

# Numbering of atoms in *myo*-inositol\*

## Recommendations 1988

A relaxation of previous recommendations on the numbering of the atoms of *myo*-inositol is suggested, so that substituents are not necessarily numbered so that the smallest possible locant is used. This allows an alternative designation to be used, when authors wish, to bring out structural relationships.

### INTRODUCTION

Present recommendations on the numbering of cyclitols [1] lead to the designations and numbering shown in structures I, II and III, namely *myo*-inositol, 1*L*-*myo*-inositol 1-phosphate (the compound formed from glucose 6-phosphate in the biosynthesis of inositol), and 1*D*-*myo*-inositol 1-phosphate (the constituent of phospholipids and inositol polyphosphates). Thus phosphorylation on O-1 of *myo*-inositol leads to 1*L*-*myo*-inositol 1-phosphate, whereas phosphorylation on O-3 alters the numbering of the carbon chain, reversing C-1 to C-3, and so leads to 1*D*-*myo*-inositol 1-phosphate.

The reason for this is that recommendation I-4 [1] first allocates the locants 1, 2, 3 and 5 to the four hydroxyl groups that are on one side of the ring, without specifying the starting point. It then allocates the lowest possible locant to the substituted one, so that phosphates II and III are both 1-phosphates. The prefix *D* or *L* is then assigned according to recommendation I-10 [1]: if the ring numbering appears clockwise when the substituent at the lowest numbered chiral centre (here C-1) is away from the viewer (i.e. when the rings drawn are viewed from above), the compound is 1*D*. (The 1 indicates that C-1 is the chiral centre used.)

For achiral compounds, e.g. *myo*-inositol itself, the numbering is defined as that that gives 1*L*. Hence such compounds, e.g. *myo*-inositol with identical substituents on positions 1, 3, 4 and 6, have to be allotted 1*L* or 1*D* designations to give the locants specific meanings.

### PROPOSAL FOR STEREOSPECIFIC NUMBERING

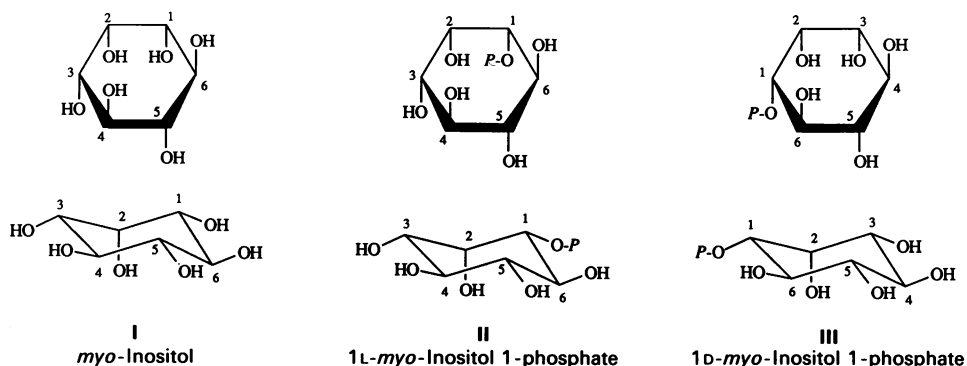
Klashchitskii *et al.* [2] have suggested stereospecific numbering for *myo*-inositol, as has proved successful for glycerol derivatives [3], and Parthasarathy & Eisenberg [4] have advocated such a system. It would overcome the difficulty that phosphorylation at O-1 gives 1*L*-*myo*-inositol 1-phosphate whereas phosphorylation at O-3 alters the numbering of the carbon chain to give 1*D*-*myo*-inositol 1-phosphate.

Such stereospecific numbering would be a minimal change from existing practice, and would leave the numbering of all the inositol bis- and tris-phosphates unchanged; it would also change the name of the product of the reaction catalysed by the enzyme classified as EC 5.5.1.4 (currently with recommended name *myo*-inositol 1-phosphate synthase) to an inositol 3-phosphate instead of 1*L*-*myo*-inositol 1-phosphate, and its relationship to the other derivatives would be clearer. Despite these advantages, we are advised that stereospecific numbering would be confusing to many who are not concerned with metabolic pathways, would obscure enantiomeric relationships, and would disrupt existing usage and indexing.

### PRESENT RECOMMENDATION

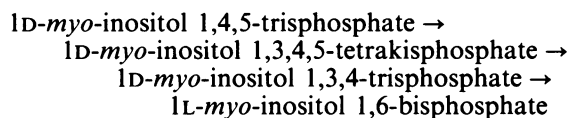
#### Relaxation of lowest-locant rule

The advantages of stereospecific numbering can be obtained by relaxing the rule that a substituent must have

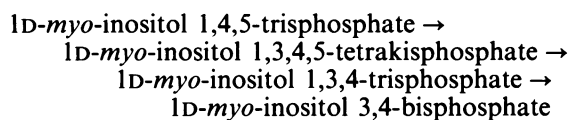


\* These are recommendations of the Nomenclature Committee of the International Union of Biochemistry (NC-IUB), whose members are H. B. F. Dixon (Chairman), C. R. Cantor, C. Liébecq (representing the IUB Committee of Editors of Biochemical Journals), N. Sharon, P. Venetianer and J. F. G. Vliegthart. NC-IUB thanks the following for expert advice during the preparation of these recommendations: S. J. Angyal (Australia), C. P. Downes (U.K.), F. Eisenberg, Jr. (U.S.A.), R. F. Irvine (U.K.), R. H. Michell (U.K.), R. Parthasarathy (India) and V. I. Shvets (U.S.S.R.). NC-IUB also thanks members of the IUPAC-IUB Joint Commission on Biochemical Nomenclature (JCBN) and former members of NC-IUB and JCBN, namely J. R. Bull, A. Cornish-Bowden, P. Karlson, K. L. Loening, G. P. Moss, J. Reedijk, E. J. Van Lenten and E. C. Webb, for consultation. Comments may be sent to any member of NC-IUB, or to its secretary, A. Cornish-Bowden, CNRS-CBM, 31 chemin Joseph-Aiguier, B.P. 71, F-13402 Marseille Cedex 9, France.

the lowest possible locant. Thus a compound that by the priority rules belongs to the 1L series may be given the 1D numbering if this shows relationships that the author wishes to stress. As the prefix 1D will be present, no ambiguity results. We suggest that this should be done whenever it is convenient in biochemical work. Thus 1L-*myo*-inositol 1-phosphate may be called 1D-*myo*-inositol 3-phosphate if it is desired to point out the 1,3 relationship to 1D-*myo*-inositol 1-phosphate. Consider, for example, the following metabolic pathway [5,6]:

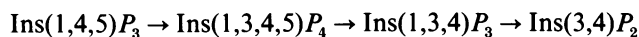


It is not immediately obvious that the last step is hydrolysis at C-1, but this becomes easier to follow if the pathway is written as follows (as was done in the original work [5,6]):



#### The symbol Ins

The symbol Ins was previously given to inositol [3]. Its use is largely confined to biochemical work, and we further suggest that it should be taken to mean *myo*-inositol with the numbering of the 1D configuration unless the prefix L is explicitly added. (This is similar to recommendation 3AA-3.3 in the recommendations on amino acid nomenclature [7] that in biochemical work the symbol Ala refers to L-alanine.) Hence the above pathway may be symbolized as follows:



#### NUMBERING OF ATOMS IN THE CHAIR CONFORMATION

As the numbering of atoms in *myo*-inositol can become especially confusing when the Haworth

projections used for defining the different forms are converted into diagrams representing the normal chair conformations of the molecules, we draw attention to 'Agranoff's turtle' [9], a useful mnemonic advice for avoiding the confusion.

#### REFERENCES

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