chem-bla-ics

CDK Molecules in RDF

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Yesterday, I finally got around to starting a branch on adding RDF support to the CDK; in particular, write the CDK data model ontology in OWL and serialization to and from RDF using the ontology. The framework is now set up, but I have yet to formalize all bits and pieces of the CDK data model in classes and properties. Just as a preview, here is what a very basic bit of CDK model in RDF looks like (N3 format):

```
@prefix cdk:     <http://cdk.sourceforge.net/model.owl#> .

<http://cdk.sf.net/model/atom/1>
      a       cdk:Atom ;
      cdk:symbol "C" .

<http://cdk.sf.net/model/molecule/1>
      a       cdk:Molecule ;
      cdk:hasAtom  .
```

Still rather verbose, but very flexible. I have even been thinking of an XHTML+RDFa writer...