Subject: Why are molecules drawn right to left?
Posted by memcop on Fri, 19 Sep 2014 00:32:21 GMT
View Forum Message <> Reply to Message

For example if I enter 5-fluoro-2,3,6-trimethyloctane the first group is on the right end...is there an option to draw the molecule regularly, left to right?

Subject: Re: Why are molecules drawn right to left?
Posted by thomas on Fri, 19 Sep 2014 19:46:54 GMT
View Forum Message <> Reply to Message

The name has nothing to do with the orientation of the drawing.
After the name has been translated into a molecule graph, atom coodinates
are generated by locating small rigid fragments first, assigning reasonable coordinates
to their atoms and then combining these fragments in a way that there are no colliding atoms.
What is left or right or top or bottom is not relevant for the algorithm.

Thomas