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## NOMENCLATURE OF PRENOLS

(Recommendations 1986)

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# Nomenclature of prenols (Recommendations 1986)

The prenols are a group of alcohols containing one or more isoprene units, and are, with their esters, the biological precursors of the isoprenoids, a variety of compounds including terpenes and steroids that contain much of the carbon skeleton intact. The new recommendations do not replace any existing document, but set out to systematize existing practice, and to supplement it by paying full attention to the important stereochemistry of the prenols. The general terms are discussed and recommendations for indicating stereochemistry are made. Short-chain prenols that have established trivial names are listed, and the relationship of the prenols to the simplest juvenile hormones is indicated.

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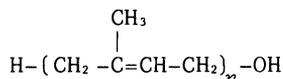
### REFERENCES

## INTRODUCTION

Present practice in the nomenclature of prenols takes little account of the important stereochemistry of these compounds. We therefore believe that a review of existing practice, with recommendations for specifying stereochemistry, should be helpful. Some of the recommendations have been used in Enzyme Nomenclature [1].

## GENERAL TERMS

Pr-1. Prenol. The term prenol, already widely used (e.g. refs. 2,3,5,6), is recommended to describe the structure shown in formula I. It originated as a contracted name for isoprenoid alcohol (i.e. suffix -ol) [2].



### I

The carbon atoms along the main chain are numbered from C-1, the atom that carries the hydroxyl group (C-15.11 of ref. 8). The methyl group carried by atom C-3 contains atom C-3<sup>1</sup>, that carried by atom C-7 contains atom C-7<sup>1</sup>, etc.

### Note

This use of superscript numbers is based on section TP-2.1 of the recommendations for the nomenclature of tetrapyrroles [9]. In the printing of these recommendations in the European Journal of Biochemistry the relevant paragraph was accidentally transposed to the caption of Table 2.

The repeating C<sub>5</sub>H<sub>8</sub> unit (inside the brackets of structure I) is termed an isoprene unit or an isoprene residue. Prenols and their esters are precursors of a variety of compounds, including terpenes and steroids, that have much of the carbon skeleton intact. Such compounds are known as isoprenoids.



3. Although large numbers of stereoisomers could arise if each newly added residue (Fig. 1) could be either cis or trans, the commonest prenyls are confined to four main groups (Fig. 2), as follows: (i) all-trans-prenols, (ii) ditrans, polycis-prenols, (iii) tritrans, polycis-prenols, and (iv) all-cis-prenols. The symbols W, T and C that appear in Fig. 2, together with a fourth symbol S, provide a convenient set for compactly representing polyprenol structures.

In group (i), the term 'all-trans' means that all the residues except the  $\omega$ -residue have the trans configuration. In groups (ii) and (iii) the trans residues are grouped next to the  $\omega$ -residue. Group (iv) is less well characterized, but probably exists as precursors of natural rubber.

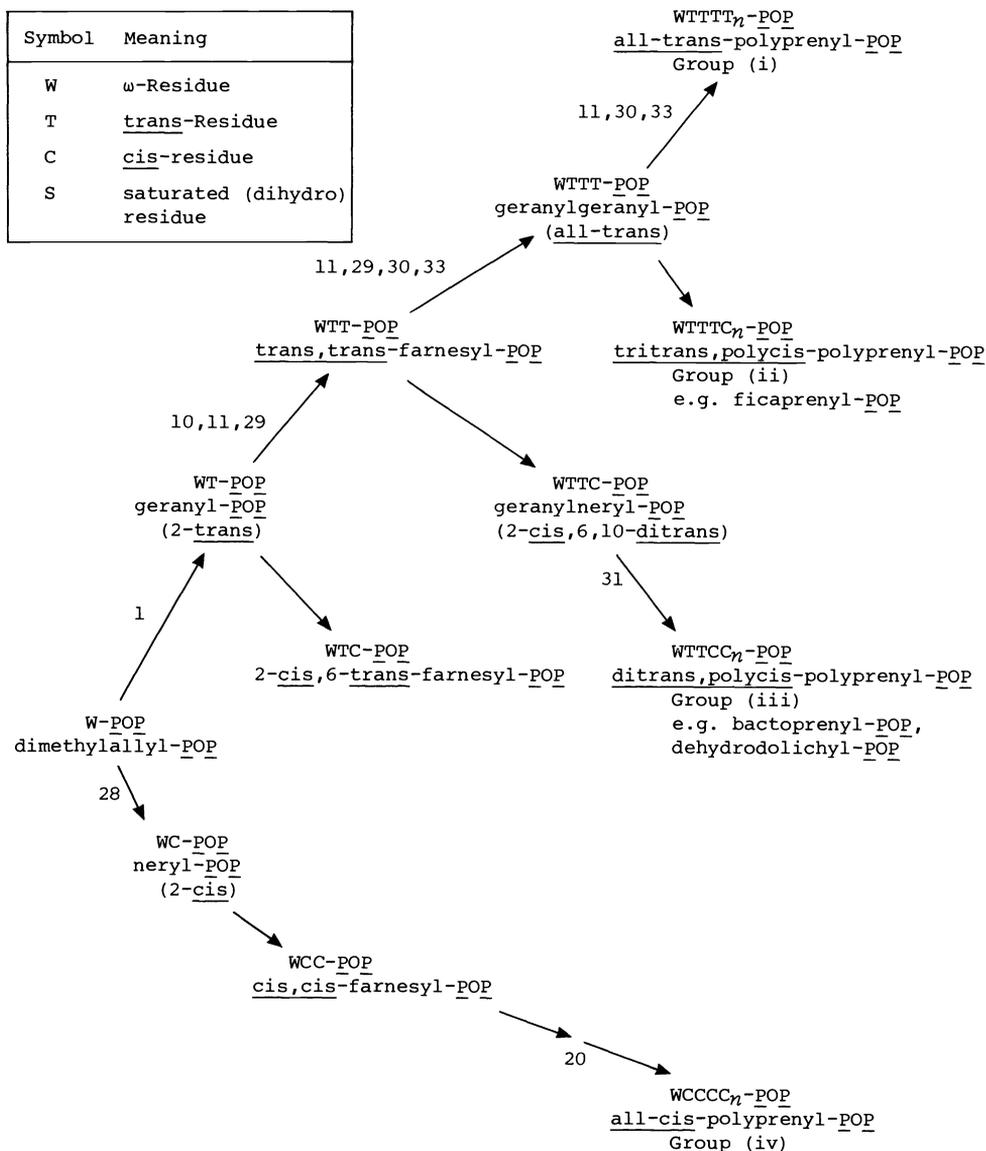


Fig. 2. Stereochemistry of polyprenol biosynthesis

Each arrow shows a transformation of the type given in Fig. 1. Upward sloping arrows represent trans additions of a unit from isopentenyl diphosphate (section Pr-9), and downward sloping arrows represent cis additions. An arabic numeral adjacent to an arrow indicates that an enzyme catalysing the reaction has been characterized and listed under that number in group EC 2.5.1 of Enzyme Nomenclature [1], e.g. EC 2.5.1.11 catalyses the conversion of geranyl-POP into trans, trans-farnesyl-POP. The groups given in the right-hand column refer to the main classes of polyprenols as listed in section Pr-6, note 3. Where locants are included the prefixes appear in locant order (section Pr-8), not in left-to-right order (section Pr-6). In the symbolic representations, W represents an  $\omega$ -residue, T a trans residue, and C a cis residue.

4. The recommendation to cite stereochemical prefixes in the reverse order from their locants is contrary to normal recommendations. We make it because (1) it is already widely used, (2) it corresponds to the left-to-right order in most drawings of formulas and symbolic representations of prenols and their diphosphates, and (3) it names first the double bonds formed first in biosynthesis.

#### Example

all-trans-Nonaprenol is the plant product solanesol, which contains nine isoprene units, eight of which are trans, the ninth being the  $\omega$ -residue.

Pr-7. Multiplicative prefixes. The prefix poly- may be replaced by an appropriate multiplicative prefix; e.g. the bacterial product bactoprenol can be called ditrans,octa-cis-undecaprenol rather than ditrans,polycis-undecaprenol.

#### Note

If this recommendation is followed it is not advisable to omit the multiplicative prefix indicating the total number of residues, even though it contains redundant information. In ditrans,octacis-undecaprenol, for example, a prenol with one  $\omega$ , two trans and eight cis residues must have eleven residues in all.

### SPECIFIC COMPOUNDS

Pr-8. Trivial names. Several short-chain prenols are known by trivial names. For example, the diphosphates with one to five residues are named as follows:

Number of residues	Stereochemistry	Trivial name
1	(none)	dimethylallyl diphosphate
2	<u>trans</u>	geranyl diphosphate
	<u>cis</u>	neryl diphosphate
3	<u>2-trans,6-trans</u>	farnesyl diphosphate
	<u>2-cis,6-trans</u>	
	<u>2-trans,6-cis</u>	
	<u>2-cis,6-cis</u>	
4	<u>2-trans,6-trans,10-trans</u>	geranylgeranyl diphosphate
	<u>2-cis,6-trans,10-trans</u>	geranylneryl diphosphate
5	<u>2-trans,6-trans,10-trans,14-trans</u>	geranylarnesyl diphosphate
	<u>2-cis,6-trans,10-trans,14-trans</u>	
	<u>2-trans,6-cis,10-trans,14-trans</u>	
	<u>2-cis,6-cis,10-trans,14-trans</u>	

Dimethylallyl diphosphate (strictly 3,3-dimethylallyl diphosphate), geranyl diphosphate and neryl diphosphate are entirely specified by name, and need no further stereochemical designation. Dimethylallyl is the trivial name for 3-methylbut-2-enyl. The name dimethylallyl does not conform to ref. 8, and is ambiguous if used outside biochemical contexts.

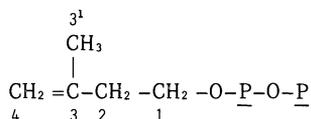
The name farnesyl diphosphate covers four  $C_{15}$  stereoisomers. It is confusing that they have been designated trans,trans, cis,trans, trans,cis and cis,cis, with the first designator applying to C-2 and the second to C-6 [16], i.e. the reverse order from that used for poly-prenols (recommendation Pr-6). We therefore recommend that locants should be used to minimize confusion, e.g. 2-cis,6-trans-farnesyl diphosphate; this becomes trans,cis when lengthened to form the  $\omega$ -terminus of a polyprenol.

Two  $C_{20}$  prenyl groups have been named geranylgeranyl and geranylneryl; in them the second isoprene residue from the oxygen atom is always trans, i.e. the group is 6-trans. The use of these terms is so widespread and well established that it would probably be damaging to recommend changes. Other compounds should be named according to sections Pr-4 to Pr-7, e.g. dicis,trans-tetraprenyl diphosphate for the compound with 2-trans-6,10-dicis stereochemistry.

#### Note

We see no harm in using the polyprenol system (sections Pr-4 to Pr-7) for  $C_{20}$  compounds (i.e. naming them as tetraprenols). This usage eliminates the inconsistency of reversing the order of stereochemical designators for compounds of fewer than five residues.

Pr-9. Isopentenyl diphosphate. An important isomer of dimethylallyl diphosphate is isopentenyl diphosphate (structure III), the diphosphate of 3-methylbut-3-en-1-ol (isopentenyl alcohol). It is the universal building block of isoprenoids; a prenyl diphosphate reacts with it to lose diphosphate and grow longer by one residue (Figs. 1 and 2). Its name should be retained.



### III

#### Notes

1. The CH<sub>2</sub>= group of isopentenyl alcohol contains C-4 [see recommendation C-13.11(b) of ref. 8]. This is convenient, as C-4 of isopentenyl diphosphate is the precursor of C-4 of a lengthened prenyl (Fig. 1).
2. The name isopentenyl is recommended only for biochemical use; it does not conform to ref. 8 and is ambiguous outside biochemical and prenyl contexts. Isopentenyl is the trivial name for 3-methylbut-3-enyl.

Pr-10. Relationship between polyprenols and isoprenoids. The derived isoprenoids are named as follows:

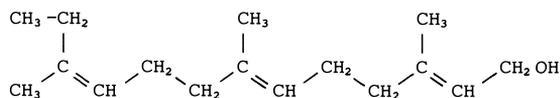
Number of residues	Prenol precursor (as diphosphate, etc.)	Terpenoid class
1	dimethylallyl alcohol	hemiterpenoid
2	geraniol or nerol	monoterpenoid
3	farnesol	sesquiterpenoid
4	geranylgeraniol	diterpenoid
5	geranylfarnesol	sesterterpenoid
6	farnesol*	triterpenoid*
8	geranylgeraniol†	tetraterpenoid or carotenoid†
many		rubber ( <u>all-cis</u> ) gutta percha ( <u>all-trans</u> )

\*Triterpenoids are formed from squalene, which is derived from two farnesyl diphosphate precursor molecules.

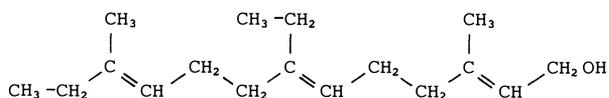
†Carotenoids are formed from phytoene, which is derived from two geranylgeranyl diphosphate precursor molecules.

Pr-11. Juvenile hormones. Farnesol is the prenyl that corresponds to the carbon skeleton of the simplest juvenile hormone. Other members of this group of compounds have an ethyl instead of a methyl group at C-3 and/or C-7 and/or C-11. These may be specified as methyl-substituted farnesol derivatives where the stereospecificity of the ω-isoprene unit (where relevant) is indicated by which methyl group is substituted.

#### Examples



ditrans-11<sup>1</sup>-methylfarnesol



ditrans-7<sup>1</sup>,12-dimethylfarnesol

Pr-12. Dolichol. Dolichols are a group of prenyl derivatives. The term, already widely used (e.g. ref. 2), is recommended for compounds of structure I in which *n* is greater than 4 and in which the residue that carries the hydroxyl group is saturated, i.e. 2,3-dihydropolyprenols. As dolichols are derivatives of prenyls the collective term prenyl should not be used without qualification to include dolichols.

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