

CDK Molecules in RDF

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Abstract

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.

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chem-bla-ics

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...