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Chemical Editing...

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Abstract

As you might have seen, we, Uppala and the EBI, are working on the next generation JChemPaint. JChemPaint is an editor, and therefore, consists of a model (IChemModel), a view (IRenderer) and a controller (IController). See the many posts in Gilleain's blog.

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As you might have seen, we, Uppala and the EBI, are working on the next generation JChemPaint. JChemPaint is an editor, and therefore, consists of a model (`IChemModel`), a view (`IRenderer`) and a controller (`IController`). See the many posts in Gilleain's blog.
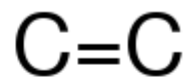
For the renderer I have set up a wiki page which I'll be hacking in the next days, which shows how a `IChemObject` content should be rendered in JChemPaint. It looks like:

```
IAtom atom0 = builder.newAtom("C");
IAtom atom1 = builder.newAtom("C");
IBond bond = builder.newBond(atom0, atom1, IBond.Order.DOUBLE);
```
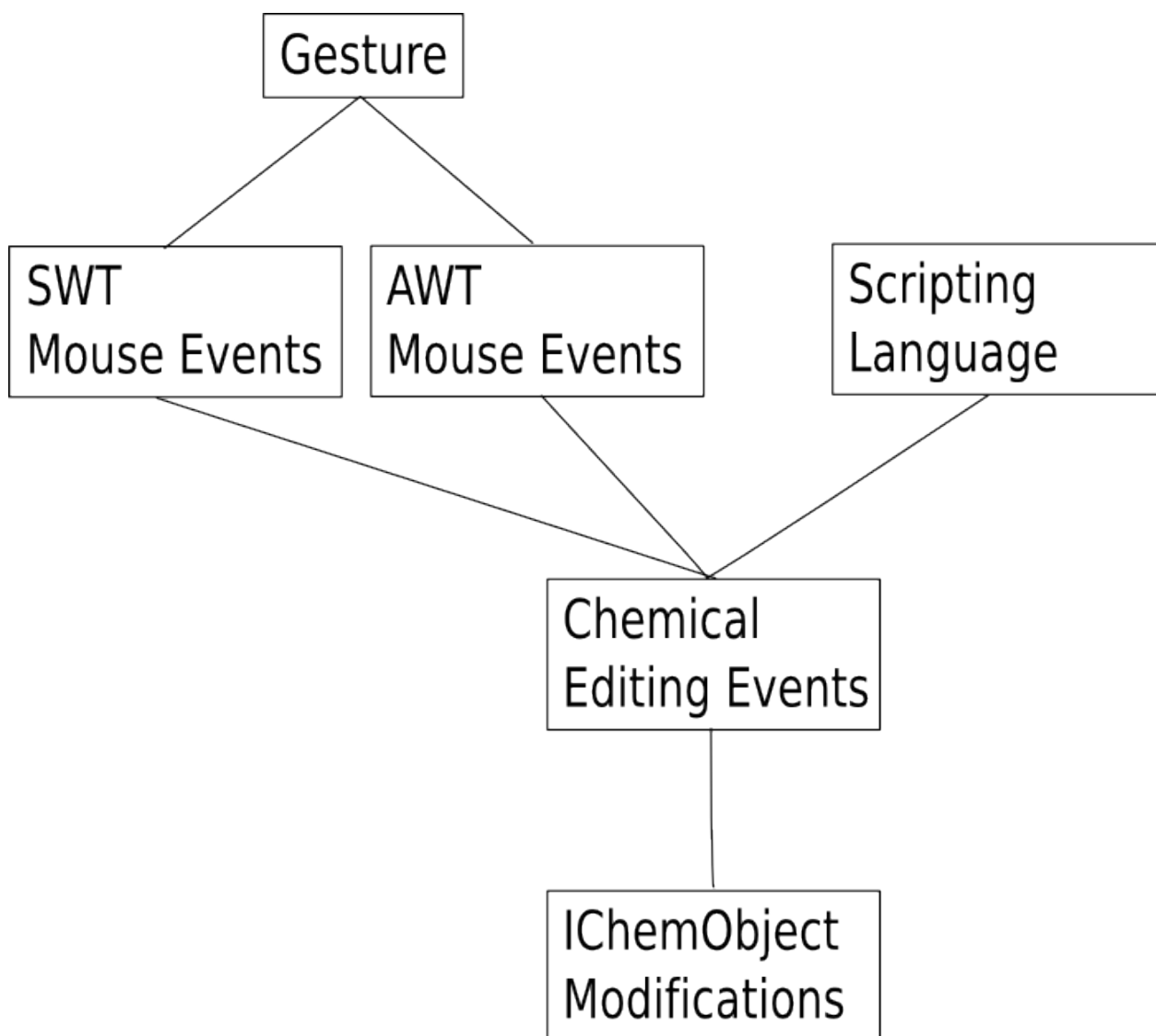C=C

```
IAtom atom0 = builder.newAtom("C");
IAtom atom1 = builder.newAtom("C");
IBond bond = builder.newBond(atom0, atom1, IBond.Order.TRIPLE);
```
C≡C

```
IAtom atom0 = builder.newAtom("C");
atom0.setFormalCharge(1);
```
C⊕

The `IController` is a rather important part too, and like the `IRenderer` bit of JChemPaint, needs a major overhaul. The new design, discussed by Gilleain here and here, should, IMHO, look like:

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In this diagram, the gestures can come from any input device, mouse, tracking ball, Wiimote, and will result in events in some widget library (SWT, AWT shown). The old JChemPaint, converted the Swing `MouseEvent`'s directly into `IChemObject` modifications, making the code incompatible with SWT. This is why the *Chemical Editing Events* layer must be added.

Events in this layer look like `addAtom(attachementAtom, coordinates)` and `setFormalCharge(atom, newCharge)`. The link to scripting should be clear now, and will help use write unit tests for this layer.