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NOTE ON THE CONFORMATION OF CHAIN MOLECULES

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NOTE ON THE CONFORMATION OF CHAIN MOLECULES

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SUMMARY — Auctor disceptat de opportunitate utendi novis quibusdam vocabulis quae a IUPAC (International Union Pure and Applied Chemistry) proposita sunt.

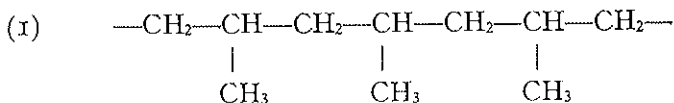
Many researchers working in the field of stereochemistry have been using terms *cis*, *gauche*, *trans* to identify different conformational isomers. They may be abbreviated as *c*, g^+ , g^- , *t* according as the torsion angles are 0° , $\pm 60^\circ$ and 180° . These terms have been used for many years and are convenient, particularly, for the conformational study of chain molecules. (See Table 1). In addition to these some authors proposed to introduce a term *skew* (s^+ and s^-) in the case of $sp^3 - sp^2$ electronic configurations.

Recently the IUPAC Commission on the Nomenclature of Organic Chemistry proposed Tentative Rules for Fundamental Stereochemistry (See IUPAC Information Bulletin 35).

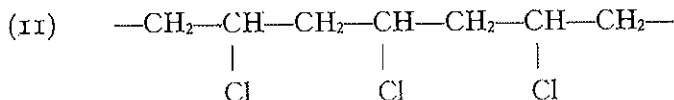
Paper presented on April 17th, 1970, during the Plenary Session of the Pontifical Academy of Sciences.

I) According to Rule E-6.6, conformations are described as synperiplanar (sp), synclinal (sc), anticlinal (ac), or anti-periplanar (ap) according as the torsion angle is 0° , $\pm 60^\circ$, $\pm 120^\circ$, or $\pm 180^\circ$. We understand this rule is practical in some cases, but at the same time we are afraid that this rule may be inconvenient to many physico-chemical treatments, particularly to those of chain molecules.

For example, if we consider such chain molecules as:



and



we have to use different notations for the same conformation: (See Table I). Furthermore, one letter abbreviations: *c*, *g*, *s*, or *t* will be more convenient than two letter abbreviations: sp, sc, ac, or ap.

TABLE I — *Notations for chain conformations*

| Chain | Notation widely used | Notation due to Rule E-6.6 |
|-------|------------------------------------|---|
| (i) | Extended zigzag syndiotactic chain | |
| I | tttttt | (ap) (ap) (ap) (ap) (ap) (ap) |
| II | tttttt | (sc) ⁺ (sc) ⁻ (sc) ⁻ (sc) ⁺ (sc) ⁺ (sc) ⁻ |
| (ii) | Three-fold isotactic helix | |
| I | tggtg | (ap) (sc) (ap) (sc) (ap) (sc) |
| II | tggtg | (sc) (ap) (sc) (ap) (sc) (ap) |

2) This Tentative Rule cannot be used without the knowledge of the bond nature of the rotation axis, for which a clear-cut classification was made as a single bond, a double bond or a bond of partial order. However, it should be borne in mind that we can often determine the conformation without the knowledge of the bond nature. This is also the case for a conformation in the excited molecular states in which not only physical chemists but also organic chemists are interested. Furthermore, even for single bonds we have different kinds which affect the conformations.

We appreciate the efforts of the Commission Members very much, but before changing the terms widely used so far, we hope the Members would consider the different situations in various areas.