Novel cyclic analogues of the Hendrickson ‘POP’ reagent

Kathryn E. Elson, A Ian D. Jenkins B,C and Wendy A. Loughlin A

A School of Science, Griffith University, Brisbane, Queensland, 4111, Australia.
B Natural Product Discovery, Griffith University, Brisbane, Queensland, 4111, Australia.
C Author to whom correspondence should be addressed (e-mail: I.Jenkins@griffith.edu.au).

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

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

\[ [A] = \frac{[\text{4-nitrobenzyl alcohol}]}{\text{at time t}} = \left(\frac{\% \text{4-nitrobenzyl alcohol at time t}}{100}\right) \times \left[\text{initial 4-nitrobenzyl alcohol}\right] \]

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/CH$_3$CN 1:1.

\[ y = 0.73036 - 0.00046774x \quad R = 0.99451 \]

\[ \ln\left(\frac{[A]}{[A]_0}\right) \]

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

\[ y = -0.44536 - 0.0032455x \quad R = 0.99086 \]
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.