

This Week's Citation Classic™

CC/NUMBER 30
JULY 23, 1984

Klyne W & Prelog V. Description of steric relationships across single bonds.
Experientia 16:521-3, 1960.
[Westfield College, London, England and Eidgenössische Technische Hochschule,
Zürich, Switzerland]

A general system for specification of conformation—an important feature of molecular structure—was proposed in this paper. [The SC[®] indicates that this paper has been cited in over 675 publications since 1960.]

Vladimir Prelog
Laboratorium für Organische Chemie
Eidgenössische Technische
Hochschule Zürich
CH-8092 Zürich
Switzerland

May 16, 1984

"At the time when 'conformation' had become an important stereochemical concept and conformational analysis a much used heuristic method, conformations were specified either numerically by torsional (dihedral) angles of identified atoms or atomic groupings around a single bond, or often graphically by stereoforulae, e.g., by Newman projections. Various typical conformations were also given special names: eclipsed, staggered, planar, gauche, s-cis, s-trans, etc.

"In the 1950s, the late Bill Klyne from Westfield College, London, and I used to meet often either in England or Switzerland to discuss stereochemical problems, including, of course, the problem of conformational nomenclature. We arrived at the conclusion that the first thing needed was to invent a rule by which the relative position of two arbitrarily chosen ligands of two single-bonded atoms could be unambiguously defined. A conformation can then be specified by the smallest torsional angle of those ligands which have the highest rank according to se-

quence rules proposed by Cahn, Ingold, and me.¹⁻⁴

"For the first purpose, we divided all torsional angles into two enantiomorphous classes and proposed a convention by which they are specified by descriptions (+) = P and (-) = M. We persuaded the IUPAC-IUB Commission on Biochemical Nomenclature to accept this convention, but not all chemists agree with it. Dickerson and Geis write in their book about this decision: 'According to traditional sources there are two types of sin, sins of omission and sins of commission. This is most definitely a sin of Commission.'⁵

"Since very often only averaged, assumed, or inaccurate values of torsional values are available, we divided the two enantiomorphous classes of torsional angles into four subclasses: syn-planar ($0^\circ \pm 30^\circ$, sp), syn-clinal ($60^\circ \pm 30^\circ$, sc), anti-clinal ($120^\circ \pm 30^\circ$, ac), and anti-periplanar ($180^\circ \pm 30^\circ$, ap). After discussing these conventions with several colleagues, we published them (with reluctance!) in the Swiss journal *Experientia*.

"Many chemists (unfortunately not all!) find our classification convenient for writing and talking about molecular structure and especially for discussing the steric course of chemical and biochemical reactions. One can save quite a lot of trivial drawings by using it.

"I, Cahn, and Ingold,^{3,4} and Helmenchen^{6,7} found the descriptions M and P also useful for specification of stereoisomers which are due to hindered rotation around single bonds (atropisomers).

"I believe all this is the reason our paper became a *Citation Classic*."

1. Cahn R S, Ingold C K & Prelog V. The specification of asymmetric configuration in organic chemistry. *Experientia* 12:81-94, 1956.
2. Prelog V. Citation Classic. Commentary on *Experientia* 12:81-94, 1956. *Current Contents/Physical, Chemical & Earth Sciences* 22(50):18, 13 December 1982.
3. Cahn R S, Ingold C K & Prelog V. Spezifikation der molekularen Chiralität. *Angew. Chem.* 78:413-47, 1965.
4., Specification of molecular chirality. *Angew. Chem. Int. Ed.* 5:385-415, 1965.
(Cited 680 times.)
5. Dickerson R E & Geis I. *The structure and action of proteins*. New York: Harper & Row, 1969. p. 24.
6. Prelog V & Helmenchen G. Grundlagen des CIP-Systems und Vorschläge zu einer Revision. *Angew. Chem.* 94:614-31, 1982.
7., Basic principles of the CIP-system and proposals for a revision. *Angew. Chem. Int. Ed.* 21:567-83, 1982.