
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 179 times
 - 2) [mapping.png](#), downloaded 300 times
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