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.