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A PROPOSAL FOR THE DESIGNATION OF CONFORMATIONS

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The recent determination of the detailed conformation of many ring compounds (1), particularly using n.m.r. spectroscopy, raises the problem of describing conformations in a text without reference to diagrams. This leads to the use of various descriptions of conformations such as the well established chair and boat to the more recent half chair, skew, butterfly and, for five membered rings, envelope. In most cases, however, such descriptions are ambiguous, there being for example two chair, six boat and six skew conformations for each six membered ring, ten envelope conformations for a five membered ring, and eight non-planar conformations for even a four membered ring.

A system for designating conformations has been in use for some years in the carbohydrate field (2) and is frequently used in publications concerning the two chair conformations of pyranose rings. It is, however, completely arbitrary and only applies to boat and chair conformations of glycopyranoses. Its extension to cover skew and half chair conformations (3) is difficult to use without constant reference to diagrams in which the conformations are defined.

The system for designating conformations described here is applicable to rings containing four, five or six atoms and is probably of use for seven and eight membered rings. It can be used for carbocyclic rings, heterocyclic rings including carbohydrates, and rings containing endo or exo cyclic double bonds. Application to fused rings is possible without extra rules.

Rules

1. Each ring is assigned a letter, T (tetra), P (penta), S (sexa) or H (hepta) depending on whether it contains four, five, six or seven atoms.
2. The ring is arranged so that when viewed from above the numbering of the ring increases in a clockwise direction. The normally accepted numbering system should be used for this purpose.
3. A reference plane is picked containing as many atoms as possible (usually 3 or 4). Where more than one plane is possible the one containing the atoms with the lowest numbers is chosen.

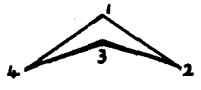
3(a). In carbohydrate rings the hetero-atom should be considered to be numbered O and given precedence over all other atoms for the purpose of picking the reference plane.

4. The numbers of the atoms above the reference plane are placed in front of the ring size letter, and those of the atoms below the plane after the letter. The numbers of atoms in the reference plane are not given.

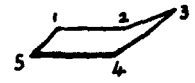
Examples

In these examples the numbers of the atoms in the reference plane are given in parentheses but would not normally be shown at all.

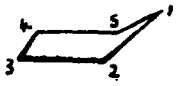
(123) 4 T



(123) T 4

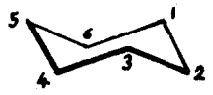


(1245) 3 P

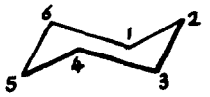


(2345) 1 P

} envelope conformations



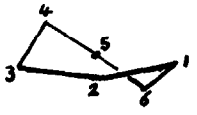
(1245) 3 S 6



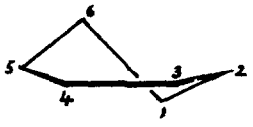
(1245) 6 S 3

} mirror image chairs

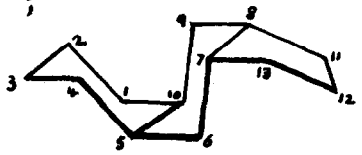
(1256) S 3 4 boat conformation



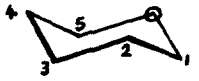
(1235) 4 S 6 skew conformation



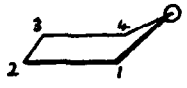
(2345) 6 S 1 half chair conformation



(1245); (5689); (8 11 12 13) 3 S 10; 10 S 7; p 7



(0134) 2 S 5 pyranose C1 conformation



(1234) O P furanose envelope conformation

Subsidiary advantages of this system are:-

(1) Corresponding conformations of enantiomorphs are given by reversing the position of the numbers relative to the ring size letter.

(ii) The two chair conformations of a six membered ring are the same except that the position of the numbers is reversed relative to the letter.

(iii) Conformations can often be visualised without drawing diagrams.

(iv) A mistake in selecting the plane of reference when there is more than one possibility does not prevent the reader from drawing the correct conformation.

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