1,4-Addition of Lithium Diisopropylamide to Unsaturated Esters:
Role of Rate-Limiting Deaggregation, Autocatalysis,
Lithium Chloride Catalysis and Other Mixed Aggregation Effects

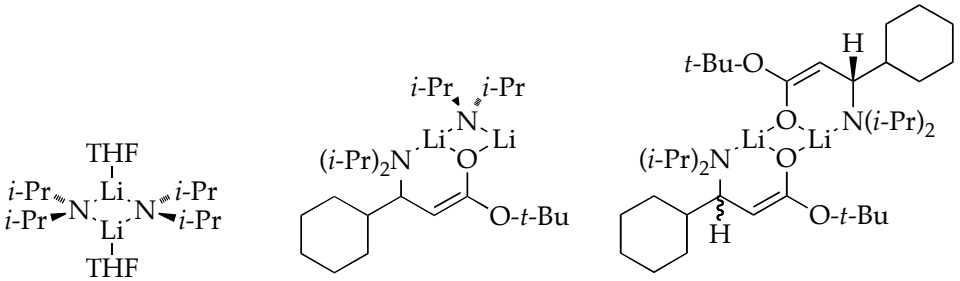
Yun Ma, Alexander C. Hoepker, Lekha Gupta, Marc F. Faggin,
and David B. Collum

Contribution from the Department of Chemistry and Chemical Biology
Baker Laboratory, Cornell University
Ithaca, New York 14853-1301

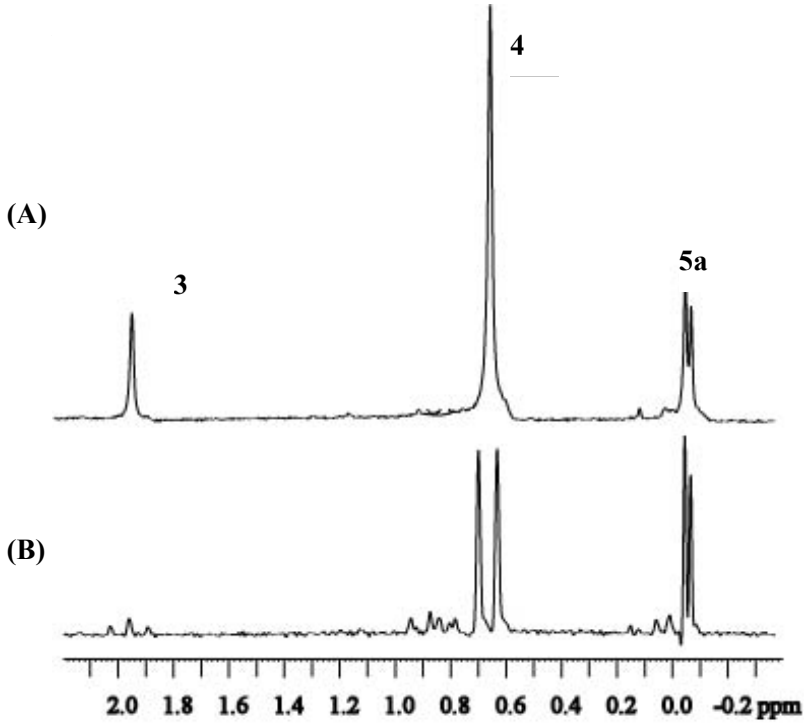
Supporting Information

Solution Structures

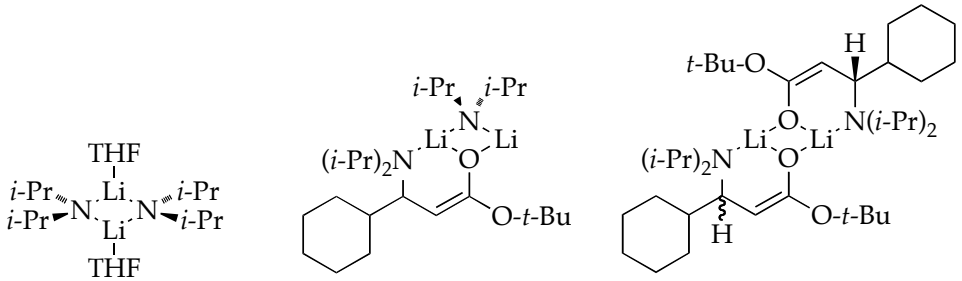
Uncatalyzed 1,4-Additions



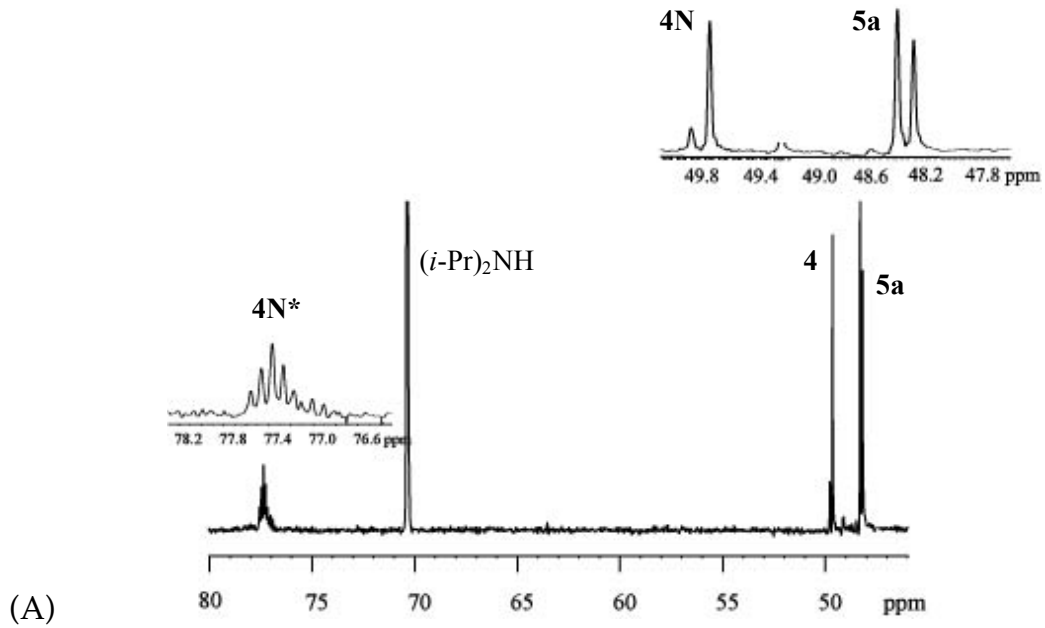
3 **4** **5a**



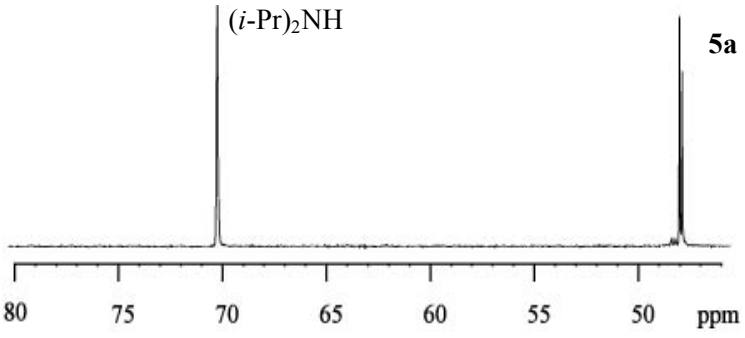
I. ^{6}Li NMR spectra of LDA with 0.50 equiv ester **1** in THF after aging at -55 ◦C for 60 min: (A) 0.10 M [^{6}Li]LDA; (B) 0.10 M [^{6}Li,^{15}N]LDA.



3 **4** **5a**



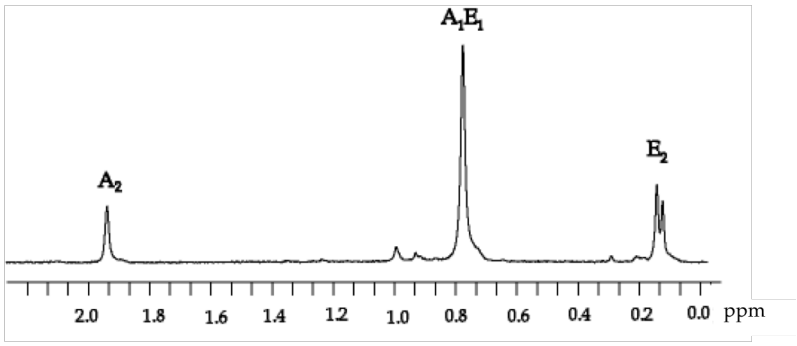
(A)



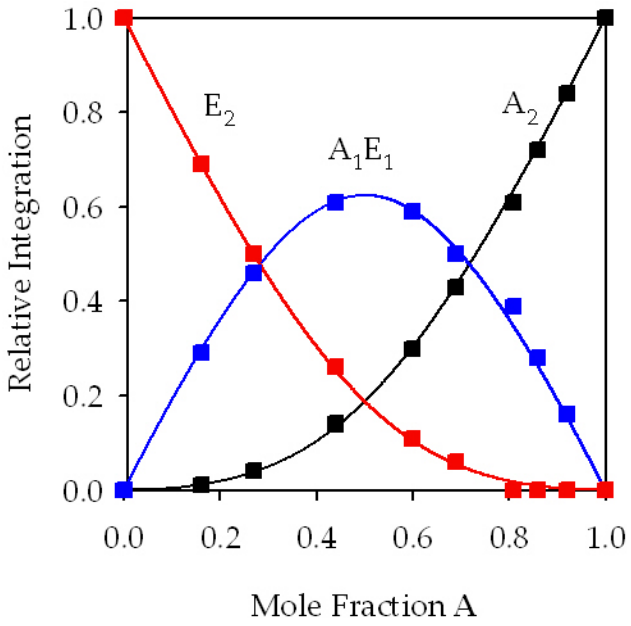
(B)

II. ^{15}N NMR spectra of 0.10 M [^{6}Li,^{15}N]LDA with ester **1** in THF after aging at -55 ^{o}C for 60 min: (A) 0.50 equiv ester **1**; (B) 0.90 equiv ester **1**.

(A)



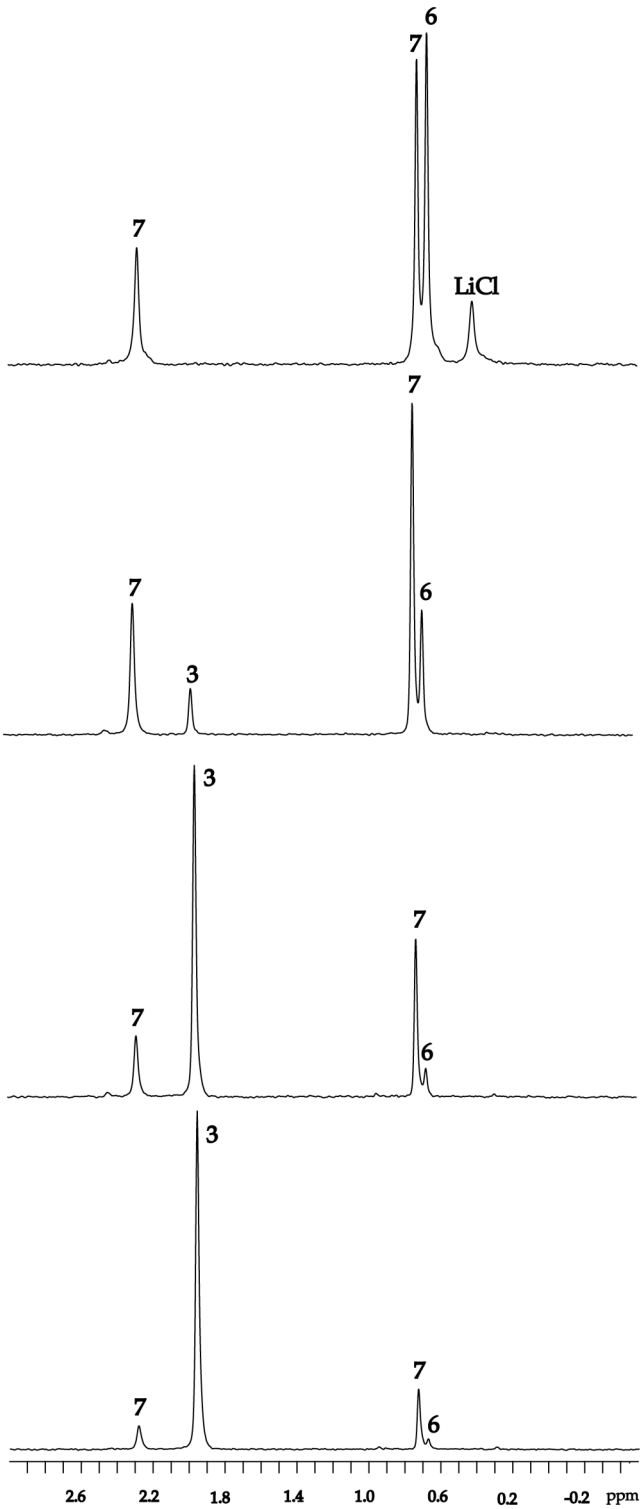
(B)



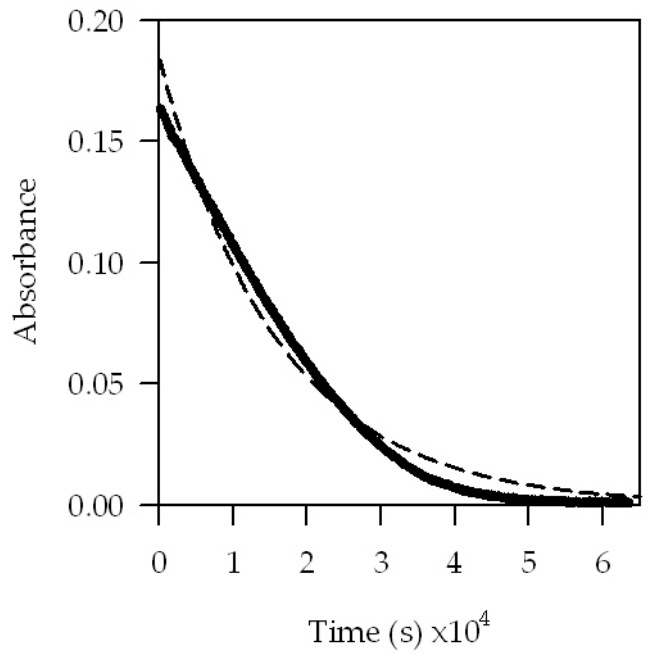
(C)

Calc. X_A	E_2	A_1E_1	A_2
1.00	0.00	0.00	1.00
0.84	0.16	0.00	0.92
0.72	0.28	0.00	0.86
0.61	0.39	0.00	0.81
0.43	0.50	0.06	0.69
0.30	0.59	0.11	0.60
0.14	0.61	0.26	0.44
0.04	0.46	0.50	0.27
0.01	0.29	0.69	0.16
0.00	0.00	0.00	1.00

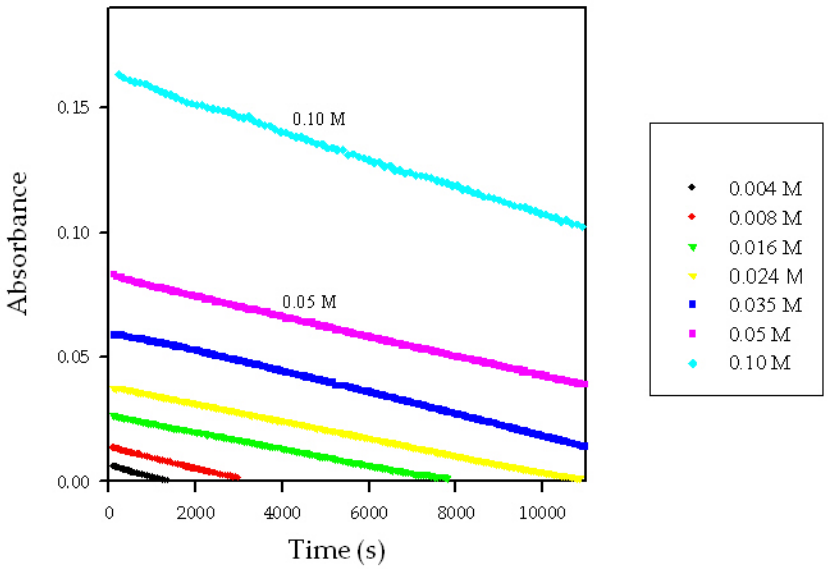
III. (a) Representative ^{6}Li NMR spectrum of a 60:40 mixture of [^{6}Li]**5** and[^{6}Li]**3** showing homodimers (A_2 and E_2) and mixed dimer [^{6}Li]**4** (AE); (b) Plot of the relative integration vs the mole fraction of [^{6}Li]**3**, [^{6}Li]**4**, and [^{6}Li]**5**; (c) measured mole fractions of each aggregate.



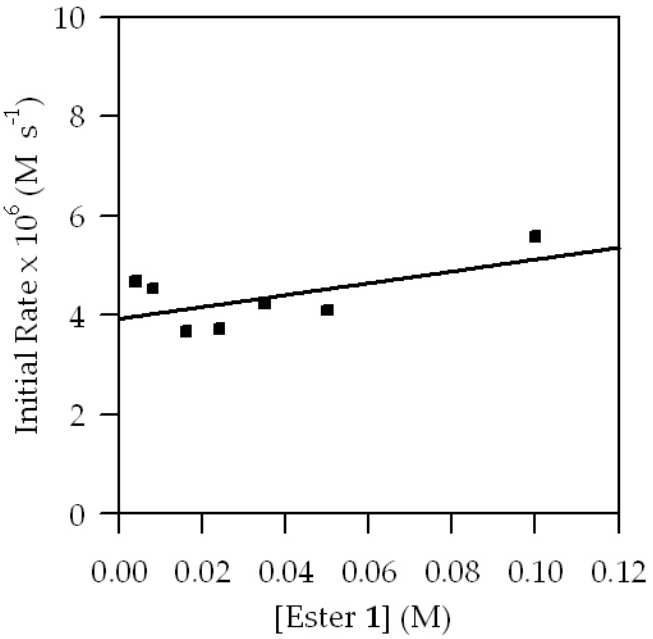
IV. ^{6}Li NMR spectra of [^{6}Li]LDA (0.10 M) with [^{6}Li]LiCl in 12.2 M THF at -110 °C: (A) 0.05 M [^{6}Li]LiCl; (B) 0.025 M [^{6}Li]LiCl; (C) 0.01 M [^{6}Li]LiCl; (D) 0.005 M [^{6}Li]LiCl. LiCl has been characterized as a dimer in THF solution.



V. Plot showing IR absorbance of ester **1** vs time for the 1,4-addition of ester **1** (0.10 M) with LDA (0.10 M) at -78 °C. The dashed line shows the results of a first-order fit ($y = ae^{bx}$).

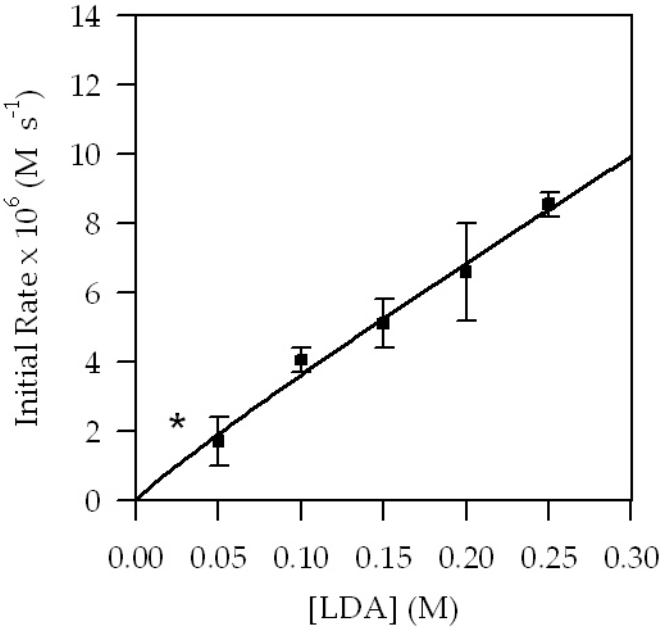


VI. Plot showing the IR absorbance of ester **1** vs time for different initial concentrations of ester **1**



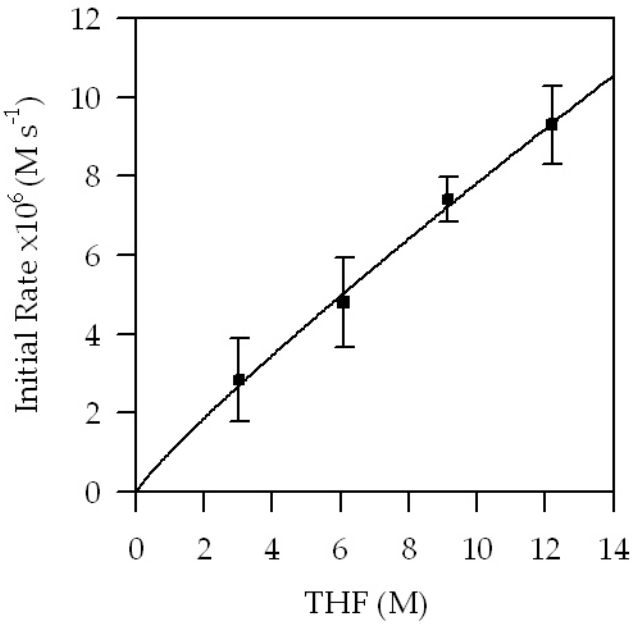
VII. Plot of initial rates vs [**1**] for the 1,4-addition of LDA (0.10 M) to ester **1** in THF (6.10 M) at -78 °C. The curve depicts an unweighted least-squares fit to y = *k*[ester **1**] + *k′* (*k* = (1.2 ± 1) x 10^{-5}, *k′* = (3.9 ± 0.4) x 10^{-6}).

[**1**] (M)	y x 10^6 ($M^{-1}.s^{-1}$)
0.004	4.68 ± 1
0.008	4.54 ± 2
0.016	3.68 ± 1
0.024	3.72 ± 1
0.035	4.23 ± 2
0.050	4.10 ± 1
0.10	5.58 ± 3



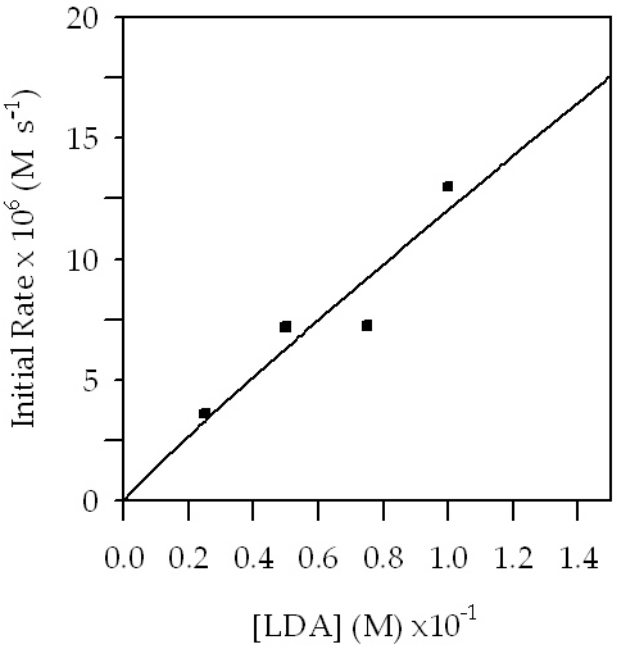
VIII. Plot of initial slopes vs [LDA] in THF (6.10 M) for the 1,4-addition of ester **1** (0.004 M) at -78 °C. The curve depicts an unweighted least-squares fit to $y = k[\text{LDA}]^n$ ($k = (3.1 \pm 0.4) \times 10^{-6}$, $n = 0.92 \pm 0.03$).

[LDA] (M)	$y_1 \times 10^6$ ($M^{-1}.s^{-1}$)	$y_2 \times 10^6$ ($M^{-1}.s^{-1}$)	$y_3 \times 10^6$ ($M^{-1}.s^{-1}$)
0.025	2.00 ± 0.03		
0.05	1.16 ± 0.01	2.21 ± 0.01	
0.10	3.88 ± 0.02	4.30 ± 2E-3	0.091 ± 2E-3
0.15	5.60 ± 0.02	4.61 ± 8E-3	0.209 ± 7E-3
0.20	7.57 ± 0.01	5.69 ± 8E-3	0.31 ± 1E-2
0.25	8.81 ± 0.03	8.25 ± 2E-2	



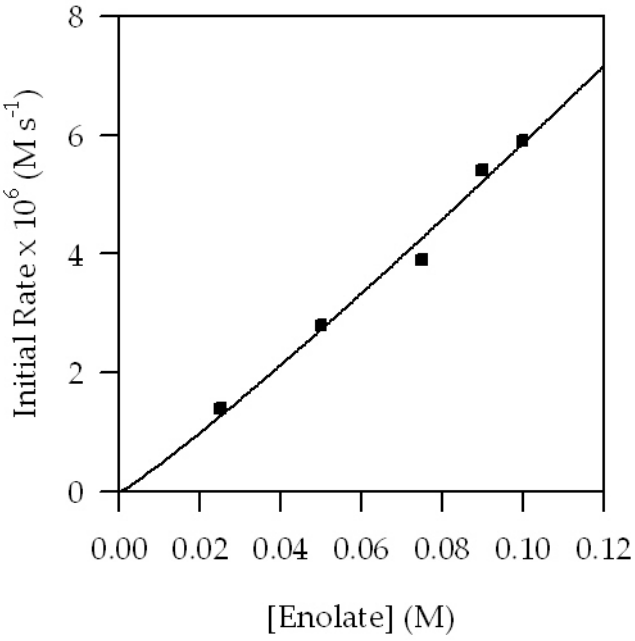
VIV. Plot of initial slopes vs [THF] for the 1,4-addition of LDA (0.10 M) to ester **1** (0.004 M) in hexane at -78 °C. The curve depicts an unweighted least squares fit to $y = k[LDA]^n + k'$ ($k = (8.1 \pm 0.2) \times 10^{-7}$, $n = 0.95 \pm 0.03$), $k' = (4.05 \pm 0.04) \times 10^{-7}$).

[THF] (M)	$y_1 \times 10^6$ ($M^{-1}.s^{-1}$)	$y_2 \times 10^6$ ($M^{-1}.s^{-1}$)
3.01	3.58 ± 0.03	2.09 ± 0.01
6.10	3.62 ± 0.02	5.62 ± 0.04
9.15	7.8 ± 0.05	7.05 ± 0.01
11.20	8.6 ± 0.04	9.5 ± 0.03



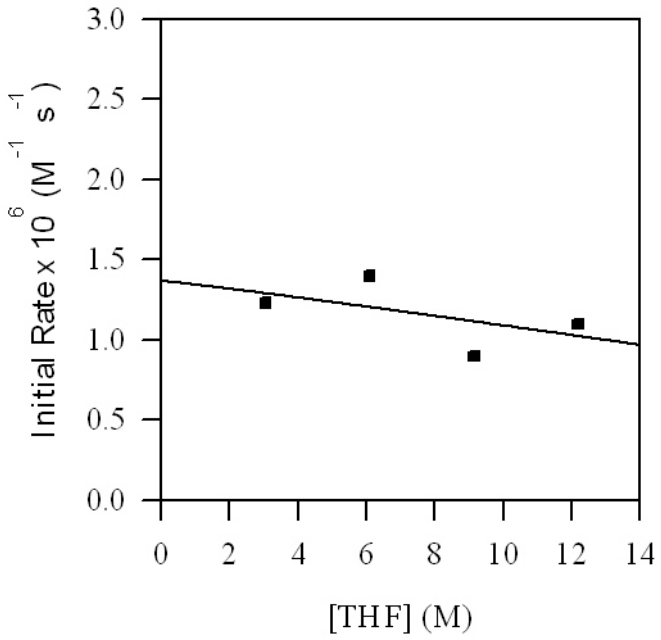
X. Plot of initial slopes vs [LDA] for the condensation of LDA dimer **3** (0.10 M) with enolate dimer **5a** (0.025M) in THF (6.10 M) at -78 °C. The curve depicts an unweighted least-squares fit to $y = k[\mathrm{LDA}]^n$ ($k = (1.0 \pm 0.3) \times 10^{-4}$, $n = 0.93 \pm 0.24$).

[LDA] (M)	$y_1 \times 10^6$ ($M^{-1}.s^{-1}$)
0.025	0.36 ± 0.02
0.05	0.72 ± 0.01
0.75	0.73 ± 0.03
0.1	13.7 ± 0.1



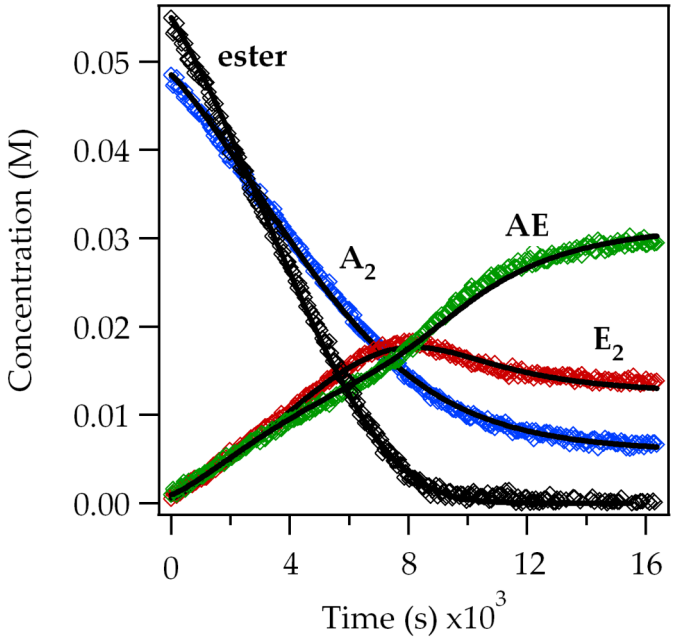
XI. Plot of initial slopes vs the concentration of enolate **5** for the condensation of LDA dimer **3** (0.10 M) with enolate dimer **5a** (0.025M) in THF (6.10 M) at -78 °C. The curve depicts an unweighted least-squares fit to $y = k[\text{enolate}]^n$ ($k = (7.4 \pm 0.3) \times 10^{-5}$, $n = 1.10 \pm 0.14$).

[Enolate] (M)	$y_1 \times 10^6$ ($M^{-1}.s^{-1}$)
0.025	1.40 ± 0.02
0.050	2.82 ± 0.01
0.075	3.90 ± 0.03
0.090	5.41 ± 0.03
0.100	5.94 ± 0.02



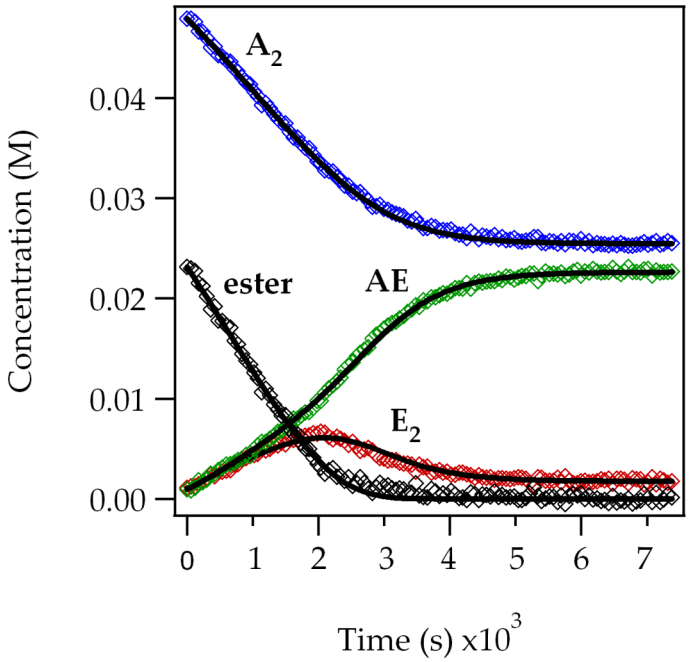
XII. Plot of initial slopes vs [THF] for the 1,4-addition of LDA (0.10 M) to enolate **3** (0.01M) in hexane at -78 °C. The curve depicts an unweighted least squares fit to y = k[THF] + k' (k = (1.1 $\pm$ 0.1) x 10^{-7}, n = 0.95 $\pm$ 0.03), k' = (-2,37 $\pm$ 0.04) x 10^{-9}).

[THF] (M)	y_1 x 10^6 ($M^{-1}.s^{-1}$)
3.05	1.23 $\pm$ 0.01
6.10	1.40 $\pm$ 0.01
9.15	0.92$\pm$ 0.02
12.20	1.10$\pm$ 0.03



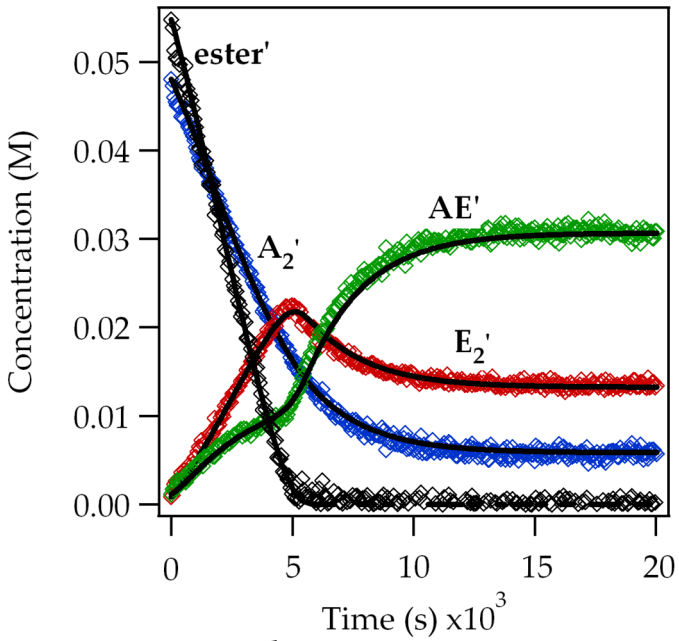
XIII. Parametric fit to eqs 17-22 of the time-dependent concentrations measured by ^{6}Li NMR spectroscopy using 0.05 M **3** (0.10 *normal*), 0.05 M **1** in 6.1 M THF at -78 °C. Ester = **1**; A_2 = LDA dimer **3**; E_2 = enolate dimer **5a**; AE = enolate mixed dimer **4**. Best-fit values of the rate constants (95% confidence) are as follows:

k_1 = 3.6914e-005 ± 9.5e-007
k_{-1} = 2190 ± 883
k_2 = 126.33 ± 14.4
k_3 = 0.19969 ± 0.0164
k_{-3} = 1.5147 ± 0.483
k_4 = 1318.1 ± 143
k_{-4} = 0.00038533 ± 1.67e-005
k_5 = 225.12 ± 80.7
k_{-5} = 0.0084579 ± 0.00324



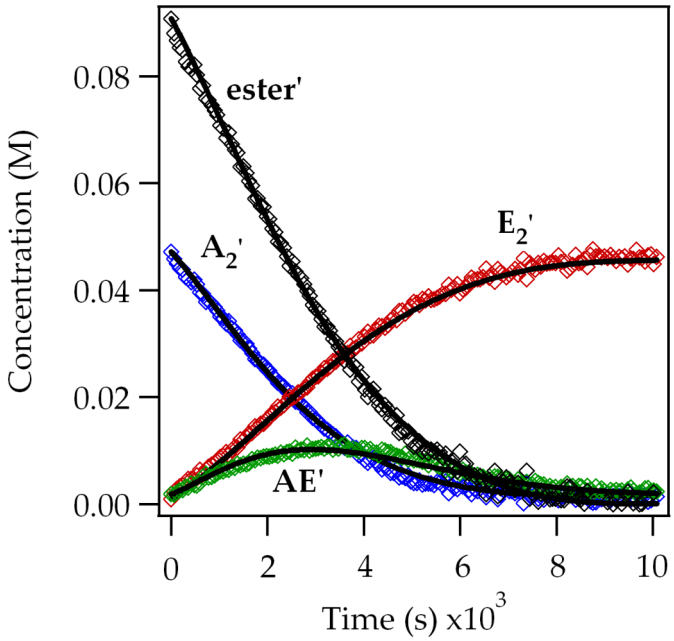
XIV. Parametric fit to eqs 17-22 of the time-dependent concentrations measured by ^{6}Li NMR spectroscopy using 0.05 M **3** (0.10 *normal*), 0.025 M **1** in 6.1 M THF at -78 °C. Ester = **1**; A_2 = LDA dimer **3**; E_2 = enolate dimer **5a**; AE = enolate mixed dimer **4**. Best-fit values of the rate constants (95% confidence) are as follows:

k_1 = 7.8377e-005 ± 2.98e-006
k_{-1} = 547.7 ± 212
k_2 = 94.857 ± 29.9
k_3 = 0.34822 ± 0.0583
k_{-3} = 1.3158 ± 1.05
k_4 = 1261.1 ± 270
k_{-4} = 0.0006229 ± 0.000154
k_5 = 429.27 ± 206
k_{-5} = 0.0087171 ± 0.00339



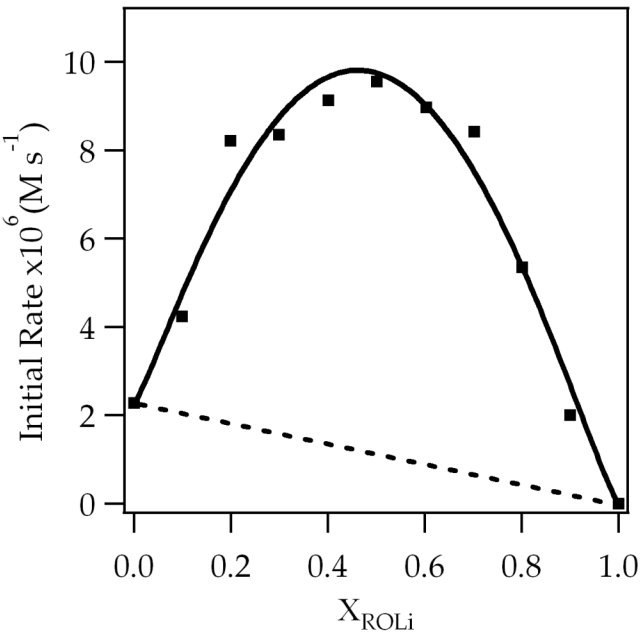
XV. Parametric fit to eqs 17-22 of the time-dependent concentrations measured by ^{6}Li NMR spectroscopy using 0.05 M **3** (0.10 *normal*), 0.05 M **12** in 6.1 M THF at -78 °C. Ester = **12**; A_2 = LDA dimer **3**; E_2 = enolate dimer of **12**; AE = enolate mixed dimer . Best-fit values of the rate constants (95% confidence) are as follows:

k_1 = 7.0944e-005 ± 3.87e-006
k_{-1} = 267.46 ± 471
k_2 = 223.44 ± 1.1e+003
k_3 = 0.33594 ± 0.0308
k_{-3} = 0.84648 ± 11.3
k_4 = 910.74 ± 131
k_{-4} = 0.00051948 ± 3.04e-005
k_5 = 451.57 ± 81.1
k_{-5} = 0.0080254 ± 0.000959



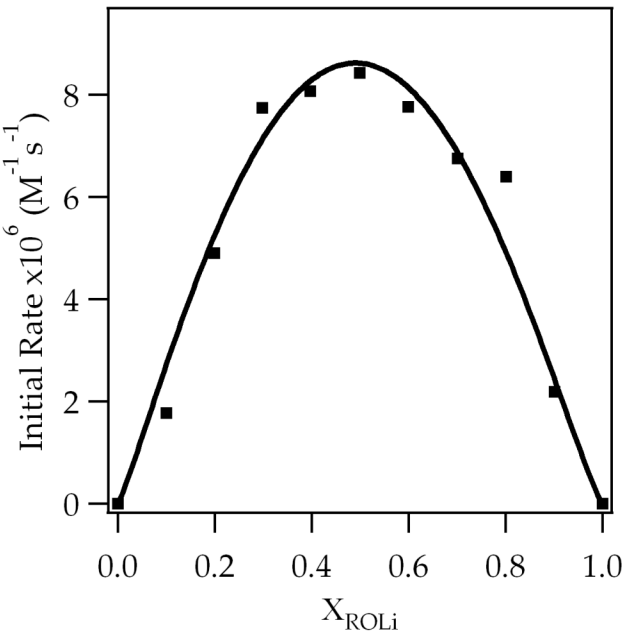
XVI. Parametric fit to eqs 17-22 of the time-dependent concentrations measured by ^{6}Li NMR spectroscopy using 0.05 M **3** (0.10 *normal*), 0.10 M **12** in 6.1 M THF at -78 °C. Ester = **12**; A_2 = LDA dimer **3**; E_2 = enolate dimer of **12**; AE = enolate mixed dimer. Best-fit values of the rate constants (95% confidence) are as follows:

k_1 = 0.00011944 ± 2.61e-006
k_{-1} = 7415.7 ± 599
k_2 = 962.34 ± 209
k_3 = 0.46237 ± 0.0395
k_{-3} = 18.327 ± 0.467
k_4 = 83.523 ± 4.44
k_{-4} = 0.00054909 ± 7.49e-006
k_5 = 280.11 ± 57.1
k_{-5} = 0.0069795 ± 0.00172



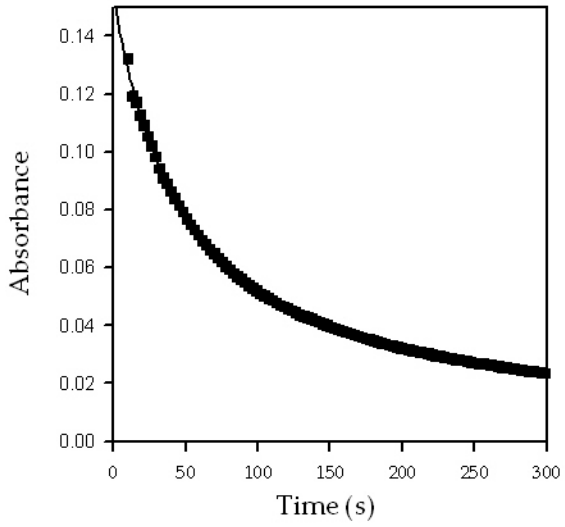
XVII. Plot of initial rate (y_1) versus X_{ROLi} for the serial injection of ten aliquots of ester **1** (0.01 M final concentrations) to 0.10 M LDA in 6.1 M THF/hexanes co-solvent at -78 °C. The dashed line depicts the theoretical initial rates in the absence of autocatalysis. The curve depicts an unweighted least squares fit to $y_1 = k[X_{ROLi}]^n[1 - X_{ROLi}]^m + k'[1 - X_{ROLi}]^{1.0}$, $n = 1.15 \pm 0.20$), $m = (1.20 \pm 0.18) \times 10^{-7}$, $k = (4.40 \pm 1.16) \times 10^{-5}$), $k' = (2.25 \pm 6.71) \times 10^{-6}$.

X_{ROLi}	$y_1 \times 10^{-6}$ ($M^{-1} \cdot s^{-1}$)
0.00	2.28
0.10	4.24
0.20	8.22
0.30	8.35
0.40	9.13
0.50	9.56
0.60	8.97
0.70	8.42
0.80	5.35
0.90	2.00
1.00	0.00

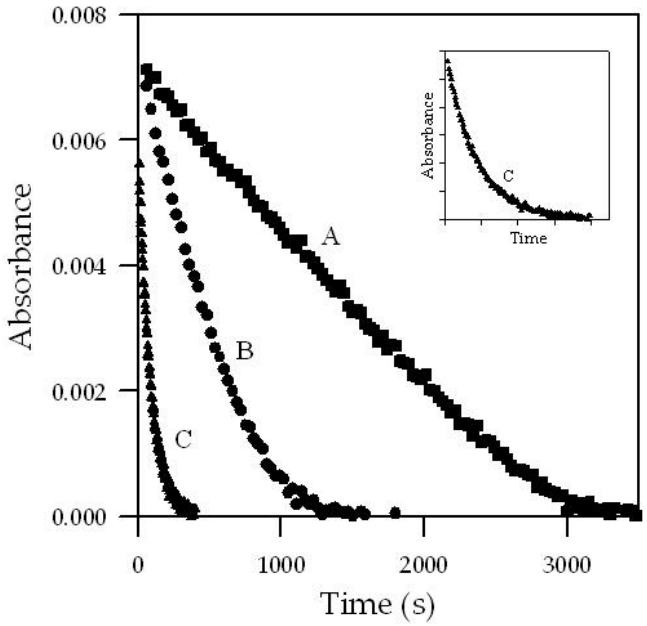


XVIII. Plot of initial rate (y_1) versus X_{ROLi} for the serial injection of ten aliquots of ester **1** (0.01 M final concentrations) to 0.10 M LDA in 6.1 M THF/hexanes co-solvent at -78 °C. The initials rate have been corrected to only include rates effected by autocatalysis. The curve depicts an unweighted least squares fit to $y_1 = k[X_{ROLi}]^n[1 - X_{ROLi}]^m$, $n = 1.15 \pm 0.16$), $m = (1.20 \pm 0.16) \times 10^{-7}$, $k = (4.41 \pm 1.05) \times 10^{-5}$), $k' = (2.25 \pm 6.71) \times 10^{-6}$.

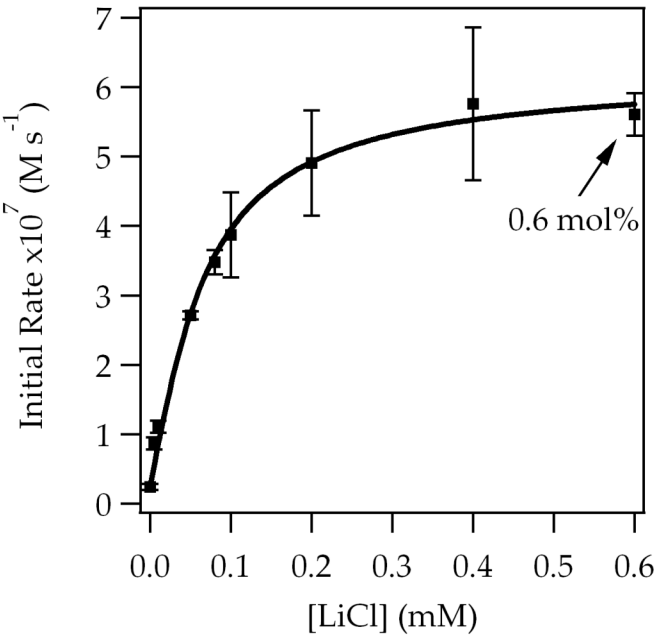
X_{ROLi}	$y_1 \times 10^{-6}$ ($M^{-1} \cdot s^{-1}$)
0.00	0.00
0.10	1.77
0.20	4.90
0.30	7.74
0.40	8.07
0.50	8.42
0.60	7.76
0.70	6.75
0.80	6.39
0.90	2.19
1.00	0.00



XIX. Plot showing IR absorbance of ester **1** vs time for the 1,4-addition of LDA (0.10 M) to equimolar ester **1** (0.10 M) in THF (6.10 M) with hexane cosolvent at -78 °C containing 1.0 mol % LiCl. The curve corresponds to a least squares fit to the second order functionm, $f(x) = a/(1 + bx)$.

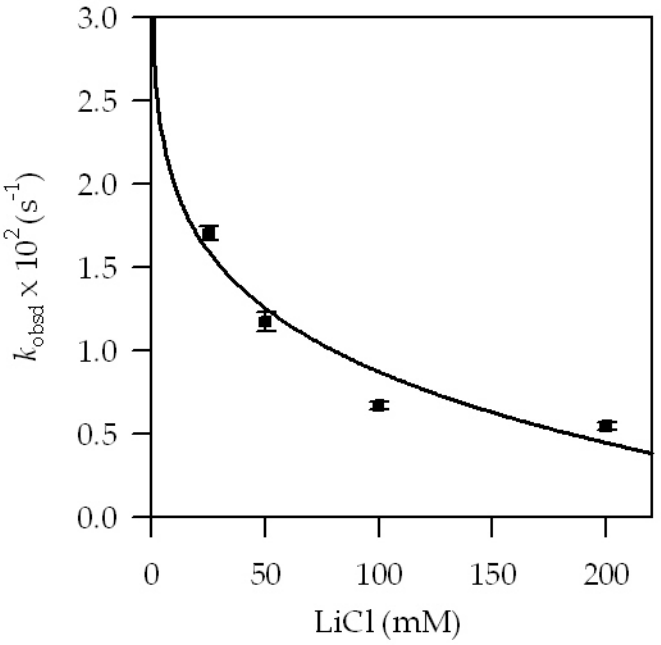


XX. Plot of IR absorbance vs time in THF (6.10 M) for the 1,4-addition of LDA (0.10 M) to ester **1** (00M) at -78 °C in the presence of LiCl. (A) no LiCl; (B) 0.01 mol % LiCl; (C) 0.4 mol % LiCl.



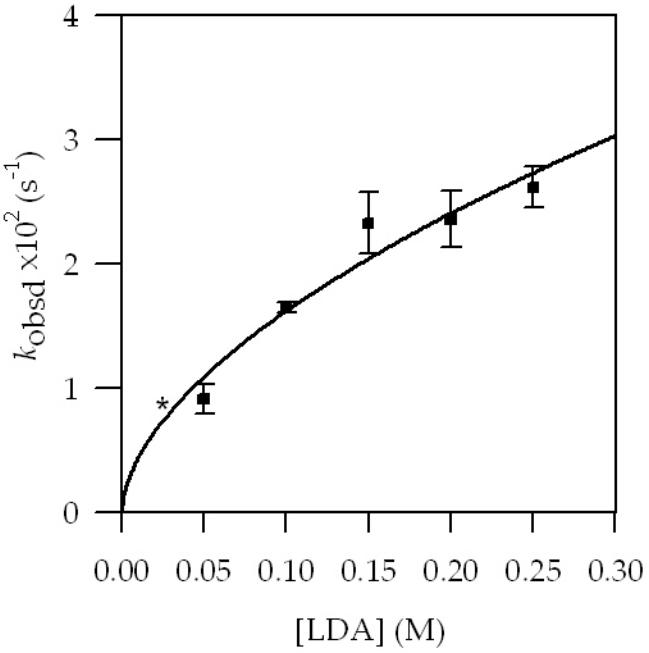
XXI. Plot of initial rates vs [LiCl] for the 1,4-addition of LDA (0.10 M) to ester **1** (0.004 M) in THF (6.1 M) at -78 °C.

LiCl (mM)	y_1 x 10^{-6} ($M^{-1}.s^{-1}$)	y_2 x 10^{-6} ($M^{-1}.s^{-1}$)	y_3 x 10^{-6} ($M^{-1}.s^{-1}$)	y_3 x 10^{-6} ($M^{-1}.s^{-1}$)
0.0001	1.88	2.22	2.07	3.06
0.005	8.7			
0.01	11.1			
0.05	26.8	2.74		
0.08	33.9	35.7		
0.10	44.9	36.2	34.9	
0.20	49.1	44.3	53.8	
0.40	63.2	52.0		
0.60	57.6	54.5		



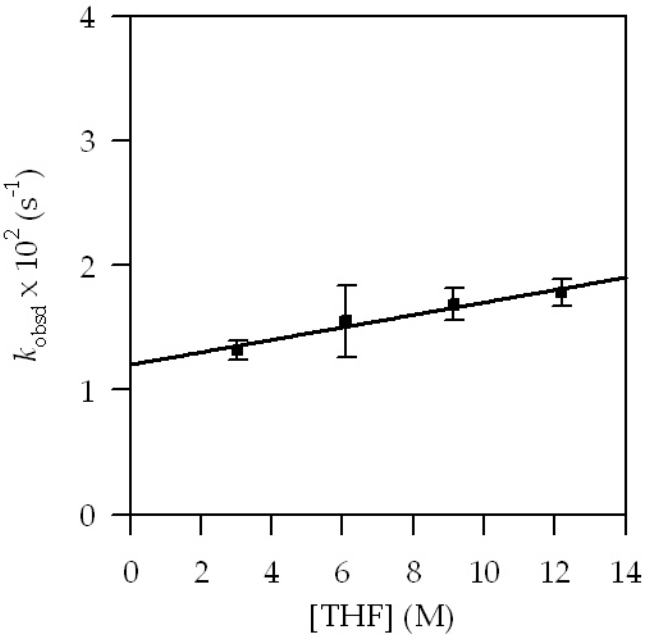
XXII. Plot of k_{obsd} vs [LiCl] for the 1,4-addition of LDA (0.10 M) to ester **1** (0.004 M) in THF (6.10 M) at -78 °C. The curve depicts an unweighted least squares fit to $y = k[LDA]^n + k'$ (k = (-1.74 ± 0.08) x 10^{-2}, n = (-1.60 ± 0.02), k' = (4.50 ± 0.02) x 10^{-2}.

[LiCl] (%)	$k_{obsd\ 1}$ x 10^2 (s^{-1})	$k_{obsd\ 2}$ x 10^2 (s^{-1})	k_{obsd} (avg) x 10^4 (s^{-1})
25	1.67 ± 0.03	1.73 ± 0.02	1.70 ± 0.01
50	1.21 ± 0.01	1.13 ± 0.04	1.17 ± 0.03
100	0.68 ± 0.02	0.65 ± 0.08	0.67 ± 0.02
200	0.56 ± 0.01	0.53 ± 0.02	0.64 ± 0.02



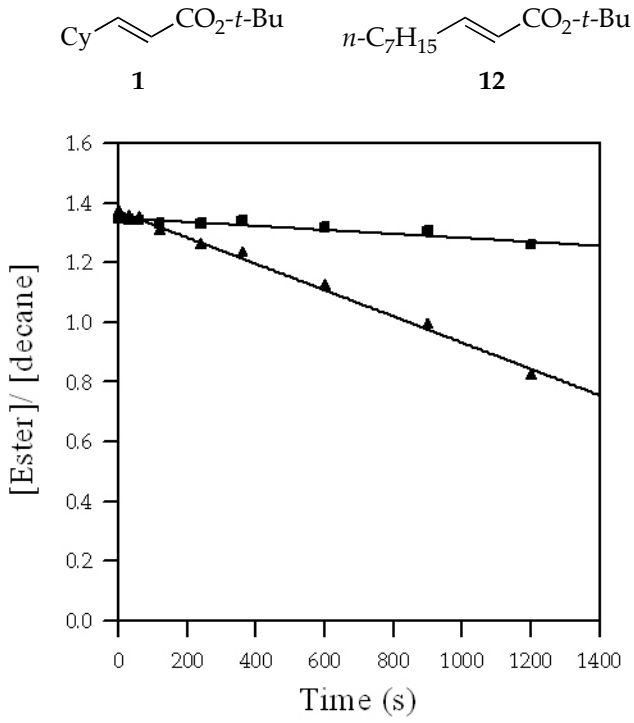
XXIII. Plot of k_{obsd} vs [LDA] for the 1,4-addition of in LDA (0.10 M) ester **1** (0.004 M) with LDA (0.10 M) in [THF] in hexane cosolvent at -78 °C. The curve depicts an unweighted least squares fit to y = k[LDA]^n + k' (k = (6.0 ± 0.1) x 10^{-7}, n = 0.57 ± 0.08).

[LDA] (M)	$k_{obsd\ 1}$ x 10^2 (s^{-1})	$k_{obsd\ 2}$ x 10^2 (s^{-1})	k_{obsd3} x 10^2 (s^{-1})
0.025	0.83 ± 0.02		
0.05	0.83 ± 0.03	1.01 ± 0.04	9.8 ± 0.04
0.10	1.62 ± 003	1.68 ± 0.03	1.72 ± 0.03
0.15	2.15 ± 0.02	2.50 ± 0.08	
0.20	2.20 ± 0.07	2.52 ± 0.03	
0.25	2.73 ± 0.02	2.50 ± 0.02	

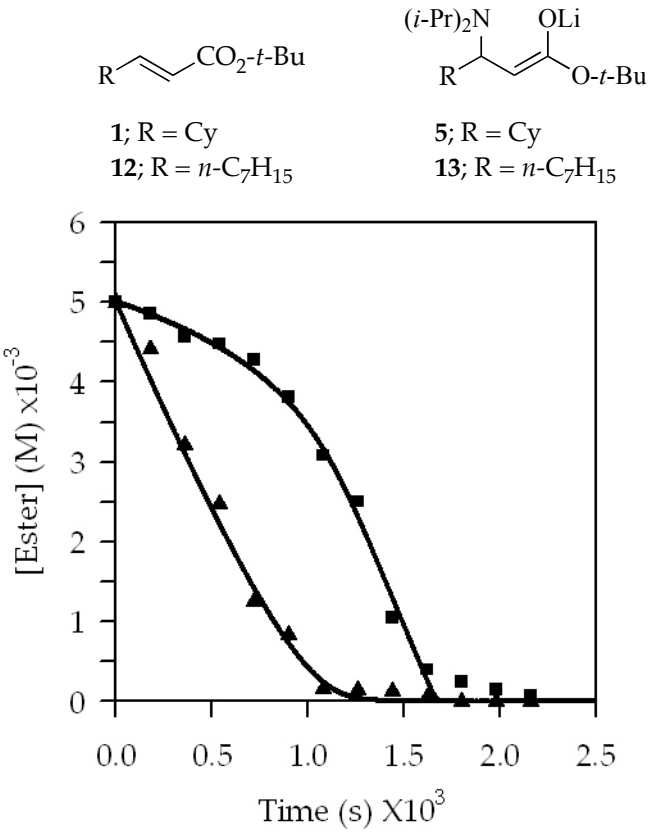


XXIV. Plot of k_{obsd} vs [THF] in hexane cosolvent for the 1,4-addition of [LDA] (0.10 M) to ester **1** (0.004 M) in the presence of 1% LiCl at -78 °C. The curve depicts an unweighted least-squares fit to y = -*k*[THF] + *k*′ (*k* = (5.0 ± 0.01) x 10^{-4}, *k*′ = (1.2 ± 0.1) x 10^{-2}).

[THF] (M)	y_1 x 10^{-2} (abs.s^{-1})	y_2 x 10^{-2} (abs.s^{-1})
3.01	1.27 ± 0.02	1.41 ± 0.01
6.10	1.67 ± 0.03	1.76 ± 0.01
9.15	1.96 ± 0.01	1.95 ± 0.02
11.20	1.92 ± 0.02	1.69 ± 0.03

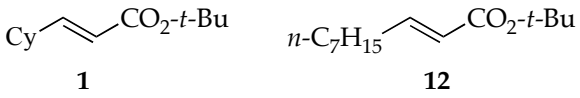


XXV. Plot of concentration vs time for the uncatalyzed 1,4-addition of a mixture of esters **1** and **12** (0.05 M each) to LDA (0.10 M) in THF (6.10 M) at -78 °C. Results are analyzed by GC relative to a decane internal standard. The slopes correspond to $k_1/k_{12} = 7.1$ (■) Ester **1**; (▲) Ester **12**.

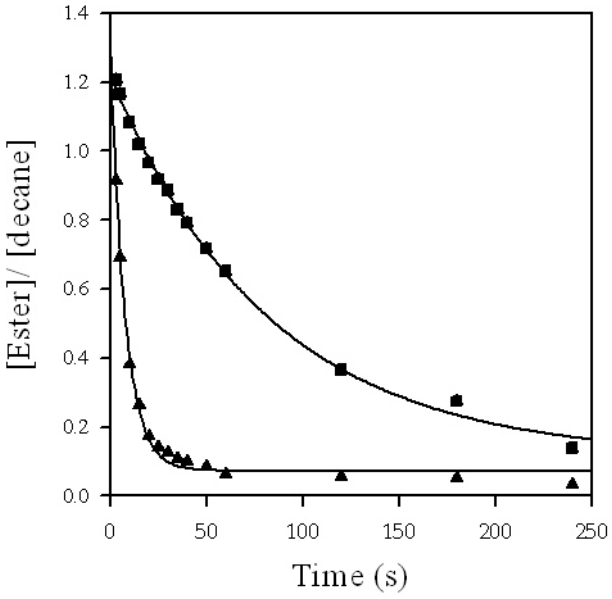


XXVI. Plot of concentration vs time for the uncatalyzed 1,4-addition of a mixture of esters **1** and **12** (0.005 M each) to LDA (0.10 M) in THF (6.10 M) at -78 °C. Results are analyzed by GC relative to a decane internal standard. (■) Ester **1**; (▲) Ester **12**. The curves in correspond to numerical integration to the highly simplified model as follows:

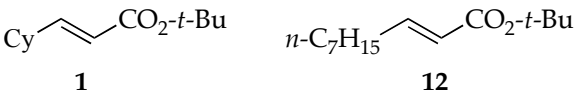
$$\tfrac{1}{2}\,A_2 \rightleftharpoons A$$
$$A + \mathbf{1} \longrightarrow \mathbf{5}$$
$$A + \mathbf{12} \longrightarrow \mathbf{13}$$



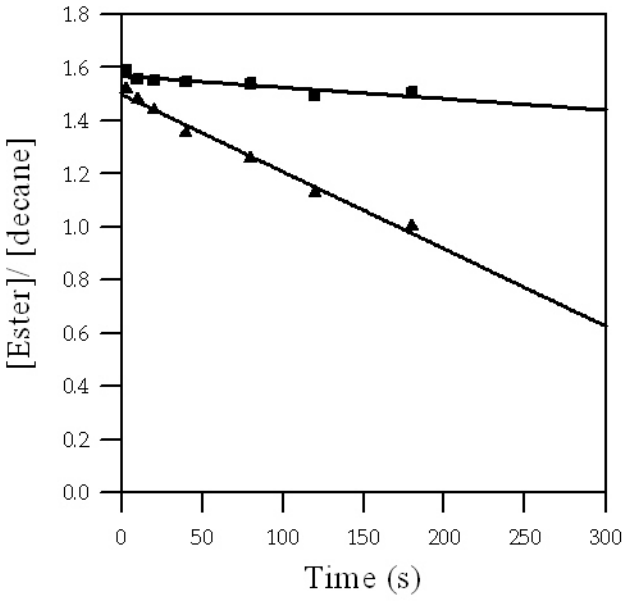
1 **12**



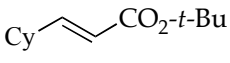
XXVII. Plot of concentration vs time for the LiCl catalyzed (1.0 mol %) 1,4-addition of LDA (0.10 M) to a mixture of esters **1** and **12** (0.05 M each) to LDA in THF (6.10 M) at -78 ºC. Results are analyzed by GC relative to a decane internal standard. The rate correspond to $k_1/k_{12} = 6.9$. (■) Ester **1**; (▲) Ester **12**.



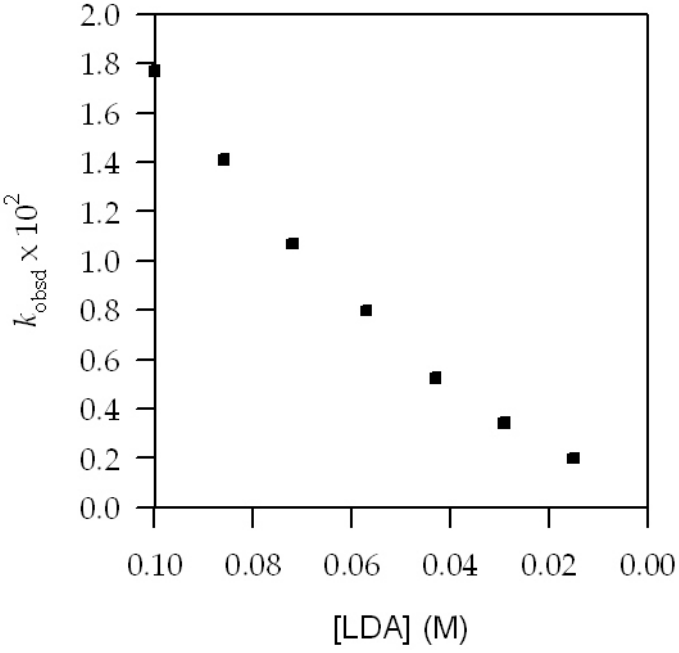
1 **12**



XXVIII. Plot of concentration vs time for the 1,4-addition of LDA (0.10 M) to a mixture of esters **1** and **12** (0.05 M each) to LDA (0.10 M) in THF (6.10 M) at -78 ºC in the presence of lithium enolate **5** (50.0 mol %)). Results are analyzed by GC relative to a decane internal standard. The slopes correspond to $k_1/k_{12} = 7.1$. (■) Ester **1**; (▲) Ester **12**.



1



XXIX. Plot of initial rate vs [LDA] in THF (6.10 M) on serially injecting ester **1** and (0.014 M) in LDA (0.10 M) in presence of 1.0% LiCl at -78 °C.

[LDA] (M)	$y_1 \times 10^{-2}$ (abs.s^{-1})
0.10	1.77
0.086	1.41
0.072	1.07
0.057	0.80
0.043	0.53
0.029	0.34
0.015	0.20

XXX. Derivation of expression for fitting LiCl saturation curve (eq 13 in manuscript):

Scheme 1

$$A_2 + LiCl \underset{k_{-1}}{\overset{k_1}{\rightleftharpoons}} 2A + LiCl$$

$$A + ester \xrightarrow{k_2} product$$

The rate of consumption of ester and its initial rate ($rate_{init}$) are defined as:

$$-\frac{d[ester]}{dt} = k_2[A][ester] \quad (1)$$

Applying the steady-state approximation to monomer A,

$$\frac{d[A]}{dt} = 2k_1[A_2][LiCl_T] - 2k_{-1}[A]^2[LiCl_T] - k_2[A][ester] = 0 \quad (2)$$

solving for [A] using the quadratic equation,

$$[A] = \frac{1}{4k_{-1}[LiCl_T]}(\sqrt{k_2^2[ester]^2 + 16k_1k_{-1}[A_2][LiCl_T]^2} - k_2[ester]) \quad (3)$$

and substituting eq 4 into eq 2 gives:

$$-\frac{d[ester]}{dt} = \frac{k_2[ester]}{4k_{-1}[LiCl_T]}(\sqrt{k_2^2[ester]^2 + 16k_1k_{-1}[A_2][LiCl_T]^2} - k_2[ester]) \quad (4)$$

where [ester] and $[A_2]$ are evaluated at t=0. To account for the LiCl-free pathway as outline below:

$$A_2 \underset{k_{-1}}{\overset{k_1}{\rightleftharpoons}} 2A$$

$$A + ester \xrightarrow{k_2} product$$

We add a constant c to eq 4 that reflects the initial rate without LiCl. The constant is determined experimentally rather than as an adjustable parameter.

$$-\frac{d[ester]}{dt} = \frac{k_2[ester]}{4k_{-1}[LiCl_T]}(\sqrt{k_2^2[ester]^2 + 16k_1k_{-1}[A_2]_0[LiCl_T]^2} - k_2[ester]) + c \quad (5$$

XXXI. Derivation of expression for fitting incremental addition curves depicted in Figures IX and X:

In a serial injection experiment, the amount of [ester] injected remains constant, but the concentration of LDA and ROLi **5** varies with each successive injection. Hence, the initial rate of consumption of ester **1** is defined as:

$$-\Delta[\text{ester}_0]/\Delta t = k[\text{ROLi}]^n[\text{LDA}]^m \quad (1)$$

Writing the concentrations in terms of mole fractions:

$$-\Delta[\text{ester}_0]/\Delta t = k[X_{\text{ROLi}}]^n[X_{\text{LDA}}]^m \quad (2)$$

where $X_{\text{ArLi}} = \text{N}_{\text{ROLi}}/(\text{N}_{\text{ROLi}} + \text{N}_{\text{LDA}})$ (N stands for normality)

Also, $X_{\text{LDA}} = 1 - X_{\text{ROLi}}$ (3)

Substituting eq 3 into eq 2 gives:

$$-\Delta[\text{ester}_0]/\Delta t = k[X_{\text{ROLi}}]^n[1 - X_{\text{ROLi}}]^m \quad (4)$$

Equation 4 is used to fit the serial injection curve depicted in Figure X. The initial rates y_i only reflect the effects of autocatalysis. To account for the uncatalyzed rate, we must add the rate term associated with LDA aggregation. It is given by the following expression (disregarding solvent effects):

$$-\Delta[\text{ester}_0]/\Delta t = k'[X_{\text{LDA}}]^{1.0} \quad (5)$$

or,

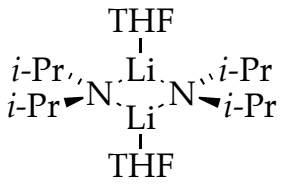
$$-\Delta[\text{ester}_0]/\Delta t = k'[1 - X_{\text{ROLi}}]^{1.0} \quad (6)$$

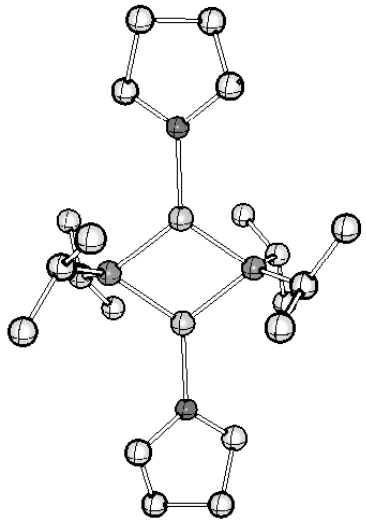
Adding expression 6 to equation 4 gives:

$$-\Delta[\text{ester}_0]/\Delta t = k[X_{\text{ROLi}}]^n[1 - X_{\text{ROLi}}]^m + k'[1 - X_{\text{ROLi}}]^{1.0} \quad (7)$$

Equation 7 describes the initial rate of the uncatalyzed and autocalyzed pathways combined. It is used to fit the serial injection curve depicted in Figure IX.

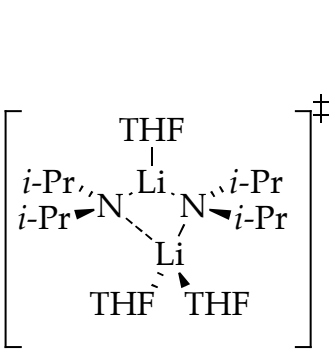
XXXII. Calculations:

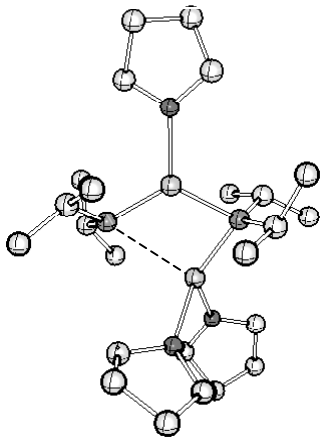




3
G = -1063.135499
(-78 °C)

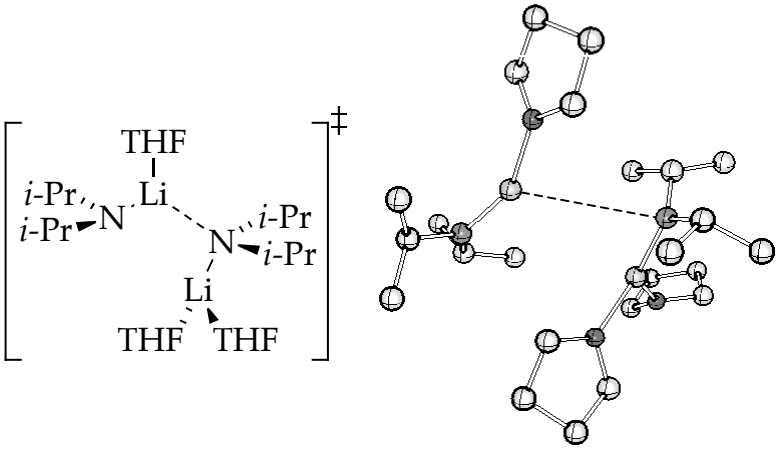
Atom	X	Y	Z	Atom	X	Y	Z
Li	-1.194627	-0.007825	0.022332	H	-1.500486	-3.820717	-0.761885
N	0.013907	1.643769	0.077205	C	0.932582	-1.814844	-2.212451
C	0.196558	2.410032	1.319032	H	1.876607	-1.339195	-1.919069
C	1.159764	1.707079	2.290512	H	1.147416	-2.498388	-3.043457
H	2.159075	1.604292	1.849772	H	0.264859	-1.033240	-2.596749
H	1.262404	2.264200	3.230548	H	1.002689	-3.335209	-0.721109
H	0.802179	0.701928	2.550069	O	3.182976	-0.015444	-0.127663
C	-1.131524	2.719155	2.048700	C	4.032339	-1.143606	0.199177
H	-1.598978	1.790545	2.404654	C	5.437966	-0.758062	-0.271094
H	-0.983501	3.376104	2.917980	C	5.411742	0.774063	-0.154916
H	-1.838550	3.216969	1.374689	C	3.984087	1.095274	-0.593500
H	0.658344	3.392275	1.104388	H	3.902781	1.157446	-1.686665
Li	1.194600	0.007938	0.022158	H	3.572808	2.009642	-0.160821
N	-0.013962	-1.643687	0.077247	H	6.162143	1.270000	-0.777688
C	-0.196637	-2.409858	1.319127	H	5.571005	1.083108	0.884979
C	1.131405	-2.718766	2.048953	H	5.590704	-1.057380	-1.314703
H	1.598735	-1.790078	2.404863	H	6.219980	-1.226951	0.333343
H	0.983363	-3.375653	2.918275	H	3.991648	-1.300598	1.282899
H	1.838548	-3.216575	1.375059	H	3.630188	-2.031035	-0.296809
C	-1.160039	-1.706940	2.290445	C	-0.277970	2.554246	-1.035528
H	-2.159328	-1.604365	1.849606	C	-0.932408	1.814820	-2.212599
H	-1.262680	-2.263956	3.230543	H	-1.876483	1.339255	-1.919253
H	-0.802631	-0.701703	2.549918	H	-1.147122	2.498323	-3.043671
H	-0.658276	-3.392178	1.104519	H	-0.264714	1.033138	-2.596792
C	0.278101	-2.554233	-1.035377	C	0.961585	3.312183	-1.569417
C	-0.961328	-3.312344	-1.569312	H	1.655983	2.609117	-2.049010
H	-1.655760	-2.609392	-2.049018	H	0.685387	4.074299	-2.312169
H	-0.684990	-4.074495	-2.311978	H	1.500736	3.820562	-0.761989
H	-1.002510	3.335320	-0.721398	H	-6.220074	1.226032	0.334511
O	-3.182976	0.015599	-0.128112	H	-5.592104	1.056795	-1.314054
C	-3.983928	-1.095127	-0.594129	H	-5.569779	-1.083823	0.885463
C	-5.411404	-0.774615	-0.154519	H	-6.162035	-1.270817	-0.776806
C	-5.438354	0.757507	-0.270589	H	-3.903299	-1.156675	-1.687391
C	-4.032490	1.143719	0.198539	H	-3.572024	-2.009558	-0.162195
H	-3.991063	1.301394	1.282122	H	-3.630993	2.030985	-0.298285





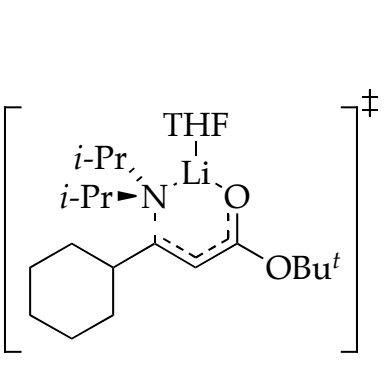
6
G = -1295.456449
(-78 °C)

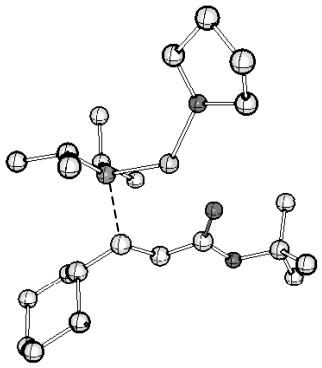
Atom	X	Y	Z	Atom	X	Y	Z
C	0.636461	1.802019	-2.288673	C	-0.228490	-3.982087	0.385700
N	0.822011	1.650311	-0.845433	H	-1.269985	-3.797777	0.102697
Li	1.509939	-0.037022	-0.014373	H	0.122300	-4.863948	-0.166914
N	0.286781	-1.501106	0.742168	H	-0.216642	-4.238917	1.449715
Li	-1.146230	-0.270797	-0.032281	C	0.690582	-2.553474	-1.453263
O	-2.510661	1.057607	0.794776	H	1.362710	-1.735653	-1.742380
C	-2.337956	2.465455	0.532152	H	1.043009	-3.459209	-1.963223
C	-2.432389	3.108190	1.912554	H	-0.308431	-2.317014	-1.841562
C	-3.519611	2.258037	2.608278	H	1.685699	-3.068606	0.349498
C	-3.489760	0.913150	1.840339	C	0.174180	-1.670666	2.199914
H	-3.182299	0.065610	2.458766	C	1.392000	-2.317572	2.901757
H	-4.466721	0.683652	1.395180	H	2.284188	-1.691893	2.772302
H	-3.319955	2.124170	3.675140	H	1.205622	-2.416944	3.979311
H	-4.503762	2.728962	2.513868	H	1.623810	-3.316002	2.517617
H	-1.472274	3.009721	2.429465	C	-0.077981	-0.320020	2.884625
H	-2.689185	4.170776	1.868346	H	-0.890699	0.233692	2.405983
H	-3.147604	2.816828	-0.128143	H	-0.334522	-0.458221	3.943108
H	-1.372289	2.558508	0.028097	H	0.816931	0.312346	2.839767
O	-2.826029	-1.121251	-1.159407	H	-0.692228	-2.316303	2.459782
C	-3.370205	-2.445604	-0.949735	O	3.539508	-0.424249	-0.080401
C	-4.859373	-2.384226	-1.339020	C	4.465644	0.420610	-0.807038
C	-5.158347	-0.876746	-1.333203	C	5.845577	0.108709	-0.229752
C	-3.822443	-0.297125	-1.791052	C	5.707807	-1.380081	0.120532
H	-3.714339	-0.353768	-2.883831	C	4.268910	-1.449874	0.635618
H	-3.649180	0.730217	-1.469606	H	3.779447	-2.410189	0.455585
H	-5.991110	-0.597334	-1.985685	H	4.219378	-1.228689	1.708550
H	-5.387610	-0.532409	-0.318163	H	5.826596	-1.996423	-0.778642
H	-5.013832	-2.797044	-2.341993	H	6.432293	-1.723139	0.865379
H	-5.488963	-2.950056	-0.645975	H	6.651578	0.317555	-0.939656
H	-3.223505	-2.695854	0.105007	H	6.026795	0.699619	0.676360
H	-2.809624	-3.164728	-1.555670	H	4.149812	1.457471	-0.677231
C	0.657291	-2.754042	0.069113	H	4.409965	0.168246	-1.872591
H	2.533919	2.936276	-0.843762	C	1.578011	2.774401	-0.291109
C	-0.555892	0.969153	-2.774494	C	1.976020	2.495264	1.167560
H	-1.479919	1.305108	-2.290136	H	2.604451	1.599818	1.261741
H	-0.697773	1.050809	-3.860567	H	2.538744	3.334121	1.596772
H	-0.412035	-0.094191	-2.545512	H	1.079821	2.343049	1.781508
C	1.880444	1.442510	-3.140188	C	0.875046	4.159259	-0.322210
H	2.121643	0.375543	-3.036146	H	0.035927	4.191469	0.384163
H	1.720468	1.649978	-4.208251	H	1.574962	4.957822	-0.038812
H	2.756911	2.019299	-2.824130	H	0.487522	4.405706	-1.316147
H	0.391623	2.848661	-2.556343				



7
G = -1295.449326
(-78 °C)

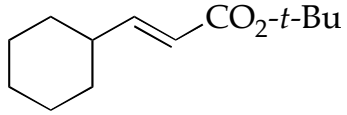
Atom	X	Y	Z	Atom	X	Y	Z
C	1.998047	-2.440567	1.794156	C	-4.708315	0.542008	2.247373
N	2.597024	-1.667569	0.720492	C	-3.935206	-0.572849	3.006501
Li	2.253942	0.099387	0.331597	C	-3.390356	-1.472232	1.884782
O	2.798805	1.907549	0.160525	H	-2.396985	-1.882114	2.076383
C	3.596110	2.622805	1.137194	H	-4.082621	-2.298466	1.663307
C	4.004805	3.927200	0.451212	H	-3.111371	-0.144585	3.584534
C	2.814595	4.186622	-0.486461	H	-4.571267	-1.133158	3.698051
C	2.459154	2.777163	-0.955734	H	-4.311158	1.528683	2.500369
H	1.400680	2.626251	-1.174614	H	-5.776931	0.542976	2.481639
H	3.062815	2.473831	-1.820858	H	-5.307965	-0.331767	0.325113
H	1.974986	4.622928	0.066035	H	-4.239966	1.092047	0.139970
H	3.058061	4.851435	-1.320296	C	-1.083484	2.749563	0.267657
H	4.176077	4.735048	1.168690	C	-2.286546	3.702730	0.500577
H	4.925151	3.783779	-0.126933	H	-3.181195	3.138427	0.797732
H	4.438994	1.986329	1.420906	H	-2.067548	4.436533	1.290003
H	2.974619	2.806838	2.022167	H	-2.532406	4.264777	-0.405909
N	-1.245827	1.724573	-0.743670	C	-0.703776	2.106274	1.610442
Li	-1.718222	-0.075010	-0.386750	H	0.210430	1.508748	1.508255
O	-1.343436	-1.812615	-1.241548	H	-0.536428	2.856716	2.393657
C	-2.388815	-2.767475	-1.539990	H	-1.502502	1.436699	1.958447
C	-1.776508	-3.762833	-2.528083	H	-0.242736	3.436500	0.004067
C	-0.293922	-3.742903	-2.126949	C	-1.356089	2.250631	-2.097705
C	-0.073274	-2.269730	-1.792301	C	-0.610623	1.347453	-3.101344
H	0.709032	-2.091370	-1.046473	H	-1.030563	0.332678	-3.075100
H	0.140518	-1.680431	-2.692647	H	-0.696806	1.715443	-4.132732
H	-0.123837	-4.365250	-1.240745	H	0.453204	1.268715	-2.849725
H	0.373953	-4.092912	-2.919160	C	-2.812049	2.416777	-2.609699
H	-2.236843	-4.753100	-2.456690	H	-3.406367	3.045259	-1.940900
H	-1.898301	-3.404771	-3.557259	H	-2.850910	2.859948	-3.615897
H	-3.251434	-2.226191	-1.940535	H	-3.301501	1.432983	-2.660008
H	-2.688886	-3.259844	-0.606650	H	-0.883428	3.254537	-2.162195
O	-3.293908	-0.617086	0.735168	C	3.779414	-2.292483	0.146704
C	-4.463548	0.222651	0.760167	C	4.584309	-1.257681	-0.655042
H	3.842666	-2.764098	2.947767	H	4.923837	-0.438645	-0.007548
H	1.882263	-3.510708	1.517365	H	5.467294	-1.702042	-1.131043
H	4.466308	-2.668062	0.933125	H	3.964659	-0.828124	-1.458429
C	0.581794	-1.921058	2.086352	C	3.475723	-3.505478	-0.766721
H	-0.054602	-2.002832	1.196914	H	2.940900	-3.179989	-1.669081
H	0.107715	-2.475530	2.907521	H	4.395678	-4.016968	-1.083558
H	0.616481	-0.862253	2.384633	H	2.849787	-4.243697	-0.252317
C	2.812960	-2.427484	3.111071	H	2.368762	-3.083373	3.873731
H	2.856045	-1.407383	3.516514				

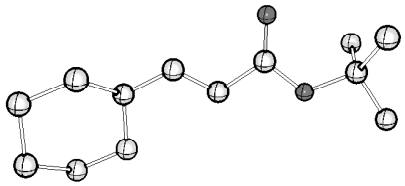




11
G = -1190.331832
(-78 °C)

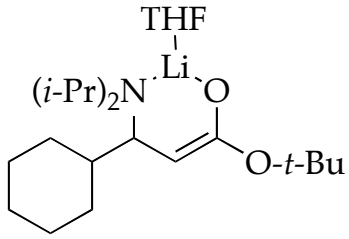
Atom	X	Y	Z	Atom	X	Y	Z
C	-0.739888	-2.750404	-0.054074	H	1.816202	4.320208	-1.815578
N	-0.507839	-1.460706	0.634981	H	3.494621	4.397447	-1.243583
Li	1.236478	-0.650569	0.121604	H	2.745740	2.822043	-1.603325
O	1.436727	1.089791	-0.524605	C	1.809288	5.140134	0.808286
C	0.510425	1.834540	-0.080053	H	2.732514	5.729816	0.816126
C	-0.834195	1.449058	0.084763	H	1.069146	5.659038	0.190738
C	-1.317812	0.227027	-0.414493	H	1.422855	5.084520	1.831218
H	-0.757954	-0.166002	-1.255995	O	2.953151	-1.535020	-0.114578
C	-2.817526	0.024066	-0.567149	C	3.963712	-0.890801	-0.926256
C	-3.657203	0.304267	0.693171	C	4.486549	-2.001437	-1.831026
C	-5.155660	0.073566	0.436227	C	4.483304	-3.207447	-0.875948
C	-5.666091	0.911626	-0.745099	C	3.245353	-2.950471	0.000407
C	-4.830968	0.657492	-2.008645	H	3.411136	-3.192901	1.055074
C	-3.334031	0.887826	-1.748747	H	2.365059	-3.499102	-0.349308
H	-3.155192	1.946588	-1.519371	H	5.393057	-3.208322	-0.265111
H	-2.753980	0.665307	-2.654587	H	4.428089	-4.168638	-1.394856
H	-5.172642	1.303495	-2.828081	H	5.476142	-1.781417	-2.242299
H	-4.987583	-0.379080	-2.343121	H	3.794947	-2.164528	-2.665760
H	-6.725200	0.695614	-0.937337	H	3.480471	-0.057827	-1.438451
H	-5.606804	1.978497	-0.482600	H	4.755730	-0.498791	-0.272921
H	-5.730853	0.303777	1.342486	C	-0.769432	-1.554279	2.085099
H	-5.326745	-0.992465	0.222829	H	-1.831441	-1.785660	2.287228
H	-3.508567	1.344824	1.013489	C	-0.466773	-0.235374	2.811593
H	-3.314946	-0.331174	1.516830	H	0.583068	0.061548	2.676144
H	-2.990095	-1.020273	-0.848793	H	-1.088359	0.585821	2.456673
H	-1.474617	2.117655	0.648215	H	-0.636929	-0.357407	3.888461
O	0.757371	3.114854	0.317368	C	0.056113	-2.668730	2.774112
C	2.076529	3.734253	0.257379	H	1.130538	-2.504878	2.610589
C	3.070975	2.993969	1.162160	H	-0.123267	-2.656064	3.856145
H	3.279284	1.993371	0.780650	H	-0.189704	-3.672586	2.414776
H	4.011686	3.554557	1.218540	H	0.022975	-3.465229	0.309530
H	2.666812	2.907458	2.177062	C	-0.493957	-2.649278	-1.570931
C	2.565502	3.817193	-1.194476	H	-0.456261	-3.653590	-2.009848
H	-2.942475	-2.875678	-0.169176	H	-1.286969	-2.100602	-2.089510
H	-2.105152	-4.425380	-0.325859	H	0.460192	-2.155353	-1.798958
H	-2.260608	-3.661368	1.257305	C	-2.091960	-3.459734	0.195228

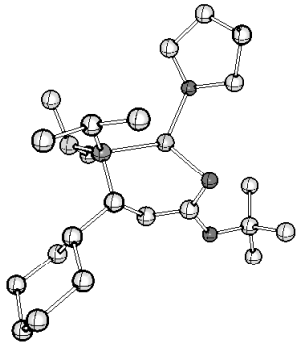




1
G = -658.796394
(-78 °C)

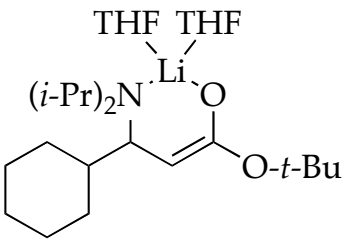
Atom	X	Y	Z	Atom	X	Y	Z
C	2.387451	-0.333797	-0.526491	C	4.702317	-0.895512	0.395076
C	0.933100	-0.711275	-0.481571	C	3.197961	-1.196567	0.474386
C	-0.107160	0.088146	-0.211800	H	2.833266	-0.990483	1.490877
C	-1.489421	-0.451957	-0.204575	H	3.011922	-2.261554	0.284998
O	-1.787466	-1.610305	-0.437212	H	5.241229	-1.491174	1.142719
O	-2.364625	0.535105	0.096694	H	5.081823	-1.210782	-0.588209
C	-3.814444	0.290584	0.166741	H	6.064952	0.797171	0.480805
C	-4.336694	-0.156746	-1.203256	H	4.726809	0.886725	1.621860
H	-3.935840	-1.133711	-1.477121	H	4.366345	2.524655	-0.204991
H	-5.430616	-0.218365	-1.176935	H	4.537311	1.259741	-1.416629
H	-4.055697	0.570718	-1.972777	H	2.306431	1.460041	0.680203
C	-4.124942	-0.729876	1.267745	H	-4.110211	2.407198	-0.232859
H	-3.697023	-0.402702	2.221825	H	0.004102	1.145502	0.004311
H	-5.210428	-0.813995	1.393581	H	0.707380	-1.759291	-0.683160
H	-3.722619	-1.712924	1.018890	C	2.681020	1.160209	-0.309466
C	-4.368542	1.669947	0.534289	C	4.186339	1.458749	-0.393154
H	-5.459421	1.627818	0.621861	C	4.991347	0.599791	0.593233
H	-3.956654	2.009652	1.490213	H	2.135469	1.761658	-1.047548
H	2.748213	-0.604484	-1.534716				

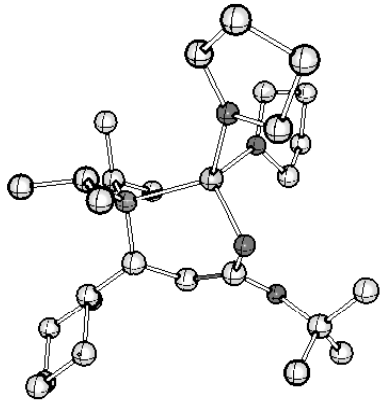




5·THF
G_{B3LYP} = -1190.344333
G_{MP2} = -1186.25046
(-78 °C)

Atom	X	Y	Z	Atom	X	Y	Z
C	-0.546335	-2.466533	-1.001785	H	3.132061	4.603567	-1.401570
N	-0.590506	-1.470430	0.120830	H	2.463374	3.000961	-1.818827
Li	1.212498	-0.410991	0.170977	C	1.570854	5.071326	0.819589
O	1.329604	1.121256	-0.890535	H	2.446197	5.730212	0.790782
C	0.461143	1.699140	-0.134920	H	0.742558	5.570103	0.305764
C	-0.673130	1.093409	0.376637	H	1.281330	4.920263	1.864937
C	-1.283383	-0.131085	-0.260560	O	2.977118	-1.235616	0.369323
H	-1.050138	-0.076215	-1.327332	C	4.054104	-0.609040	-0.378794
C	-2.851254	-0.135503	-0.181494	C	4.819571	-1.771978	-1.001569
C	-3.502115	0.364257	1.129056	C	4.729403	-2.833405	0.106964
C	-5.035662	0.257030	1.072596	C	3.317997	-2.610653	0.667602
C	-5.607318	1.058781	-0.104475	H	3.254710	-2.762917	1.749869
C	-4.960860	0.627656	-1.428007	H	2.578726	-3.255653	0.178610
C	-3.426367	0.679728	-1.363122	H	5.483661	-2.640948	0.878481
H	-3.088526	1.721247	-1.267195	H	4.872639	-3.855231	-0.256214
H	-3.009155	0.308024	-2.309291	H	5.848466	-1.505680	-1.260604
H	-5.322990	1.256206	-2.252281	H	4.314698	-2.117251	-1.911406
H	-5.275505	-0.401076	-1.661137	H	3.590452	0.081666	-1.084574
H	-6.697903	0.942775	-0.156352	H	4.684483	-0.042160	0.318736
H	-5.413293	2.128587	0.062720	C	-1.048403	-2.052477	1.423778
H	-5.468239	0.609491	2.018193	H	-2.148302	-2.076488	1.446959
H	-5.328945	-0.799147	0.971170	C	-0.568750	-1.200224	2.611965
H	-3.239129	1.416059	1.294649	H	0.525130	-1.254112	2.704699
H	-3.126559	-0.188569	1.996754	H	-0.836672	-0.149305	2.511045
H	-3.189688	-1.170221	-0.316388	H	-0.999257	-1.589439	3.542952
H	-1.251596	1.670100	1.085437	C	-0.581905	-3.498155	1.670622
O	0.627184	3.012706	0.264473	H	0.509595	-3.587326	1.604107
C	1.882022	3.727405	0.147254	H	-0.871484	-3.786275	2.687245
C	2.998543	3.005682	0.914799	H	-1.031087	-4.226829	0.990014
H	3.226606	2.046366	0.448085	H	-0.006330	-3.323063	-0.590473
H	3.909842	3.615792	0.925905	C	0.311482	-1.992610	-2.188843
H	2.693114	2.830762	1.953143	H	0.437615	-2.828394	-2.887874
C	2.253264	3.950712	-1.326187	H	-0.136850	-1.165318	-2.745275
H	1.421657	4.435502	-1.849684	H	1.308796	-1.672796	-1.869639
H	-1.719002	-3.854343	-2.187891	C	-1.896529	-3.003375	-1.518563
H	-2.543302	-3.352657	-0.706708	H	-2.445174	-2.247590	-2.089614





5·(THF)$_2$
G_{B3LYP} = -1422.691459
G_{MP2} = -1417.830597
(-78 °C)

Atom	X	Y	Z	Atom	X	Y	Z
Li	1.151303	-0.438243	-0.052861	C	-3.905727	-0.121155	1.264706
N	-0.809879	-1.490165	0.229151	C	-5.424628	-0.369692	1.271721
C	-0.758339	-2.651128	-0.731470	C	-6.126828	0.367889	0.124947
H	0.108549	-3.231436	-0.398276	C	-5.505123	-0.010929	-1.225532
C	-0.443404	-2.236260	-2.180000	C	-3.984317	0.205231	-1.232016
H	-0.076524	-3.116104	-2.724111	H	-3.759704	1.277980	-1.155161
H	-1.328886	-1.879109	-2.715757	H	-3.572197	-0.124077	-2.195747
H	0.317839	-1.454784	-2.227285	H	-5.969551	0.566168	-2.036251
C	-1.954297	-3.631097	-0.745068	H	-5.722114	-1.069773	-1.434698
H	-2.816208	-3.219032	-1.278383	H	-7.202821	0.148670	0.127712
H	-1.659020	-4.548873	-1.269475	H	-6.026964	1.452650	0.279029
H	-2.283368	-3.918470	0.257967	H	-5.846110	-0.061663	2.237857
C	-1.713655	-0.335314	-0.243696	H	-5.617982	-1.449446	1.179112
C	-1.255316	1.038012	0.177175	H	-3.727623	0.945638	1.451128
C	-0.133641	1.610247	-0.360657	H	-3.454336	-0.662449	2.101595
O	0.737148	1.033031	-1.118180	H	-3.475224	-1.602373	-0.205182
O	0.110568	2.931149	0.055243	C	-1.019587	-1.948457	1.636652
C	0.478396	3.930747	-0.927524	H	-2.053487	-2.310686	1.758906
C	1.973940	3.833985	-1.270816	C	-0.795162	-0.830067	2.667691
H	2.187933	2.867643	-1.729334	H	0.257005	-0.531059	2.679168
H	2.265843	4.638085	-1.958576	H	-1.386623	0.060743	2.467253
H	2.576891	3.932615	-0.359990	H	-1.058627	-1.209395	3.663474
C	-0.384907	3.802156	-2.190779	C	-0.088684	-3.115025	2.022526
H	-1.448085	3.818868	-1.927937	H	0.960210	-2.858141	1.824975
H	-0.184257	4.636066	-2.873913	H	-0.185083	-3.306308	3.097010
H	-0.170929	2.865985	-2.713255	H	-0.314760	-4.052370	1.507191
C	0.184640	5.257593	-0.216355	O	2.303474	0.099338	1.557045
H	0.462155	6.109249	-0.848413	C	3.389026	-0.635127	2.156942
H	-0.880205	5.334053	0.027104	C	4.122176	0.352839	3.075448
H	0.752913	5.320515	0.718249	C	3.023272	1.376783	3.403169
H	-1.885048	1.656183	0.804044	C	2.262645	1.450629	2.082234
H	-1.549024	-0.379373	-1.321889	H	2.749423	2.123975	1.367644
C	-3.261812	-0.533436	-0.079397	H	1.214324	1.739165	2.164469
H	4.952794	-1.040376	-3.403845	H	3.418768	2.348445	3.714022
H	2.577851	-0.578468	-2.971330	H	2.371532	1.001656	4.201298
H	3.333164	0.402138	-1.701668	H	4.943636	0.839674	2.536732
C	3.132171	-2.779119	-1.164477	H	4.542392	-0.135425	3.959894
H	3.585283	-3.043996	-0.201223	H	2.963917	-1.474831	2.722312
H	2.290166	-3.455272	-1.347825	H	4.023909	-1.035956	1.360509
H	5.004166	-3.454199	-2.103241	O	2.642006	-1.425784	-1.066654
H	3.690958	-3.121664	-3.241474	C	3.243254	-0.609314	-2.098825
H	5.319391	-1.054830	-1.667311	C	4.561032	-1.308150	-2.418018
C	4.160445	-2.788876	-2.308949				

XXXIII. Full citation for reference 25 in manuscript:
Gaussian 03, Revision B.04, Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Montgomery, Jr., J. A.; Vreven, T.; Kudin, K. N.; Burant, J. C.; Millam, J. M.; Iyengar, S. S.; Tomasi, J.; Barone, V.; Mennucci, B.; Cossi, M.; Scalmani, G.; Rega, N.; Petersson, G. A.; Nakatsuji, H.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Klene, M.; Li, X.; Knox, J. E.; Hratchian, H. P.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Ayala, P. Y.; Morokuma, K.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Zakrzewski, V. G.; Dapprich, S.; Daniels, A. D.; Strain, M. C.; Farkas, O.; Malick, D. K.; Rabuck, A. D.; Raghavachari, K.; Foresman, J. B.; Ortiz, J. V.; Cui, Q.; Baboul, A. G.; Clifford, S.; Cioslowski, J.; Stefanov, B. B.; Liu, G.; Liashenko, A.; Piskorz, P.; Komaromi, I.; Martin, R. L.; Fox, D. J.; Keith, T.; Al-Laham, M. A.; Peng, C. Y.; Nanayakkara, A.; Challacombe, M.; Gill, P. M. W.; Johnson, B.; Chen, W.; Wong, M. W.; Gonzalez, C.; and Pople, J. A.; Gaussian, Inc., Wallingford CT, 2004.

II. *Gaussview*, Version 3.09, Dennington II, R.; Keith, T.; Millam, J.; Eppinett, K.; Hovell, W. L.; Gilliland, R.; Semichem, Inc.; Shawnee Mission, KS, 2003.