in contrast to regular practices of substitutive nomenclature that the propionic principal group is unexpressed. In these rules a subordinate group may be cited as a suffix. Compare IUPAC Rule C-10.3.

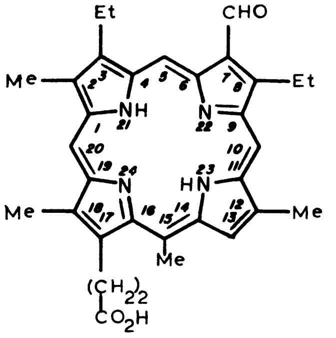
[b] If it is necessary to specify the absolute stereochemistry of this molecule, it should be indicated by *R* or *S* in accord with TP-0.3.

[c] For systematic numbering see TP-1.1 and TP-1.7.

[d] Alternatively a name based on ring fusion principles could be formed, but see footnote d, TP-1.3.

[e] Not Pyrroporphyrin-15-carboxylic acid. Phylloporphyrin ranks higher than pyrroporphyrin in Table 2.

7.



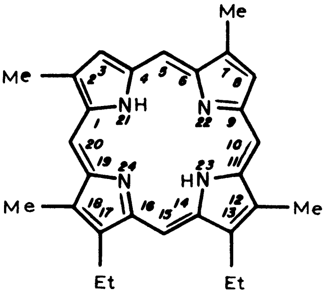
Semisystematic: 7^1-Oxophylloporphyrin

Systematic: 8,13-Diethyl-12-formyl-3,7,-
17,20-tetramethylporphyrin
2-propionic acid

Fischer: Rhodinporphyrin *g*$_3$

TP-3.2. Subtractive Nomenclature. The prefix "de" followed by the name of a substituent group is used to denote the removal of that substituent from the semisystematic parent porphyrin[a] and its replacement by the appropriate amount of hydrogen as in organic nomenclature.[b] These prefixes combined with a multiplicative prefix denote the loss of a corresponding number of substituents or atoms. "Dehydro" denotes the loss of one hydrogen atom. The "de" prefix is nondetachable from the name of the substituent group to which it refers.[c] Simple subtractive prefixes are alphabetized disregarding the multiplying prefixes, di, tri, tetra, penta, etc. When there is a choice, as low locants as possible are selected for the subtractive prefixes as in systematic substitutive nomenclature.[d]

Example:



Semisystematic: 3,8-Dideethyletioporphyrin III

Systematic:[e] 3,7-Diethyl-2,8,12,17-
tetramethylporphyrin

Fischer: Deuteroetioporphyrin IX

TP-3.3. Combinations of Substitutive and Subtractive Operations. The subtractive operations of TP3.2 may be combined with the operations of substitution of TP-3.1 to denote the removal of a group or atom from a position in the parent porphyrin and subsequent substitution at any position. The subtractive prefixes are alphabetized among the substitutive prefixes. As low locants as possible are selected for substitutive and subtractive prefixes considered together in one series. If this is not decisive, then the numbering is chosen that assigns the lowest locant to the first cited substituent or subtractive prefix. When a porphyrin structure can be considered as a derivative of two or more trivially named parent porphyrins listed in Tables 2 and 3, and shown in Appendix 1, the name that requires the fewest number of subtractive and substitutive operations combined is preferred. If this is not decisive, then the name that requires the smaller number of subtractive prefixes is preferred.

---

[a] Further development of guidelines for choice of the trivially named parent porphyrin, its numbering, and limits of application of these operations is needed.

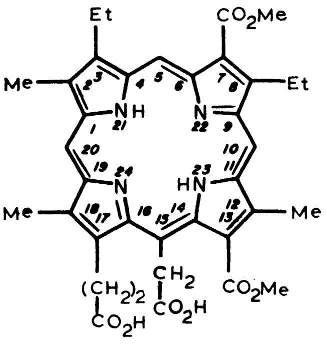
[b] See IUPAC Rule C-41.

[c] See IUPAC provisional Rules F-4.10 and F-4.13.

[d] See IUPAC Rule C-15.11(d) and (e).

[e] See TP-1.7 for formation of the systematic name.

Example:



Semisystematic: 7-Demethyl-7-(methoxycarbonyl)rhodoporphyrin-15-acetic acid 13-methyl ester[a]

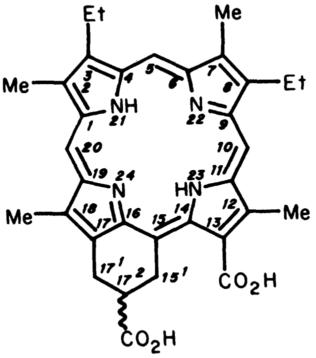
Systematic: 20-(Carboxymethyl)-8,13-diethyl-12,18,bis(methoxycarbonyl)-3,7,17-trimethylporphyrin-2-propionic acid

Fischer: Rhodinporphyrin g_8 (as one of its dimethyl esters)

TP-3.4. Additional ring formation. Compounds closely related to the trivially named porphyrins of Rule TP-2 but in which an additional ring has been formed by means of a direct link between two atoms of the parent structure are named by prefixing "cyclo" preceded by the locants of the positions joined by the new bond.[b] Alternatively such compounds may be named according to the provisions for fused rings in Rule TP-1.3.

Examples

1.

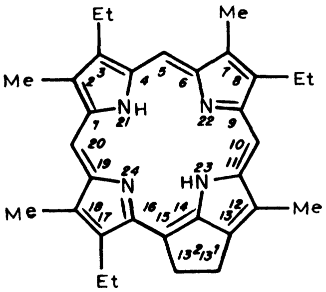


Semisystematic:[c] $15^1,17^2$-Cyclophylloporphyrin-13-carboxylic acid

Systematic[c,d]: 8,13-Diethyl-$2^2,2^3$-dihydro-3,7,12,17-tetramethyl-2^1H-benzo[*at*]porphyrin-2^2,18-dicarboxylic acid

Fischer: Neoporphyrin 4

2.



Semisystematic: 13^2,15-Cycloetioporphyrin III, or 17^2-Decarboxy-13^1-deoxophytoporphyrin

Systematic:[d] 7,12,18,Triethyl-$2^1,2^2$-dihydro-3,8,13,17-tetramethylcyclopenta[*at*]porphyrin

Fischer: Deoxophylloerythroetioporphyrin

---

[a] Alternate formats for naming this diester should be considered such as 7-carboxy-7-demethylrhodoporphyrin-15-acetic acid 7,13-dimethyl ester, or 13-methyl 7-demethyl-7-(methoxycarbonyl)-rhodoporphyrin-15-acetate. Present IUPAC nomenclature rules are not definitive in this respect.

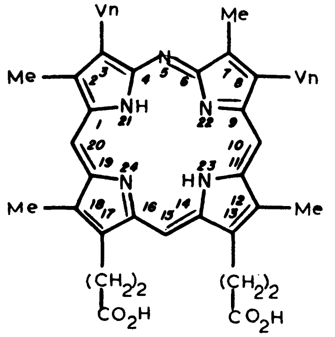
[b] See IUPAC provisional Rule F-4.1.

[c] If it is necessary to specify the absolute stereochemistry of this molecule, it should be by *R* or *S* according to TP-0.3.

[d] See TP-1.3 for the systematic name and numbering of the fundamental ring.

TP-3.5. Skeletal Replacement of Substituted Porphyrins.[a] Trivially named porphyrins in which one or more of the atoms in the porphyrin ring nucleus have been replaced by atoms of other elements are named by prefixing to the trivial name, the appropriate locants with corresponding multiplicative and replacement prefixes. Where there is a choice due to the symmetry of substituents, the replacing atoms are numbered in line with IUPAC Rule B-4.

Example:



Semisystematic: 5-Azaprotoporphyrin

Systematic:[a] 2,7,12,18-Tetramethyl-3,8-divinyl-5-azaporphyrin-13,17-dipropionic acid

RULE TETRAPYRROLES 4. REDUCED PORPHYRINS INCLUDING CHLORINS

TP-4.1. Unsubstituted Reduced Porphyrins. The most common reduced porphyrins are dihydroporphyrins in which saturated carbon atoms are located at the nonfused carbon atoms of one of the pyrrole rings. The parent compound of this series is called *chlorin*, which, defined in terms of the unsubstituted porphyrin ring, is 2,3-dihydroporphyrin (see Fig. 7). Tetrahydroporphyrins in which the saturated carbon atoms are located at nonfused carbon atoms of two diagonally opposite pyrrole rings are bacteriochlorins: tetrahydroporphyrins with adjacent pyrrole rings reduced in this way are called isobacteriochlorins. Hexahydroporphyrins in which the nitrogen atoms and four meso positions are saturated are porphyrinogens. The unsubstituted bacteriochlorin, isobacteriochlorin and porphyrinogen ring system are shown together with their systematic names and numbering in Figs. 8, 8a and 9 respectively. Further hydrogenated derivatives of these specially named structures are to be named systematically as hydroporphyrins in preference to hydrochlorins, hydrobacteriochlorins, hydroisobacteriochlorins or hydroporphyrinogens. Other unsubstituted reduced porphyrin ring systems are also to be named systematically according to TP-1.7.

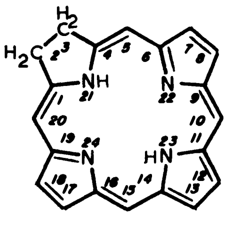


Fig. 7. Chlorin
2,3-Dihydroporphyrin[b].

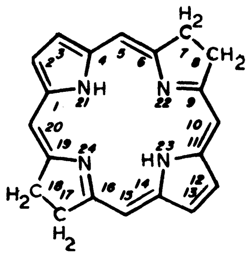


Fig. 8. Bacteriochlorin
7,8,17,18-Tetrahydroporphyrin[c].

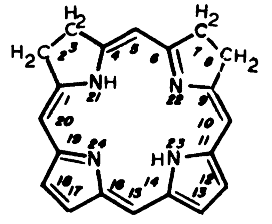


Fig. 8a. Isobacteriochlorin
2,3,7,8-tetrahydroporphyrin[b].

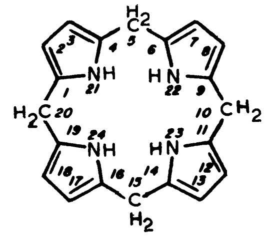


Fig. 9. Porphyrinogen
5,10,15,20,22,24-Hexahydroporphyrin[b].

---

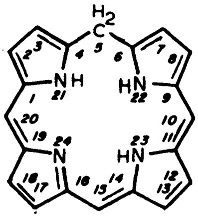
[a] See TP-1.4 and TP-1.5 for systematic names and numbering of skeletally replaced fundamental porphyrin systems.

[b] The presence of hydrogen atoms at positions 21 and 23 is implied by the name "porphyrin".

[c] The 2,3,12,13-tetrahydroporphyrin with implied hydrogen atoms at 21 and 23 is not structurally possible.

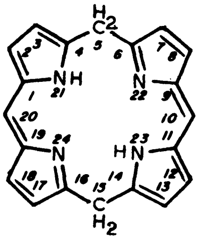
Examples:

1.



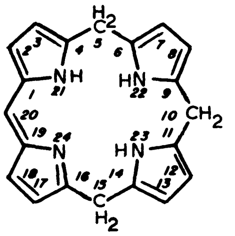
5,22-Dihydroporphyrin
(formerly named phlorin)

2.



5,15-Dihydroporphyrin
(formerly porphodimethene)

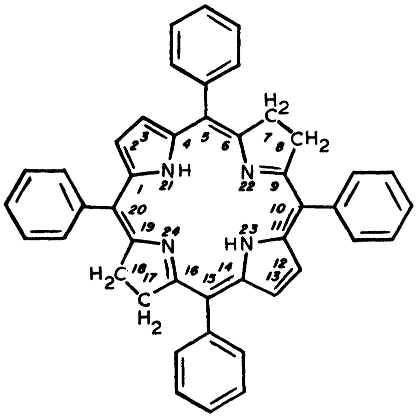
3.



5,10,15,20-Tetrahydroporphyrin
(formerly porphomethene)

TP-4.2 Substituted Reduced Porphyrins. Systematic Chlorin Names. Derivatives of chlorins and other reduced porphyrins may be named systematically based on one of the parent rings chlorin, bacteriochlorin, porphyrinogen, or porphyrin shown in Figs. 7, 8, 9 and 2 respectively.[a] Substituents are expressed by prefixes or suffixes as in organic nomenclature.[b]

Example:[c]



5,10,15,20-Tetraphenylbacteriochlorin

---

[a] See also Appendix 1.

[b] See also TP-1.7.

[c] For more examples see TP-4.4.

TP-4.3. Substituted Reduced Porphyrins and Close Relatives of the Chlorophylls. Trivial Names and Numbering.

TP-4.3.1. The four trivial names listed in Table 4 may be used to name 17,18-dihydro derivatives of the four corresponding trivially named porphyrins in Table 2. These names may also be used to form semisystematic names as directed in TP-4.4. 17,18-Dihydro derivatives of other trivially named porphyrins are named systematically as directed in TP-4.2.

Table 4. Trivially named substituted chlorins corresponding to 17,18-dihydro derivatives of trivially named porphyrins

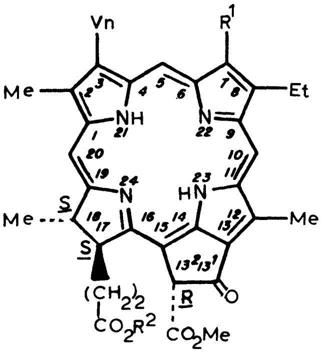
Trivial name	Rank No.	Substituents and locants								
		2	3	7	8	12	13	15	17	18
Phyllochlorin	2	Me	Et	Me	Et	Me	H	Me	Cet,H	Me,H
Phytochlorin	4	Me	Et	Me	Et	Me	$-C(O)$——	CH_2-	Cet,H	Me,H
Pyrrochlorin	1	Me	Et	Me	Et	Me	H	H	Cet,H	Me,H
Rhodochlorin	3	Me	Et	Me	Et	Me	$-CO_2H$	H	Cet,H	Me,H

TP-4.3.2. Additional trivial names used to name chlorins, bacteriochlorins and porphyrins may be derived from the common chlorophyll names listed in TP-8.4 and Appendix 1. Compounds that may be formally derived by demetallation of the corresponding substituted naturally occurring chlorophyll shown in TP-8.4 are called pheophytins (if the ester of the 17-propionic acid group is phytyl) or pheofarnesins (if the ester of the 17-propionic acid group is farnesyl). In naming such compounds, the word "pheophytin" (or "pheofarnesin") replaces "chlorophyll" in the original name.[a] Thus demetallation of bacteriochlorophyll *a* gives bacteriopheophytin *a*.

Compounds that are demetallated and also possess a free propionic acid or acrylic acid residue at position 17 are called pheophorbides,[b] and the names are related to those of the chlorophyll in the same way. Thus, on demetallation and hydrolysis of the phytyl ester, chlorophyll *a* gives pheophorbide *a*.

Examples:

1.



Pheophytin *a* $R^1 = -CH_3$; R^2 = phytyl[c]

Pheophytin *b* $R^1 = -CHO$; R^2 = phytyl[c]

Pheophorbide *a* $R^1 = -CH_3$; $R^2 = -H$

Pheophorbide *b* $R^1 = -CHO$; $R^2 = -H$

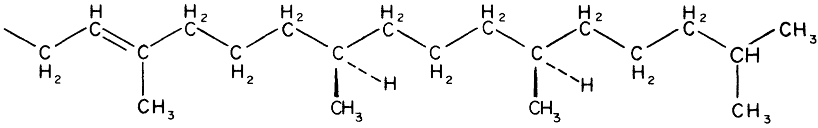
Pheophorbide *a* methyl ester $R^1 = -CH_3$; $R^2 = -CH_3$

---

[a] At present this method is limited to the phytyl and farnesyl ester groups. Even though a geranylgeranyl ester has been reported for bacteriochlorophyll, no trivial name has been accepted for the demetallation analog.

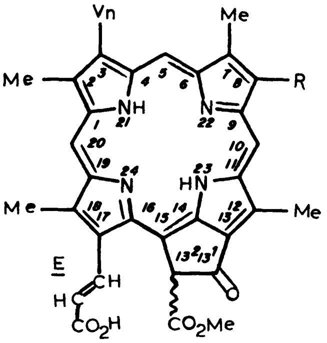
[b] The ending "-ide" should not be confused with its meaning by IUPAC Rule C-84.3 in which it would designate an anion formed by removal of a proton from a carbon atom.

[c] Phytyl =



(2*E*)-(7*R*,11*R*)-3,7,11,15-tetramethyl-2-hexadecenyl.

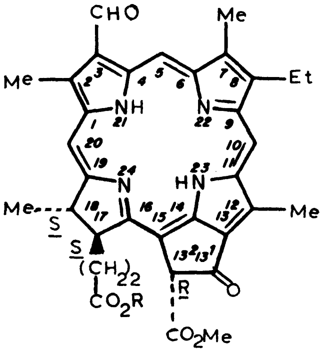
2.



[a,b]Pheophorbide *c_1* R = $-CH_2CH_3$

[a,b]Pheophorbide *c_2* R = $-CH=CH_2$

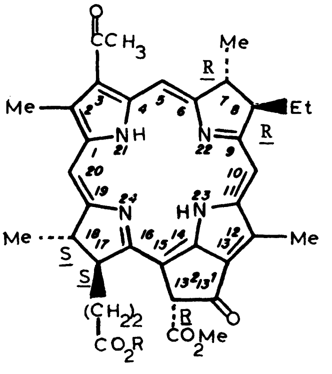
3.



Pheophytin *d* R = phytyl

Pheophorbide *d* R = -H

4.



Bacteriopheophytin *a* R = phytyl

Bacteriopheofarnesin *a* R = farnesyl[c]

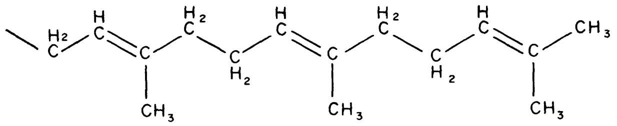
Bacteriopheophorbide *a* R = -H

---

a. Chlorophylls *c_1* and *c_2* (which have a free acrylic acid residue at C-17) on demetallation yield the pheophorbides *c_1* and *c_2*, and are porphyrins rather than chlorins.

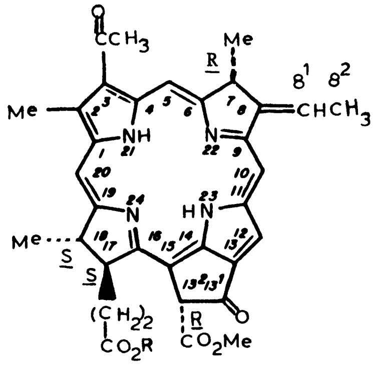
b. The configuration of the double bond is *E*, and is to be implied by these names. If it is necessary to specify the absolute configuration at C-13^2, it should be indicated by *R* or *S* according to TP-0.3.

c. *trans*,*trans*-Farnesyl is



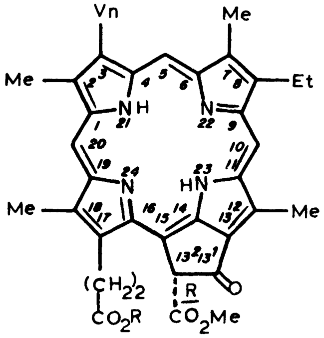
(2*E*,6*E*)-3,7,11-trimethyl-2,6,10-**dodecatrienyl**

5.



Bacteriopheophytin *b*[a] R = phytyl

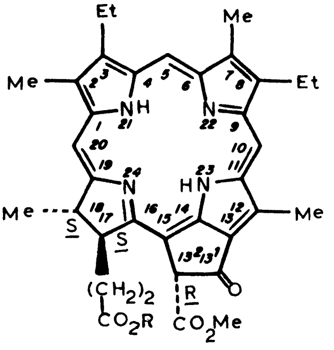
6.



17,18-Didehydropheophytin *a*[b] R = phytyl

17,18-Didehydropheophorbide *a*[b] R = -H

7.



Mesopheophytin *a* R = Phytyl

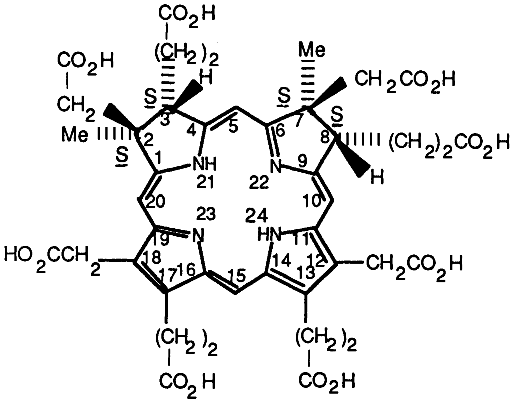
Mesopheophorbide *a* R = -H

---

[a] If it is necessary to specify the sterochemistry of the 8(8^1) double bond, it should be indicated by *E* or *Z* according to TP-0.3.

[b] The names protopheophytin *a* and protopheophorbide *a* would be derived according to this rule from the Fischer name, protochlorophyll *a*. However "protochlorophyll a" is not included in the list of chlorophyll names in TP-8.4 because its substitution pattern differs from that of protoporphyrin (an ethyl group at position 8 is a vinyl group in protoporphyrin). Hence "protopheophytin *a*" and "protopheophorbide *a*" are not acceptable names in this document. These structures are easily named using the subtractive prefix "didehydro" combined with derivative terms, pheophytin *a* or pheophorbide *a* based on the parent structure, chlorophyll *a*.

TP-4.3.3. The compound shown below, an isobacteriochlorin (see TP-4.1) encountered along the biosynthetic pathway to corrinoids, is called sirohydrochlorin [13].

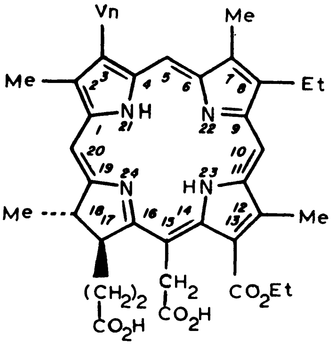


Sirohydrochlorin

TP-4.4. Substituted Chlorins. Semisystematic Chlorin Names. As an alternative to systematic chlorin names formed according to TP-4.2, chlorin derivatives closely related to the four trivially named chlorins in Table 4 of TP-4.3.1 may be named semisystematically. Subtractive and/or substitutive prefixes (or suffix) are combined with the appropriate trivial name. The procedures for forming semisystematic porphyrin names in TP-3 are followed.

Examples:

1.

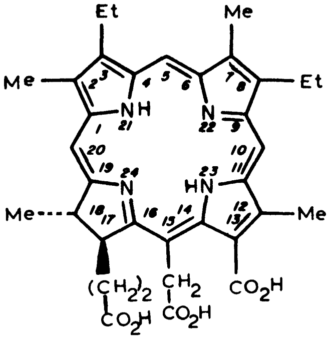


Semisystematic: $3^1,3^2$-Didehydrorhodochlorin-15-acetic acid 13-ethyl ester

Systematic: (2*S*,3*S*)-20-(Carboxymethyl)-18-(ethoxycarbonyl)-13-ethyl-3,7,12,17-tetramethyl-8-vinylchlorin-2-propionic acid

Fischer: Chlorin e_6 (as a monoethyl ester)

2.

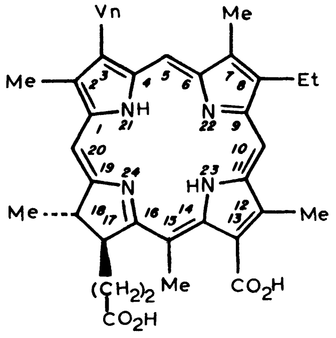


Semisystematic: Rhodochlorin-15-acetic acid

Systematic: (2*S*,3*S*)-18-Carboxy-20-(carboxymethyl)-8,13-diethyl-3,7,12,17-tetramethylchlorin-2-propionic acid

Fischer: Mesochlorin e_6

3.

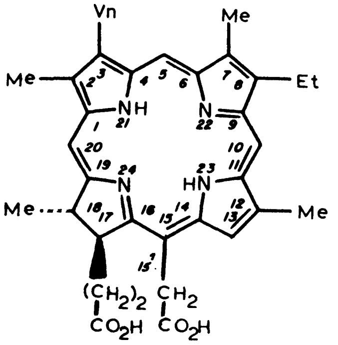


Semisystematic: 3^1,3^2-Didehydro-15-methylrhodochlorin

Systematic: (2*S*,3*S*)-18-Carboxy-13-ethyl-3,7,12,17,20-pentamethyl-8-vinylchlorin-2-propionic acid

Fischer: Chlorin e_4

4.

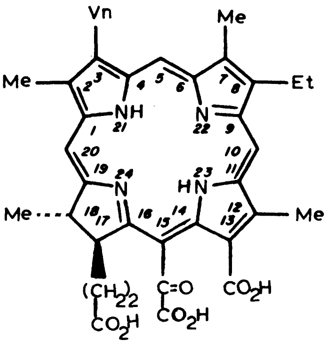


Semisystematic: 3^1,3^2-Didehydrophyllochlorin-15^1-carboxylic acid

Systematic: (2*S*,3*S*)-20-(Carboxymethyl)-13-ethyl-3,7,12,17-tetramethyl-8-vinylchlorin-2-propionic acid

Fischer: Isochlorin e_4

5.

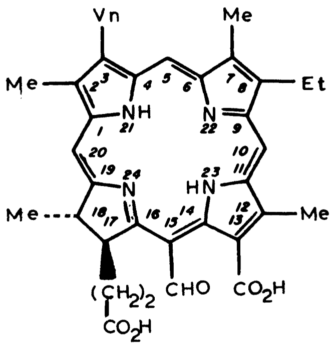


Semisystematic: 3^1,3^2-Didehydrorhodochlorin-15-glyoxylic-acid

Systematic: (2*S*,3*S*)-18-Carboxy-13-ethyl-3,7,12,17-tetramethyl-20-oxalo-8-vinylchlorin-2-propionic acid

Fischer: Purpurin 7

6.



Semisystematic: 3^1,3^2-Didehydro-15-formylrhodochlorin

Systematic: (2*S*,3*S*)-18-Carboxy-13-ethyl-20-formyl-3,7,12,17-tetramethyl-8-vinylchlorin-2-propionic acid

Fischer: Purpurin 5

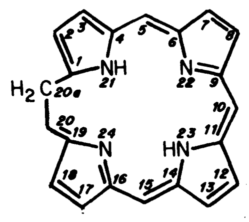
RULE TETRAPYRROLES 5. RING-EXPANDED AND RING-CONTRACTED SYSTEMS

TP-5.1. Ring Expansion. Inclusion of a methylene group (-CH_2-) into a porphyrin ring sector is indicated by the prefix "homo" in accord with the guidelines established for natural products.[a] The homo prefix is preceded by a locant indicating the position of the inserted group. A locant for the inserted group is generated by adding the letter "a" to the locant of the highest possible numbered atom of the ring-sector that is not a bridgehead or junction[b] to which the group is added.

To denote ring expansion of the fundamental porphyrin nucleus, "homo" immediately precedes "porphyrin". To denote ring expansion of a trivially named porphyrin or reduced porphyrin, "homo" immediately precedes the appropriate trivial name.

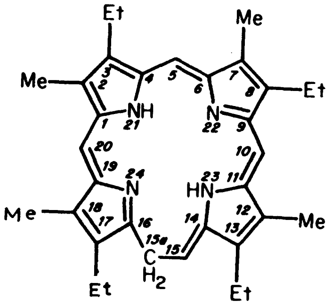
Examples:

1.



20a-Homoporphyrin

2.

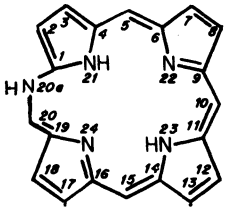


15a-Homoetioporphyrin III

TP-5.2. Skeletal Replacement of Ring-expanded Systems. Replacement prefixes with appropriate locants are added in front of the name of the ring-expanded porphyrin.[c]

Examples:

1.



20a-Aza-20a-homoporphyrin

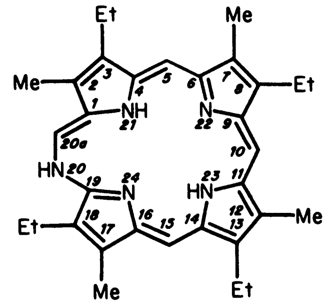
---

a. IUPAC, "Nomenclature of Organic Chemistry, Sections A, B, C, D, E, F and H, 1979 edition." Pergamon, 1979, Rule F-4.13

b. Bridgehead and junction atoms are excluded to avoid ambiguity.

c. General practice varies in related areas such as steroids and natural products as to the relative placement of ring modifying and skeletal replacement prefixes. Further study is needed. See IUPAC provisional Rule F-4.5.

2.



20*H*-20-Aza-20a-homoetioporphyrin I[a]

TP-5.3. Ring-contracted systems. The trivial names "corrin" and "corrole" [7] are retained for the ring-contracted structures shown in Figs. 10 and 11 respectively.[b] Skeletal replacement analogs are named by prefixing the appropriate locants with multiplicative and replacement prefixes to the parent name "corrole".[c] Other ring-contracted porphyrins are named systematically according to the rules for naming heterocycles.[d,e]

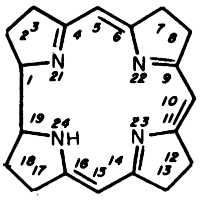


Fig. 10. Corrin.

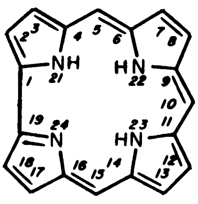
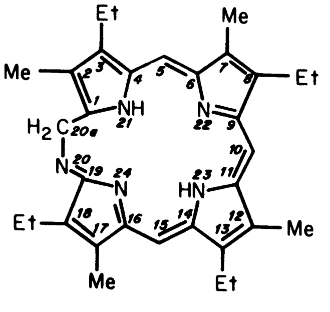


Fig. 11. Corrole.

---

a. "Indicated hydrogen" distinguishes this structure from the closely related one:



20-Aza-20a-homoetioporphyrin I

Because atom 19 is a bridgehead, the locant 19a may be ambiguous.

b. For other trivial names such as cobyrinic acid, cobinic acid and vitamin B-12 that are retained for substituted derivatives of these ring systems, see IUPAC-IUB Commission on Biochemical Nomenclature, "Nomenclature of Corrinoids, Rules Approved 1975." *Pure Appl. Chem.* 48, 495-502 (1976).

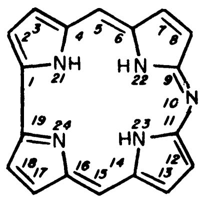
c. As for skeletal replacement in porphyrins, replacement of saturated nitrogen atoms of corrin and corrole precede replacement of the unsaturated nitrogen atoms. See TP-1.5.

d. See IUPAC Rules B-1 to B-15.2.

e. The ring contraction prefix "nor", recommended for natural products in IUPAC provisional Rule F-4.4, at present denotes only the loss of a methylene ($-CH_2-$) group from a ring system. Generally, ring contraction by use of "nor" has been restricted to saturated systems such as steroids. Extension of the meaning of "nor" to indicate loss of either a methylene ($-CH_2-$) or methyne ($-CH=$) group needs further study with regard to indication of hydrogen present in the ring, priority of citation and numbering of heteroatoms and other ring modifying prefixes.

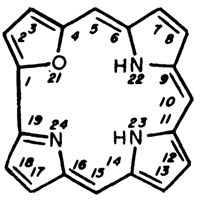
Examples:

1.



10-Azacorrole

2.



21-Oxacorrole

TP-5.4. The pentapyrrolic macrocycle Fig. 12 is called sapphyrin [8], and is numbered as shown.

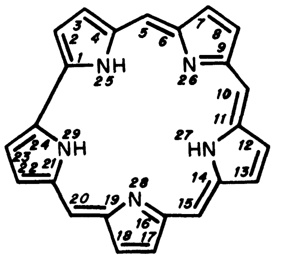


Fig. 12. Sapphyrin.

RULE TETRAPYRROLES 6. LINEAR TETRAPYRROLES

TP-6.1. Fundamental System. The structure in Fig. 13 is called "bilane". It is defined without oxygen substituents, and is numbered (omitting C-20) to agree with the numbering of the unsubstituted porphyrin ring system (see Fig. 2). Unless otherwise specified it is implied that each nitrogen atom of bilane (Fig. 13) is saturated.

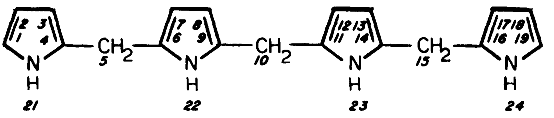


Fig. 13. Bilane[a] (trivial name bilinogen)

TP-6.2. Unsubstituted Oxidised Bilanes. Unsubstituted oxidised bilanes may be named semisystematically on the basis of the bilane structure in Fig. 13. The number of additional double bonds involving the carbon bridges is indicated by changing the ending '-ane' to '-ene' (1 such additional double bond, total 9 double bonds), and '-adiene' (2 such additional double bonds, total 10 double bonds). The system with one further double bond (total 11 double bonds) has already been defined [9] as bilin (Fig. 14) and this name is used in preference to bilatriene. The location of the additional double bonds for the bilene and biladiene names is indicated by the letters *a*, *b*, or *c* corresponding to the bridge positions 5, 10 and 15 respectively.

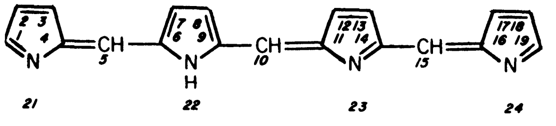


Fig. 14. Bilin (22*H*-form drawn conventionally)

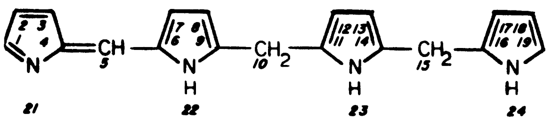
---

[a] The use of bilane in biochemical literature is established although it does not follow the guidelines set forth in IUPAC Rule F-3.

Where it is necessary to specify the stereochemistry of the 4(5)-, 5(6)-, 9(10)-, 10(11)-, 14(15)- and/or 15(16)-double bonds, it should be indicated by *E* or *Z* according to TP-0.3.

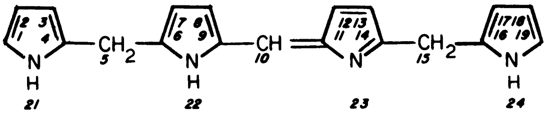
Examples:[a]

1.



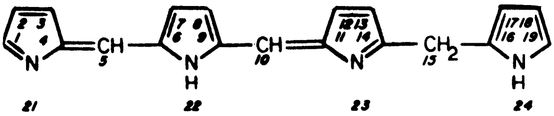
Bilene-*a*

2.



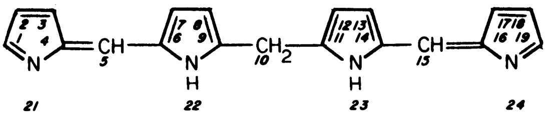
Bilene-*b*

3.



Biladiene-*ab*

4.



Biladiene-*ac*

The name 1,19-secocorrin (Fig. 15) defined previously [9] may be used in place of 1,2,3,7,8,12,13,17,18,19-decahydrobilin. Secocorrin names are derived systematically from the corrin nomenclature.[b]

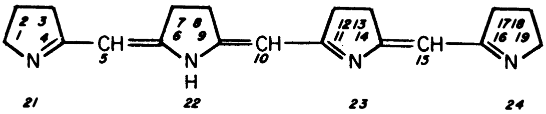


Fig. 15. 1,19-Secocorrin (22*H*-form drawn)

TP-6.3. Semisystematic Nomenclature. Substituted linear tetrapyrroles may be named on the basis of the fundamental bilane structure (Fig. 13) and the less saturated systems defined in TP-6.2. The appropriate parent is selected according to the number, and location, of the C,C-double bonds involving C-5, C-10 and/or C-15. All substituents are expressed by prefixes and/or suffixes as in systematic nomenclature.[c] Positions of substituents are determined in accord with IUPAC Rule C-15.11(b) to (e) based, where relevant, on the 22*H* form.

---

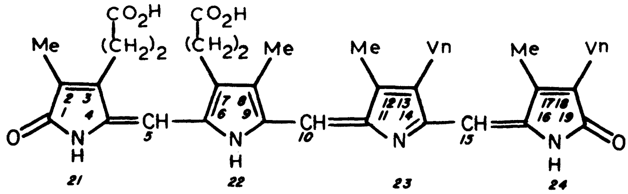
[a] The use of bilene and biladiene in biochemical literature is established although they do not follow the guidelines set forth in IUPAC Rule F-3.

[b] IUPAC-IUB Commission on Biochemical Nomenclature, "Nomenclature of Corrinoids, Rules Approved 1975." *Pure Appl. Chem.* 48, 495-502 (1976).

[c] Common biochemical practice favors the expression of the ketone function as a suffix in contradistinction to the usual hierarchy of functions in systematic nomenclature which favors the expression of the acid function as a suffix.

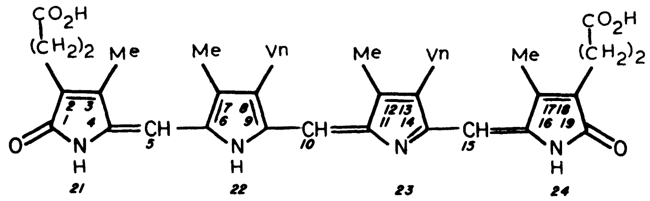
Examples:[a]

1.



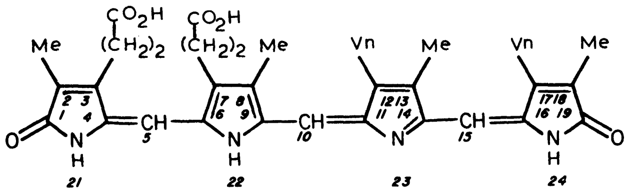
3,7-Bis(2-carboxyethyl)-2,8,12,17-tetramethyl-13,18-divinylbilin-1,19(21*H*,24*H*)-dione (biliverdin IXβ)

2.



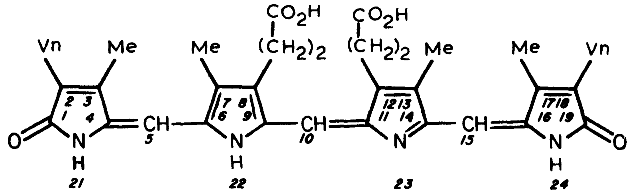
2,18-Bis(2-carboxyethyl)-3,7,12,17-tetramethyl-8,13-divinylbilin-1,19(21*H*,24*H*)-dione (biliverdin IXγ)

3.



3,7-Bis(2-carboxyethyl)-2,8,13,18-tetramethyl-12,17-divinylbilin-1,19(21*H*,24*H*)-dione (biliverdin IXδ)[b]

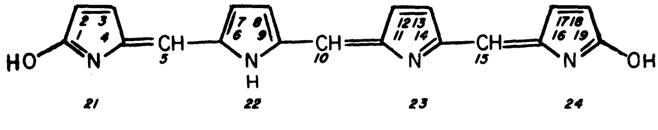
4.



8,12-Bis(2-carboxyethyl)-3,7,13,17-tetramethyl-2,18-divinylbilin-1,19(21*H*,24*H*)-dione (biliverdin IIIα)

---

[a] The linear tetrapyrrole structures shown in examples 1-5 are formally tautomeric with the corresponding bilin-1,19-diols.



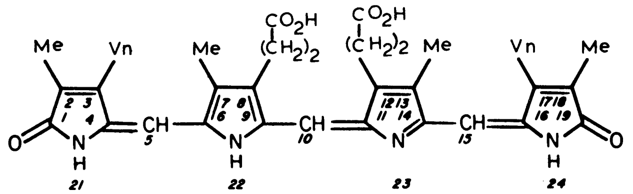
Bilin-1,19-diol

However, present evidence indicates that the bislactam form predominates and most naturally occuring linear tetrapyrroles are named on the basis of the bislactam (i.e. -1,19-dione) tautomer.

---

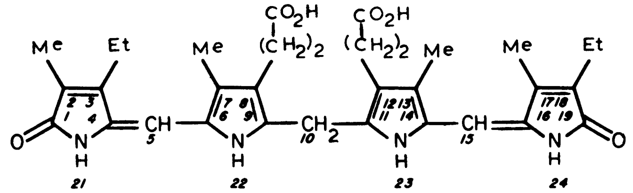
[b] Note that the systematic orientation and numbering differ from that accepted for the trivial name, biliverdin IXδ.

5.



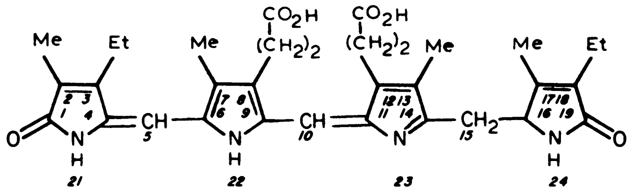
8,12-Bis(2-carboxyethyl)-2,7,13,18-tetramethyl-3,17-divinylbilin-1,19(21*H*,24*H*)-dione (biliverdin XIIIα)

6.



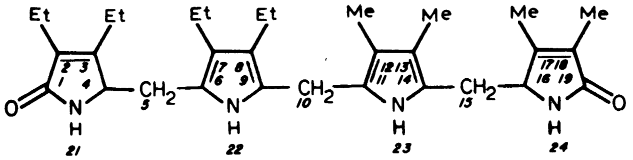
8,12-Bis(2-carboxyethyl)-3,18-diethyl-2,7,13,17-tetramethylbiladiene-*ac*-1,19(21*H*,24*H*)-dione (mesobilirubin, see Fig. 19)[a]

7.



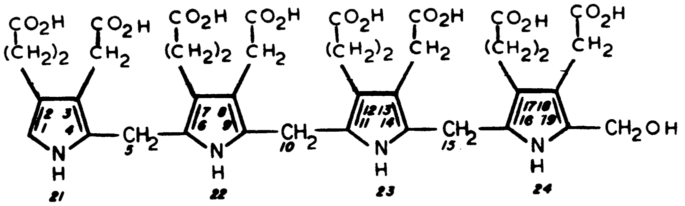
8,12-Bis(2-carboxyethyl)-3,18-diethyl-2,7,13,17-tetramethylbiladiene-*ab*-1,19(16*H*,21*H*)-dione (15,16-dihydromesobiliverdin, see example 1, TP-6.5)

8.



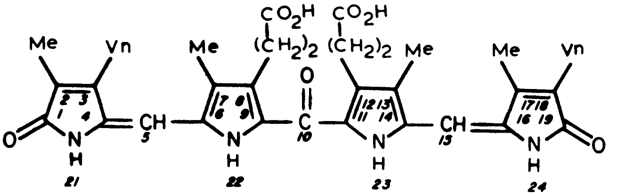
2,3,7,8-Tetraethyl-12,13,17,18-tetramethylbilane-1,19(4*H*,16*H*)-dione

9.



3,8,13,18-Tetrakis(carboxymethyl)-19-hydroxymethylbilane-2,7,12,17-tetrapropionic acid

10.



8,12-Bis(2-carboxyethyl)-2,7,13,17-tetramethyl-3,18-divinylbiladiene-*ac*-1,10,19(21*H*,24*H*)-trione

---

[a] Note that the systematic orientation and numbering differ from that accepted for the trivial name, mesobilirubin.

TP-6.4. Trivial Names. Seven trivial names and associated locants are retained for naming the substituted linear tetrapyrroles shown in Fig. 16-22.[a] The side chains may be numbered using the locant of the point of substitution on the bilane system with a following superscript numeral as for trivially named porphyrins in TP-2.1.

These recommended trivial names may be used to form names for modified derivatives as directed in TP-6.5. However, positional isomers of these trivially named structures are named according to TP-6.3.

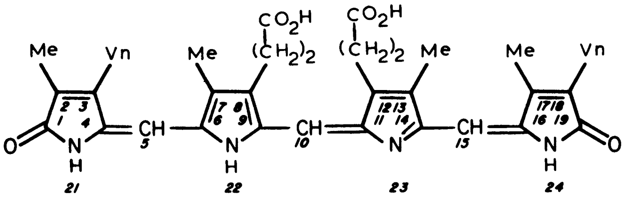


Fig. 16. Biliverdin (biliverdin IXα).

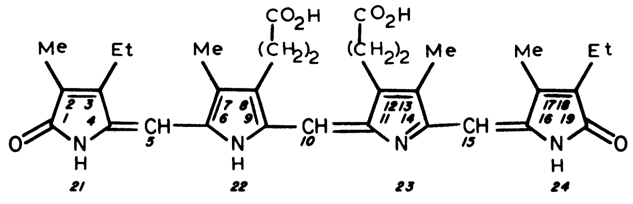


Fig. 17. Mesobiliverdin (mesobiliverdin IXα).

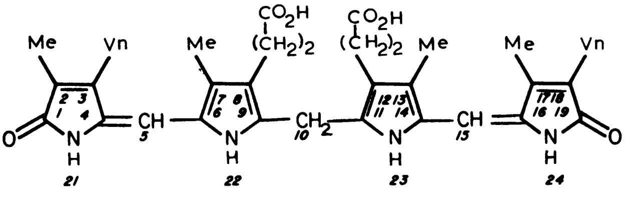


Fig. 18. Bilirubin (bilirubin IXα).[b]

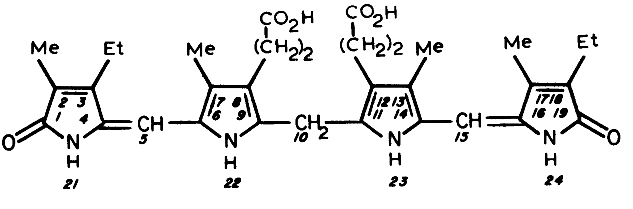


Fig. 19. Mesobilirubin (mesobilirubin IXα).

---

a. In the recommended nomenclature the Roman numeral and Greek letter (that in the Fischer system refer in a formal way to the substitution pattern and to the position of cleavage of the corresponding porphyrin respectively) have been dropped. Thus biliverdin was formerly biliverdin IXα. Because the vast majority of references are to this common substitution pattern, it has become common practice to drop the IXα designation.

b. X-ray crystallography has shown that the natural compound has the configuration (4Z,15Z). See R. Bonnett, J. E. Davies and M. B. Hursthouse, *Nature* 262, 326 (1976).

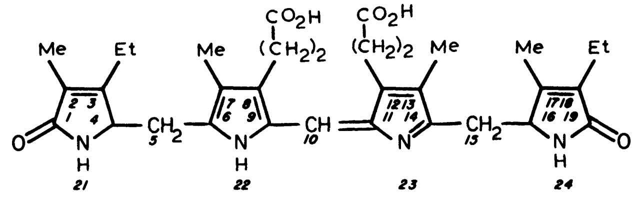


Fig. 20. Urobilin (urobilin IXα [10]).[a]

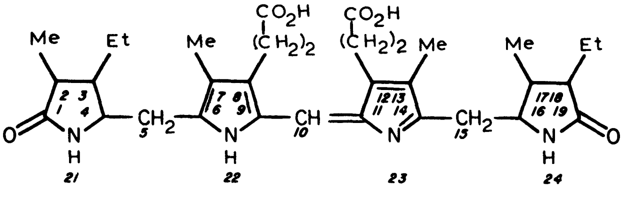


Fig. 21. Stercobilin (stercobilin IXα).[a]

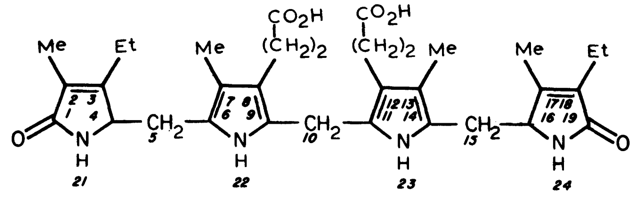
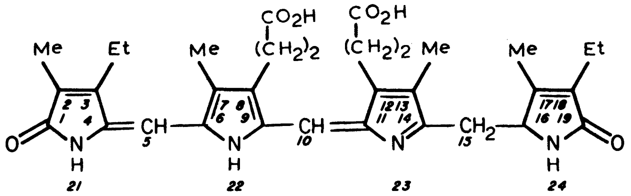


Fig. 22. Urobilinogen (mesobilirubinogen IXα; urobilinogen IXα).[a]

TP-6.5. Modified Trivial Names. As an alternative to the semisystematic nomenclature of TP-6.3, substituted bilins closely related to the trivially named bilin structures shown in Figs. 16-22, in which only a few substituents differ or that differ only in degree of saturation, may be conveniently named on the basis of the recommended trivial names. The subtractive prefix "de," and the substitutive prefixes and suffixes may be used as for porphyrin derivatives in TP-3.1 through TP-3.3. When sites of saturation are known to be either one of two possible locations, the lowest possible locants are cited, followed in parentheses by the italic word "or" and the alternate locants.

Examples:

1.



15,16-Dihydromesobiliverdin (formerly mesobiliviolin IXα)[a,b,c]

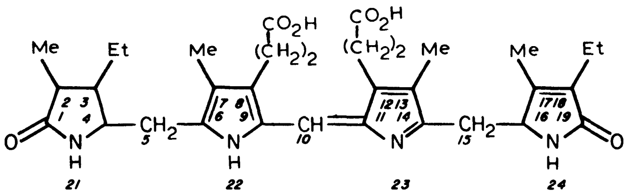
---

a. If it is necessary to indicate the absolute configuration of any of the chiral centers, this should be indicated by *R* or *S* in accord with TP-0.3.

b. Where sites of saturation are indefinite, the name would be 4,5(*or* 15,16)-dihydromesobiliverdin.

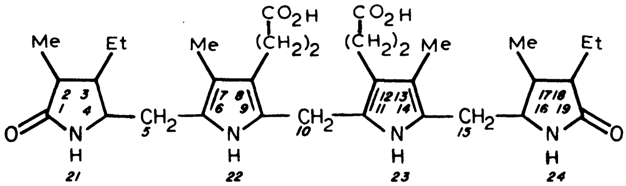
c. Note that, in many cases, the older trivial names do not distinguish between isomeric possibilities. "Mesobiliviolin IXα" may refer to two possible isomers [11].

2.



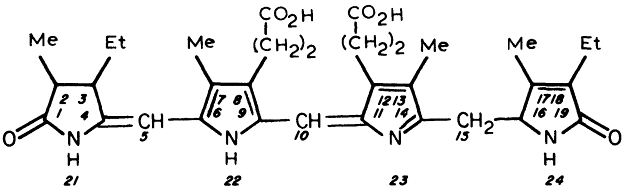
2,3-Dihydrourobilin (formerly half-stercobilin IXα)[a]

3.



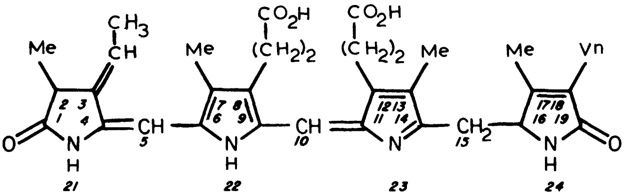
10,23-Dihydrostercobilin (formerly stercobilinogen IXα)[a]

4.



2,3,15,16-Tetrahydromesobiliverdin (formerly mesobilirhodin IXα)[a,b]

5.



$3,3^1,18^1,18^2$-Tetradehydro-2,3,15,16-tetrahydromesobiliverdin (phycoerythrobilin preferred to phycobiliviolin)[a,c,d,e]

---

[a] If it is necessary to indicate the absolute configuration of any of the chiral centers, this should be indicated by *R* or *S* in accord with TP-0.3.

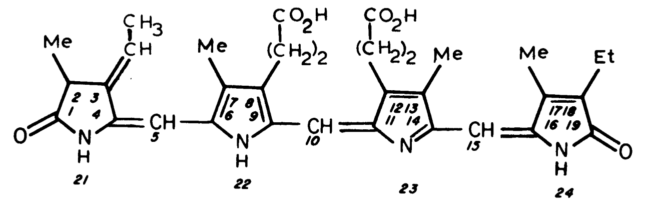
[b] The name "mesobilirhodin IXα" may refer to two possible isomers [12].

[c] Two sets of trivial names have arisen for the bilinoids derived from algal biliproteins. (W. Rüdiger, *Fortschritte der Chemie organischer Naturstoffe* 29, 60 (1971); D. J. Chapman, W. J. Cole, and H. W. Siegelman, *J. Am. Chem. Soc.* 89, 5976 (1967); H. L. Crespi, L. J. Boucher, G. D. Norman, J.J. Katz and R. C. Dougherty, *J. Am. Chem. Soc.* 89, 3642 (1967)). While the semisystematic names based on mesobiliverdin in examples 5 and 6 are preferred, if a trivial name is to be used, phycoerythrobilin and phycocyanobilin would be better choices than phycobiliviolin and phycobiliverdin because the violins are muted in these recommendations.

[d] Aplysioviolin is the monomethyl ester of this structure, *Angew. Chem., Int. Ed.* 9, 473 (1970).

[e] The stereochemistry of the $3(3^1)$-double bond may be indicated by *E* or *Z* in accord with TP-0.3.

6.



$3,3^1$-Didehydro-2,3-dihydromesobiliverdin (phycocycanobilin preferred to phycobiliverdin)[a,b]

RULE TETRAPYRROLES 7. RELATIVES OF LINEAR TETRAPYRROLES

TP-7.1. Linear Tripyrroles. By analogy with the nomenclature of bilins, the nomenclature of linear tripyrroles is based systematically on the most unsaturated system known, which is called tripyrrin and shown in Fig. 23. Unless otherwise stated it is implied that the nitrogen atom at position 16 (e.g. in Fig. 23) is saturated.

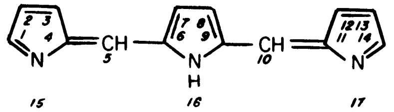
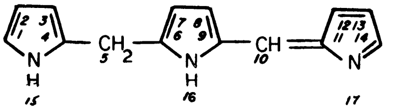


Fig. 23. Tripyrrin

Reduced tripyrrins are named as dihydro, tetrahydro etc. derivatives:

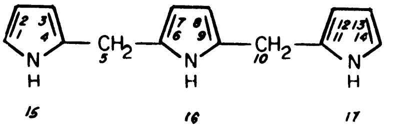
Examples:

1.



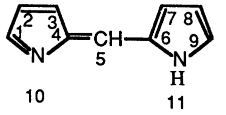
5,15-Dihydrotripyrrin

2.



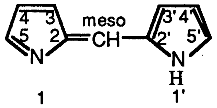
5,10,15,17-Tetrahydrotripyrrin[c]

TP-7.2. Dipyrroles. It is possible to extend this nomenclature to the related dipyrrole systems, as shown below. Dipyrromethane is retained as a trivial name, and dipyrrin is introduced as a trivial name: as elsewhere in this document the names refer to systems with 2,2'-bridged pyrrole nuclei. Unless otherwise specified, it is implied that the nitrogen atom at position 11 is saturated.

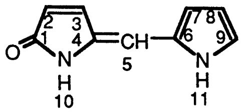


Dipyrrin

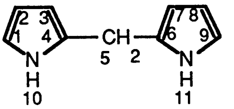
(Formerly:



dipyrromethane
pyrromethene)



Dipyrrin-1(10*H*)-one (Formerly: pyrromethenone)



5,10-Dihydrodipyrrin
Dipyrromethane

(Formerly: 2,2'-dipyrrolylmethane,
dipyrrylmethane, pyrromethane)

---

[a] If it is necessary to indicate the absolute configuration of any of the chiral centers, this should be indicated by *R* or *S*.

[b] The sterochemistry of the $3(3^1)$- double bond may be indicated by *E* or *Z* in accord with TP-0.3.

[c] This structure is called tripyrrane in the Fischer system.

RULE TETRAPYRROLES 8. METAL COORDINATION COMPLEXES

TP-8.1. General Description. The common structural pattern for metal coordination complexes in this series consists of a metal ion coordinated to a roughly planar tetrapyrrole, acting as a tetradentate dianionic ligand, and, possibly, to one or two axial ligands, as illustrated in Fig. 24.

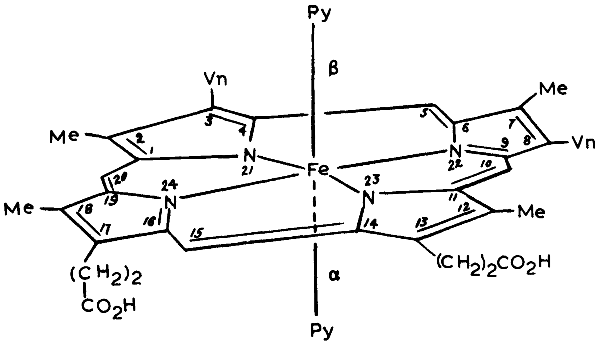


Fig. 24. A protohemochrome[a] as an example of a tetrapyrrole coordination complex containing a tetrapyrrole terradentate dianionic ligand and two pyridine molecules as axial ligands.

The tetrapyrrolic ligand is oriented with the numbering clockwise when seen from above (see TP-1.2, TP-1.7 and TP-2.1). The axial ligands above and below the plane are then designated by the use of β and α respectively, in analogy with established custom for other groups of compounds.[b,c,d] For example, hemoglobin coordinates with oxygen on the α face of the protoheme system.

Coordination of the four central nitrogen atoms (N-21, N-22, N-23, N-24) is the common structural pattern, and need not be specifically designated, but may be designated as instructed in Inorganic Rule 7.33 or D-2.38 if desired. When the charge on the tetrapyrrolic ligand is not specified it is understood that it carries a formal negative charge of two units. For systems that do not conform to the common structural pattern see TP-9.2.

TP-8.2. Coordination Nomenclature. The Rules for Coordination Compounds[e] are followed, except that stereochemical configuration of axial ligands, if any, may be designated, where known, by the use of α and β as in TP-8.1, Fig. 24. The names of ligands precede the name of the metal, the ligands being cited in alphabetical order. Enclosing marks are employed as described in Inorganic Rule 7.3 and D-2.21 of the Rules for Coordination Compounds.[f]

---

a. See TP-8.4.3 for definition.

b. Because the assignment of α and β is dependent on the direction of numbering of substituents, they are defined only in a relative sense. For example, the α side of mesoporphyrin named systematically as 7,12-diethyl-3,8,13,17-tetramethylporphyrin-2,18-dipropionic acid is the β side of mesoporphyrin named and numbered according to the trivial system.

c. IUPAC-IUB Commission on Biochemical Nomenclature, "Nomenclature of Corrinoids, Rules Approved 1975". *Pure Appl. Chem.* 48, 495-502 (1976).

d. IUPAC Commission on the Nomenclature of Organic Chemistry and IUPAC-IUB Commission on Biochemical Nomenclature. "1971 Definitive Rules for Nomenclature of Steroids." *Pure Appl. Chem.* 31, 284-322 (1972).

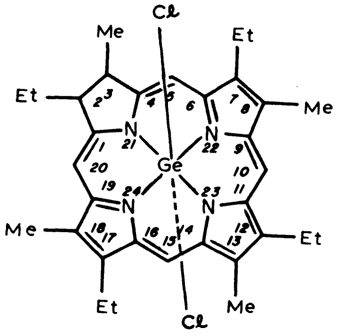
e. IUPAC, "Nomenclature of Inorganic Chemistry, Definitive Rules 1970" 2nd ed. Butterworths, 1971 also published in *Pure Appl. Chem.* 28, 39 (1971), Section 7; IUPAC, "Nomenclature of Organic Chemistry, Sections A, B, C, D, E, F and H, 1979 edition" Pergamon, 1979, Section D-2.

f. An essential result is that organic anions, including macrocyclic anions, are placed in brackets. The names of inorganic anions are not bracketed except in special cases [e.g. when the name contains a numerical prefix e.g. (triphosphato)]. When a neutral molecule is coordinated its name is used unchanged, and is brakceted, except, on both counts, for the following common neutral ligands: water (becomes aqua), ammonia (becomes ammine), nitric oxide (becomes nitrosyl), and carbon monoxide (becomes carbonyl).

For coordination complexes of the common structural pattern decribed in Rule TP-8.1 the macrocycle name takes the ending *"ato"*.[a] Thus chlorin becomes chlorinato, porphyrin becomes porphyrinato, bilirubin becomes bilirubinato and mesoprophyrin diethyl ester becomes mesoporphyrinato diethyl ester. The name of the metal follows, and is itself followed by its oxidation number (Roman numeral in brackets), or its Ewens-Bassett number[b] to indicate the charge on the entire coordination complex (instead of an oxidation number) as recommended in Inorganic Rule 7.22 or Rule D-2.23.

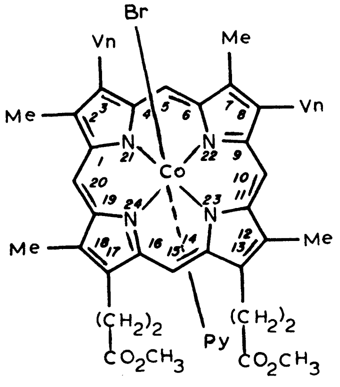
Examples: (Py = pyridine)

1.



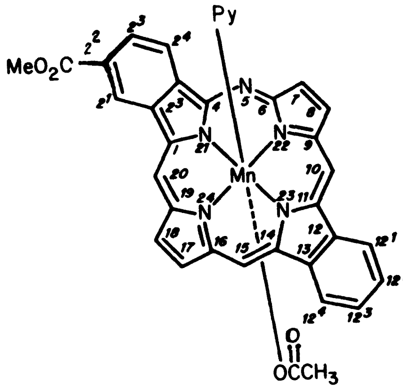
Dichloro(2,7,12,17-tetraethyl-2,3-dihydro-3,8,13,18-tetramethyl porphyrinato)germanium(IV)

2.



β-Bromo(protoporphyrinato dimethyl ester)-α-(pyridine)cobalt(III)
or
β-Bromo[dimethyl 3,7,12,17-tetramethyl-8,13-divinylporphyrin-2,18-dipropionato(2-)]-α-(pyridine)cobalt(III)

3.



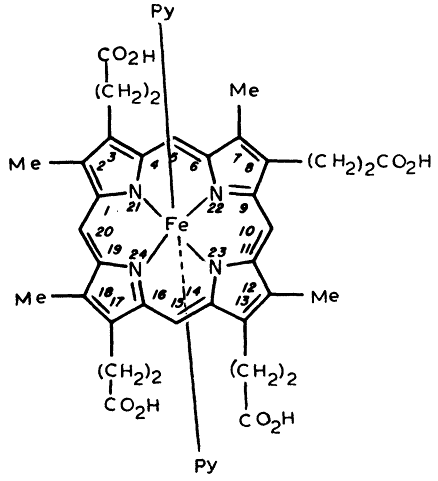
α-(Acetato)[2^2-(methoxycarbonyl)dibenzo[*b,l*]-5-azaporphyrinato] -β-(pyridine)manganese(III)

---

a. The designation of the charge on the ligand such as (2-) is often not specified.

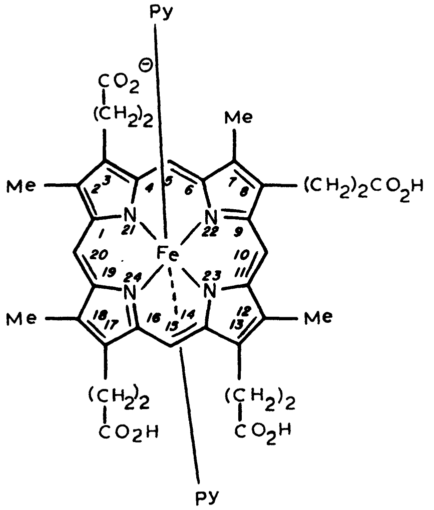
b. See Inorganic Rule 2.252 for definition.

4.



(Coproporphyrinato III)bis(pyridine)iron(II)[a]
or
Bis(pyridine)(3,8,13,17-tetramethylporphyrin-2,7,12,18-tetrapropionato)
iron(II)

5.



[Coproporphyrinato(6-) III] bis(pyridine)iron(III)
or
Bis(pyridine)[3,8,13,17-tetramethylporphyrin-2,7,12,18-tetrapropionato-(3-)]iron(III)

---

[a] Practice varies as to whether the protons of the acid groups are formally removed from the ligand or are retained in naming such coordination complexes. If they are retained for this coordination complex, the name is based on iron. If they are removed, a hexaanionic ligand results, and the precise name of the anion would be [coproporphyrinato(6-) III N^{21},N^{22},N^{23},N^{24}] bis(pyridine)ferrate(4-).

TP-8.3. Alternative Order of the Components of the Name: (Alternative to TP-8.2). Since the macrocyclic name is frequently complex and unwieldy the alternative order of components: (axial ligands)-metal-tetrapyrrolic ligand is introduced here for use in naming tetrapyrrole metal coordination complexes. This form of name, although not encompassed by the established IUPAC coordination rules, has the additional advantage that confusion between axial ligands and substituents on the macrocyclic ligand cannot easily arise.

The axial ligands are cited in alphabetical order and with enclosing marks as before (Rule TP-8.2.). The name of the metal follows, and is itself followed by the oxidation number (Roman numeral in parentheses) or the Ewens Bassett number. After a space the name of the tetrapyrrole ligand is given, ending in "ate":[a] it is not bracketed.

The structures drawn in Rule TP-8.2. are named as follows on the basis of this alternative procedure:

1. Dichlorogermanium(IV) 2,7,12,17-tetraethyl-2,3-dihydro-3,8,13,18-tetramethylporphyrinate
2. β-Bromo-α-(pyridine)cobalt(III) protoporphyrinate dimethyl ester
3. α-(Acetato)-β-(pyridine)manganese(III) 2^2-(methoxycarbonyl)dibenzo[*b*,*l*]-5-azaporphyrinate
4. Bis(pyridine)iron(II) coproporphyrinate III
5. Bis(pyridine)iron(III) coproporphyrinate(3-) III

TP-8.4. Trivial Names. Because of their natural occurrence the magnesium and iron coordination complexes are associated with an extensive trivial nomenclature.

TP-8.4.1. Nine trivial names may be used to name the chlorophyll structures as indicated in Figs. 25, 26, 27, and 28.

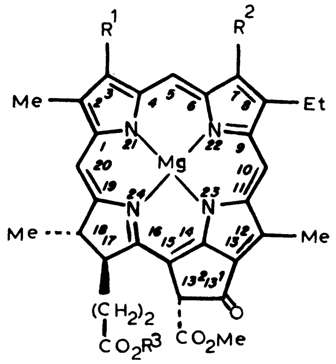
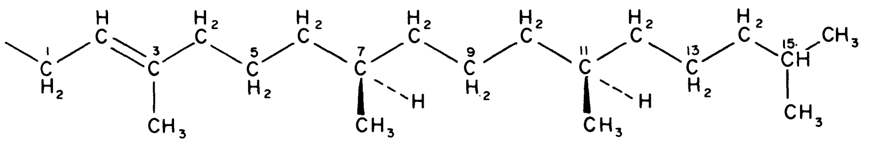


Fig. 25.	Chlorphyll *a*	R^1 = Vn	R^2 = Me	R^3 = phytyl[b]
	Chlorophyll *b*	R^1 = Vn	R^2 = -CHO	R^3 = phytyl
	Chlorophyll *d*	R^1 = -CHO,	R^2 = Me	R^3 = phytyl
	Mesochlorophyll *a*	R^1 = Et	R^2 = Me	R^3 = phytyl
	Chlorophyllide *a*	R^1 = Vn	R^2 = Me	R^3 = -H.

---

[a] The use of the "ate" ending here is not sanctioned by any current organic nomenclature rule in IUPAC Sections A,B,C,D or in the IUPAC inorganic rules. In the organic rules, "ate" refers to an anion derived by loss of a proton from a functional group (see IUPAC Rules C-84.1 and C-84.2). In the inorganic nomenclature rules "ate" denotes the loss of a proton from an acid group, or the presence of an anionic coordination center (see Inorganic Rule 3.223).

[b] Phytyl = (2*E*)-(7*R*,11*R*)-3,7,11,15-tetramethyl-2-hexadecenyl



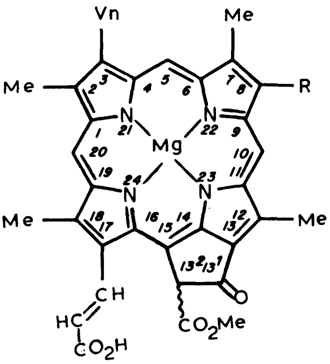


Fig. 26.[a] Chlorophyll c_1 R = Et

Chlorophyll c_2 R = Vn.

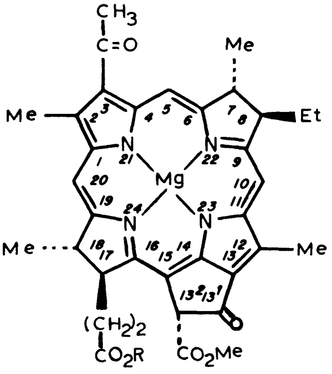


Fig. 27. Bacteriochlorophyll *a*[b] R = phytyl.

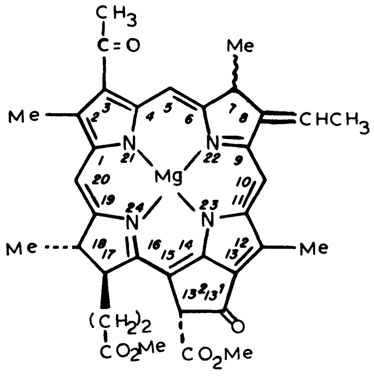


Fig. 28. Bacteriochlorophyll *b*[c,d] R = phytyl.

---

[a] The double bond at C-17^1 is *E* which is implied by these names. However, if the absolute configuration is known at C-13^2, it may be expressed by *R* or *S* placed in front of these names. See TP-0.3.

[b] Bacteriochlorophyllide *a* (*all-trans*)-geranylgeranyl ester has also been reported, and called bacteriochlorophyll *gg*: J. J. Katz, H. H. Strain, A. L. Harkness, M. H. Studier, W. A. Svec, T. R. Janson and B. T. Cope, *J. Am. Chem. Soc.* 94, 7938 (1972).

[c] The stereochemistry of the 8(8^1) double bond may be designated by *E* or *Z* in accord with TP-0.3.

[d] The structure of bacteriochlorophyll *b* has been formulated by H. Scheer, W. A. Svec, B. T. Cope, M. H. Studier, R. G. Scott and J. J. Katz, *J. Am. Chem. Soc.* 96, 3714 (1974).

TP-8.4.2. Alternatively, the structures represented in Figs. 25, 27 and 28 may be named semisystematically as magnesium(II) coordination complexes of pheophytins, bacteriopheophytins or mesopheophytin, respectively.[a,b] Chlorophyll c_1 and c_2 may be named semisystematically as $3^1,3^2,17^1,17^2$-tetradehydro-13^2-(methoxcarbonylphytoporphyrinato) and $3^1,3^2,8^1,8^2,17^1,17^2$-hexadehydro-$13^2$-(methoxycarbonyl)phytoporphyrinato magnesium(II) coordination complexes, respectively. Chlorophyll structures containing a free propionic acid residue at position C-17 are called chlorophyllides. They may be named semisystematically as magnesium(II) coordination complexes of pheophorbides.

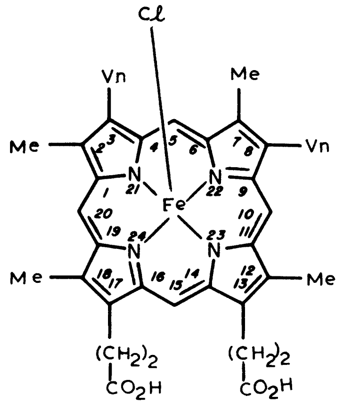
TP-8.4.3. Similarly terms for iron coordination complexes may be defined and interrelated as follows:

Iron Coordination Complexes

heme	:	an iron porphyrin coordination complex
ferroheme	:	an iron(II) porphyrin coordination complex
ferriheme	:	an iron(III) porphyrin coordination complex
hemochrome	:	a low-spin iron porphyrin coordination complex with one or more strong field axial ligands (e.g. pyridine)
ferrohemochrome	:	an iron(II) hemochrome
ferrihemochrome	:	an iron(III) hemochrome
hemin	:	a chloro(porphyrinato)iron(III) coordination complex. For example protohemin = chloro(protoporphyrinato)iron(III) or chloroiron(III) protoporphyrinate
hematin	:	a hydroxo(porphyrinato)iron(III) coordination complex.[c]

Examples:

1.



Protohemin
or
Chloro(protoporphyrinato)iron(III)

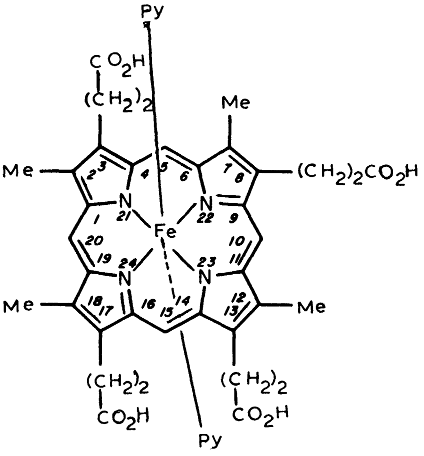
---

a. See TP-4.3.2 for pheophytin and pheophorbide names.

b. See TP-2.1 Fig. 5 for phytoporphyrin structure.

c. Such compounds appear to be isolated as the μ-oxo anhydro dimers (μ-oxo dimers). Examples are given in Rule TP-9.5.

2.



Bis(pyridine)coproferrohemochrome III
or
(Coproporphyrinato III)bis(pyridine)iron(II)

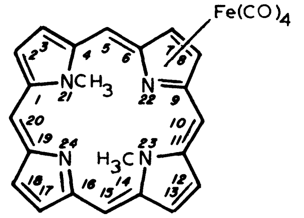
RULE TETRAPYRROLES 9. METAL COORDINATION COMPLEXES—LESS COMMON STRUCTURAL TYPES

Although most of the metal coordination complexes in this series fall under Rule TP-8.1, other structural types do occur, and seem likely to increase. These are named using the Rules for Coordination Compounds[a,b] as illustrated below, where the number in brackets after the side heading refers to the appropriate part of those rules.

TP-9.1. Coordination Complexes of Unknown Structure (Inorganic Rule 7.41). Where the detail of structure is unknown the name, in the extended form "metal complex of free base" (e.g. the zinc coordination complex of bilirubin), indicates stoichiometric composition only.

TP-9.2. Coordination other than at Central Nitrogen (Inorganic Rules 7.33, 7.34, 7.513 and D-2.38, D-2.39.). All earlier examples assume coordination to central nitrogen atoms (Rule TP-8.1). Coordination to other sites must be specifically designated as shown below:

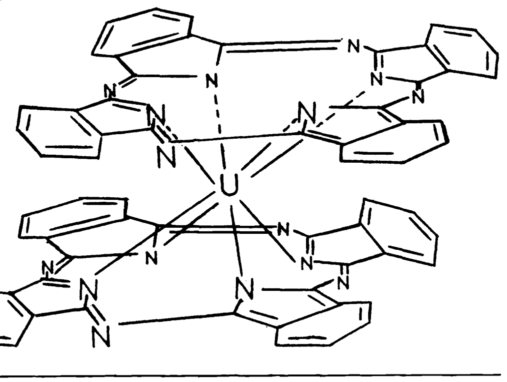
Example:



Tetracarbonyl[7-8-η-(21,23-dimethylporphyrin)]iron(0)
(η is read as hapto)

TP-9.3. Mononuclear Metal Coordination Complexes with Two Tetrapyrrolic Ligands

Example:



Bis(phthalocyaninato)uranium(IV)
or
Uranium(IV) bisphthalocyaninate

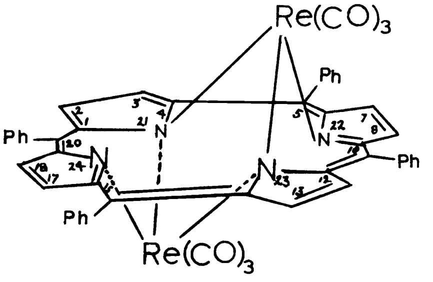
---

[a] IUPAC, "Nomenclature of Inorganic Chemistry, Definitive Rules 1970" 2nd ed. Butterworths, London 1971 also published in *Pure Appl. Chem.* 28, 39(1971), Section 7.

[b] IUPAC, "Nomenclature of Organic Chemistry, Sections A, B, C, D, E, F and H, 1979 edition" Pergamon, 1979, Section D-2.

TP-9.4. Porphyrin as a Bridging Ligand (Inorganic Rule 7.6)

The bridging ligand is given the prefix μ, and if, in addition, certain *atoms* function as bridges, this symbol is repeated to indicate these, as shown in the following example:



μ-[5,10,15,20-Tetraphenylporphyrinato-(2-)-N^{22},N^{24},μ-N^{21},μ-N^{23}]-bis-[tricarbonylrhenium(I)]

or

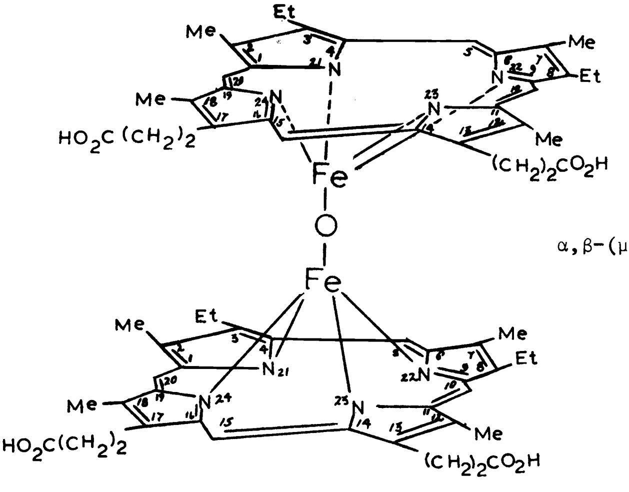
Bis[tricarbonylrhenium(I)] μ-[5,10,15,20-tetraphenylporphyrinate(2-)-N^{22},N^{24},μ-N^{21},-μ-N^{23}]

Less symmetrically substituted molecules of this type can be named by using the locant designators given in Inorganic Rules 7.613 and 7.614 to denote the position of ligands.

TP-9.5. Axial Bridging Ligands.

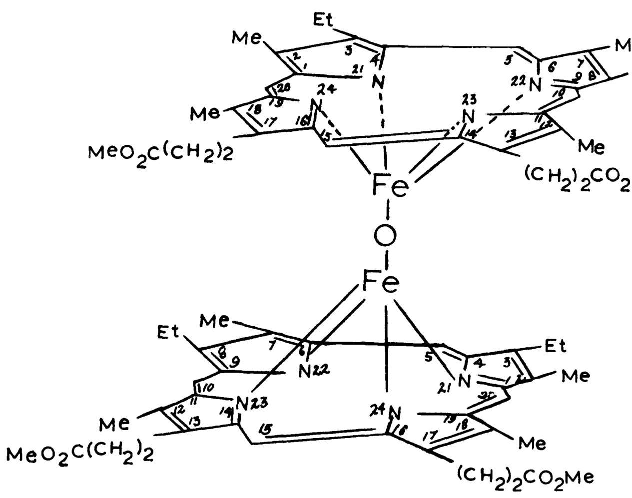
Examples:

1.



α,β-(μ-Oxo)-bis[mesoporphyrinatoiron(III)]

2.



α,α-(μ-Oxo)-bis[(mesoporphyrinato dimethyl ester)iron(III)]

or

Bis[dimethyl 7,12-diethyl-3,8,13,17-tetramethyl-2,18-porphyrindipropionato-(2-)]-β,β-(μ-oxo)-diiron[a]

(Where the stereochemical configuration is unknown the sterochemical designators α and β are omitted).

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2. R. Bonnett, Proceeding of 9th Meeting of the European Association for the Study of Liver Diseases, Hemsedal (1974) p. 212.
3. H. Fischer and H. Orth, *Die Chemie des Pyrrols*, Volume II.1, Akademische Verlagsgessellschaft, Leipzig (1937).
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13. A. R. Battersby and E. McDonald, "B_{12}" (ed. D. Dolphin) Volume 1, p.107, Wiley, New York, 1982.

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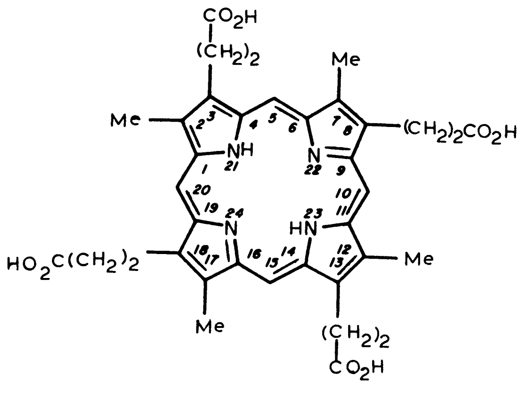
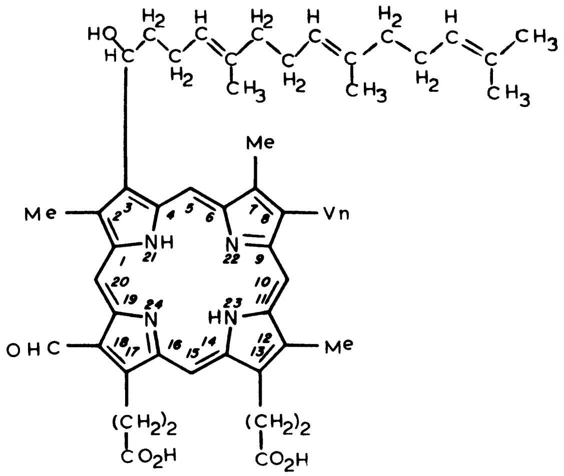
[a] Because the assignment of α and β is dependent on the direction of numbering of substituents, the α side of the trivially named mesoporphyrin is the β side when named systematically.

APPENDIX 1

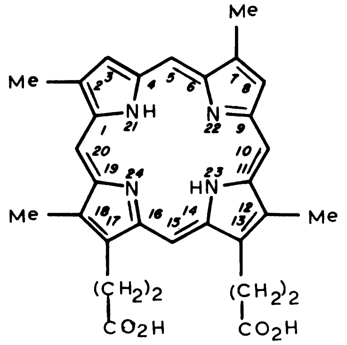
A. TRIVIALLY NAMED PORPHYRINS[a]



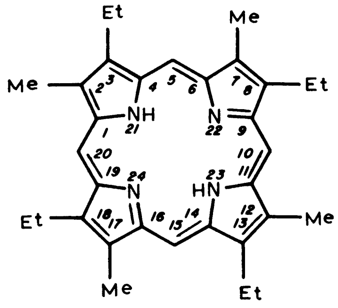
Coproporphyrin I[b]



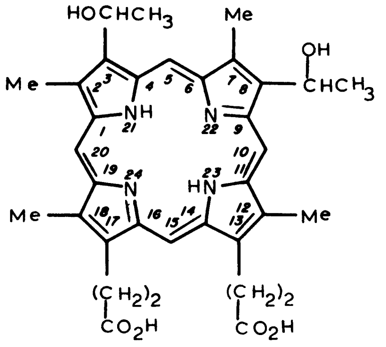
Cytoporphyrin[c]



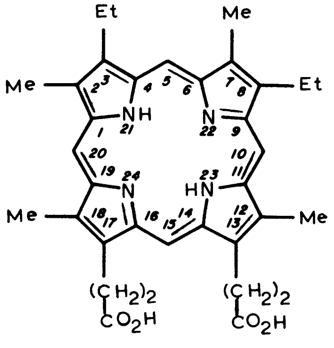
Deuteroporphyrin[c]



Etioporphyrin I[b]



Hematoporphyrin



Mesoporphyrin

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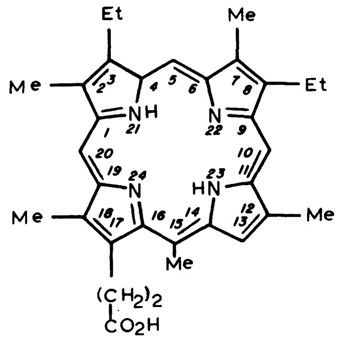
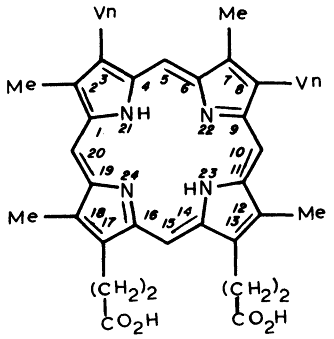
[a] The trivial names apply to the tautomeric structures also. See TP-1.1.

[b] Type I shown only. See TP-2.2 for "type nomenclature" using Roman numerals.

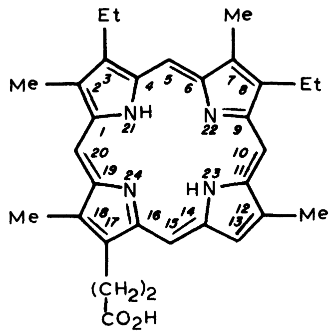
[c] Not to be confused with the isotopically labeled compound deuterioporphyrin.



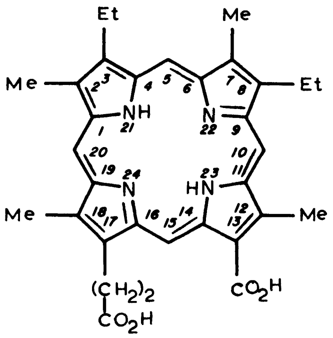
Phylloporphyrin



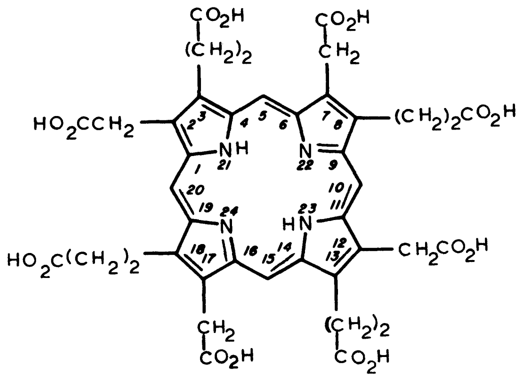
Protoporphyrin



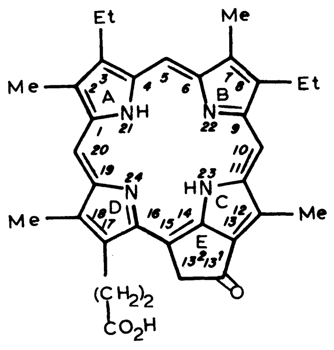
Pyrroporphyrin



Rhodoporphyrin



Uroporphyrin I[a]



Phytoporphyrin

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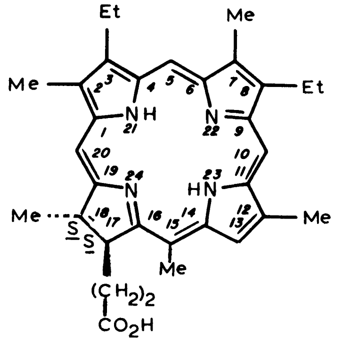
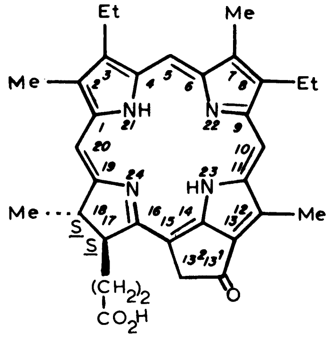
[a] Type I shown only. See TP-2.2 for "type nomenclature" using Roman numerals.

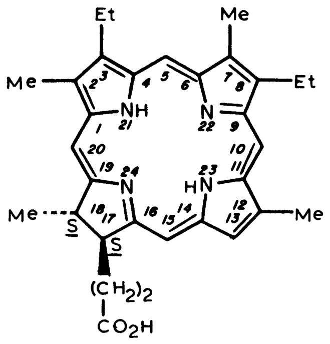
B. TRIVIALLY NAMED CHLORINS



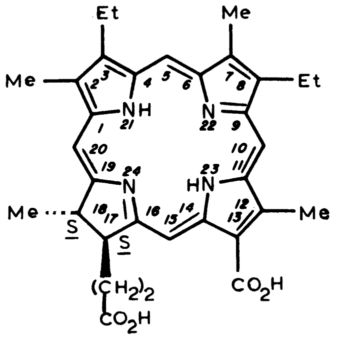
Phyllochlorin[a]



Phytochlorin

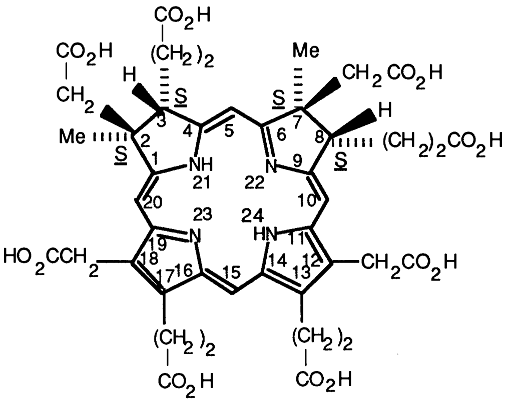


Pyrrochlorin



Rhodochlorin[a]

B′. TRIVIALLY NAMED ISOBACTERIOCHLORINS



Sirohydrochlorin

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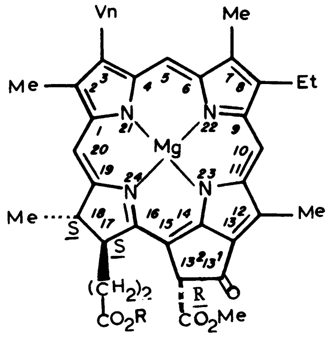
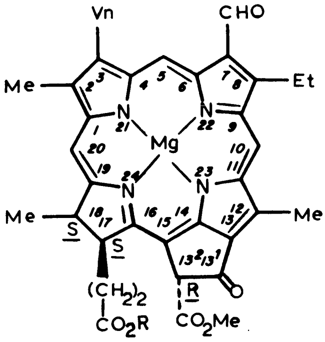
[a] Phyllochlorin and rhodochlorin have been redefined so that they are now 17,18-dihydro derivatives of the corresponding phylloporphyrin and rhodoporphyrin. These chlorin names have formerly been used in the literature to refer to the structure shown, but with vinyl groups in place of ethyl groups at position 3.

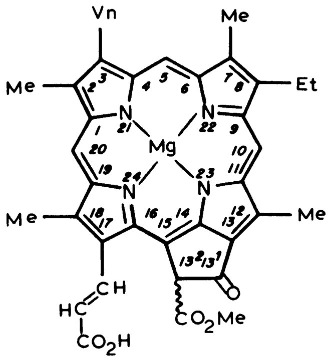
C. TRIVIALLY NAMED CHLOROPHYLLS



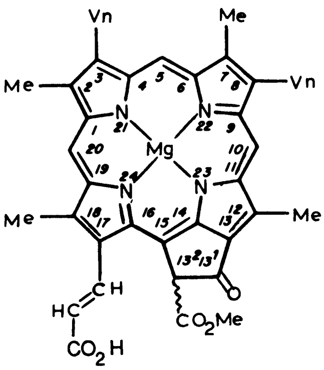
Chlorophyll *a* (R = phytyl)



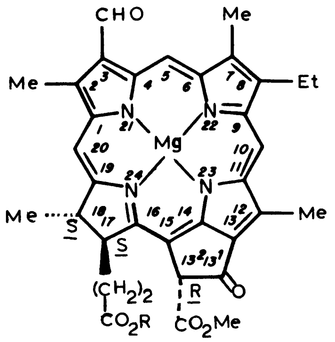
Chlorophyll *b* (R = phytyl)



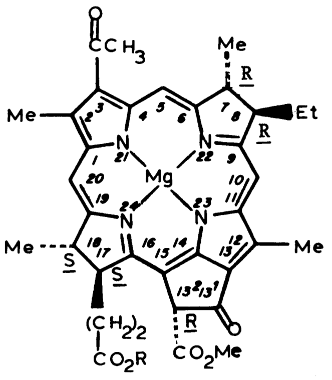
Chlorophyll c_1[a]



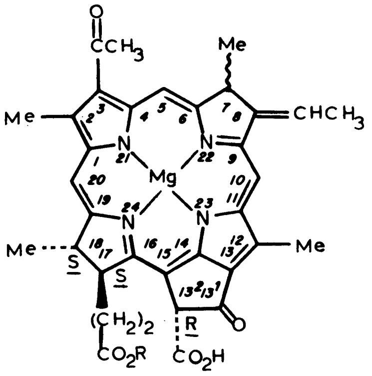
Chlorophyll c_2[a]



Chlorophyll *d* (R = phytyl)

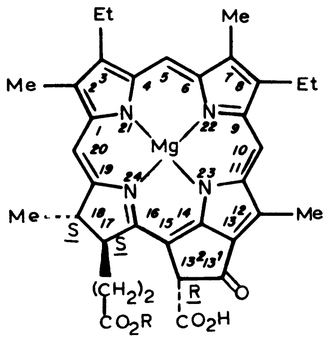


Bacteriochlorophyll *a*



Bacteriochlorophyll *b*

R = phytyl



Mesochlorophyll *a*

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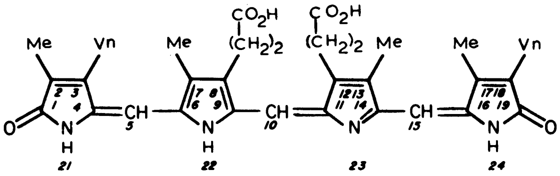
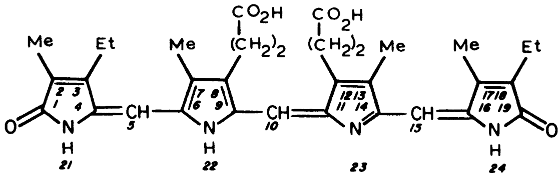
a. In contrast to the other chlorophyll structures, chlorophylls c_1 and c_2 are unsaturated at positions 17 and 18. Further they are free acids at position 17.

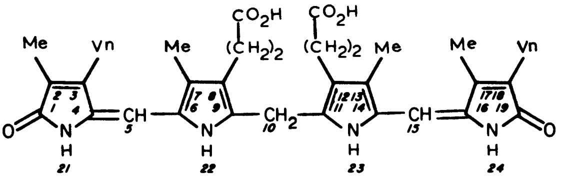
D. TRIVIALLY NAMED BILANES



Biliverdin



Mesobiliverdin



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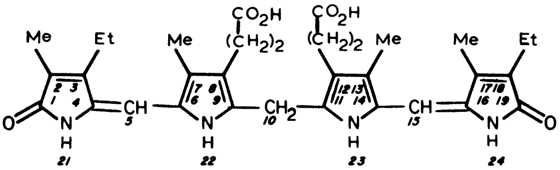
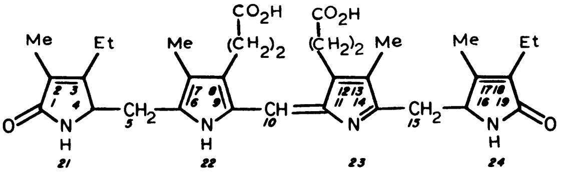
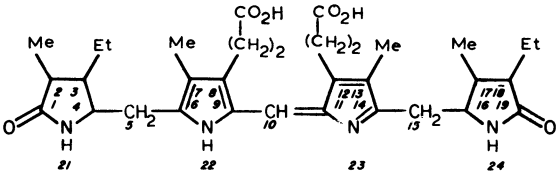


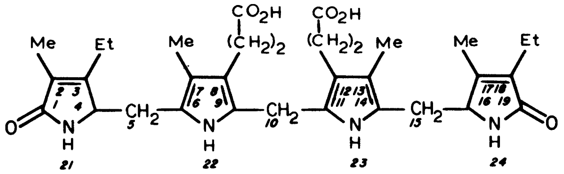
Mesobilirubin



Urobilin



Stercobilin



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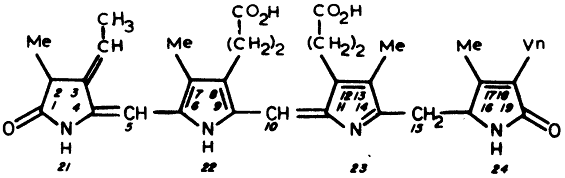
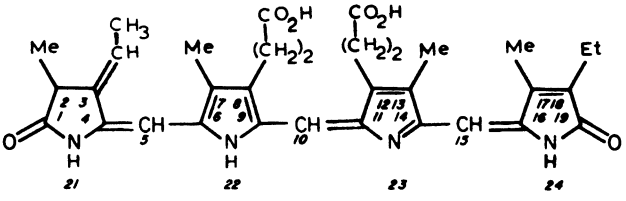
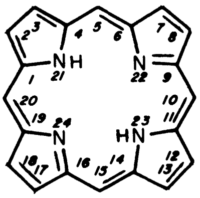


phycoerythrobilin

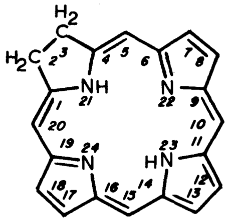


phycocyanobilin

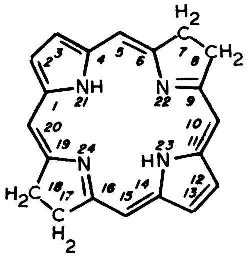
E. FUNDAMENTAL PARENTS



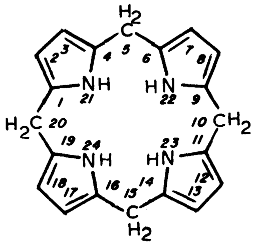
Porphyrin



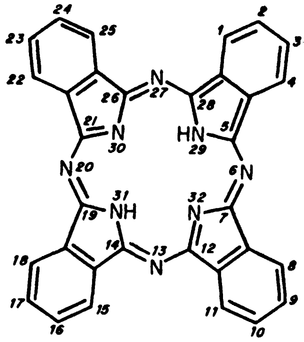
Chlorin



Bacteriochlorin



Porphyrinogen



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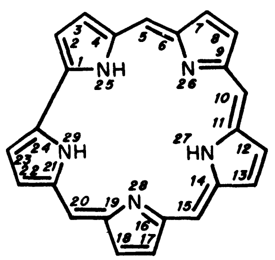
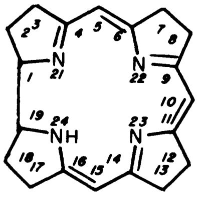
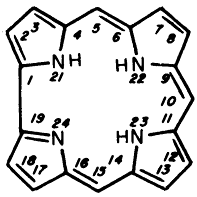


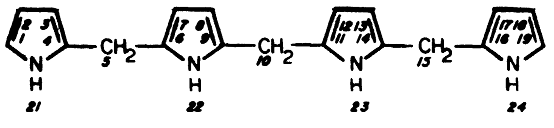
Sapphyrin



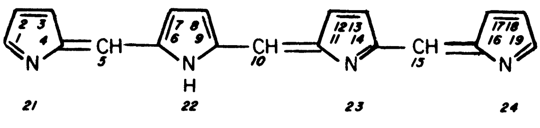
Corrin



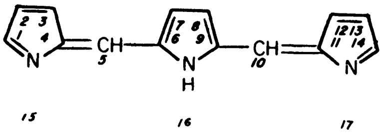
Corrole



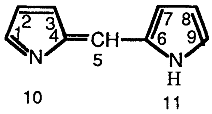
Bilane



Bilin



Tripyrrin



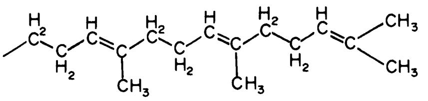
Dipyrrin

APPENDIX 2

COMPARISON OF THE NUMBERING OF THE TRIVIALLY NAMED PORPHYRINS(TNP) WITH NUMBERING BASED ON CNOC/CAS

TNP Trivial Name	Numbering Basis	2	3	7	8	12	13	15	17	18	20
1. Uroporphyrin I	TNP	Cm	Cet	Cm	Cet	Cm	Cet	--	Cm	Cet	--
	CNOC/CAS	Cet	Cm	Cet	Cm	Cet	Cm	--	Cet	Cm	--
2. Coproporphyrin II	TNP	Me	Cet	Cet	Me	Me	Cet	--	Cet	Me	--
	CNOC/CAS	Cet	Me	Me	Cet	Cet	Me	--	Me	Cet	--
3. Etioporphyrin I	TNP	Me	Et	Me	Et	Me	Et	--	Me	Et	--
	CNOC/CAS	Et	Me	Et	Me	Et	Me	--	Et	Me	--
4. Etioporphyrin II	TNP	Me	Et	Et	Me	Me	Et	--	Et	Me	--
	CNOC/CAS	Et	Me	Me	Et	Et	Me	--	Me	Et	--
5. Etioporphyrin III	TNP	Me	Et	Me	Et	Me	Et	--	Et	Me	--
	CNOC/CAS	Et	Me	Et	Me	Et	Me	--	Me	Et	--
6. Etioporphyrin IV	TNP	Me	Et	Me	Et	Et	Me	--	Et	Me	--
	CNOC/CAS	Et	Me	Et	Me	Me	Et	--	Me	Et	--
7. Cytoporphyrin	TNP	Me	R^1CHOH	Me	Vn	Me	Cet	--	Cet —	CHO	--
	CNOC/CAS	Cet	Me	Vn	Me	R^1CHOH	Me	--	—CHO	Cet	--
8. Protoporphyrin	TNP	Me	Vn	Me	Vn	Me	Cet	--	Cet	Me	--
	CNOC/CAS	Cet	Me	Vn	Me	Vn	Me	--	Me	Cet	--
9. Mesoporphyrin	TNP	Me	Et	Me	Et	Me	Cet	--	Cet	Me	--
	CNOC/CAS	Cet	Me	Et	Me	Et	Me	--	Me	Cet	--
10. Hematoporphyrin	TNP	Me	CH_3CHOH	Me	CH_3CHOH	Me	Cet	--	Cet	Me	--
	CNOC/CAS	Cet	Me	CH_3CHOH	Me	CH_3CHOH	Me	--	Me	Cet	--
11. Deuteroporphyrin	TNP	Me	-------	Me	-------	Me	Cet	--	Cet	Me	--
	CNOC/CAS	Cet	Me	Me	-------	Me	---	--	Me	Cet	--
12. Rhodoporphyrin	TNP	Me	Et	Me	Et	Me	—COOH	--	Cet	Me	--
	CNOC/CAS	Cet	Me	Me	Et	Me	Et	--	Me	—COOH	--
13. Pyrroporphyrin	TNP	Me	Et	Me	Et	Me	----	--	Cet	Me	--
	CNOC/CAS	Cet	Me	Me	Et	Me	Et	--	Me	----	--
14. Phylloporphyrin	TNP	Me	Et	Me	Et	Me	----	Me	Cet	Me	--
	CNOC/CAS	Cet	Me	Me	Et	Me	Et	--	Me	----	Me

R^1 =



Cm = $-CH_2COOH$

Cet = $-CH_2CH_2COOH$

CNOC = IUPAC Commission on Nomenclature of Organic Chemistry

CAS = Chemical Abstracts Service

Note: Cet and Cm are often abbreviated to P and A. This is acceptable provided these are defined as $CH_2CH_2CO_2H$ and CH_2CO_2H respectively.

APPENDIX 3

FISCHER TRIVIAL NAMES

The following extensions to the list of accepted trivial names are proposed as permitted: they encompass a further selection of trivial names due to Hans Fischer. They each refer to a single compound and must not be used as a basis for semisystematic nomenclature.

A. Porphyrins

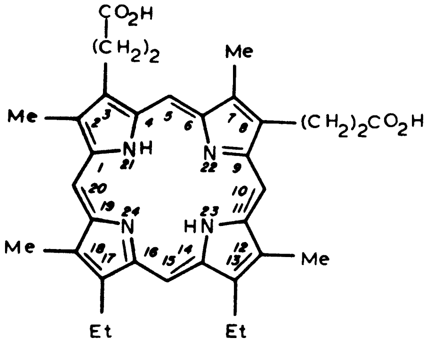
The names are illustrated for isomers of mesoporphyrin, but may also be used for deuteroporphyrin (for Et read H), haematoporphyrin (for Et read $-CH(OH)CH_3$) and protoporphyrin (for Et read $-CH{=}CH_2$).

The names all carry a Roman numeral. The name without such a numeral is already defined in Table 2, and corresponds to isomer IX in the Fischer scheme. The Roman numerals here do not mean the same as those employed in the trivial names in Table 3. Both systems are referred to as "type numbering". The start point and sequence of locant numbering used by Fischer are retained (although the locant numbers follow the 1-24 system, TP-1.2).

Comparison of the Numbering of the Fischer Trivially Named Porphyrins (TNP) with Numbering Based on CNOC/CAS Numbering Principles. Cm = $-CH_2COOH$; Cet = $-CH_2CH_2COOH$; CNOC = IUPAC Commission on the Nomenclature of Organic Chemistry; CAS = Chemical Abstracts Service.

Fischer Isomer Type Number	Numbering Basis	Substituents and Locants							
		2	3	7	8	12	13	17	18
I	TNP	Me	Et	Me	Et	Me	Cet	Me	Cet
	CNOC/CAS	Cet	Me	Cet	Me	Et	Me	Et	Me
II	TNP	Me	Cet	Me	Et	Me	Cet	Me	Et
	CNOC/CAS	Cet	Me	Et	Me	Cet	Me	Et	Me
III	TNP	Me	Et	Et	Me	Me	Cet	Cet	Me
	CNOC/CAS	Cet	Me	Me	Et	Et	Me	Me	Cet
IV	TNP	Me	Cet	Et	Me	Me	Et	Cet	Me
	CNOC/CAS	Cet	Me	Me	Cet	Et	Me	Me	Et
V	TNP	Me	Cet	Et	Me	Me	Cet	Et	Me
	CNOC/CAS	Cet	Me	Me	Et	Cet	Me	Me	Et
VI	TNP	Me	Cet	Me	Cet	Me	Et	Et	Me
	CNOC/CAS	Cet	Me	Cet	Me	Me	Et	Et	Me
VII	TNP	Me	Cet	Me	Et	Me	Cet	Et	Me
	CNOC/CAS	Cet	Me	Et	Me	Cet	Me	Me	Et
VIII	TNP	Me	Et	Me	Cet	Me	Cet	Et	Me
	CNOC/CAS	Cet	Me	Cet	Me	Et	Me	Me	Et
IX	TNP	Me	Et	Me	Et	Me	Cet	Cet	Me
	CNOC/CAS	Cet	Me	Et	Me	Et	Me	Me	Et
X	TNP	Me	Et	Me	Cet	Me	Et	Cet	Me
	CNOC/CAS	Cet	Me	Et	Me	Me	Cet	Et	Me
XI	TNP	Me	Cet	Me	Et	Me	Et	Cet	Me
	CNOC/CAS	Cet	Me	Me	Et	Et	Me	Et	Me
XII	TNP	Me	Et	Et	Me	Cet	Me	Me	Cet
	CNOC/CAS	Cet	Me	Me	Cet	Me	Et	Et	Me
XIII	TNP	Et	Me	Me	Et	Me	Cet	Cet	Me
	CNOC/CAS	Cet	Me	Et	Me	Me	Et	Me	Cet
XIV	TNP	Me	Cet	Et	Me	Et	Me	Me	Cet
	CNOC/CAS	Cet	Me	Cet	Me	Me	Et	Me	Et
XV	TNP	Me	Cet	Et	Me	Cet	Me	Me	Et
	CNOC/CAS	Cet	Me	Et	Me	Me	Cet	Et	Me

Thus mesoporphyrin VI is



B. Bilindiones

The following Fischer trivial names for bile pigments are permitted. Each refers to a single compound, and must not be used as the basis for semisystematic nomenclature. They each have a Roman numeral and a Greek letter as suffixes: the Roman numeral refers to the porphyrin structure (tabulated above) which has been formally broken at the meso bridge denoted by the Greek letter (Fischer numeration, Fig. 1). The structures and names have already been referred to in TP-6.3 and TP-6.4 and are:

biliverdin IIIα, biliverdin IXα (= biliverdin), biliverdin IXβ, biliverdin IXγ, biliverdin IXδ, biliverdin XIIIα, together with the corresponding hydrogenated derivatives (e.g. bilirubins, mesobiliverdins).

The names without a Roman numeral and Greek letter are already defined in Fig. 16-22: in each case the IXα isomer is implied. For convenience the structures of the biliverdin isomers mentioned in the previous paragraph are tabulated below.

Roman Numeral Designation	Substituents at Positions 2	3	7	8	12	13	17	18
IXα	Me	Vn	Me	Cet	Cet	Me	Me	Vn
IXβ	Me	Cet	Cet	Me	Me	Vn	Me	Vn
IXγ	Cet	Me	Me	Vn	Me	Vn	Me	Cet
IXδ	Me	Vn	Me	Vn	Me	Cet	Cet	Me
IIIα	Vn	Me	Me	Cet	Cet	Me	Me	Vn
XIIIα	Me	Vn	Me	Cet	Cet	Me	Vn	Me