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Comments on Shallenberger's Chiral Principles Contained in Structure–Sweetness Relations

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ABSTRACT

*The explanation given by Shallenberger (*Food Chem., ***12****, 1983, 89–107) of the difference in sweet taste of* D- *and* L-*amino acids as opposed to the sweet taste of enantiomeric forms of sugars is found to be in error. The chiral principles applied by Shallenberger are shortly reviewed, taking into account that the topism terminology is commonly used for comparison of groups or sides within one structure and not for comparison of two structures where isomerism terminology should be used.*

INTRODUCTION

While there are differences in the sweet taste of enantiomeric amino acids, no differences in the sweet taste of enantiomeric sugars have been found.

Shallenberger (1983) derived three chiral principles which are used in an explanation of the anomaly mentioned above. Topism terminology is used in the derivation of the chiral principles. However, this terminology is commonly used for comparison between groups or sides within one structure and not for comparison between two structures where isomerism terminology should be used (Eliel, 1980).

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THE CHIRAL PRINCIPLES

The examples are given only for the two-dimensional space.

'Principle one. Differential labeling of a regular (symmetrical) geometric structure generates a chiral structure.'

mirror line

These two structures are configurational enantiomers [not configurationally enantiotopic as used by Shallenberger (1983)].

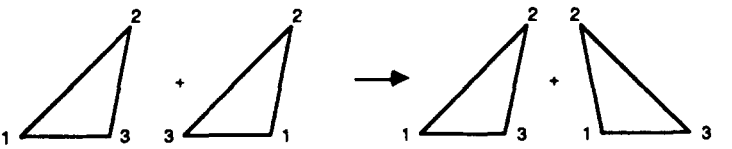
'Principle two. Skewing a regular geometrical structure forms a chiral structure.'

mirror line

These two structures are conformational enantiomers.

'Principle three. The differential labeling of a skewed structure in a given spatial continuum leads to:

(a) Configurational isomers in a given spatial continuum that become conformational isomers only in the next highest continuum.'



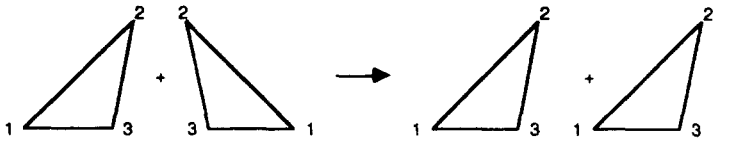
Configurational isomers Conformational isomers

Thus, configurational isomers in 2-space become conformational isomers only in 3-space [not the configurational diastereotopic isomers become conformationally diastereotopic in 3-space, as used by Shallenberger (1983)]. Here too, no topism terminology should be used in comparing two structures. This also applies for the following examples, but will not be mentioned any further.

'(b) Conformational isomers in a given spatial continuum become configurational isomers in the next highest continuum.'

This is the opposite of principle 3(a).

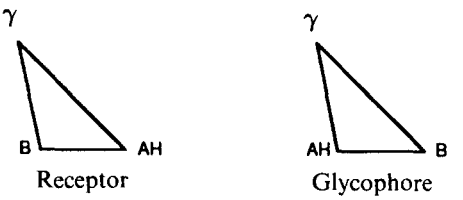
'(c) Enantiomers in a given spatial continuum, which are both configurational and conformational (conversional) enantiomers, then become congruent in the next highest spatial continuum.'



Enantiomers in 2-space become congruent only in 3-space.

The chiral nature of sweetness

The explanation of the anomaly mentioned in the first paragraph is made on the basis of the tripartite concept of sweet taste. In this model the glycophore responsible for the sweet taste, is a skewed triangle formed by a hydrogen-bond donor (AH), a hydrogen-bond acceptor (B) and a hydrophobic binding-side (γ). The receptor side is the 2-space configurational isomer of the glycophore, so that the interaction is made by two hydrogen bonds and one hydrophobic interaction.



DISCUSSION

According to Shallenberger (1983) the glycophores of enantiomeric amino acids are configurational isomers so that principle 3(a) applies to amino acids. For sugars the glycophore of the enantiomers are configurational and conformational isomers so that principle 3(c) can be applied to the sugars. This means that the glycophores of enantiomeric sugars are congruent in 3-space and in contrast with the enantiomeric amino acids no difference in sweet taste is expected.

In the derivation that the glycophores of enantiomeric amino acids are configurational isomers, the next statements are made (Shallenberger, 1983, p. 100):

'To convert a D*-amino acid to an* L*-amino acid requires that* NH_2 *and COOH be transposed about the single chiral center. The effect on the*

glycophore is to merely transpose AH and B. Hence, for the 2-space glycophore structure for the enantiomeric amino acids, the structures are configurationally diastereotopic and conformationally homotopic.'

However, the 2-space glycophore structures for enantiomeric amino acids are configurational and conformational isomers, because the 2-space glycophore structures are enantiomers. If, instead of mirror imaging, the enantiomeric amino acid is obtained by transposing NH_2 and COOH it should be noted that the 2-space glycophore structure changes skewing and labeling, not only labeling as stated by Shallenberger (1983). This means that the chiral principle 3(c) also applies to the glycophores of enantiomeric amino acids, making them congruent in 3-space.

When this is taken into account there remains no essential difference between the 2-space glycophore structures of enantiomeric amino acids and the 2-space glycophore structures of enantiomeric sugars, and no explanation of the anomaly as mentioned in the first paragraph can be given on the basis of the quoted chiral principles.

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REFERENCES

Eliel, E. L. (1980). *J. Chem. Educ.*, **57**, 52–55.
Shallenberger, R. S. (1983). *Food Chem.*, **12**, 89–107.