TIMELESS CLASSICS: ON THE APPLICABILITY OF BOCHVAR'S THREE-VALUED LOGIC B3 TO THE DESCRIPTION OF AN ABSOLUTE CONFIGURATION IN STEREOCHEMISTRY§ (*AUTHOR'S VIEW*)

Cite this: *INEOS OPEN*, **2021**, *4 (2)*, 68–69
DOI: 10.32931/io2110a

Received 21 December 2020,
Accepted 25 June 2021

http://ineosopen.org

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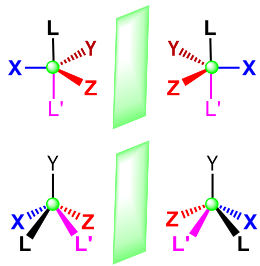
Abstract

It is shown that the absolute configuration of a chiral center can be successfully described in terms of Bochvar's three-valued logic.



Key words: absolute configuration, chiral centers, coordination polyhedra, three-valued logic.

This communication shows that a three-valued logic suggested by a prominent Soviet mathematician and quantum chemist D. A. Bochvar [1] can be used for the description of an absolute configuration—one of the fundamental concepts in stereochemistry [2].

In the early 20s century, particular attention was drawn to the extension of Aristotle's two-valued logical calculus based on two possible values: true (yes) or false (no). The first attempt was made by J. Łukasiewicz [3] who added the third value to these notions: possible. In the author's opinion, among three-valued logical systems suggested subsequently, Bochvar's three-valued logic **B3** is the most interesting one since it introduced meaningless as the third proposition. Herein, the applicability of this type of logics to stereochemistry will be demonstrated.

The types of chirality differ in the character of chiral elements (not to be confused with the crystallographic symmetry elements): center, axis, and chirality plane [4]. An absolute configuration of the molecule with a chiral center depends on the number and arrangement of ligands around this center. The chiral center can be surrounded by 4, 5, or 6 ligands. Although the coordination numbers above 6 are possible, they are rare. The corresponding polyhedra are as follows: a tetrahedron (4), trigonal bipyramid or tetragonal pyramid (5), and octahedron (6). The most popular chiral center in organic chemistry is a carbon atom with tetrahedral geometry for which the (*R*)- and (*S*)-configurations of enantiomers are defined by the well-known Cahn–Ingold–Prelog priority rules [5]. Metal complexes feature, as a rule, the coordination number of 6 and octahedral geometry.

In the 1960–1970s, E. Ruch significantly extended the chirality notion, turning to other chiral centers. Ruch's theorem [6, 7] based on the homochirality concept states that an unambiguous assignment of the configuration is possible only for chiroids of ***a*** class, in which chiral zones are separated by an achiral boundary as in a tetrahedron (T) or trigonal bipyramid (TB) (Fig. 1).

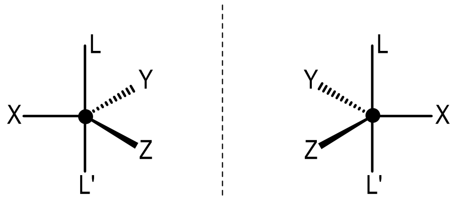


Fig. 1. Trigonal bipyramid with three different monodentate ligands in a basal plane. When L = L', a symmetry plane arises that passes between these ligands and involves the three remaining ones. It is an achiral boundary between enantiomeric chiral zones (a chiroid of ***a*** class).

An octahedron (O) and tetragonal pyramid (TP) refer to chiroids of ***b*** class, in which there are no achiral boundaries between chiral zones (Fig. 2). Therefore, there is no sense to ask about an absolute configuration of octahedral complexes which lack homochirality.

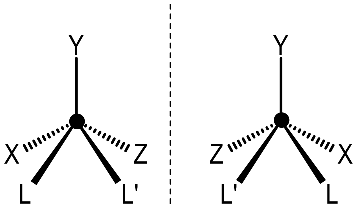


Fig. 2. Tetragonal pyramid with different monodentate ligands in a basal plane. When L = L', there is no symmetry plane; therefore, there is also no achiral boundary between chiral zones (a chiroid of ***b*** class).

Hence, the absolute configuration of a chiral center indeed complies with Bochvar's three-valued logic **B3**, according to which the answer to the question about its existence will be as follows:

– "no" when the center is no longer chiral;
– "yes" for a chiral tetrahedron or trigonal bipyramid;

− "meaningless" for a chiral octahedron or tetragonal pyramid.

Let me note also that, for the coordination number of 5, two polyhedra refer to different classes of chiroids. This means that, upon reversible intramolecular conversion between them (TB ↔ TP), if it is possible, a stereochemical result will not be obvious: the absolute configuration may appear and disappear. In the chemical sense, the mentioned equilibrium must lead to racemization.

Acknowledgements

This work was supported by the Ministry of Science and Higher Education of the Russian Federation.

I would also like to mention a landmark prediction of the group of D. A. Bochvar about the stability of fullerene C_{60} which substantially opened the way to nanochemistry [D. A. Bochvar, E. G. Gal'pern, *Dokl. AN SSSR*, **1973**, *209*, 610–612].

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§ Dedicated to the memory of Prof. D. A. Bochvar (1903–1998) who headed the Laboratory of Quantum Chemistry of INEOS RAS.