Automated Determination of Oxidation Number on an in-silico basis using Electronegativity through a Semantic Markup system in XML

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Abstract

A methodology to determine the oxidation numbers of every atom in a chemical structure is arrived on in-silico basis. This method involves a structure markup system developed in XML, where the electron environment of every atom is encoded explicitly. The calculation of oxidation number is achieved automatically through a structure editor, ChemEd utilizing the electronegativity attributes of every atom in the structure markup.

References


**Index Terms**

Computer Science

Applied Sciences

**Keywords**

Oxidation Number, XML, Chemical Bonding, Chemical Structure, Electronegativity.