The barrier to enantiomerization of *N*-Boc-2-lithopyrrolidine: the effect of chiral and achiral diamines

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Electronic Supplementary Information



Figure 1. Chromatogram of (N)-Boc-2-trimethylsilylpyrrolidine run on a β -Cyclodextrin capillary column. The colum temperature was programmed as follows:- Initial Temperature T = 70 °C for 5 mins, followed by a gradient of 5 °C/min until T = 200 °C, maintained for 10 mins β -cyclodextrin column. The regulator pressures were: H₂ = 6psi; N₂ = 52 psi; Air = 50 psi.

Kinetic data were fitted to Equation 1, the integrated rate equation for a 1st order process relaxing to equilibrium:-

0.5 ln [T –2R] = -kt Equation 1

T = total initial concentration of stannane

R =concentration of 4-(R)- at time, t.

k = rate constant for enantiomerization

Graphs plotting equation 1 for the racemisation of 4-(S) to 4-(R) with each of three ligands at four different temperatures are given below:-



t/seconds \rightarrow

Figure 2. 1st order rate plots for the racemization of *N*-BOC-2-Li-pyrrolidine in the presence of TMEDA.



Figure 3. 1st order rate plots for the racemization of *N*-Boc-2-Li-pyrrolidine in the presence of sparteine.



Figure 4. 1st order rate plots for the racemization of *N*-Boc-2-Li-pyrrolidine in the presence of bispidine.



Figure 5. Eyring plots for the enantiomerization of *N*-Boc-2-Li-pyrrolidine in the presence and absence of diamines. Data for ether and ether/hexane are duplicated from ref. 8 for comparison, with one extra data point in the ether plot to assure continuity between experimentalists.