INTERNATIONAL UNION OF
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NOMENCLATURE OF QUINONES WITH ISOPRENOID SIDE-CHAINS

Rules (1973)

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BUTTERWORTHS

IUPAC–IUB COMMISSION ON
BIOCHEMICAL NOMENCLATURE[2]

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Rules (1973)[1]

1. INTRODUCTION

The biologically active quinones with isoprenoid or phytyl 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 numbers (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 3*) 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 (phytyl or derived phytyl, 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 *Figure 1*.

These Rules are concerned solely with the naturally occurring compounds of these types and with those compounds formed (e.g. by cyclization) from

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[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[3].

The present Rules differ from the 1964 Tentative Rules[3] principally in the deletion of the alternative Proposal II (see 3.3.1) from the latter. Comments on and suggestions for future revisions may be sent to any member of CBN[2].

Reprints of these Rules and of other Recommendations of the IUPAC–IUB Commission on Biochemical Nomenclature[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, Tenn. 37830, USA.

[2] O. Hoffmann-Ostenhof (Chairman), W. E. Cohn (Secretary), A. E. Braunstein, B. L. Horecker, P. Karlson, B. Keil, W. Klyne, C. Liébecq, E. C. Webb.

[3] The 1964 'Tentative Rules' replaced Rule V-4 of the 'Rules for the Nomenclature of Vitamins' [*J. Amer. Chem. Soc.* **82**, 5581 (1960)] and were published in IUPAC *Information Bulletin No. 25*, February 1966, page 24, also in *Biochim. Biophys. Acta*, **107**, 5 (1965) and in several other journals.

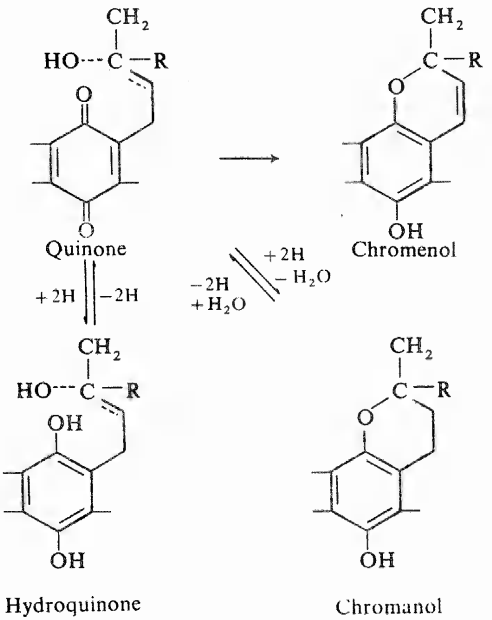


Figure 1

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.

2. RULES

2.1. Designation of length of side-chains

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

2.1.2. An isoprene unit is designated 'prenyl'[4]. The hexahydrotetraprenyl side-chain (cf. *Table 3*) is termed 'phytyl'[5].

2.1.3. The oxygen-containing ring of a chromenol or chromanol incorporates three of the five carbon atoms of the first prenyl of the corresponding (non-cyclized) quinone or hydroquinone. The number of intact prenyls to be designated is therefore reduced by one to reflect the actual number of prenyls remaining.

2.2. Trivial names for groups of quinones

2.2.1. 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_2, vitamins K_1 and K_2, and coenzyme Q are replaced by appropriate chemical names.

2.2.2. Because it is desirable to retain links with the older names, the

[4] 'Prenyl' is 3-methyl-2-butenyl (IUPAC Rule A-3.5).

[5] 'Phytyl' is (*E*)-(7*R*,11*R*)-3,7,11,15-tetramethyl-2-hexadecenyl (IUPAC Rule A-75.1).

chemical names or abbreviations recommended have been selected with that in mind.

2.2.3. The group names shown in *Table 1* are recommended.

Table 1

Quinoid nucleus	Side-chain[4,5,6]	Class name	Abbreviation
2,3,5-Trimethylbenzoquinone	Multiprenyl	Tocoquinone	
2,3-Dimethylbenzoquinone	Multiprenyl	Plastoquinone	PQ
2,3-Dimethoxy-5-methylbenzoquinone	Multiprenyl	Ubiquinone	Q
2-Methylnaphthoquinone	Multiprenyl	Menaquinone*	MK
2-Methylnaphthoquinone	Phytyl	Phylloquinone	K

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

2.2.4. The corresponding hydroquinones, chromenols and chromanols are named by replacing the suffix 'quinone' with 'quinol', 'chromenol' and 'chromanol', respectively; e.g. *ubiquinone* becomes *ubiquinol*, *ubichromenol* and *ubichromanol*.

2.2.5. 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.

2.2.6. A reduced and cyclized tocopherolquinone, a chromanol, is a **tocopherol**. The tocopherols may also be regarded as methylated tocols (**tocol** is 2-methylbenzopyran-6-ol or 2-methyl-6-chromanol). When the side-chain is triprenyl rather than substituted phytyl, such chromanols are termed **tocotrienols**, the triene referring to the three double bonds in the side-chain. (See 2.3.2.) The oxidation of these to the 1,4-benzoquinone form yields **tocotrienolquinones**.

2.2.7. The abbreviations for tocopherol, tocopherolquinone, tocotrienol and tocotrienolquinone 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. 2.3.2 and *Table 3*)
2,3,5-Trimethyltocotrienolquinone	2,3,5-TQ-3

[6] 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 prenyl groups.

2.2.8. The hydroquinones may be abbreviated by the addition of H_2 to the abbreviation of the quinone. If an abbreviation of a chromanol or chromenol is required, it is suggested that the suffixes *al* and *el*, respectively, be added to the abbreviation of the quinone (e.g. PQ-3-*al* for plastochromanol-3).

2.3. Designation of individual members of each group

2.3.1. In its earlier deliberations[1], the Commission recognized that there were two schools of thought concerning the designation 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 tocoquinone and by the abbreviations Q and K (or MK), and proposed that the different members should be designated -quinone-*n* (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 coenzyme Q series.

The Commission favours the first proposal, summarized in *Table 2*. In many cases *n* may be omitted from the abbreviation, especially in chemical equations.

Table 2

Name	Abbreviation
Tocoquinone-*n*	
Plastoquinone-*n*	PQ-*n*
Ubiquinone-*n*	Q-*n*
Menaquinone-*n*	MK-*n*
Phylloquinone	K

2.3.2. According to these recommendations, *5,7,8-trimethyltocotrienol*, also known as α-tocotrienol and ζ_1-tocopherol, may be designated *tocochromanol-3*. It is recommended that 5,7,8-trimethyltocotrienol be used when the relationship with tocols and toco-enols (with vitamin E activity) is relevant, and tocochromanol-3 when the relationship with the quinones with isoprenoid side-chains (K and Q series) is more important. Similarly, *7,8-dimethyltocotrienol*, also known as γ-tocotrienol and η-tocopherol, may be designated *plastochromanol-3*.

2.3.3. Saturation of one or more (but not all) of the double bonds in a multiprenyl side-chain should be indicated in the following 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 indicated 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 abbreviated if necessary (e.g. in tables) to II-H_2; I, II, III-H_6, etc.

[7] The Greek-letter prefixes for the tocopherols are defined in the CBN 1965 reference given in footnote 3 and in a 1973 revision of that document (in preparation). The latter includes the stereochemical description and designation of the tocopherols; it also recommends against the use of Greek letters in the names and abbreviations of the tocotrienols and their quinones.

NOTE: Arabic numerals should not be employed for the *units*, because such numerals are generally employed for individual *atoms*.

3. SUMMARY AND EXAMPLES

The Recommended Trivial Names (in **boldface**) and abbreviations for some naturally occurring quinones of the vitamins E and K and coenzyme Q series and related compounds are displayed in *Table 3*. Older and superseded names, marked by a dagger, are listed for convenience; their use is not recommended.

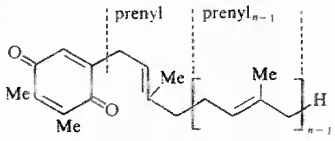
Table 3

Summary of chemical relationships and nomenclature of some biologically active quinones with isoprenoid side-chains, including vitamins E and K and co-enzyme Q

[Recommended names are in **boldface** type.]

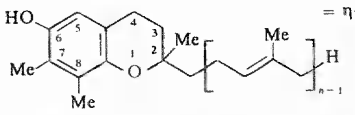
Aromatic nucleus	Side-chain	Trivial name(s)	Abbrevs.	Cyclized form	Trivial names	Abbrevs.
1,4-Naphthoquinone, 2-methyl-	3-(prenyl)$_n$	**Menaquinone**-*n* *Prenylmenaquinone-*n* *n* = 10: vitamin K_2(50)† *n* = 7: vitamin K_2(35)† *n* = 6: vitamin K_2(30)†	MK-*n* *MQ-*n*	2*H*-Naphtho[1,2-*b*]pyran-6-ol, (2,5-substituted)	**Menachromenol**-(*n* − 1)	MK-*n*-el
*Menaquinone (Menadione)						
	3-Phytyl	**Phylloquinone** *Phytylmenaquinone = Vitamin K_1(20)†	K *PMQ	same	**Phyllochromenol**	K-el
1,4-Benzoquinone, 2,3-dimethoxy--5-methyl-	6-(prenyl)$_n$	**Ubiquinone**-*n* *n* = 10: coenzyme Q_{10}† = ubiquinone-50† *n* = 6: coenzyme Q_6† = ubiquinone-30†	Q-*n* Q-10 Q-6	7,8-dimethoxy-2*H*-chromen-6-ol (2,5-substituted)	**Ubichromenol**-(*n* − 1) *n* = 10: ubichromenol-9 = ubichromenol (50)†	Q-*n*-el
1,4-Benzoquinone, 2,3,5-trimethyl-	6-(prenyl)$_n$	**Tocoquinone**-*n* *n* = 10: vitamin E_2(50)† *n* = 4: cf. 2,3,5-trimethyl-tocotrienolquinone			**Tocochromanol**-(*n* − 1)	

1,4-Benzoquinone, 2,3-dimethyl- 6-(prenyl)$_n$



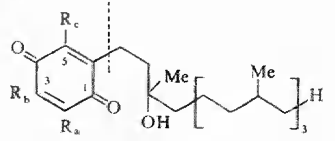
Plastoquinone-*n* PQ-*n*

n = 9: plastoquinone† PQ-9
= Kofler's quinone†
= plastochromenol-8 PQ-8-el
= solanochromene†



Plastochromanol-(n − 1) PQ-*n*-al
Plastochromanol-3 = PQ-3-al
7,8-dimethyltocotrienol 7,8-T-3
= γ-tocotrienol†
= η-tocopherol†

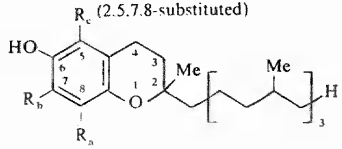
1,4-Benzoquinone, (2,3,5-substituted) 6-'phytyl'



***x*-Tocopherolquinone(s)** *x*-TQ

x	R_a	R_b	R_c	
α	Me	Me	Me	(oxidized vit. E)
β	Me		Me	
γ	Me	Me		(cf. plastoquinone)
δ	Me			

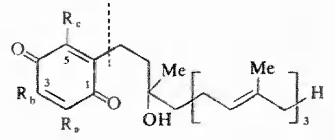
Cyclized, reduced form
Chroman-6-ol
(Benzopyran-6-ol)
(R_c (2.5.7.8-substituted)



***x*-Tocopherol(s)** *x*-T
Tocol: $R_a = R_b = R_c$ = H

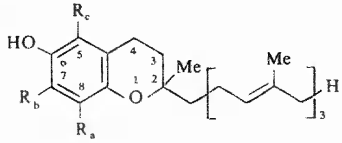
α($R_a = R_b = R_c$ = Me) =
5,7,8-trimethyltocol
= vitamin E†

6-'tetraprenyl'



***x*-Tocotrienolquinone(s)** *x*-TQ-3

x =		
2,3,5-trimethyl- = α†-(cf. tocoquinone-4)	2,3,5-TQ-3	
2,5-dimethyl- = β†-	2,5-TQ-3	
2,3-dimethyl- = γ†- (cf. plastoquinone-4)	2,3-TQ-3	
2-methyl = δ†-		



***x*-Tocotrienol(s)** *x*-T-3

x =	
5,7,8-trimethyl = tocochromanol-3 = α-tocotrienol† = ζ_1-tocopherol†	5,7,8-T-3
5,8-dimethyl = ε-tocopherol†	5,8-T-3
7,8-dimethyl = plastochromanol-3 = γ-tocotrienol† = η-tocopherol†	7,8-T-3 PQ-3-al

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* Proposed by Committee on Nomenclature of IUNS [*Nutr. Abstracts and Reviews*, **40**, 395 (1970)], where differing from those recommended here.
† Names previously used (see para. 1 in Introduction), not recommended.