Subject: Re: Pentavalent carbonyl issue (urea formation?)
Posted by thomas on Sat, 24 Jun 2023 14:53:12 GMT
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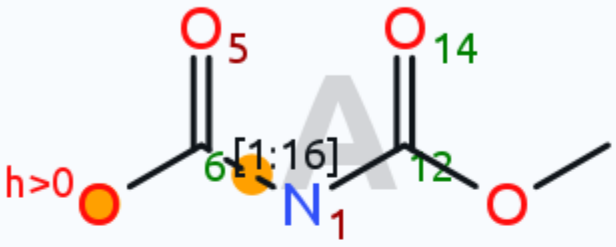
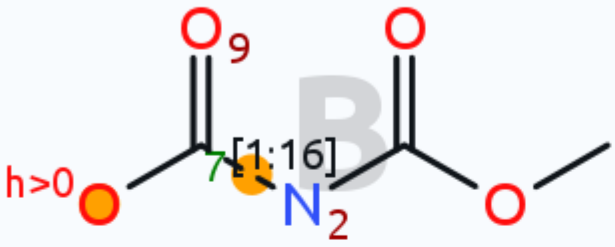
Thank you for the files. To me it seems that your atom mapping is incorrect. The reactants fragments consisting out of a carbonyl group with attached bridge bond to nitrogen should not break bonding in the reaction, thus they should appear in the product the same way with the same mapping numbers. I have attached the updated macro file, which seems to work fine now.

The upper reaction shows your original mapping, the lower one shows the updated mapping:

File Attachments

1) correctedMacro.dwam, downloaded 462 times
2) mapping.png, downloaded 785 times


O
5
O
14
h>0
6
[1:16]
12
N
1
O
A


O
9
O
h>0
7
[1:16]
N
2
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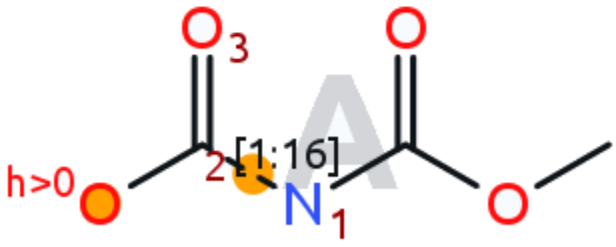
O
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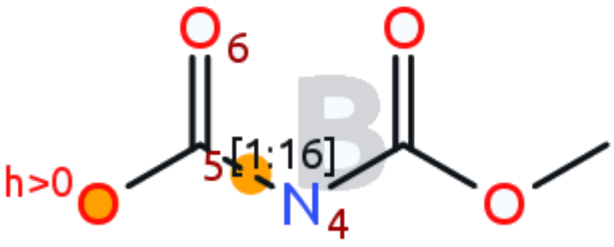
O
6
O
h>0
5
[1:16]
N
4
O
B