IUPAC Provisional Recommendations

Provisional Recommendations are drafts of IUPAC recommendations on terminology, nomenclature, and symbols, made widely available to allow interested parties to comment before the recommendations are finally revised and published in IUPAC's journal *Pure and Applied Chemistry*. Full text is available online.

Glossary of Terms Used in Developmental and Reproductive Toxicology

The primary objective of this Glossary of Terms Used in Developmental and Reproductive Toxicology is to give clear definitions for those who contribute to studies relevant to these disciplines in toxicology, or who must interpret them, but are not themselves reproductive physiologists or physicians. This applies especially to chemists who need to understand the literature of reproductive and teratogenic effects of substances without recourse to a multiplicity of other glossaries or dictionaries. The Glossary includes terms related to basic and clinical reproductive biology and teratogenesis, insofar as they are necessary for a self-contained document, and particularly terms related to diagnosing, measuring, and understanding the effects of substances on the embryo, fetus, and the male and female reproductive systems. The glossary consists of about 1200 terms as primary alphabetical entries and includes Annexes of common abbreviations and examples of chemicals with known effects on human reproduction and development. The authors hope that among the groups who will find this glossary helpful are, in addition to chemists, toxicologists, pharmacologists, medical practitioners, risk assessors, and regulatory authorities. In particular, the Glossary should facilitate the worldwide use of chemical terminology in relation to occupational and environmental risk assessment.

Comments by **30 April 2016.**

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How to Name Atoms in Phosphates, Polyphosphates, their Analogues, and Transition State Analogues for Enzyme-catalysed Phosphoryl Transfer Reactions

Procedures are proposed for the naming of individual atoms, N, P, O, etc., in phosphate esters, amidates, thiophosphates, polyphosphates, their mimics, and analogues of transition states for enzyme-catalysed phosphoryl transfer reactions. Their purpose is to enable scientists in very different fields, e.g. biochemistry, biophysics, chemistry, computational chemistry, crystallography, molecular biology, NMR, etc., to share standard protocols for the labelling of individual atoms in complex molecules. This will facilitate clear and unambiguous descriptions of structural results and scientific intercommunication concerning them. At the present time, perusal of the Protein Data Bank (PDB) and other sources shows that there is a limited degree of commonality in nomenclature but a large measure of irregularity in more complex structures. There appears to be no common ground with nomenclature used in computational work or in NMR. The recommendations described herein adhere to established practice as closely as possible, in particular to IUPAC and IUBMB recommendations, and to "best practice" in the PDB, especially to its atom labelling of amino acids, and particularly to Cahn-Ingold-Prelog rules for stereochemical nomenclature. They are designed to work in complex enzyme sites for binding phosphates, but also to have utility for non-enzymatic systems. Above all, the recommendations are designed to be clear, easy to assimilate, and convenient to use.

Comments by **30 June 2016.**

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Comprehensive Definition of Oxidation State

Oxidation state (OS) is a simple numerical attribute of an atom in a compound, which aids the systematic descriptive chemistry of the elements, scales trends in properties, and tracks key chemistry changes in reactions. Lacking a comprehensive definition, OS has so far been defined via algorithms for its calculation or with postulated values. This document provides a definition of OS based on ionic approximation of chemical bonds. Associated with the definition's underlying principle of bond-electron allegiance, two general algorithms are outlined for OS determination in a molecule, ion, or a solid, described by a Lewis formula or a bond graph. Typical origins of ambiguous OS values are pointed out, and the relationship between OS and the d-electron configuration of transition metals is commented on.

Comments by **31 May 2016.**

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