## Making an imPAC

## Abbreviations of polymer names and guidelines for abbreviating polymer names (IUPAC **Recommendations 2014)**

Jiasong He, et al Pure and Applied Chemistry, 2014 Volume 86, Issue 6, pp 1003-1015

Abbreviations are commonly used by authors of manuscripts to avoid repetition of lengthy polymer names, and for the benefit of the editors and readers of scientific and professional journals and other written material. People working within industry use a well-established ISO list of abbreviations of polymer names which contains more than 100 entries (138 in ISO 1043-1:2011). In fact, mainly selected on the basis

of the scale of production, the ISO abbreviations are used in industry, standards, trade, and legislation. On the other hand, scientific and professional journals in the polymer field deal with hundreds of polymers annually, including many new ones, some with complicated structures. Thus, IUPAC has also recognized the importance of abbreviations and has published recommendations on the use of common abbreviations for polymer names.

This document provides some basic rules and guidelines regarding the use and creation of abbreviations for the names of polymers. An extended list of currently used abbreviations for polymers and polymeric materials is appended.

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## Toward a comprehensive definition of oxidation state (IUPAC Technical Report)

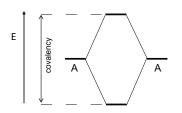
Pavel Karen, Patrick McArdle, and Josef Takats Pure and Applied Chemistry, 2014 Volume 86, Issue 6, pp 1017-1081

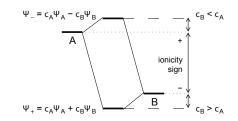
A generic definition of oxidation state (OS) is: "The OS of a bonded atom equals its charge after ionic approximation." In the ionic approximation, the atom that contributes more to the bonding molecular orbital (MO) becomes negative. This sign can also be estimated by comparing Allen electronegativities of the two bonded atoms, but this simplification carries an exception when the more electronegative atom

is bonded as a Lewis acid. Two principal algorithms are outlined for OS determination of an atom in a compound: one based on composition, the other on topology. Both provide the same generic OS because both the ionic approximation and structural formula obey rules of stable electron configurations. A sufficiently simple empirical formula yields OS via the algorithm of direct ionic approximation (DIA) by these rules. The topological algorithm works on a

Lewis formula (for a molecule) or a bond graph (for an extended solid) and has two variants. One assigns bonding electrons to more electronegative bond partners, the other sums an atom's formal charge with bond orders (or bond valences) of sign defined by the ionic approximation of each particular bond at the atom. A glossary of terms and auxiliary rules needed for determination of OS are provided, illustrated with examples, and the origins of ambiguous OS values are pointed out. An electrochemical OS is suggested with a nominal value equal to the average OS for atoms of the same element in a moiety that is charged or otherwise electrochemically relevant.

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The essence of the adopted ionic approximation based on how the valence orbitals participate in the bonding MO. The mixing coefficients  $c_{\mathrm{A}}$  and  $c_{\mathrm{B}}$ refer to the atomic-orbital wavefunctions  $\psi_{\mathrm{A}}$  and  $\psi_{\mathrm{B}}$  in a MO as linear combination of atomic orbitals (MO-LCAO) approach.