# New Aspects of Isomerism and Isomerisation
## Discovery of the Sixth and Final Form of Stereoisomerism and a Unified and Systematic Framework for All Isomerism

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Stereochemistry has been thought complete for the last 60 years following Pasteur's description of chirality in 1848, the notion of *cis-trans* isomerism about a double bond in 1890, atropisomerism in 1914, inversion at tetrahedral N, and at 5-coordinate P, both in the 1960's.

Our discovery in 2018 of the sixth, and definitively the last, form of stereoisomerism, which we called **akamptisomerism**, showed that there were still aspects of isomerism that were unknown. This is a significant problem for the discovery of new chemical compounds by both synthetic design and by artificial intelligence and it also has great significance in patent law.

This lead us the think long, hard, and deeply about the subject and we found several new, and we think very important, features of isomerism that substantially overcome the previous limitations.

We have developed a conceptual framework capable of describing the full scope of stereoisomerism and associated concerted unimolecular rearrangement processes ($R_{st}^c 1$) arising at a single atomic centre of arbitrary coordination number and which is also capable of describing torsions about bonds unlike the previous models. We call our model the Polytopal Formalism of stereochemistry.

Isomerism is composed of two mutually exclusive sub-categories: stereoisomerism and constitutional isomerism. Conceptionally, the scope of stereoisomerism deals with *permutations* of spatial arrangements of atoms or groups. Similarly constitutional isomerism deals with the *permutations* of bonds. Notwithstanding this, to date, these two sub-categories of isomerism have been strictly treated independently resulting in a chasm dividing them.

We have developed a method for generating and cataloging all structures and concerted-unimolecular reaction mechanisms associated with constitutional isomerism and isomerization. It applies the Combinatorics/Graph Theory mathematics of the Polytope Formalism of stereoisomerism and thereby **provides a common approach to model both main branches of isomerism**. We illustrate this concept by application to porphyrin systems, but this approach is broadly applicable to many chemical systems.

Our work also shows that there are substantial deficiencies in present chemical nomenclature.

Of particular importance is the fact that as the Polytopal Formalism strictly defines a finite and complete set of allowed unimolecular reaction pathways between any two genera of a chemical system, its use is thereby also a **powerful tool for the elucidation of concerted unimolecular reaction mechanisms**.