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

Durairaj Vijayasarathi
Department of Chemistry
Kanchi Mamunivar
Centre for Post Graduate Studies
Puducherry- 605 008, India

Panneerselvam Vinoth
Department of Chemistry
Pondicherry Engineering College
Puducherry- 605 008, India

Asok Kumar Jana
Department of Chemistry
Kanchi Mamunivar
Centre for Post Graduate Studies
Puducherry- 605 008, India

Punnaivanam Sankar
Department of Chemistry
Pondicherry Engineering College
Puducherry- 605 008, India

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.

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

1. INTRODUCTION
Oxidation number (ON) of an atom is a measure of the degree of oxidation of an atom in a molecule[1]. The oxidation number of an atom in a compound is considered as a hypothetical charge of the corresponding atomic ion[2]. It is arrived by heterolytically cleaving the bonds associated with the atoms of different electronegativity and allocating the electrons to the atom with higher electronegativity whereas, the bonds between like atoms are cleaved homolytically[2,3].

The oxidation number is normally used in naming compounds[4] like Iron (II) Sulphate, Iron (III) Sulphate etc. Since the oxidation number shows the number of electrons lost or gained or shared as a result of chemical bonding in molecules, it is also used to identify the oxidation state of any atom in oxidation, reduction, and in redox reactions[5]. Bentley et al[6] reported the method of oxidation number determination using relative electronegativity and its significance in metabolic redox reactions. It is useful especially in understanding the reaction mechanisms in a complex metabolic pathway and to arrive at an inference about an oxidation reaction. A related study reported by Halkides[7] reveals the significance of the oxidation number in biochemistry. The oxidation number also plays a key role in coordination chemistry and organometallic compounds[8].

There are two different methods recommended for determining the oxidation number by IUPAC[4], one is a rule based method in which ON is determined by using the electrons allocated around the atoms. It is calculated as an imaginary charge arising on an atom by counting the electrons around that atom according to a set of rules[4]. The second method is based on the relative electronegativity of atoms bonded to each other in the molecule. According to this method it is possible to calculate the oxidation numbers automatically with the information about the electronegativity of the atom and its electronic environment in the structure. The basic requirement for this determination is the details of electronic status around every atom such as unpaired electron status, shared electron status, unshared electron status, vacant status etc. This kind of electronic information about every atom in the existing structure representation systems like CT, Mole file, InChI, SMILES, CML etc. are either not available or not explicit. Recently it is reported that the electronic environment of every atom in the structure can be encoded using XML markup[9-13]. This markup system describes the chemical structures with a deeper semantics by including the electronic details around every atom explicitly. The semantics about the electrons are encoded with appropriate number of <electronLink> XML tags representing the valence electrons of every atom. These attributes are used to arrive at the information about the type of bonding such as ionic, covalent, co-ordinate covalent and polar covalent in a chemical structure.

A methodology to determine the oxidation numbers of every atom in chemical structures using the semantic structure markup system[11] is reported here. This study demonstrates the determination of oxidation number of atoms in a structure description using the electronegativity data associate to the atom in the markup. The study involves the structure editor ChemEd[11] developed and reported earlier to encode the chemical structures in XML along with the details of electronic status around atoms[11].

2. METHOD
The structure markup system describes the semantics about the electrons using <electronLink> element with appropriate attributes inside <atom> element. The <atom> element is described with necessary attributes to signify appropriate elements in Periodic Table.

```
<atom id="a1" atNo="6" block="p" group="14" name="Carbon" symbol="C" charge="0" chargeCount="0" state="neutral"
atomicMass="12.01" electroNegativity="2.55">
        <electronLink id="a1e1" title="s" electronStatus="uPair" type="2s" spin="1" charge="0" chargeCount="0"/>
        <electronLink id="a1e2" title="p1" electronStatus="uPair" type="2px" spin="1" charge="0" chargeCount="0"/>
        <electronLink id="a1e3" title="p2" electronStatus="uPair" type="2py" spin="1" charge="0" chargeCount="0"/>
        <electronLink id="a1e4" title="p3" electronStatus="uPair" type="2pz" spin="1" charge="0" chargeCount="0"/>
</atom>

<atom id="a1" atNo="7" block="p" group="15" name="Nitrogen" symbol="N" charge="0" chargeCount="0" state="neutral"
atomicMass="14.01" electroNegativity="3.04">
        <electronLink id="a1e1" title="s" electronStatus="lPair" type="2s" spin="2" charge="0" chargeCount="0"/>
        <electronLink id="a1e2" title="p1" electronStatus="uPair" type="2px" spin="1" charge="0" chargeCount="0"/>
        <electronLink id="a1e3" title="p2" electronStatus="uPair" type="2py" spin="1" charge="0" chargeCount="0"/>
        <electronLink id="a1e4" title="p3" electronStatus="uPair" type="2pz" spin="1" charge="0" chargeCount="0"/>
</atom>

<atom id="a1" atNo="15" block="p" group="15" name="Phosphorus" symbol="P" charge="0" chargeCount="0" state="neutral"
atomicMass="30.98" electroNegativity="2.19">
        <electronLink id="a1e1" title="s" electronStatus="lPair" type="3s" spin="2" charge="0" chargeCount="0"/>
        <electronLink id="a1e2" title="p1" electronStatus="uPair" type="3px" spin="1" charge="0" chargeCount="0"/>
        <electronLink id="a1e3" title="p2" electronStatus="uPair" type="3py" spin="1" charge="0" chargeCount="0"/>
        <electronLink id="a1e4" title="p3" electronStatus="uPair" type="3pz" spin="1" charge="0" chargeCount="0"/>
        <electronLink id="a1e5" title="d1" electronStatus="vacant" type="3dxy" spin="0" charge="0" chargeCount="0"/>
        <electronLink id="a1e6" title="d2" electronStatus="vacant" type="3dyz" spin="0" charge="0" chargeCount="0"/>
        <electronLink id="a1e7" title="d3" electronStatus="vacant" type="3dzx" spin="0" charge="0" chargeCount="0"/>
        <electronLink id="a1e8" title="d4" electronStatus="vacant" type="3dx2-y2" spin="0" charge="0" chargeCount="0"/>
        <electronLink id="a1e9" title="d5" electronStatus="vacant" type="3dz2" spin="0" charge="0" chargeCount="0"/>
</atom>
```

Fig 1: XML Code Snippet showing the electronic details for Carbon, Nitrogen and Phosphorous atom descriptions

All the atoms represented by the Periodic Table elements are described in XML and stored as an XML library. The atomic description for Carbon, Nitrogen and Phosphorous from the fundamental XML base used for the structure markup is shown in Figure 1.

In the atom description shown in Figure 1, the semantics about the atom is associated to the <atom> XML element with the appropriate attributes and the respective values. It is to be noted that the electronegativity values are included using 'electroNegativity' attributes of the respective <atom> XML elements. The electronic details of Carbon atom is described with four <electronLink> elements for the <atom> XML element. The semantics necessary and sufficient to describe the valence electrons are marked with suitable attributes. The semantics about the electrons like unpaired status, lone paired status, bond paired status and vacant status are explicitly marked for every atom with the attribute 'electronStatus'. The values viz. "uPair", "lPair", "bPair" and "vacant" are used to denote the respective status of electrons associated to every atom. It is seen from the Figure 1 that there are four <electronLink> elements for Carbon atom description. The 'electronStatus' for all the four is shown with the value of "uPair" indicating the electronic status for all the four electrons described for Carbon atom is unpaired i.e. "uPair" <electronLink> elements. In the case of Nitrogen again there are four <electronLink> elements. Among them three are unpaired and one is a lone pair as indicated by the attribute value "lPair" for the respective 'electronStatus' attribute. Accordingly it can be considered that the Nitrogen atom is associated with one 'lPair' <electronLink> and three 'uPair' <electronLink> elements. In a similarly way the Phosphorous atom is associated with nine <electronLink> elements to incorporate the semantic for one lone pair, three unpaired electrons and five vacant *d*-orbital electrons. This indicates that the Phosphorous atom is described with one 'lPair' <electronLink>, three 'uPair' <electronLink> elements and five 'vacant' <electronLink> elements. The semantics also includes the provision to encode the type of orbital, spin status and the charge status on the <electronLink>. The ChemEd structure editor works on this fundamental XML to encode the chemical structure drawn on the screen and generates a more detailed structure description format in XML with rich semantics markup during the structure construction. The ON is automatically calculated by the system and is encoded in the XML description. The structure markup for Carbon and Nitrogen atoms in the structure of Methylamine is shown in Figure 2 and the XML markup is shown in Figure 3.

The XML structure description generated by ChemEd shows the oxidation number of every atom in the structure. This is arrived from the electronegativity data and the semantics of bonded electrons and lone pair electrons. The method involves the counting of total number of valance electrons, bonded electrons and non-bonded electrons in terms of the respective <electronLink>'s. Then the ON is computed by a simple formula. This achieved automatically through an algorithm detailed below:

In case of an atom 'A' bonded to another atom 'X' through a chemical bond, the total number of valance electrons 'V_A' is calculated by counting the 'uPair' <electronLink>'s and 'lPair' <electronLink>'s associated to the atom 'A' described in the XML library. This is represented in the form of an equation (1).

$$V_A = [(\text{'uPair' <electronLink> of atom A}) + 2(\text{'lPair' <electronLink> of atom A})] \quad (1)$$

Further, for the calculation of ON using the electronegativity of bonded atoms, the pair of bonded electrons 'B_A' along a chemical bond is to be counted as the electrons of the atom with higher electronegativity. A zero count is allocated for the atom with lesser electronegativity. Accordingly in the A-X bond, if 'A' atom is more electronegative than 'X' atom then a count of two is allocated to the atom 'A'. Otherwise a zero count is allotted for it. This can be obtained by counting the 'bPair' <electronLink>'s of atom 'A' and comparing the electronegativity of atom 'A' with that of atom 'X'. If the electronegativity values of both the atoms 'A' and 'X' are equal, then the electronegativity difference becomes zero.

In such a situation the bonded electrons are counted by equally sharing them between the two atoms. This is represented in equation (2).

$$B_A = n \text{ (`bPair' <electronLink> of atom A)} \quad (2)$$

Where,

n = 2 for electronegativity of A > electgronegativity of X

n = 1 for electronegativity of A = electgronegativity of X

n = 0 for electronegativity of A < electgronegativity of X

The non-bonded electron (N_A) for the atom 'A' can be calculated as double the number of 'lPair' <electronLink>'s as shown in the equation (3).

$$N_A = 2(\text{`lPair' <electronLink> of atom A}) \quad (3)$$

By combining the three equations (1), (2), (3) and considering the possibilities of more than one bonds to a central atom for which the ON is calculated the equation (4) is used.

$$ON_A = V_A - (\sum B_A + N_A) \quad (4)$$

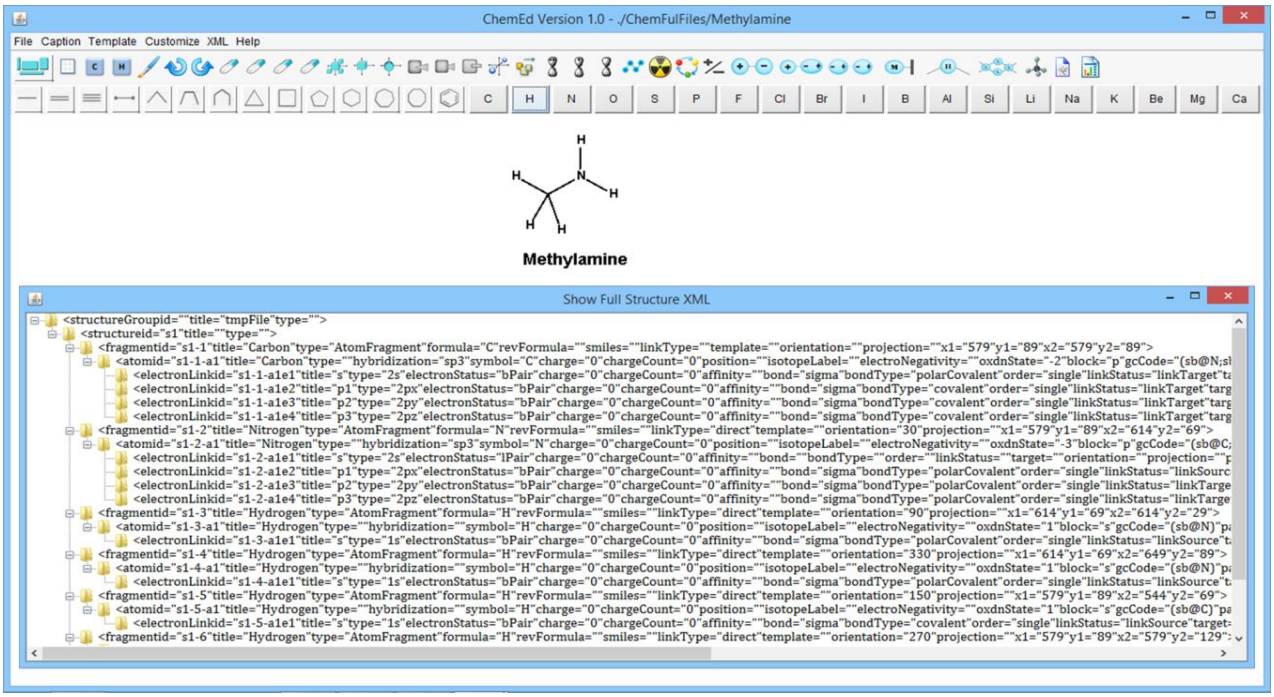

Fig 2: The Structure markups for Methylamine structure in ChemEd Editor

```
<atom id="s1-1-a1" title="Carbon" type="" hybridization="sp3" symbol="C" charge="0" chargeCount="0" position="" isotopeLabel="" electroNegativity="2.55"
        oxdnState="-2" block="p" gcCode="(sb@N;sb@H;sb@H;sb@H)" notation="C(00)(4sh)" partCharge="-" partChargeVal="0.56" x="0" y="0">
        <electronLink id="s1-1-a1e1" title="s" type="2s" electronStatus="bPair" charge="0" chargeCount="0" affinity="" bondType="polarCovalent" bond="sigma"
        order="single" linkStatus="linkTarget" target="s1-2-a1e2" orientation="30" projection="" priority="1.7" gcCode="sb@N" notation="(+δ)hp" partCharge="+"
        partChargeVal="0.49" x1="0" y1="0" x2="35" y2="-20"/>
        <electronLink id="s1-1-a1e2" title="p1" type="2px" electronStatus="bPair" charge="0" chargeCount="0" affinity="" bondType="covalent" bond="sigma"
        order="single" linkStatus="linkTarget" target="s1-5-a1e1" orientation="150" projection="" priority="1.1" gcCode="sb@H" notation="(-δ)hp" partCharge="-"
        partChargeVal="0.35" x1="0" y1="0" x2="-35" y2="-20"/>
        <electronLink id="s1-1-a1e3" title="p2" type="2py" electronStatus="bPair" charge="0" chargeCount="0" affinity="" bondType="covalent" bond="sigma"
        order="single" linkStatus="linkTarget" target="s1-6-a1e1" orientation="270" projection="" priority="1.1" gcCode="sb@H" notation="(-δ)hp" partCharge="-"
        partChargeVal="0.35" x1="0" y1="0" x2="14" y2="40"/>
        <electronLink id="s1-1-a1e4" title="p3" type="2pz" electronStatus="bPair" charge="0" chargeCount="0" affinity="" bondType="covalent" bond="sigma"
        order="single" linkStatus="linkTarget" target="s1-7-a1e1" orientation="240" projection="" priority="1.1" gcCode="sb@H" notation="(-δ)hp" partCharge="-"
        partChargeVal="0.35" x1="0" y1="0" x2="-20" y2="35"/>
</atom>
<atom id="s1-2-a1" title="Nitrogen" type="" hybridization="sp3" symbol="N" charge="0" chargeCount="0" position="" isotopeLabel="" electroNegativity="3.04"
        oxdnState="-3" block="p" gcCode="(sb@C;sb@H;sb@H)" notation="N(00)(1lp;3sh)" partCharge="-" partChargeVal="2.17" x="35" y="-20">
        <electronLink id="s1-2-a1e1" title="s" type="2s" electronStatus="lPair" charge="0" chargeCount="0" affinity="" bondType="" bond="" order="" linkStatus=""
        target="" orientation="" projection="" priority="" gcCode="" notation="(00)lp" partCharge="" partChargeVal="" x1="35" y1="-20" x2="35" y2="-20"/>
        <electronLink id="s1-2-a1e2" title="p1" type="2px" electronStatus="bPair" charge="0" chargeCount="0" affinity="" bondType="polarCovalent" bond="sigma"
        order="single" linkStatus="linkSource" target="s1-1-a1e1" orientation="210" projection="" priority="1.6" gcCode="sb@C" notation="(-δ)hp" partCharge="-"
        partChargeVal="0.49" x1="35" y1="-20" x2="0" y2="0"/>
        <electronLink id="s1-2-a1e3" title="p2" type="2py" electronStatus="bPair" charge="0" chargeCount="0" affinity="" bondType="polarCovalent" bond="sigma"
        order="single" linkStatus="linkTarget" target="s1-3-a1e1" orientation="90" projection="" priority="1.1" gcCode="sb@H" notation="(-δ)hp" partCharge="-"
        partChargeVal="0.84" x1="35" y1="-20" x2="35" y2="-60"/>
        <electronLink id="s1-2-a1e4" title="p3" type="2pz" electronStatus="bPair" charge="0" chargeCount="0" affinity="" bondType="polarCovalent" bond="sigma"
        order="single" linkStatus="linkTarget" target="s1-4-a1e1" orientation="330" projection="" priority="1.1" gcCode="sb@H" notation="(-δ)hp" partCharge="-"
        partChargeVal="0.84" x1="35" y1="-20" x2="70" y2="0"/>
</atom>
```

Fig 3: The XML Code Snippet for Carbon and Nitrogen atoms in Methylamine structure

3. RESULT AND DISCUSSION

The proposed method of arriving at the oxidation numbers of every atom in the structure description in XML is described with the structures of two simple molecules namely Methane (CH_4) and Carbon tetrachloride (CCl_4). The output of ChemEd for these two molecules is shown in Figure 4. The XML descriptions for Carbon atom in Methane structure and Chlorine atom in Carbon tetrachloride is provided in Figure 5 and Figure 6 respectively.

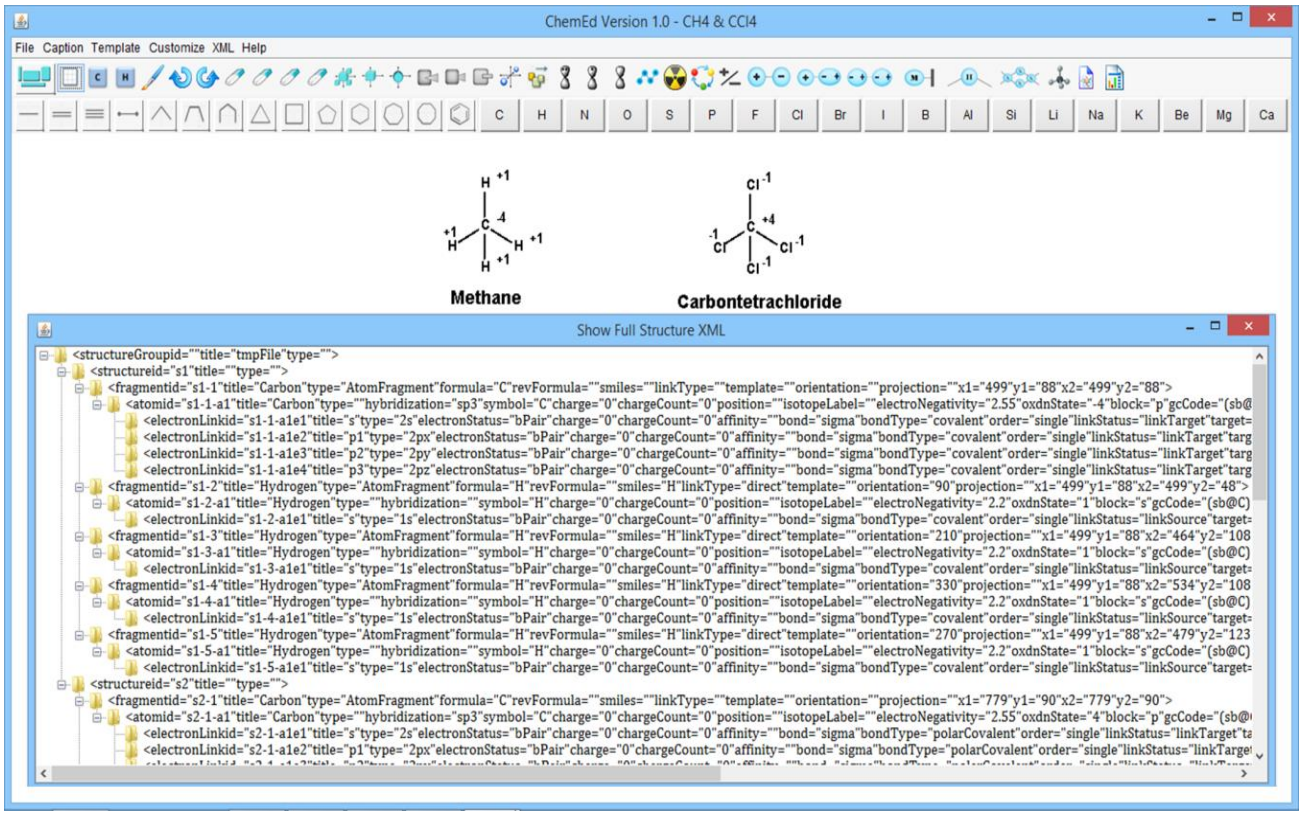

Fig 4: Oxidation Numbers of every atom in the structures of Methane (CH_4) and Carbon tetrachloride (CCl_4) on ChemEd Editor

```
<atom id="s1-1-a1" title="Carbon" type="" hybridization="sp3" symbol="C" charge="0" chargeCount="0" position="" isotopeLabel="" electroNegativity="2.55" oxdnState="-4" block="p" gcCode="(sb@H;sb@H;sb@H;sb@H)" notation="C(00)(4sh)" partCharge="-" partChargeVal="1.40" x="0" y="0">
        <electronLink id="s1-1-a1e1" title="s" type="2s" electronStatus="bPair" charge="0" chargeCount="0" affinity="" bondType="covalent" bond="sigma" order="single" linkStatus="linkTarget" target="s1-2-a1e1" orientation="90" projection="" priority="1.1" gcCode="sb@H" notation="(-δ)hp" partCharge="-" partChargeVal="0.35" x1="0" y1="0" x2="0" y2="-40"/>
        <electronLink id="s1-1-a1e2" title="p1" type="2px" electronStatus="bPair" charge="0" chargeCount="0" affinity="" bondType="covalent" bond="sigma" order="single" linkStatus="linkTarget" target="s1-3-a1e1" orientation="210" projection="" priority="1.1" gcCode="sb@H" notation="(-δ)hp" partCharge="-" partChargeVal="0.35" x1="0" y1="0" x2="-35" y2="20"/>
        <electronLink id="s1-1-a1e3" title="p2" type="2py" electronStatus="bPair" charge="0" chargeCount="0" affinity="" bondType="covalent" bond="sigma" order="single" linkStatus="linkTarget" target="s1-4-a1e1" orientation="330" projection="" priority="1.1" gcCode="sb@H" notation="(-δ)hp" partCharge="-" partChargeVal="0.35" x1="0" y1="0" x2="35" y2="20"/>
        <electronLink id="s1-1-a1e4" title="p3" type="2pz" electronStatus="bPair" charge="0" chargeCount="0" affinity="" bondType="covalent" bond="sigma" order="single" linkStatus="linkTarget" target="s1-5-a1e1" orientation="240" projection="" priority="1.1" gcCode="sb@H" notation="(-δ)hp" partCharge="-" partChargeVal="0.35" x1="0" y1="0" x2="0" y2="40"/>
</atom>
```

Fig 5: The XML description for Carbon atom in the structure of Methane

```
<atom id="s2-2-a1" title="Chlorine" type="" hybridization="sp3" symbol="Cl" charge="0" chargeCount="0" position="" isotopeLabel=""
electroNegativity="3.16" oxdnState="-1" block="p" gcCode="(sb@C)" notation="Cl(00)(3lp;5vp;1sh)" partCharge="-" partChargeVal="0.61" x="280" y="-38">
        <electronLink id="s2-2-a1e1" title="s" type="3s" electronStatus="lPair" charge="0" chargeCount="0" affinity="" bondType="" bond="" order=""
linkStatus="" target="" orientation="" projection="" priority="" gcCode="" notation="(00)lp" partCharge="" partChargeVal="" x1="280" y1="-38" x2="280"
y2="-38"/>
        <electronLink id="s2-2-a1e2" title="p1" type="3px" electronStatus="lPair" charge="0" chargeCount="0" affinity="" bondType="" bond=""
order="" linkStatus="" target="" orientation="" projection="" priority="" gcCode="" notation="(00)lp" partCharge="" partChargeVal="" x1="280" y1="-38"
x2="280" y2="-38"/>
        <electronLink id="s2-2-a1e3" title="p2" type="3py" electronStatus="lPair" charge="0" chargeCount="0" affinity="" bondType="" bond=""
order="" linkStatus="" target="" orientation="" projection="" priority="" gcCode="" notation="(00)lp" partCharge="" partChargeVal="" x1="280" y1="-38"
x2="280" y2="-38"/>
        <electronLink id="s2-2-a1e4" title="p3" type="3pz" electronStatus="bPair" charge="0" chargeCount="0" affinity="" bondType="polarCovalent"
bond="sigma" order="single" linkStatus="linkSource" target="s2-1-a1e1" orientation="270" projection="" priority="1.6" gcCode="sb@C" notation="(-δ)hp"
partCharge="-" partChargeVal="0.61" x1="280" y1="-38" x2="280" y2="2"/>
        <electronLink id="s2-2-a1e5" title="d1" type="3dxy" electronStatus="vacant" charge="0" chargeCount="0" affinity="" bondType="" bond=""
order="" linkStatus="" target="" orientation="" projection="" priority="" gcCode="" notation="(00)vp" partCharge="" partChargeVal="" x1="280" y1="-38"
x2="280" y2="-38"/>
        <electronLink id="s2-2-a1e6" title="d2" type="3dyz" electronStatus="vacant" charge="0" chargeCount="0" affinity="" bondType="" bond=""
order="" linkStatus="" target="" orientation="" projection="" priority="" gcCode="" notation="(00)vp" partCharge="" partChargeVal="" x1="280" y1="-38"
x2="280" y2="-38"/>
        <electronLink id="s2-2-a1e7" title="d3" type="3dzx" electronStatus="vacant" charge="0" chargeCount="0" affinity="" bondType="" bond=""
order="" linkStatus="" target="" orientation="" projection="" priority="" gcCode="" notation="(00)vp" partCharge="" partChargeVal="" x1="280" y1="-38"
x2="280" y2="-38"/>
        <electronLink id="s2-2-a1e8" title="d4" type="3dx2-y2" electronStatus="vacant" charge="0" chargeCount="0" affinity="" bondType="" bond=""
order="" linkStatus="" target="" orientation="" projection="" priority="" gcCode="" notation="(00)vp" partCharge="" partChargeVal="" x1="280" y1="-38"
x2="280" y2="-38"/>
        <electronLink id="s2-2-a1e9" title="d5" type="3dz2" electronStatus="vacant" charge="0" chargeCount="0" affinity="" bondType="" bond=""
order="" linkStatus="" target="" orientation="" projection="" priority="" gcCode="" notation="(00)vp" partCharge="" partChargeVal="" x1="280" y1="-38"
x2="280" y2="-38"/>
</atom>
```

Fig 6: The XML description for a Chlorine atom in the structure of Carbon tetrachloride

The Carbon atom in Methane is more electronegative (EN = 2.55) than Hydrogen (EN = 2.20) atom. The system assigns 8 bonded electrons (four C-H bonds) to the Carbon atom and 0 bonded electrons to Hydrogen atoms. The Carbon atom is described with four <electronLink> elements of bonded electron status and 0 non-bonded electrons in the XML markup. The Hydrogen atom is marked with only one <electronLink> with bonded electrons status. Accordingly oxidation number for Carbon atom is calculated as -4 as per the equation (4) mentioned above (4-(8+0) = -4). Similarly the oxidation number of every Hydrogen atom is calculated as +1 from (1-(0+0) = +1).

In the structure of Carbon tetrachloride molecule, there are four Chlorine atoms bonded to the same carbon atom. The Chlorine is more electronegative (EN = 3.16) than Carbon (EN = 2.55) in this case. As per the above equation (4) the bonded electrons are assigned to the Chlorine atom and no bonded electrons to Carbon atom. Chlorine is captured with nine <electronLink> elements with one bonded electron status and six non-bonded (three lone pairs) electron status. The remaining five <electronLink> are used to indicate the vacant d-orbital electrons. The oxidation number for Chlorine atom is calculated as -1 from the equation (7-(2+6) = -1). For Carbon atom the oxidation number is calculated as +4 as per the equation (4-(0+0) = +4). This resultant oxidation number of every atom is calculated automatically immediately after the structure is completed and is encoded with attribute named as "oxdnState" assigned to <atom> tag in the XML descriptions of the chemical structure drawn in ChemEd editor.

The proposed approach is suitable to capture the oxidation numbers of the atoms in the structures of unstable intermediates too as shown in Figure 7.

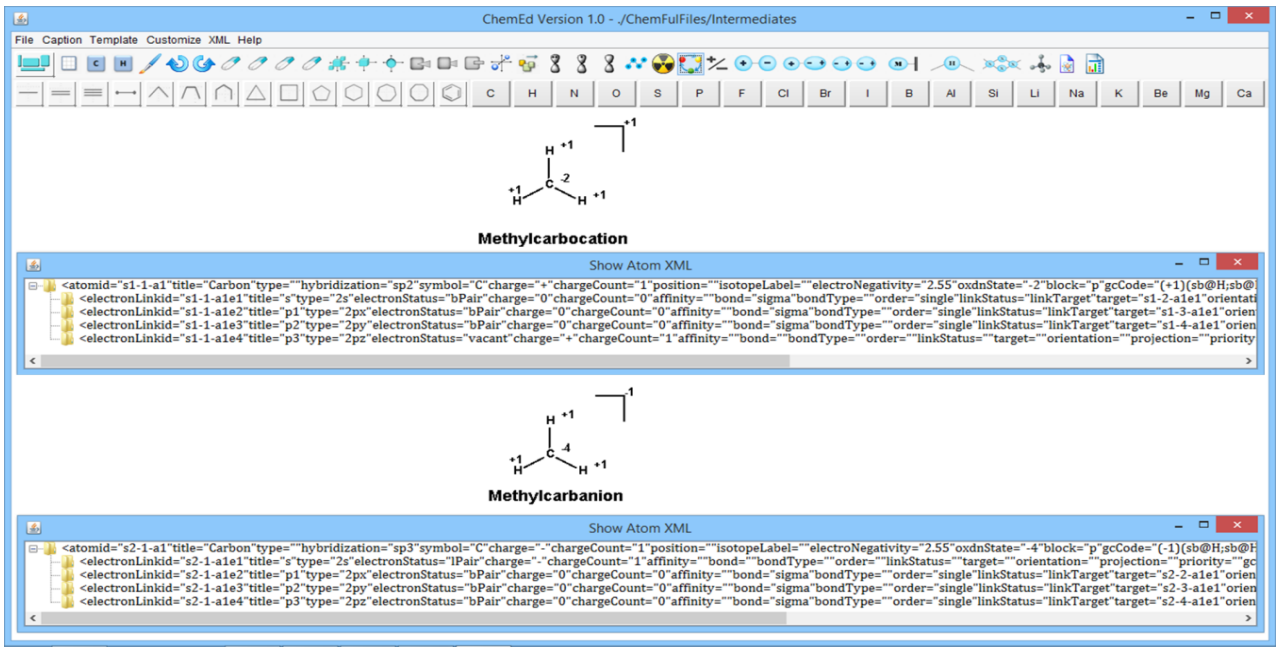

Fig 7: Oxidation Number shown by ChemEd editor for the intermediates Methyl carbocation and Methyl carbanion

The suitability of the method in calculating the oxidation numbers of a biomolecule with the structure of Viracept, an Anti HIV agent[14] is illustrated in Figure 8.

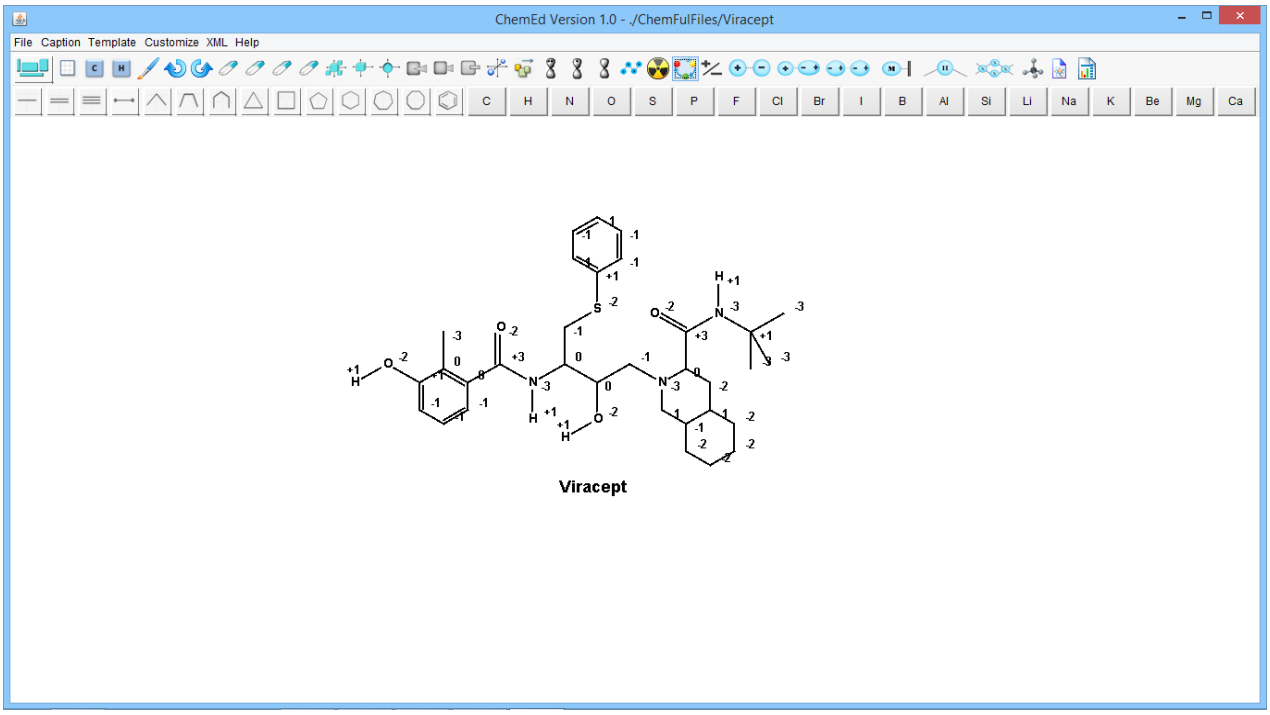

Fig 8: Structure of a biomolecule Viracept showing the Oxidation Number of all atoms

The application of the proposed methodology is demonstrated with a metabolic redox reaction in citric acid cycle[15] in Figure 9. In the metabolic redox reaction the conversion of Isocitrate to α-ketoglutarate the changes in the ON of encircled carbon atoms are captured on both reactant and product side. It is seen from the Figure 9, that the ON of carbon atom bearing the hydroxyl group in Isocitrate is changing from 0 to +2 in the *α*-ketoglutarate indicating that two electron are lost by that carbon atom. Hence it can be inferred as an oxidation process and that information is captured and shown in Figure 9 as reported by the ChemEd editor.

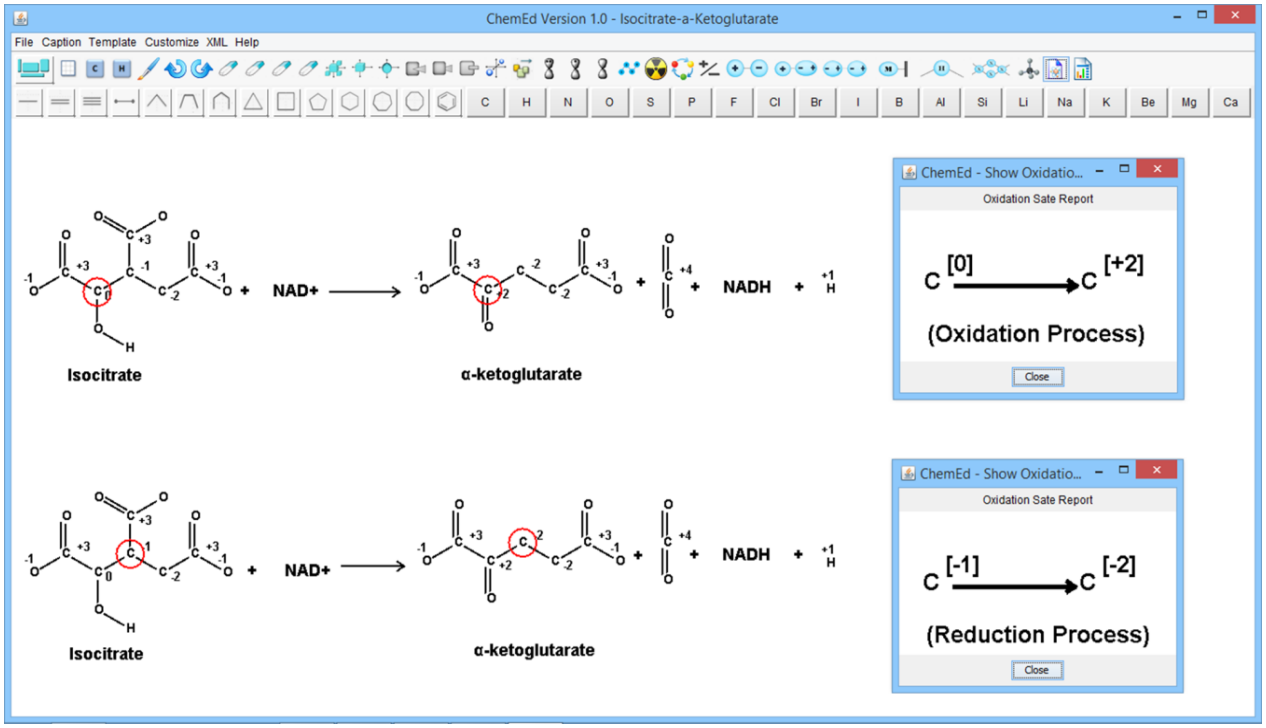

Fig 9: Oxidation Numbers of Selected Carbon atoms in the conversion of Isocitrate to α-ketoglutarate of Citric acid cycle

Similarly for the third carbon in the conversion of Isocitrate to α-ketoglutarate, the ON of next carbon atom in Isocitrate changes from -1 to -2 in the *α*-ketoglutarate due to a gain of one electron in the process. This can be inferred as a reduction process and the same is captured by the editor and shown in the Figure 9. Subsequently it is also possible to conclude the situation of redox condition on the same molecule.

4. CONCLUSION

The proposed methodology utilizes the electron information described explicitly for every atom in the structure as an XML markup. Accordingly the system is capable of arriving at the oxidation numbers based on the valence electron status around every atom in a semantic XML format. This approach makes the system open and useful in the automatic determination of oxidation number of every atom in a chemical structure using the electron information and the electronegativity. The existing structure description formats are not explicit in describing the electronic information. The advantage of the system is that the semantic description of chemical structures in a reaction sequence is suitable for the evolving Semantic Web concepts. The demonstration on biological reaction sequences is suitable for building intelligent applications on reaction modeling as well as for the prediction of biological reaction mechanism on *in-silico* basis. The applicability of the proposed methodology may bring support in the *in-silico* drug discovery also.

5. ACKNOWLEDGMENTS

The authors P.S. and D.V. acknowledge the financial support by the Department of Science & Technology (DST), New Delhi, India (Project No. SR/S1/OC-86/2009).

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