Orbital Development Kit

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Representation Types

Quantum Chemistry
- Detailed, accurate
- Scales badly

Chemical Graph
- Scales OK
- No electrons
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Orbital Development Kit
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Why?

- More in line with how we think about molecules
- Organometallics
- Stereochemistry at an atomic level
- Explicit information
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Worst of both worlds?
Methane I

sp3 hybridization
Counting electrons

Oxidation states and filled orbitals
Lone Pairs

Oxidation states and filled orbitals

[Diagram of a molecule with lone pairs and oxidation states]
Atom types: from the CDK

Web Ontology Language

<at:AtomType rdf:ID="C.minus.sp3">
  <at:formalCharge>-1</at:formalCharge>
  <at:hasElement rdf:resource="&elem;C"/>
  <at:formalNeighbourCount>3</at:formalNeighbourCount>
  <at:lonePairCount>1</at:lonePairCount>
  <at:piBondCount>0</at:piBondCount>
  <at:hybridization rdf:resource="&at;sp3"/>
</at:AtomType>
Atom types

Osp3.getOrbitalTypes()

```java
public List<IOrbitalType> getOrbitalTypes() {
    List<IOrbitalType> orbitals =
        new ArrayList<IOrbitalType>();
    orbitals.add(LonePair.getInstance(Sp3.getInstance()));
    orbitals.add(LonePair.getInstance(Sp3.getInstance()));
    orbitals.add(SingleElectron.getInstance(Sp3.getInstance()));
    orbitals.add(SingleElectron.getInstance(Sp3.getInstance()));
    return orbitals;
}
```
Water

Oxidation states and filled orbitals
Water

MoleculeFactory factory = new MoleculeFactory();

IAAtom oxygen = factory.addAtom(Osp3.getInstance());

for (int i=1; i<=2; i++) {
    IAtom hydrogen = factory.addAtom(Hs.getInstance());
    factory.bind(
        oxygen.getFreeSingleElectron(Sp3.getInstance()),
        hydrogen.getFreeSingleElectron(S.getInstance())
    );
}

IMolecule immutable = factory.getImmutable();
Water

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Zeise’s Salt

Beyond the Chemical Graph
Zeise’s Salt

`IMolecularOrbital piBond = factory.bind(`
carbons[0].getFreeSingleElectron(Pz.getInstance()),
carbons[1].getFreeSingleElectron(Pz.getInstance())
);
IAtom platinum = factory.addAtom(Ptsp.getInstance());

factory.bind(`
    platinum.getFreeEmpty(Dsp.getInstance()),
    piBond
);`
I/O: Resource Description Framework

Molecules
:mol1 a odk:Molecule ;
  odk:hasAtom :atom4 , :atom3 , :atom1 , :atom5 , :atom2 ;

Atoms
:atom3 a odk:Atom ;
  odk:hasAtomType at:Hs ;
  odk:hasOrbital :orbital6 .

Orbitals
:orbital8 a odk:Orbital ;
  odk:hasElectronCount "1" ;
  odk:hasOrbitalType ot:S .

Overlaps
:overlap10 a odk:Overlap ;
  odk:binds :overlap6 , :orbital16 .
Conclusions

- Atom types are expressed in more detail
- Electron counting is explicit
- We can represent organometallics
- (De)serialization from/into RDF
Where to?

- descriptor calculation (QSAR)
- fingerprints (database searching)
- bridge to the CDK
- ...

...
The Details

- http://www.citeulike.org/user/egonw/tag/papers
- http://chem-bla-ics.blogspot.com
- http://egonw.github.com
- waveto: egon.willighagen@googlewave.com