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Research Article

Encoding valence electron configuration, hybridization and geometry of atomic entities with a semantic markup system

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Abstract

Hybridization and geometry of various atomic entities belong to *s*-block, *p*-block, *d*-block and *f*-block elements are determined through a unique AXLE code programmed in Java. The AXLE code describes valence electronic configuration of atomic orbitals of atom entities individually. The hybridization and geometry of atom entities based on AXLE information are visualized in a GUI along with their elemental properties. The system generates a report in XML with the details of electronic environment, bonding status, hybridization and its geometry for neutral and various ionic states of atomic entities.

Keywords: *Atomic orbitals; AXLE code; hybridization; geometry; Extensible Markup Language.*

Introduction

Atom entity is a constitutionally or isotopically distinct species of an atom identifiable as a separately distinguishable entity. The individual atom entities are distinguished based on their valence electron configuration, orbital hybridization and chemical bonding possibilities[1]. Accordingly an atom can be exhibited with different atom entities. For example a Carbon atom in its ground state configuration is an atom entity of Carbon. Carbon atom in sp^3 hybridized state is another atom entity. Similarly carbon atom in different bonding environment is also considered as different entities of carbon atom. The entities of an atom also arise due to the number of lone pair orbitals and vacant electron orbitals. Singlet and doublet carbenes are two distinguishable entities. Consequently an atom can be exhibited with different atom entities with respect to the difference in their valence electron configuration, orbital hybridization and chemical bonding. Similarly all the other atom of elements of Periodic Table can be exhibited with several atom entities. Since the atom entities are characterized with respect to bonding environment, identifying them in chemical structures become significant. It is possible to associate proper geometry for each and every atom entity through its hybridization. The geometry of atomic entities is purely based on its valence electronic configuration. The molecular geometry depends on the geometry of central atom of the molecule.[2] Hence the atomic entity geometry can be related to the molecular geometry.

There are several theories to describe the molecular geometry [C A COULSON; HUHEEY INORGANIC CHEM;HOUSECUFT INORGANIC CHEMISTRY;GILLEPSE INORG STEROCHEM] such as Valence Shell Electron Pair Repulsion theory (VSEPR), Crystal Field Theory (CFT), Ligand Field Theory (LFT), Molecular Orbital theory (MO), Ligand Close Packing theory (LCP),etc., supported with experimental techniques such as IR spectroscopy, X-ray Crystallography, Raman spectroscopy, Microwave spectroscopy, etc. The VSEPR theory is derived from Valence Bond theory and is applied on Lewis structures [ref].In VSEPR theory the bonding electron and lone pair electron plays major role in the determination of geometry of molecules. The method adopted in VSEPR is AXE method, in which 'A' represents central atom, 'X' represents number of bonding electrons and 'E' denotes number of lone pair of electrons. By this method the lone pair electron in valence shell orbital of a molecule determines the geometry.

The involvement of vacant orbitals is imperative in determining the molecular geometry in certain cases (D.Xue,C.Sun and X.Chen hybridization; C E Housecroft and AG Sharp Inorganic Chem; R J Gillespie fifty years; X. Dongfeng, S. Congting, C.Xiaoyan, hybridized) [10, 13, 16, 17]. For example, the square planar geometry of ICl_4^- molecule is explained by AXE method with a notation as 'AX_4E_2' which is derived from Lewis Octet [ref]. The code 'AX_4E_2'represents 4 bonded electron pairs and 2 lone pair electrons around the central atom. Evidences are there which proves the accountability of vacant *d*- and *f*-orbitals in determining the hybridization of atom entity. For example CrH_6, VH_5, YCl_3, $La(NO_3)_3$, $CeCl_3$, etc. the geometry around the central atom can be ascertained by considering the vacant *d*-orbitals also (D.Xue,C.Sun and X.Chen hybridization; R J Gillespie fifty years; X. Dongfeng, S. Congting, C.Xiaoyan, hybridized valence electrons).

This is taken into consideration in the development of AXLE code which describes vacant electron link status, in addition to bond pair electron link (X) and lone pair electron link (L) present in the valence electronic configuration explicitly. This method predicts the geometry of atom entity to perceive the molecular geometry. The system generated AXLE code for ICl_4^- is 'IL2Ep2Ed5', corresponding hybridization is p^2d^2 with square planar geometry which is well coincide with the evidence for vacant *p*- and *d*-orbital participation in detailing the geometry of molecule.

The developed AXLE code in XML semantic markup system focused on the ground state valence electronic configuration of atom entities in predicting the atomic entity geometry. Chemical structural information are encoded with several formats (P. Murray-Rust, and H. S. Rzepa, Markup Languages; P. Murray-Rust, H.S. Rzepa, Chemical Markup)[21-28] such as Connection Table (A. Dalby, J.G. Nourse, W.D. Hounshell, A.K.I. Gushurst) [22] (CTab), Molfile (A. Dalby, J.G. Nourse, W.D. Hounshell, A.K.I. Gushurst)[22], SMILES (D. Weininger, SMILES, a chemical language; D. Weininger, A. Weininger, J. L. Weininger, SMILES. 2. Algorithm; D. Weininger, SMILES. 3. DEPICT. Graphical depiction) [23-25], InChI (The IUPAC International Chemical; InChI TRUST, http://www.inchi-trust.org)[26, 27] and CML (P. Murray-Rust, H.S. Rzepa, Chemical Markup)[28]. The detailed electron information is not explicit in the available formats. As the handling of chemical information in web media demanded the chemical structural information to be described in terms of markup languages, CML (Chemical Markup Language) evolved. In CML the structural information is described based on the Extensible Markup Language (XML) (W3C, Extensible Markup Language (XML))[29] technology. The XML framework allows the description of chemical information with domain specific XML elements along with necessary attributes to attach semantics. A format which can detail the valence electronic configuration of atomic entities reported earlier (P. Sankar, S. Jerome Pastal Raj and P. Vinoth, In-silico; D. Vijayasarathi, P. Sankar, Encoding of Fundamental; P. Vinoth and P. Sankar, Encoding of coordination; P. Sankar, G. Aghila, Design; P. Sankar, G. Aghila, Ontology Aided; P. Sankar, A. Krief, G. Aghila, Model Tool to; P. Sankar, A. Krief, D. Vijayasarathi, A conceptual)[5-7, 30-33] is able to encode the valence electronic environment of every atomic entity in the periodic table. Based on this explicit information the encoding of hybridization, geometry and elemental properties of every atomic entity in periodic table is achieved.

It is found that the ground state valence electronic configuration is enough is suitable for the prediction of hybridization and geometry (P. Sankar, S. Jerome Pastal Raj and P. Vinoth, In-silico; D. Vijayasarathi, P. Sankar, Encoding of Fundamental; P. Vinoth and P. Sankar, Encoding of coordination; Hsin-Yi Liao, Mei-Yin Yen, Computational; M. Sohma, M. Kawaguchi, Magnetic and structural aspects)[5-9]. Hence, in this work the ground state valence electronic configuration of all the entities are created as XML markup system which helps in the visualization of valence electronic configuration of each and every atom entities, in continuation to that respective AXLE code is generated for the same. This AXLE code information predicts the hybridization as well as geometry through proper algorithm. Based on theoretical studies as a guide (D. Xue, C. Sun, and X. Chen, Hybridization)[10] the hybridization and geometry at atomic level is designed.

Results and Discussion

Encoding of hybridization and geometry of atomic entities is ascertained through AXLE code in semantic structure markup system. An

atom has several instances of atomic entities of neutral and ionic states. In case of nitrogen atom, it has 15 atom entity instances that are developed earlier (D. Vijayasarathi, P. Sankar, Encoding of Fundamental) [6]. It comprises both stable and unstable entities. In the case of neutral nitrogen atom entity it possesses one lone pair and three unpair electron links. Likewise each and every atom in the Periodic Table has atom entity class and this is compiled as an XML frame in their ground state valence electronic configuration. This supports the generation of AXLE code for the respective atom entity which in turn reveals the hybridization status along with geometry through an algorithm.

A structured XML frame for atom is already developed in chemical structure editor ChemEd (P. Sankar, A. Krief, G. Aghila, Model Tool)[32]. In the present work XML frame for atom entity is arrived with the <atomEntity> and <electronLink> XML elements. <electronLink> briefly describes the valence electron link status of the specific atom entity. And one can know the electronic status explicitly from the XML report.

There is a consequence in utilizing the ground state or excited state valence electronic configuration of atom entity in the construction of chemical structure. Anomaly the excited state valence electronic configuration of some atomic entities is not suitably explained in the formation of chemical structure (P. Sankar, S. Jerome Pastal Raj and P. Vinoth, In-silico; Hsin-Yi Liao, Mei-Yin Yen, Computational; M. Sohma, M. Kawaguchi, Magnetic and structural aspects)[5, 8, 9]. This can be rectified by utilizing the ground state valence electronic configuration of atom entities in the semantic structure markup system.

In this work hybridization and geometry of atomic entities visualized through AXLE code which details the electronic environment of atomic entities. AXLE represents atomic symbol, bond pair electron link status, lone pair electron link status and vacant electronic link status of atomic orbitals respectively. Based on AXLE code information the hybridization nature of atomic entities and corresponding geometry is predicted by this system in *in-silico* manner. The system shows various type of hybridization of atomic orbitals for neutral and different ionic states of atomic entities along with their spatial arrangements. Electronic environment of hybrid orbitals specifically identified with color scheme i.e., black represents *Bond Pair ElectronLink* (X), orange represents *Lone Pair ElectronLink* (L), dark green represents *Vacant s ElectronLink* (Es), dark pink represents *Vacant p ElectronLink* (Ep), purple represents *Vacant d ElectronLink* (Eid), light pink represents *Outer Vacant d ElectronLink* (Eod), light green represents *Vacant f ElectronLink* (Ef).

The "ChemAt - Atom Entity Editor" is programmed in Java, which describes the hybridization and geometry of all atom entities (in their neutral and ionic states) present in periodic table. The electronic configuration of atomic entities is encoded in <atomEntity> XML element with appropriate attributes. These attributes are an unique 'id' for atomic entities, 'atNo' which represents the atomic number of specific atomic entities, 'block' and 'group' attributes tells about the position of atomic entities in the periodic table, 'symbol' attribute defines the symbol of atomic entities, 'axleCode' attribute describes the AXLE code for specific atomic entity, 'hybridization' and 'geometry' attributes depicts the status of hybridization and geometry of atomic entities pictured in the display panel. The neutral and different ionic states of atomic entities can be viewed from 'state' attribute and other additional attributes such as 'charge', 'chargeCount', 'electroNegativity' and spatial orientation defines the elemental information of atom entities. The knowledge of electronic environment of hybrid atomic orbital known from <electronLink> XML element with attributes such as 'id', 'title', 'type', 'electronStatus', 'hybridStatus', 'spin', 'charge', 'chargeCount', 'bond', 'order', 'orientation' and 'multiBondId'.

A GUI is developed to visualize the hybridization and geometry of atomic entities based on their ground state valence electronic configuration (Figure 1). Graphical User Interface is divided into four compartments, such as Display panel, Atom Entity selection panel, Property panel and Report panel at the center, left, right and bottom portions respectively (Figure 1). Display panel, which is the central panel of GUI, consists of three tabbed panes such as atom, orbital and periodic table tab panes. The hybridization and geometry of specific atomic entities can be visualized by selecting that atom from the periodic table which

is present in the periodic table tab pane of display panel. The orbital tab pane of display panel pictures the electronic arrangement of hybrid atomic orbitals. Atom tab pane shows the geometry of atoms and also describes the hybridization and electronic status of each and every atom. The hybridization and geometry of atomic entities for its neutral and various ionic states can be visualized by selecting the appropriate oxidation state that is arranged in the form of button array at the bottom of display panel. The button array restricted with familiar ionic states of atomic entities. The right hand side of display panel shows few examples of molecules related to atomic geometry. The left panel in the GUI is Atomic entities selection panel in that chemical element are arranged as *s*, *p*, *d* & *f* blocks and displayed in tree view with the support of chemical ontology. One can select an atomic entity that belongs to corresponding group of *s*, *p*, *d* and *f* block elements from this tree view. The property panel which is at right panel in GUI displays the selected elemental properties of atomic entities whose geometry is depicted by the system. Report panel is the bottom panel of GUI where the system triggered a semantic rich report of electronic status, bond order, hybridization and geometry of atomic entities in XML explicitly.

Geometry of *s*-block atom entities

Based on ground state valence electronic environment the hybridization of atomic orbitals explained with appropriate attributes of XML elements through AXLE code which in turn details the hybridization nature and geometry of respective atomic entities in the periodic table. AXLE code details the valence electronic environment of atomic orbitals.

In *s*-block elements, the geometry of all the possible entities are arrived through AXLE code, For Beryllium atom, there are seven possible Beryllium entities (D. Vijayasarathi, P. Sankar, Encoding of Fundamental)[6], the AXLE code for one of the Beryllium entity, Be(0) of ground state valence electronic configuration is $2s^2$ $2p^0$, after hybridization is 'BeX2Ep2', indicates the valence orbital status of hybrid orbitals as 'Be' represents the symbol of atomic entity, 'X2' denotes two bond pair electronlink and 'Ep2' represents two vacant *p*-orbital electron link. Based on this information the system generates the hybridization as *sp* and linear geometry through a logical algorithm and it is pictured in GUI (Figure 1) along with their few examples and elemental properties. The corresponding report is generated in XML description for the Beryllium atom entity is provided in XML Code 1.

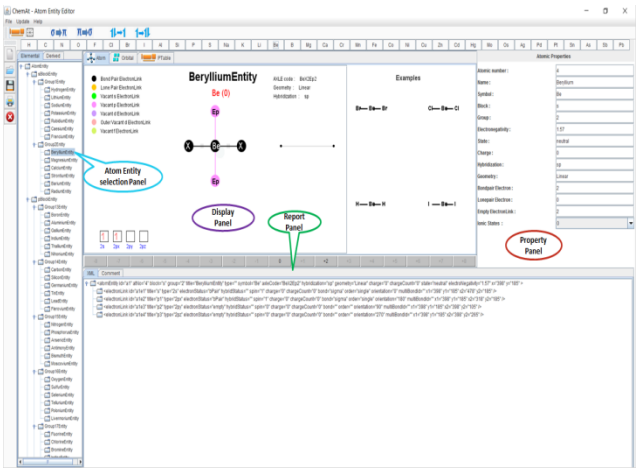

Figure: GUI illustrating encoding details of Beryllium (0) Entity

```
<?xml version="1.0"?>

<atomEntity id="a1" atNo="4" block="s" group="2" title="BerylliumEntity" type="" symbol="Be" axleCode="BeX2Ep2" hybridization="sp" geometry="Linear" charge="0" chargeCount="0" state="neutral" electroNegativity="1.57" x="398" y="185">

<electronLink id="a1e1" title="s" type="2s" electronStatus="bPair" hybridStatus="" spin="1" charge="0" chargeCount="0" bond="sigma" order="single" orientation="0" multiBondId="" x1="398" y1="185" x2="478" y2="185"/>

<electronLink id="a1e2" title="p1" type="2px" electronStatus="bPair" hybridStatus="" spin="1" charge="0" chargeCount="0" bond="sigma" order="single" orientation="180" multiBondId="" x1="398" y1="185" x2="318" y2="185"/>

<electronLink id="a1e3" title="p2" type="2py" electronStatus="empty" hybridStatus="" spin="0" charge="0" chargeCount="0" bond="" order="" orientation="90" multiBondId="" x1="398" y1="185" x2="398" y2="105"/>

<electronLink id="a1e4" title="p3" type="2pz" electronStatus="empty" hybridStatus="" spin="0" charge="0" chargeCount="0" bond="" order="" orientation="270" multiBondId="" x1="398" y1="185" x2="398" y2="265"/>

</atomEntity>
```

XML Code 1: XML description for Beryllium (0) Entity

Similarly, the +2 ionic state of Beryllium entity is selected using ionic state button array the corresponding valence in Figure along with the system generated XML description.

electronic environment displayed as $2s^0$ $2p^0$ in display panel of GUI. The same is depicted as 'BeEs1Ep3' in AXLE code along with its sp^3 hybridization and tetrahedral geometry as shown

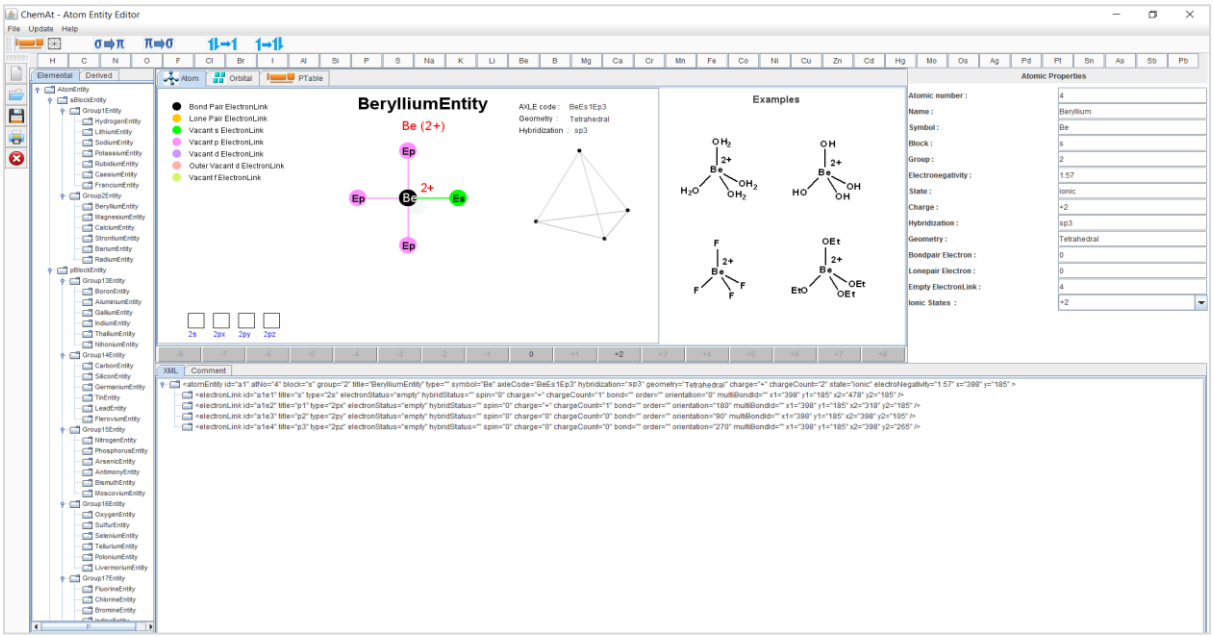

Figure: Encoding details of Beryllium (2+) Entity

The snippet of AXLE code information along with the hybridization and geometry of few *s*- block atomic entities such as Be (0), Mg (0), Na (0), Rb (0), Ca (2+), K (1+), Ba (2+), Li (1+) and Sr (2+) are shown in Table 1.

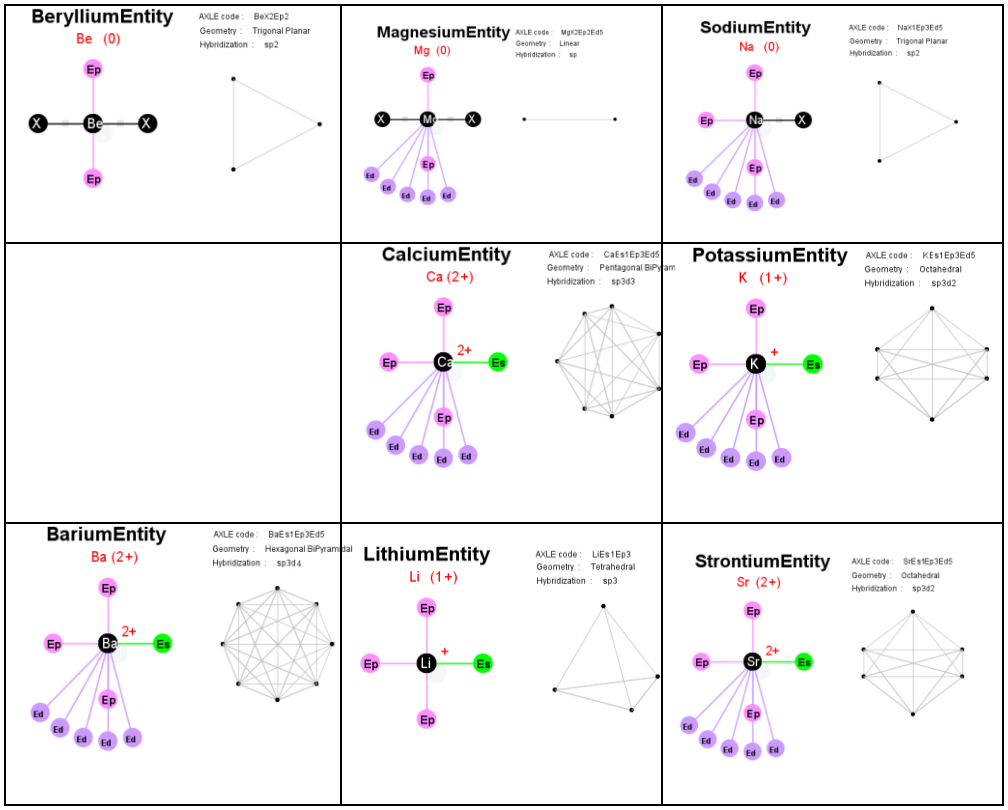

Table: Representative *s*- block atom entities

Geometry of *p*-block atom entities

For Carbon atom, there are 24 possible carbon entities(D. Vijayasarathi, P. Sankar, Encoding of Fundamental Chemical) [6], the geometry of all the possible entities are arrived through AXLE code, here the encoding details C (0) entity is shown in Figure 3 whose AXLE code is 'CX4' for sp^3 hybridization and tetrahedral geometry along with their properties and few representative examples of molecule structure.

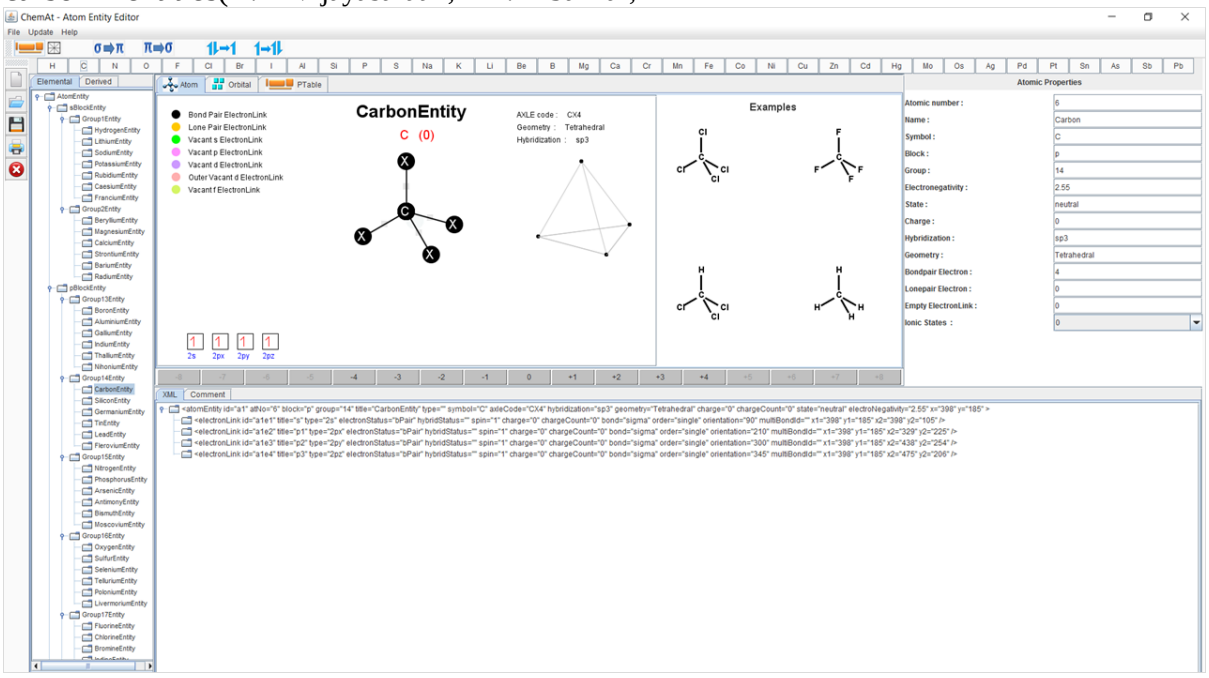

Figure: Encoding details of Carbon (0) Entity

There is option in the GUI to change the bond *sigma* to *pi* vice versa. The change of bond is allowed only for the possible valence electronic environment. For carbon entity by selecting the *sigma* to *pi* bond option from tool bar two of the *sigma* bond turns into *pi* bond and the resultant AXLE code for this entity is 'CX2', its corresponding geometry is linear (Figure 4). Also the electron link status of an entity can be changed into lonepair to unpair link vice versa. This option is utilized to vary the orbital environment suitable for hybridization.

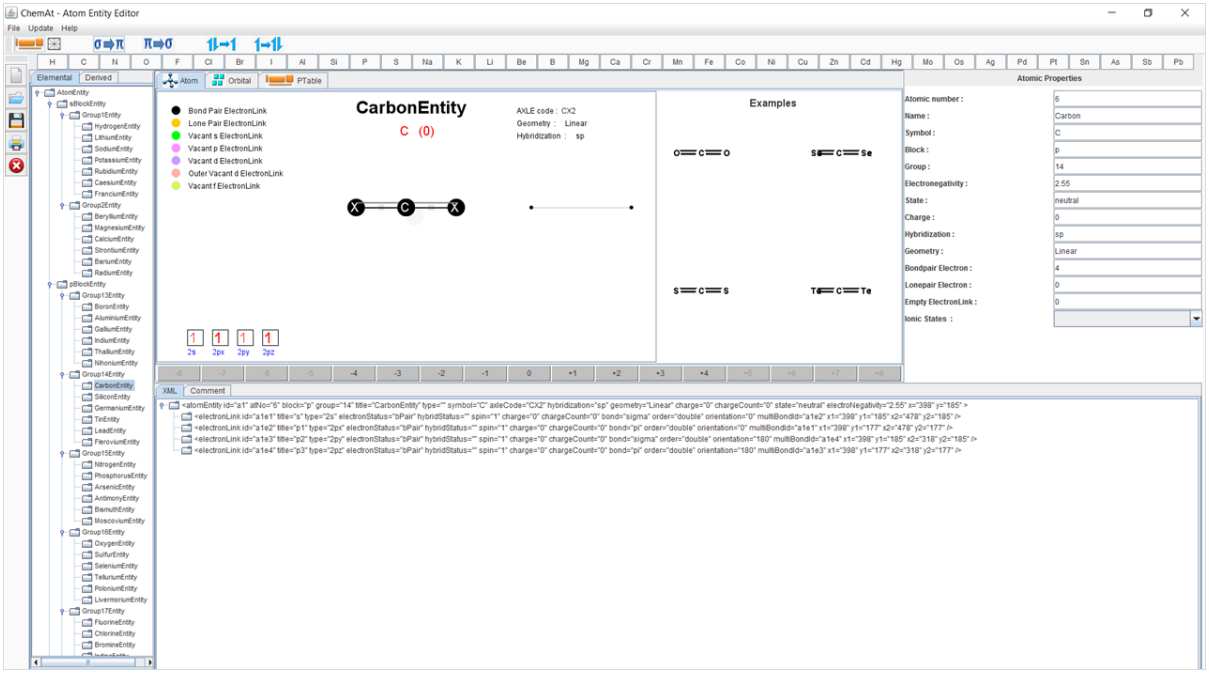

Figure: Encoding details of *sigma* to *pi* bond change in Carbon (0) Entity

The AXLE code information along with the hybridization and geometry of few *p*-block atom entities screen shot is shown in Table 2.

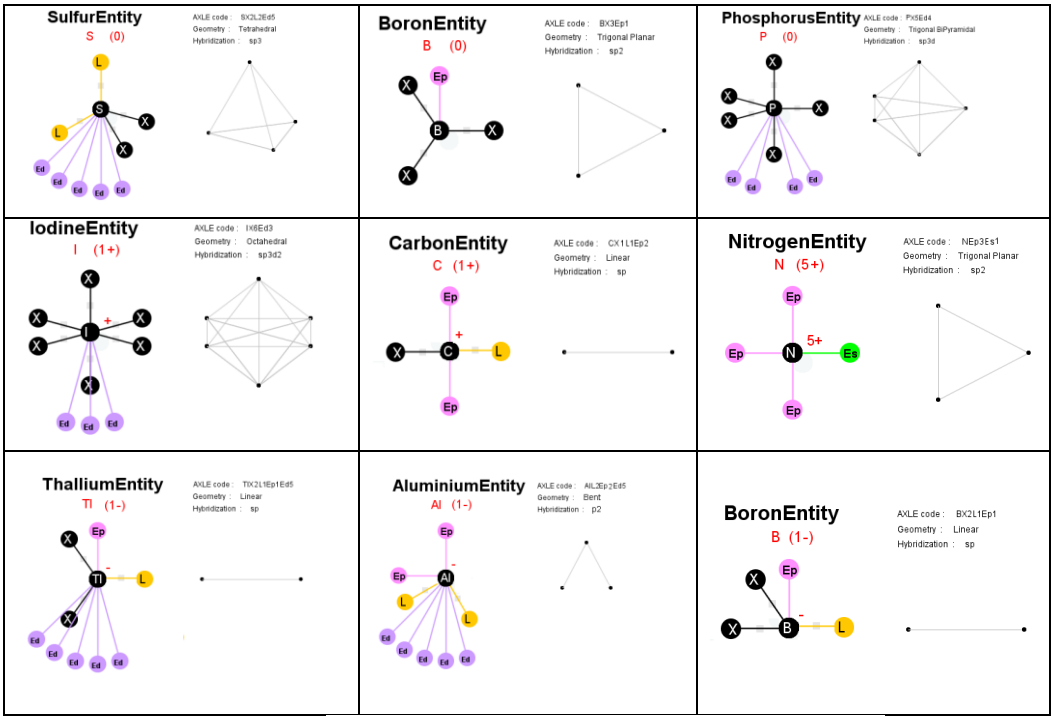

Table: Representative *p*-block atom entities

Geometry of *d*-block atom entities

Transition metal atom entities orbital hybridization occurs with *s* and *p* valence orbitals in addition to inner and outer valence *d*-orbitals. The orbital hybridization of *d*-block atom entities results *dsp* and *spd* pattern. For example Ni^{2+} entity has *sp*, sp^2, sp^3, sp^3d, sp^3d^2, *dsp*, dsp^2, etc., hybridization. All these possibilities can be predicted with the help of developed AXLE code information which includes the valence electronic status such as unpair, lonepair and empty electron link. The system generated AXLE code in case of Ni^{2+} entity is 'NiX2L3Es1Ep3Eod5' in which

'Es1Ep3Eod5' represents vacant *s*-, *p*- and *d*-valence orbital respectively involves in sp^3d^2 hybridization results octahedral geometry. In addition to this, AXLE code also briefs out the valence orbital electronic environment of Ni^{2+} entity, as 'X2' represents presence of two bond pair electrons; 'L3' denotes presence of three lone pair electrons. Encoding details of Ni (2+) entity is given in Figure 5. The AXLE code information along with the hybridization and geometry of few *d*- block atom entities are shown in Table 3.

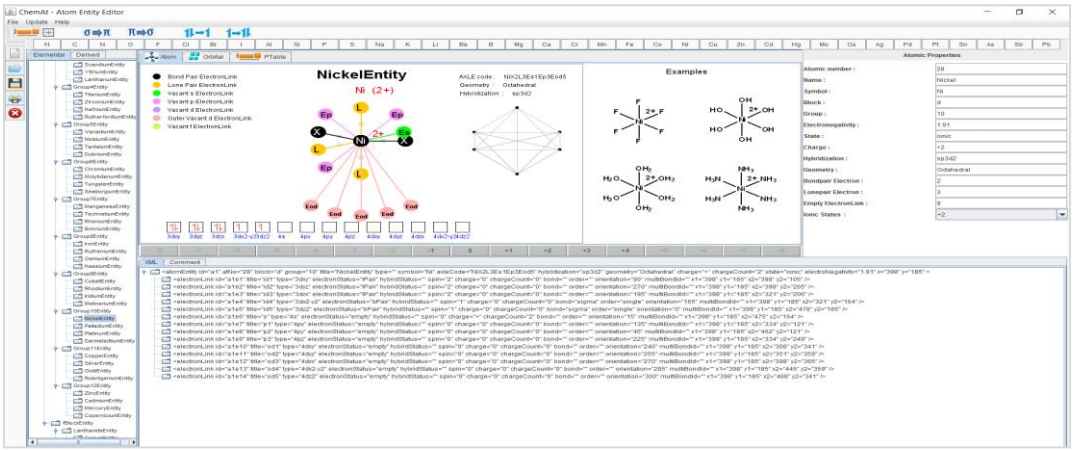

Figure : Encoding details of Nickel (2+) Entity

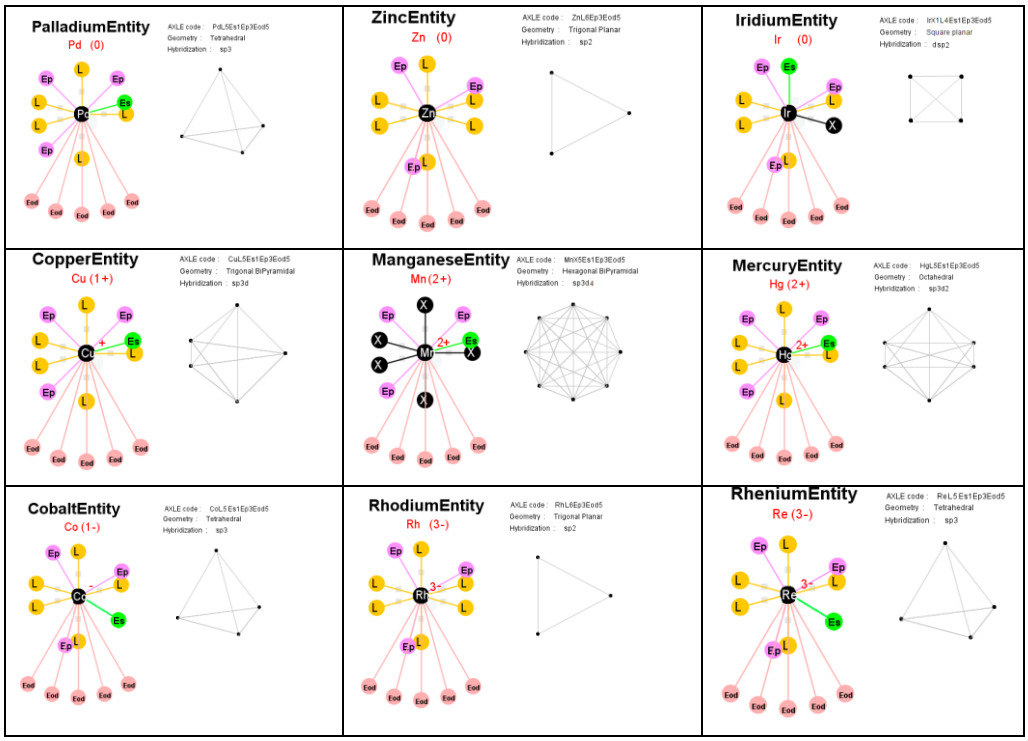

Table : Representative *d*- block atom entities

Geometry of *f*-block atom entities

Orbital hybridization takes place in $4f^{0\text{-}14}\ 5d^{0\text{-}1}\ 6s^{0\text{-}2}\ 6p^0$ and $5f^{0\text{-}14}\ 6d^{0\text{-}1}\ 7s^{0\text{-}2}\ 7p^0$ valence electrons (P. Sankar, S. Jerome Pastal Raj andP. Vinoth, In-silico bonding schemes; X. Dongfeng, S. Congting, C. Xiaoyan, Hybridized valence; R. E. Connick, and Z. Z. Hugus Jr, The Participation)[5, 17, 34] of *f*-block atomic entities results *spdf* pattern of hybridization with appropriate geometry ascertained through AXLE code. For Ce (4+) entity the AXLE code is

'CeEs1Ep3Ed5Ef7' and the corresponding hybridization is d^2sp^3 with octahedral geometry also the system generated elemental properties shown in Figure.

The AXLE code information, hybridization and geometry of few *f*- block atomic entities are shown in Table 4.

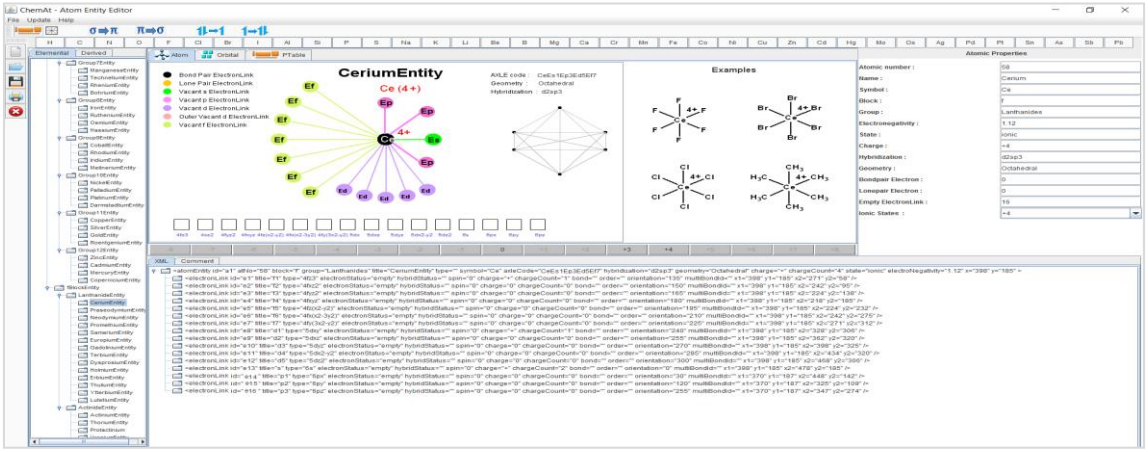

Figure : Encoding details of Cerium (4+) Entity

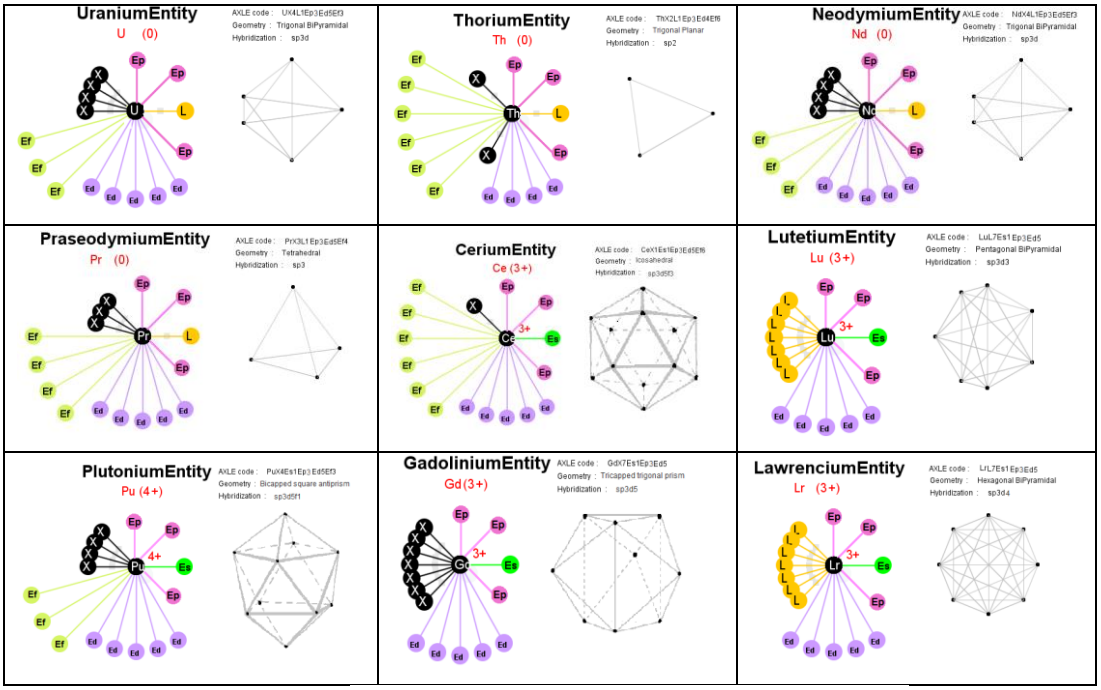

Table: Representative *f*- block atom entities

The hybridization and geometry of all the possible atom entities in the Periodic Table is arrived in GUI with AXLE code concept. Also each and every atom entity is visualized with a system generated report in XML explicitly along with their elemental properties.

Conclusion

Hybridization and geometry of atomic entities are encoded with a unique AXLE code. Atomic orbital hybridization controls the structure and reactivity hence the understanding of hybridization tendency is significant(I. V.

Alabugin, S. Bresch, and G. P. dos Gomes) [4]. Atomic orbital hybridization is convenient in determining the coordination number of central atom of rare earth elements (R. J. Gillespie and R. S. Nyholm, Inorganic)(R. J. Gillespie and R. S. Nyholm, Inorganic Stereochemistry)[14]. This study frames platform for the development of bonding nature, molecular geometry and chemical reactivity in modeling via computer simulation. This is also very much helpful to convert the classroom atmosphere interesting for young minds when they are studying the hybridization and geometry concepts.

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