

chem-bla-ics

new Atom(Elements.CARBON);

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Keywords

Cdk

Abstract

Something I have not completely comfortable with about the CDK in the past, is the way Atom's are constructed:

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Something I have not completely comfortable with about the [CDK](#) in the past, is the way [Atom](#)'s are constructed:

```
IAtom carbon = new Atom("C");
```

Not that it is horrible code, but the CDK has an [Element](#) too. Why not reuse that? However, until revision 6755 there were not constructors that allowed something like the following:

```
IAtom carbon = new Atom(new Element("C"));
```

This afternoon I have hacked in constructors for [ChemObject](#), [Element](#), [Isotope](#), [AtomType](#), [Atom](#) and [PseudoAtom](#) that allow to be constructed from its interface, or the interface of one of its superclasses.

Additionally, in revision 6753, I added [cdk.config.Elements](#) with static [IElements](#) for all elements up to atomic number 116, taken from the [Blue Obelisk Data Repository](#). Therefore, I can now also write:

```
IAtom carbon = new Atom(Elements.CARBON);
```