contained papers from winners of the 2016 IUPAC-SOLVAY International Award for Young Chemists.

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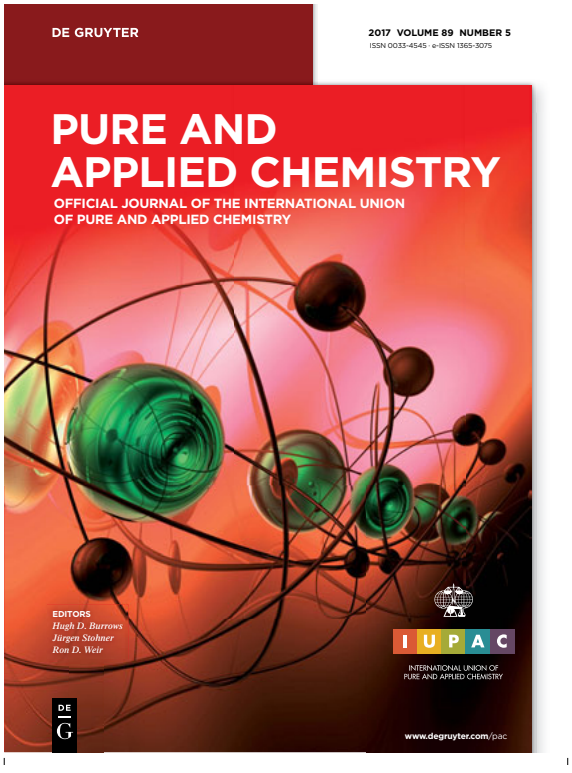

How to name atoms in phosphates, polyphosphates, their derivatives and mimics, and transition state analogues for enzyme-catalysed phosphoryl transfer reactions (IUPAC Recommendations 2016)

G. Michael Blackburn, Jacqueline Cherfils, Gerard P. Moss, *et al.*

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Procedures are proposed for the naming of individual atoms, P, O, F, N, and S in phosphate esters, amidates, thiophosphates, polyphosphates, their mimics, and analogues of transition states for enzyme-catalyzed phosphoryl transfer reactions. Their purpose is to enable scientists in very different fields, *e.g.*, biochemistry, biophysics, chemistry, computational chemistry, crystallography, and molecular biology, to share standard protocols for the labelling of individual atoms in complex molecules. This will facilitate clear and unambiguous descriptions of structural results, as well as 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. The recommendations described here adhere to established practice as closely as possible, in particular to IUPAC and IUBMB recommendations and to "best practice" in the PDB, especially to the 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 easy to comprehend and user-friendly.

https://doi.org/10.1515/pac-2016-0202

A critical review of the proposed definitions of fundamental chemical quantities and their impact on chemical communities (IUPAC Technical Report)

Roberto Marquardt, Juris Meija, Zoltan Mester, *et al.*

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In the proposed new SI, the kilogram will be redefined in terms of the Planck constant and the mole will be redefined in terms of the Avogadro constant. These redefinitions will have some consequences for measurements in chemistry. The goal of the Mole Project (see www.iupac.org/project/2013-048-1-100) was to compile published work related to the definition of the quantity 'amount of substance', its unit the 'mole', and the consequence of these definitions on the unit of the quantity mass, the kilogram. The published work has been reviewed critically with the aim of assembling all possible aspects in order to enable IUPAC to judge the adequateness of the existing definitions or new proposals. Compilation and critical review relies on the broadest spectrum of interested IUPAC members. Recommendation presenting the new definition of the mole will be published early 2018.

https://doi.org/10.1515/pac-2016-0808