Subject: Why are molecules drawn right to left? Posted by memcop on Fri, 19 Sep 2014 00:32:21 GMT

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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