Subject: Set Bond Properties for Combinatorial Library
Posted by sn on Mon, 21 Jun 2021 13:45:16 GMT
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Hi everyone,

I draw virtual reactions which have bond properties(setting the atom bridge), so that I could use a variety of reactants.

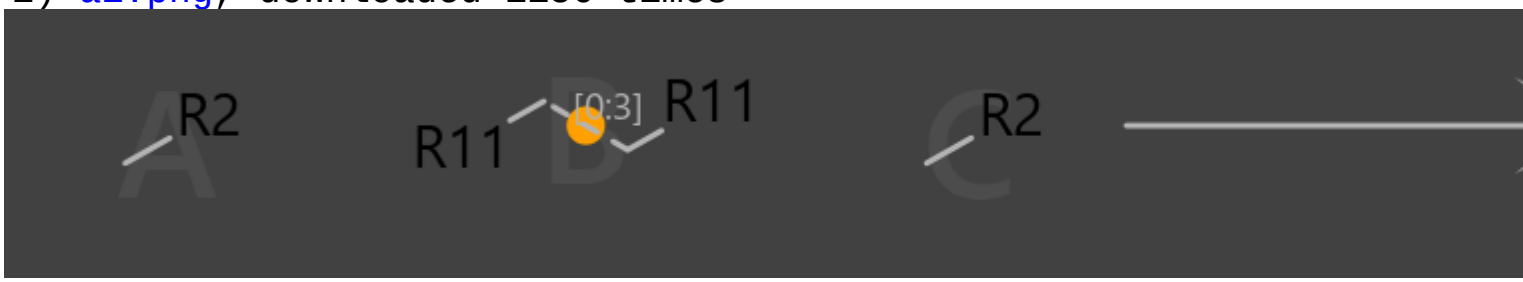
But the bond in reactant transforms to another bond in the product automatically.
ex: "linear chain" to "cyclic chain"

What I would like to do would be to then keep the bond properties between the reactant and product.

Is there any way to do this that would keep the bond properties in the virtual reaction?

Warm Regards,
sn

File Attachments
1) a1.png, downloaded 1156 times



Subject: Re: Set Bond Properties for Combinatorial Library
Posted by thomas on Mon, 28 Jun 2021 19:52:26 GMT
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Hi sn,

it seems that you can just remove the bridge bond from generic product to avoid creating cyclic products.

I also have updated the development version to skip bridge bonds of generic products.
Thus, your virtual reactions should work after updating as they are.

Thomas