

Novel cyclic analogues of the Hendrickson ‘POP’ reagent

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Accessory Materials

Calculations for the kinetic study of 4-nitrobenzyl 4-nitrobenzoate formation using (1)-(4)

Total volume = 150 mL (solvent) + diisopropylethylamine (1.74 mL) + triflic anhydride (0.34 mL) = 152.08 mL = 0.15208 L

$[A]_0 = [\text{initial 4-nitrobenzyl alcohol}] = \text{moles} / \text{vol (L)} = 0.002 / 0.15208 = 0.01315 \text{ M}$

$[A] = [\text{4-nitrobenzyl alcohol}] \text{ at time } t = (\% \text{ 4-nitrobenzyl alcohol at time } t / 100) * [\text{initial 4-nitrobenzyl alcohol}]$

Pseudo first order conditions were achieved using 5 eq. 4-nitrobenzoic acid in 150 mL solvent at 0°C.

Rate constant (k) = - gradient (m).

$T_{1/2} = \ln 2 / k$

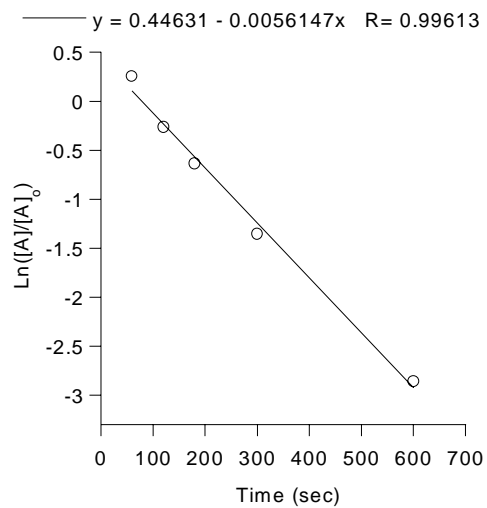


Figure A1. First order plot of the Hendrickson reagent (1) in DCM/toluene 1:1.

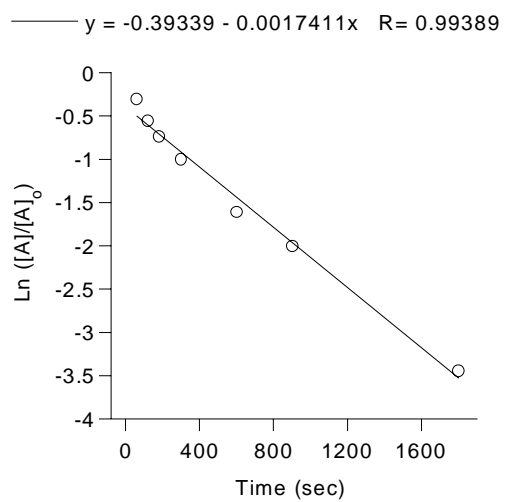


Figure A2. First order plot for Hendrickson reagent (1) in DCM.

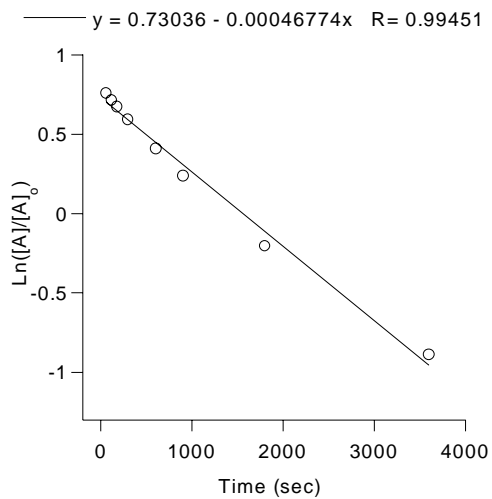


Figure A3. First order plot of the Hendrickson reagent (1) in DCM/CH₃CN 1:1.

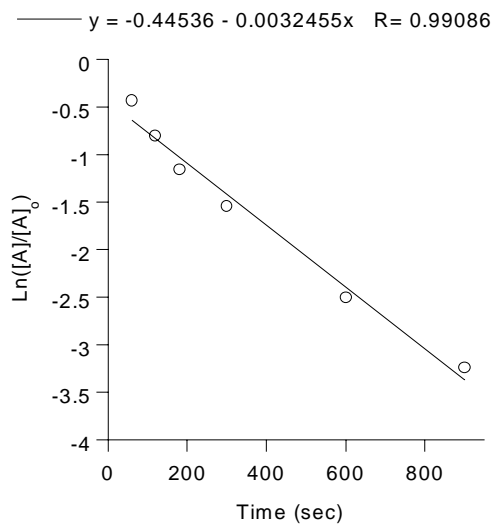


Figure A4. First order plot of five membered cyclic 'POP' (2) in DCM.

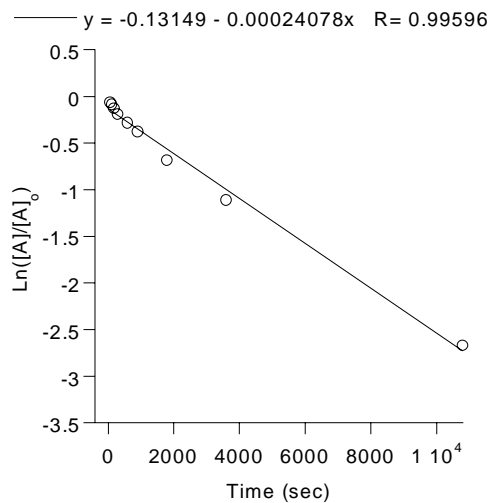


Figure A5. First order plot of six membered cyclic 'POP' (3) in DCM.

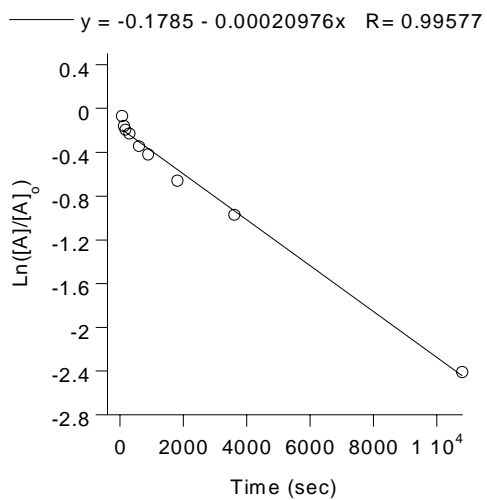


Figure A6. First order plot of seven membered cyclic 'POP' (4) in DCM.