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The Biochemical Journal is published and distributed by the Biochemical Society. It is published twice monthly, alternate issues being devoted to Molecular Aspects and to Cellular Aspects of biochemistry. It is planned that in 1975 eight volumes, each volume being made up of three issues, will be published according to the following schedule:

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Biochemical Society Transactions. This is now a separate publication (see below). Volume 3 will be published in 1975, in six parts.

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Papers submitted should be written concisely. Special attention is directed to the sections below concerning the preparation of the typescript. Typescripts that are not concise or do not conform to the conventions of the Biochemical Journal will be returned to the authors for revision. If a paper that has been returned to an author for revision is not resubmitted within one month, it will, on resubmission, be deemed to be a new paper and the date of receipt altered accordingly. A revised paper containing a significant amount of new material will also be redated.

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Papers should be headed by a concise but informative full title, by the names of the authors (preferably with one forename in full for each author) and by the name and address of the establishment where the work was performed. Details of financial support appear in the acknowledgements at the end of the paper.

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The Nomenclature of Corrinoids

(1973 Recommendations)

IUPAC-IUB Commission on Biochemical Nomenclature

1. The corrinoids are a group of compounds containing four reduced pyrrole rings joined into a macrocyclic ring by links between their α-positions; three of these links are formed by a one-carbon unit (methylidyne radicals) and the other by a direct Cα-Cα bond. They include various B-12 vitamins; factors, and derivatives based upon the skeleton of corrin, C₁₂H₁₆N₄ (structure I). The atoms are numbered and the rings are lettered as shown in structure I. The numbering is thus the same as that of the porphyrin nucleus, number 20 being omitted to preserve the identity.

△ Note. The name “corrin” was proposed by those who established its structure because it is the core of the vitamin B-12 molecule; the letters “co” of corrin are not derived from the fact that vitamin B-12 contains cobalt. However, this does not apply to the “cob” terms below, all of which do contain “co” for cobalt.

△ 2. Some important corrinoids that are more unsaturated than corrin itself are derivatives of octadehydrocorrin. This has sometimes been called tetradehydrocorrin because it has four additional double bonds. Although this could be indicated by the prefix “tetrakis(didehydro),” “octadehydro” is preferred.

The octadehydrocorrin system IA has the trivial name corrole.

3. Many important corrinoids have a regular pattern of substituents on the methylene carbon atoms of the reduced pyrrole rings and a cobalt atom in the center of the macrocyclic ring. The heptacarboxylic acid II is named cobyrinic acid. The carboxyl groups are designated by the locants a to g, as shown in II.4 Cobyrinic a,b,c,d,e,g-hexaamide, formerly referred to as Factor V₁, is named cobyrinic acid. Substituents on the side chains may be designated by appropriate locants, e.g., 7β₁-methylcobyrinic acid, if —CH(CH₃)CO₂H replaces —CH₂CO₂H at C-7β of cobyrinic acid.

4. The compound III (R=OH, R'=H), which is the amide formed by combination of cobyrinic acid with d-1-amino-2-propanol at position f, is named cobinie

*Revision of the 1965 document (1) of the Commission on Biochemical Nomenclature (CBN) of the International Union of Pure and Applied Chemistry (IUPAC) and the International Union of Biochemistry (IUB), approved by CBN, IUPAC, and IUB in 1973 and published by permission of IUPAC and IUB. Significant changes from the 1965 version (1) are indicated by △ in the margin. An appendix on abbreviations has been added.

Comments on and suggestions for future revisions of these Recommendations may be sent to any member of CBN.

Reprints of this publication may be obtained from W. E. Cohn, Director, NAS-NRC Office of Biochemical Nomenclature, Oak Ridge National Laboratory, Box Y, Oak Ridge, Tennessee 37830, U.S.A.

* Members of the Commission are: O. Hoffmann-Ostenhof (Chairman), W. E. Cohn (Secretary), A. E. Braunstein, B. L. Horecker, P. Karlson, B. Keil, W. Klyne, C. Liébeeq, E. C. Webb, and W. J. Whelan.

The names cobyrinic acid, cobinic acid, cobamic acid, and cobalamin, and names derived from them, imply the relative and absolute configurations shown in the structural formulas. α and β are used as in Steroid Nomenclature (2) and the IUPAC E-Rules (3) to indicate stereochemical configuration. Epimers at C-3, C-8, and C-13 may be designated as, e.g., 13-epicobalamin.
acid;* its hexaamide (III; R=H₂N, R'=-H) is named cobinamide.⁴

5. The compound III (R=OH, R'=-H) and additionally linked, as stated in 7 above, by a bond between the N-3 and the cobalt (in position α).⁴ They may be named as cobamides, as above, or according to the pattern:

(ligand in Coβ position, if any) - cobalamin. (Xb)

Examples:

Coα-[α-(5,6-dimethylbenzimidazolyl)]-Coβ-cyanocobamide, also known as vitamin B-12, is termed cyanocobalamin.

Coα-[α-(5,6-dimethylbenzimidazolyl)]-Coβ-aquacobamide, also known as vitamin B-12a, is termed aquacobalamin.

Coα-[α-(5,6-dimethylbenzimidazolyl)]-Coβ-hydroxocobamide, also known as vitamin B-12b, is termed hydroxocobalamin.

Note: aquacobalamin is the conjugate acid of hydroxocobalamin.

Coα-[α-(5,6-dimethylbenzimidazolyl)]-Coβ-nitritocobamide, also known as vitamin B-12c, is termed nitritocobalamin.

10. Anion(s) associated with the corrinoids is(are) stated in the usual way after the name of the (cationic) corrinoid, e.g., cobamic dichloride (not dichlorocobamic acid).

11. The state of oxidation of the cobalt may be specified, when necessary, as follows:

vitamin B-12 cyanocob(III)alamin

vitamin B-12r cob(II)alamin⁵

vitamin B-12s cob(I)alamin⁵

12. Displacement of the ribosyl-bound aglycon base from its normal coordinate bonding to position α of the cobalt by another ligand (or by water) may be indicated by placing the name and locant of the replacing ligand before the corrinoid name and enclosing the modified corrinoid name (see Section 6) in parentheses. (See also Section 7.)

Example:

Coα-aqua-Coβ-methyl(2-methyladenyl-

* The previous document (1) erred in prefixing “cyano” to these names.

A 6. Glycosyls and nucleotides (which are N-glycosyl derivatives at C-1 of the ribofuranose unit) of cobamides are named by adding the name of the appropriate aglycon radical (ending in “yl”) as a prefix to the name of the corrinoid allotted according to 1–5, e.g., aglyconylcobamide (VI).

A 7. Most of the important natural products in this series have aglycon radicals containing an imidazole nucleus, one N of the latter being covalently bonded to the ribose while the other is coordinately bonded to what is, by this attachment, defined as the cobalt-α position. The latter situation (VII) is assumed to exist unless otherwise indicated. When another ligand occupies the cobalt-α position, it and its locant may be indicated by, e.g., (Co-α ligand) - aglyconylcobamide (VIII). The absence of a “Coα-ligand” term, as in the cobalamins (Sec. 9), indicates that the aglycon radical attached to the ribose occupies the cobalt-α position as well.

8. Cobamides bearing a ligand in the cobalt-β position [which implies Co(III)] may be named as follows:

(Coα-ligandyl)-(Coβ-ligandyl)-

(aglyconylcobamide). (IX)

or, if the aglycon is attached to the cobalt-α position, as indicated in Section 7,

aglyconyl-(Coβ-ligandyl)cobam ide (Xa)

In a cobalamin (see 9 below), the latter becomes simply

ligandylecobalamin (Xb)

See also Section 15.

9. Cobalamins.⁴ A cobalamin is a cobamide in which 5,6-dimethylbenzimidazole is the aglycon attached by a glycosyl link from its N-1 to the C-1 of the ribose
cobamide), in which the 2-methyladenyl residue is attached to the ribose residue but is not coordinately bound to the cobalt atom, having been displaced by water. Methyl occupies the Coβ position.

13. Modified, derived or related compounds are named systematically from the largest of the compounds I, II, or III that is contained in them.

Examples:
- cobyricin acid \(a, b, c, d, e, g\)-hexaamide \(f\)-2-hydroxyethylamide;
- 3, 8, 13, 17-tetraethyl-1, 2, 2, 5, 7, 7, 12, 12, 15, 17, 18-undecamethylcobalticorrin dichloride (for the dichloride of fully decarboxylated cobyricin acid);
- 12α-carboxycobyricin acid (for cobyricin acid in which the 12α-methyl group has been replaced by \(-\text{CH}_2\text{CO}_2\text{H}\)).

14. Replacement of the cobalt atom in compounds II or III by another metal or by hydrogen is indicated by replacing “co” in the “cob” part of the name with the name or the root of the name of the replacing metal followed by “o” or “i” according to its valence (e.g., cupri, cupro, zinco). When cobalt is replaced by hydrogen, “hydrogeno” replaces “co.”

Examples:
- ferrobamic acid
- hydrogenobamic acid

See Note to Section 1 concerning corrin. This replacement nomenclature does not apply to corrole (Section 2).

15. Cofactor forms. The coenzymatically active forms of the B-12 vitamins (Section 12) and their analogs possess an organic ligand, either methyl or 5′-deoxy-5′-adenosyl, attached to the β position of the cobalt by a carbon-to-cobalt bond, i.e., in the position of the CN in formula IV. These adducts (4) should be named according to the pattern:

\[\text{Co}α-(\text{radical in } \alpha \text{ position})-\text{Co}β-(\text{ligand in } \beta \text{ position})(\text{corrinoid name})\]

\[\Delta\]

* For brevity, 5′-deoxy-5′-adenosyl may be replaced by adenosyl, with definition, as is commonly seen in S-adenosylmethionine. The intermediate form, 5′-deoxyadenosyl, should not be used.

Examples:
- \(\text{Co}α-[\alpha-(5, 6\text{-dimethylbenzimidazolyl})]-\text{Co}β\)-adenosylcobamide, for the compound formerly known as “coenzyme B-12.”
- \(\text{Co}α-[\alpha-(5, 6\text{-dimethylbenzimidazolyl})]-\text{Co}β\)-methylcobamide or methylcobalamin, for the compound involved in several reactions, including methionine biosynthesis, where a methyl group is ligated to the cobalt in the β position.

16. Summary. The trivial names applied to corrinoids of varying complexity are perhaps confusing to the nonspecialist, and it seems desirable to tabulate (in outline) how they are interrelated (Table I).

NOTES ON FORMULAS

1. In formulas II and III, the corrin nucleus is represented as being roughly in the plane of the paper. Bonds joining peripheral substituents to the nucleus are shown by the same convention as in the steroid series (2), i.e., full (heavy) lines are bonds lying above the plane of the ring system, while dashed (broken) lines are bonds lying below this plane.

2. Formulas II, III, and IV represent the true absolute stereochemical configuration of the structures as determined by X-ray work (5, 6). The CN is in the β-position of the cobalt, the ribose-bound heterocyclic base in the α-position, in formula IV. When adenine is the heterocyclic base, it is usually bound to the ribose by its N-7, the opposite from what is seen in the nucleic acids.

3. Formula V represents the absolute stereochemical configuration of the ribofuranose residue. For convenience in comparing it with formula IV, it is written with the α-substituent at C-1 above the plane of the ring (i.e., the reverse of the usual carbohydrate method) (7).
TABLE I

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<td>Skeleton (porphyrin nucleus minus C-20)</td>
<td>Corrin (I)</td>
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<td>3</td>
<td>1, with standard side chains and with cobalt</td>
<td>Heptaacid</td>
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<tr>
<td>4</td>
<td>3, with D-1-amino-2-propanol at position f</td>
<td>Cobyric acid</td>
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<td>5</td>
<td>4, with D-ribofuranose 3-phosphate at position 2</td>
<td>Cobyrinic acid (II)</td>
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<td>7</td>
<td>5, with heterocyclic base attached by N-</td>
<td>Cobyric acid (III)</td>
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<td>9</td>
<td>Many &quot;B₁₂&quot; vitamins and derivatives, in</td>
<td>Cobinamide</td>
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<td>15</td>
<td>&quot;B₁₂ coenzymes&quot;, compounds in which a further</td>
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<td>organic group (X-yl) is β-ligated to cobalt</td>
<td>Aglyconylecobamide (VI)</td>
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<td>(Sections 9, 15)</td>
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<td>X-ylcobalamin;</td>
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<td></td>
<td></td>
<td>(Coα-ligandyl)-</td>
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<td>(Coβ-X-yl)cobamide (X)</td>
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(1) Corrin

(2) Heptaacid, hexaamide

(a) HO₃C–CH₂
(b) CO₂H
(c) CH₃–CH₂–CO₂H
(d) CH₃
(e) CH₃–CH₂–CO₂H
(f) HO₂C–CH₂–CH₂
(g) HO₃C–CH₂

Corrin (I)

Cobyric acid (II)
Cobyric acid (III)
Cobyric acid (III-V)
Aglyconylecobamide (VI)
Cobalamin
X-ylcobalamin;
(Con-ligandyl)-
(Con-X-yl)cobamide (X)

1975
**NOMENCLATURE OF CORRINIOIDS**

IV. Sketch based on Hodgkin et al. (5). Detail of substituents on corrin nucleus (except side chain at C-17) is omitted for the sake of clarity.

IV. Vitamin B-12

V. \( \alpha \)-d-Ribofuranose 3-phosphate residue

VI. Aglyconylcobamide (III: \( R' = P \)-Rib-aglycon).
VII. Aglyconylcobamide, with aglyconyl ligated to cobalt (IV without CN and with dimethylbenzimidazole as aglycon).

VIII. (Coα-Ligandyl)-aglyconylcobamide (ligand has "displaced" aglycon of VII).

IX. (Coα-Ligandyl)- (Coβ-ligandyl)aglyconylcobamide (VIII with additional ligand in Coβ position).

X. (a) Aglyconyl-(Coβ-ligandyl)cobamide (VII with additional ligand in Coβ position; IV with dimethylbenzimidazole as aglycon, CN as Coβ ligand). (b) Ligandylcobalamin (if aglycon is dimethylbenzimidazole as in IV, and with CN as Co,B ligand).

REFERENCES

APPENDIX: ABBREVIATIONS FOR CORRINIOIDS
This appendix was inspired by the burgeoning literature concerning corrinoid compounds, many of which have long and unwieldy names—a fact that has led to a variety of ad hoc abbreviations that in turn has led to difficulties for the reader.

Many individuals, including, but not limited to those whose names appear in the references, have assisted in the development of the system and symbols here proposed. They are not here named, but a special acknowledgment is made of the assistance of B. M. Babor to CBN in the construction of this appendix.

In accordance with several preceding CBN documents (1-3), as well as with standard chemical practice, the abbreviations are constructed by assembling symbols representing the various radicals involved, rather than from combinations of letters drawn haphazardly from the complete names of the compounds. The use of symbols reflects the actual structure of a compound and facilitates the writing of equations for
its chemical transformations. In particular, the use of DBC, DMBC, etc., is discouraged, as is the use of B-12 (except as vitamin B-12), coenzyme B-12, and “factor” terms.

I. Names and Symbols

<table>
<thead>
<tr>
<th>Names</th>
<th>Symbols</th>
</tr>
</thead>
<tbody>
<tr>
<td>corrin</td>
<td>of Crn</td>
</tr>
<tr>
<td>free acid</td>
<td>(for the hexamid)</td>
</tr>
<tr>
<td>cobyric acid</td>
<td>Cby</td>
</tr>
<tr>
<td>cobiinic acid</td>
<td>Cbi</td>
</tr>
<tr>
<td>cobamic acid</td>
<td>Cba</td>
</tr>
<tr>
<td>cobalamnin</td>
<td>Cbl</td>
</tr>
</tbody>
</table>

II. Designation of Substituents Attached to Cobalt

Ligands coordinated to the \( \alpha \) and \( \beta \) position of the cobalt (below and above the plane of the corrin residue, respectively, as shown in structure IV) are represented by terms that precede the symbol for the corrinoid residue. If the positions of the ligands are unknown or not specified, the two terms representing the ligands in the \( \alpha \) and \( \beta \) position are enclosed in one set of parentheses and are separated by a comma. If the positions are known and specified, the \( \alpha \) ligand precedes and is set apart by parentheses; the \( \beta \) is enclosed (separately) only if its complexity may make it ambiguous. If the ligands are identical, a single term followed by the subscript 2 is used.

A. Anion substituents. The chemical symbol for the anion is used. Aqua is abbreviated aq. Examples.

\[(\text{Me})\text{aqCbi} \ \text{(methyl)aquocobinamide}\ (4) \text{ (methyl in } \alpha \text{ position)}\]
\[(\text{CN})\text{MeCbi} \ \text{(cyanomethylcobinamide) (methyl in } \beta \text{ position)}\]
\[(\text{CN}, \text{aq})\text{Cbi} \text{ or (aq,CN)Cbi cyanooaquocobinamide (ligand location unspecified)}\]

B. Alkyl substituents.

1. Primary substituents are designated by

\[\text{A cobalamin is a cobamidine in which } 5,6-\text{dimethylbenzimidazole is covalently bonded to the ribose in } \alpha\text{-glycosidic linkage; it is thus a dimethylbenzimidazolylcobamidine and can be symbolized as such. However, it is often convenient to have a short symbol for this complex, hence Cbl. Cbl is recommended in place of the former B_{12} or B-12 for chemical use.}\]

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naming the alkyl group\(^8\) without denoting the position attached to the cobalt, as it is always 1. Examples:

\[(\text{aq})\text{EtCbi} \ \text{(aqua)ethylcobinamide}\]
\[(\text{CN})\text{(2-OAcBu)}\text{Cbi} \ \text{(cyano)(2-acetoxybutyl)-cobinamide}\]

2. Secondary substituents are named similarly, except that the position attached to the cobalt is given by a locant suffixed to the name of the alkyl group (as in the \(-x\)-yl name). Examples.

\[(\text{aq})(\text{Bu}-2)\text{Cbi} \text{ or (aq)}\text{But^\*Cbi (aqua)(a.ee-bu)lycobinamide (5)}\]
\[(\text{aq})(3-\text{OAcBu}-2)\text{Cby} \ \text{(aqua)(3-acetoxybutyl)-lycobinamide}\]

3. Alicyclic groups are indicated by a small “\(c\)” before the symbol for the alkyl residue. In these compounds, cobalt is always assumed to be substituted in position 1 of the ring. Examples:

\[(\text{aq})\text{eHxCbi} \ \text{(aqua)cyclohexylecobinamide (5)}\]
\[(\text{CN})(2-\text{HOePe})\text{Cby} \ \text{(cyanoc)(2-hydroxyeyelo-pentyl)cobinamide}\]

4. 5’-Deoxy-5’-adenosyl in the \( \beta \) coordination position, as in “coenzyme B-12,” is represented by the symbol Ado for “adenosyl,” \(6\) a 2’-deoxyadenosine residue by dAdo (3). Unusual deoxyadenosine residues can be indicated by superscripts (e.g., \(d^4\)Ado, \(d^4\)Ado). See C below.

C. Cobamides of the cobalamin\(^7\) type. As the symbol Cbl designates \(\alpha-(5,6\)-dimethylbenzimidazolyl)cobamide [cob(III)alamin], only those cobamides having this base utilize Cbl. Those containing another base are named as cobamides, utilizing the symbol Cba. Hence, Cbl is preceded by only a single term, the one representing the \( \beta \)-substituent. Examples are in Table IA.

Notes:

i. The hyphenation in the case of secondary alkyl substituents and similar situations of potential confusion may make it necessary to enclose the \( \beta \)-substituent in parentheses, or set it off by a hyphen.

ii. If the replacing base (in \( \alpha \) position) is unspecified, the term (?\() is used, e.g., (\(?)\text{MeCba}. The term (OH/base) indicates that the ribose residue is not attached to the \(\text{Co-x}\)-linked base.

\(\) Symbols for alkyl groups are Me, Et, Pr, Pr\(^\prime\), Bu, Bu\(^\prime\), Bu\(^\prime\), Pe, Hx, Hp, . . . .
TABLE IA

<table>
<thead>
<tr>
<th>Compound</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>CN-Cbl</td>
<td>cyanocob(III)alamin (vitamin B-12)</td>
</tr>
<tr>
<td>AdoCbl</td>
<td>adenosylecob(III)alamin (6, 7)</td>
</tr>
<tr>
<td>PrCbl</td>
<td>n-propylocob(III)alamin; methyl-, etc., similarly (8, 9)</td>
</tr>
<tr>
<td>(Ade)(Pr-2)Cba or (Ade)Pr-Cba&lt;sup&gt;a&lt;/sup&gt;</td>
<td>Coα-[α-(aden-9-yl)]-Coβ-isopropylcobamide</td>
</tr>
<tr>
<td>(Bza)MeCba&lt;sup&gt;b&lt;/sup&gt;</td>
<td>Coα-(α-benzimidazolyl)-Coβ-methylcobamide</td>
</tr>
<tr>
<td>2-(MeOOC)EtCbl</td>
<td>Coα-[α-(aden-7-yl)]-Coβ-adenosylcobamide (10)</td>
</tr>
<tr>
<td>(Ado-7)AdoCba&lt;sup&gt;a&lt;/sup&gt;</td>
<td>Coα-[α-(aden-7-yl)]-Coβ-adenosylcobamide (10)</td>
</tr>
<tr>
<td>(2-SHAdo-7)AdoCba&lt;sup&gt;a&lt;/sup&gt;</td>
<td>Coα-[α-(2-thiaaden-7-yl)]-Coβ-adenosylcobamide (11)</td>
</tr>
<tr>
<td>(5-MeOBza)MeCba</td>
<td>Coα-(5-methoxybenzimidazolyl)-Coβ-methylcobamide&lt;sup&gt;c&lt;/sup&gt; (12, 13)</td>
</tr>
<tr>
<td>(2-MeAdo-7)CN-Cba&lt;sup&gt;a&lt;/sup&gt;</td>
<td>Coα-[α-(2-methylenaden-7-yl)]-Coβ-cyanocobamide (11, 14)</td>
</tr>
<tr>
<td>(Ade)CN-Cba&lt;sup&gt;a&lt;/sup&gt;</td>
<td>Coα-[α-(aden-9-yl)]-Coβ-cyanocobamide (pseudovitamin B-12)</td>
</tr>
<tr>
<td>(Ade)OH-Cba&lt;sup&gt;a&lt;/sup&gt;</td>
<td>Coα-[α-(aden-9-yl)]-Coβ-hydroxocobamide (hydroxypseudovitamin B-12)</td>
</tr>
<tr>
<td>(Ade)MeCba&lt;sup&gt;a&lt;/sup&gt;</td>
<td>Coα-[α-(aden-9-yl)]-Coβ-methylcobamide</td>
</tr>
<tr>
<td>[4-(Ade-9)Bu]Cbl&lt;sup&gt;c&lt;/sup&gt;</td>
<td>[4-(aden-9-yl)butyl]cob(III)alamin (6)</td>
</tr>
<tr>
<td>(6MeSPur)AdoCba</td>
<td>Coα-(α-6-methylthiopurinyl)-Coβ-adenosylcobamide (15)</td>
</tr>
</tbody>
</table>

<sup>a</sup> Ade alone represents adenine bonded to the ribosyl moiety through its 7 position (i.e., a 7-α-D-ribofuranosyladenine). Bonding to the cobalt is thus through N-9. When these positions are reversed, Ade-7 and aden-7-yl are used (i.e., the locant specifies the N linked to cobalt).

<sup>b</sup> Bza = benzimidazolyl.

<sup>c</sup> As this is a cobalamin, the adenine residue is not in the Coα position, but is attached (-9-yl) to a but-4-yl residue that is in turn linked to the β position of the cobalt. Named as a cobamide, it would be (Me<sub>2</sub>Bza)[4-(Ade-9)Bu]Cba.

<sup>d</sup> Factor III<sub>m</sub> (15, 16).

iii. If the α-substituent (the “base”) is displaced from the cobalt by another ligand, but remains attached to the ribosyl residue, the same system is used. Example:

<table>
<thead>
<tr>
<th>Compound</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>(2-MeAdo/aq)MeCba</td>
<td>Coα-aqua-Coβ-methyl(2-methyladenylcobamide)</td>
</tr>
<tr>
<td>(Ade/CN)CN-Cba</td>
<td>Coα-cyano-Coβ-cyano-(adenylcobamide) or dicyanoadenylcobamide</td>
</tr>
</tbody>
</table>

In abbreviating cobalamin derivatives, the base need not be specified. Replacement of the base by another Coα ligand is indicated by merely adding to the abbreviation a term corresponding to the replacing ligand. Examples:

<table>
<thead>
<tr>
<th>Compound</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>(OH)MeCbl</td>
<td>Coα-hydroxo-Coβ-methylcobalamin or Coα-hydroxo-Coβ-methyl(dimethylbenzimidazolylcobamide)</td>
</tr>
<tr>
<td>(CN)₂Cbl</td>
<td>Coα-cyano-Coβ-cyanocobalamin or dicyanocobalamin</td>
</tr>
</tbody>
</table>

iv. Cobalt valences of II or I may be indicated by superscripts (e.g., Cbl<sup>II</sup>).

III. Designation of Alterations and Substitutions on the Corrin Ring

Substituents on the ring itself are represented by symbols following the symbol for the corrinoid, with locants indicating the positions of the substituents. Epimerization is indicated in a similar manner. Symbols representing replacements on the carboxyl groups at the periphery of the corrin residue follow those that designate substituents directly on the ring. The location of the substituent is indicated by the letter corresponding to the carboxyl group that carries it. Examples:

<table>
<thead>
<tr>
<th>Compound</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>CN-Cbl(13-epi)</td>
<td>cyano(13-epi)cobalamin</td>
</tr>
<tr>
<td>CN-Cbl(13epi-eOH)</td>
<td>Coα-(α-5,6-dimethylbenzimidazolyl)-Coβ-cyano(13-epi)cobamic a,b,c,d,g-pentaamide</td>
</tr>
<tr>
<td>Ado-Cbl(10-Cl)</td>
<td>adenosyl-10-chlorocobalamin (aq) AdoCbl(ε-PhNH)</td>
</tr>
<tr>
<td>(CN)Cl-Cby(8-NH-c-lactam)</td>
<td>(CN)₂Cby(OMe)</td>
</tr>
</tbody>
</table>

If the location of the carboxyl substituent(s) is unknown, a term of the following structure should be used:

(a:g-X)
group, and $n$ refers to the number of carboxyl groups substituted. Examples:

\[(CN)\text{aq}Cby[a;g-(NH\text{aq})]_n \text{cyanooacobyrinic acid pentaamide (14)}\]

\[(CN)\text{aq}Cby[10-Cl-a;g-(NH\text{aq})]_4 \text{10-chloro derivative of the above}\]

\[IV. \text{ Replacement of Cobalt by Other Metals (18, 19)}\]

Corrinoids containing metals other than cobalt are symbolized by placing the symbol of the replacing metal in square brackets preceding and attached to the symbol of the corrinoid. Thus, a hydrogenocobamide utilizes \([H]Cba\), a nickelocobalamin \([Ni]Cbl\), a zinccobinamide \([Zn]Cbi\), etc. Phenylcupribamide \((19, 20)\) could be indicated as \((Ph)[Cu]Cba^+\). I, II, and III may be added as superscripts when needed.

\[V. \text{ Isotopic Labeling}\]

A labeled position is indicated in the usual fashion \((21)\), e.g.,

\[(Bza)\text{Me}[^{15}C]Cba \text{ Co}^\alpha - (\alpha - \text{benzimidazolyl}) - Co\beta-\text{methyl}[^{15}C]\text{cobamide}\]

\[(Bza)[^{14}C]MeCba \text{ Co}^\alpha-(\alpha\text{-benzimidazolyl})-Co\beta-[^{14}C]\text{methylcobamide}\]

\[([4-^3H]Bza)MeCba \text{ Co}^\alpha-(\alpha - [4-^3H]\text{benzimidazolyl})-Co\beta-\text{methylcobamide}\]

\[VI. \text{ Metallocorrins}\]

As corrin contains no metal (the name "corrin" being derived from "core", not "cobalt"), complexes of metals with corrin require specification of both terms. Example: Cu$^{111}$Crn for copper(II) corrin.

\[REFERENCES\]

1. IUPAC-IUB Commission on Biochemical Nomenclature (1972) Arch. Biochem. Biophys. 150, 1; and in other journals.
2. IUPAC-IUB Commission on Biochemical Nomenclature (1972) Arch. Biochem. Biophys. 151, 597; and in other journals.
21. "Instructions to Authors" (1972) J. Biol. Chem. 247, 4; and elsewhere.

Acknowledgement. We are indebted to the Editors and Publishers (Academic Press) of Archives of Biochemistry and Biophysics for permission to reproduce these Recommendations photographically.
All Tentative Rules and Proposals of the IUPAC-IUB Commission of Biochemical Nomenclature (CBN) are available from Waldo E. Cohn, Director, NRC Office of Biochemical Nomenclature, Oak Ridge National Laboratory, Box Y, Oak Ridge, Tenn. 37830, U.S.A.

1. Abbreviations and Symbols for Chemical Names of Special Interest in Biological Chemistry [see Biochem. J. (1966) 101, 1–7 (extended by items 6, 11 and 15 below)].

2. Nomenclature of Vitamins, Coenzymes and Related Compounds: Trivial Names of Miscellaneous Compounds of Importance in Biochemistry, Nomenclature of Quinones with Isoprenoid Side Chains, Nomenclature and Symbols for Folic Acid and Related Compounds, Nomenclature of Corrinoids. Tentative Rules [see Biochem. J. (1967) 102, 15–22 (but see items 10 and 22 below)].

3. Abbreviated Designation of Amino Acid Derivatives and Peptides [see Biochem. J. (1967) 102, 23–27 (superseded by item 15 below)].


9. Revised Tentative Rules for Nomenclature of Steroids [see Biochem. J. (1969) 113, 5–28 (for amendments see item 16 below)].


16. Amendments to Rules for Nomenclature of Steroids [see Biochem. J. (1972) 127, 613–617 (amendments to item 9 above)].


22. The Nomenclature of Corrinoids. Recommendations [this document (supersedes section in item 2 above)].

A document, OBN-5, describing the (American) NRC Office of Biochemical Nomenclature, and listing other rules affecting biochemical nomenclature, is available from its Director, Dr. Waldo E. Cohn [see also J. Chem. Doc. (1967) 7, 72–73; (1969) 9, 235–241].

1975
IUPAC-IUB Commission on Biochemical Nomenclature (CBN)

Nomenclature of Tocopherols and Related Compounds

Recommendations (1973)¹

The structure of natural \( \alpha \)-tocopherol, the most potent natural source of vitamin-E activity, was elucidated in 1938; at the same time, the first synthesis of a biologically active product of similar structure was reported. Work in the following years revealed the existence in nature of a whole family of structurally related compounds with qualitatively identical biological action.

Recommendations for the nomenclature of the vitamins, including the tocopherols, were published by CBN in 1966 [1]; in this document, the configuration of the natural \( \alpha \)-tocopherol as \( 2R,4'E,8'S \) is mentioned in a footnote, followed by the sentence “The designation of other stereoisomers is under consideration”.

From the work of Iler and his coworkers [2a,2b] we are now in a position to describe unequivocally the configuration of all compounds of this class. However, to devise a nomenclature of the tocopherols taking into account the stereochemistry turned out to be a more difficult task than originally assumed. This was caused by the fact that some of the practically important tocopherols are mixtures of diastereoisomers. So far, no system of designation for mixtures of diastereoisomers has ever been devised, but the importance of the tocopherol mixtures is such that a system of designation is needed.

Traditionally, the symbols \( \delta \), \( l \) and \( dl \) have been used for distinguishing the compounds, but these signs, originally indicating the direction of the rotation of plane-polarized light passing through solutions of the compounds, do not accord with the present IUPAC rules for stereochemistry (E-Rules) [3]. To replace them, as suggested for similar cases, by the signs (\(+\)), (\(-\)), and (\( \pm \)) is not advisable because, in tocopherols, the rotation effects are extremely small and the direction of the rotation is frequently dependent on the solvent used; furthermore these signs do not give any information on the stereochemistry of the compounds.

The IUPAC-IUB Commission on Biochemical Nomenclature (CBN), at its meeting in January 1972, decided to publish a special document, extending Section M-3 of the 1966 Rules [1], to provide a system for the designation of the various stereoisomeric tocopherols and mixtures thereof. The present Recommendations are based on drafts prepared by W. Klyne and O. Hoffmann-Ostenhof after consultation with several active workers in the field, with the IUPAC-Commission on the Nomenclature of Organic Chemistry (CNOC), and with Committee 1-I on Nomenclature of the International Union of Nutritional Sciences (IUNS). The last-named committee proposed another tentative system for the designation of the tocopherols [4]; however, this system did not meet with complete agreement from CBN.

RECOMMENDATIONS

Replacing Section M-3 of [1].

1.1 Vitamin E. The term vitamin E should be used as the generic descriptor for all tocol and tocotrienol derivatives qualitatively exhibiting the biological activity of \( \alpha \)-tocopherol. This term should be used in derived terms such as vitamin-E deficiency, vitamin-E activity, vitamin-E antagonist.

1.2 Tocol. The term tocol is the trivial designation for 2-methyl-2-(\( 4',8',12' \)-trimethyltridecyl)chroman-6-ol (I, \( R^1 = R^2 = R^3 = H \)).

1.3 Tocopherol. The term tocopherol should be used as a generic descriptor for all mono, di, and trimethyltocols. Thus, this term is not synonymous with the term vitamin E.

![Diagram](image)

1. Compound I (\( R^1 = R^2 = R^3 = Me \)), known as \( \alpha \)-tocopherol, is designated \( \alpha \)-tocopherol or 5,7,8-trimethyltocol. For the designation of the configuration of \( \alpha \)-tocopherol see Rules 11 to 13².

2. Compound II (\( R^1 = R^2 = R^3 = Me \)), known as \( \beta \)-tocopherol, is designated \( \beta \)-tocopherol or 5,8-dimethyltocol.

3. Compound III (\( R^1 = R^2 = Me \); \( R^3 = H \)), known as \( \gamma \)-tocopherol, is designated \( \gamma \)-tocopherol or 7,8-dimethyltocol.

4. Compound IV (\( R^1 = H \); \( R^2 = R^3 = Me \)), known as \( \delta \)-tocopherol, is designated \( \delta \)-tocopherol or 8-methyltocol.

5. Compound V (\( R^1 = R^2 = H \); \( R^3 = Me \)), known as \( \gamma_2 \)-tocopherol, is designated \( \gamma_2 \)-tocopherol or 7,8-\( \delta \)-dimethyltocol.

6. Compound VI (\( R^1 = R^2 = R^3 = H \)), 2-methyl-2-(\( 4',8',12' \)-trimethyltridecyl-3',7',11'-triényl)chroman-6-ol, is designated tocotrienol (naturally occurring tocotrienols, so far as it is known at present, have the \( all-trans \) configuration).

² The name \( \alpha \)-tocopherol should never be used without a stereochemical designation whenever referring to a specific material.
Table. List of the trivial names for some α-tocopherols

| Description of Product | Configuration | Trivial names recommended | other
|------------------------|--------------|---------------------------|--------|
| 1. The compound having the configuration shown in the next column, exemplified by the only isomer of α-tocopherol as yet found in nature | 2R,4′R,8′R | RRR-α-tocopherol | [d]-α-tocopherol
| 2. The isomer epimeric only at 8′-Rα-8′-Rβ-tocopherol | 2S,4′R,8′R | 2-epi-α-tocopherol | |
| 3. Semisynthetic α-tocopherol, such as can be produced from natural phyto- | 2R,4′R,8′R and 2S,4′R,8′R (mixture not necessarily in equal proportions) | 2-ambo-α-tocopherol | |
| 4. Totally synthetic α-tocopherol, such as can be produced from synthetic phyto- or isophyto- | a mixture (not necessarily equimolar) of all four possible racemates (i.e., of all the four pairs of enantiomers) | all-rac-α-tocopherol | [dl]-α-tocopherol
| 5. Semisynthetic α-tocopherol, obtained by hydrogenation of (2R)-5,7,8-trimethyltocotrienol | a mixture (not necessarily equimolar) of the four isomers 2R,4′R,8′R; 2R,4′S,8′R; 2R,4′R,8′S; 2R,4′S,8′S | 4′-ambo-8′-ambo-α-tocopherol | |

* Not to be used in indexing without cross-reference to the recommended names.

7. Compound II (R′2 = R2 = R3 = Me), formerly known as ζ1 or ζ2-tocopherol, is preferably designated 5,7,8-trimethyltocotrienol. Other names are α-tocotrienol and tocotrienol-3β, cf. [5], para 3.3.2.

8. Compound II (R′2 = R2 = Me; R3 = H), formerly known as η-tocopherol, is preferably designated 5,8-dimethyltocotrienol. Another name is δ-tocotrienol.

9. Compound II (R′2 = H; R2 = R3 = Me), formerly known as γ-tocopherol, is preferably designated 7,8-dimethyltocotrienol. Other names are γ-tocotrienol and plastochromanol-3.

10. Compound II (R′2 = R2 = H; R3 = Me) is preferably designated 8-methyltocotrienol. Another name is δ-tocotrienol.

11. The only naturally occurring stereoisomer of α-tocopherol hitherto discovered has the configuration 2R, 4′R,8′R according to the sequence-rule system [3]. Its semisystematic name is therefore (2R,4′R,8′R)α-tocopherol. The same principle can be applied to all other individual stereoisomers of tocopherols.

12. Trivial names are sometimes required to indicate briefly the configuration of important stereoisomers of α-tocopherol and especially of mixtures of such stereoisomers. Some of these materials are of considerable commercial and therapeutic importance. The use of the following trivial designations for the most important materials of this class is recommended.

   a) The above mentioned α-tocopherol with the configuration 2R,4′R,8′R should be called RRR-α-tocopherol.
   b) The diastereoisomer of RRR-α-tocopherol, being its epimer at C-2, should be called 2-epi-α-tocopherol.
   c) A mixture of RRR-α-tocopherol and 2-epi-α-tocopherol, obtained by synthesis using natural phyto- or isophytol, should be called 2-ambo-α-tocopherol. Formerly it was believed that such material is a mixture of the two epimers in equimolar proportions. However, this is most probably not the case. Asymmetric reactions, like the one involved in the partial synthesis, would only by chance lead to the formation of equimolar amounts of the two possible epimers or—in other cases—enantiomers. The actual ratio obtained in such a reaction is strongly dependent on parameters like temperature, solvent, catalysts present, etc., which means that this ratio in 2-ambo-α-tocopherol may differ from one synthesis to the other. The acetate of 2-ambo-α-tocopherol is the present international standard for vitamin E activity [7].
   d) The reduction product of natural 5,7,8-tocotrienol, in which the double bonds at 3′,7′, and 11′ are hydrogenated and two new asymmetric centers are created at C-4′ and C-8′, is a mixture of four diastereoisomeric α-tocopherols, having the configuration 2R,4′R,8′R; 2R,4′S,8′R; 2R,4′R,8′S; and 2R,4′S,8′S. The material should be called 4′-ambo-α-tocopherol.
   e) The totally synthetic vitamin E, obtained from totally synthetic phyto- or isophytol as starting material, is a mixture of four racemates in unspecified proportions. It should be called all-rac-α-tocopherol.

13. Traditionally the two compounds of greatest practical importance of this class, RRR-α-tocopherol and all-rac-α-tocopherol are commonly described as d-α-tocopherol and dl-α-tocopherol, respectively, using symbols normally no longer accepted in organic nomenclature [3]. In this case, however, it seems unrealistic to suggest discarding this nomenclature completely. It is proposed that these prefixes should be permitted for the time being in a slightly altered form (lower-case roman in brackets; i.e. [d] and [dl] instead of lower-case italics), as purely trivial prefixes to trivial names for these commercially produced particular compounds. In indexing, however, such designations should be cross-referenced to the names recommended above (in 12a, 12c).

Recommended and other trivial names are listed in the Table.

---

6 From "ambo", Latin for "both".
7 A more complete name would be 2-ambo-(4′R,8′R)-α-tocopherol, but in order to keep trivial names short it is to be assumed that the configuration at each center in the tocopherols is R unless stated otherwise. The term α-tocopherol, by itself a generic descriptor without stereochemical implication, thus obtains a stereochemical meaning when preceded by a stereochemical prefix like ambo or epi.
8 International vitamin standards are the responsibility of the World Health Organization.
ACKNOWLEDGEMENT. We are indebted to the Editors and Publishers (Springer-Verlag) of the European Journal of Biochemistry for permission to reproduce these Recommendations photographically.

All Tentative Rules and Proposals of the IUPAC-IUB Commission of Biochemical Nomenclature (CBN) are available from Waldo E. Cohn, Director, NRC Office of Biochemical Nomenclature, Oak Ridge National Laboratory, Box Y, Oak Ridge, Tenn. 37830, U.S.A.

1. Abbreviations and Symbols for Chemical Names of Special Interest in Biological Chemistry [see Biochem. J. (1966) 101, 1-7 (extended by items 6, 11 and 15 below)].

2. Nomenclature of Vitamins, Coenzymes and Related Compounds: Trivial Names of Miscellaneous Compounds of Importance in Biochemistry, Nomenclature of Quinones with Isoprenoid Side Chains, Nomenclature and Symbols for Folic Acid and Related Compounds, Nomenclature of Corrinoids. Tentative Rules [see Biochem. J. (1967) 102, 15-22 (but see items 10, 22 and 23 below)].

3. Abbreviated Designation of Amino Acid Derivatives and Peptides [see Biochem. J. (1967) 102, 23-27 (superseded by item 15 below)].


9. Revised Tentative Rules for Nomenclature of Steroids [see Biochem. J. (1969) 113, 5-28 (for amendments see item 16 below)].


15. Symbols for Amino Acid Derivatives and Peptides. Recommendations [see Biochem. J. (1972) 126, 773-780 (supersedes item 3 above; for corrections see Biochem. J. (1973) 135, 9)].

16. Amendments to Rules for Nomenclature of Steroids [see Biochem. J. (1972) 127, 613-617 (amendments to item 9 above)].


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22. The Nomenclature of Corrinoids. Recommendations [see Biochem. J. (1975) 147, 1–10 (supersedes section in item 2 above)].

23. Nomenclature of Tocopherols and Related Compounds. Recommendations [this document (replaces M-3 of item 2 above)].

A document, OBN-5, describing the (American) NRC Office of Biochemical Nomenclature, and listing other rules affecting biochemical nomenclature, is available from its Director, Dr. Waldo E. Cohn [see also J. Chem. Doc. (1967) 7, 72–73; (1969) 9, 235–241].
Nomenclature of Quinones with Isoprenoid Side-Chains

Recommendations (1973)\(^1\)

IUPAC-IUB COMMISSION ON BIOCHEMICAL NOMENCLATURE (CBN)\(^2\)

The biologically active quinones with isoprenoid or phytol side-chains include members of the vitamins K and E and coenzyme Q families. The various trivial names given these substances as they were discovered and investigated do not reflect the close chemical relationships among them. Particularly confusing has been the use of numerical subscripts as series num-

\(^1\) At its meeting in April 1961, the IUPAC Commission for the Nomenclature of Biological Chemistry appointed a Subcommittee, consisting of K. Folkers, D. E. Green, O. Isler, C. Martius, R. A. Morton, and E. C. Slater, to report on the standardization of the nomenclature of the quinones with an isoprenoid side chain. The Subcommittee met once in April 1963, and otherwise carried out its activities by correspondence. In June 1964, it reported to the IUPAC-IUB Commission on Biochemical Nomenclature, which adopted the report, with minor modifications, at its meeting in September 1964 and published it as Tentative Rules in 1965.

\(^2\) The present Recommendations differ from the 1964 Tentative Rules principally in the deletion of the alternative Proposal II (see 3.1) from the latter. Comments on and suggestions for future revisions may be sent to any member of CBN (see footnote 2).

Reprints of these Recommendations and of other Recommendations of the IUPAC-IUB Commission on Biochemical Nomenclature (see footnote 2) may be obtained from W. E. Cohn, Director, NRC (USA) Office of Biochemical Nomenclature, Biology Division, Oak Ridge National Laboratory, Box Y, Oak Ridge, TN 37830 (USA).

\(^3\) The 1966 "Tentative Rules" replaced Rule V-4 of the "Rules for the Nomenclature of Vitamins" (J. Am. Chem. Soc. 82, 5581, 1965), and were published in IUPAC Information Bulletin No. 25, February 1966, page 24, and also in Arch. Biochem. Biophys. 118, 505 (1967) and in several other journals.

bers (e.g., vitamin K\(_2\)), as indicators of the number of isoprene units (e.g., coenzyme Q\(_2\)), and to show that a side-chain in a vitamin E is the same as in a vitamin K (e.g., E\(_2\) and K\(_2\)).

An inspection of the chemical structures involved (Table III) indicates that there are three types of quinone nuclei (1,4-naphthoquinone, methyl-substituted 1,4-benzoquinone, methyl- and methoxy-substituted 1,4-benzoquinone) and two types of side-chains (phytol or derived phytol, multi-isoprenyl). On reduction, the quinones yield the corresponding hydroquinones, and each of these has an isomer formed by ring closure; these are known as chromenols and chromanols, respectively. The interrelationships are shown in Fig. 1.

These recommendations are concerned solely with the naturally occurring compounds of these types and with those compounds formed (e.g., by cyclization) from them, with respect to (a) designation of the length of the isoprenoid side chains, (b) trivial names for each group of quinones, and (c) designation of individual members of each group.

RECOMMENDATIONS

1 Designation of Length of Side-chains

1.1 The number of isoprene units, not the number of carbon atoms, is chosen as the basis of side-chain designation.

1.2 An isoprene unit is designated "prenyl." The hexahydrotetraprenyl side-chain (cf. Table III) is termed "phytyl."\(^4\)

1.3 The oxygen-containing ring of a chromenol or chromanol incorporates three

\(^4\) "Prenyl" is 3-methyl-2-butenyl (IUPAC Rule A-3.5).

\(^5\) "Phytol" is \((E)-(\tau R,11R)-3,7,11,15\)-tetramethyl-2-hexadecenyl (IUPAC Rule A-75.1).
1,4-benzoquinone form yields tocotrienol-
quinones.

2.7 The abbreviations for tocopherol,
tocopherolquinone, tocotrienol and tocot-
rienolquinone are, respectively, T, TQ,
T-3, and TQ-3. Each is prefixed with the
appropriate Greek letter or numerals;7
thus, for example:

α-tocopherol α-T
β-tocopherolquinone β-TQ
7,8-dimethyltocotrienol 7,8-T-3 (or PQ-3-al; cf. 3.2 and
Table III)
2,3,5-trimethyltocotrienolquinone 2,3,5-TQ-3

2.8 The hydroquinones may be abbre-
viated by the addition of H₂ to the abbre-
viation of the quinone. If an abbreviation of a
chromanol or chromenol is required, it is
suggested that the suffixes al and el, re-
spectively, be added to the abbreviation of
the quinone (e.g., PQ-3-al for plasto-
chromanol-3).

3 Designation of Individual Members of
- Each Group

3.1 In its earlier deliberations,1 the
Commission recognized that there were
two schools of thought concerning the des-
ignation of the individual members of each
group of quinones. One school considered
that the links with vitamin E, coenzyme Q,
and vitamin K are retained sufficiently by
the name tocopherine and by the abbre-
viations Q and K (or MK), and pro-
posed that the different members should
be designated -quinone-ν (abbreviation X-
n), where n is the number of intact isoprene
units in the side-chain. The other school
considered it necessary to retain E, Q, and
K as a part of the name and to designate
the number of isoprene units by the lower
subscript n, as was the practice in the co-
enzyme Q series.

The Commission favors the first pro-
posal, summarized in Table II. In many
cases, n may be omitted from the abbrevia-
tion, especially in chemical equations.

3.2 According to these recommenda-
tions, 5,7,8-trimethyltocotrienol, also
known as α-tocotrienol and δ-tocopherol,
may be designated tocochromanol-3. It is
recommended that 5,7,8-trimethyltocotri-
енol be used when the relationship with
tocols and toco-enols (with vitamin E ac-
tivity) is relevant, and tocochromanol-3
when the relationship with the quinones
with isoprenoid side-chains (K and Q se-
ries) is more important. Similarly, 7,8-di-
methyltocotrienol, also known as γ-
tocotrienol and η-tocopherol, may be desig-
nated plastochromanol-3.

3.3 Saturation of one or more (but not
all) of the double bonds in a multiprenyl
side-chain should be indicated in the fol-
lowing way:
a. The isoprene units are designated by
Roman numerals (I, II, III, etc.) starting
from the quinone or chroman nucleus.
b. Additional hydrogen atoms are indi-
cated by the prefixes dihydro, tetrahydro,
hexahydro, etc., with the Roman numerals
of the units that are reduced, e.g., II-
dihydro...; I, II, III-hexahydro...
c. These abbreviations may be abbrevi-
ated if necessary (e.g., in tables) to II-H₄; I,
II, III-H₆, etc.

Note. Arabic numerals should not be
employed for the units, because such
numerals are generally employed for indi-
individual atoms.

SUMMARY AND EXAMPLES

The recommended trivial names (under-
lined) and abbreviations for some naturally
occurring quinones of the vitamins E and
K and coenzyme Q series and related
compounds are displayed in Table III.
Older and superseded names are listed in
smaller type (and marked by a double
asterisk) for convenience; their use is not
recommended.
NOMENCLATURE OF QUINONES WITH ISOPRENOID SIDE CHAINS

<table>
<thead>
<tr>
<th>Quinoid nucleus</th>
<th>Side chain&lt;sup&gt;4, 6, 8&lt;/sup&gt;</th>
<th>Class name</th>
<th>Abbreviation</th>
</tr>
</thead>
<tbody>
<tr>
<td>2,3,5-Trimethylbenzoquinone</td>
<td>Multiprenyl</td>
<td>Tocoquinone</td>
<td>PQ</td>
</tr>
<tr>
<td>2,3-Dimethylbenzoquinone</td>
<td>Multiprenyl</td>
<td>Plastoquinone</td>
<td>Q</td>
</tr>
<tr>
<td>2,3-Dimethoxy-5-methylbenzoquinone</td>
<td>Multiprenyl</td>
<td>Ubiquinone</td>
<td>MK</td>
</tr>
<tr>
<td>2-Methylnaphthoquinone</td>
<td>Multiprenyl</td>
<td>Menaquione&lt;sup&gt;*&lt;/sup&gt;</td>
<td>K</td>
</tr>
<tr>
<td>2-Methylnaphthoquinone</td>
<td>Phytol</td>
<td>Phyloquinone</td>
<td>K</td>
</tr>
</tbody>
</table>

* It is realized that menaquinone has sometimes been used to designate the parent quinone, 2-methyl-1,4-naphthoquinone (menadione).

2 Trivial Names for Groups of Quinones

2.1 Because it is against IUPAC practice to designate chemical compounds by terms such as vitamin X or coenzyme X, and because the cyclized forms of the quinones and hydroquinones cannot easily be designated in such terms, the trivial names vitamin E<sub>2</sub>, vitamins K<sub>1</sub> and K<sub>2</sub>, and coenzyme Q are replaced by appropriate chemical names.

2.2 Because it is desirable to retain links with the older names, the chemical names or abbreviations recommended have been selected with that in mind.

2.3 The group names shown in Table I are recommended.

2.4 The corresponding hydroquinones, chromenols, and chromanols are named by replacing the suffix “quinone” with “quino-,” “chromenol,” and “chromanol,” respectively, e.g., ubiquinone becomes ubiquinol, ubichromanol, and ubichromanol.

2.5 It is realized that some confusion may arise from the fact that 6-(3-hydroxy-3,7,11,15-tetramethylhexadecanyl) 2,3,5-trimethyl-1,4-benzoquinone, the quinone form of α-tocopherol, has been referred to as α-tocoquinone in the literature. Usually, however, the name of α-tocopherylquinone has been used. It is recommended that this compound be named α-tocopherolquinone. Similarly, the analogous compounds formed by oxidation of β-, γ-, and δ-tocopherol should be named β-, γ-, and δ-tocopherolquinone, respectively.

2.6 A reduced and cyclized tocopherolquinone, a chromanol, is a tocopherol. The tocophers may also be regarded as methylated tocols (<i>tocol</i> is 2-methylbenzopyran-6-ol or 2-methyl-6-chromanol). When the side-chain is triprenyl rather than substituted phytol, such chromanols are termed tocotrienols, the triene referring to the three double bonds in the side-chain. (See 3.2). The oxidation of these to the

*Although by IUPAC Rules A-54 and C-71, governing assemblies of identical cyclic units, the prefixes ter-, quater-, ..., novi-, and deci- might seem more appropriate, the traditional terms tri-, tetra-, ..., nona- and deca- are used for the multiprenyl side chains. Because of the single locant preceding the side-chain term, this designation is unlikely to be mistaken for multiple substitution by independent prenol groups.
### TABLE III
SUMMARY OF CHEMICAL RELATIONSHIPS AND NOMENCLATURE OF SOME BIOLOGICALLY ACTIVE QUINONES WITH ISOPRENOID SIDE-CHAINS, INCLUDING VITAMINS E AND K AND COENZYME Q. (RECOMMENDED NAMES ARE UNDERLINED.)

<table>
<thead>
<tr>
<th>Aromatic nucleus</th>
<th>Side-chain</th>
<th>Trivial name(s)</th>
<th>Abbrevs.</th>
<th>Cyclized form</th>
<th>Trivial names</th>
<th>Abbrevs.</th>
</tr>
</thead>
<tbody>
<tr>
<td>1,4-Naphthoquinone,</td>
<td>3-(prenyl)</td>
<td>Menaquinone-α</td>
<td>MK-α</td>
<td>2H-Naphtho(1,2)pyran-6-ol</td>
<td>Menachromenol-(n-1)</td>
<td>MK-α-εl</td>
</tr>
<tr>
<td>2-methyl-</td>
<td></td>
<td>*Menaquinone-α</td>
<td>*MQ-α</td>
<td>(2,5-substituted)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>*Menaquinone (Menadione)</td>
<td></td>
<td>7: vitamin Kt(35)**</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>6: vitamin Kt(30)**</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>3-Phytyl</td>
<td></td>
<td>Phylloquinone</td>
<td>K</td>
<td></td>
<td>Phyllochromenol</td>
<td>K-εl</td>
</tr>
<tr>
<td></td>
<td></td>
<td>*Phylloquinone</td>
<td>*PMQ</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>7: vitamin Kt(20)**</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>1,4-Benzquinone,</td>
<td>6-(prenyl)</td>
<td>Ubiquinone-α</td>
<td>Q-α</td>
<td>7,8-dimethoxy-2H-chromen-6-ol</td>
<td>Ubichromenol-(n-1)</td>
<td>Q-α-εl</td>
</tr>
<tr>
<td>2,3-dimethoxy-</td>
<td></td>
<td>10: coenzyme Q10**</td>
<td>Q-10</td>
<td>(2,5-substituted)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>*-5-methyl-</td>
<td></td>
<td>6: coenzyme Qα-50**</td>
<td>Q-6</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>6: coenzyme Qα-30**</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>1,4-Benzquinone,</td>
<td>6-(prenyl)</td>
<td>Tocororine-α</td>
<td>Q-α</td>
<td>7,8-dimethoxy-2H-chromen-6-ol</td>
<td>Tocochromenol-(n-1)</td>
<td></td>
</tr>
<tr>
<td>2,3,5-trimethyl-</td>
<td></td>
<td>n = 10: vitamin Eα(50)**</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>n = 4: cf. 2,3,5-trimethyl-</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>tocotrienolquinone</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
# Table III continued

<table>
<thead>
<tr>
<th>Aromatic nucleus</th>
<th>Side-chain</th>
<th>Trivial name(s)</th>
<th>Abbrevs.</th>
<th>Cyclized form</th>
<th>Trivial names</th>
<th>Abbrevs.</th>
</tr>
</thead>
<tbody>
<tr>
<td>1,4-Benzoquinone, 2,3-dimethyl-</td>
<td>6-(prenyl) 2,3-dimethyl-</td>
<td>Plastoquinone ( n = 9 ): plastoquinone** = Koller's quinone** = plastoquironol-8 = solanochromene**</td>
<td>PQ-9</td>
<td>Plastoquinone-9 = 7,8-dimethyl-tocotrienol = ( \gamma )-tocotrienol**</td>
<td>PQ-9 = PQ-9-8-el</td>
<td>7,8-T-3</td>
</tr>
<tr>
<td>1,4-Benzoquinone, (2,3,5-substituted)</td>
<td>6-&quot;phyl&quot;</td>
<td>( \alpha )-Tocopherolquinone(s)</td>
<td>x-TQ</td>
<td>Cyclized, reduced form</td>
<td>Chroman-6-ol (Benzyopyran-6-ol) (2,5,7,8-substituted)</td>
<td>x-T</td>
</tr>
<tr>
<td>6-&quot;tetraprenyl&quot;</td>
<td>x-( \alpha )-Tocotrienolquinone(s)</td>
<td>x-TQ-3, 2,5,3-TQ-3</td>
<td>x-TQ-3 = 5,7,8-trimethyl-1 = ( \alpha )-tocotrienol** = ( \gamma )-tocotrienol**</td>
<td>x = 5,7,8-trimethyl = ( \alpha )-tocotrienol** = ( \gamma )-tocotrienol** = ( \eta )-tocotrienol**</td>
<td>5,7,8-T-3</td>
<td></td>
</tr>
</tbody>
</table>


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Acknowledgement. We are indebted to the Editors and Publishers (Academic Press) of Archives of Biochemistry and Biophysics for permission to reproduce these Recommendations photographically.

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