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Subject: Re: Pentavalent carbonyl issue (urea formation?)

Posted by [padster](#) on Fri, 23 Jun 2023 18:02:09 GMT

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Sure thing, attached are four .dwar files with one structure each for one cycle and the .rxn file:

I'm not sure how to provide a macro to be honest

### File Attachments

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- 1) [Cycle1.dwar](#), downloaded 202 times
  - 2) [Cycle2.dwar](#), downloaded 190 times
  - 3) [Cycle3.dwar](#), downloaded 194 times
  - 4) [Cycle4.dwar](#), downloaded 170 times
  - 5) [4 macrocycle disulphide.rxn](#), downloaded 187 times
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