Structures and Reactivities of Sodiated Evans Enolates: Role of Solvation and Mixed Aggregation on the Stereochemistry and Mechanism of Alkylations

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1. Aging effect

1. Aggregation study

3. Solvation study

5. Alkylation kinetics

6. Quaternization reaction

7. Aldol reaction

8. Aza-aldol Reaction

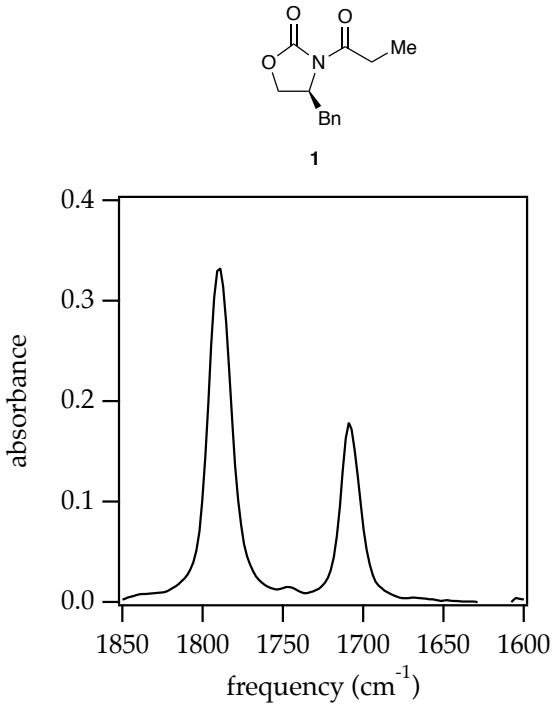


Figure S1. IR spectrum of 0.10 M **1** in toluene recorded at –78 °C.

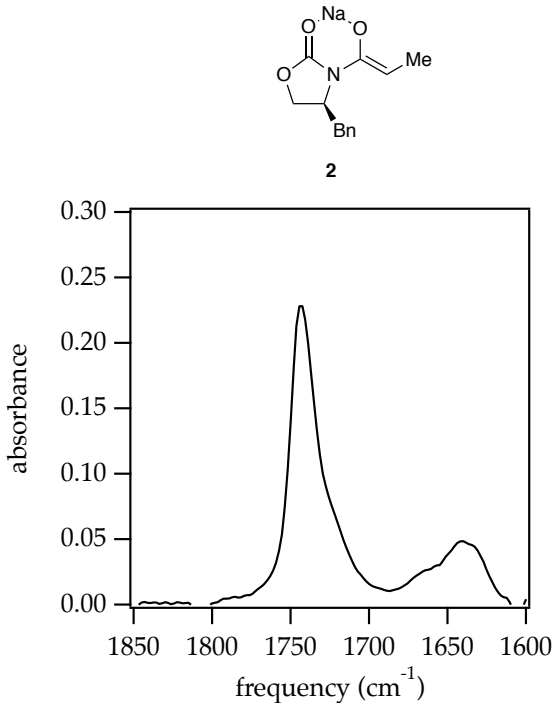


Figure S2. IR spectrum of 0.10 M **2** in 1.0 M TMEDA/toluene recorded at –78 °C.

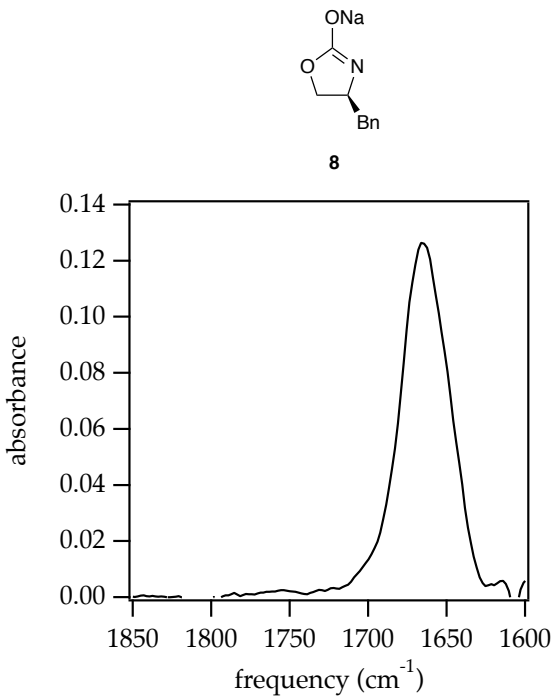
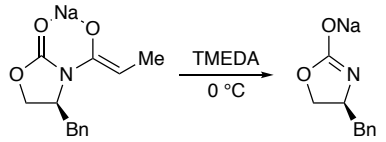
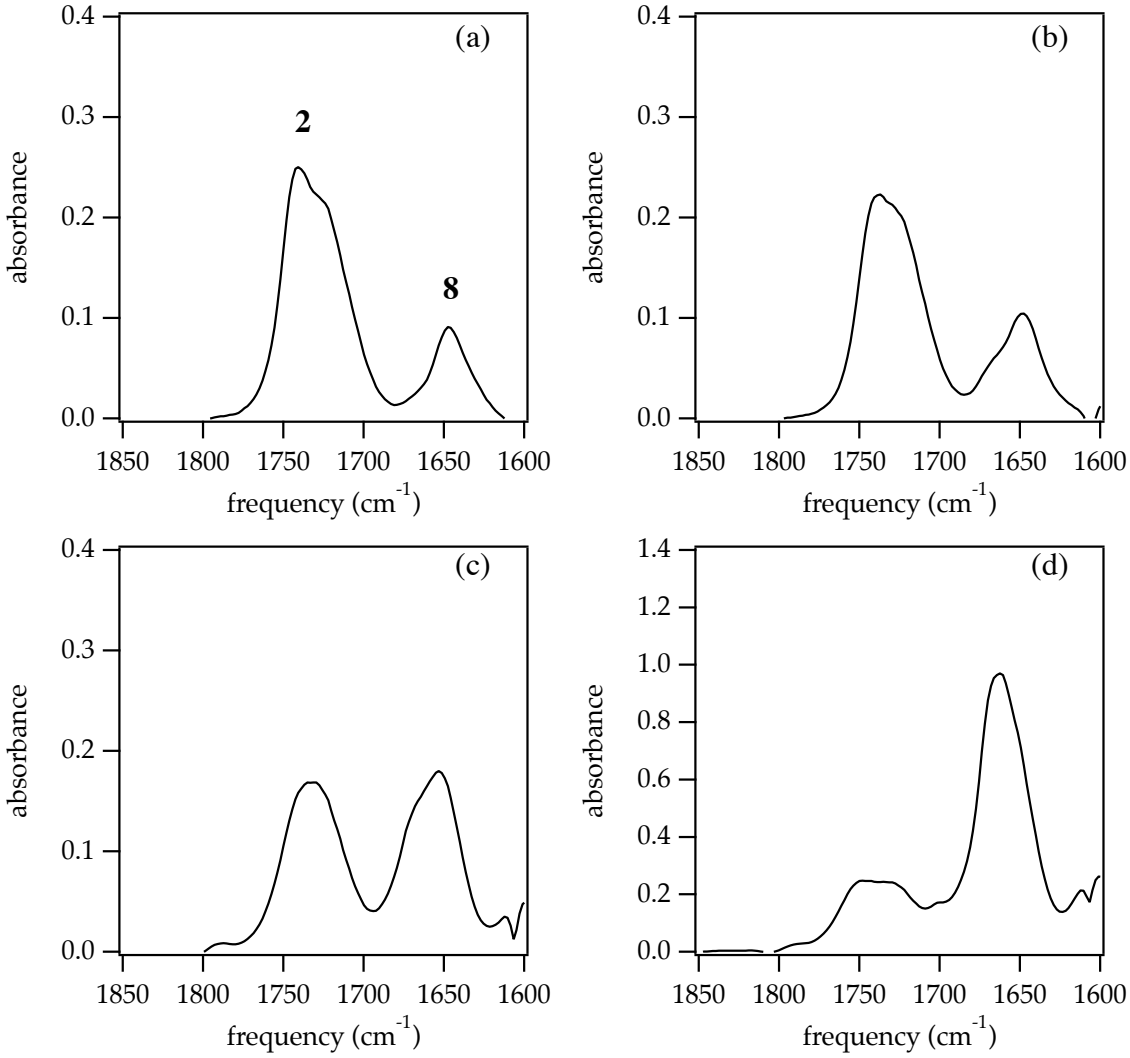


Figure S3. IR spectrum of 0.10 M **8** in 1.0 M TMEDA/toluene recorded at –78 °C.


Na
O
O
O
N
Me
Bn
TMEDA
0 °C
ONa
O
N
Bn

2 **8**


(a)
(b)
(c)
(d)
2
8
absorbance
frequency (cm-1)
0.0
0.1
0.2
0.3
0.4
0.6
0.8
1.0
1.2
1.4
1850
1800
1750
1700
1650
1600

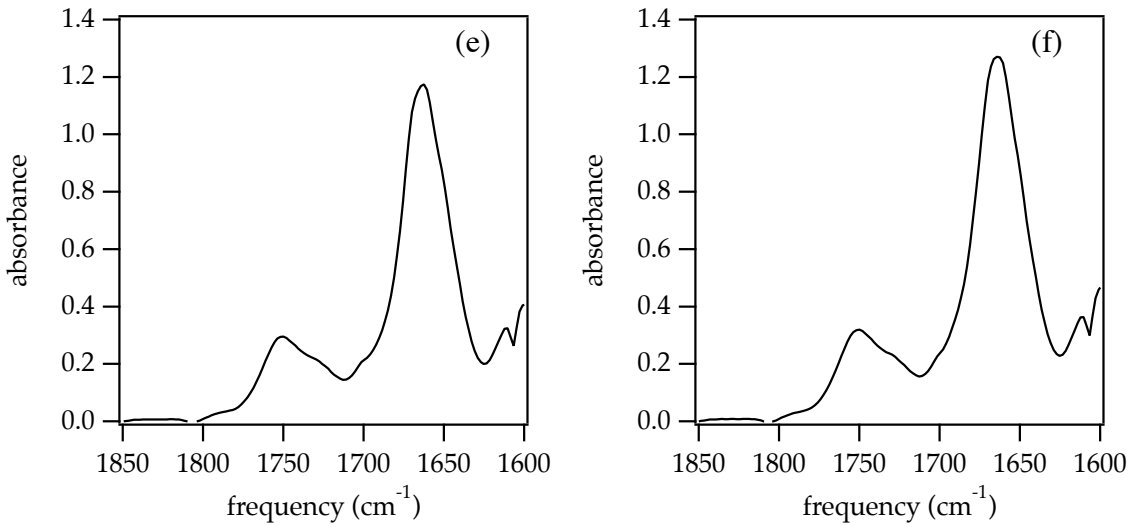


Figure S4. IR spectra of 0.10 M **2** and 0.050 M NaHMDS in 1.0 M TMEDA/toluene recorded at 0 °C after (a) 1 min; (b) 15 min; (c) 45 min; (d) 1.5 h; (e) 2.5 h; (f) 4 h. Nearly instantaneous enolate formation is followed by decomposition to give deacylated product **8**.

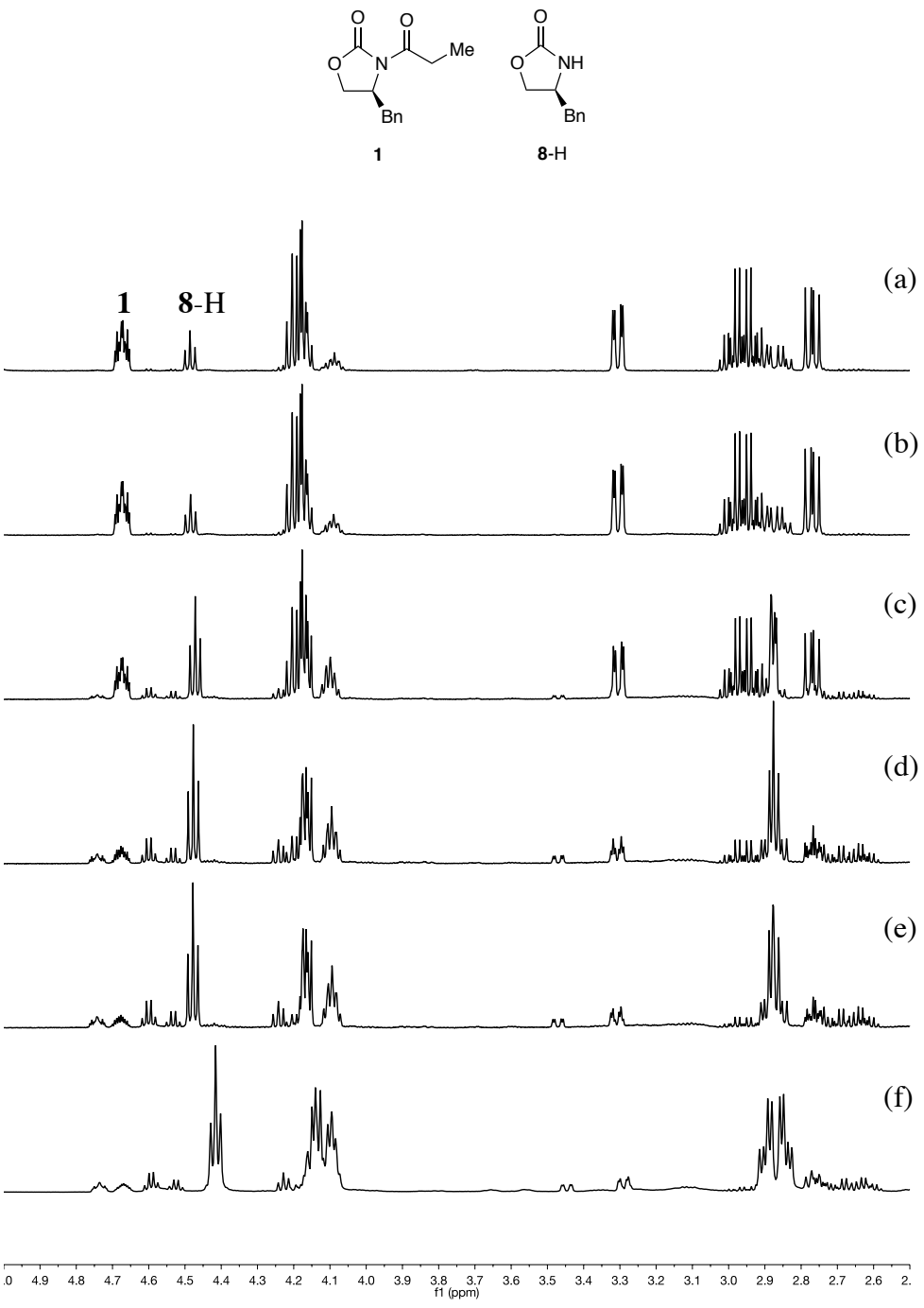


Figure S5. ^{1}H NMR spectra in $CDCl_3$ recorded at 25 °C of 0.10 M **2** and 0.050 M NaHMDS in 1.0 M TMEDA/toluene quenched with HCl (conc.), after aging at 0 °C for: (a) 1 min; (b) 15 min; (c) 45 min; (d) 1.5 h; (e) 2.5 h; (f) 4 h. Spectra show quenched enolate (starting material **1**) is gradually converted into quenched decomposition product (deacylated oxazolidinone).

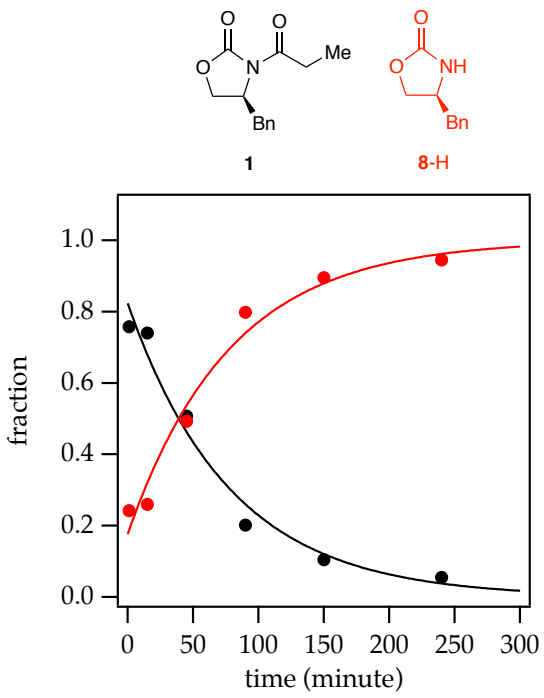


Figure S6. Plot of the fraction of **1** in quenched samples of enolate **2** versus time of aging at 25 °C. $y = a * e^{-bx}$, $a = 0.98 \pm 0.03$, $b = 0.016 \pm 0.001$.

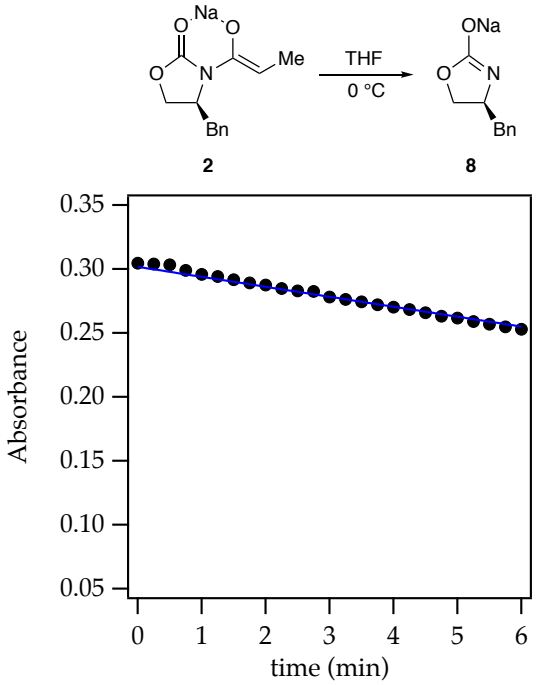


Figure S7. Plot showing loss of enolate **2** (0.10 M) with 0.050 M excess NaHMDS in THF at 0 °C. $y = a * (1 + bx)$, $a = 0.3017 \pm 0.0004$, $b = 0.0258 \pm 0.0001$. Decomposition of enolate **2** in THF is faster than in TMEDA/toluene ($k_{THF/TMEDA} = 1.6$).

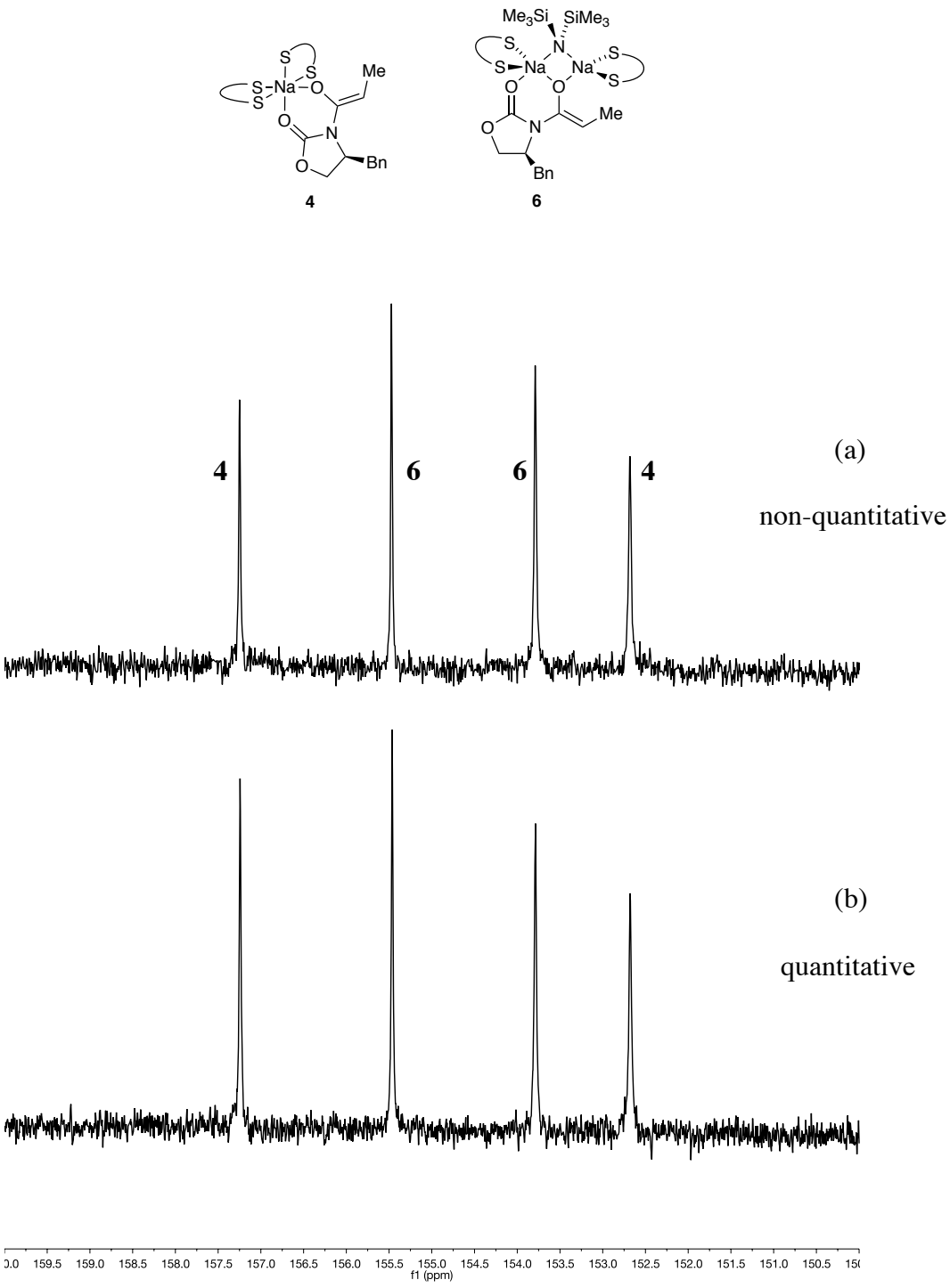


Figure S8. ^{13}C NMR spectra of 0.20 M **4** and 0.10 M NaHMDS in 1.0 M TMEDA/toluene recorded at –80 °C. The qualitative spectrum (a) is acquired with 1.0 s relaxation delay and 11.75 pulse width. The quantitated spectrum is acquired with 30 s. relaxation delay and 22 pulse width. The experiment shows the integrations are ±<10%.

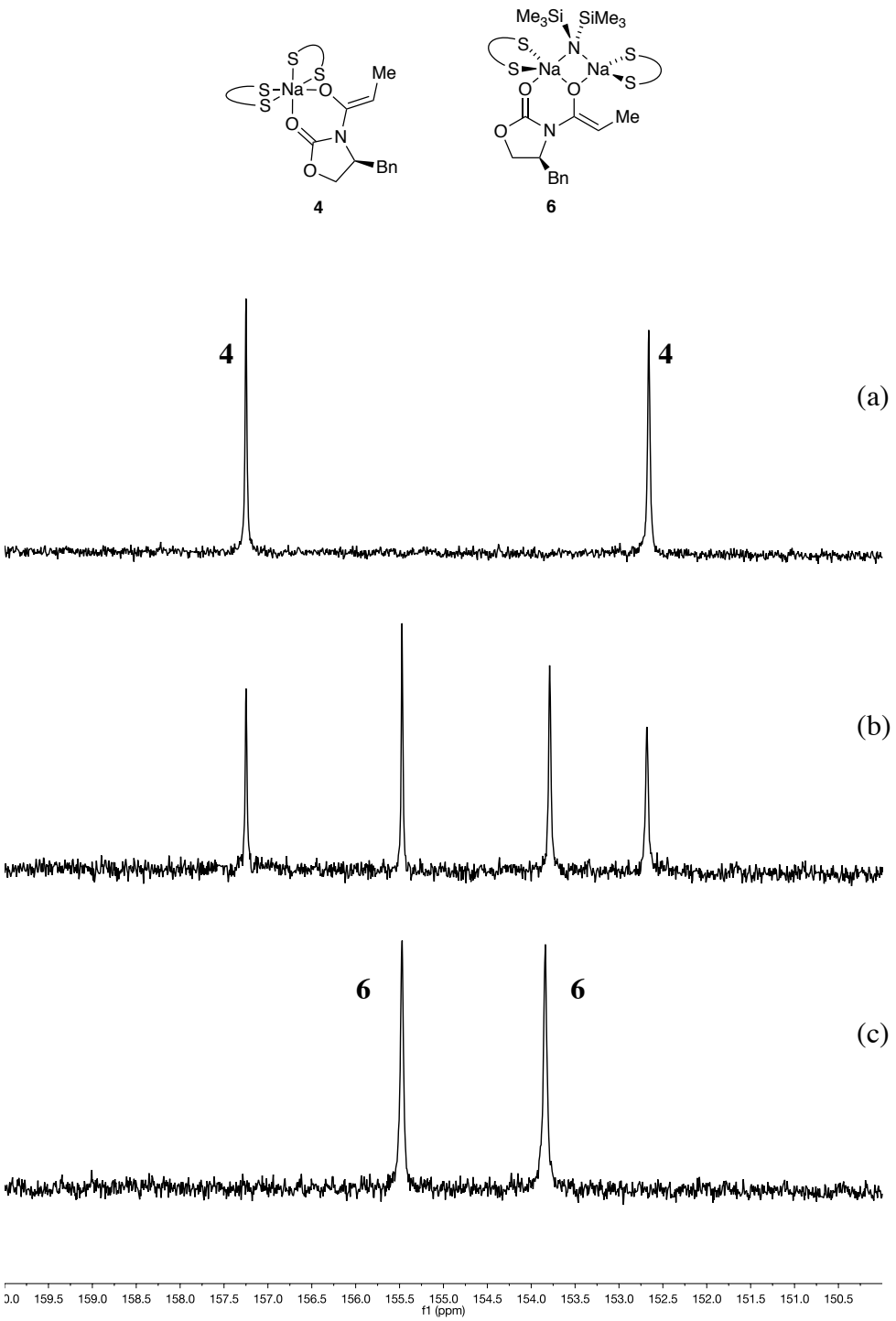


Figure S9. ^{13}C NMR spectra of 0.20 M **4** in 1.0 M TMEDA/toluene recorded at –80 °C with (a) no NaHMDS; (b) 0.10 M NaHMDS; (c) 0.20 M NaHMDS. The experiment shows enolate **2** is converted quantitatively to mixed aggregate **6**

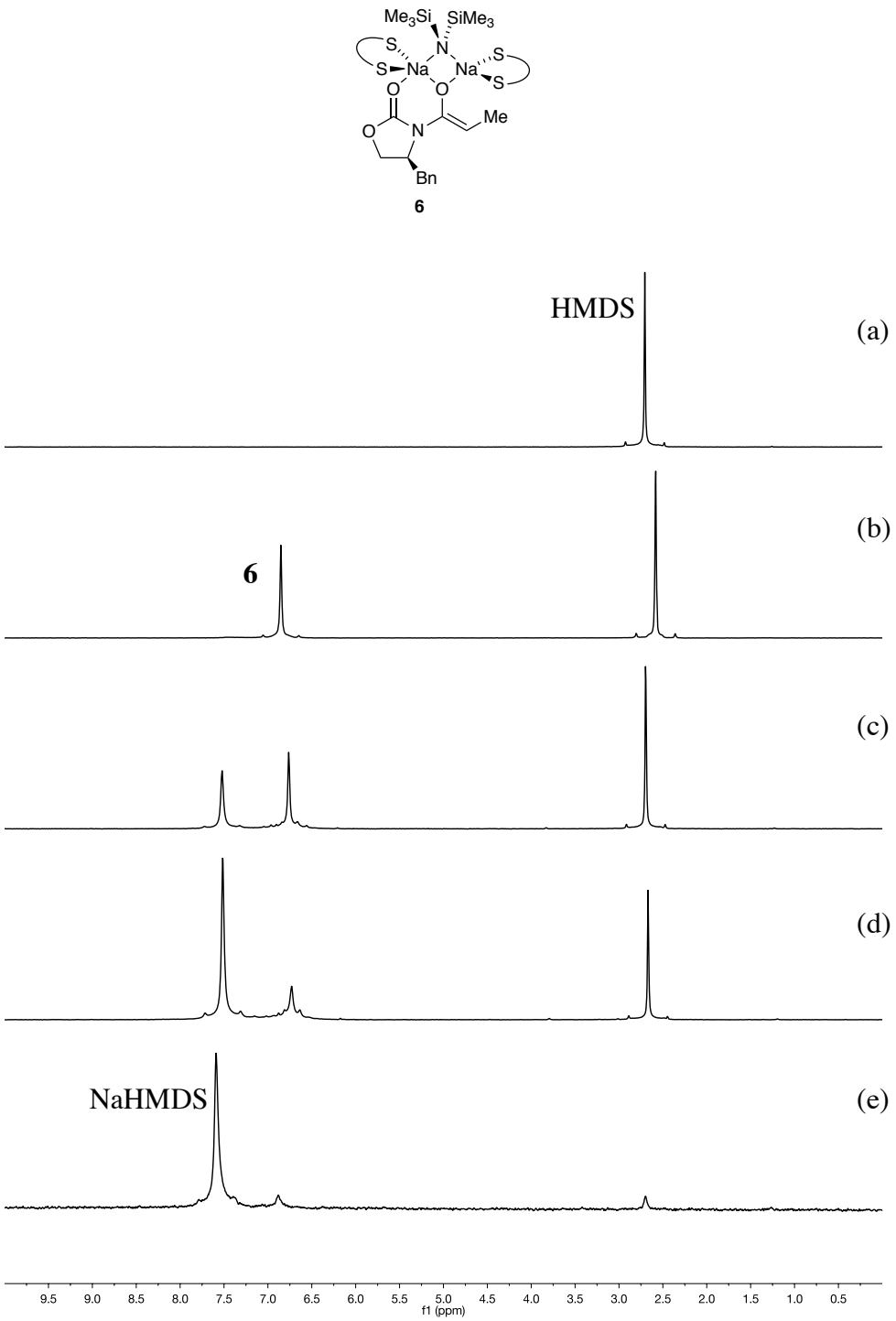


Figure S10. ^{13}C NMR spectra of 0.20 M **4** in 1.0 M TMEDA/toluene recorded at –80 °C with (a) no excess NaHMDS; (b) 0.20 M excess NaHMDS; (c) 0.40 M excess NaHMDS; (d) 0.80 M NaHMDS; (e) no enolate and 1.0 M NaHMDS. Enolate monomer not shown. HMDS (2.7 ppm), NaHMDS (7.6 ppm) and mixed aggregate **6** (6.9 ppm, TMS carbon) are as labeled.

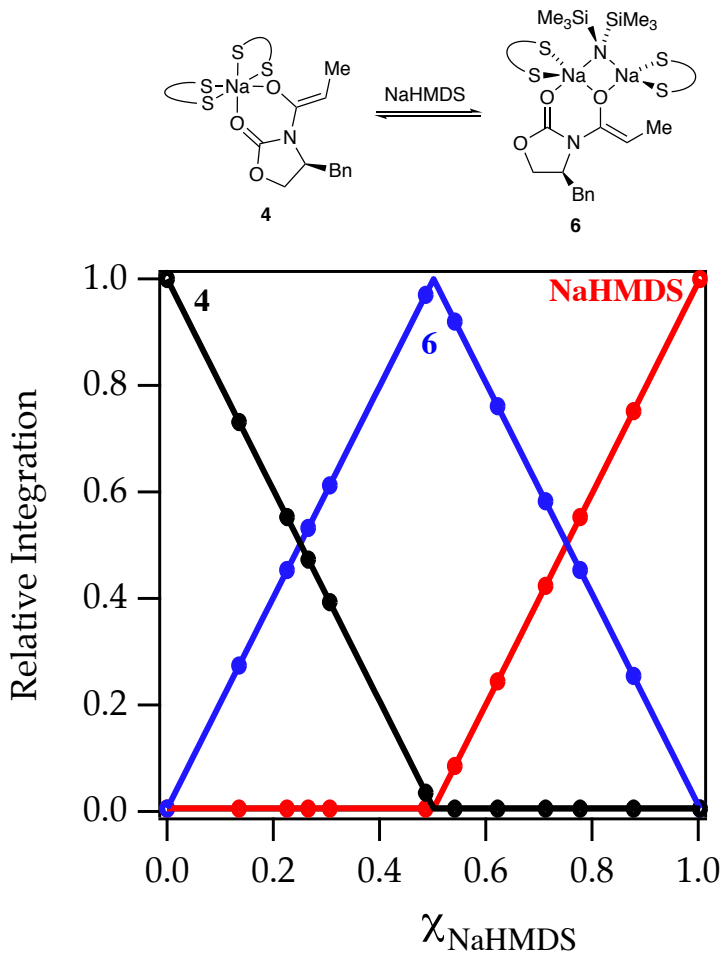


Figure S11. Job plot showing the relative integrations versus the measured mole fraction of NaHMDS, χ_{NaHMDS}, in mixtures of NaHMDS and enolate **4** (0.30 M total titer) in 0.60 M TMEDA/toluene recorded at –80 °C. The curves represent a parametric fit to a dimer-based model.

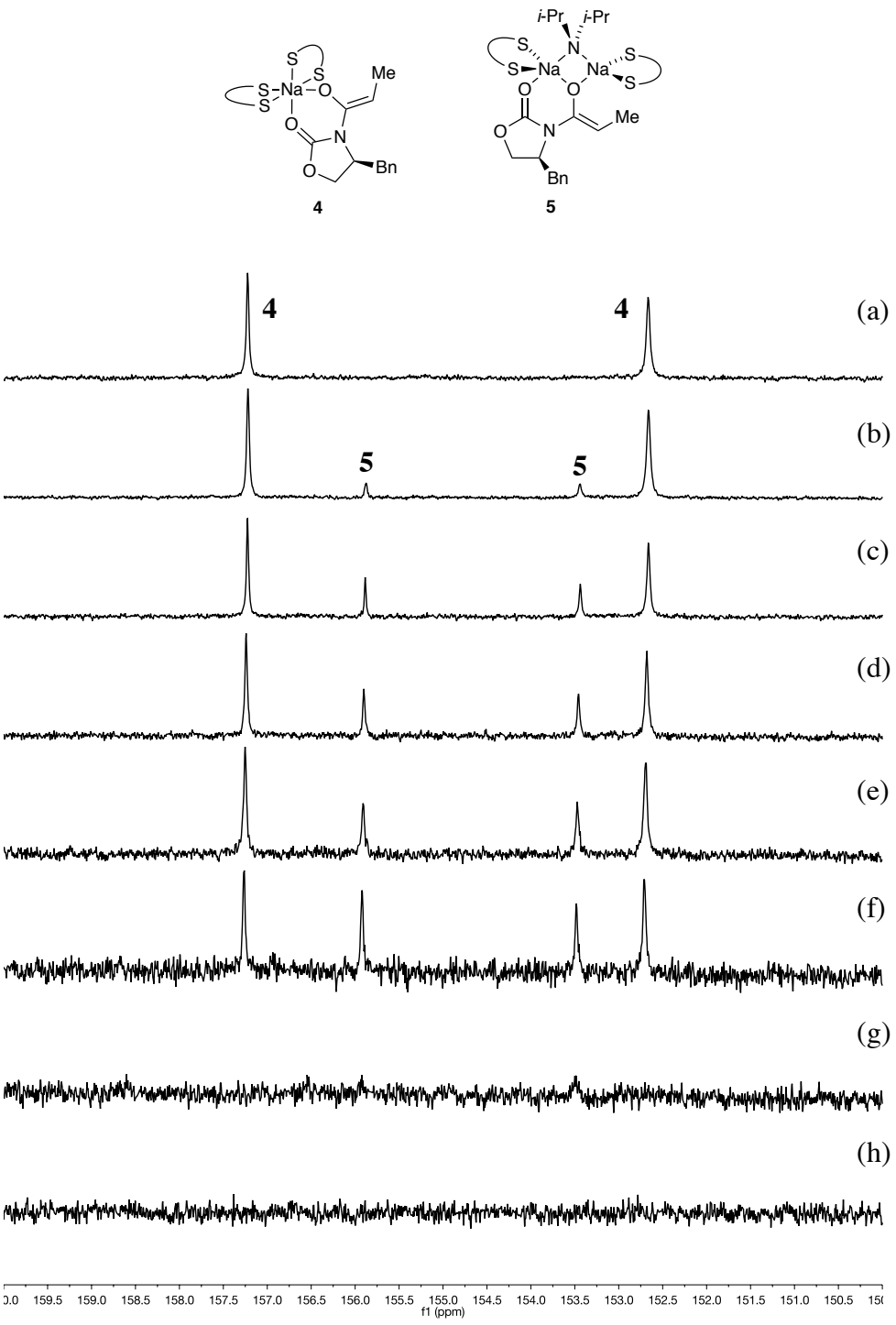


Figure S12. ^{13}C NMR spectra of enolate **4** and NaDA (0.40 M total titer) in 1.0 M TMEDA/toluene recorded at –80 °C. The samples contain (a) 0.40 M **4**; (b) 0.35 M **4** and 0.050 M NaDA; (c) 0.30 M **4** and 0.10 M NaDA; (d) 0.25 M **4** and 0.15 M NaDA; (e) 0.20 M **4** and 0.20 M NaDA; (f) 0.15 M **4** and 0.25 M NaDA; (g) 0.10 M **4** and 0.30 M NaDA; (h) 0.050 M **4** and 0.35 M NaDA.

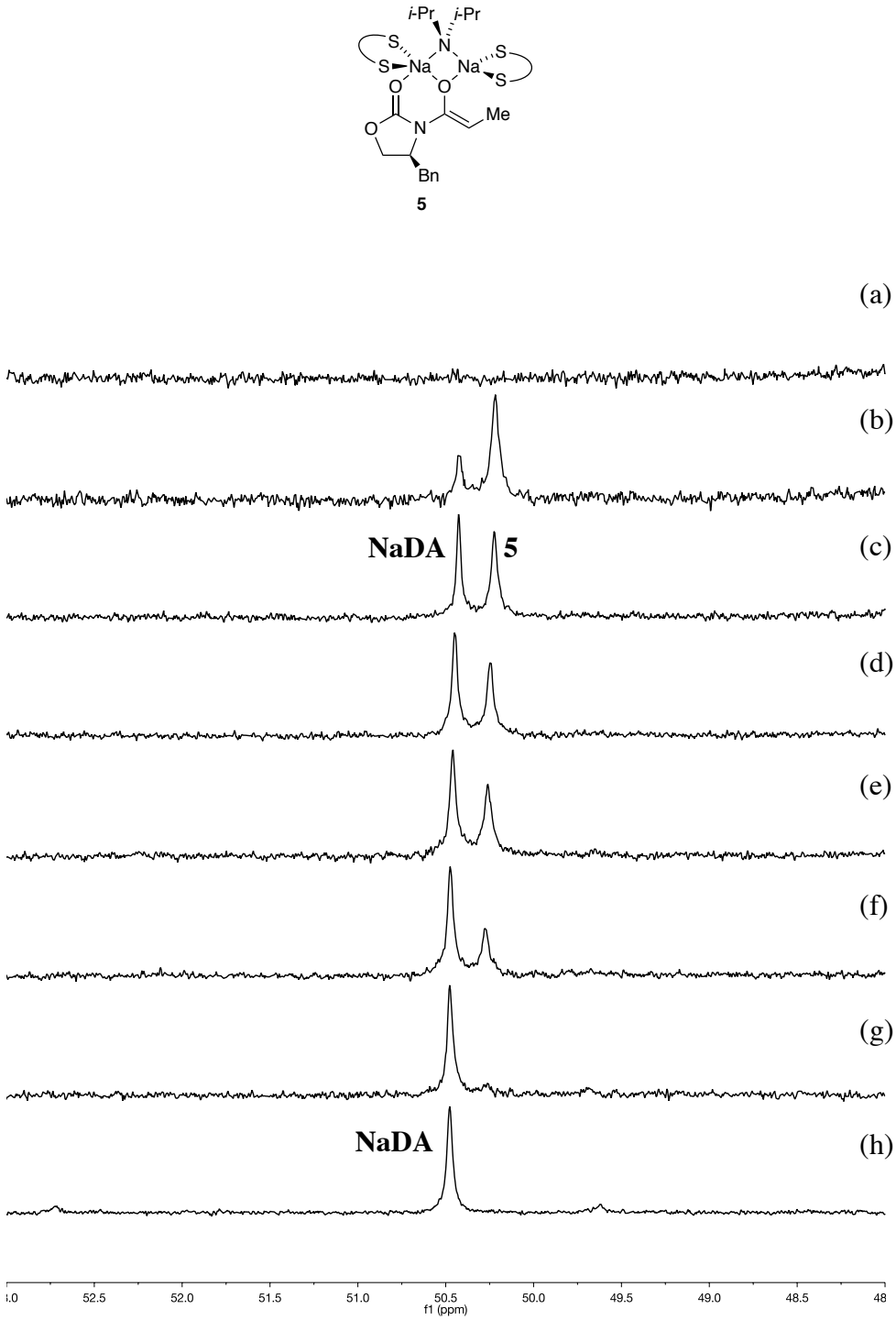


Figure S13. ^{13}C NMR spectra of enolate **4** and NaDA (0.40 M total titer) in 1.0 M TMEDA/toluene recorded at –80 °C. The samples contain (a) 0.40 M **4**; (b) 0.35 M **4** and 0.050 M NaDA; (c) 0.30 M **4** and 0.10 M NaDA; (d) 0.25 M **4** and 0.15 M NaDA; (e) 0.20 M **4** and 0.20 M NaDA; (f) 0.15 M **4** and 0.25 M NaDA; (g) 0.10 M **4** and 0.30 M NaDA; (h) 0.050 M **4** and 0.35 M NaDA. Free and bound NaDA (methine carbon) are illustrated.

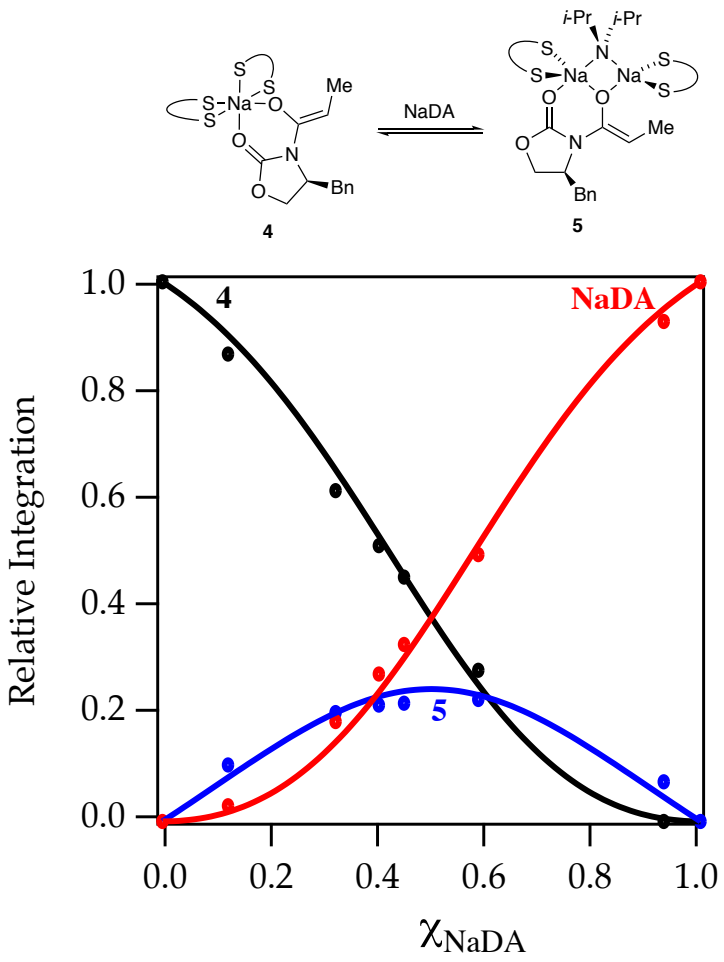


Figure S14. Job plot showing the relative integrations versus the measured mole fraction of NaDA, χ_{NaDA}, for mixtures of NaDA and enolate **4** (0.40 M total titer) in 1.0 M TMEDA/toluene recorded at –80 °C. The data comes from Figures S12 and S13.

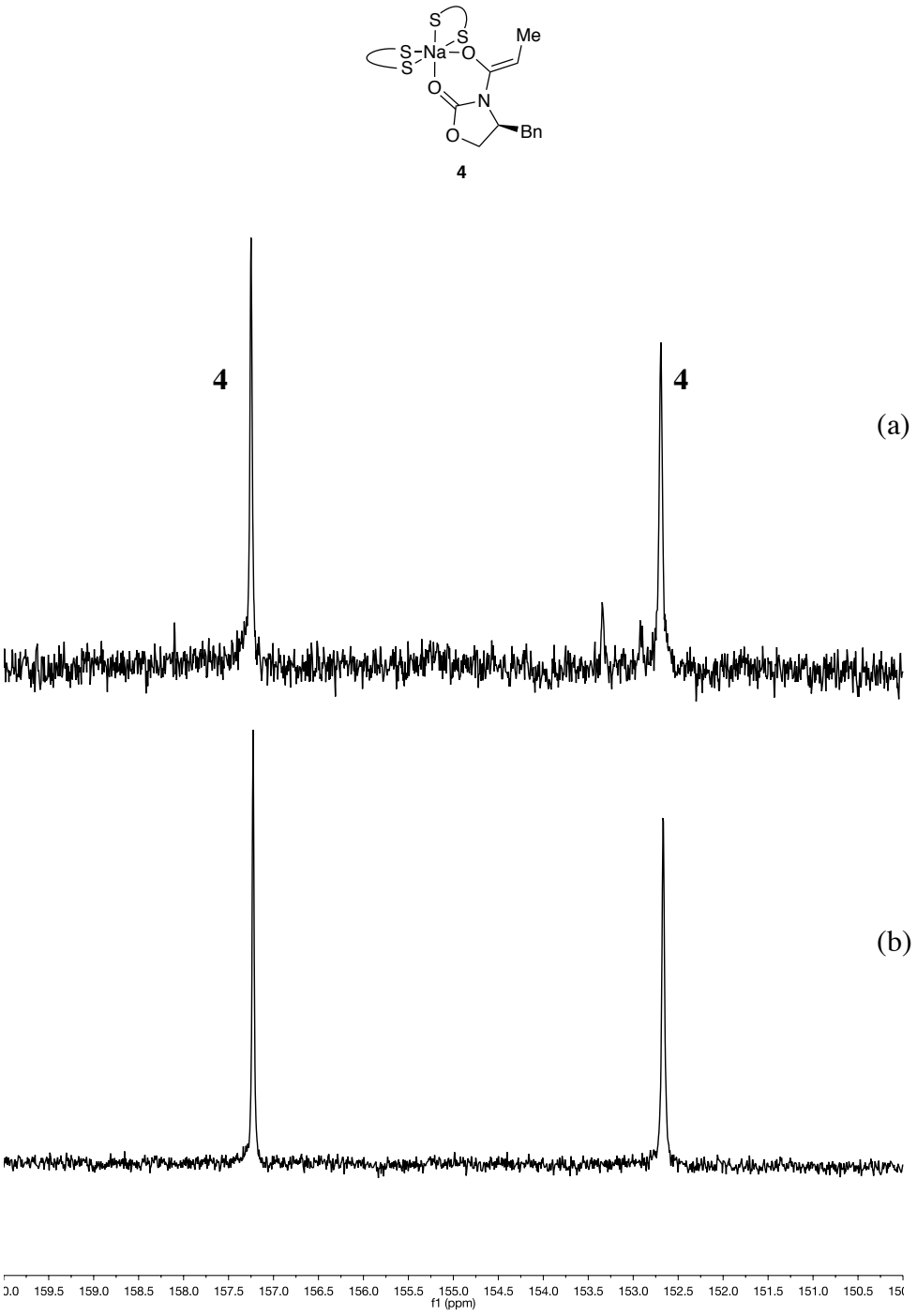


Figure S15. ^{13}C NMR spectra of enolate **4** (0.20 M) in 1.0 M TMEDA/toluene recorded at –80 °C generated from (a) 0.20 M NaHMDS; (b) 0.20 M NaDA. The experiment shows the spectrum of **4** is base independent.

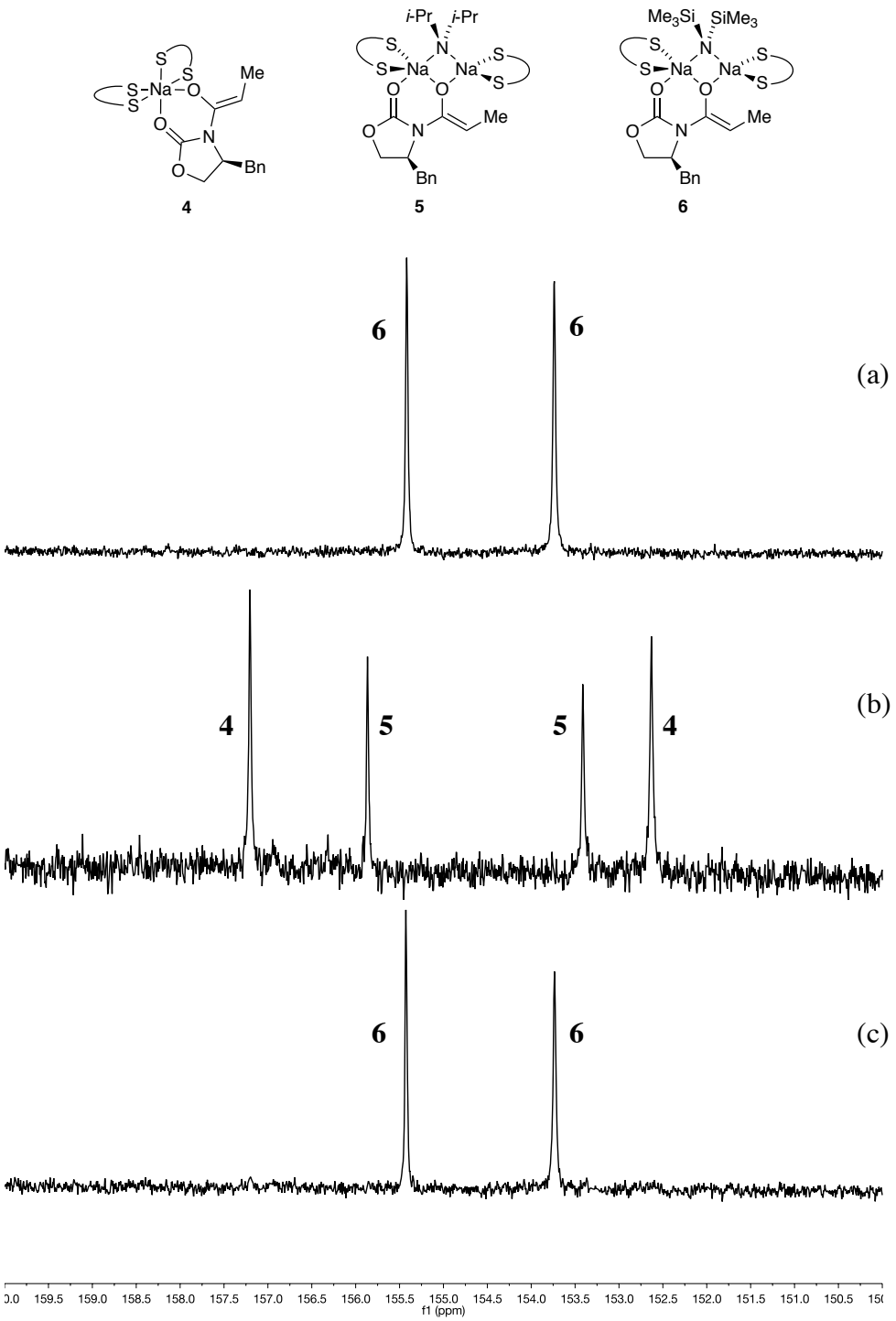


Figure S16. ^{13}C NMR spectra in 1.0 M TMEDA/toluene at –80 °C of (a) 0.20 M **6**; (b) 0.20 M NaDA and 0.20 M **4**; (c) 0.20 M NaHMDS, 0.20 M NaDA and 0.20 M **4**. The experiment shows NaHMDS forms mixed dimer **6** quantitatively whereas NaDA mixed dimer **5** non-quanitatively. Spectrum (c) shows a competition of NaDA and NaHMDS affords only the NaHMDS-derived mixed dimer **6**.

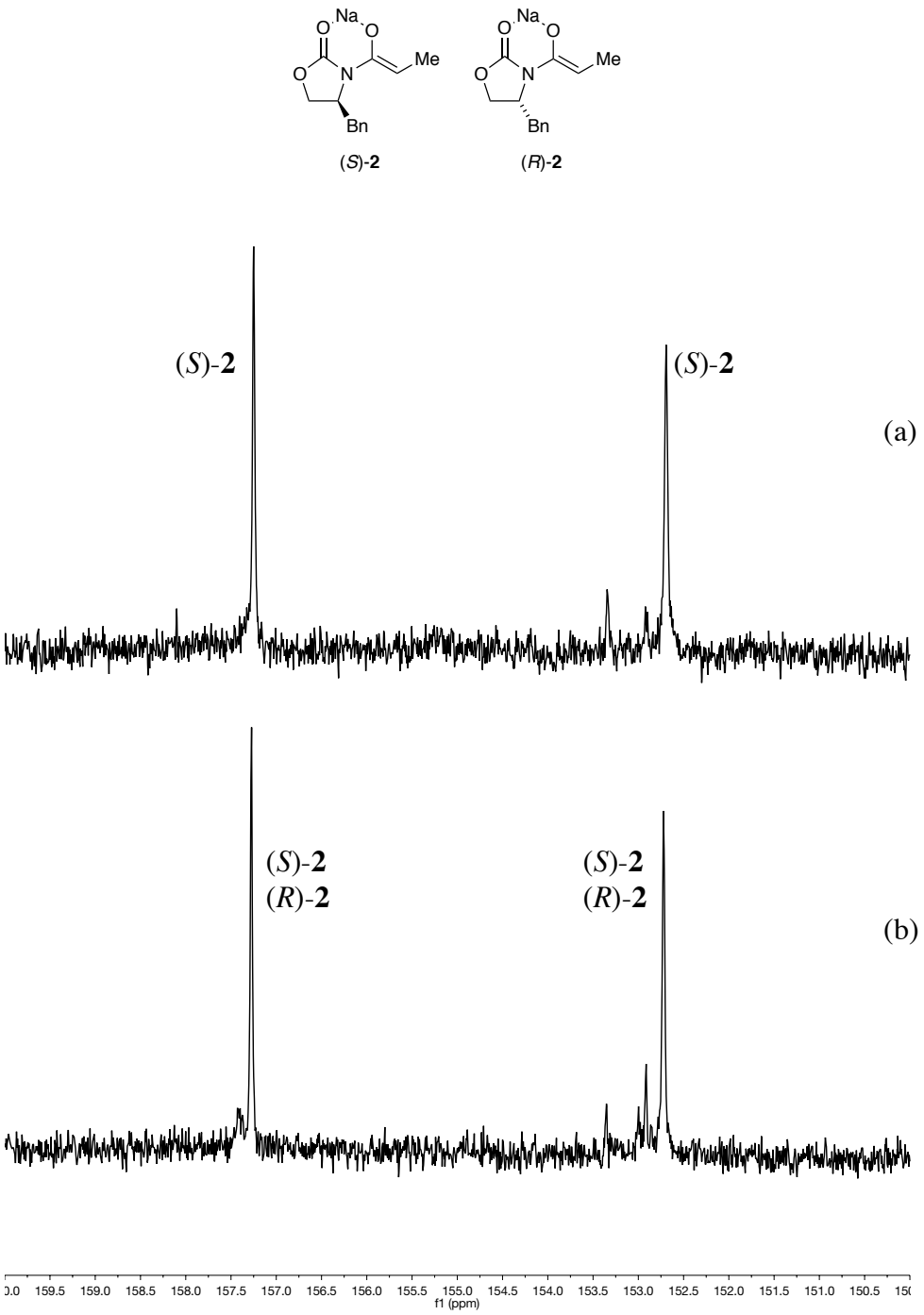


Figure S17. ^{13}C NMR spectra in 1.0 M TMEDA/toluene recorded at –80 °C of (a) 0.20 M (*S*)-**2**; (b) 0.10 M (*R*)-**2** and 0.10 M (*S*)-**2** showing no new resonances that would evidence a heteroaggregate.

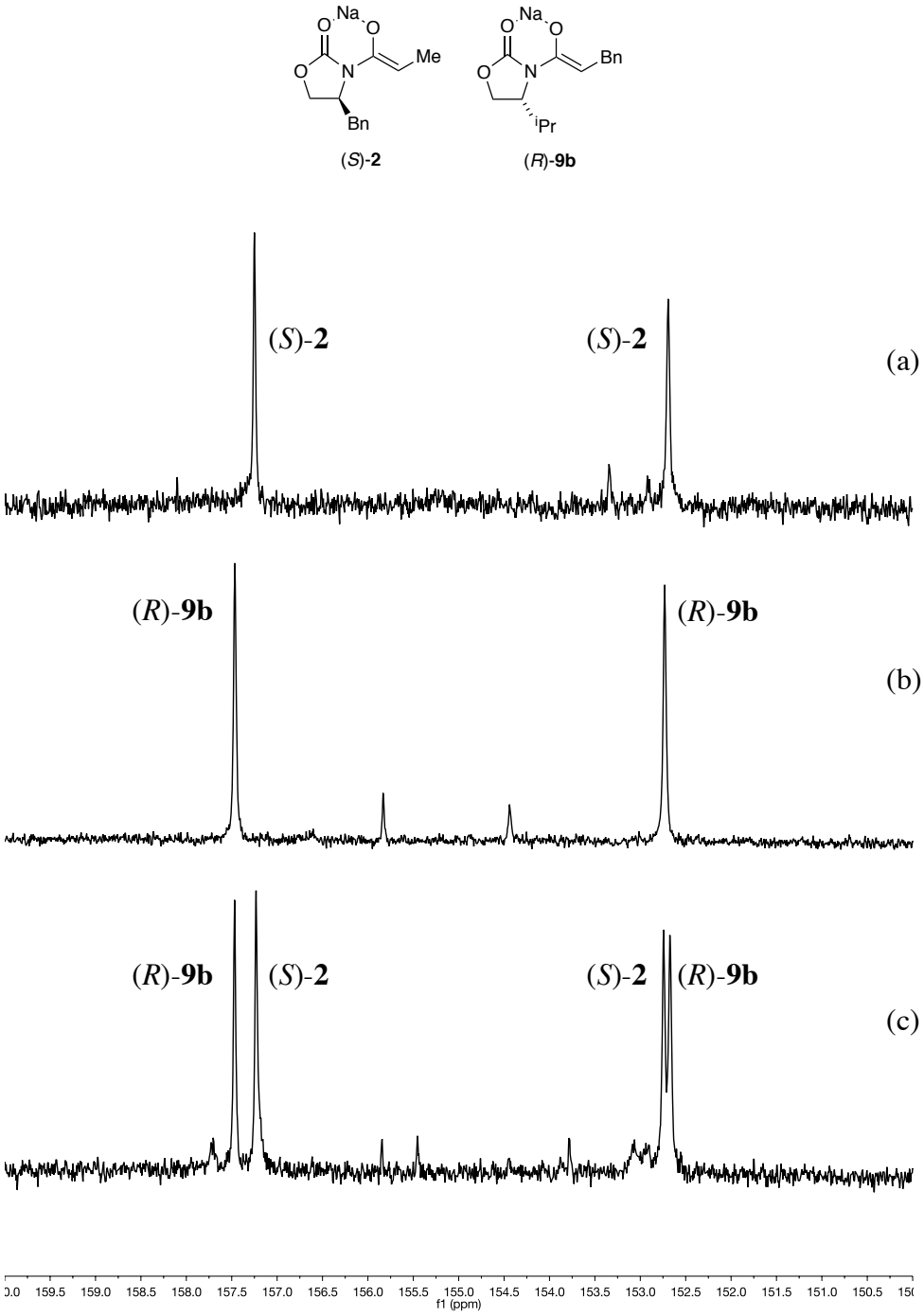


Figure S18. ^{13}C NMR spectra in 1.0 M TMEDA/toluene recorded at –80 °C of (a) 0.20 M (*S*)-**2**; (b) 0.20 M (*R*)-**9b**; (c) 0.10 M (*S*)-**2** and 0.10 M (*R*)-**9b** showing no substantial resonances that would evidence a heteroaggregate.

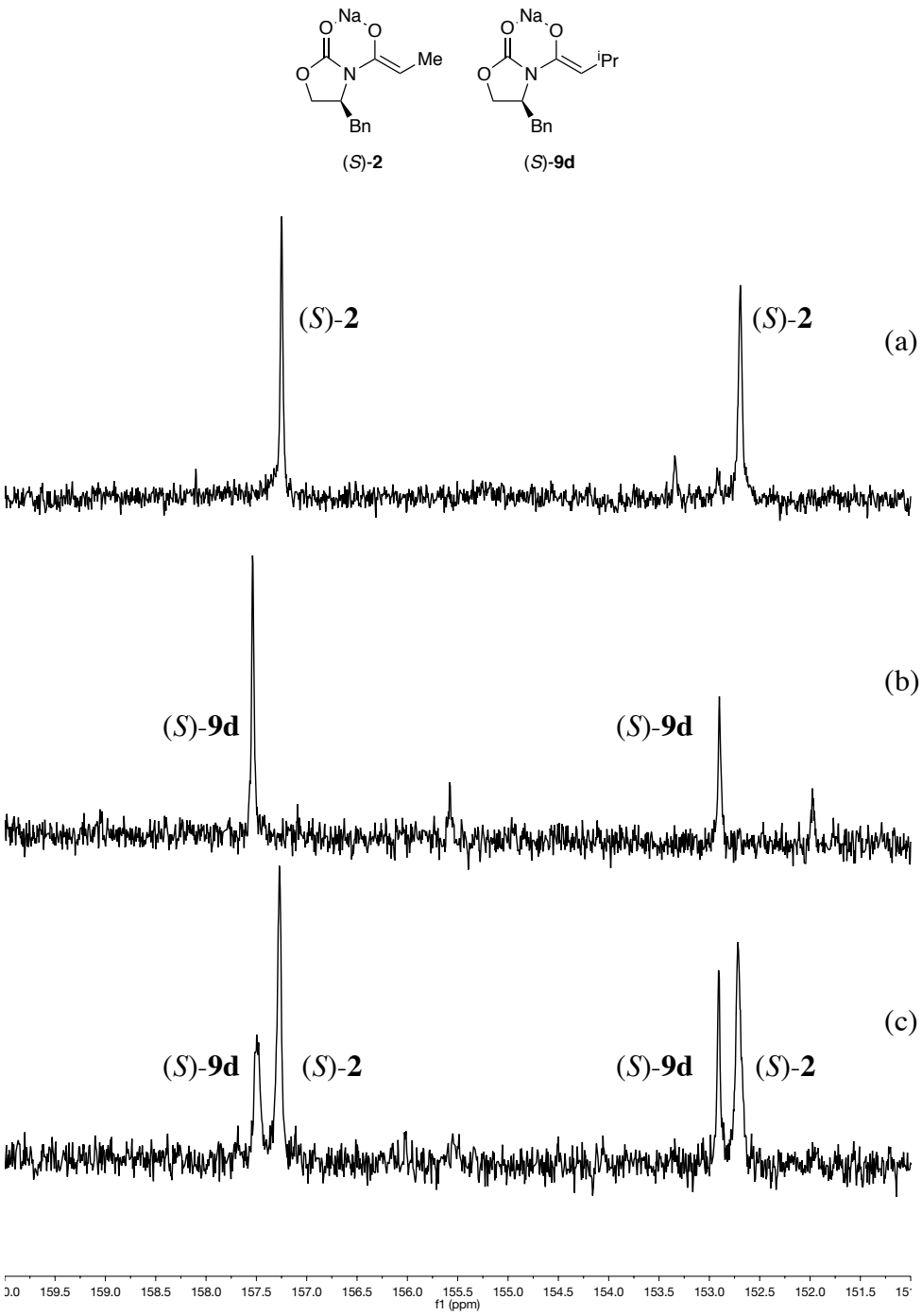


Figure S19. ^{13}C NMR spectra in 1.0 M TMEDA/toluene recorded at –80 °C of (a) 0.20 M (*S*)-**2**; (b) 0.20 M (*S*)-**9d**; (c) 0.10 M (*S*)-**2** and 0.10 M (*S*)-**9d**. No heteroaggregate is observable in (c).

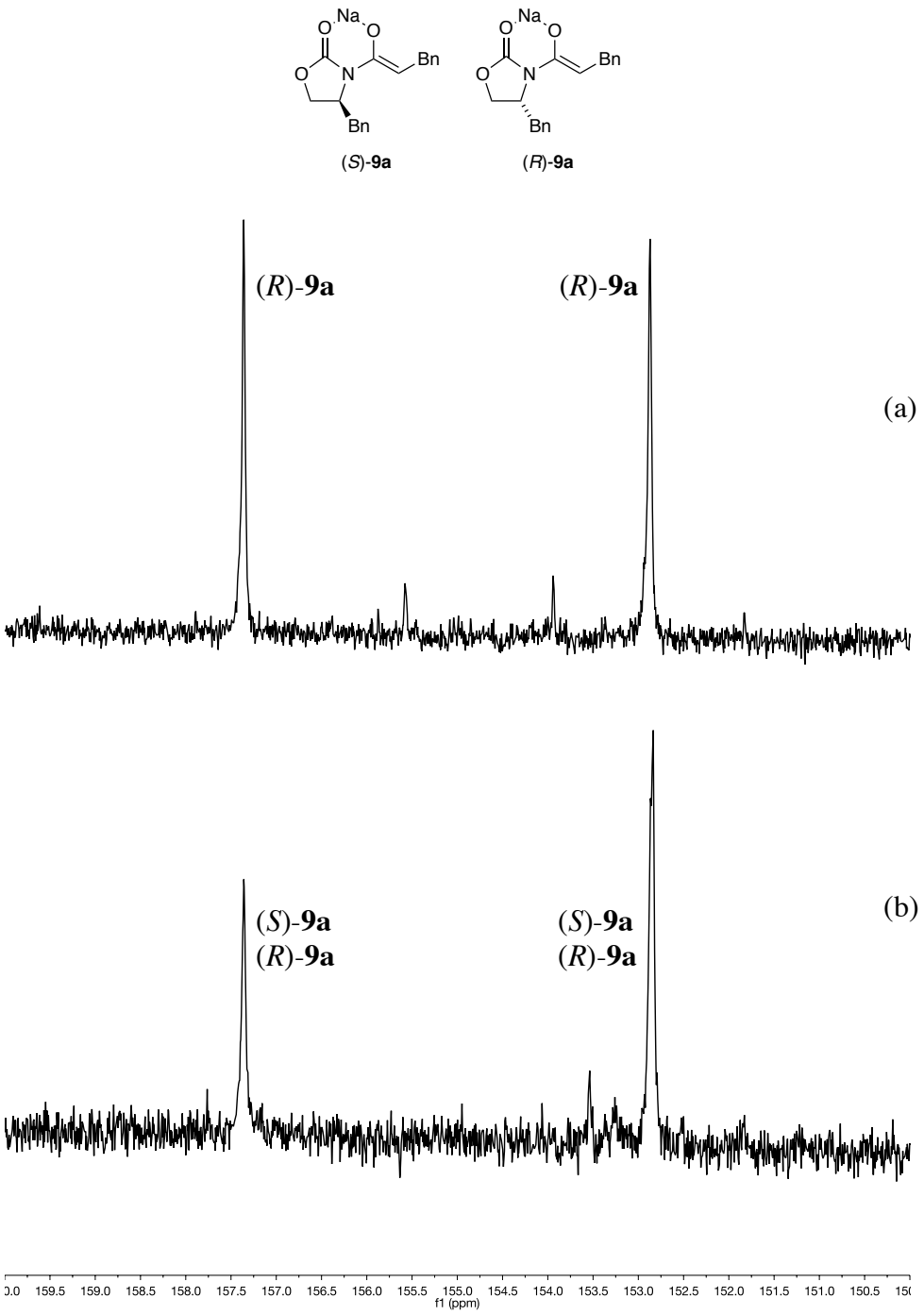


Figure S20. ^{13}C NMR spectra in 1.0 M TMEDA/toluene recorded at –80 °C of (a) 0.20 M (*R*)-**9a**; (b) 0.10 M (*R*)-**9a** and 0.10 M (*S*)-**9a**. No heteroaggregate is observable in (b).

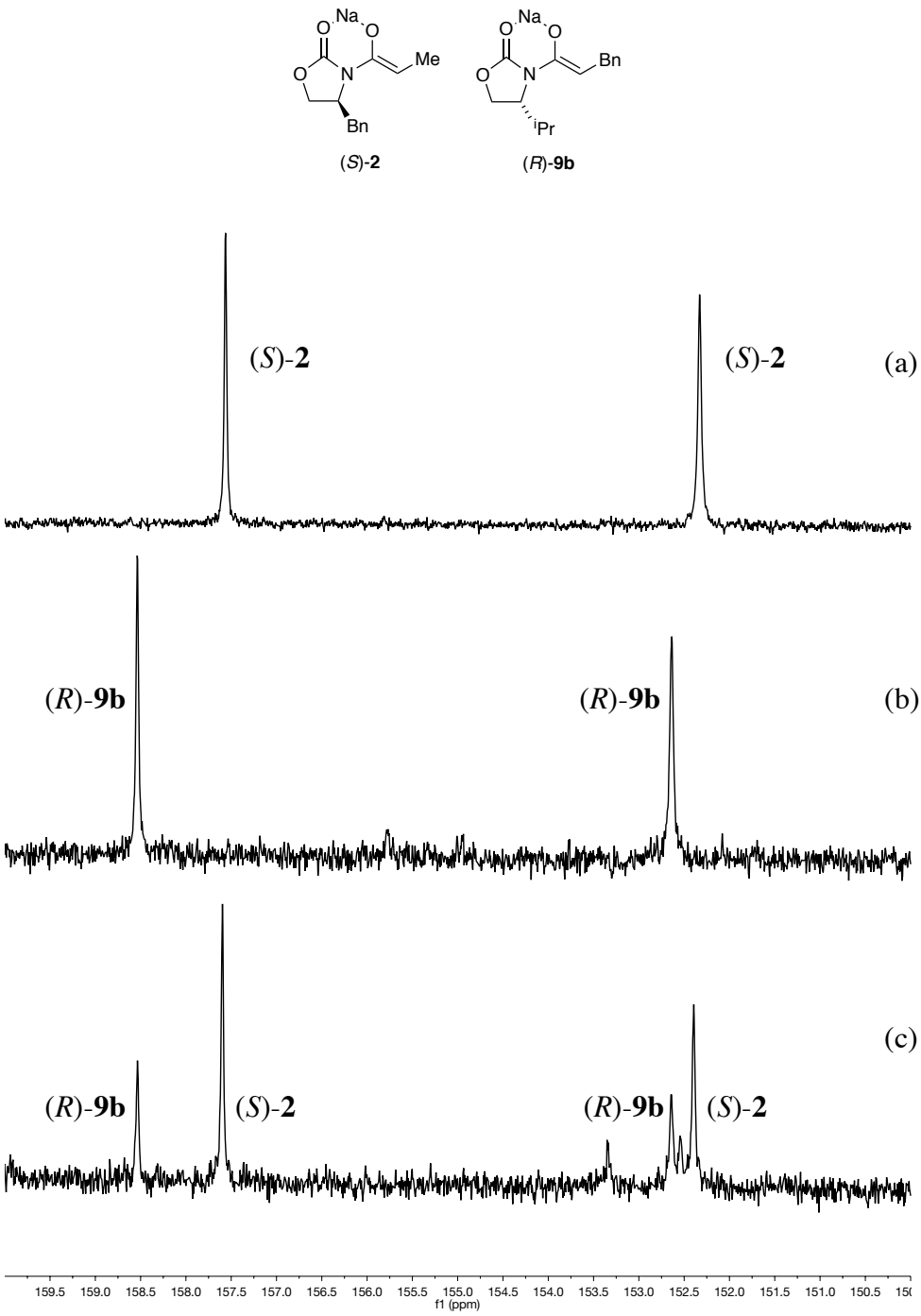


Figure S21. ^{13}C NMR spectra in 1.0 M (*S*,*S*)-TMCDA/toluene recorded at –80 °C of (a) 0.20 M (*S*)-**2**; (b) 0.20 M (*R*)-**9b**; (c) 0.10 M (*S*)-**2** and 0.10 M (*R*)-**9b**.

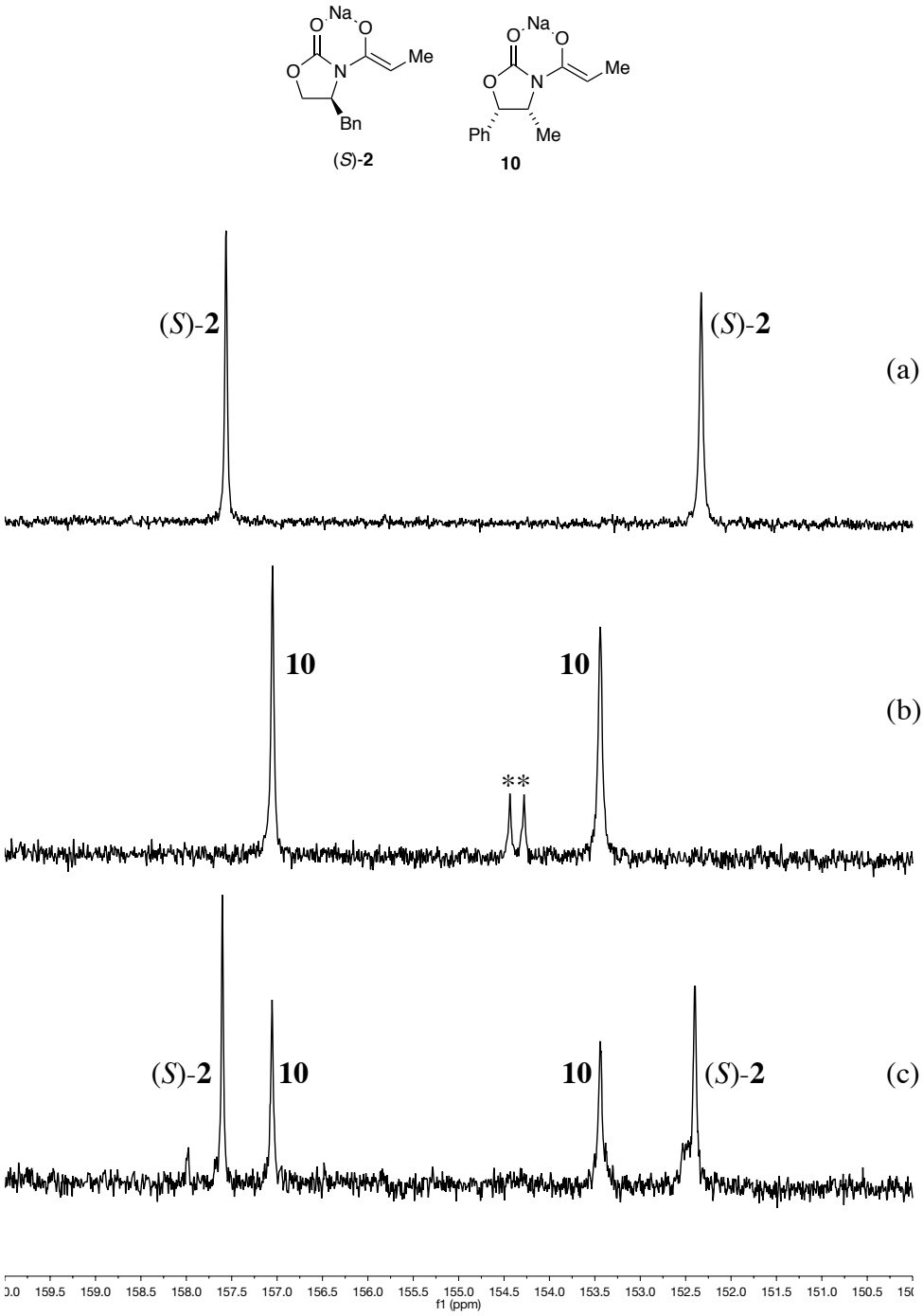


Figure S22. ^{13}C NMR spectra in 1.0 M (*S*,*S*)-TMCDA/toluene recorded at –80 °C of (a) 0.20 M (*S*)-**2**; (b) 0.20 M **10**; (c) 0.10 M (*S*)-**2** and 0.10 M **10**.
* residual mixed dimer **10**-A is present due to extra NaHMDS remaining.

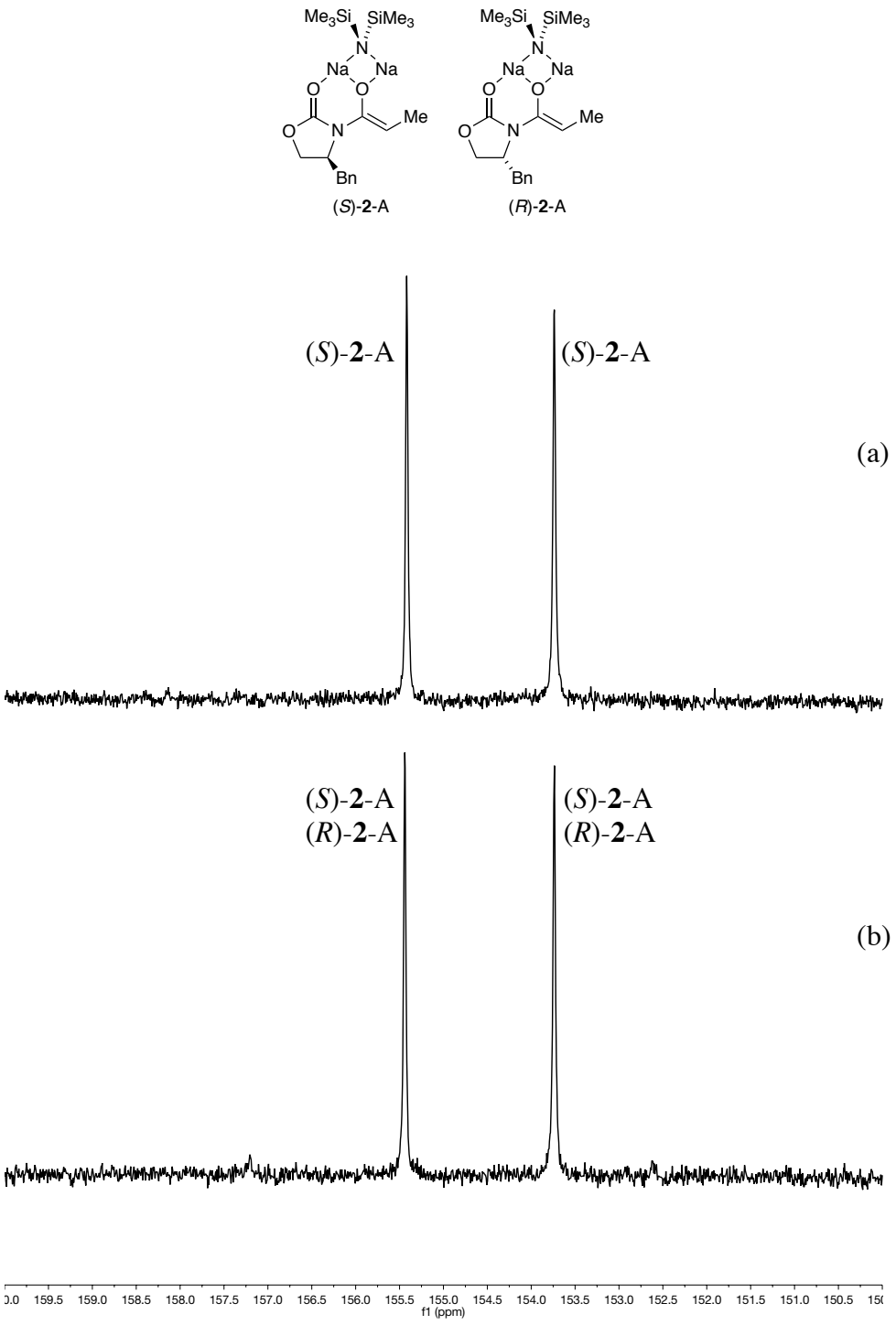


Figure S23. ^{13}C NMR spectra in 1.0 M TMEDA/toluene recorded at –80 °C of (a) 0.20 M (*S*)-**2**-A; (b) 0.10 M (*S*)-**2**-A, 0.10 M (*R*)-**2**-A. Mixing of NaHMDS mixed dimers (*S*)-**2**-A and (*R*)-**2**-A shows no new peak or chemical shift change, consistent with one enolate present in the mixed dimer.

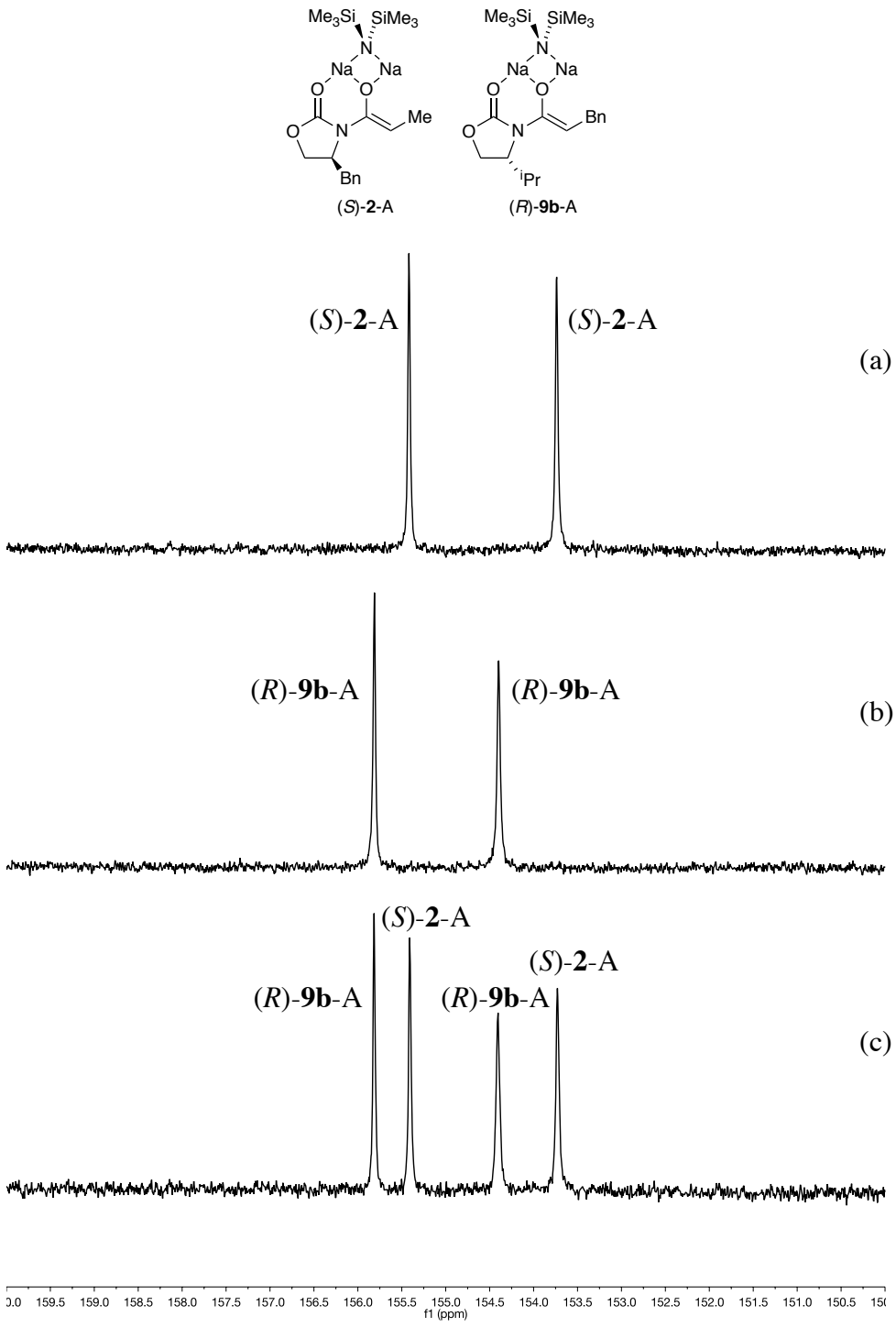


Figure S24. ^{13}C NMR spectra in 1.0 M TMEDA/toluene recorded at –80 °C of (a) 0.20 M (*S*)-**2**-A; (b) 0.20 M (*R*)-**9b**-A; (c) 0.10 M (*S*)-**2**-A, 0.10 M (*R*)-**9b**-A.

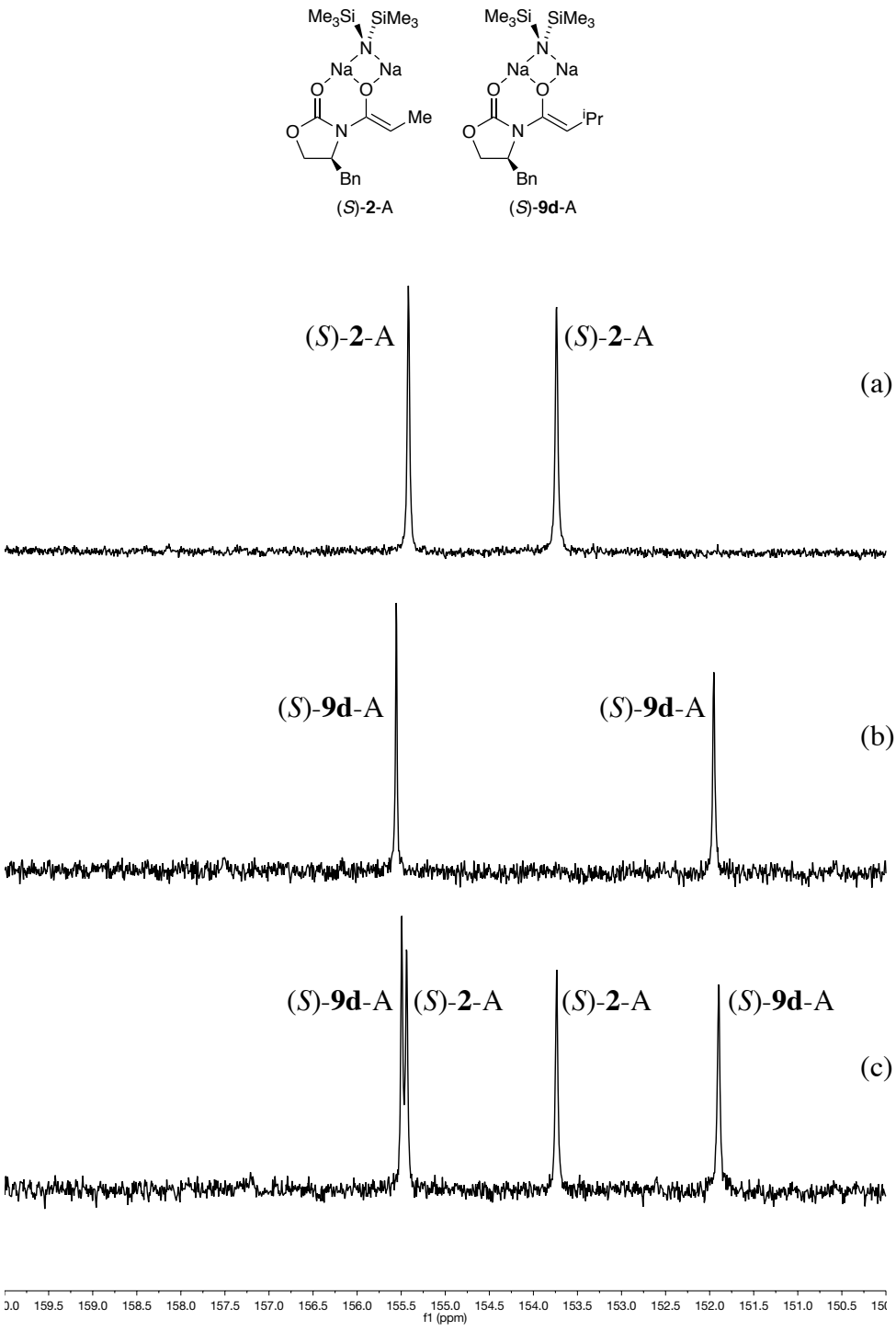


Figure S25. ^{13}C NMR spectra in 1.0 M TMEDA/toluene recorded at –80 °C of (a) 0.20 M (*S*)-**2**-A; (b) 0.20 M (*S*)-**9d**-A; (c) 0.10 M (*S*)-**2**-A, 0.10 M (*S*)-**9d**-A.

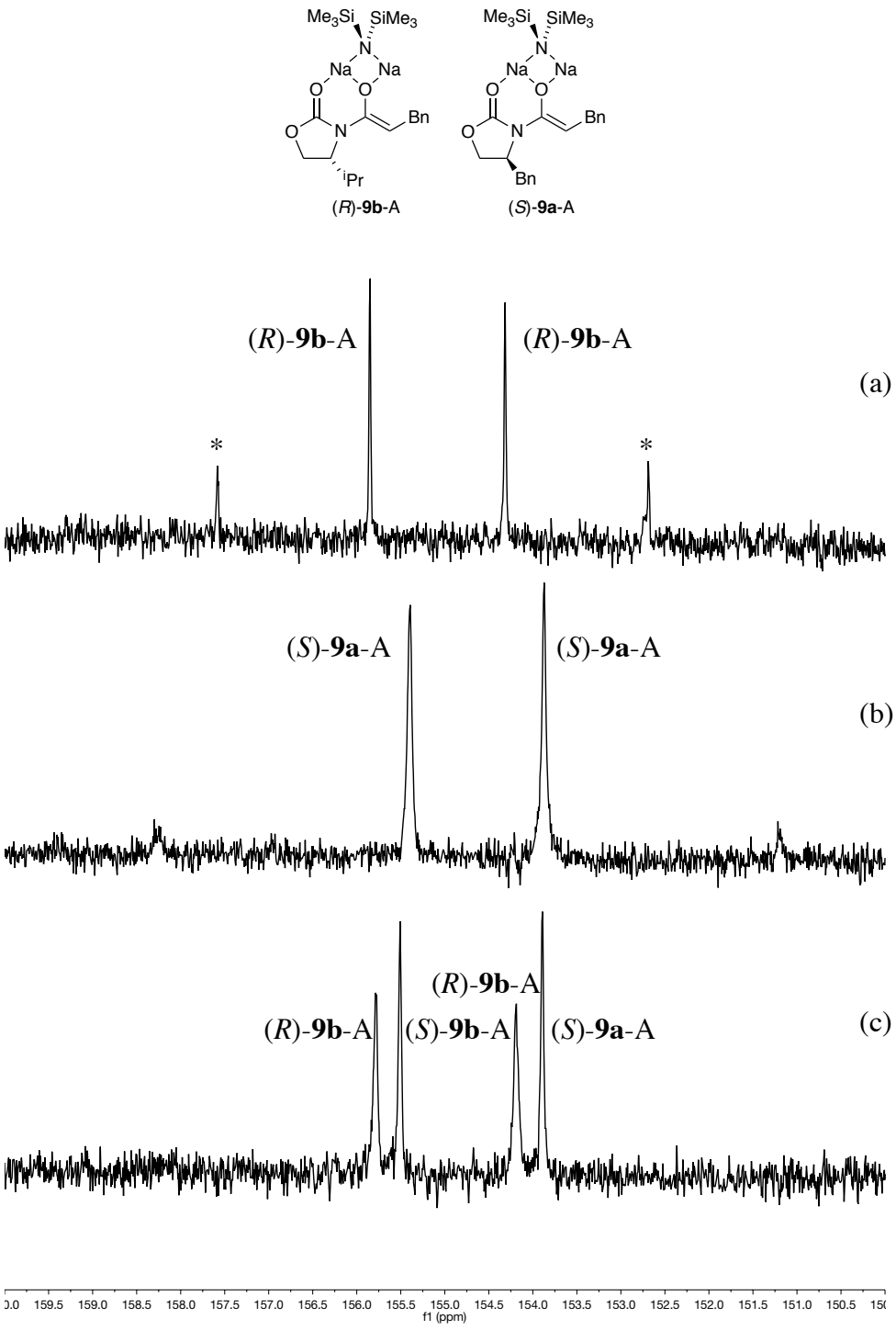


Figure S26. ^{13}C NMR spectra in 1.0 M TMEDA/toluene recorded at –80 °C of (a) 0.20 M (*R*)-**9b**-A; (b) 0.20 M (*S*)-**9a**-A; (c) 0.10 M (*R*)-**9b**-A, 0.10 M (*S*)-**9a**-A.
* homoaggregate residue.

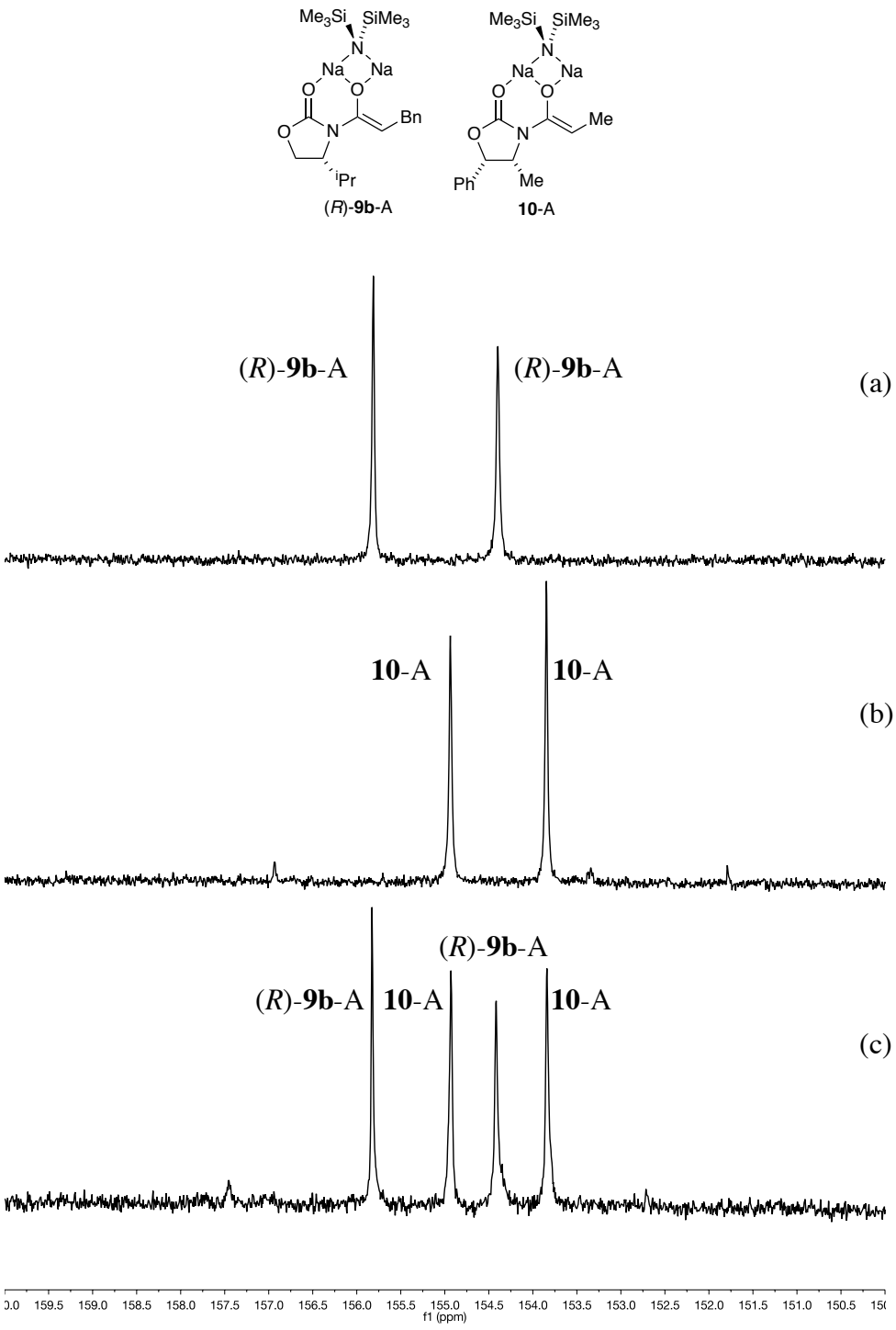


Figure S27. ^{13}C NMR spectra in 1.0 M TMEDA/toluene recorded at –80 °C of (a) 0.20 M (*R*)-**9b**-A; (b) 0.20 M **10**-A; (c) 0.10 M (*S*)-**9b**-A, 0.10 M **10**-A.

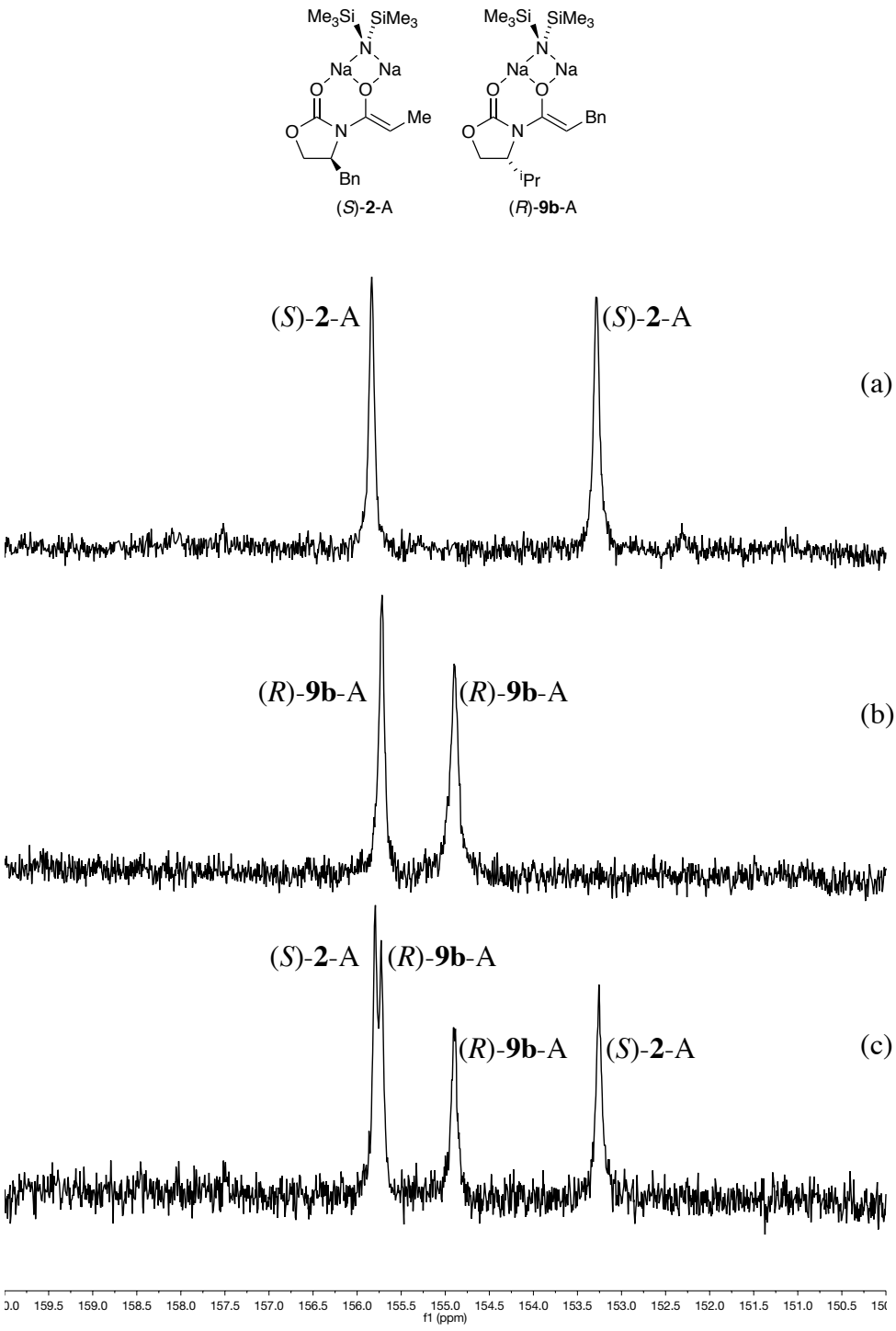


Figure S28. ^{13}C NMR spectra in 1.0 M (*S*,*S*)-TMCDA/toluene recorded at –80 °C of (a) 0.20 M (*S*)-**2**-A; (b) 0.20 M (*R*)-**9b**-A; (c) 0.10 M (*S*)-**2**-A, 0.10 M (*R*)-**9b**-A.

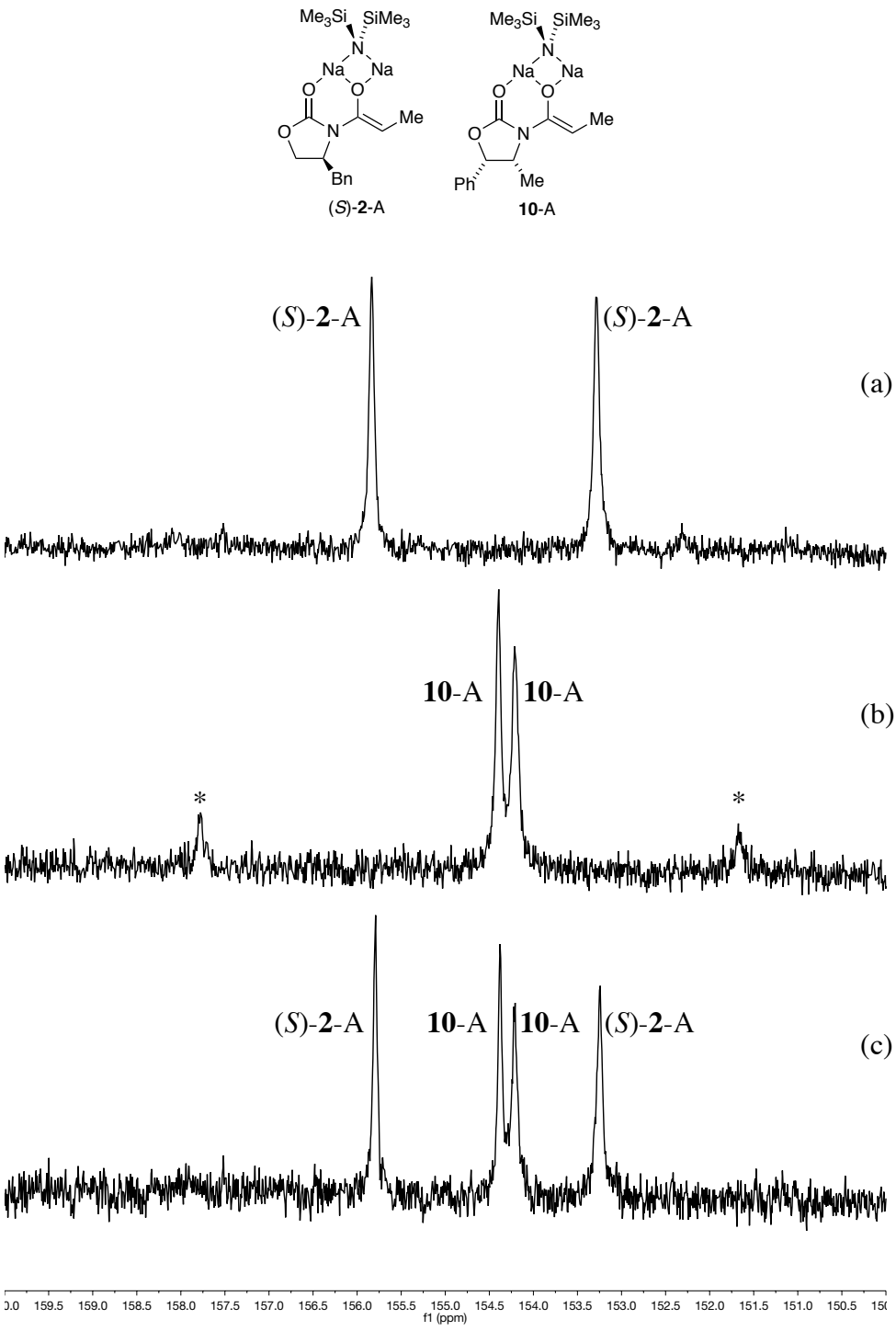


Figure S29. ^{13}C NMR spectra in 1.0 M (*S*,*S*)-TMCDA/toluene recorded at –80 °C of (a) 0.20 M (*S*)-**2**-A; (b) 0.20 M **10**-A; (c) 0.10 M (*S*)-**2**-A, 0.10 M **10**-A.
* homoaggregate residue

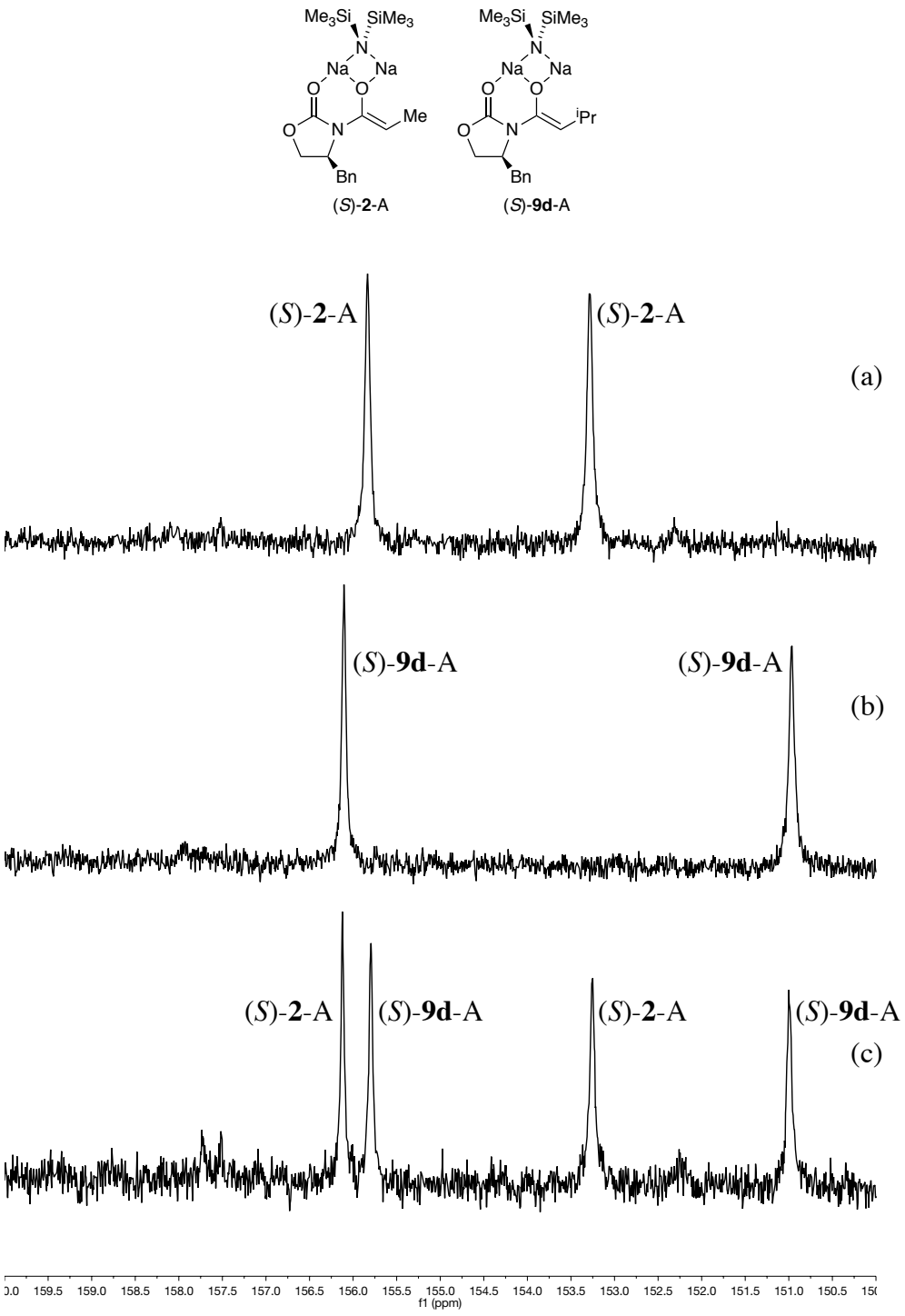


Figure S30. ^{13}C NMR spectra in 1.0 M (*S*,*S*)-TMCDA/toluene recorded at –80 °C of (a) 0.20 M (*S*)-**2**-A; (b) 0.20 M (*S*)-**9d**-A; (c) 0.10 M (*S*)-**2**-A, 0.10 M (*S*)-**9d**-A.

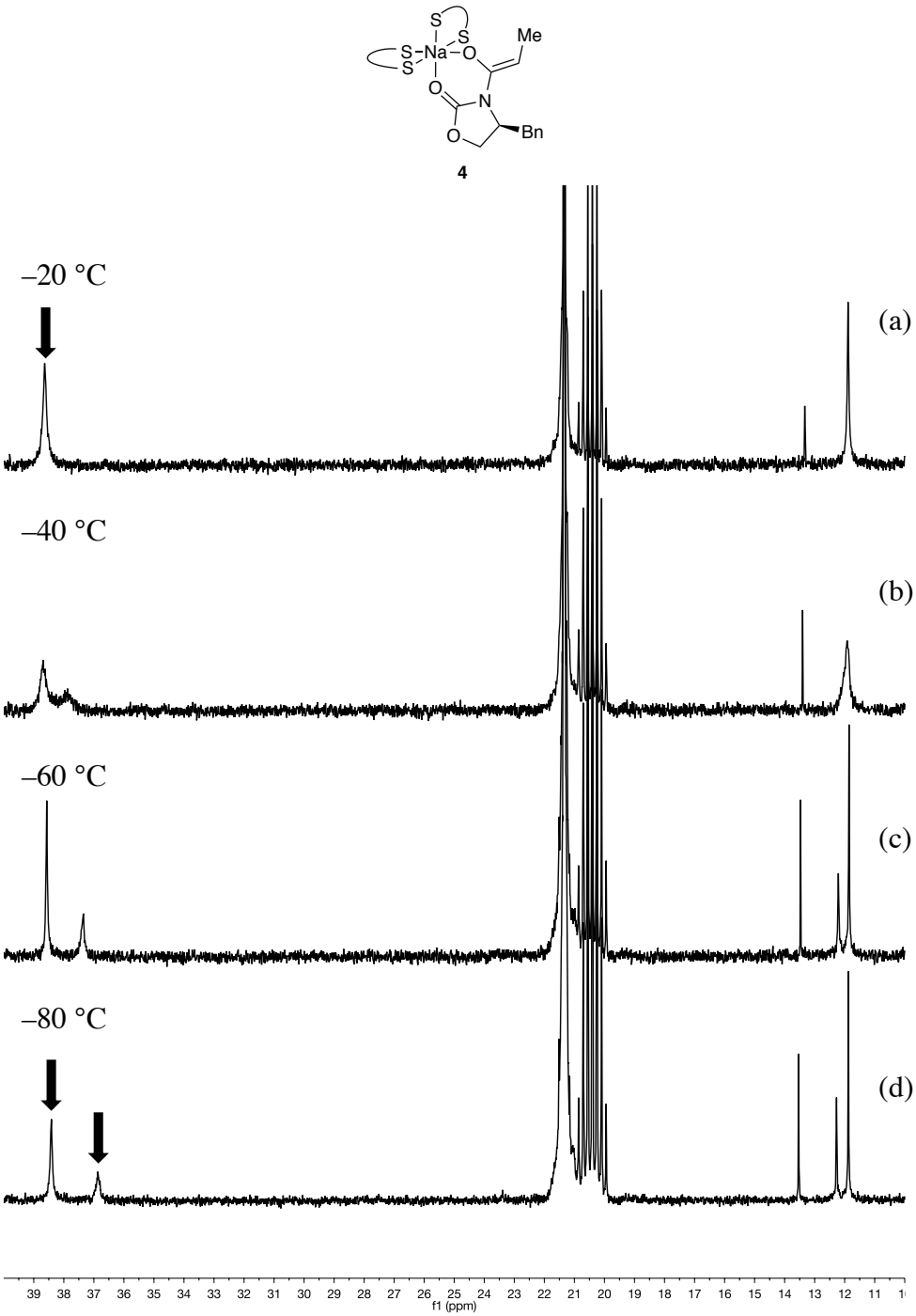


Figure S31. ^{13}C NMR spectra of 0.20 M **4** and 0.10 M NaHMDS in 1.0 M TMEDA/toluene recorded at (a) –20 °C; (b) –40 °C; (c) –60 °C; (d) –80 °C. Gradually increasing the temperature of a tube consisting of shows coalescence at approximately –20 °C.

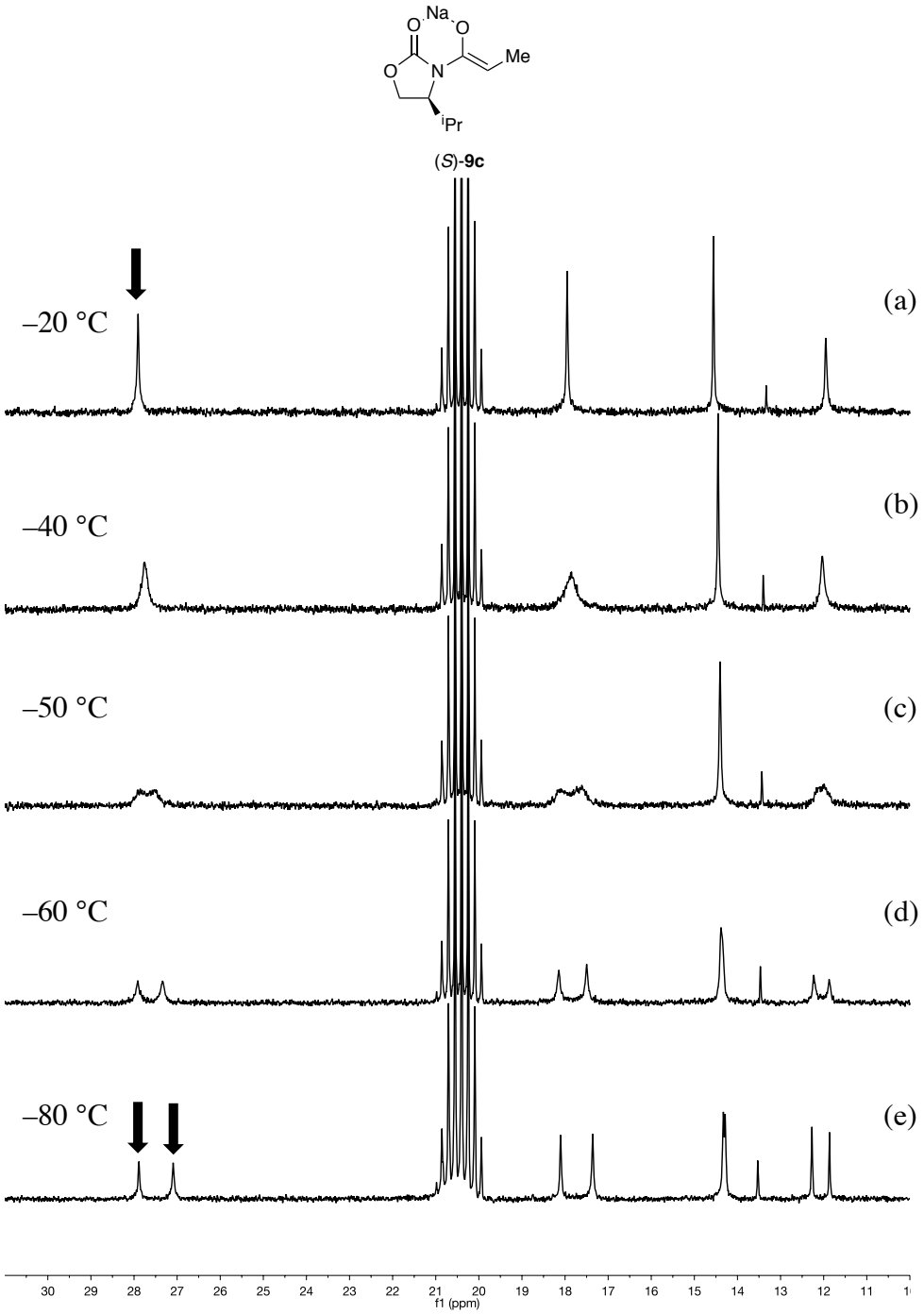


Figure S32. ^{13}C NMR spectra of 0.20 M (*S*)-**9c** and 0.10 M NaHMDS in 1.0 M TMEDA/toluene recorded at (a) –20 °C; (b) –40 °C; (c) –50 °C; (d) –60 °C; (e) –80 °C.

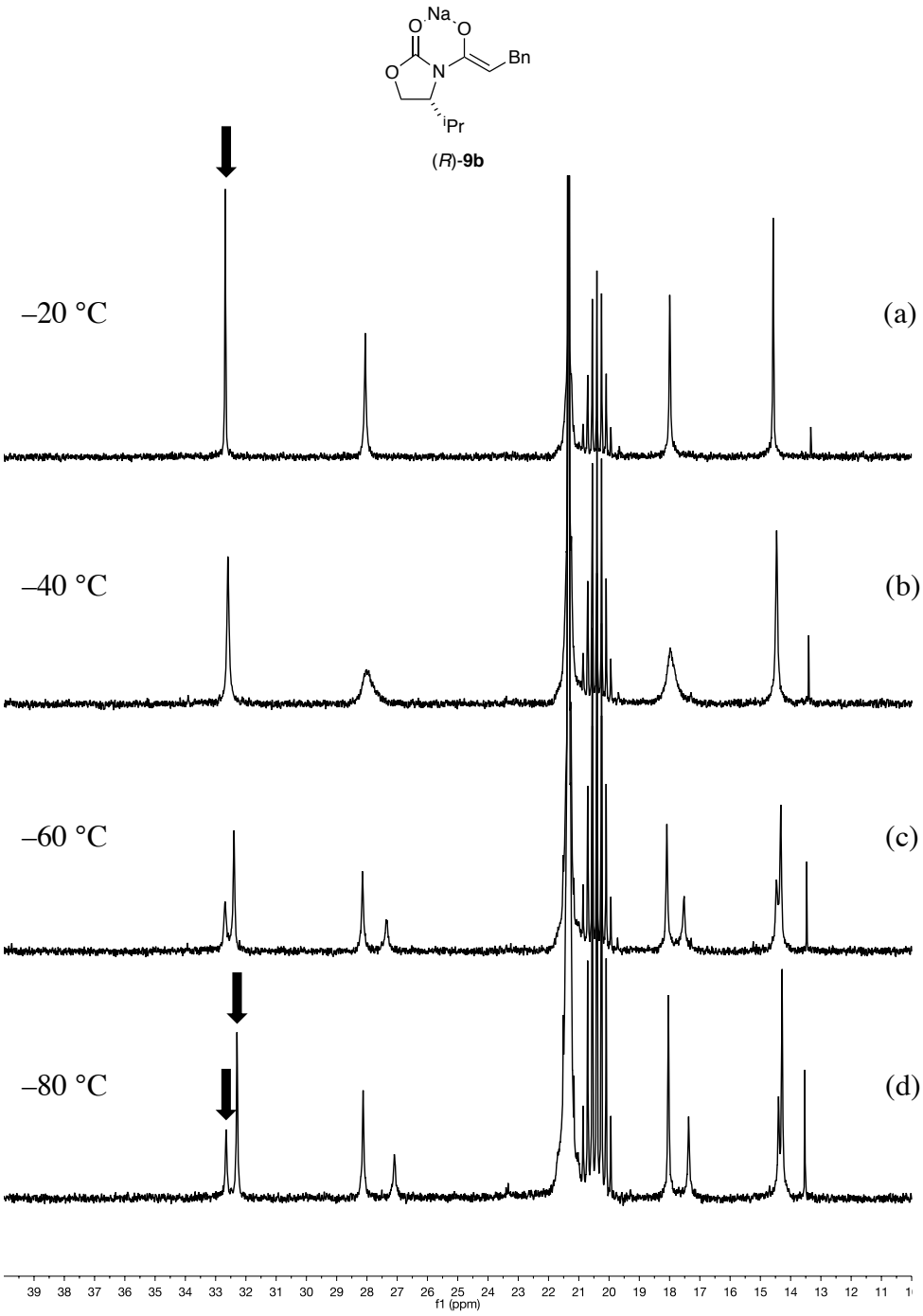


Figure S33. ^{13}C NMR spectra of 0.20 M (*R*)-**9b** and 0.10 M NaHMDS in 1.0 M TMEDA/toluene recorded at (a) –20 °C; (b) –40 °C; (c) –60 °C; (d) –80 °C.

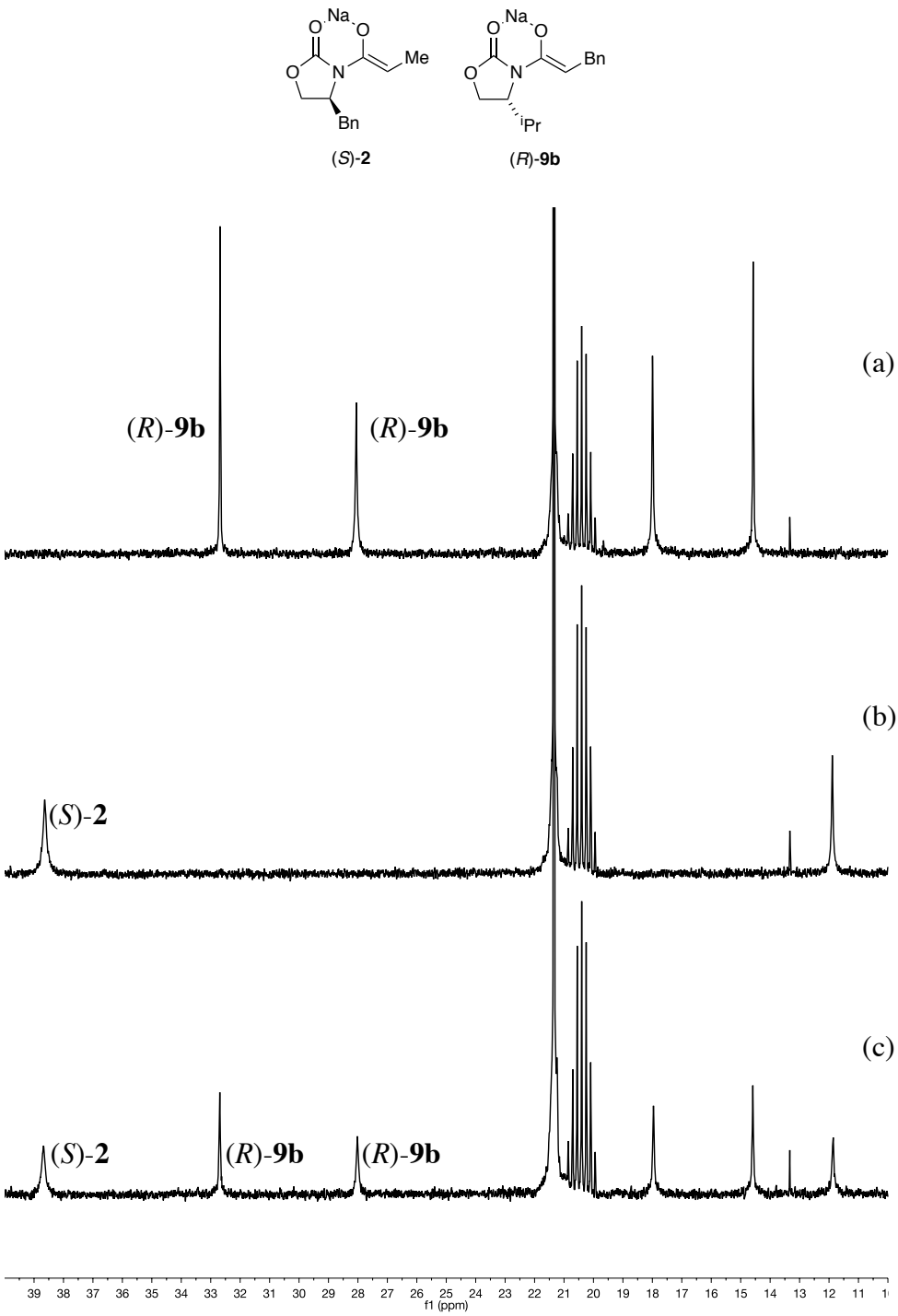


Figure S34. ^{13}C NMR spectra in 1.0 M TMEDA/toluene recorded at –20 °C of 0.10 M NaHMDS and (a) 0.20 M (*R*)-**9b**; (b) 0.20 M (*S*)-**2**; (c) 0.10 M (*R*)-**9b**, 0.10 M (*S*)-**2**. Mixing (*S*)-**2** and (*R*)-**9b** enolate at a temperature in which inter-aggregate exchange between monomer and NaHMDS mixed dimer is fast shows no chemical shift change.

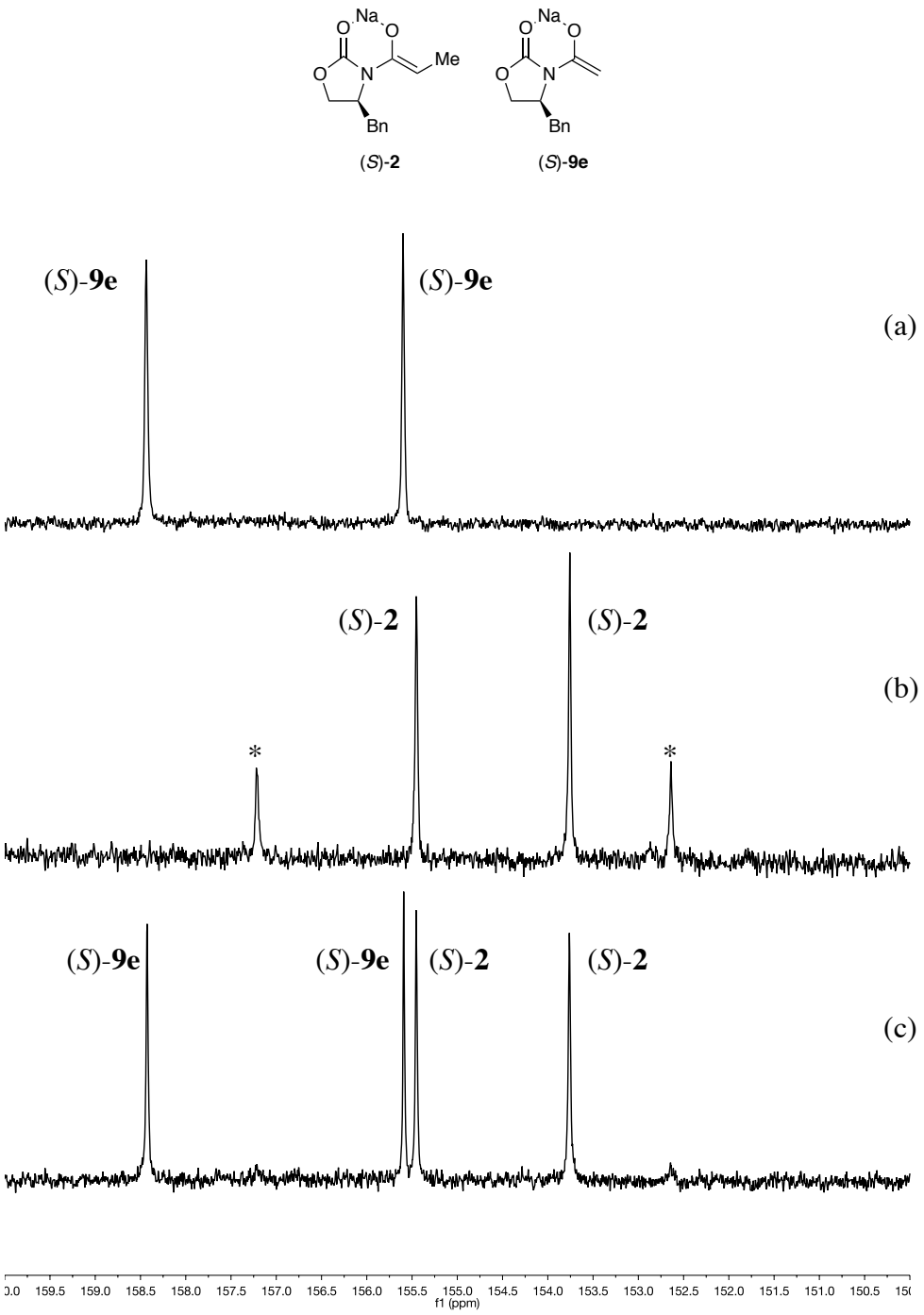


Figure S35. ^{13}C NMR spectra in 1.0 M TMEDA/toluene recorded at –80 °C of 0.10 M NaHMDS and (a) 0.20 M (*S*)-**9e**; (b) 0.20 M (*S*)-**2**; (c) 0.10 M (*S*)-**9e**, 0.10 M (*S*)-**2**. * homoaggregate residue

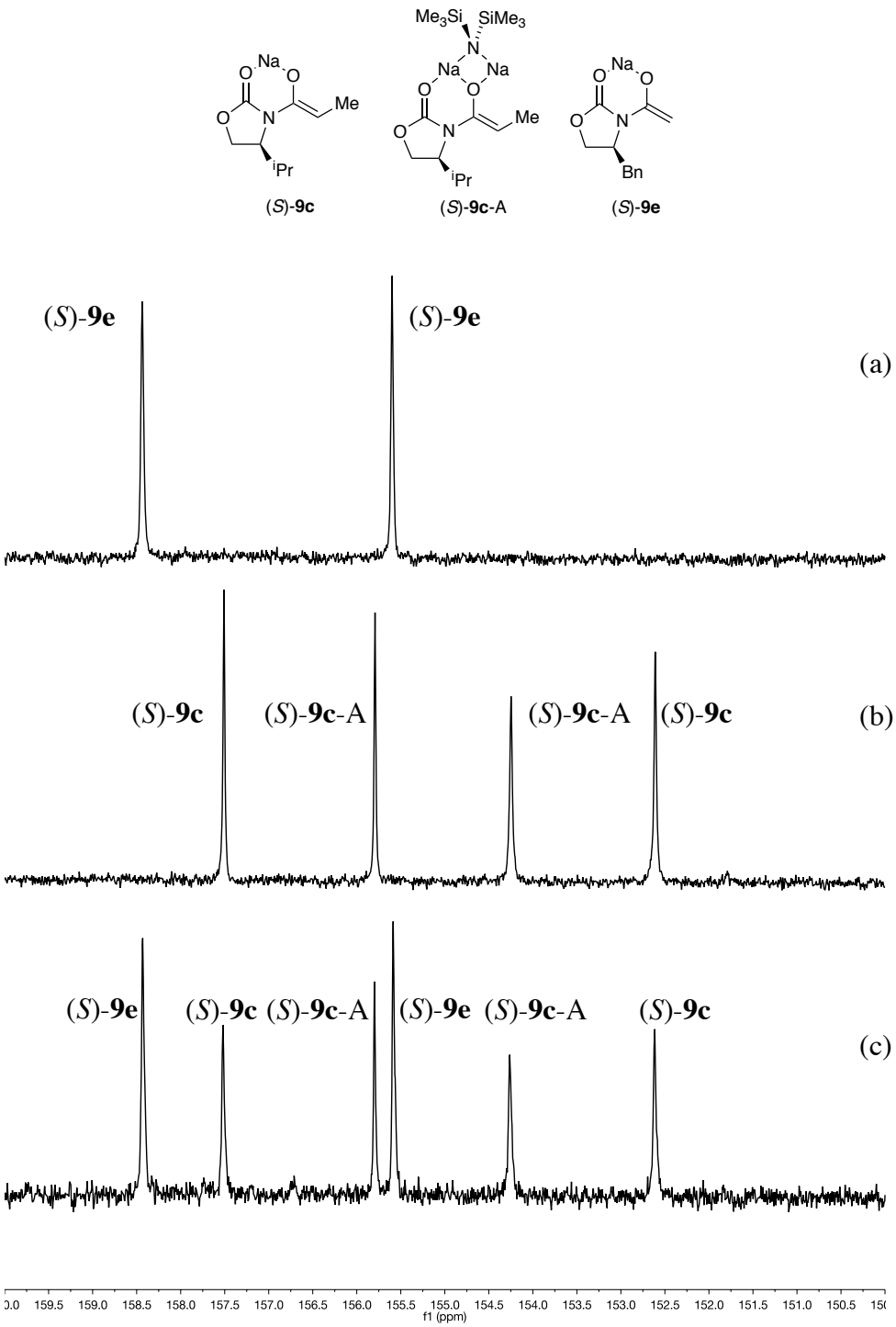


Figure S36. ^{13}C NMR spectra in 1.0 M TMEDA/toluene recorded at –80 °C of 0.10 M NaHMDS and (a) 0.20 M (*S*)-**9e**; (b) 0.20 M (*S*)-**9c**; (c) 0.10 M (*S*)-**9e**, 0.10 M (*S*)-**9c**.

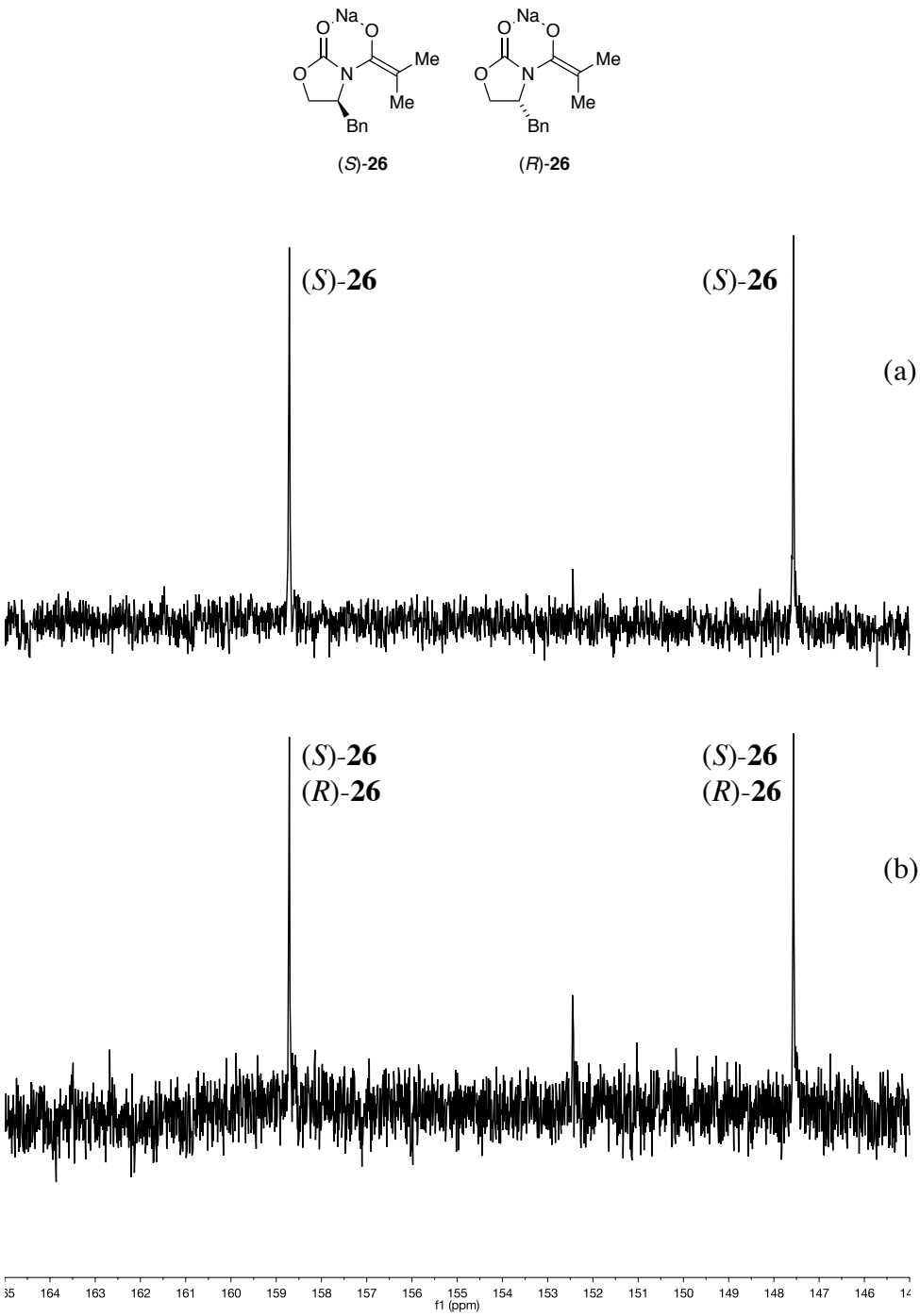


Figure S37. ^{13}C NMR spectra in 1.0 M TMEDA/toluene recorded at –80 °C of (a) 0.20 M (*S*)-**26**; (b) 0.10 M (*S*)-**26**, 0.10 M (*R*)-**26**.
The tube was aged at 0 °C for 10 minutes to complete the enolization of (*S*)-**26**, leading to some decomposition.

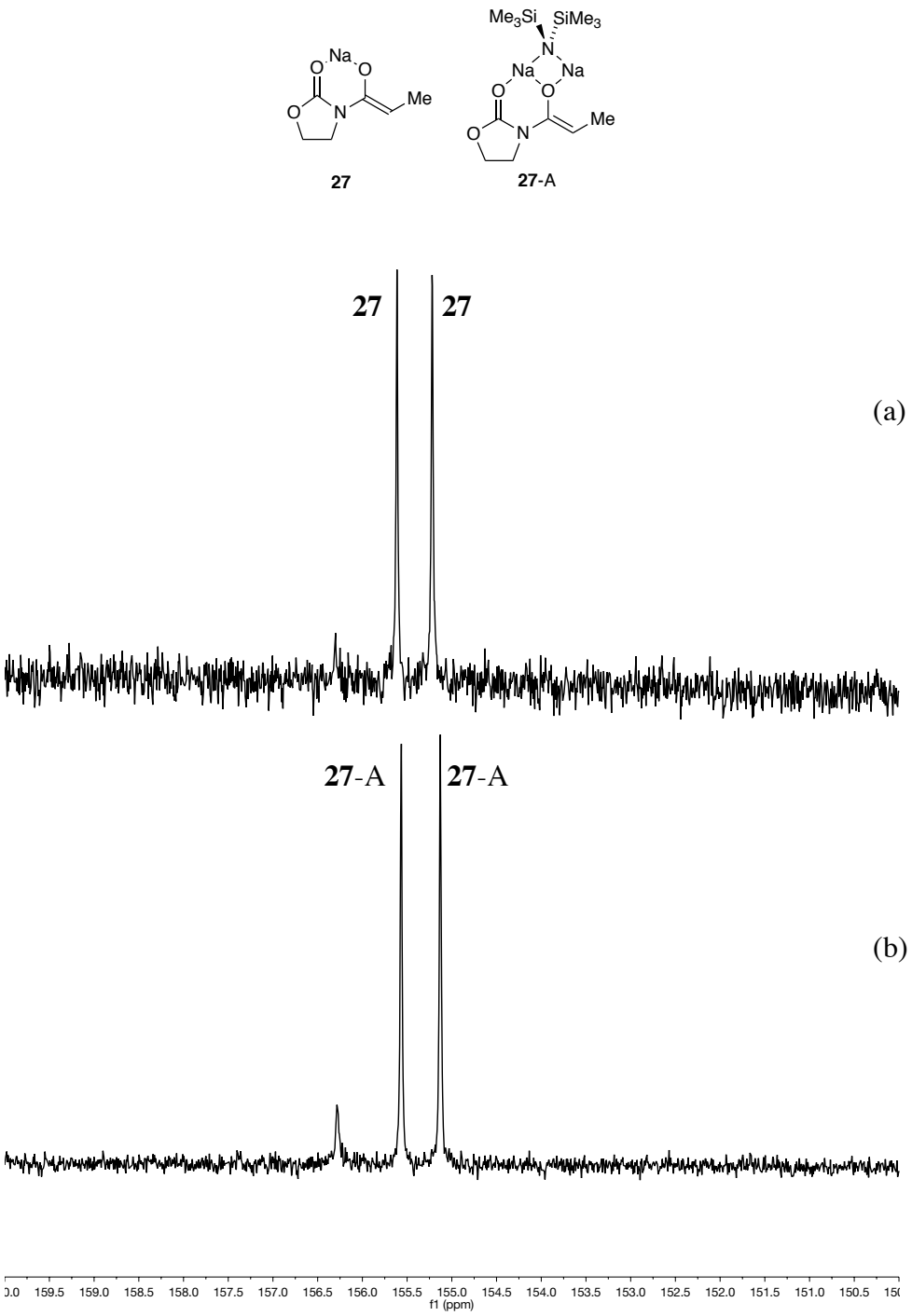


Figure S38. ^{13}C NMR spectra in 1.0 M TMEDA/toluene recorded at –80 °C of (a) 0.20 M **27**; (b) 0.20 M **27**-A.

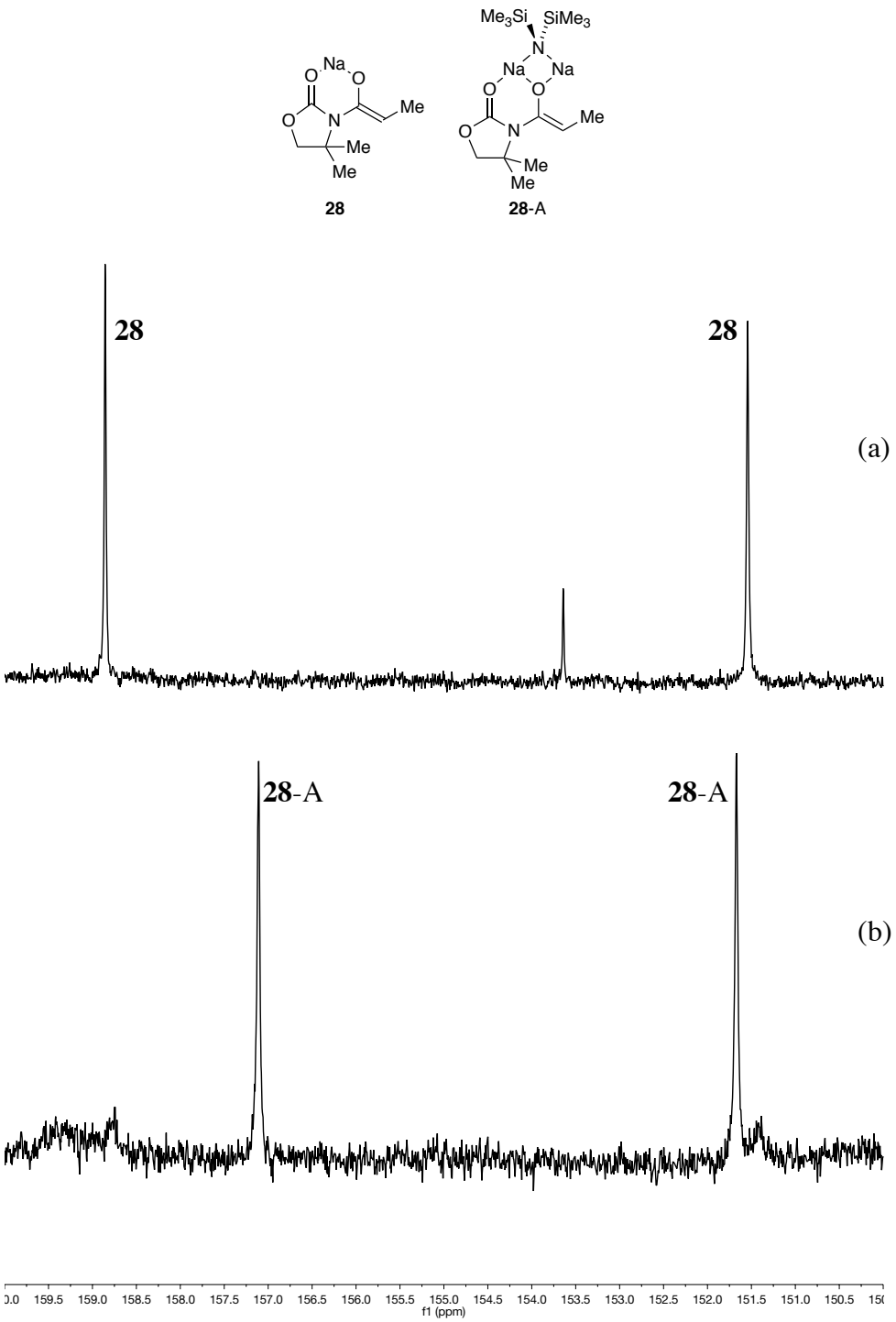


Figure S39. ^{13}C NMR spectra in 1.0 M TMEDA/toluene recorded at –80 °C of (a) 0.20 M **28**; (b) 0.20 M **28**-A.

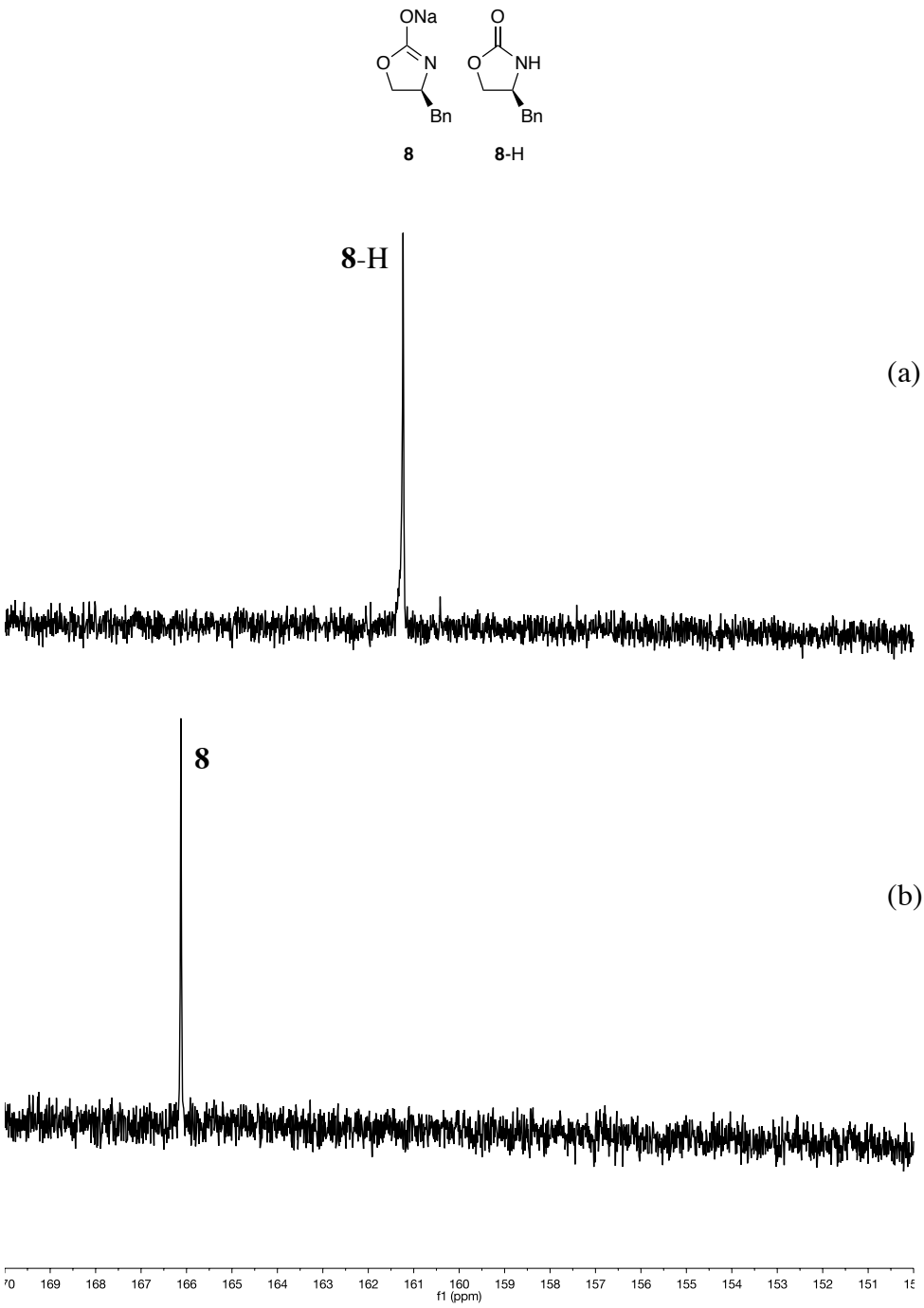


Figure S40. ^{13}C NMR spectra in 1.0 M TMEDA/toluene recorded at –80 °C of (a) 0.20 M **8**-H; (b) 0.20 M **8**. Enolate **8** often precipitates out of solution.

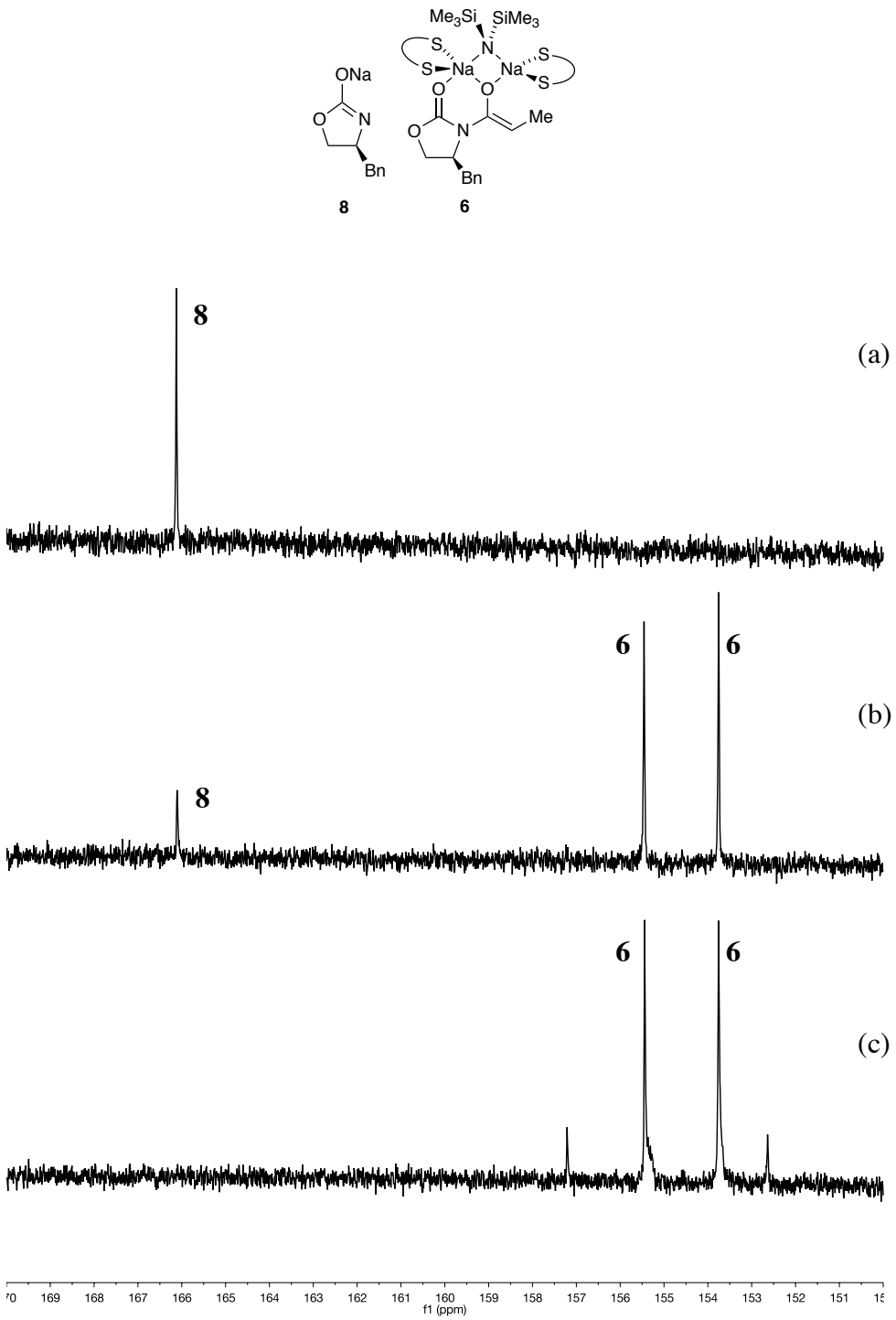


Figure S41. ^{13}C NMR spectra of (a) 0.20 M **8**; (b) 0.10 M **8** and 0.10 M **6**; (c) 0.20 M **6** and 0.10 M NaHMDS in 1.0 M TMEDA in toluene recorded at –80 °C. No evidence of mixed aggregates are observable.

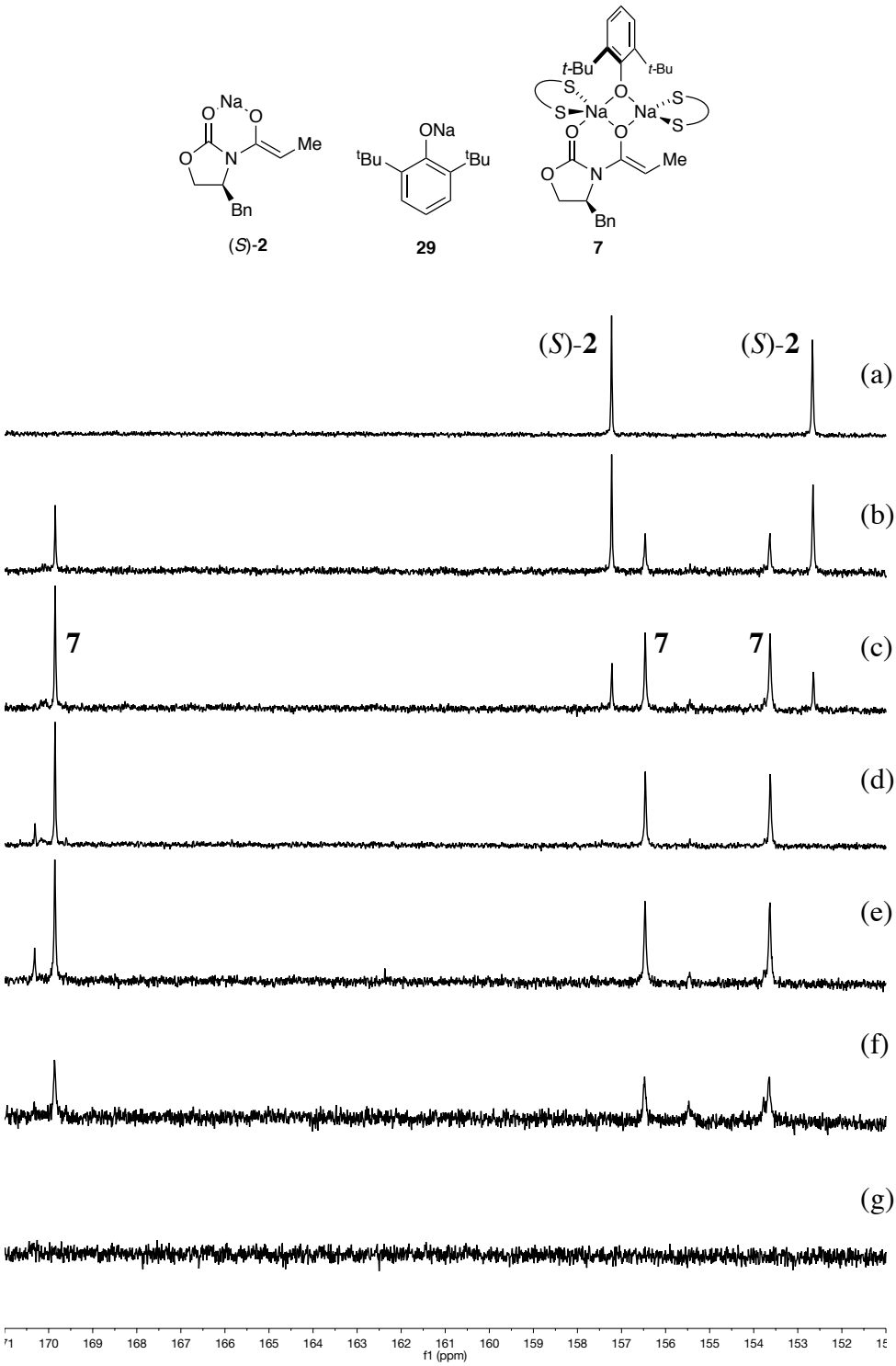


Figure S42. ^{13}C NMR spectra of (a) 0.30 M (*S*)-**2**; (b) 0.25 M (*S*)-**2** and 0.05 M **29**; (c) 0.20 M (*S*)-**2** and 0.10 M **29**; (d) 0.15 M (*S*)-**2** and 0.15 M **29**; (e) 0.10 M (*S*)-**2** and 0.20 M **29**; (f) 0.05 M (*S*)-**2** and 0.25 M **29**; (g) 0.30 M **29** in 1.0 M TMEDA in toluene recorded at –80 °C. Phenolate **29** forms a mixed dimer with (*S*)-**2** quantitatively. Phenolate **29** is insoluble in the absence of (*S*)-**2**. .

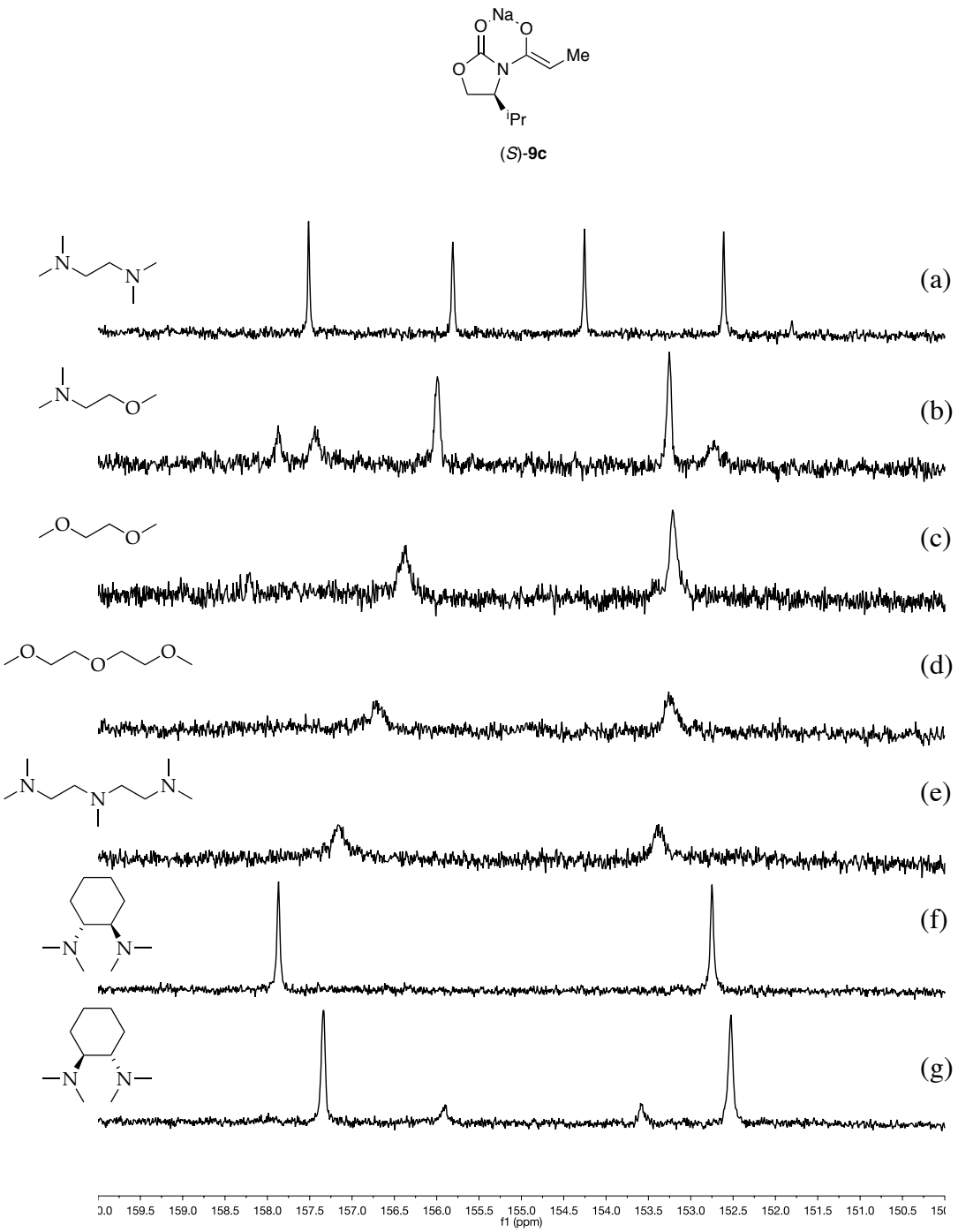


Figure S43. ^{13}C NMR spectra of 0.20 M (*S*)-**9c** and 0.10 M NaHMDS in 1.0 M (a) TMEDA; (b) *N*,*N*-dimethyl-2-methoxyethylamine; (c) DME; (d) diglyme; (e) PMDTA; (f) (*R*,*R*)-TMCDA; (g) (*S*,*S*)-TMCDA in toluene recorded at –80 °C.

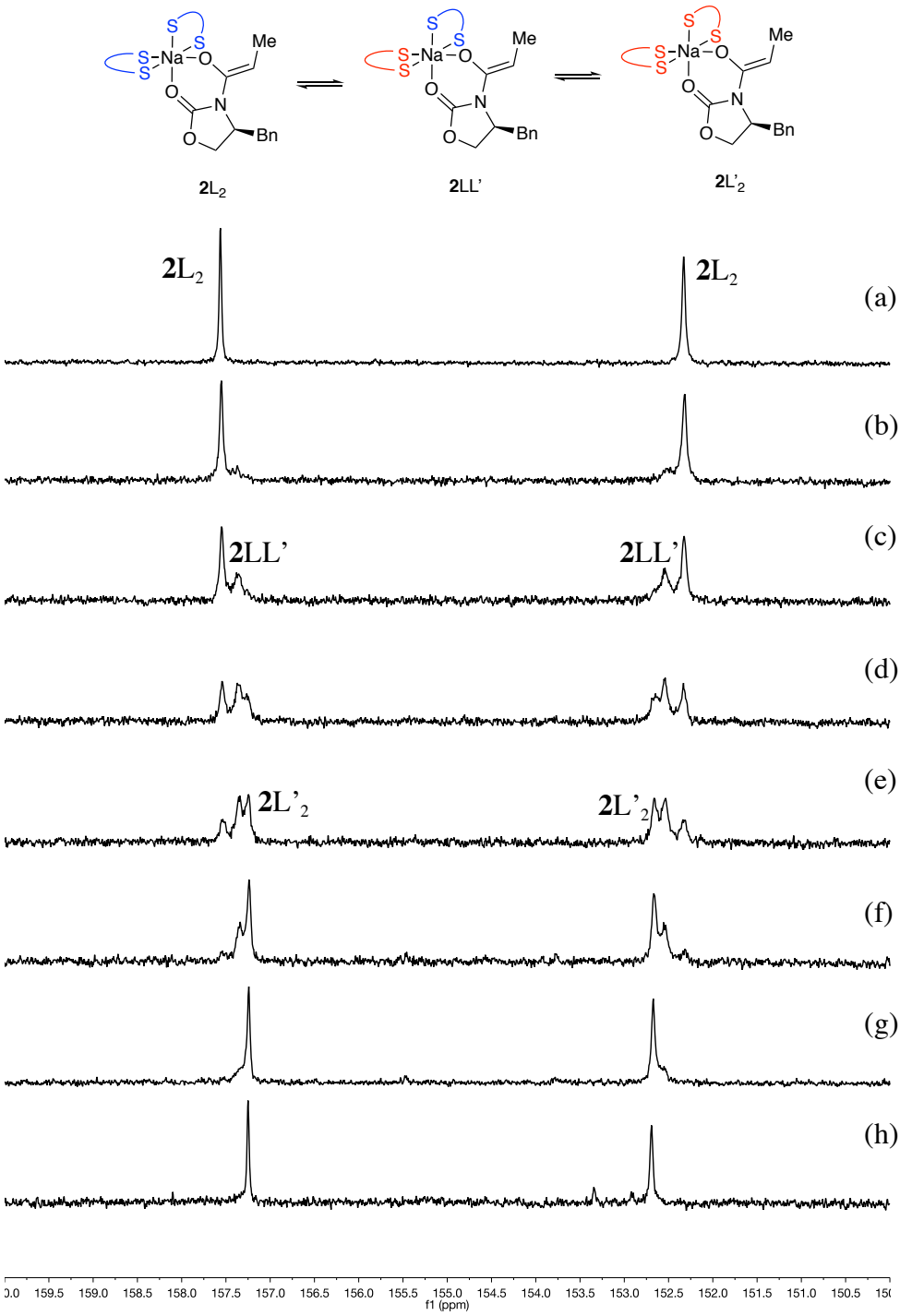


Figure S44. ^{13}C NMR spectra of 0.20 M **4** and TMEDA and (*S*,*S*)-TMCDA (1.0 total ligand titer) in toluene recorded at –80 °C. The intended mole fractions for (*S*,*S*)-TMCDA, X_B, in (a)–(h) are 0.00, 0.10, 0.20, 0.30, 0.40, 0.60, 0.80 and 1.00, respectively. L = TMEDA; L' = (*S*,*S*)-TMCDA. The experiment shows that monomer **4** forms a mixed solvate species, confirming the solvation number of the homosolvates.

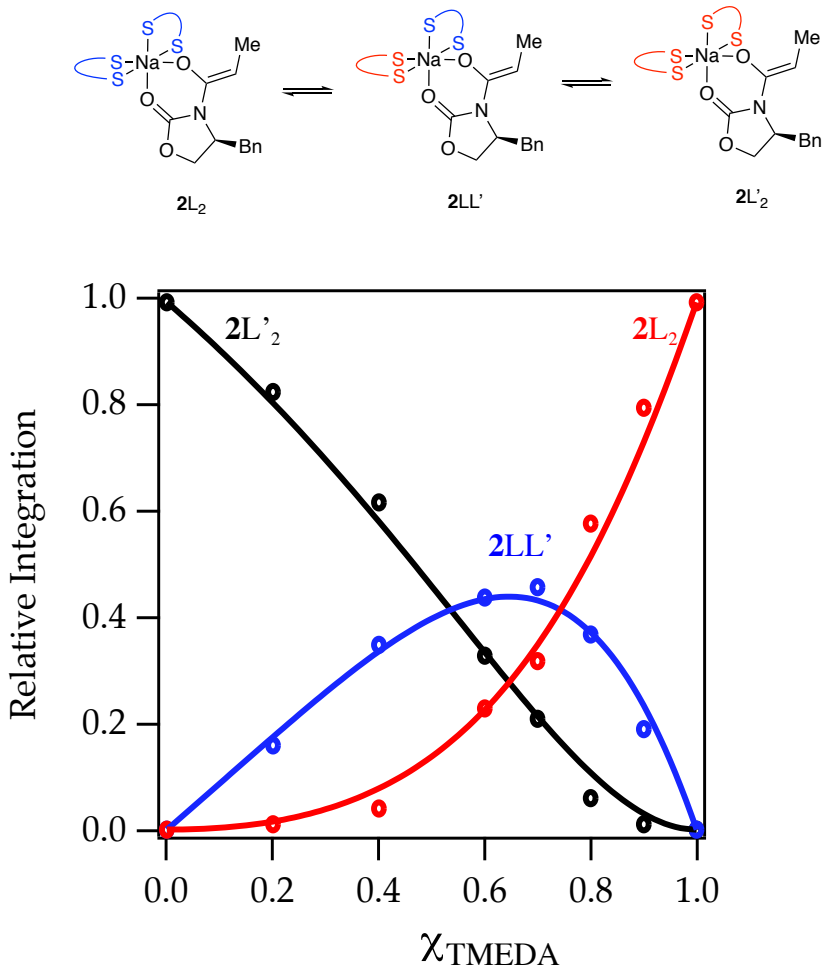


Figure S45. Job plot showing the relative integrations versus the intended mole fraction of TMEDA for 0.20 M **4** and 1.0 M total TMEDA and (*S*,*S*)-TMCDA in toluene recorded at –80 °C. The curves represent a parametric fit to a dimer model that includes provisions for relative binding affinities to the disolvated monomer. The 'shift' of the maximum for the mixed solvate from 0.50 results from the differential binding constants. L = TMEDA; L' = (*S*,*S*)-TMCDA.

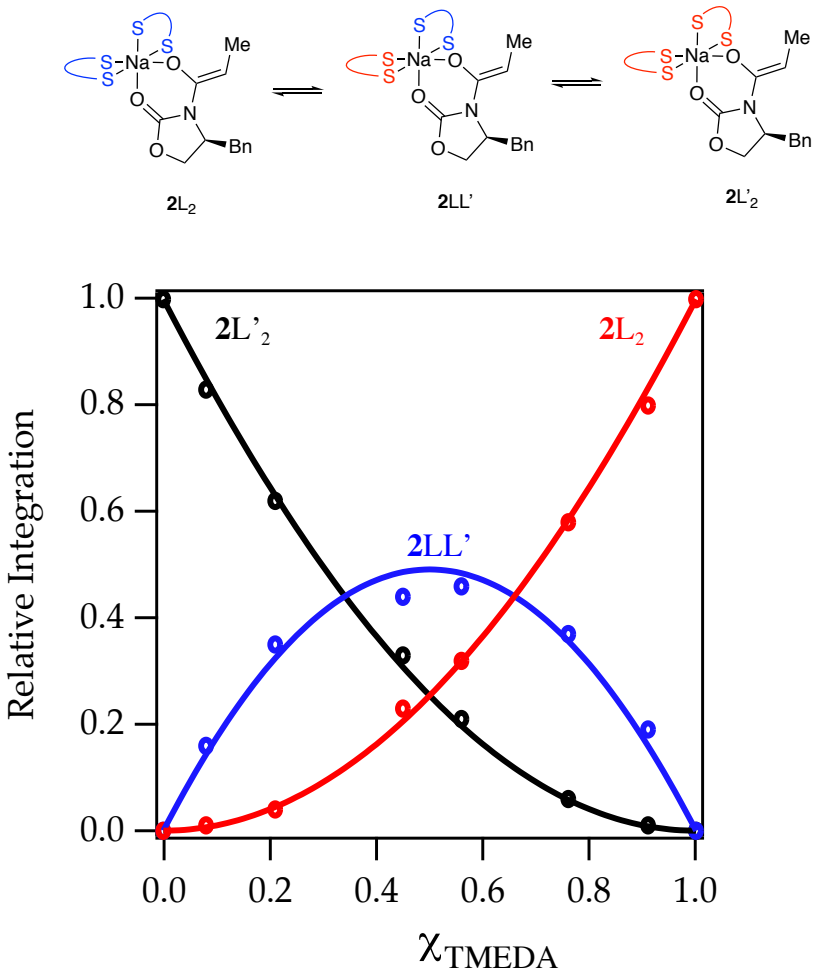


Figure S46. Job plot showing the relative integrations versus the *measured* mole fraction of TMEDA for 0.20 M **4** with added TMEDA and (*S*,*S*)-TMCDA (1.0 M total ligand titer) in toluene recorded at –80 °C. L = TMEDA; L' = (*S*,*S*)-TMCDA.

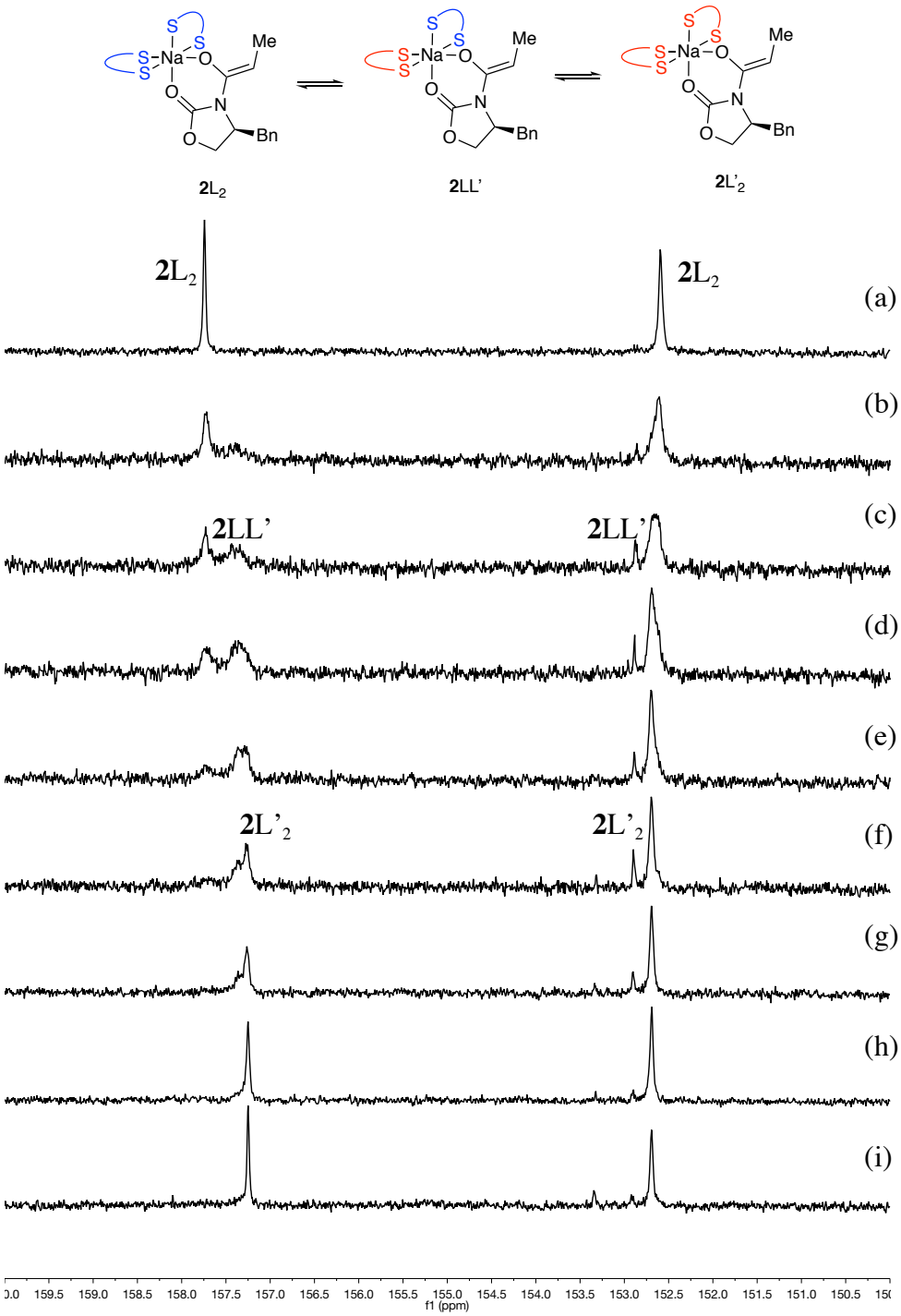


Figure S47. ^{13}C NMR spectra of 0.20 M **4** with TMEDA and (*R*,*R*)-TMCDA (1.0 M total ligand titer) in toluene recorded at –80 °C. The intended mole fractions for (*R*,*R*)-TMCDA, X_B, in (a)–(i) are 0.00, 0.10, 0.20, 0.30, 0.40, 0.50, 0.60, 0.80 and 1.00, respectively. L = TMEDA, L' = (*R*,*R*)-TMCDA.

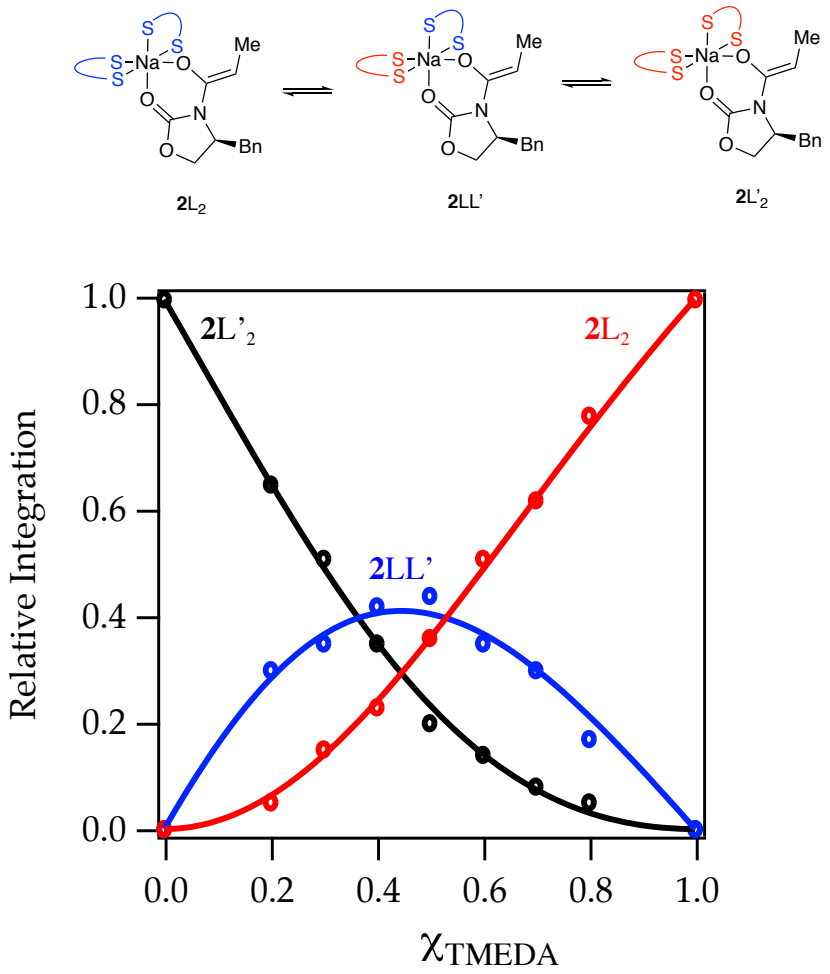


Figure S48. Job plot showing the relative integrations versus the intended mole fraction of TMEDA for 0.20 M **4** and 1.0 M total TMEDA and (*R*,*R*)-TMCDA in toluene recorded at –80 °C. L = TMEDA, L' = (*R*,*R*)-TMCDA.

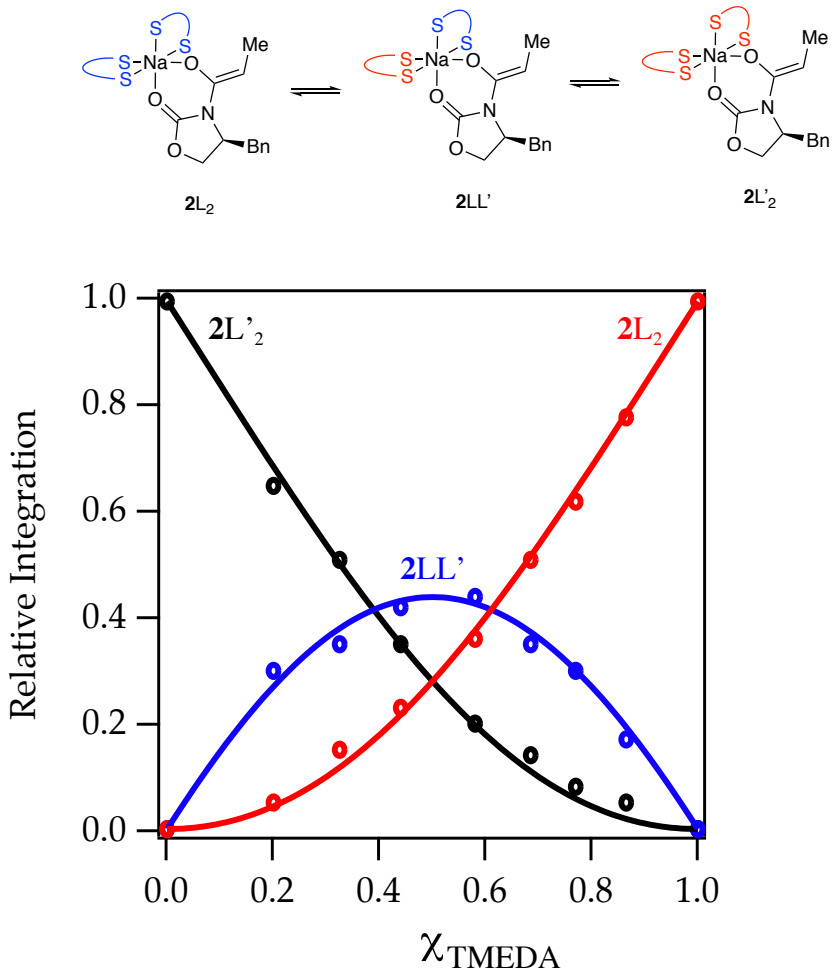


Figure S49. Job plot showing the relative integrations versus the measured mole fraction of TMEDA for 0.20 M **4** and 1.0 M total TMEDA and (*R*,*R*)-TMCDA in toluene recorded at –80 °C.

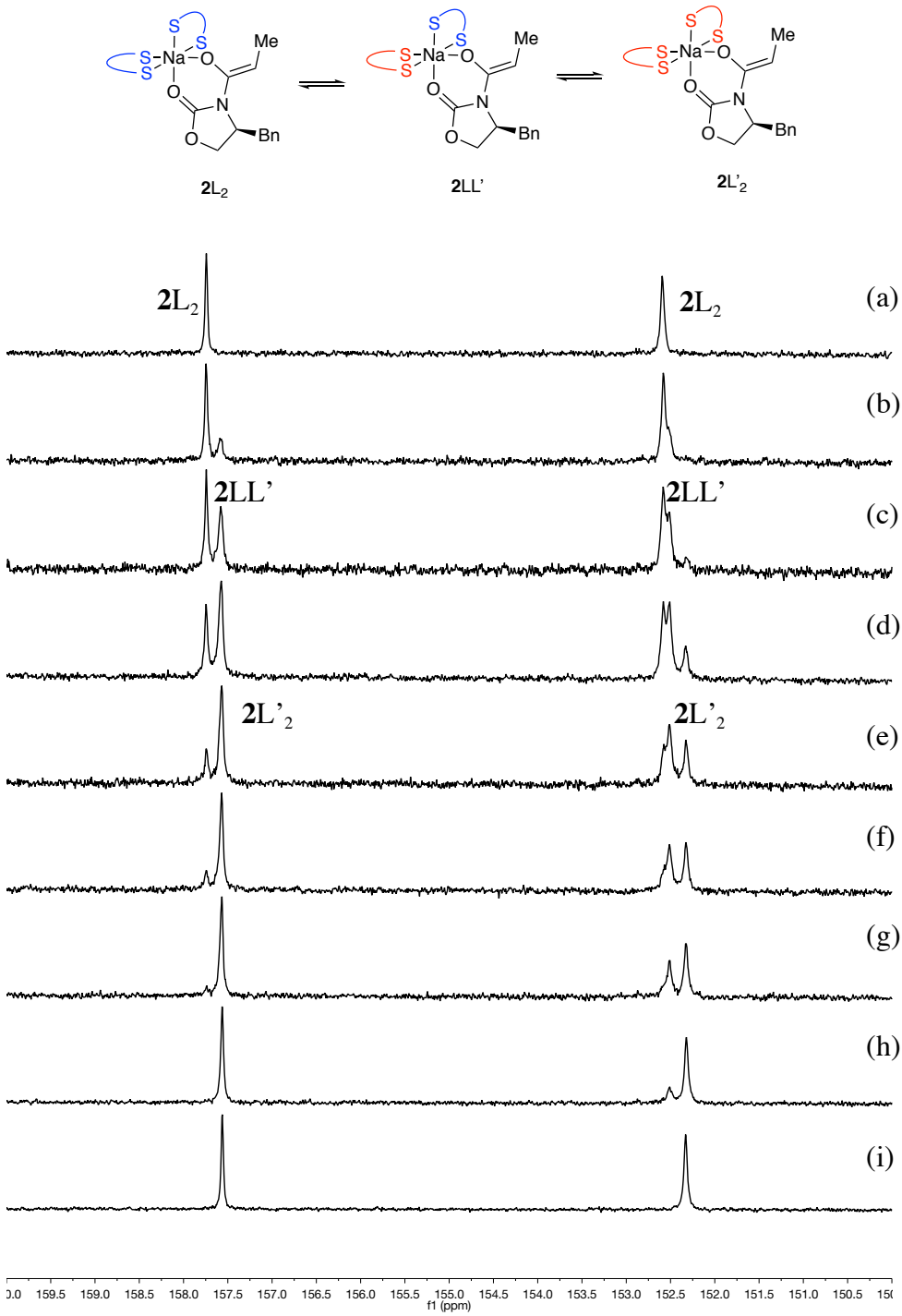
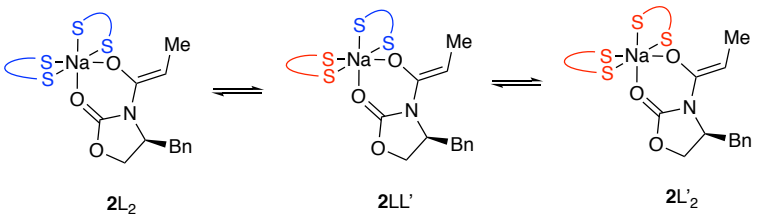


Figure S50. ^{13}C NMR spectra of 0.20 M **4** in (*S*,*S*)-TMCDA and (*R*,*R*)-TMCDA mixtures (1.0 M total ligand titer) in toluene recorded at –80 °C. The intended mole fractions for (*R*,*R*)-TMCDA, X_B, in (a)–(i) are 0.00, 0.20, 0.40, 0.50, 0.60, 0.70, 0.80, 0.90 and 1.00, respectively. L = (*S*,*S*)-TMCDA, L' = (*R*,*R*)-TMCDA.



2L_2 **2**LL' **2**L'$_2$

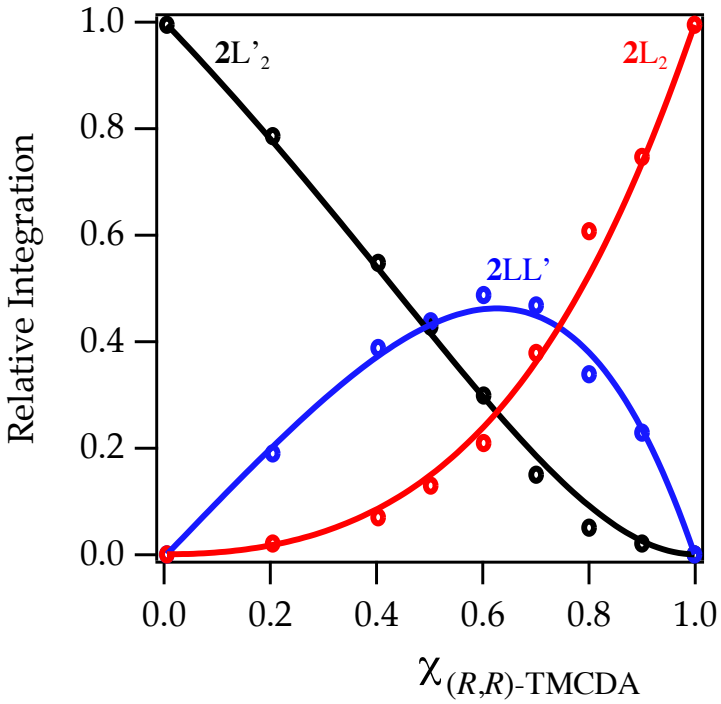


Figure S51. Job plot showing the relative integrations versus the intended mole fraction of (*R*,*R*)-TMCDA for 0.20 M (*S*)-**2** in (*R*,*R*)-TMCDA and (*S*,*S*)-TMCDA mixtures (1.0 M total ligand titer) in toluene recorded at −80 °C. L = (*S*,*S*)-TMCDA, L' = (*R*,*R*)-TMCDA. The offset of the maximum to the right shows a relative preference for binding (*S*,*S*)-TMCDA versus (*R*,*R*)-TMCDA.

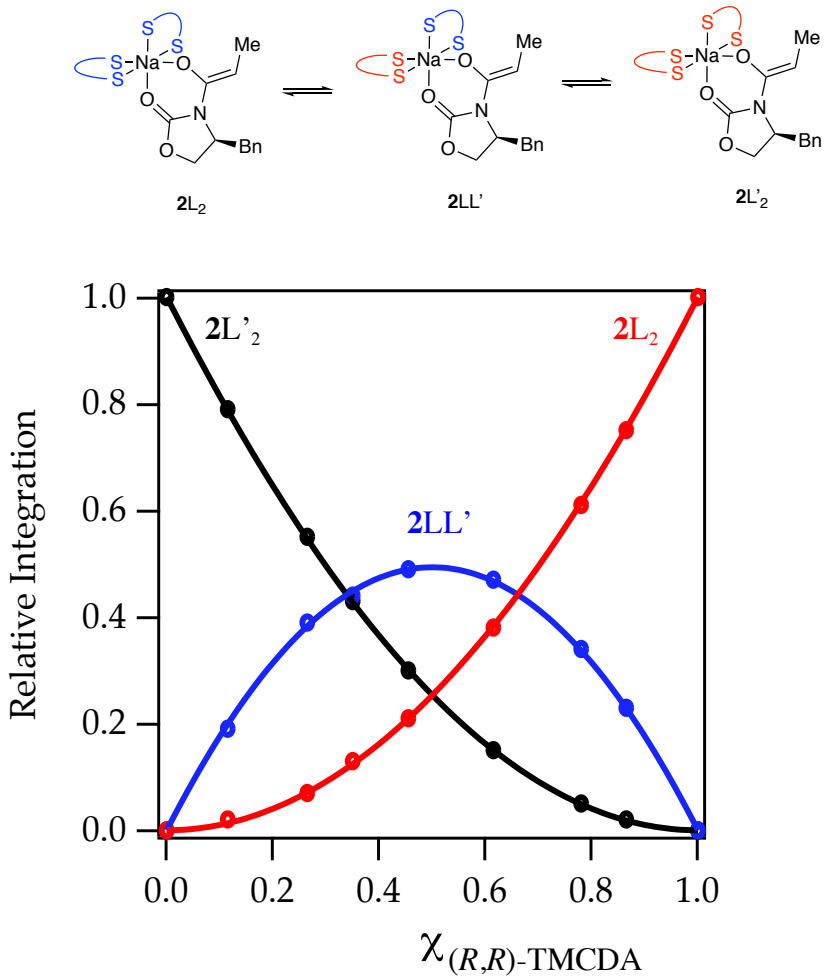


Figure S52. Job plot showing the relative integrations versus the measured mole fraction of (*R*,*R*)-TMCDA for 0.20 M (*S*)-**2** and 1.0 M total (*R*,*R*)-TMCDA and (*S*,*S*)-TMCDA in toluene recorded at –80 °C. L = (*S*,*S*)-TMCDA, L' = (*R*,*R*)-TMCDA.

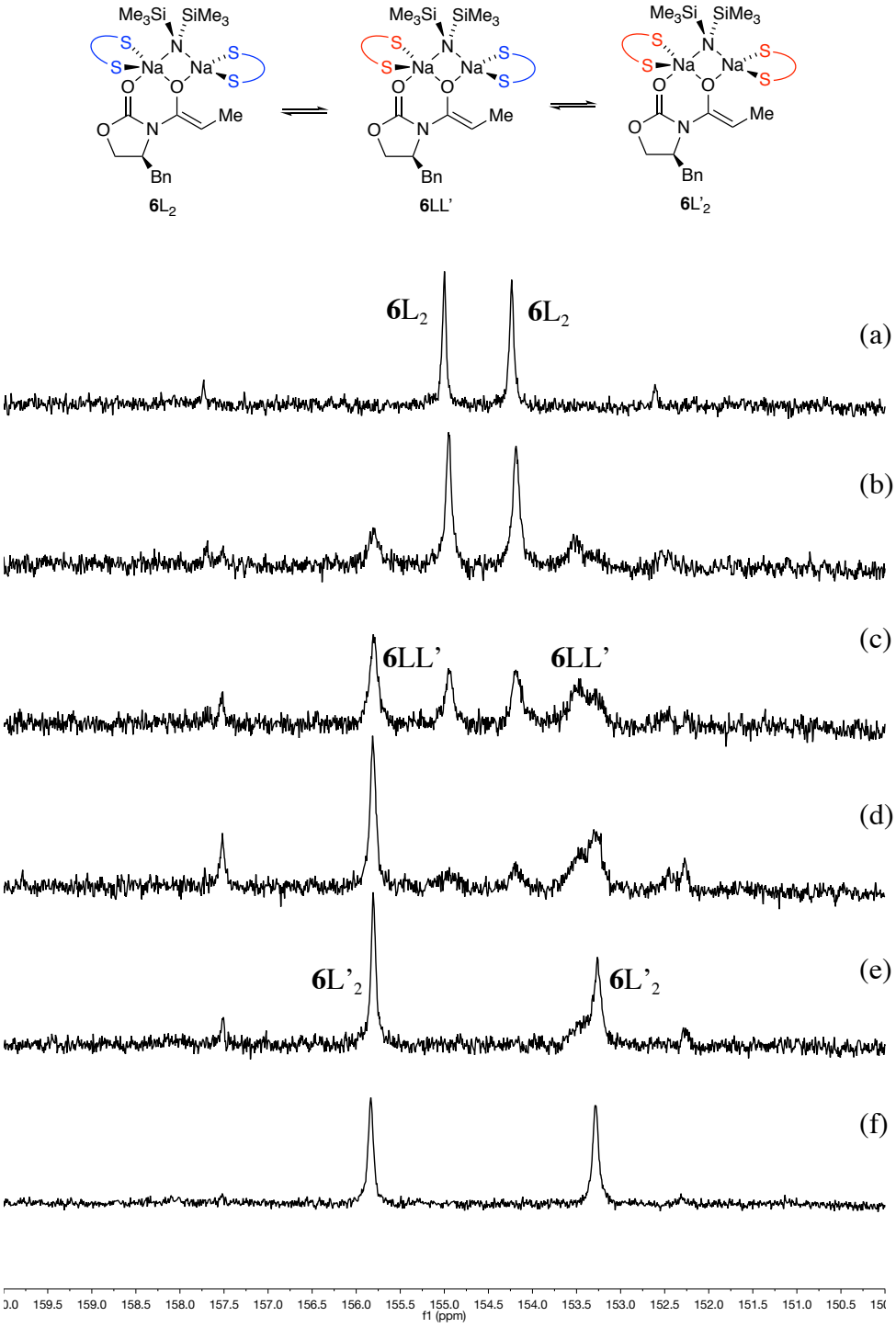


Figure S53. ^{13}C NMR spectra of 0.20 M **6** and 1.0 M (*R*,*R*)-TMCDA and (*S*,*S*)-TMCDA in toluene recorded at –80 °C. The intended mole fractions for (*S*,*S*)-TMCDA, X_B, in (a)–(f) are 0.00, 0.20, 0.40, 0.60, 0.80, and 1.00, respectively. L = (*R*,*R*)-TMCDA, L' = (*S*,*S*)-TMCDA. The experiment shows two coordinated diamines.

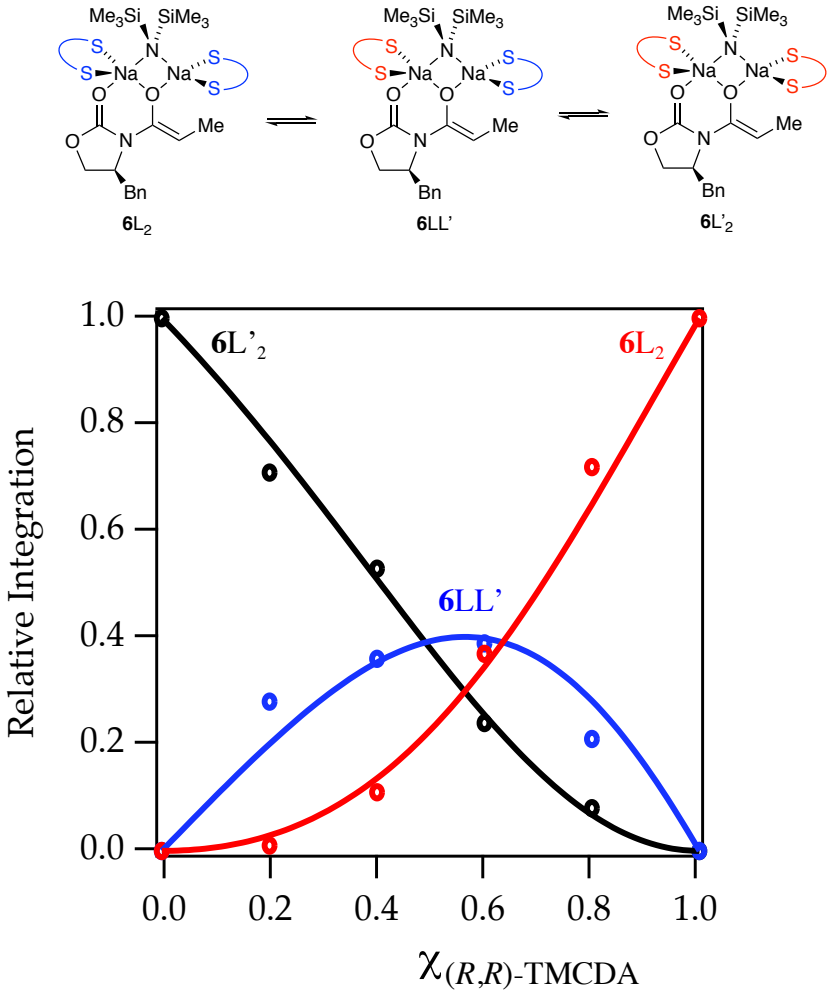


Figure S54. Job plot showing the relative integrations versus the intended mole fraction of (*R*,*R*)-TMCDA for 0.20 M **6** and 1.0 M total (*R*,*R*)-TMCDA and (*S*,*S*)-TMCDA in toluene recorded at –80 °C. L = (*R*,*R*)-TMCDA, L' = (*S*,*S*)-TMCDA. Job plot indicates a disolvated dimer and shows minor differences in relative binding constants.

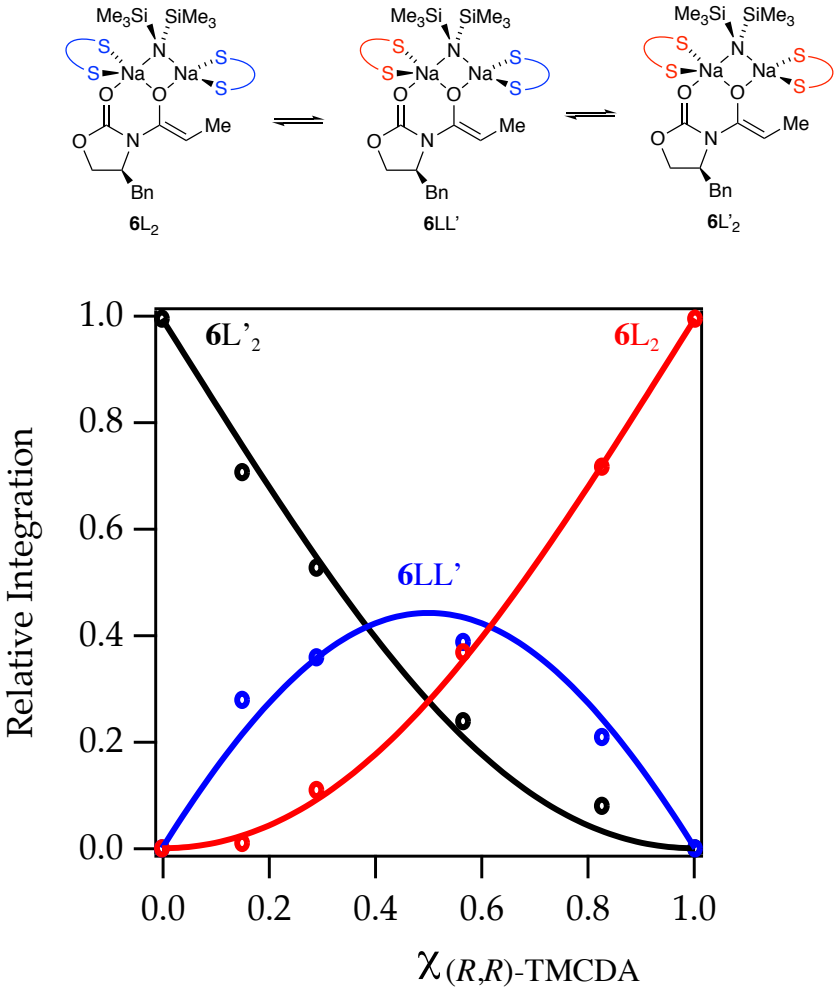


Figure S55. Job plot showing the relative integrations versus the measured mole fraction of (*R*,*R*)-TMCDA for 0.20 M **6** and 1.0 M total (*R*,*R*)-TMCDA and (*S*,*S*)-TMCDA in toluene recorded at –80 °C.
L = (*R*,*R*)-TMCDA, L' = (*S*,*S*)-TMCDA.

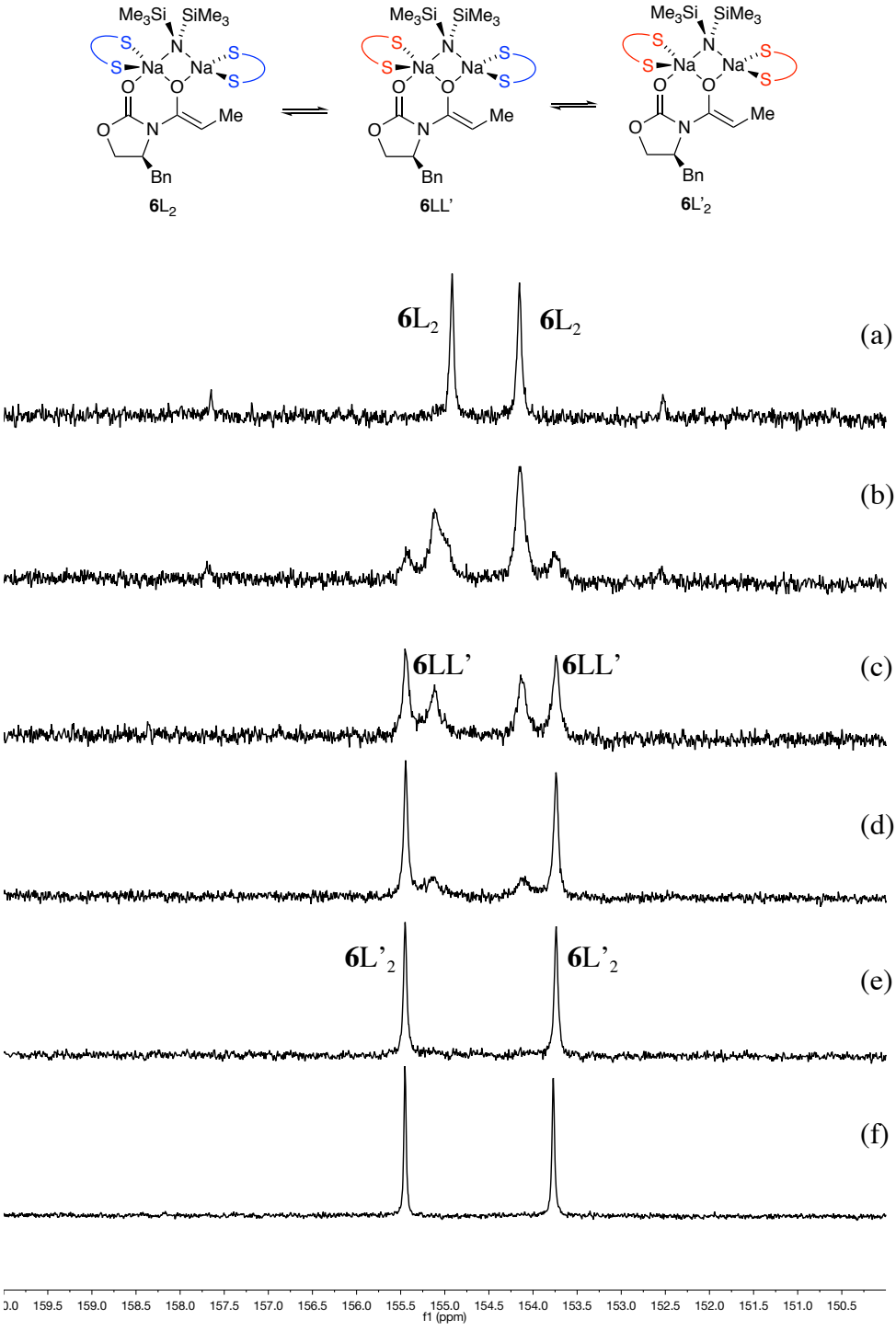


Figure S56. ^{13}C NMR spectra of 0.20 M **6** and 1.0 M (*R*,*R*)-TMCDA and TMEDA in toluene recorded at –80 °C. The intended mole fractions for TMEDA, X_B, in (a)–(f) are 0.00, 0.20, 0.40, 0.60, 0.80, and 1.00, respectively. L = (*R*,*R*)-TMCDA, L' = TMEDA.

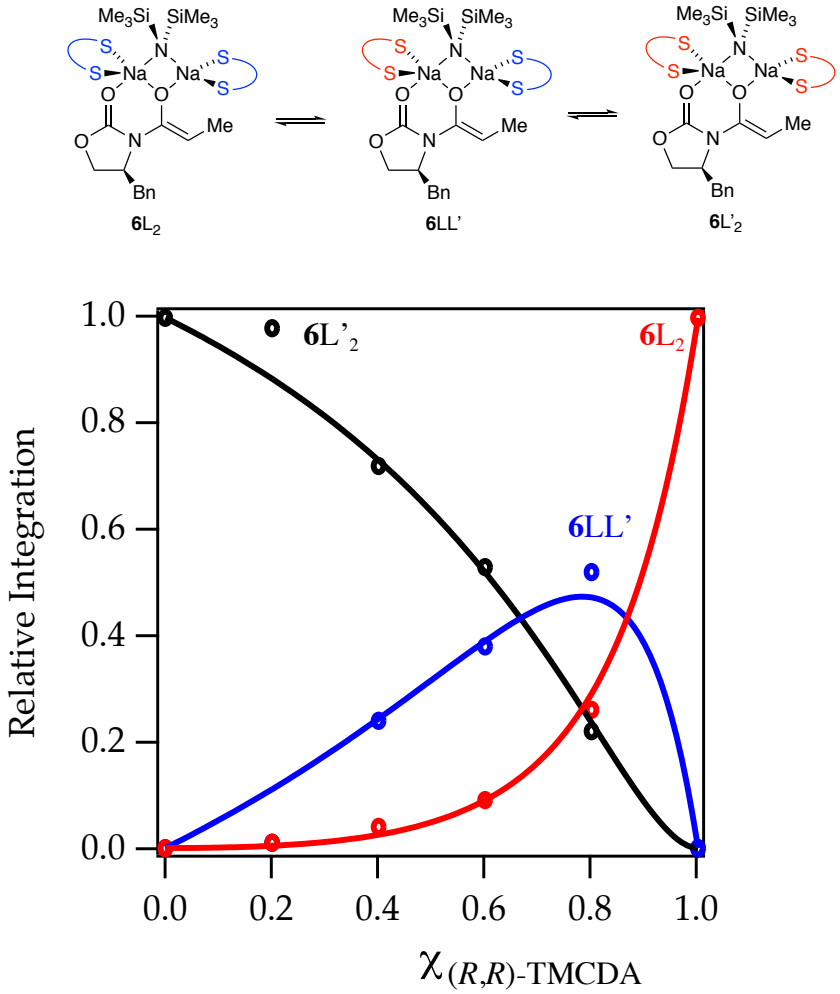


Figure S57. Job plot showing the relative integrations versus the intended mole fraction of TMEDA for 0.20 M **6** and 1.0 M total (*R*,*R*)-TMCDA and TMEDA in toluene recorded at –80 °C. The offset of the maximum to the right shows a relative preference for binding (*S*,*S*)-TMCDA versus (*R*,*R*)-TMCDA. L = (*R*,*R*)-TMCDA, L' = TMEDA.

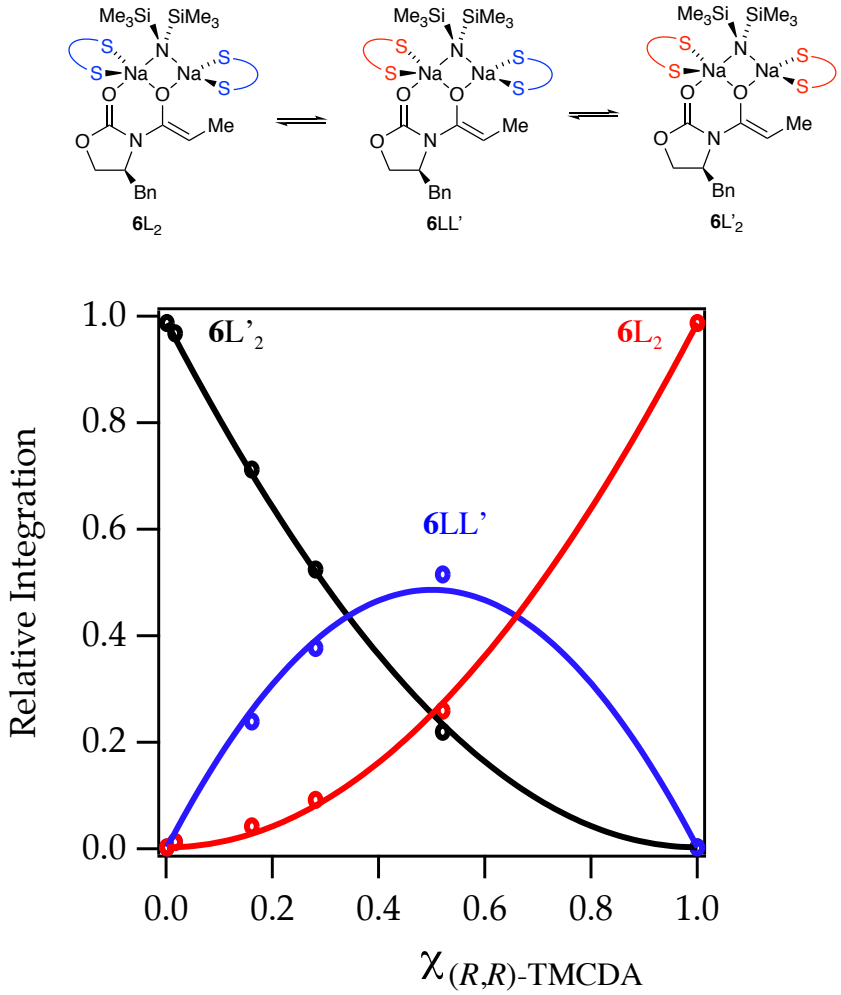


Figure S58. Job plot showing the relative integrations versus the measured mole fraction of TMEDA for 0.20 M **6** and 1.0 M total (*R*,*R*)-TMCDA and TMEDA in toluene recorded at –80 °C. The absence of data on the right half arises from strong binding affinity TMEDA has much stronger binding affinity to the mixed dimer (*R*,*R*)-TMCDA. L = (*R*,*R*)-TMCDA, L' = TMEDA.

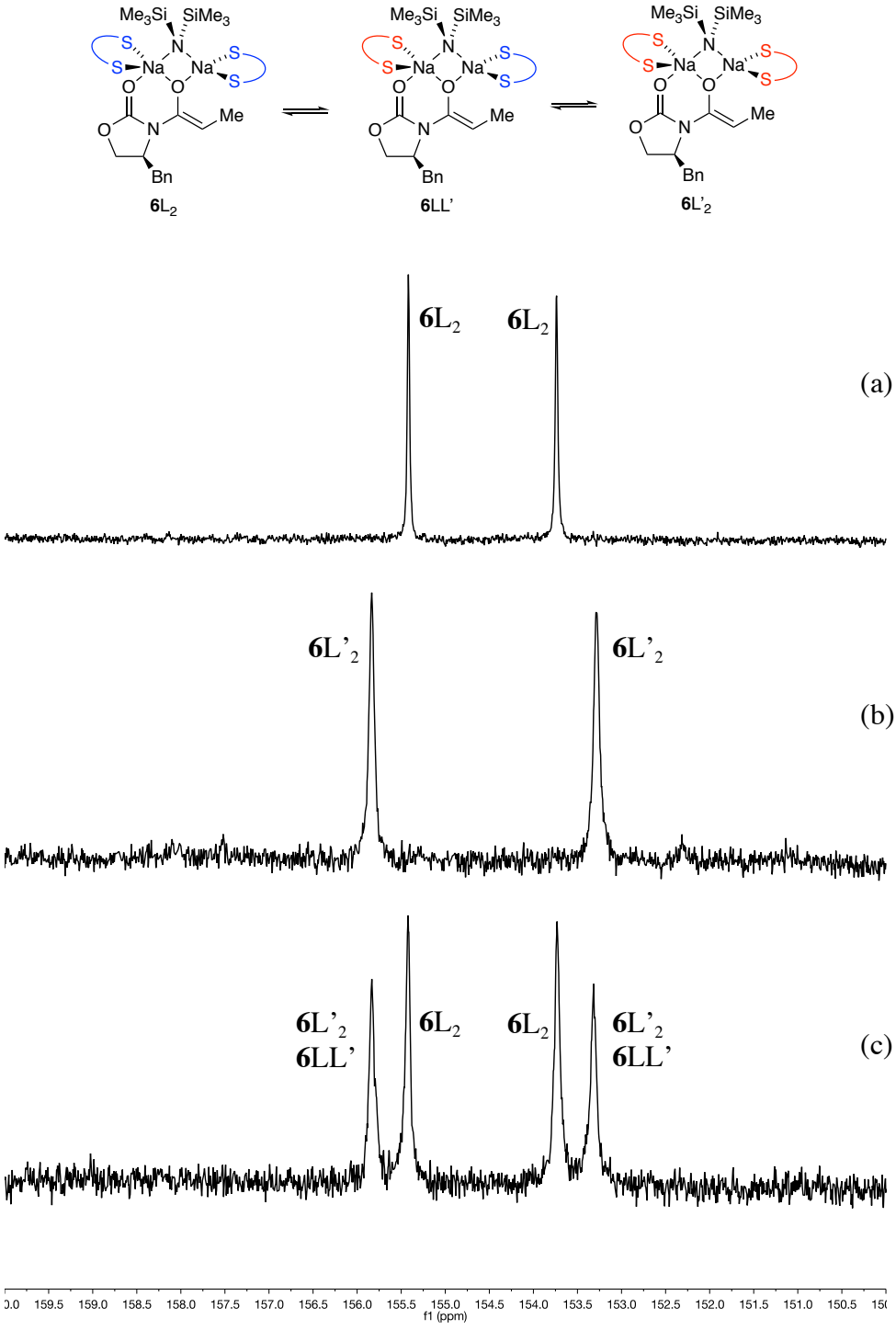


Figure S59. ^{13}C NMR spectra of 0.20 M **6** in (a) 1.0 M TMEDA; (b) 1.0 M (*S*,*S*)-TMCDA; (c) 0.5 M TMEDA and 0.5 M (*S*,*S*)-TMCDA in toluene recorded at –80 °C. A mixed solvate is not observed because, presumably owing to resonance overlaps.L = TMEDA, L' = (*S*,*S*)-TMCDA.

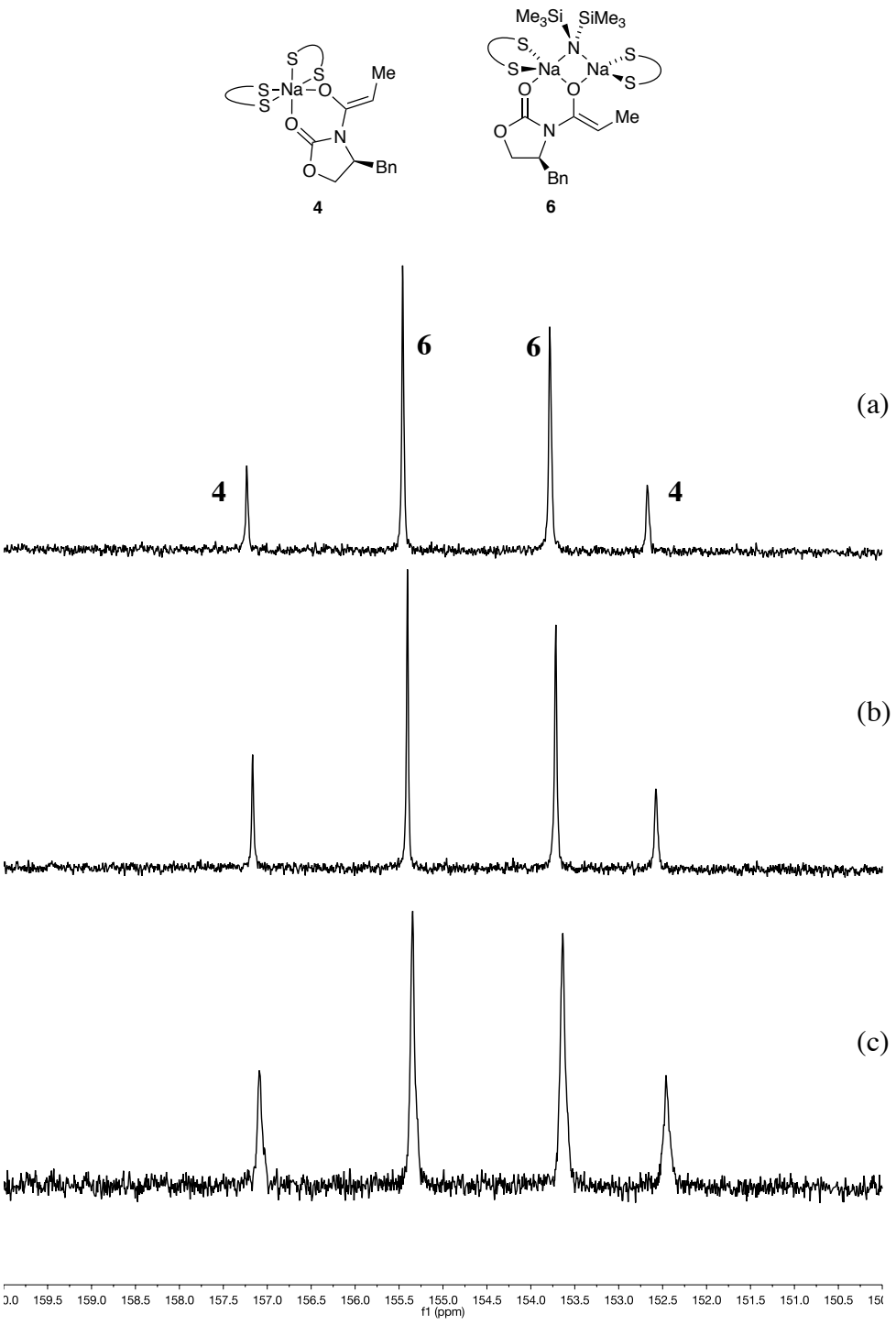


Figure S60. ^{13}C NMR spectra of 0.10 M **4**, 0.10 M **6** and (a) 0.80 M TMEDA; (b) 1.8 M TMEDA; (c) 3.0 M TMEDA in toluene recorded at –80 °C.Adding more TMEDA to a mixture of monomer and NaHMDS mixed dimer shows no ratio change because the equilibrium favoring mixed dimer is essentially quantitative.

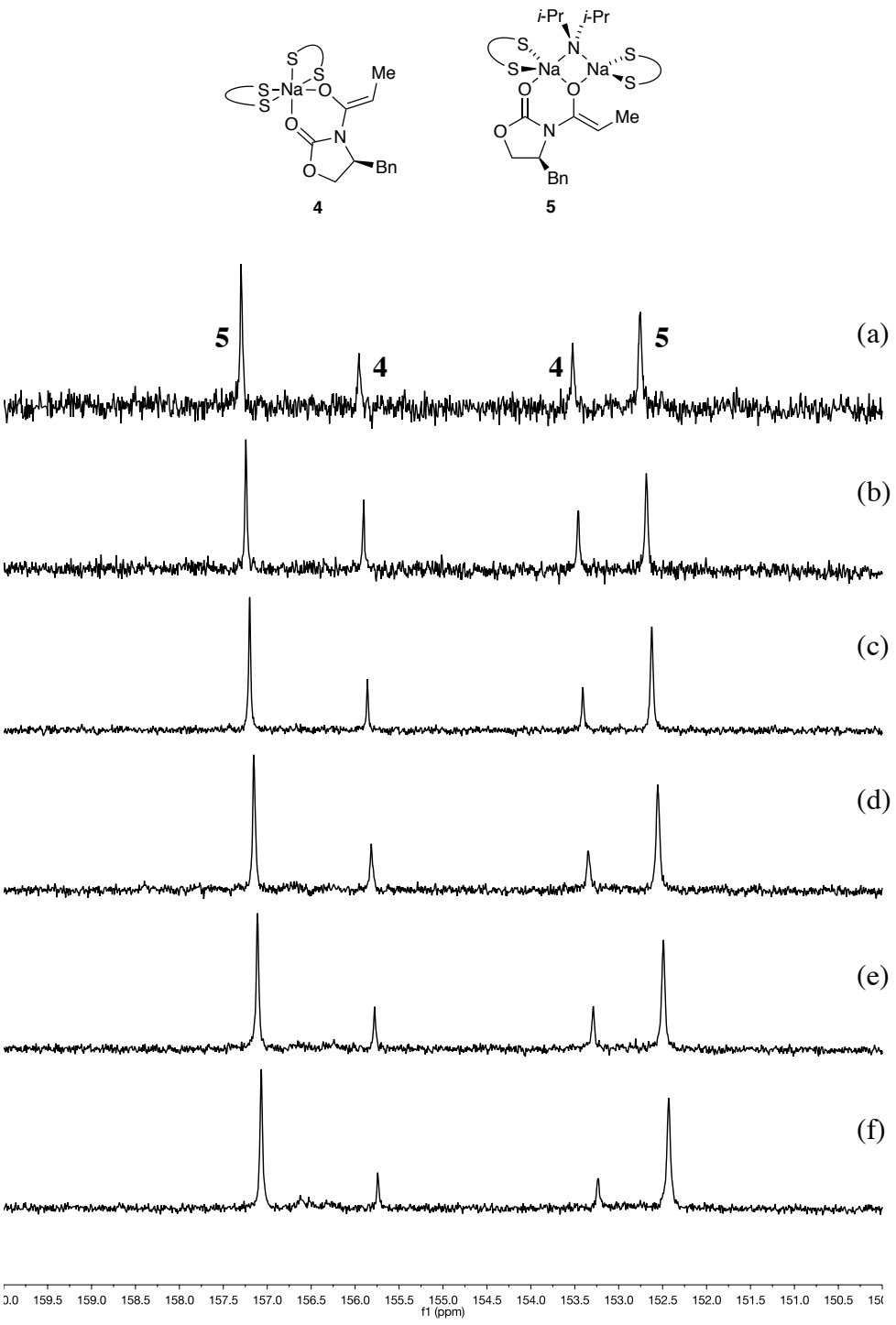


Figure S61. ^{13}C NMR spectra in toluene recorded at –80 °C of 0.20 M (*S*)-**2**, 0.10 M NaDA and (a) 0.30 M TMEDA; (b) 1.0 M TMEDA; (c) 1.6 M TMEDA; (d) 2.3 M TMEDA; (e) 3.0 M TMEDA; (f) 3.6 M TMEDA.

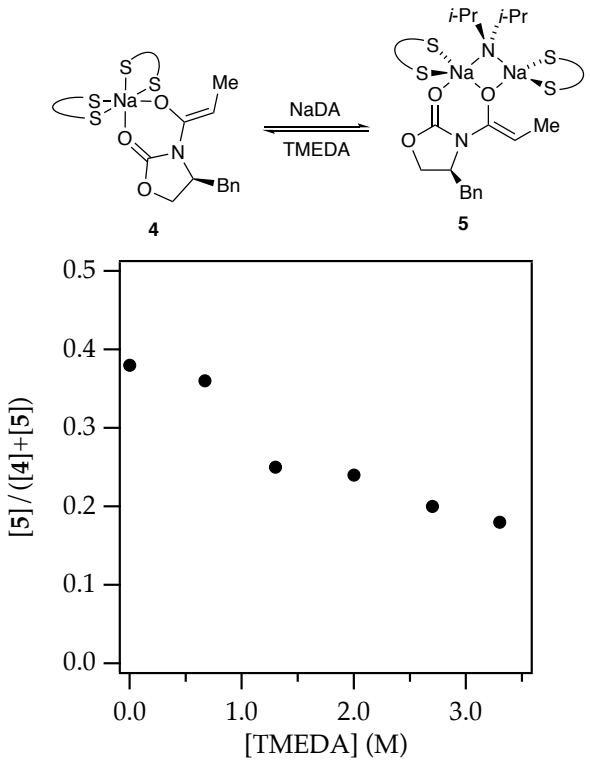


Figure S62. Plot of mixed dimer **5** proportion versus [TMEDA] in a solution of 0.20 M (*S*)-**2** and 0.10 M NaDA in TMEDA/toluene at –80 °C. Data are from Figure S61. The NaDA mixed dimer/monomer ratio decreases when raising the concentration of TMEDA, suggesting a lower per-sodium solvation number on the mixed dimer.

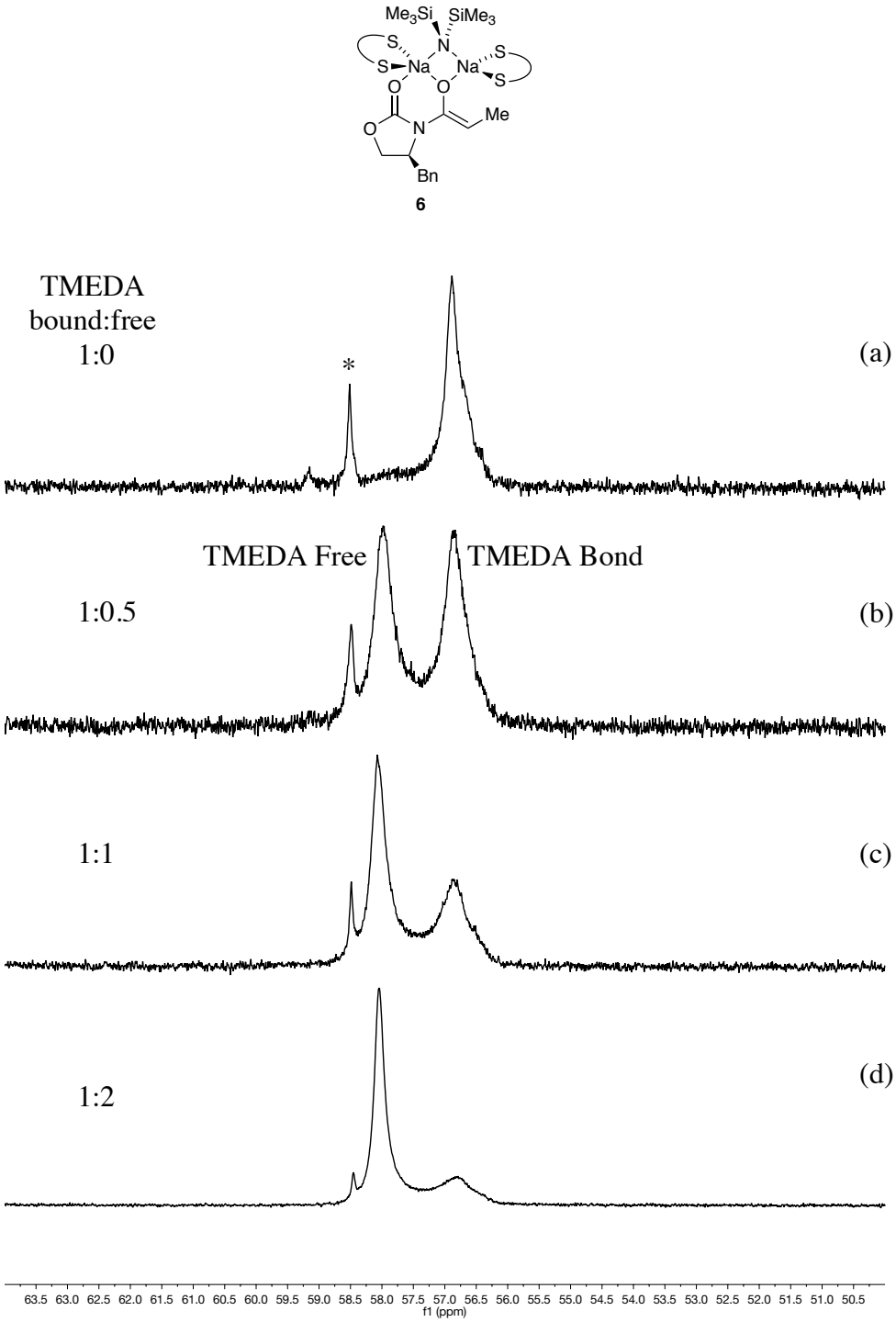


Figure S63. ^{13}C NMR spectra in toluene recorded at –80 °C of 0.20 M **6**: (a) 0.40 M TMEDA; (b) 0.60 M TMEDA; (c) 0.80 M TMEDA; (d) 1.2 M TMEDA. The ratio of free and bound TMEDA is qualitatively consistent with one ligand per sodium. *Oxazolidinone methine carbon adjacent to nitrogen.

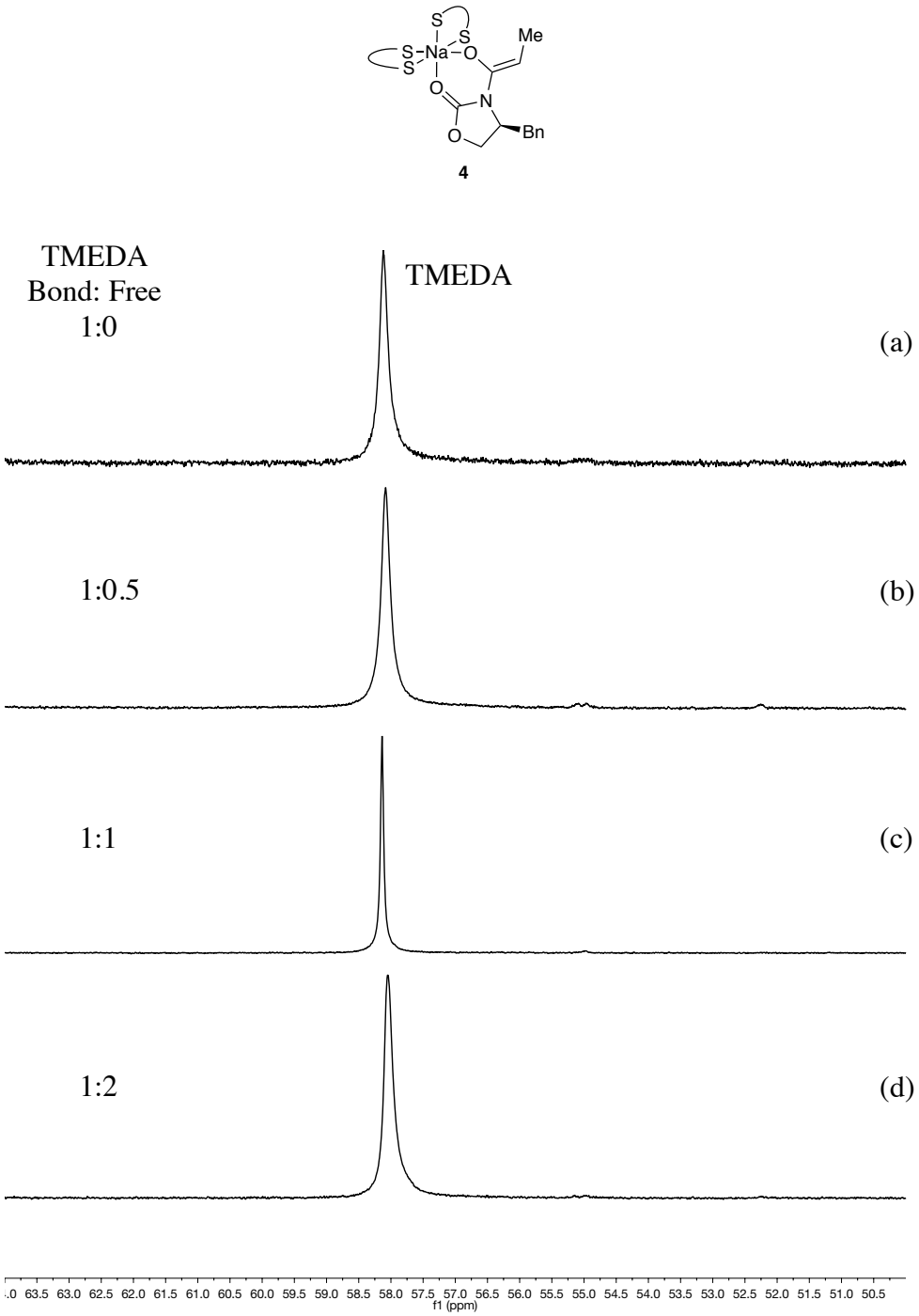


Figure S64. ^{13}C NMR spectra in toluene recorded at –80 °C of 0.20 M **4** and (a) 0.40 M TMEDA; (b) 0.60 M TMEDA; (c) 0.80 M TMEDA; (d) 1.2 M TMEDA. Free and monomer-bound TMEDA do not resolve.

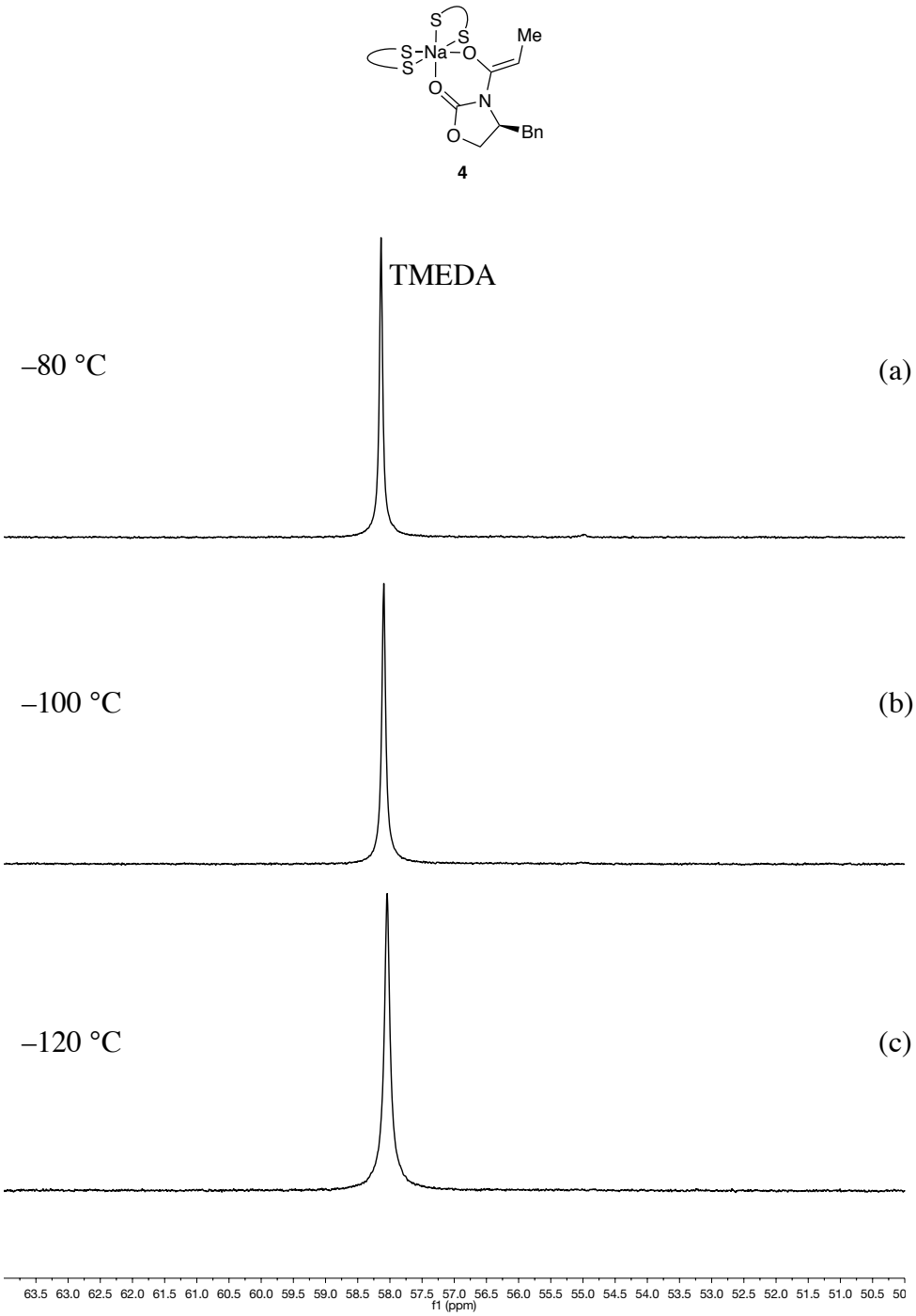


Figure S65. ^{13}C NMR spectra of 0.20 M **4** and 0.80 M TMEDA in 25% cyclopentane/toluene recorded at (a) –80 °C; (b) –100 °C; (c) –120 °C. Cooling the solution does not resolve the free and monomer-bound TMEDA.

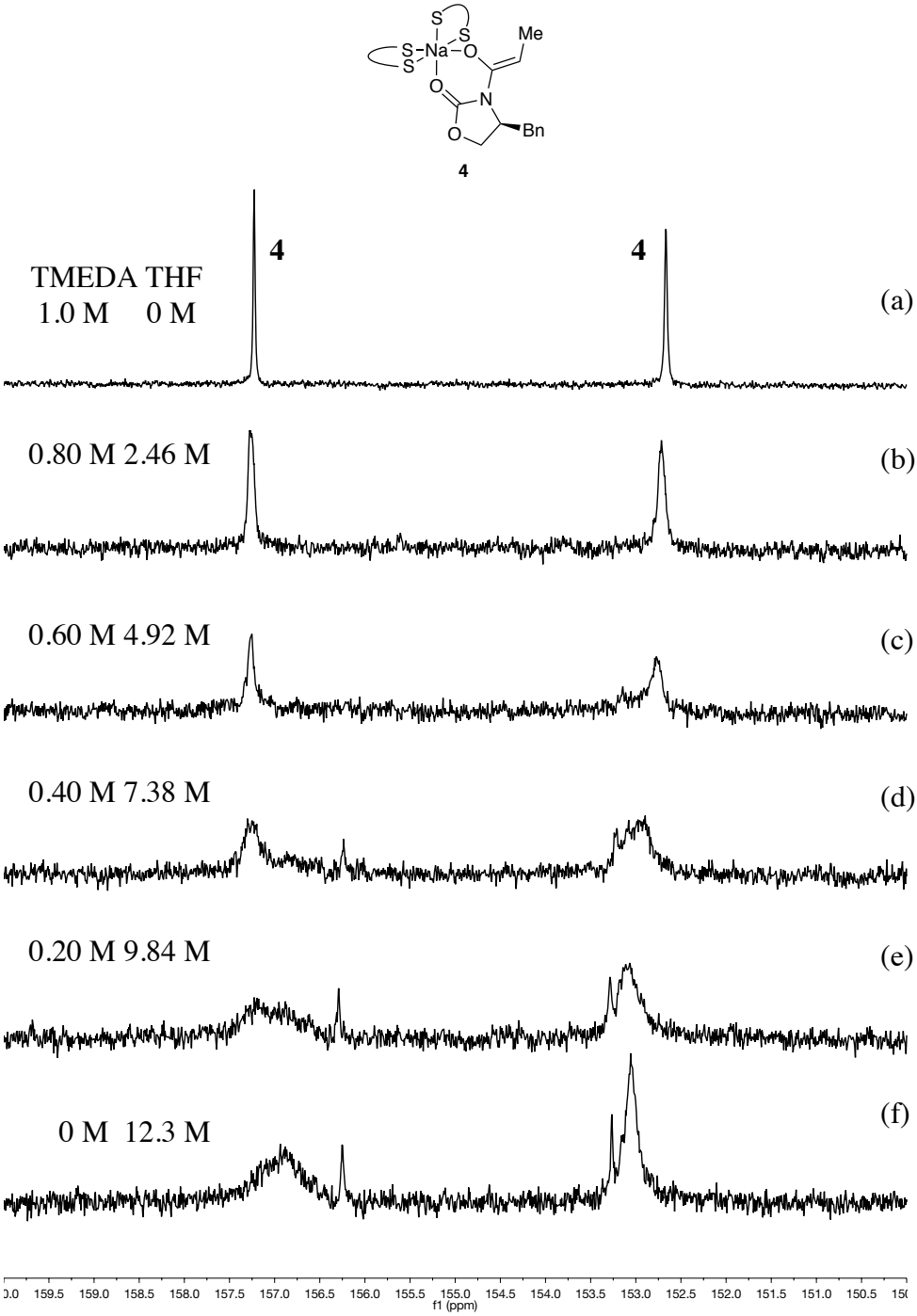


Figure S66. ^{13}C NMR spectra in toluene co-solvent recorded at –80 °C of 0.20 M **4** and (a) 1.0 M TMEDA; (b) 0.80 M TMEDA and 2.46 M THF; (c) 0.60 M TMEDA and 4.92 M THF; (d) 0.40 M TMEDA and 7.38 M THF; (e) 0.20 M TMEDA and 9.84 M THF; (f) 12.3 M THF. Gradually switching from a TMEDA/toluene solvent system to THF significantly lowers the quality of the spectra.

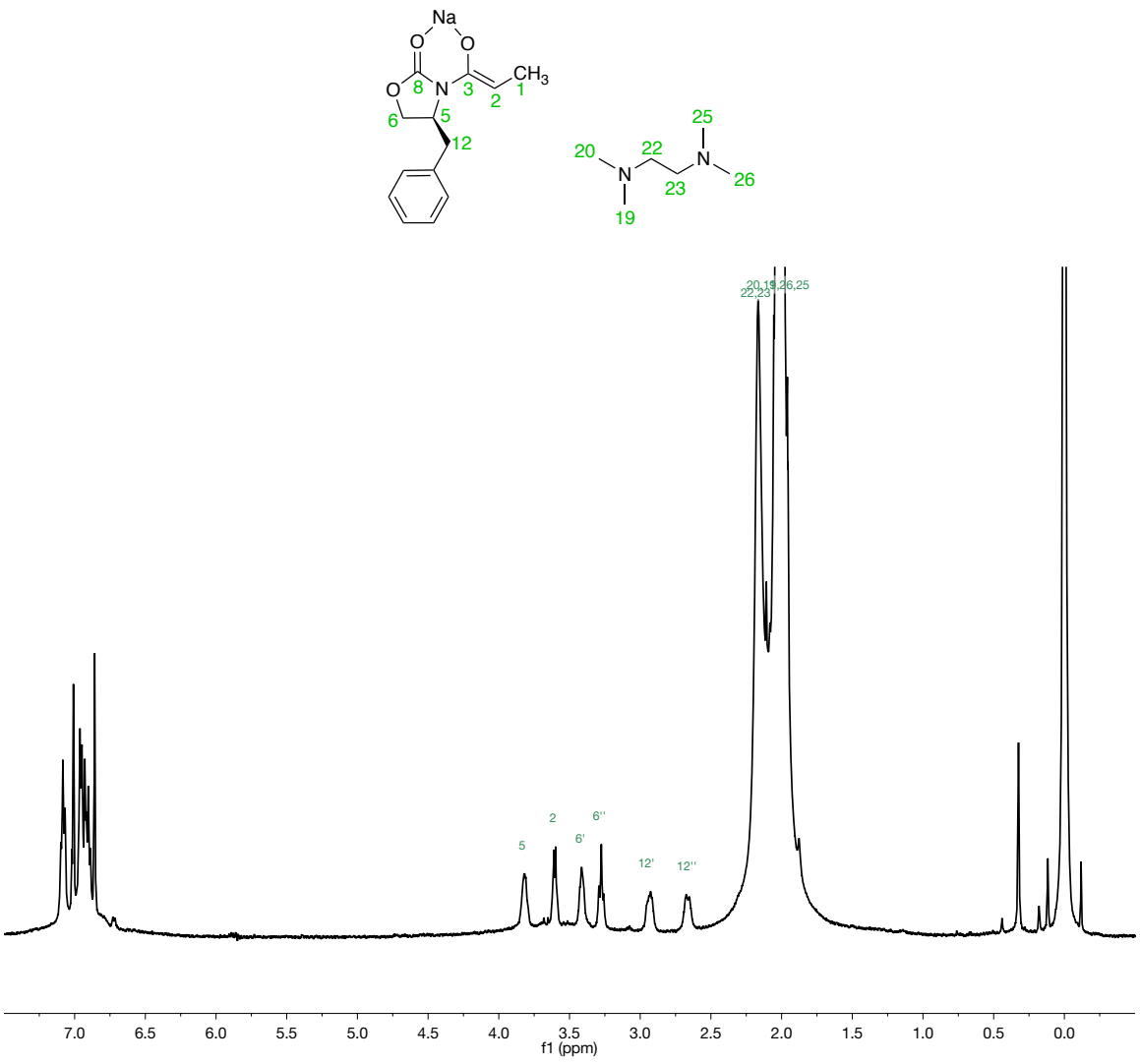


Figure S67. ^{1}H NMR spectrum of 0.20 M **4** in 0.50 M TMEDA/toluene recorded at –60 °C. The peaks are assigned by an HSQC experiment.

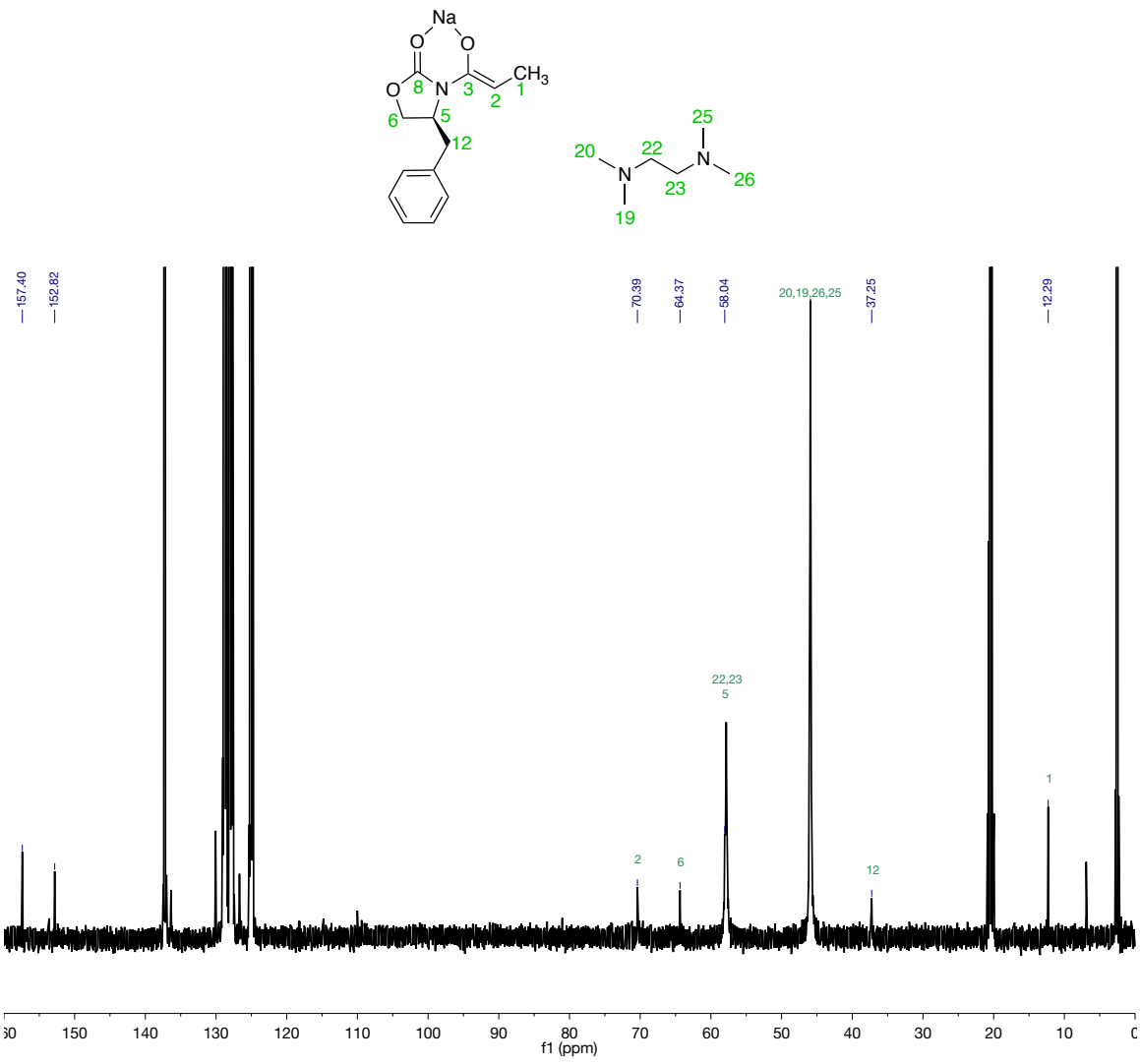
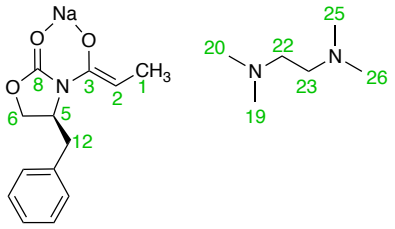


Figure S68. ^{13}C NMR spectrum of 0.20 M **4** in 0.50 M TMEDA/toluene recorded at –60 °C.

Parameter	Value
1 Solvent	toluene
2 Temperature	-60.0
3 Pulse Sequence	gHSQCAD
4 Number of Scans	2
5 Receiver Gain	30
6 Relaxation Delay	1.0000
7 Pulse Width	7.5000
8 Acquisition Time	0.1499



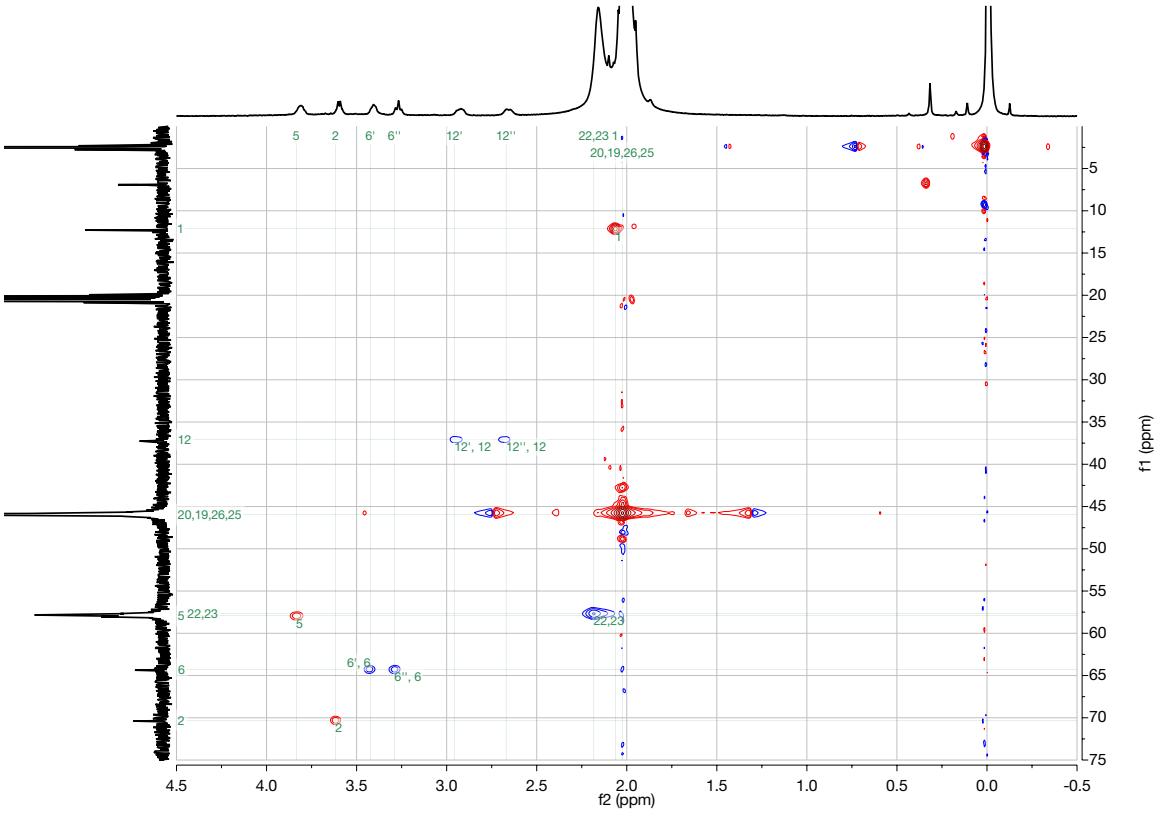


Figure S69. HSQC spectrum of 0.20 M **4** in 0.50 M TMEDA/toluene recorded at –60 °C.

Parameter	Value
1 Solvent	toluene
2 Temperature	-60.0
3 Pulse Sequence	ROESYAD
4 Number of Scans	2
5 Receiver Gain	0
6 Relaxation Delay	1.0000
7 Pulse Width	7.5000
8 Acquisition Time	0.4001

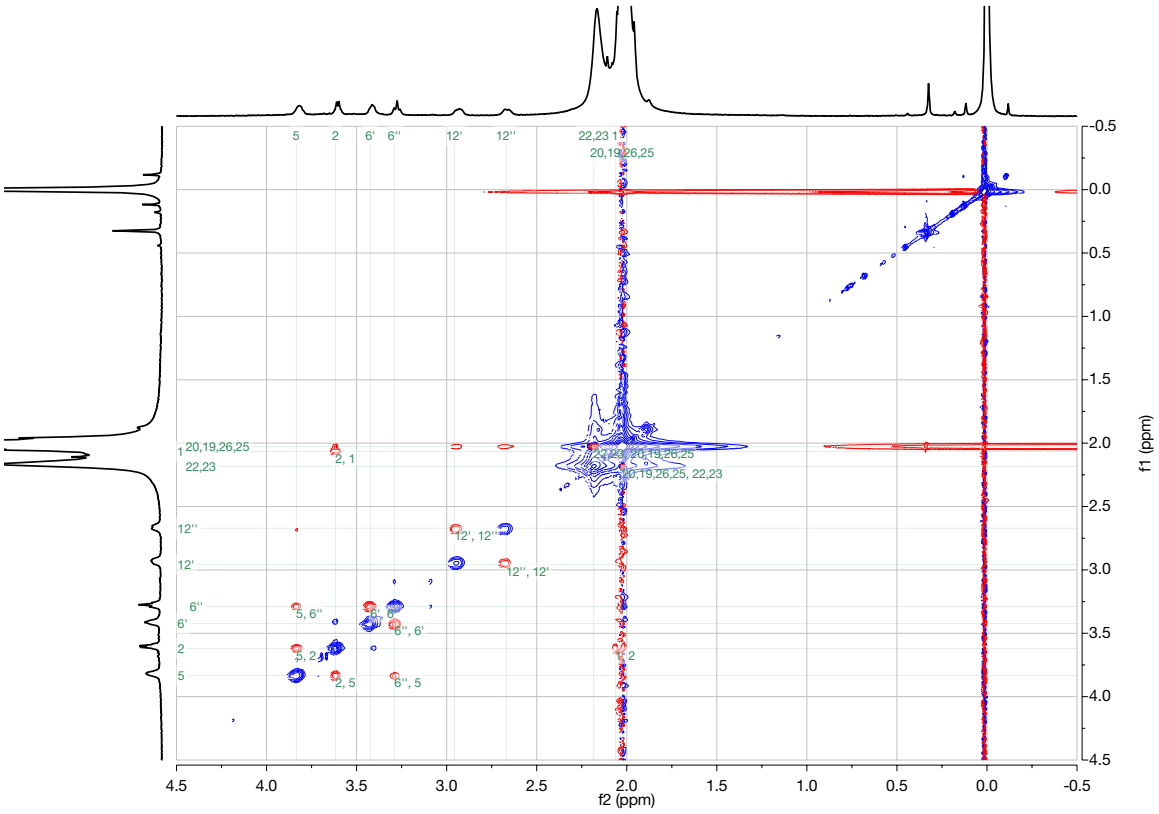


Figure S70. ROESY spectrum of 0.20 M **4** in 0.50 M TMEDA/toluene recorded at –60 °C.

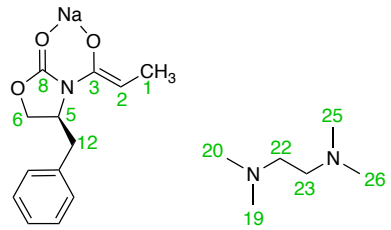


Table S1. ^{1}H and ^{13}C chemical shift assignments for monomer **4**.

Atom #	δC, ppm	δH, ppm	ROESY
1	12.13	2.06	2
2	70.29	3.62	1, 5, 19
3	152.82	-	-
5	57.93	3.83	2, 6”
6	64.26	3.42 (6’)	6”
		3.29 (6”)	5, 6’
8	157.40	-	
12	37.08	2.96 (12’)	12”, 19
		2.67 (12”)	12’, 19
19, 20, 25, 26	45.93	2.03	2, 12’, 12”, 22
22, 23	57.68	2.18	19

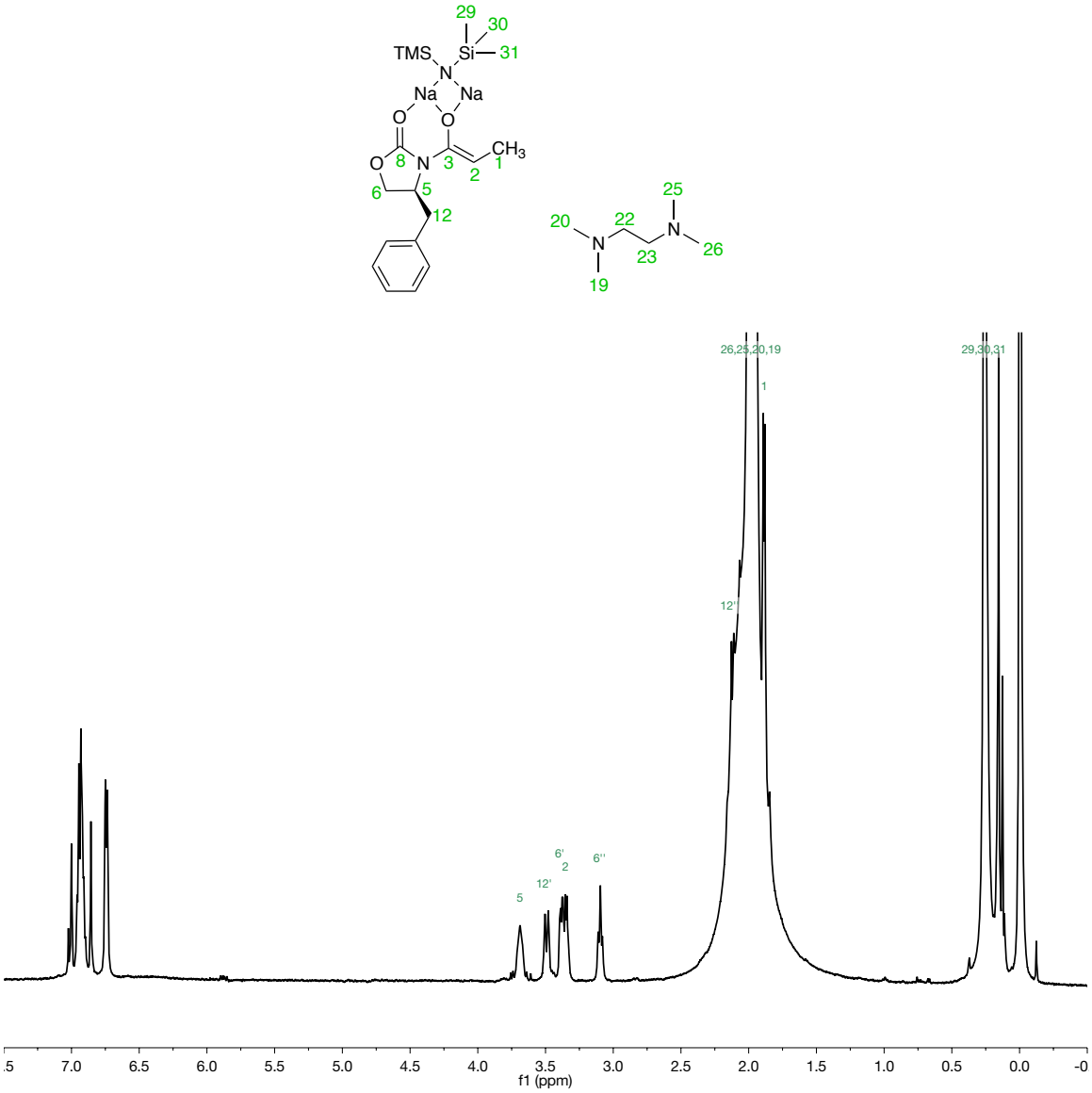


Figure S71. ^{1}H NMR spectrum of 0.20 M **6** in 1.0 M TMEDA/toluene recorded at –60 °C.

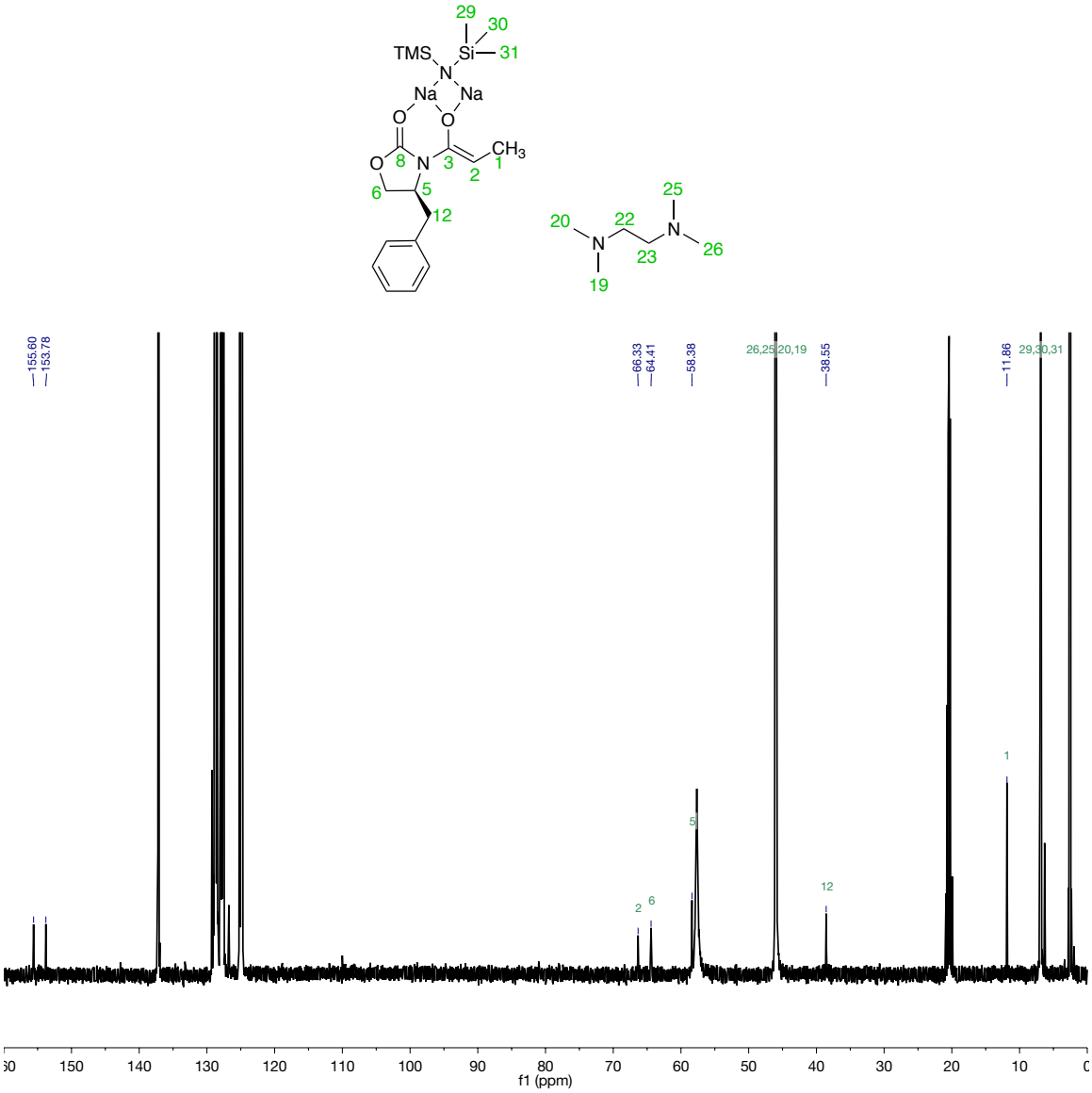
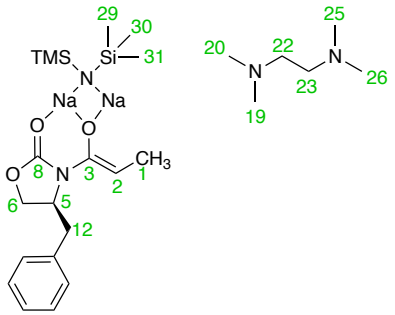


Figure S72. ^{13}C NMR spectrum of 0.20 M **6** in 1.0 M TMEDA/toluene recorded at –60 °C.

Parameter	Value
1 Solvent	toluene
2 Temperature	-60.0
3 Pulse Sequence	gHSQCAD
4 Number of Scans	2
5 Receiver Gain	30
6 Relaxation Delay	1.0000
7 Pulse Width	7.5000
8 Acquisition Time	0.1499



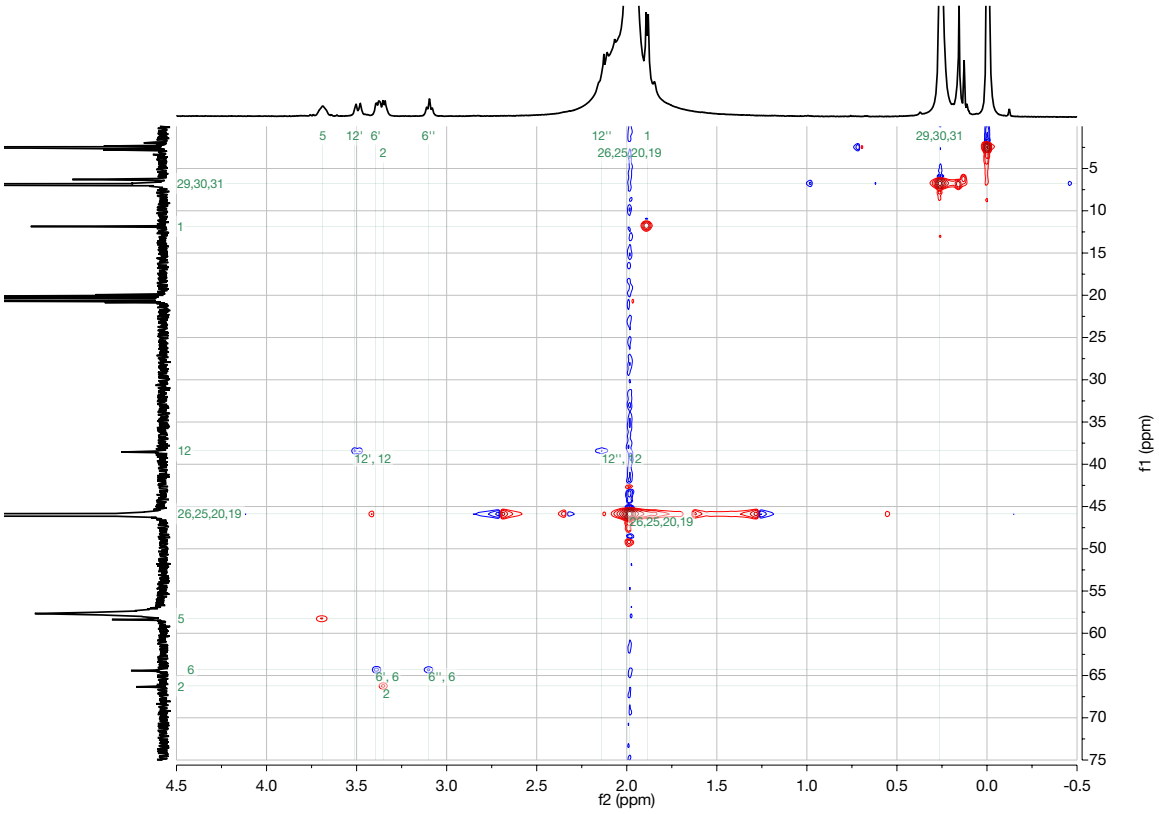
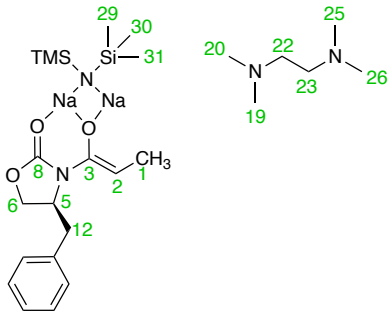


Figure S73. HSQC spectrum of 0.20 M **6** in 1.0 M TMEDA/toluene recorded at –60 °C.

Parameter	Value
1 Solvent	toluene
2 Temperature	-60.0
3 Pulse Sequence	ROESYAD
4 Number of Scans	2
5 Receiver Gain	0
6 Relaxation Delay	1.0000
7 Pulse Width	7.5000
8 Acquisition Time	0.4001



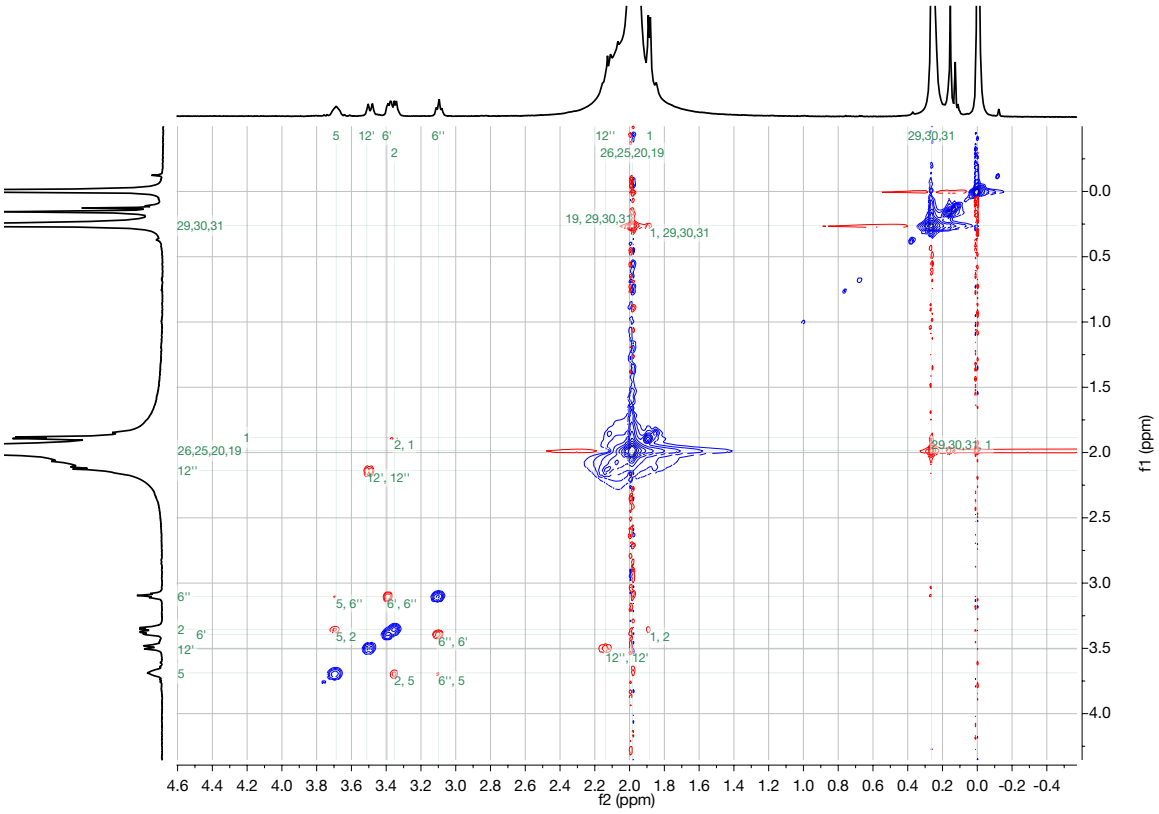


Figure S74. ROESY spectrum of 0.20 M **6** in 1.0 M TMEDA/toluene recorded at –60 °C.

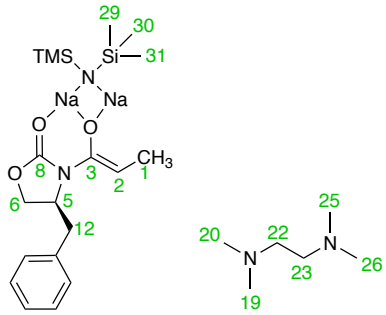


Table S2. ^{1}H and ^{13}C chemical shift assignments for mix dimer **6**.

Atom #	δC, ppm	δH, ppm	ROESY
1	11.86	1.88	2, 29
2	55.23	3.35	1, 5
3	153.78	-	-
5	58.26	3.69	2, 6”
6	64.31	3.39 (6’)	6”
		3.10 (6”)	5, 6’
8	155.60	-	-
12	38.41	3.51 (12’)	12”
		2.14 (12”)	12’
19, 20, 25, 26	45.87	1.98	29
22, 23	57.66	1.98	-
29, 30, 31	6.75	0.26	1, 19

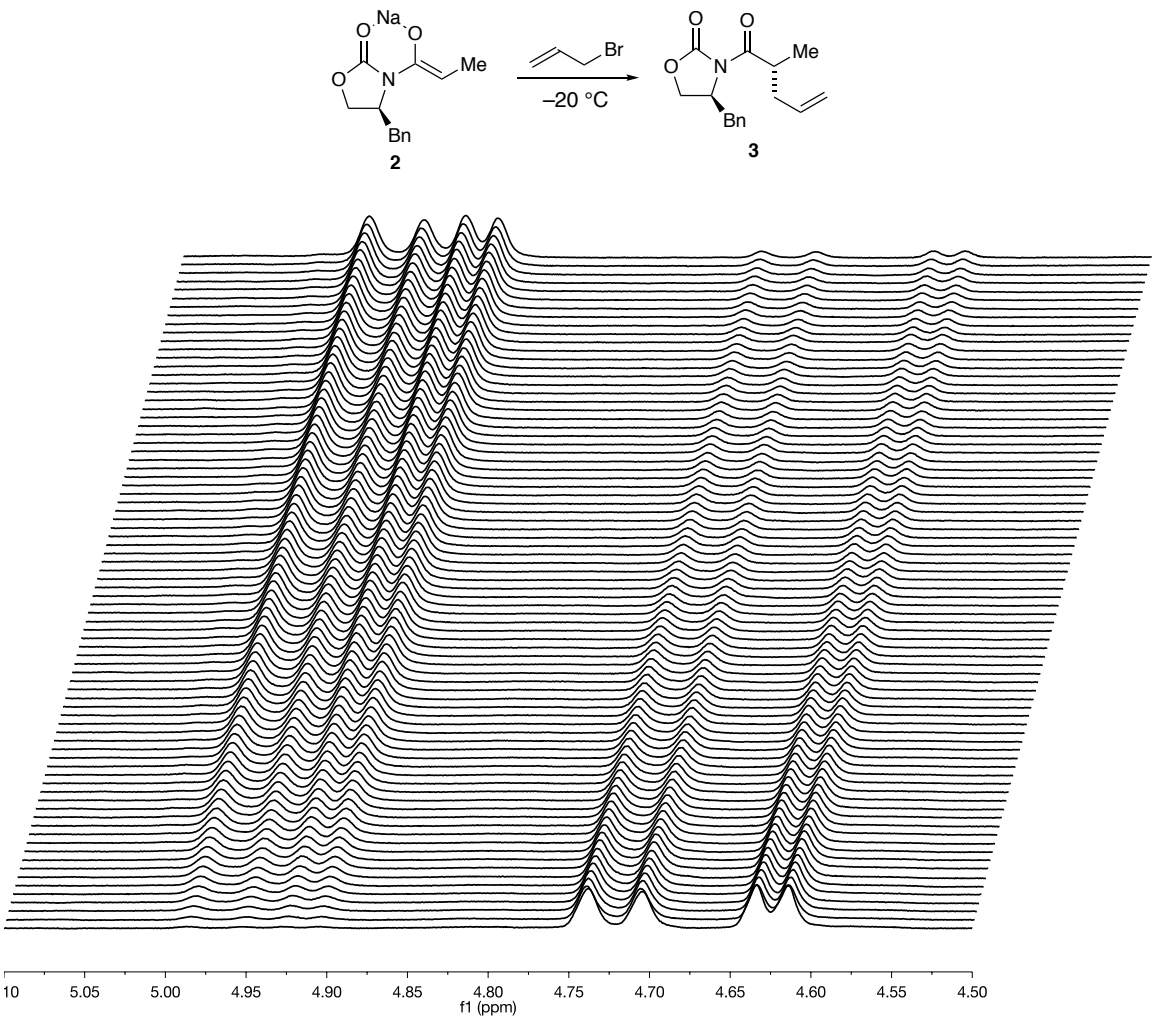


Figure S75. ^{1}H NMR spectra following reaction of 0.40 M (*S*)-**2** with 0.010 M allyl bromide in 1.0 M TMEDA/toluene recorded at –20 °C at 1 spectrum per minute. The alkylation reaction is followed to completion. Both the growth of product and decay of starting material follow a first-order function.

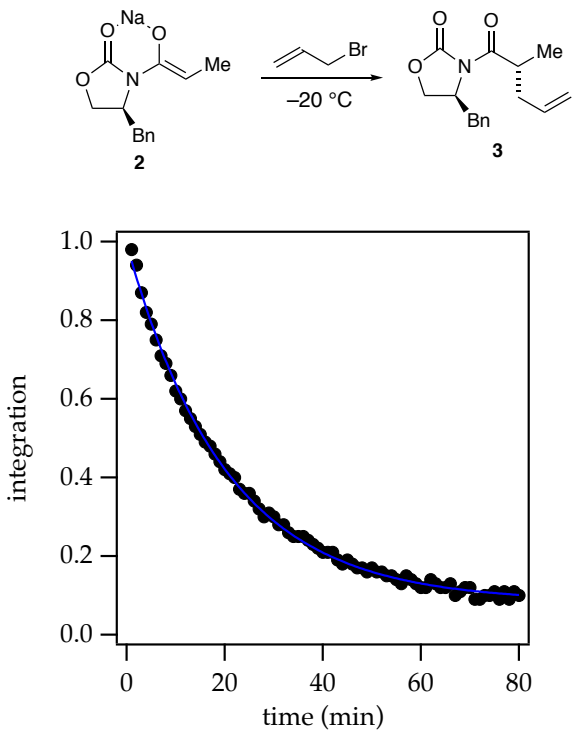


Figure S76. Plot following loss of allyl bromide in 0.40 M (*S*)-**2** and 0.010 M allyl bromide in 1.0 M TMEDA/toluene at –20 °C.

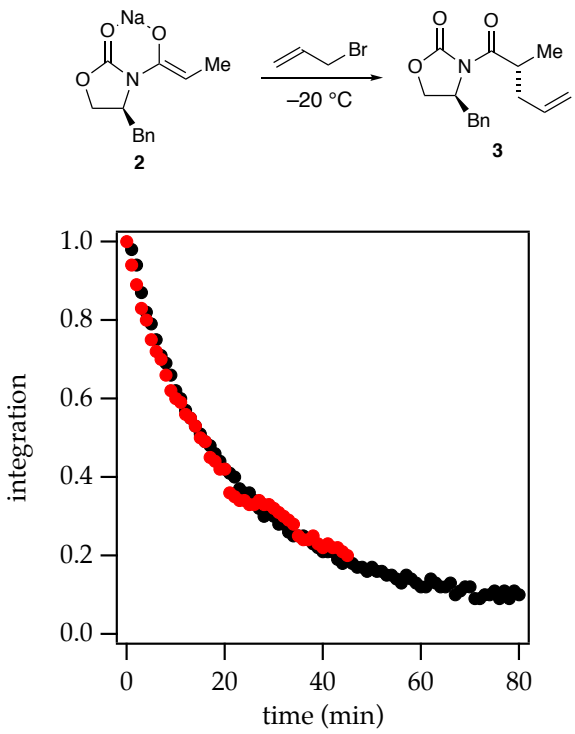


Figure S77. Plot following loss of allyl bromide in 0.40 M (*S*)-**2** and second injection of 0.010 M allyl bromide in 1.0 M TMEDA/toluene at –20 °C.

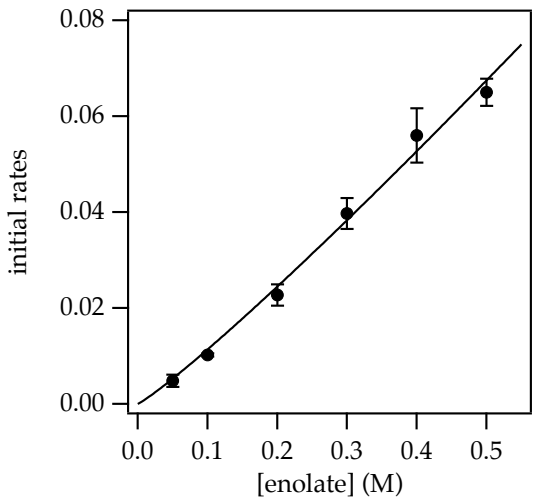


Figure S78. Plot of initial rates vs [enolate]. $y = ax^n$, $a = 0.15 \pm 0.01$, $n = 1.11 \pm 0.08$. The reaction is first order in enolate.

[(*S*)-**2**] (M)	TMEDA (M)	AllylBr (M)	Run 1	Run 2
0.050	0.10	0.010	0.0039286	0.0057692
0.10	0.20	0.010	0.01	0.010455
0.20	0.40	0.010	0.024286	0.021143
0.30	0.60	0.010	0.037429	0.042
0.40	0.80	0.010	0.052	0.06
0.50	1.0	0.010	0.063	0.067

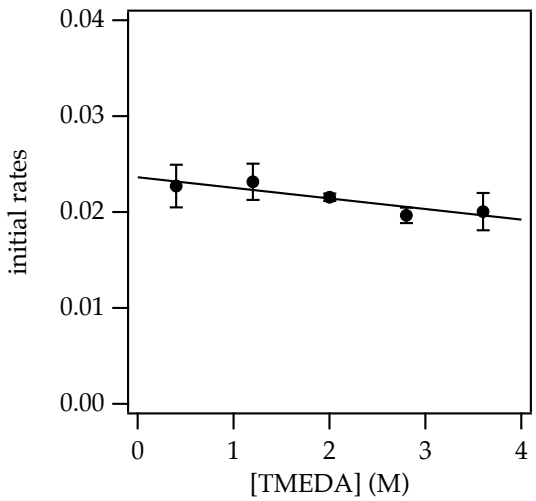


Figure S79. Plot of initial rates vs [TMEDA]. $y = ax + b$, $a = -0.0011 \pm 0.0003$, $b = 0.0236 \pm 0.0007$. The reaction is zeroth order in TMEDA.

[(*S*)-**2**] (M)	TMEDA (M)	AllylBr (M)	Run 1	Run 2
0.20	0.8	0.010	0.021143	0.024286
0.20	1.6	0.010	0.0245	0.021833
0.20	2.4	0.010	0.021818	0.021273
0.20	3.2	0.010	0.019091	0.020238
0.20	4.0	0.010	0.021429	0.018667

(4S)-4-benzyl-3-((2R)-2-methylpent-4-enoyl)-2-oxazolidinone (**3**). To a solution of NaHMDS (0.60 mmol, 110 mg) and TMEDA (1.2 mmol, 180 μL) in 4.5 mL toluene under argon at –78 °C was added **1** (0.50 mmol, 116.5 mg) in 0.50 mL toluene. After stirring for 30 minutes, allyl bromide (3.0 mmol, 260 μL) was injected, and the vessel was warmed to 0 °C. The reaction was quenched by 5.0 mL saturated NH_4Cl and extracted three times with EtOAc. The organic extracts were dried over $MgSO_4$ and concentrated in vacuo. Flash chromatography with 20% ethyl acetate in hexanes provided 132 mg (97% yield) shown by ^{1}H NMR spectroscopy to be a 20:1 diastereomeric mixture of **3** and its isomer analogous to that reported previously. ^{1}H NMR (599 MHz, $CDCl_3$) δ 7.36 – 7.31 (m, 2H), 7.30 – 7.26 (m, 1H), 7.24 – 7.20 (m, 2H), 5.83 (ddt, *J* = 17.2, 10.2, 7.1 Hz, 1H), 5.11 (dq, *J* = 17.1, 1.6 Hz, 1H), 5.07 (ddt, *J* = 10.1, 2.0, 1.1 Hz, 1H), 4.69 (ddt, *J* = 9.9, 7.6, 3.2 Hz, 1H), 4.19 (dd, *J* = 8.4, 7.7 Hz, 1H), 4.16 (dd, *J* = 9.1, 3.0 Hz, 1H), 3.87 (h, *J* = 6.8 Hz, 1H), 3.29 (dd, *J* = 13.4, 3.4 Hz, 1H), 2.70 (dd, *J* = 13.4, 9.8 Hz, 1H), 2.53 (dtt, *J* = 13.7, 6.8, 1.3 Hz, 1H), 2.24 (dtt, *J* = 14.0, 7.0, 1.2 Hz, 1H), 1.19 (d, *J* = 6.8 Hz, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 176.67, 153.26, 135.52, 135.41, 129.56, 129.09, 127.47, 117.37, 66.16, 55.55, 38.26, 38.13, 37.30, 16.59.

Schmidt, B.; Wildemann, H. *J. Chem. Soc., Perkin Trans. 1,* **2002**, 1050.

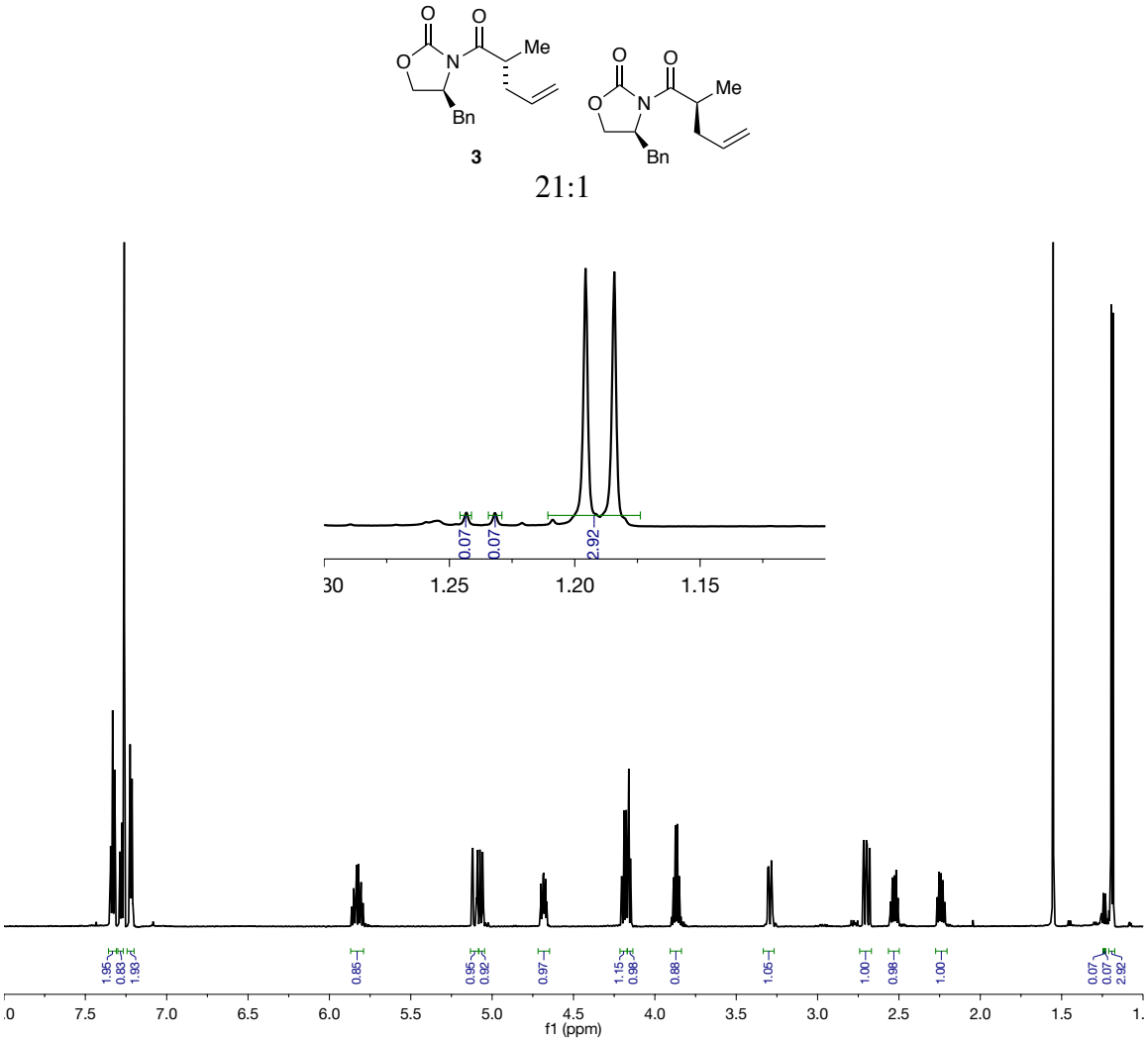


Figure S80. ^{1}H NMR spectrum of **3** prepared from monomer **4** recorded in $CDCl_3$ at rt. An isolated yield of 97% was obtained. The integration provides a selectivity of 21:1.

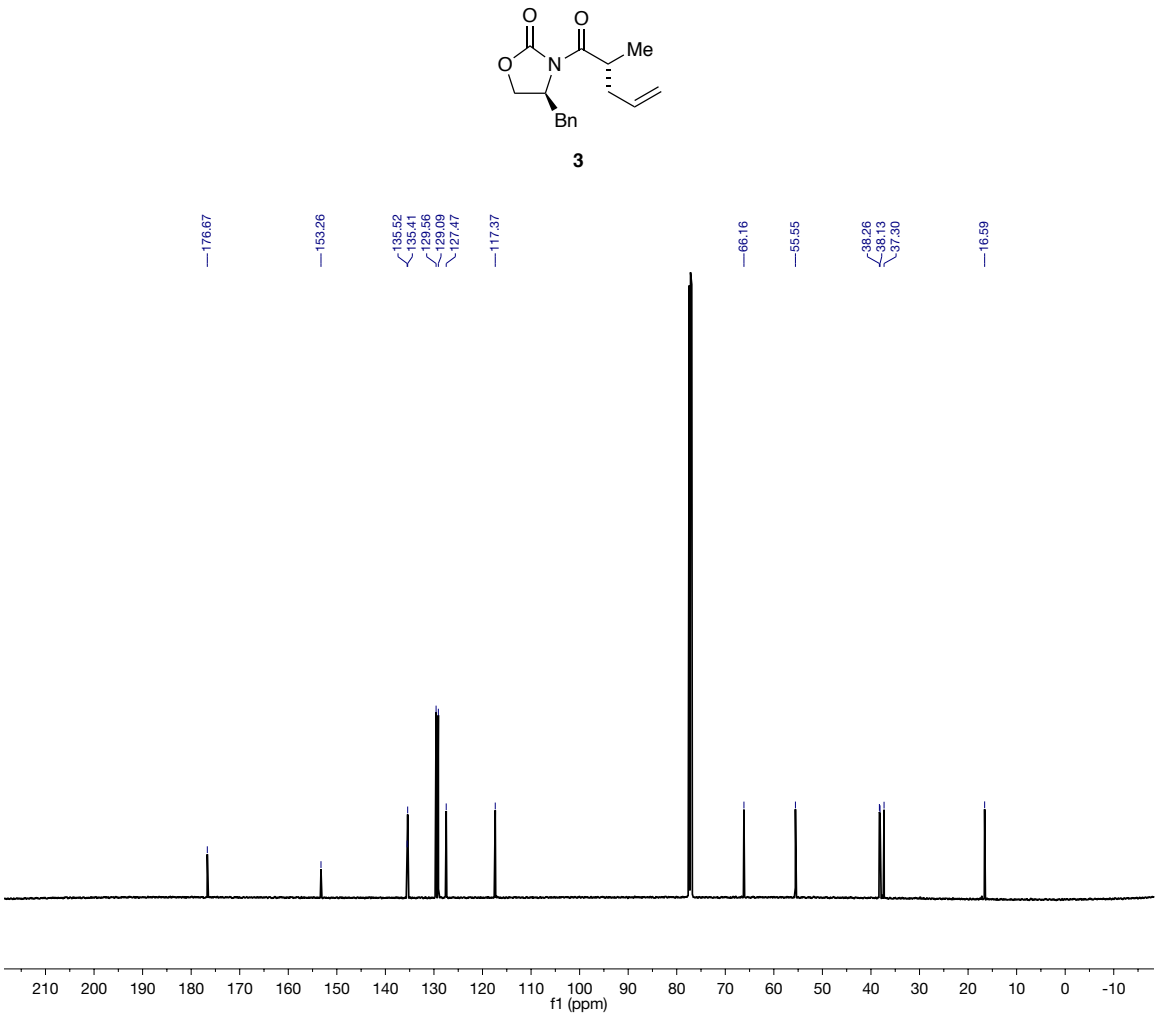


Figure S81. ^{13}C NMR spectrum ($CDCl_3$, 25 °C) of **3**.

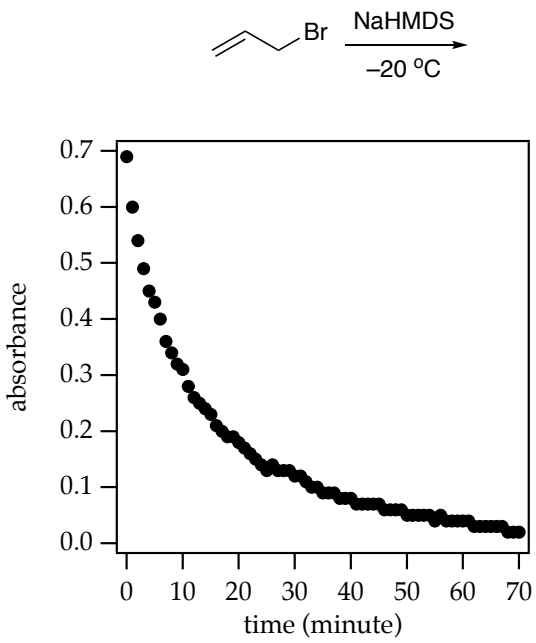


Figure S82. Plot following reaction of 0.20 M NaHMDS and 0.020 M allyl bromide in 0.40 M TMEDA/toluene recorded at –20 °C at 1 spectrum per minute. NaHMDS reacts with allyl bromide, making it difficult to study the allylation of mixed dimer **7**.

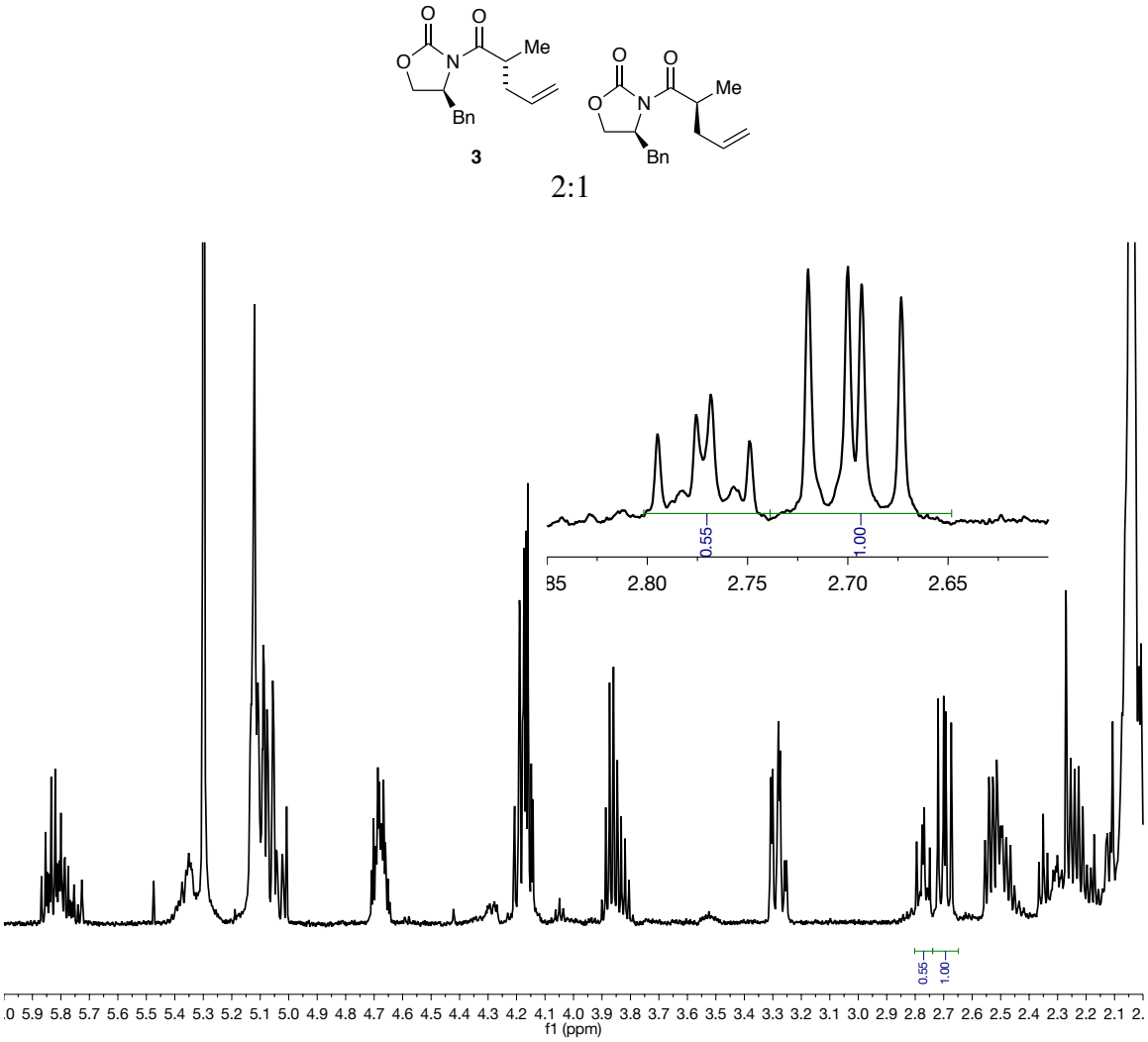


Figure S83. ^{1}H NMR ($CDCl_3$, 25 °C) spectrum of **3** prepared from **6**. The integration provides a selectivity of 2:1, significantly lower than the allylation of monomer **4**.

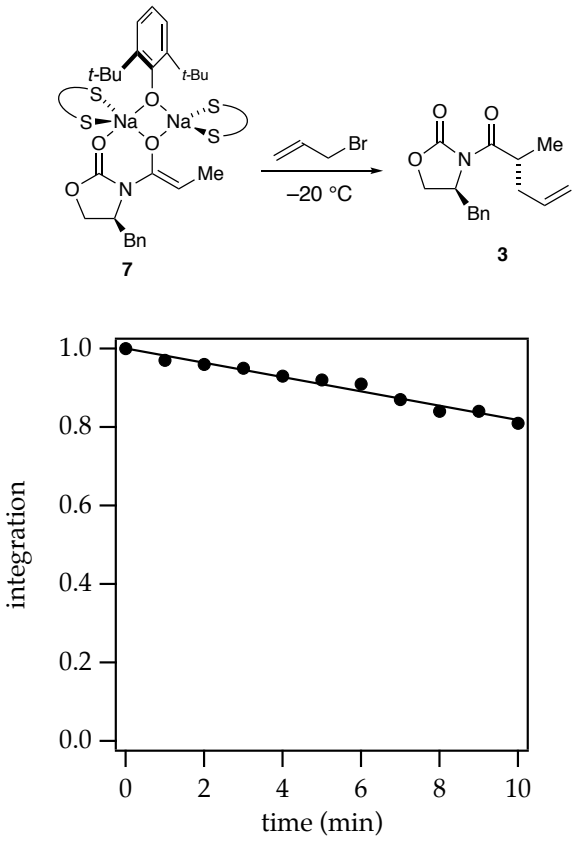


Figure S84. Plot following reaction of 0.40 M NaHMDS, 0.20 M **7**, and 0.020 M allyl bromide in 0.80 M TMEDA/toluene recorded at –20 °C at 1 spectrum per minute. $k_{obsd} = 0.0183 \pm 0.0009$. $k_7/k_4 = 0.81$. Allylation of phenolate-derived mixed dimer **7** is slightly slower than the allylation of monomer **4**.

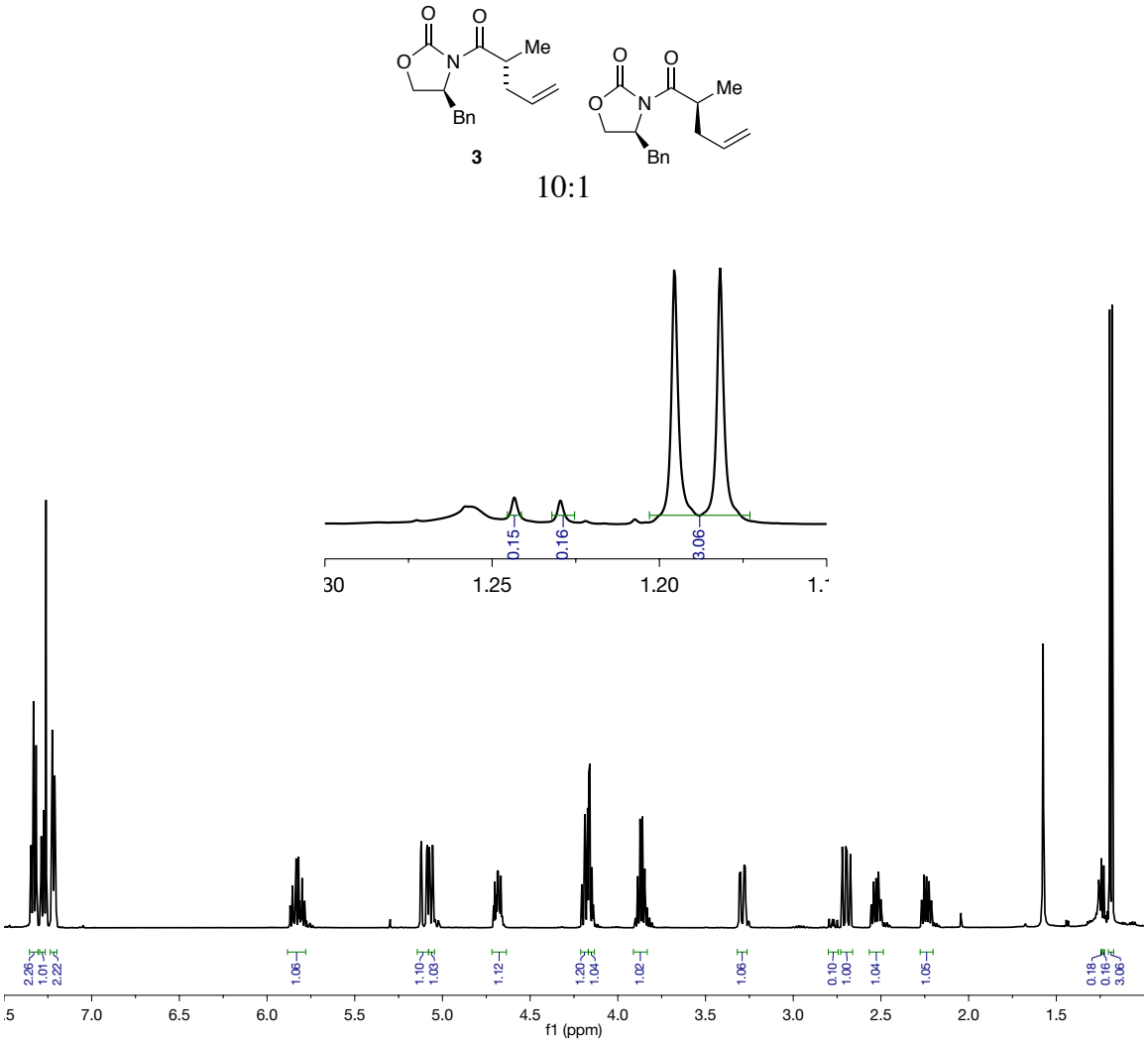


Figure S85. ^{1}H NMR spectrum ($CDCl_3$, 25 °C) of **3** prepared from **7** in $CDCl_3$ recorded at rt. An isolated yield of 86% was obtained. The integration provides a selectivity of 10:1, lower than the monomer reaction.

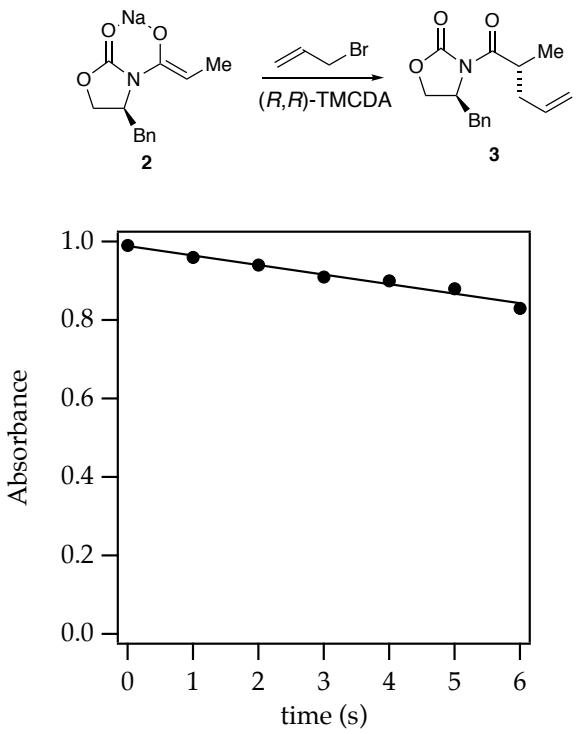


Figure S86. Plot following reaction of 0.20 M (*S*)-**2** and 0.020 M allyl bromide in 0.40 M (*R*,*R*)-TMCDA in toluene recorded at –20 °C at 1 spectrum per minute. k_{obsd} = 0.024 ± 0.002. $k_{(R,R)\text{-TMCDA}}/k_{\text{TMEDA}}$ = 1.1.

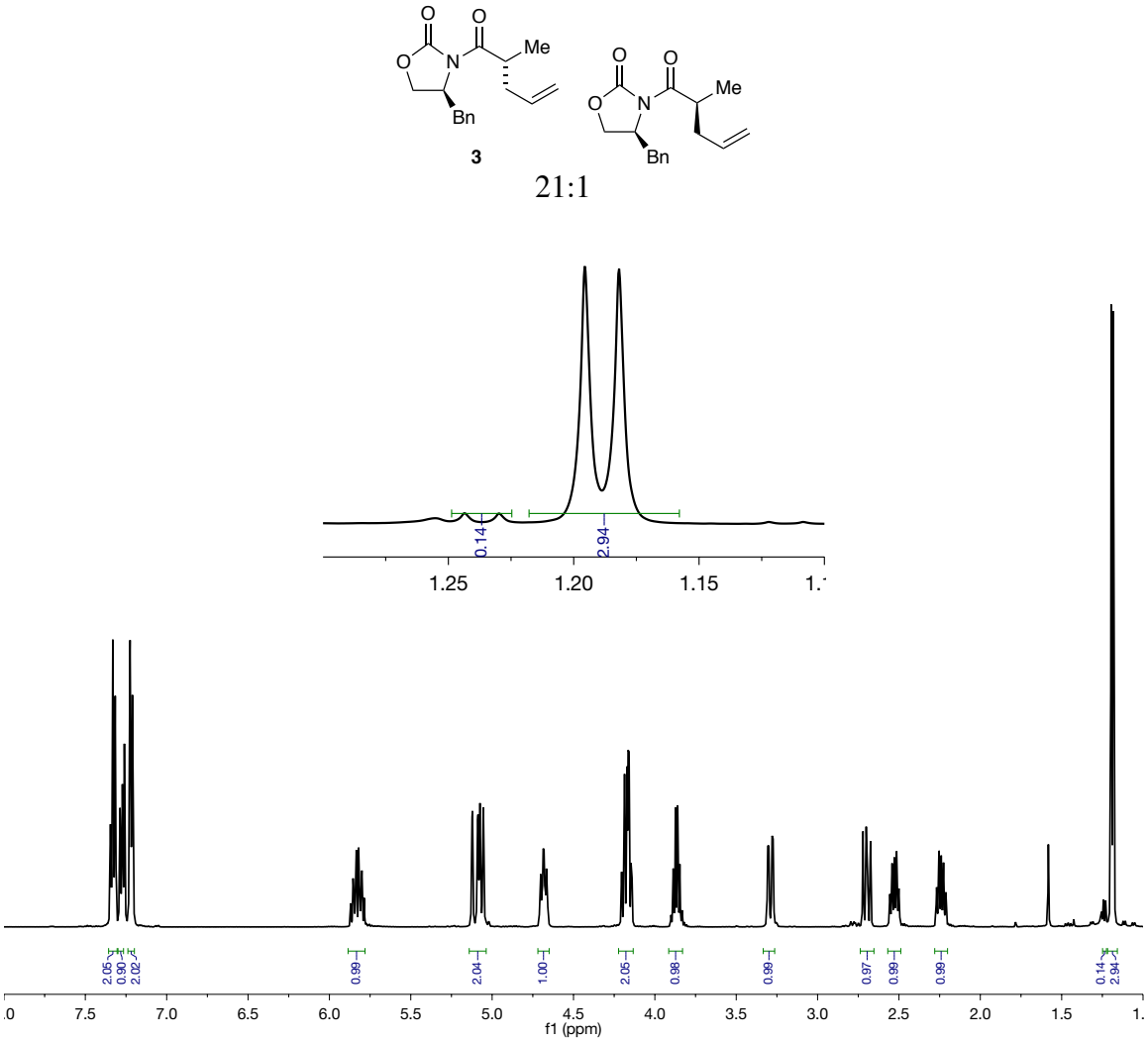


Figure S87. ^{1}H NMR spectrum ($CDCl_3$, 25 °C) of **3** prepared from **4** in (*R*,*R*)-TMCDA. An isolated yield of 87% was obtained. The integration provides a selectivity of 21:1, indistinguishable from that obtained from monomer **4**.

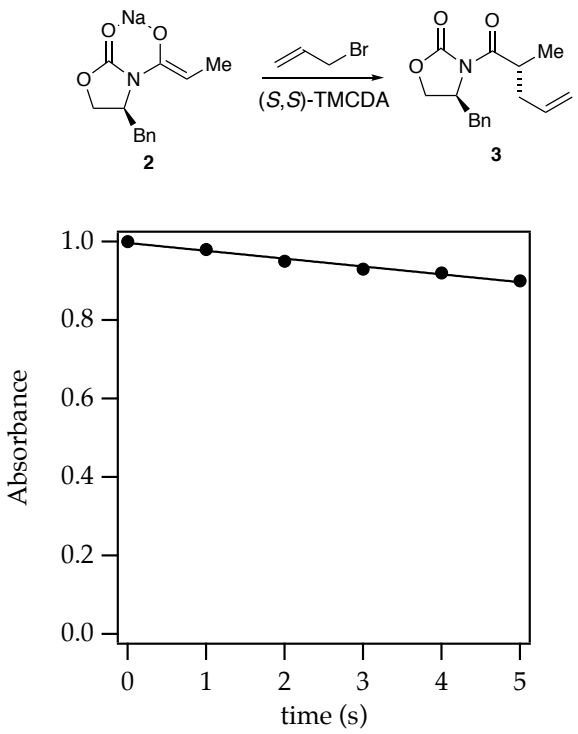


Figure S88. Plot following reaction of 0.20 M (*S*)-**2** and 0.020 M allyl bromide in 0.40 M (*S*,*S*)-TMCDA in toluene recorded at –20 °C at 1 spectrum per minute. $k_{obsd} = 0.020 \pm 0.001$. $k_{(S,S)\text{-TMCDA}}/k_{TMEDA} = 0.9$.

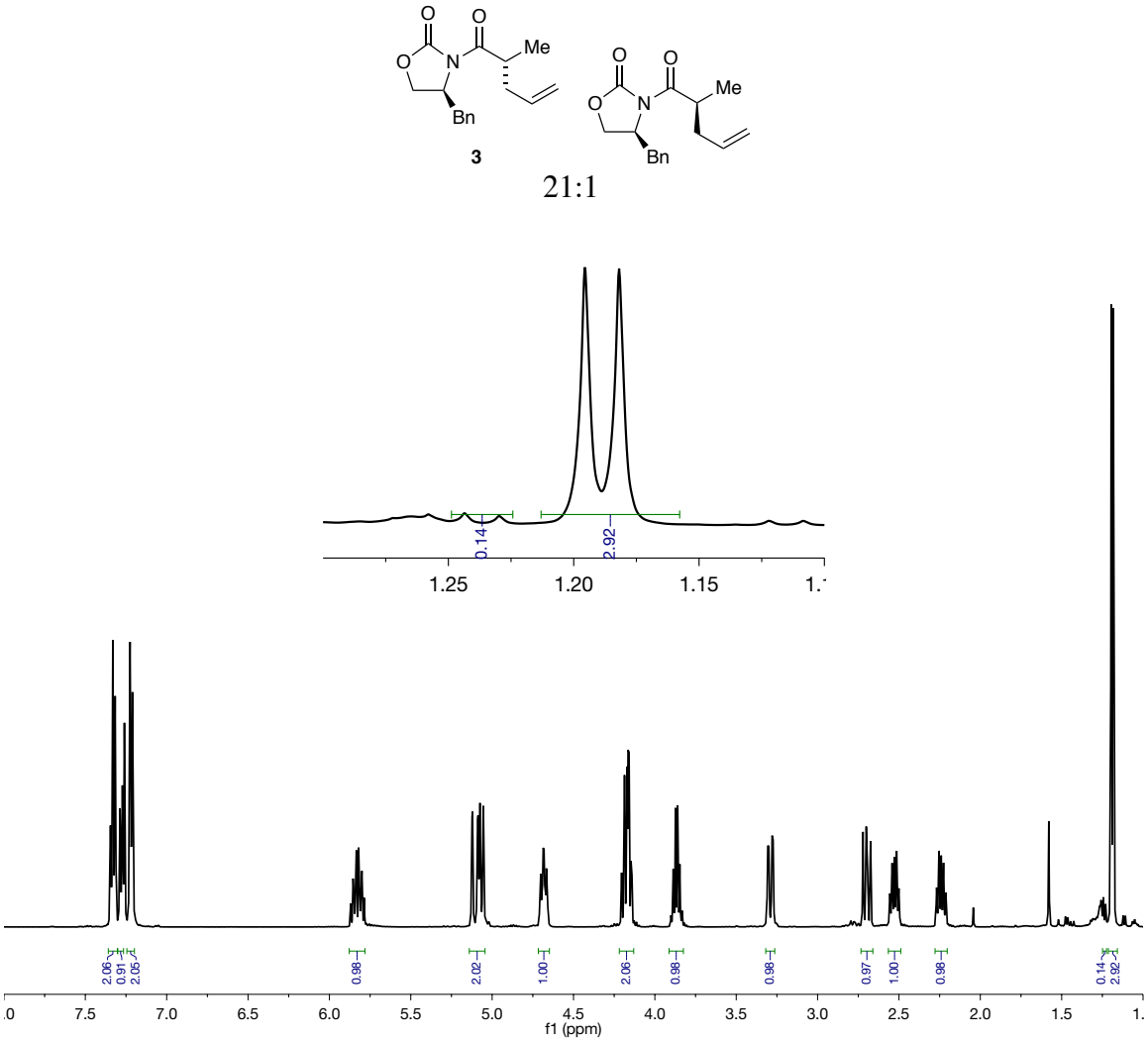


Figure S89. ^{1}H NMR spectrum ($CDCl_3$, 25 °C) of **3** prepared from **4** in (*S*,*S*)-TMCDA. An isolated yield of 90% was obtained. The integration provides a selectivity of 21:1, which is the same as that obtained from monomer **4**.

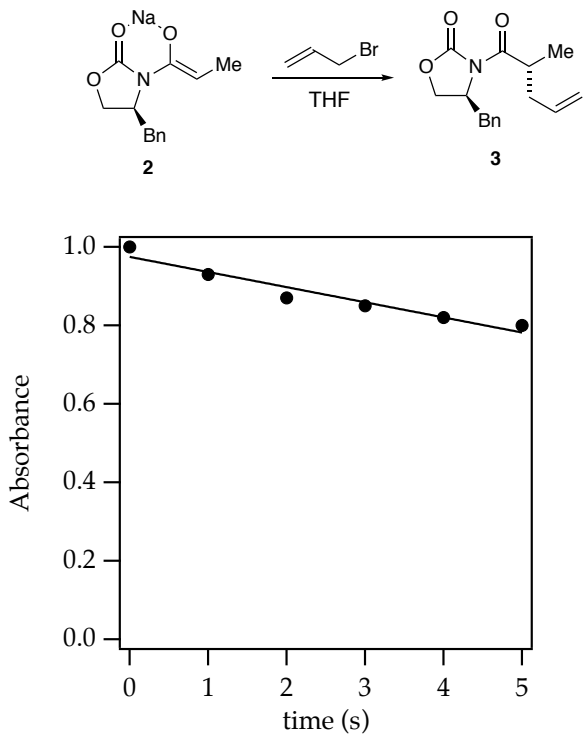


Figure S90. Plot following reaction of 0.20 M NaHMDS, 0.20 M **1** and 0.020 M allyl bromide in THF recorded at –20 °C at 1 spectrum per minute. $k_{obsd} = 0.0396 \pm 0.005$. The allylation in THF is slightly faster than in TMEDA ($k_{THF}/k_{TMEDA} = 1.7$).

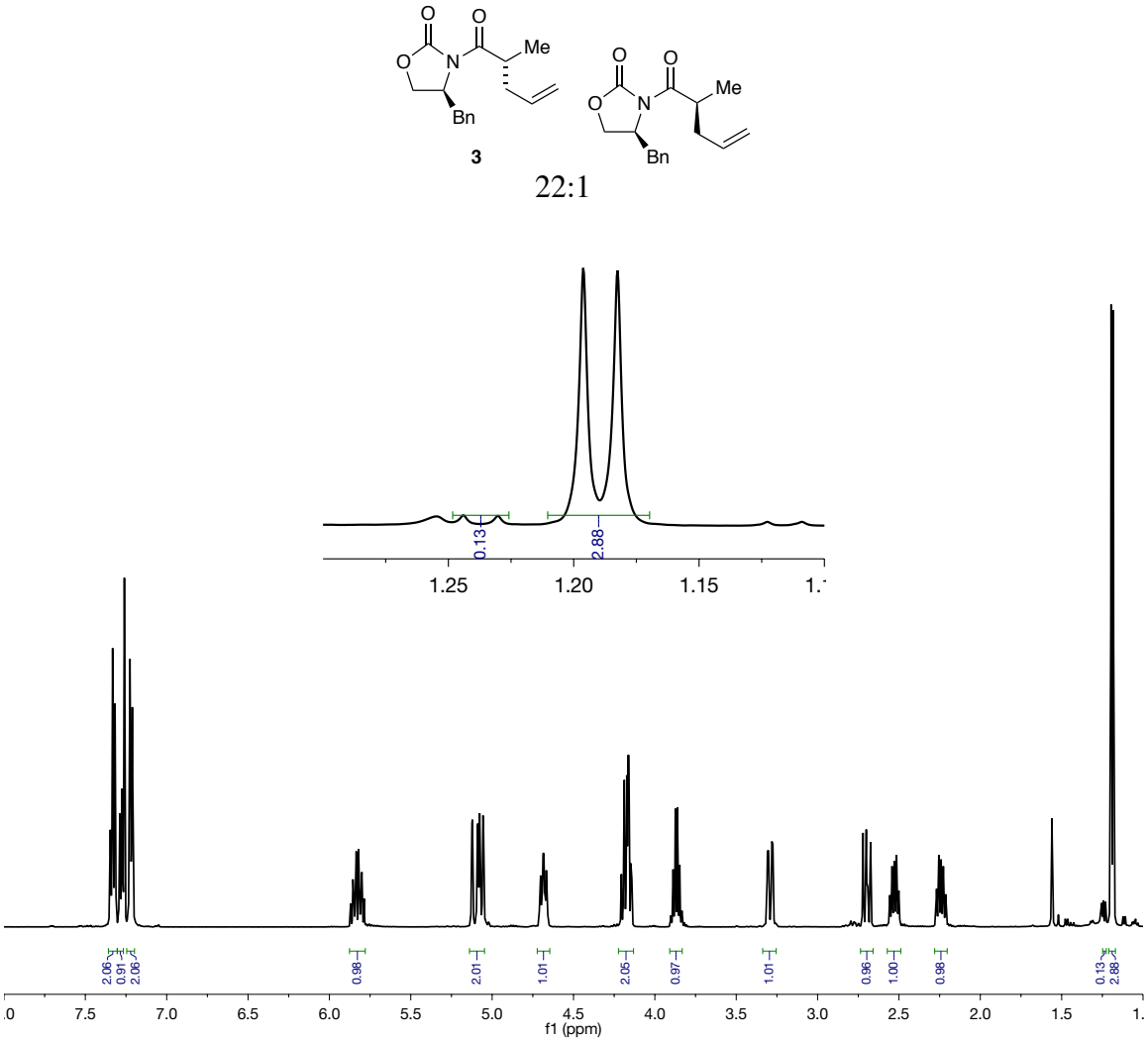


Figure S91. ^{1}H NMR spectrum ($CDCl_3$, 25 °C) of **3** prepared from (*S*)-**2** in THF
An isolated yield of 83% was obtained. The integration provides a selectivity of 22:1, same as the monomer reaction.

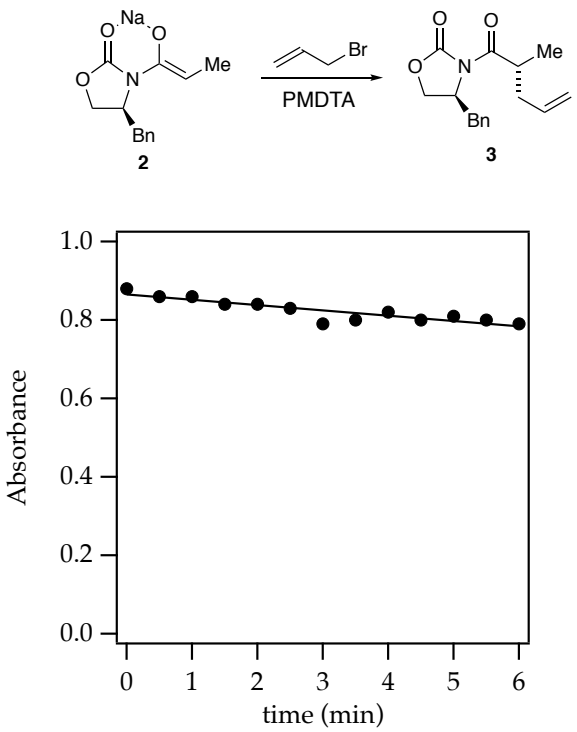


Figure S92. Plot following reaction of 0.10 M **2** and 0.10 M allyl bromide in 0.20 M PMDTA recorded at –20 °C at 1 spectrum per minute. $k_{obsd} = 0.0135 \pm 0.002$. The allylation in PMDTA is slightly faster than in TMEDA ($k_{PMDTA}/k_{TMEDA} = 1.3$).

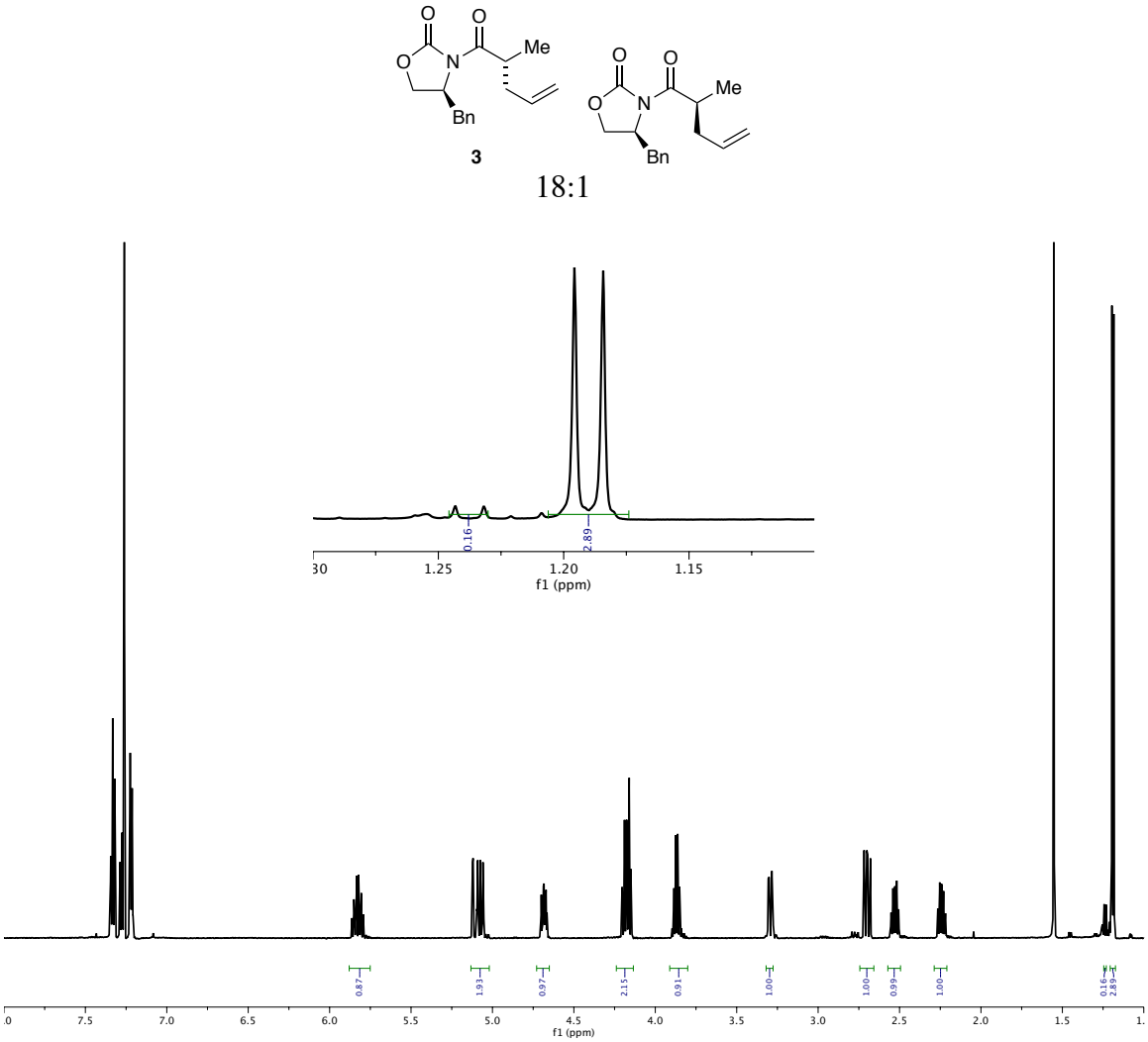


Figure S93. ^{1}H NMR spectrum ($CDCl_3$, 25 °C) of **3** prepared from (*S*)-**2** in PMDTA An isolated yield of 92% was obtained. The integration provides a selectivity of 18:1.

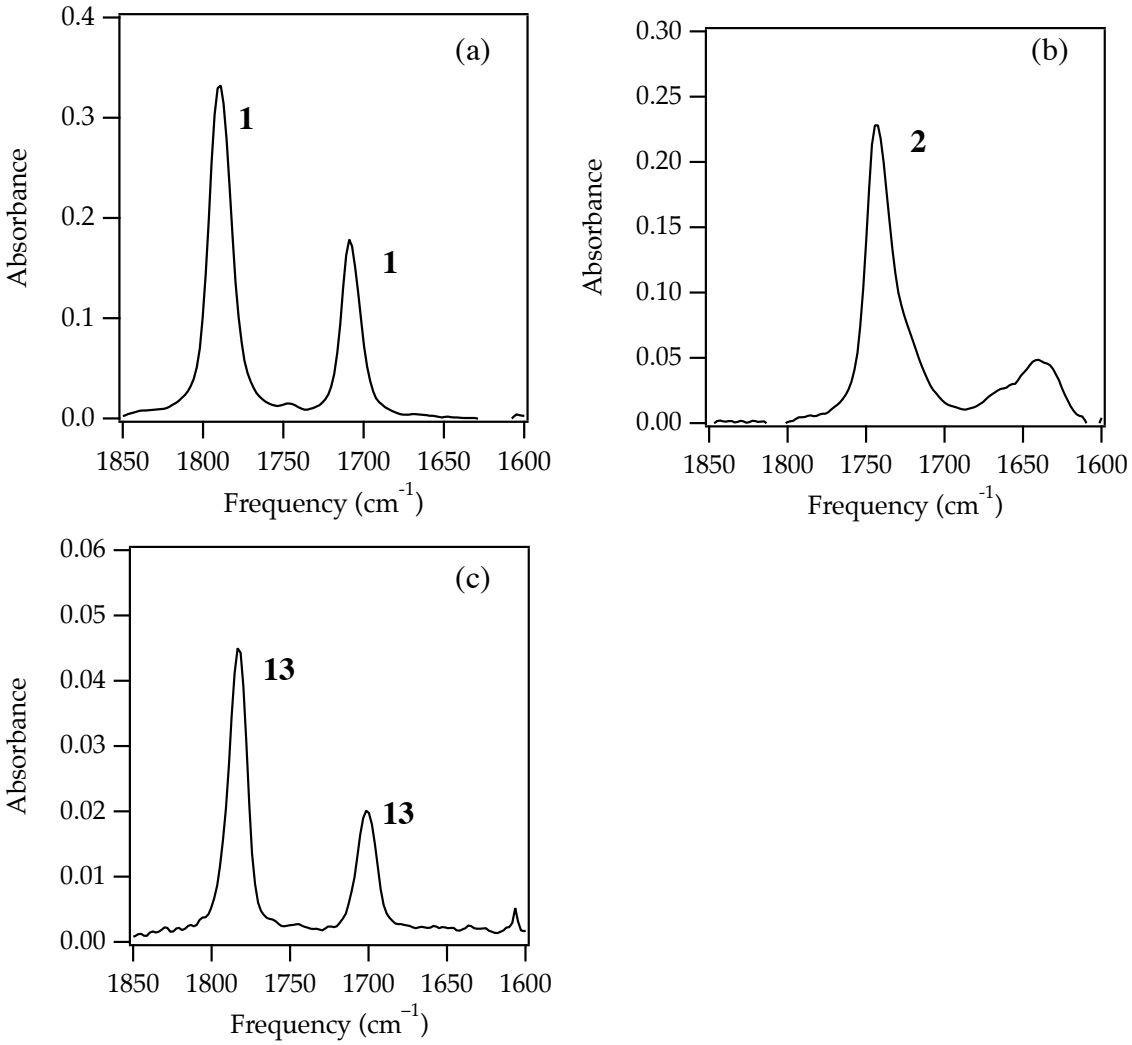


Figure S94. IR spectra of (a) 0.10 M **1** in toluene; (b) 0.10 M **2** in 1.0 M TMEDA/toluene; (c) 0.010 M **13** in toluene recorded at –78 °C.

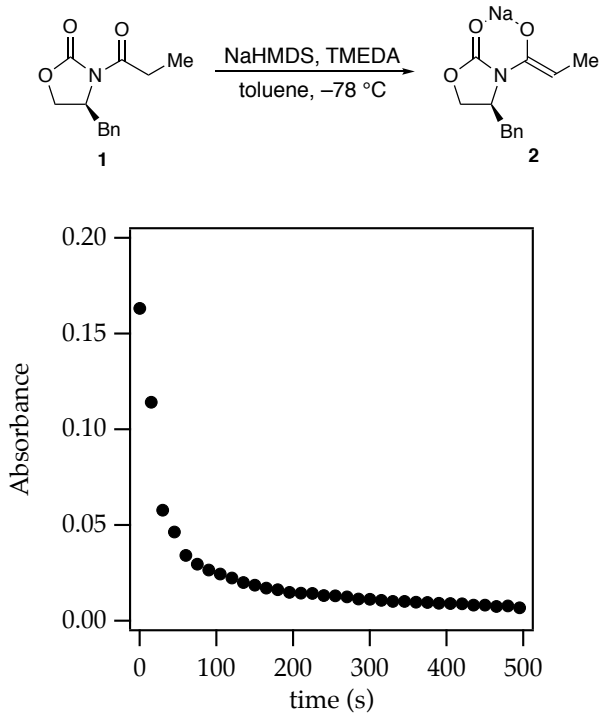


Figure S95. IR spectrum following loss of **1** in a solution of 0.10 M **1** and 0.11 M NaHMDS in 1.0 M TMEDA/toluene recorded at –78 °C.
Enolization of **1** is fast even at stoichiometric condition at low temperature.

(4S)- 4-benzyl-3-((2R)-2-methyl-3-phenylpropanoyl)-2-oxazolidinone (**13**). To a solution of NaHMDS (3.3 mmol, 605 mg) and TMEDA (6.6 mmol, 988 μL) in 5.0 mL toluene under argon at –78 °C was added **1** (3.0 mmol, 699 mg) in 1.0 mL of toluene. The reaction was stirred for 30 minutes, charged with benzyl bromide (20 mmol, 2.4 mL), warmed to 0 °C, and stirred for 0.5 h. The reaction was quenched with 5.0 mL saturated NH_4Cl and extracted three times with EtOAc. The organic extracts were dried over $MgSO_4$ and concentrated in vacuo. Flash chromatography with 20% ethyl acetate in hexanes afforded 825 mg of **13** (85% combined yield) displaying spectroscopic properties described previously.[1] ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.31 – 7.29 (m, 2H), 7.29 – 7.27 (m, 2H), 7.26 – 7.25 (m, 3H), 7.23 – 7.17 (m, 1H), 7.08 – 7.03 (m, 2H), 4.67 (ddt, *J* = 9.3, 7.9, 3.2 Hz, 1H), 4.20 – 4.08 (m, 3H), 3.15 (dd, *J* = 13.2, 7.3 Hz, 1H), 3.07 (dd, *J* = 13.5, 3.4 Hz, 1H), 2.68 (dd, *J* = 13.3, 7.6 Hz, 1H), 2.55 (dd, *J* = 13.5, 9.3 Hz, 1H), 1.19 (d, *J* = 6.8 Hz, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 176.56, 153.05, 139.18, 135.17, 129.39, 129.37, 128.90, 128.34, 127.28, 126.41, 65.89, 55.10, 39.91, 39.57, 37.71, 16.76.

Schmidt, B.; Wildemann, H. *J. Chem. Soc., Perkin Trans. 1,* **2002**, 1050.

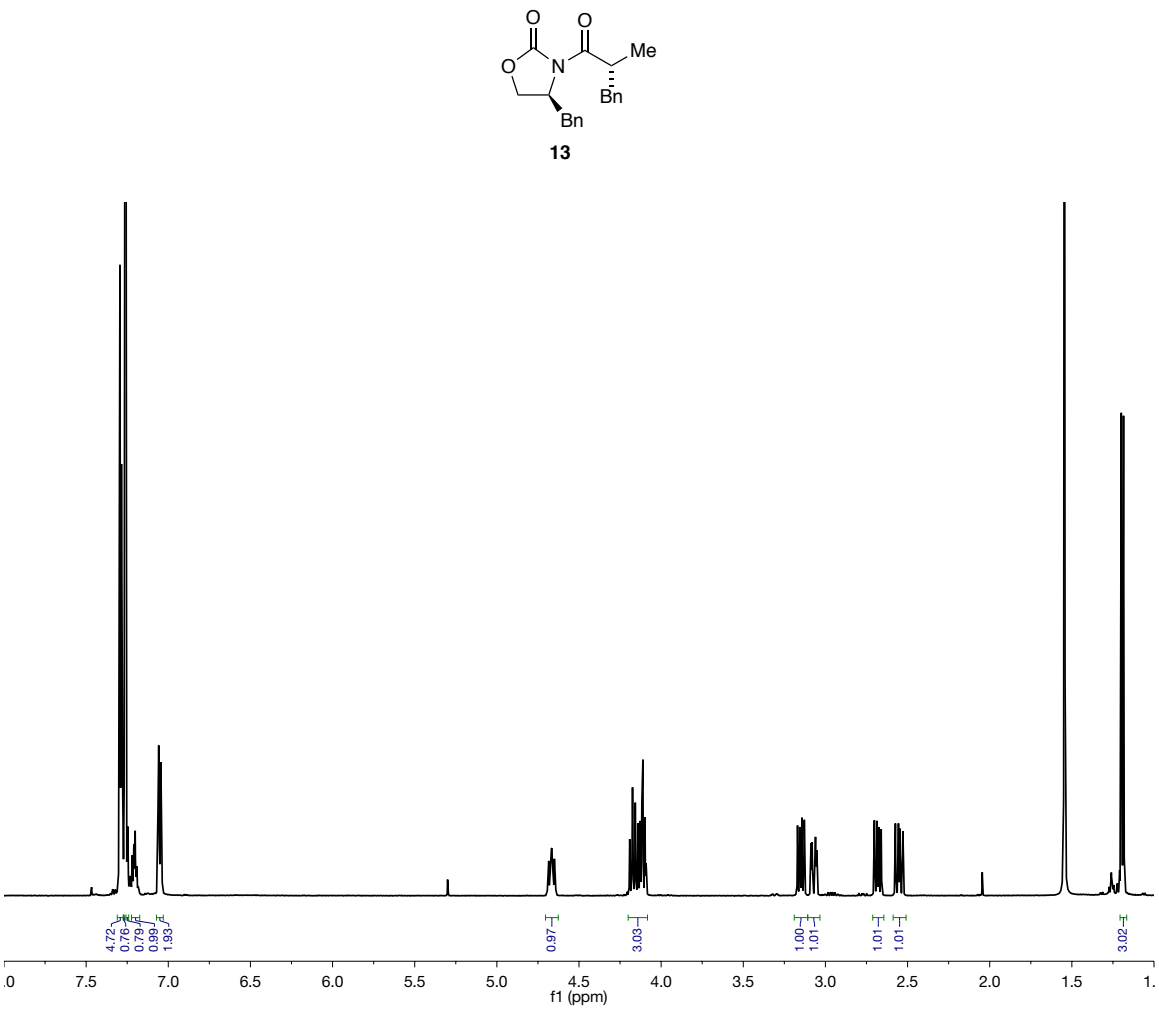


Figure S96. ^{1}H NMR spectrum ($CDCl_3$, 25 °C) of **13**.

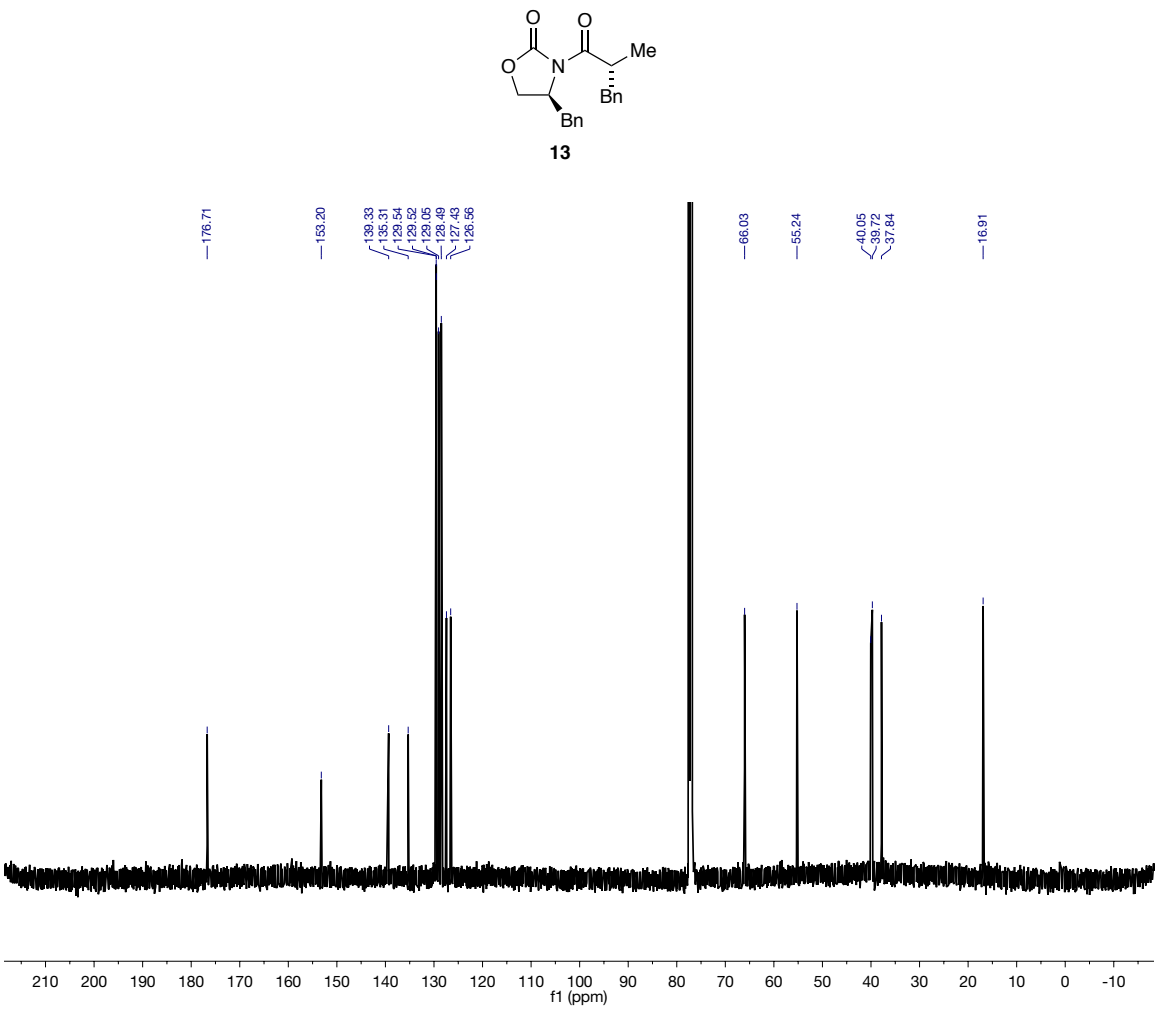


Figure S97. ^{13}C NMR spectrum ($CDCl_3$, 25 °C) of **13**.

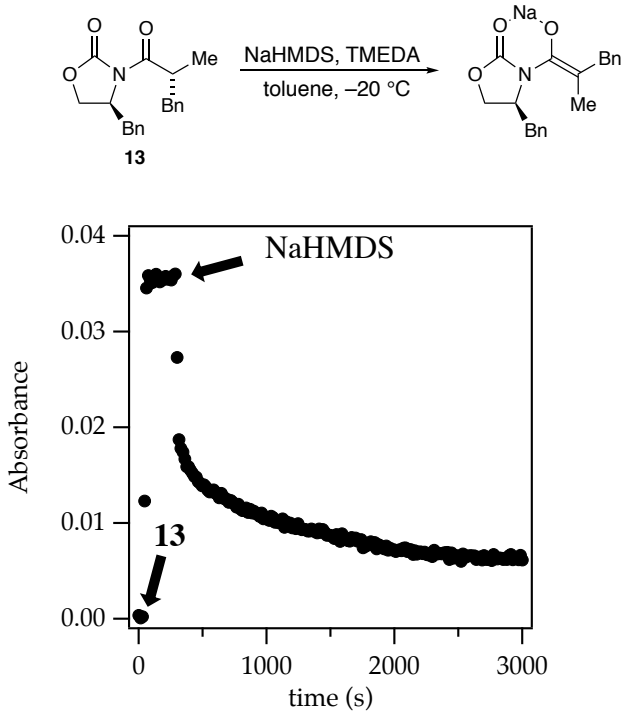


Figure S98. IR spectrum following loss of **13** in a solution of 0.010 M **13** and 0.015 M NaHMDS in 0.030 M TMEDA/toluene recorded at –20 °C.
The enolization is much slower than for non-branched enolates, demanding a higher reaction temperature which results in some deacylation.

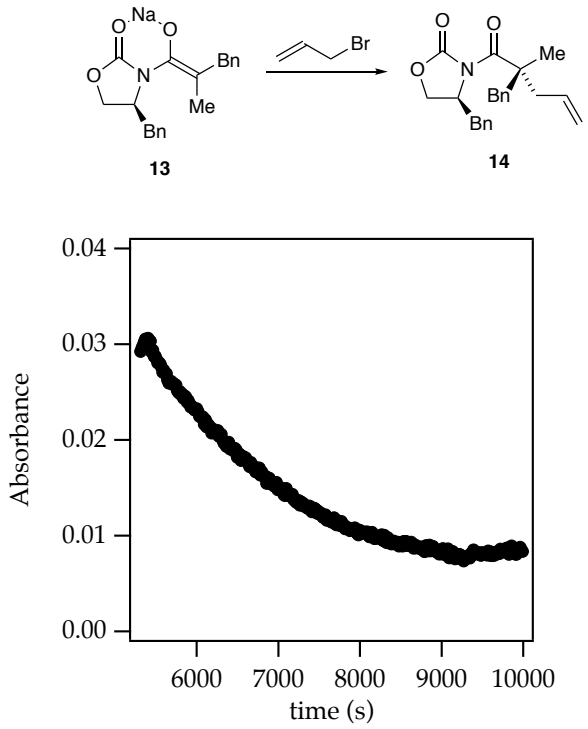


Figure S99. IR spectrum following loss of enolate **13** in a solution of 0.010 M **13**, 0.0050 M NaHMDS and 0.10 M allylbromide in 0.030 M TMEDA/toluene recorded from –20 °C to rt. The spectroscopy is often capricious owing to precipitation of NaBr disturbing the absorbance.

(*S*)-4-benzyl-3-((*S*)-2-benzyl-2-methylpent-4-enoyl)oxazolidin-2-one (**14**). To a solution of NaHMDS (0.10 mmol, 18.3 mg) and TMEDA (0.20 mmol, 30 μL) in toluene (2.0 mL) under argon was added **13** (0.070 mmol, 22.6 mg) in 0.10 mL of toluene. Reaction was stirred under argon for 1 hr at –20 °C. Allyl bromide (0.40 mmol, 35 μL) was injected, and the mixture was warmed to 0 °C over 2 hr. The reaction was quenched with 3.0 mL of saturated NH_4Cl and extracted three times with EtOAc. The organic extracts were dried over $MgSO_4$ and concentrated in vacuo. Flash chromatography with 15% ethyl acetate in hexanes afforded 13.7 mg of product (54% combined yield) shown to be an 11:1 mixture of **14** and its minor diastereomer. ^{1}H NMR (599 MHz, $CDCl_3$) δ 7.34 – 7.30 (m, 2H), 7.28 – 7.24 (m, 3H), 7.23 – 7.19 (m, 5H), 5.77 (dddd, *J* = 16.9, 10.1, 8.0, 6.7 Hz, 1H), 5.11 (dq, *J* = 17.0, 1.6 Hz, 1H), 5.06 (ddt, *J* = 10.0, 2.0, 1.0 Hz, 1H), 4.61 (ddt, *J* = 10.7, 6.7, 3.3 Hz, 1H), 4.15 – 4.10 (m, 2H), 3.61 (d, *J* = 13.6 Hz, 1H), 3.18 (dd, *J* = 13.2, 3.3 Hz, 1H), 3.12 – 3.04 (m, 2H), 2.61 (dd, *J* = 13.2, 10.6 Hz, 1H), 2.29 (ddt, *J* = 14.3, 6.7, 1.4 Hz, 1H), 1.36 (s, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 176.07, 152.77, 137.72, 135.94, 134.39, 130.58, 129.54, 129.06, 128.20, 127.38, 126.74, 118.27, 66.43, 58.32, 50.54, 42.01, 40.73, 38.01, 23.38. m/z calculated for $(M+H)^+$ 364.19072, found 364.19097.

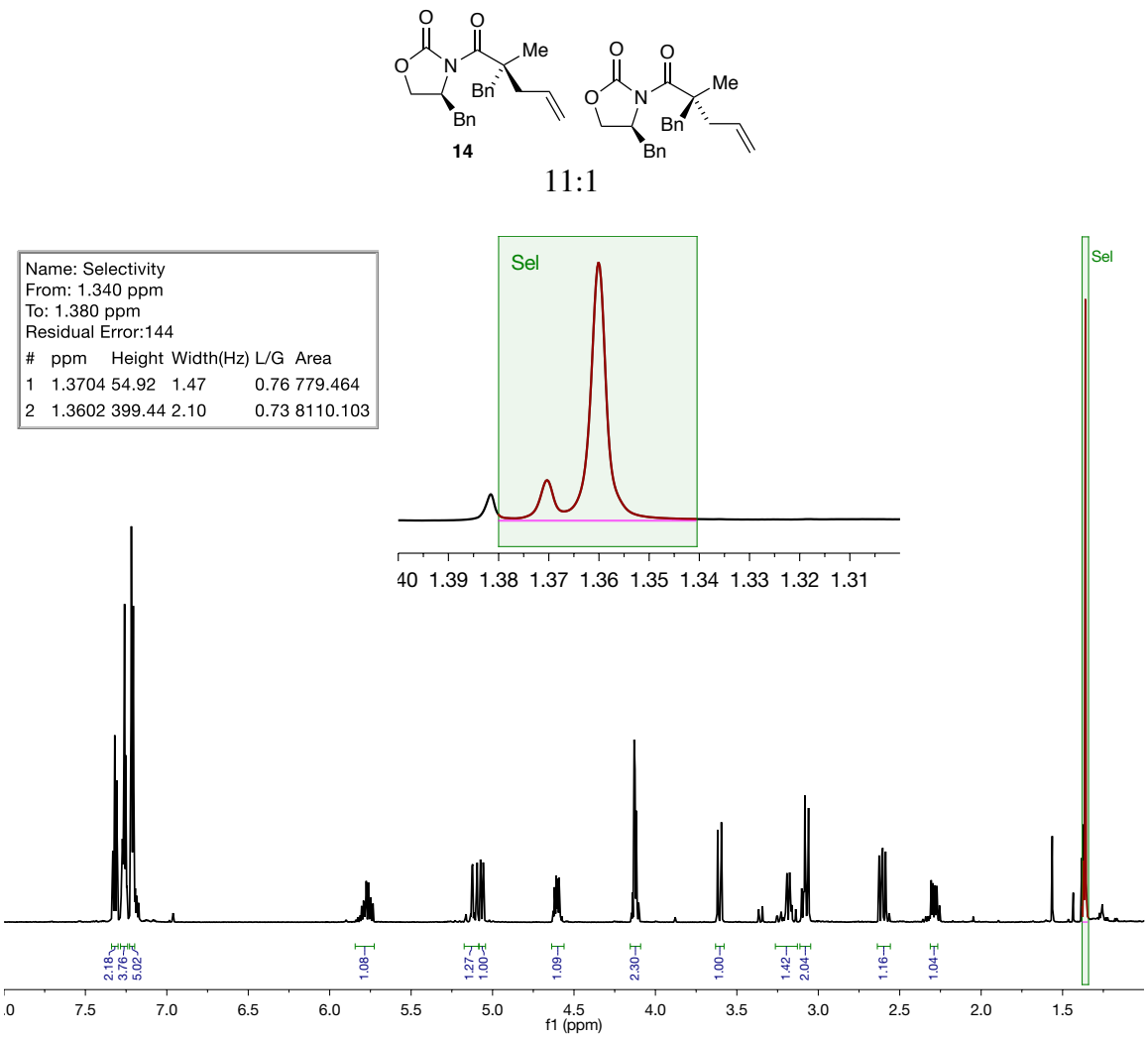


Figure S100. ^{1}H NMR spectrum ($CDCl_3$, 25 °C) of **14**. An isolated yield of 54% was obtained. The integration shows an 11:1 selectivity.

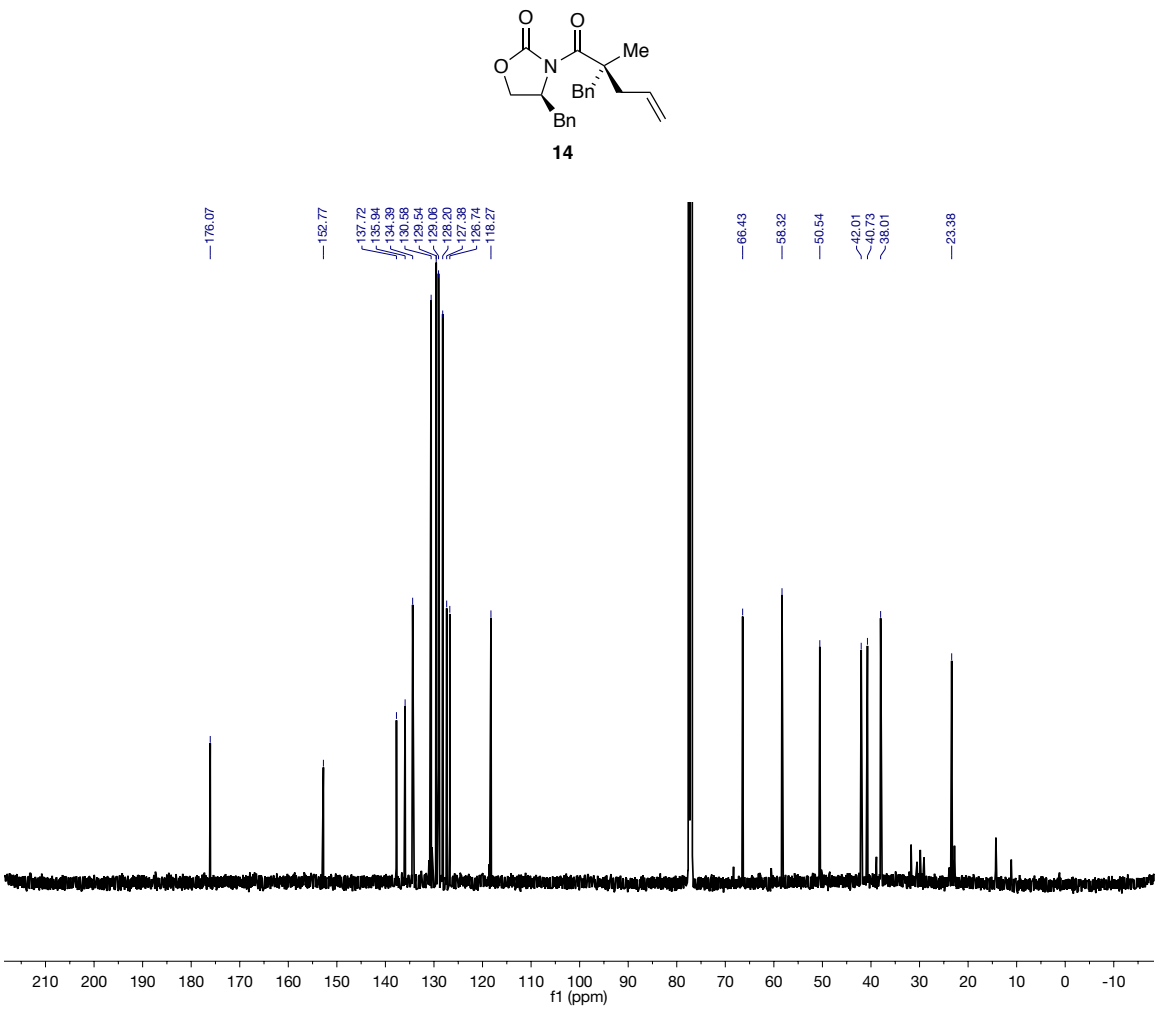


Figure S101. ^{13}C NMR spectrum ($CDCl_3$, 25 °C) of **14** in $CDCl_3$.

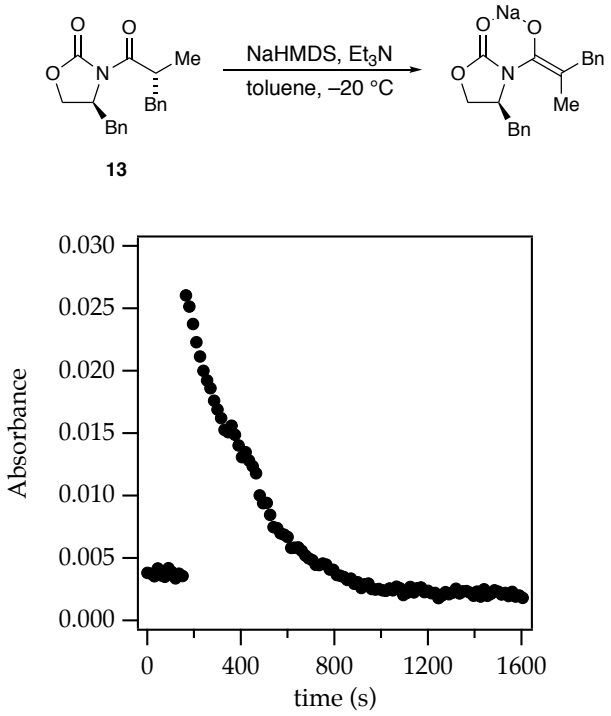
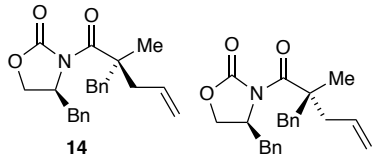


Figure S102. IR spectrum following loss of **13** in a solution of 0.010 M **13** and 0.015 M NaHMDS in 0.10 M Et_3N/toluene recorded at –20 °C. The elevated enolization rate suppresses decomposition. A new species attributed to a **13**/NaHMDS complex is observed at early time in the IR spectrum.



11:1

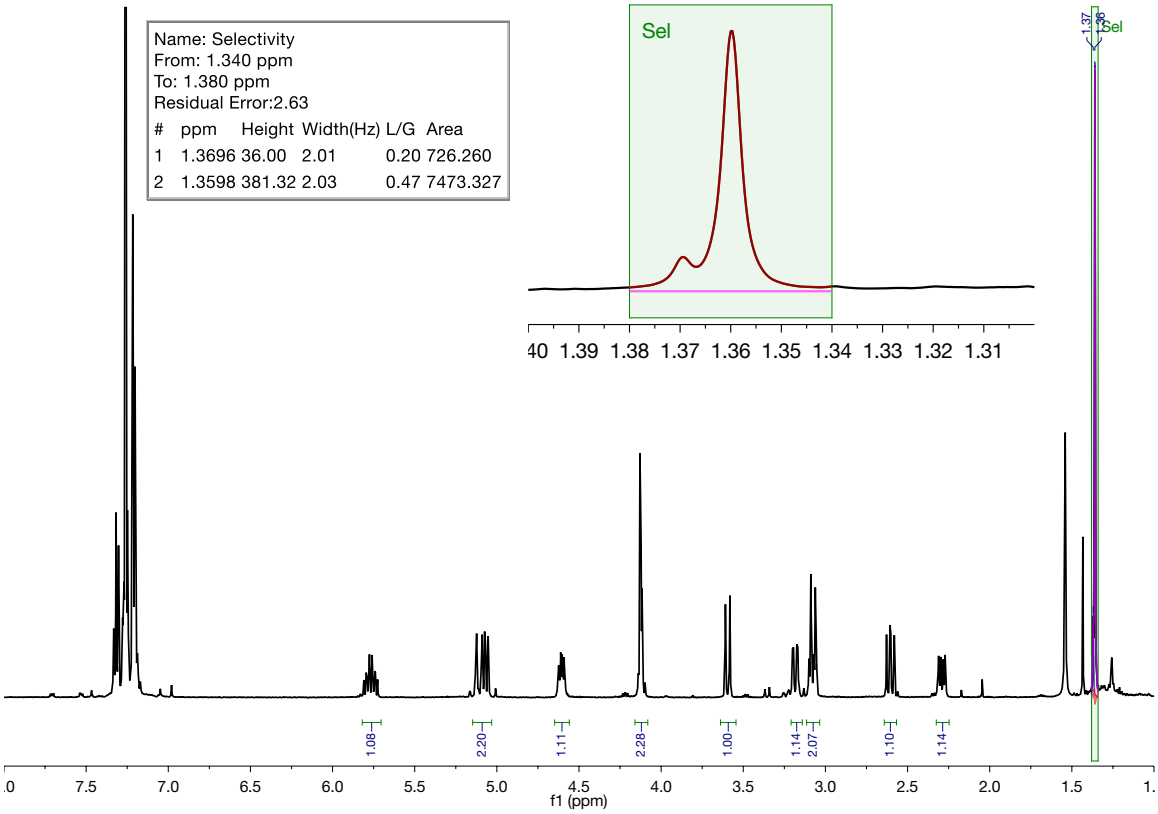


Figure S103. ^{1}H NMR spectrum ($CDCl_3$, 25 °C) of **14** prepared from Et_3N. An isolated yield of 70%was obtained. The integration shows 11:1 selectivity.

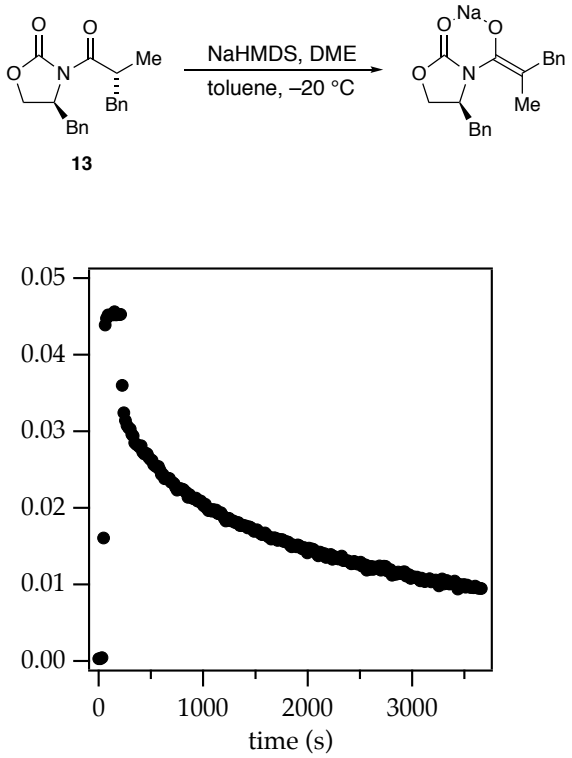
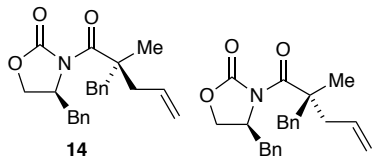


Figure S104. IR spectrum following loss of **13** in a solution of 0.010 M **13** and 0.015 M NaHMDS in 0.040 M DME/toluene recorded at –20 °C. The slower enolization is affiliated with greater decomposition.



11:1

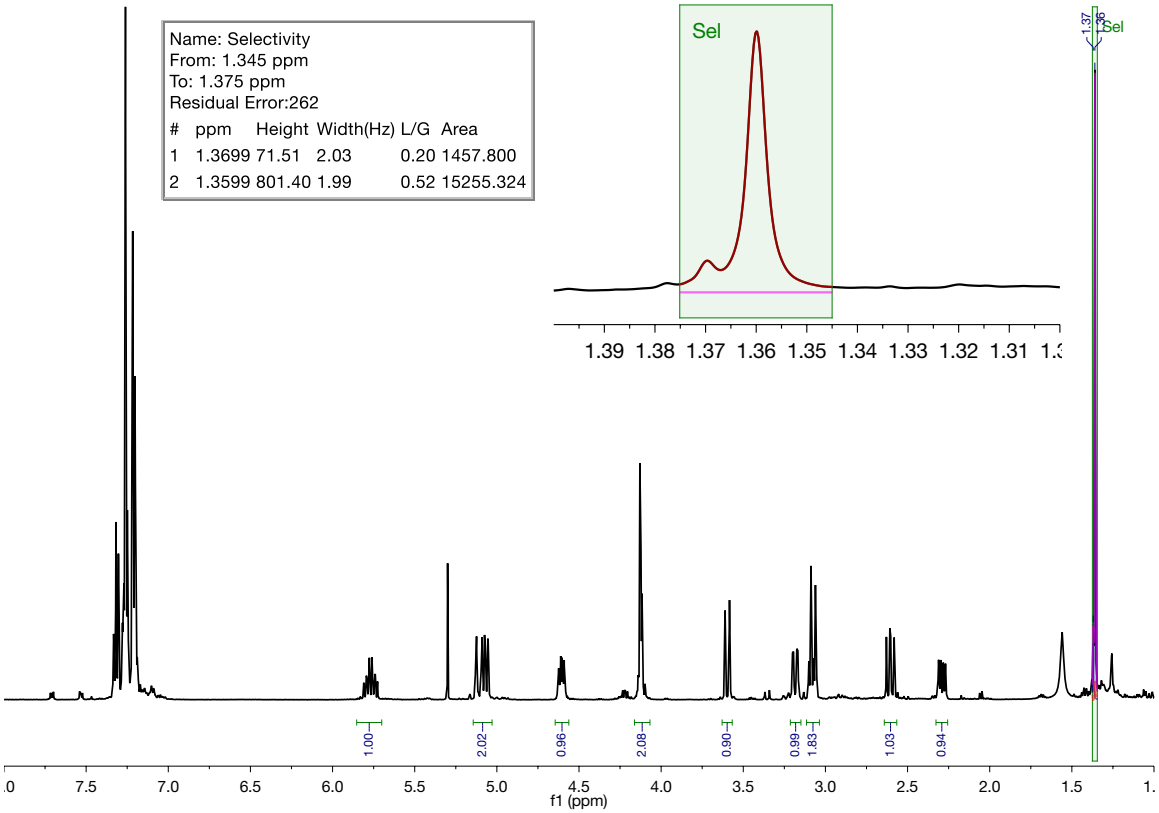


Figure S105. ^{1}H NMR spectrum ($CDCl_3$, 25 °C) of **14** prepared from **13** in DME. An isolated yield of 40% was obtained. The integration shows an 11:1 selectivity.

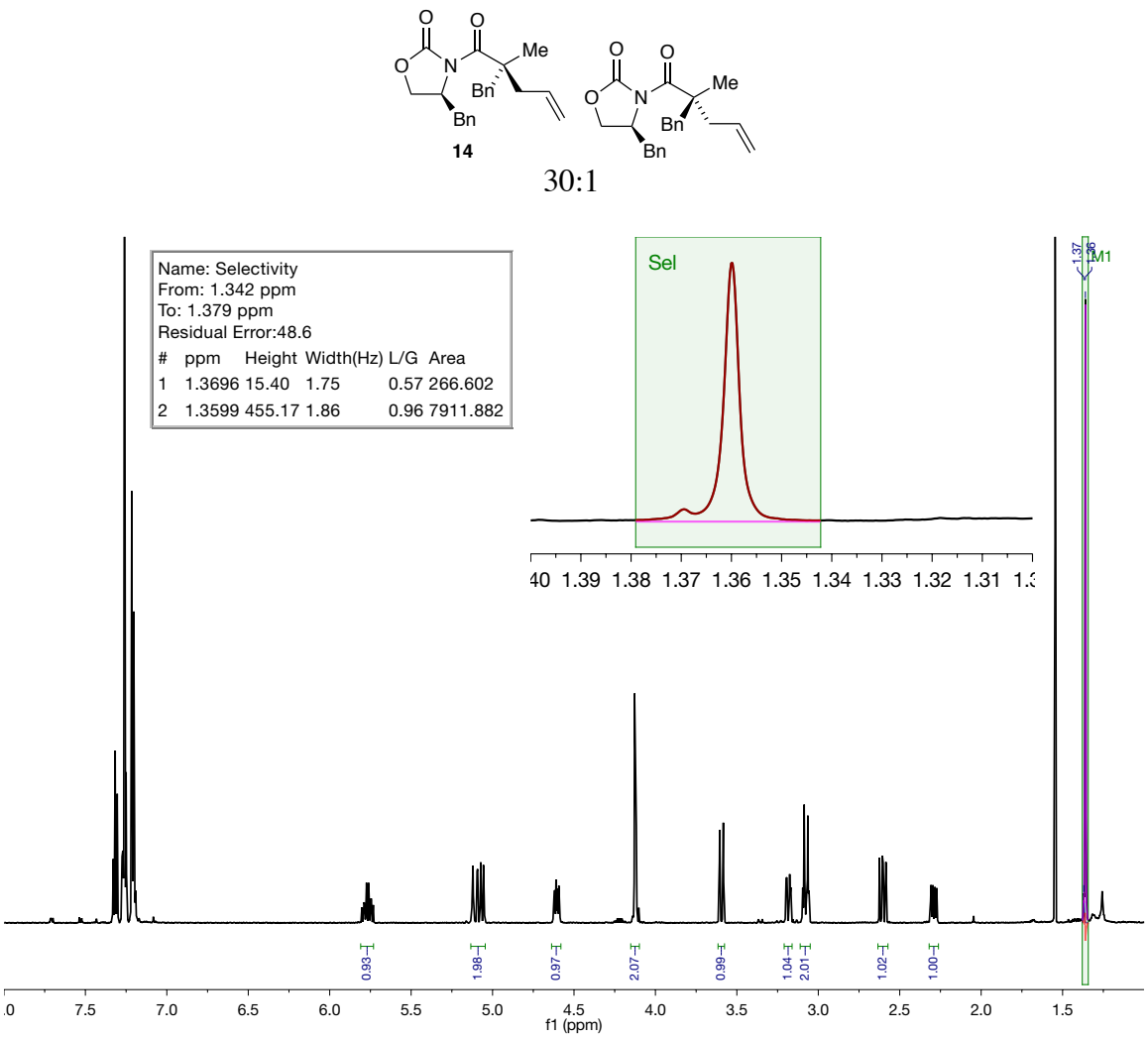


Figure S106. ^{1}H NMR spectrum ($CDCl_3$, 25 °C) of **14** prepared from **13** in (*R*,*R*)-TMCDA. An isolated yield of 40%was obtained. The integration shows a 30:1 selectivity.

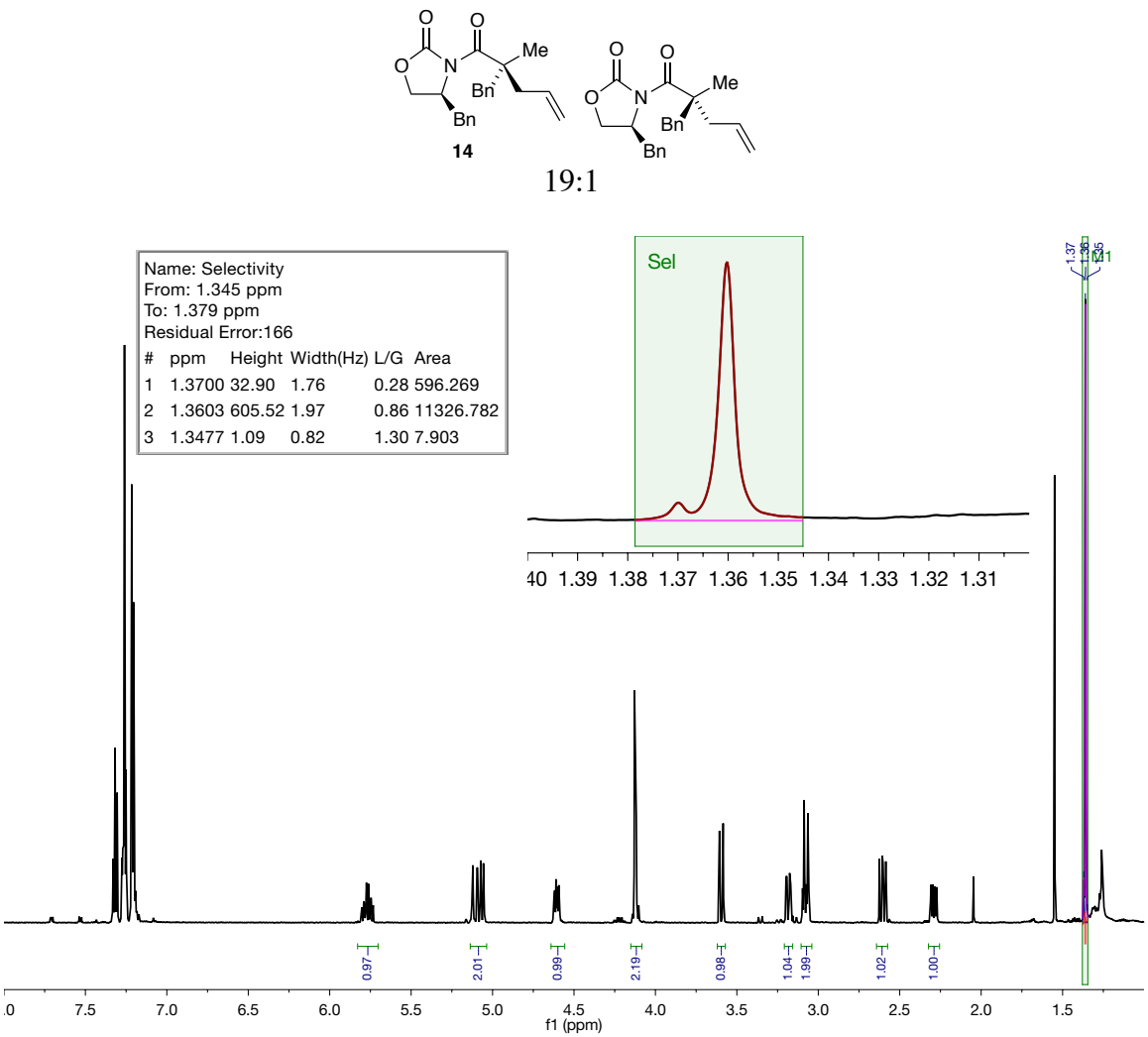


Figure S107. ^{1}H NMR spectrum ($CDCl_3$, 25 °C) of **14** prepared from **13** in (*S*,*S*)-TMCDA. An isolated yield of 52%was obtained. The integration shows a 19:1 selectivity.

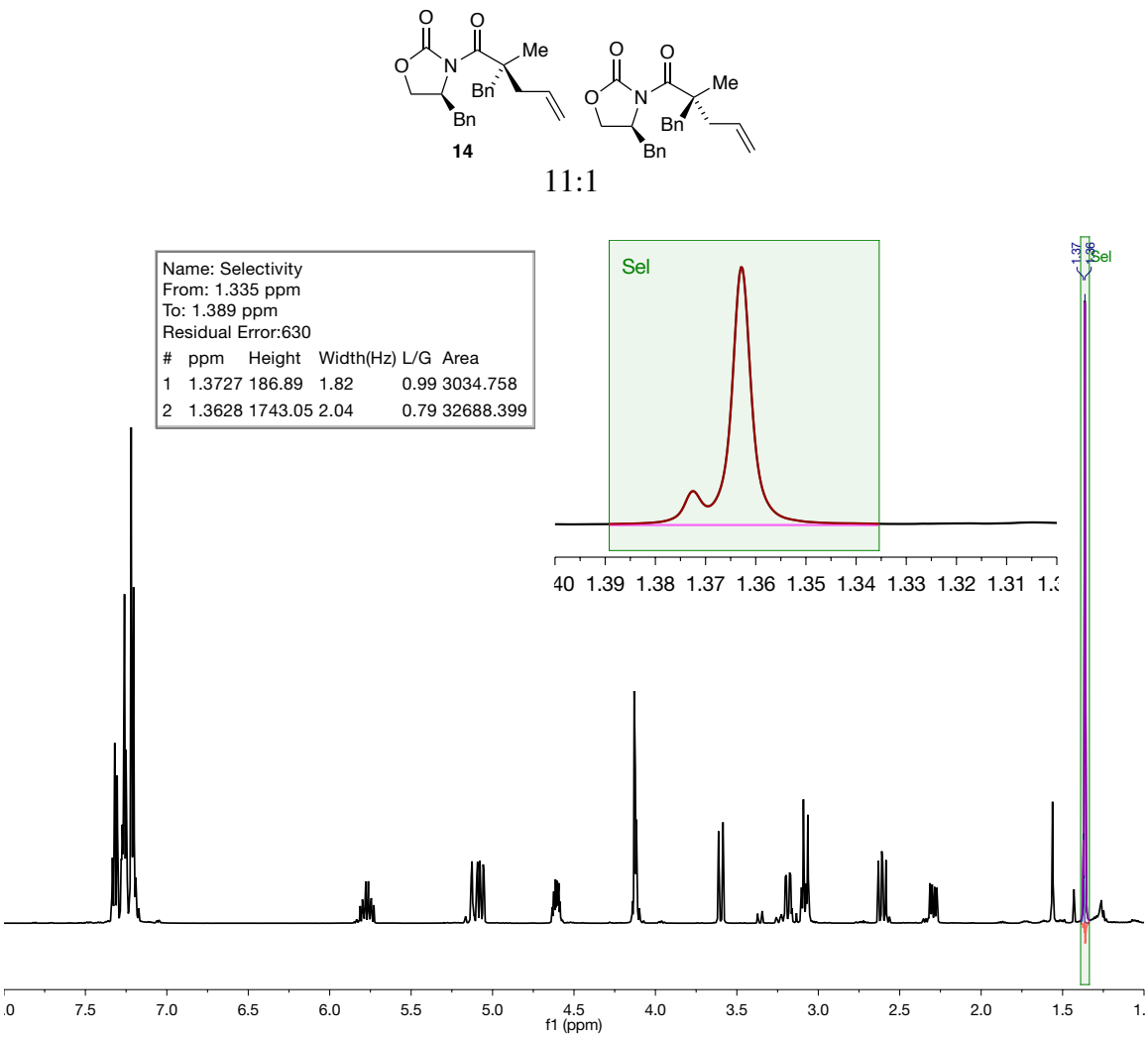


Figure S108. ^{1}H NMR spectrum ($CDCl_3$, 25 °C) of **14** prepared from **13** using Et_3N/toluene for the enolization with addition of (*R*,*R*)-TMCDA prior to alkylation. An isolated yield of 71%was obtained. The integration shows a 11:1 selectivity.

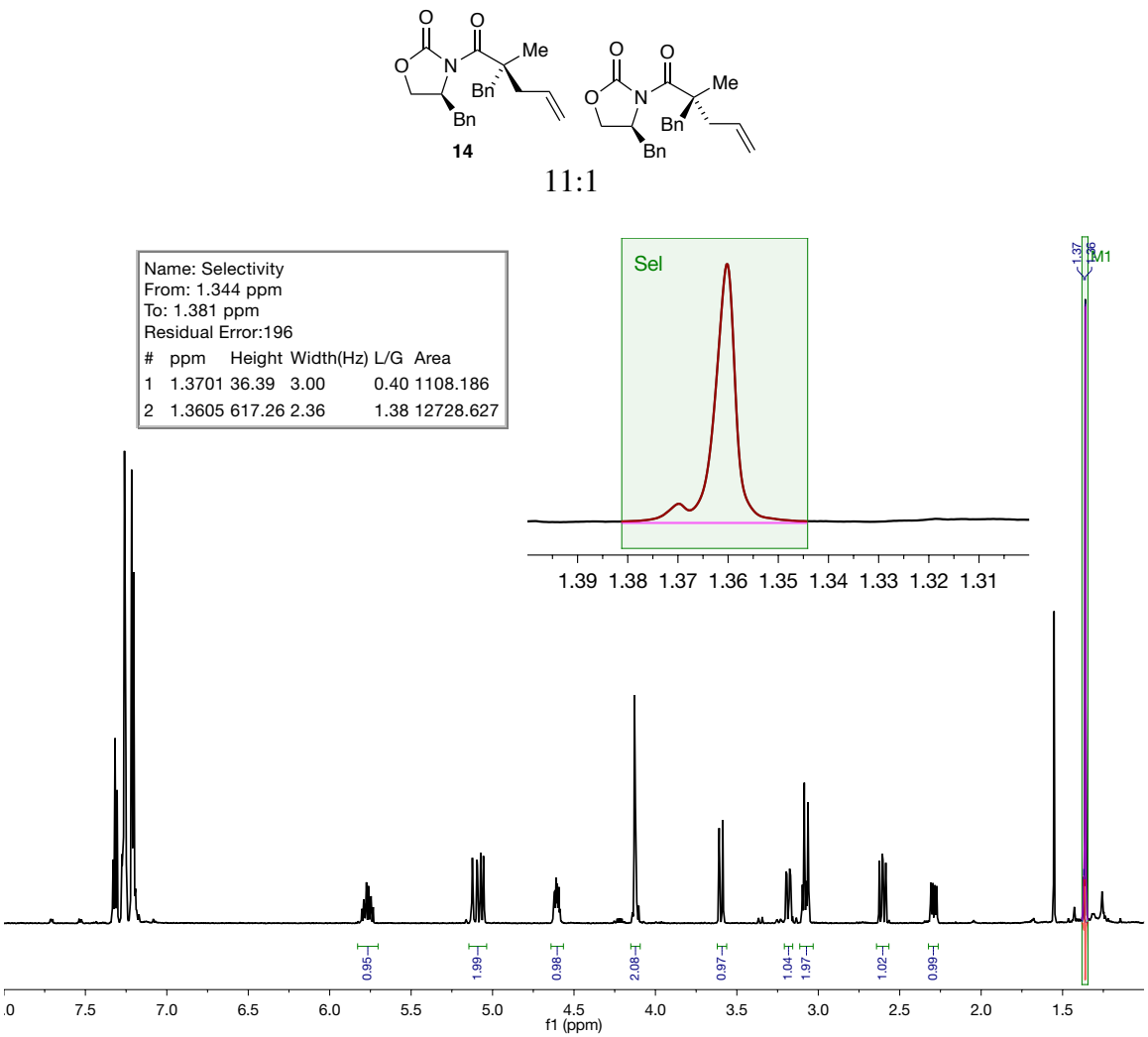


Figure S109. ^{1}H NMR spectrum ($CDCl_3$, 25 °C) of **14** prepared from **13** and **29** in TMEDA. An isolated yield of 44% was obtained. The integration shows a 11:1 selectivity.

(4S)- 4-benzyl-3-((2S)-2-methyl-3-phenylpropanoyl)-2-oxazolidinone (**15**). To a solution of (*S*)-**9a** (0.30 mmol, 92.7 mg) in THF (1.5 mL) under Ar was added NaHMDS (0.40 mmol, 73.3 mg). Reaction was stirred under at –78 °C for 30 minutes. Methyl iodide (1.0 mmol, 62 μL) was injected and the mixture was stirred for 1 hour. The reaction was quenched by saturated NH_4Cl and extracted three times with EtOAc. The organic extracts were dried over $MgSO_4$, concentrated in vacuo, and purified by flash chromatography (20% EtOAc/hexanes) to afford the desired product. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.35 – 7.30 (m, 2H), 7.30 – 7.27 (m, 2H), 7.26 – 7.24 (m, 1H), 7.24 – 7.18 (m, 5H), 4.52 (dddd, *J* = 9.8, 7.8, 3.3, 2.3 Hz, 1H), 4.16 – 4.10 (m, 1H), 4.08 (dd, *J* = 9.1, 2.5 Hz, 1H), 3.96 (ddd, *J* = 8.7, 7.7, 0.8 Hz, 1H), 3.25 (dd, *J* = 13.3, 3.4 Hz, 1H), 3.03 (dd, *J* = 13.3, 7.8 Hz, 1H), 2.78 – 2.68 (m, 2H), 1.25 (d, *J* = 6.8 Hz, 3H).

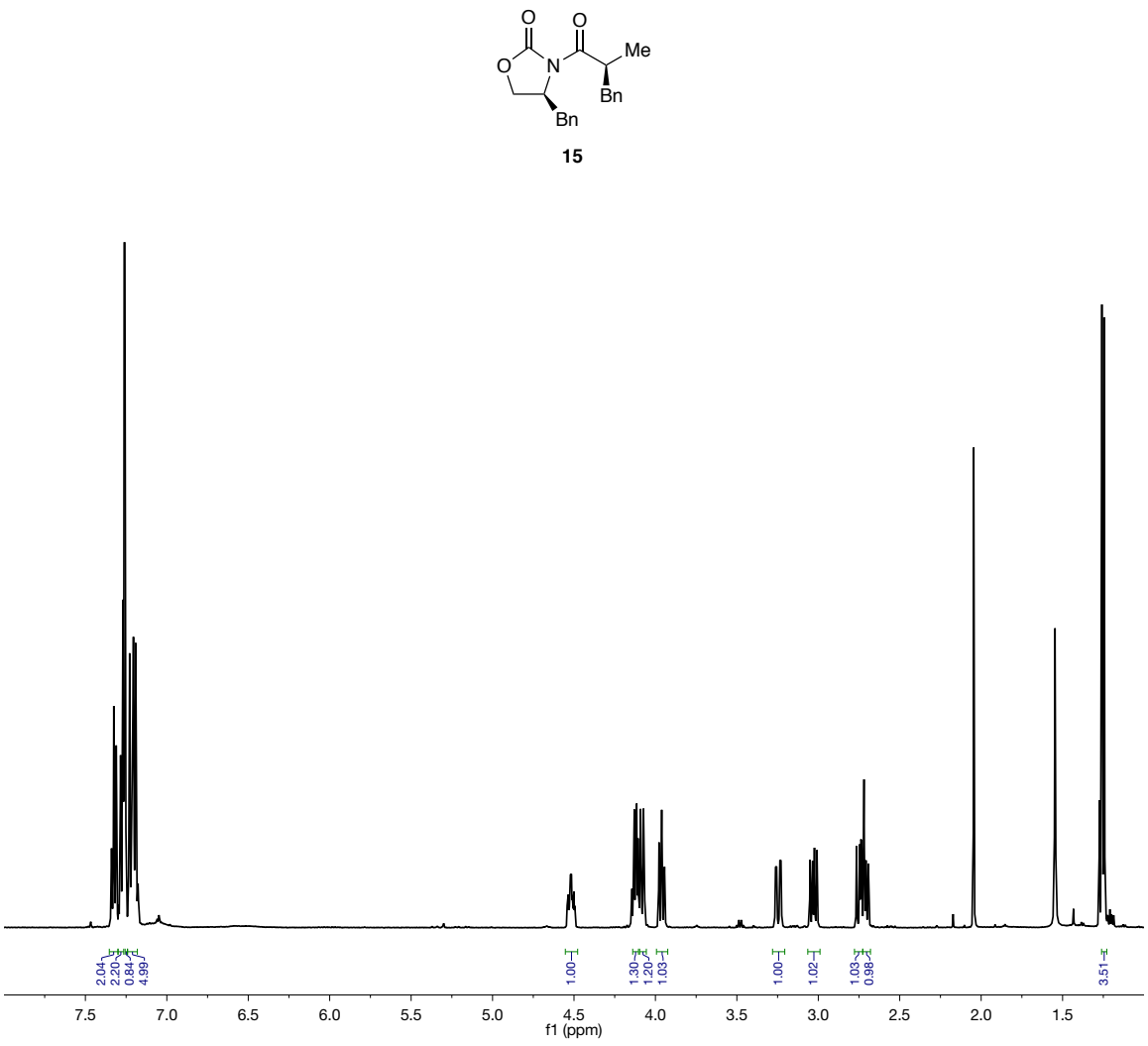


Figure S110. ^{1}H NMR spectrum ($CDCl_3$, 25 °C) of **15**.

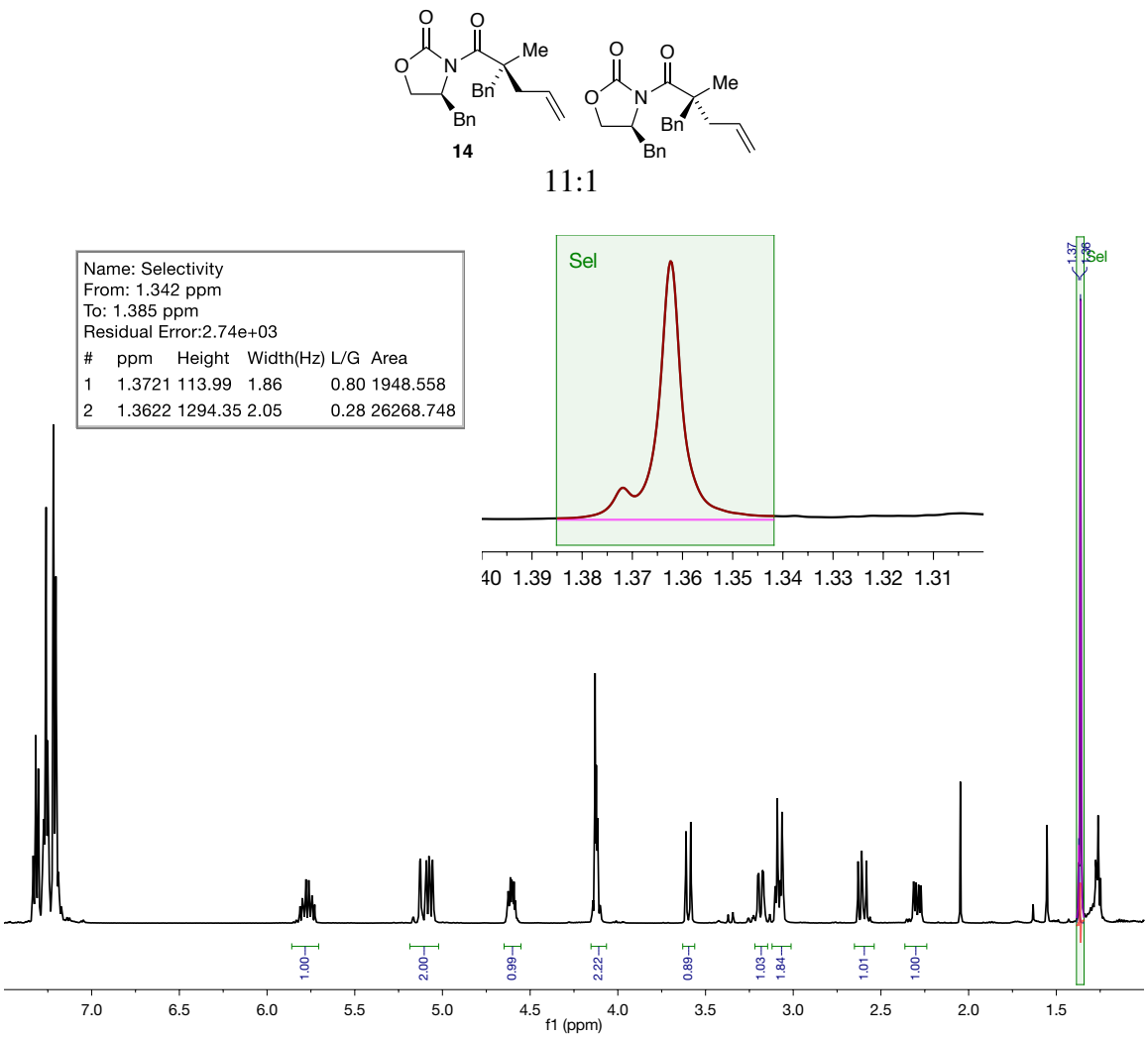
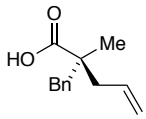


Figure S111. ^{1}H NMR spectrum ($CDCl_3$, 25 °C) of **14** prepared from **15**.
An isolated yield of 54%was obtained. The integration shows a 11:1 selectivity.

(*R*)-2-benzyl-2-methylpent-4-enoic acid (30). To a solution of **14** (0.050 mmol, 18 mg) in THF (0.45 mL) and water (0.15 mL) at 0 °C was added H_2O_2 (30%, 40 mL) dropwise and LiOH (2.4 mg) in water (0.10 mL). The reaction was warmed to 20 °C for 2 hr, cooled to 0 °C, and treated with Na_2SO_3 (56.8 mg) in water (0.3 mL) with stirring at 20 °C for 12 hr. The reaction was concentrated in vacuo, and its pH was adjusted to 13 using NaOH at 0 °C. The aqueous solution was extracted three times with CH_2Cl_2, and the pH was brought to 1 using concentrated HCl at 0 °C. The mixture was extracted three times with EtOAc, dried over $MgSO_4$, and concentrated in vacuo to afford 7 mg of product (69% combined yield). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.30 – 7.21 (m, 3H), 7.20 – 7.14 (m, 2H), 5.82 (ddt, *J* = 18.5, 9.2, 7.4 Hz, 1H), 5.17 – 5.09 (m, 2H), 3.05 (d, *J* = 13.4 Hz, 1H), 2.78 (d, *J* = 13.4 Hz, 1H), 2.53 (ddt, *J* = 13.8, 6.9, 1.3 Hz, 1H), 2.21 (ddt, *J* = 13.7, 7.7, 1.2 Hz, 1H), 1.12 (s, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 183.05, 137.33, 133.75, 130.35, 128.23, 126.77, 118.76, 47.48, 44.89, 43.33, 20.72. m/z calculated for $(M+H)^+$ 205.12231, found 205.12198. $[\alpha]^{22}$ = +12, c 0.35, CH_2Cl_2. An authentic sample was prepared using the procedure of Myers and coworkers. $[\alpha]^{22}$ = +24, c 0.5, CH_2Cl_2.

Kummer, D. A.; Chain, W. J.; Morales, M. R.; Quiroga, O.; Myers, A. G. *J. Am. Chem. Soc,* **2008**, *130*, 13231.



30

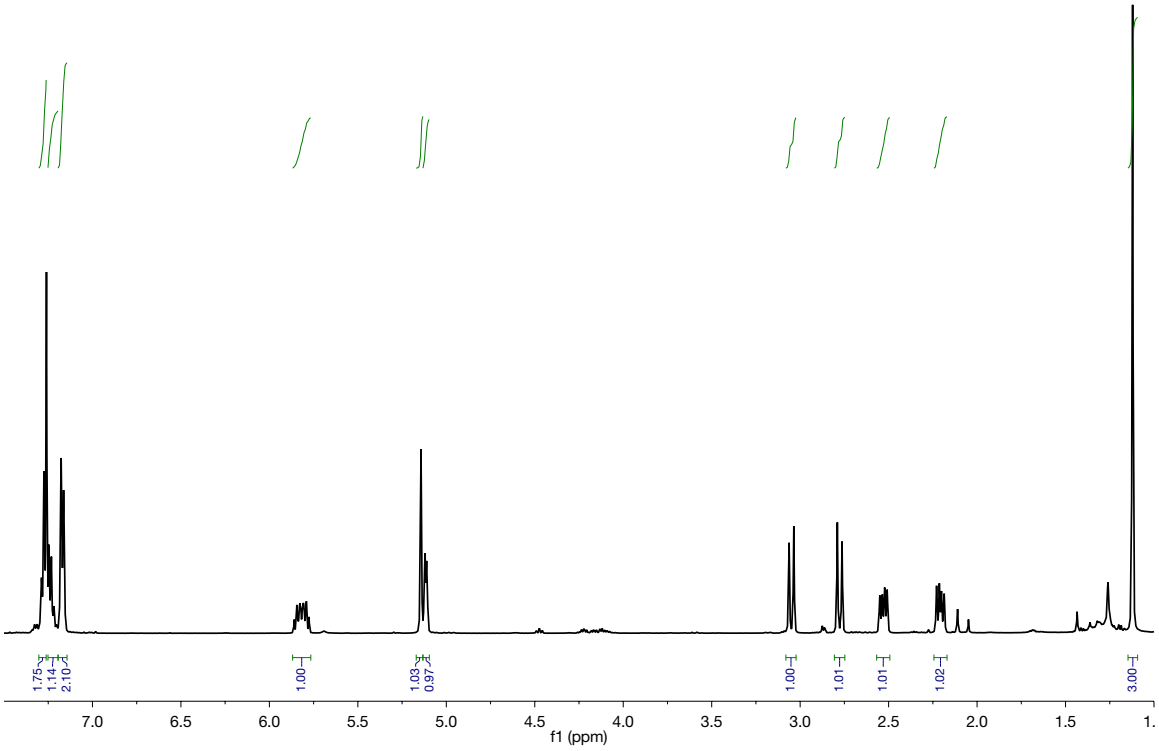


Figure S112. ^{1}H NMR spectrum ($CDCl_3$, 25 °C) of **30**.

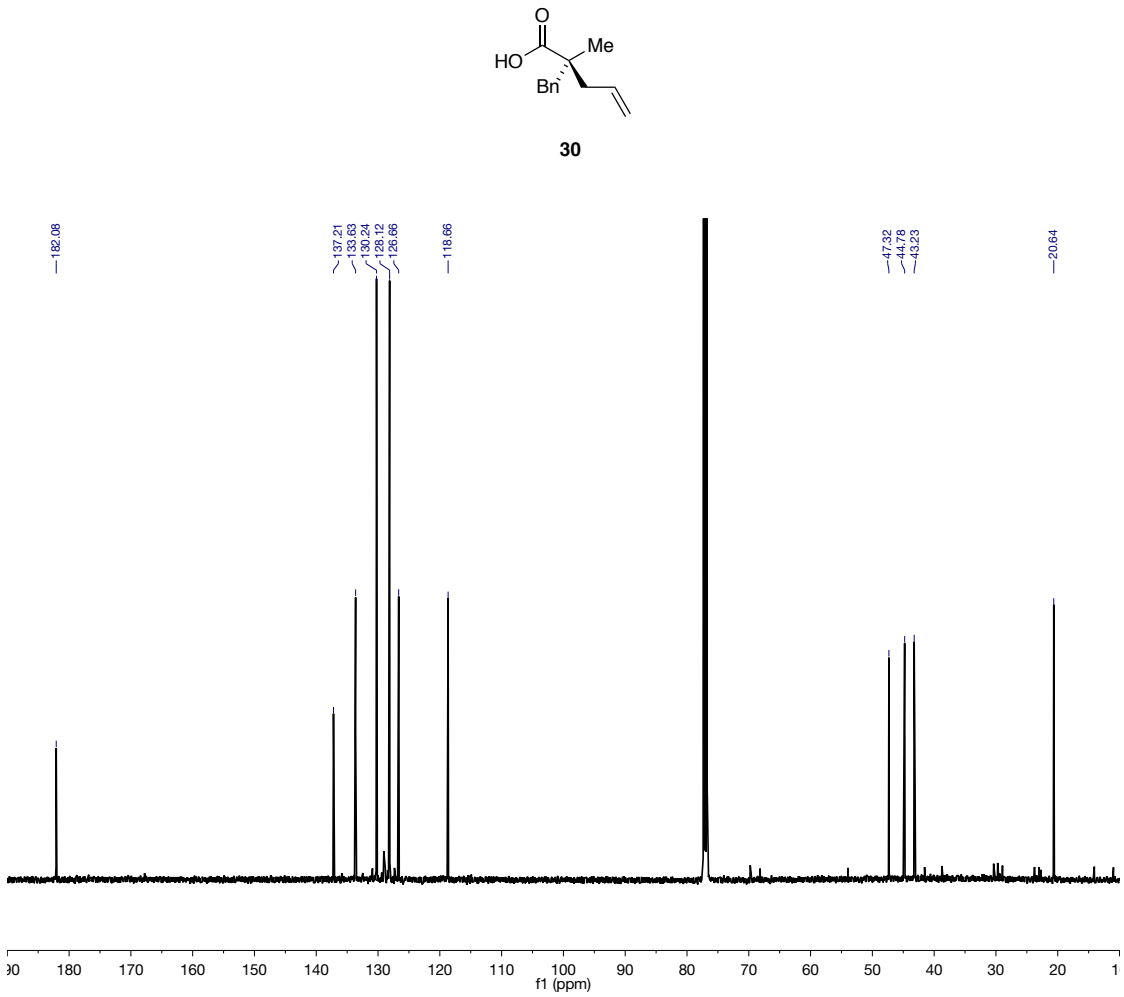


Figure S113. ^{13}C NMR spectrum ($CDCl_3$, 25 °C) of **30**.

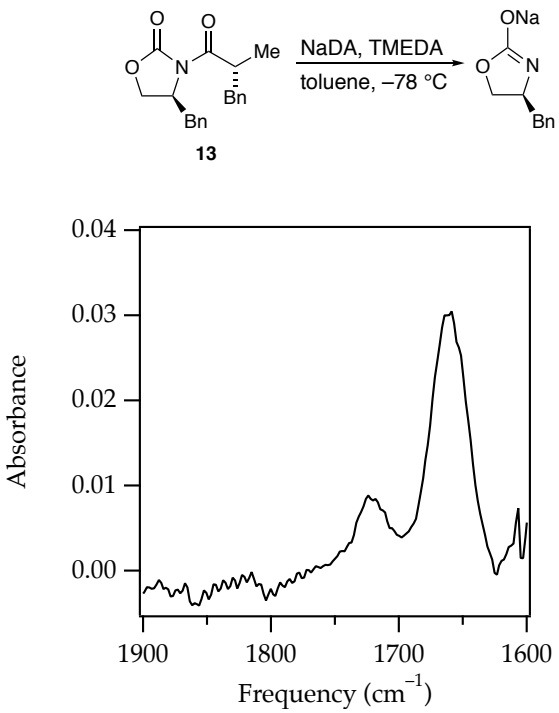


Figure S114. IR spectrum of 0.010 M **13** and 0.013 M NaDA in 0.030 M TMEDA/toluene recorded at –78 °C. Using NaDA instead of NaHMDS results in exclusively deacylated product even at –78 °C. An isolated byproduct suggests competitive deprotonation on the auxiliary.

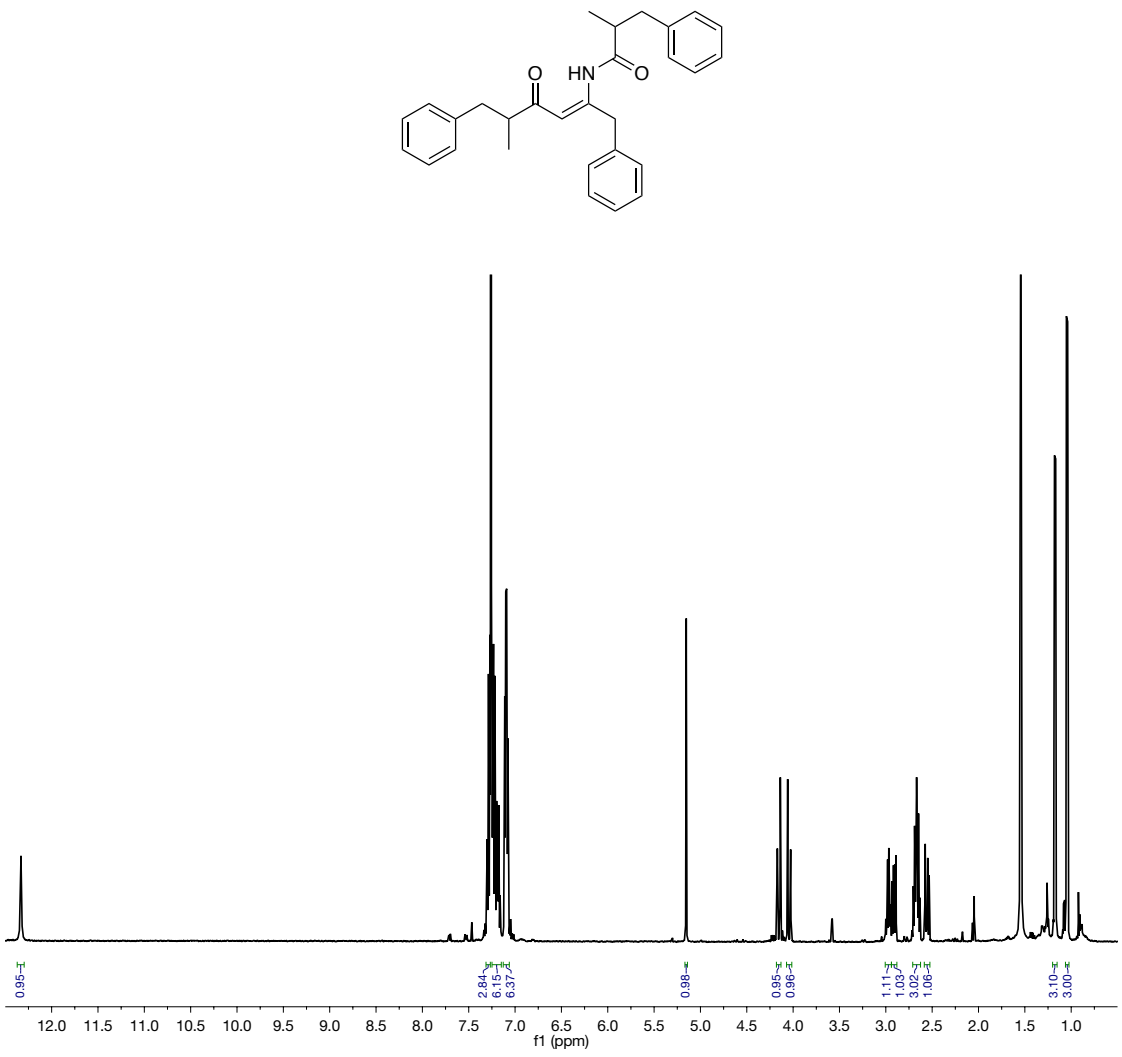


Figure S115. ^{1}H NMR spectrum ($CDCl_3$, 25 °C) of backbone decomposition product.

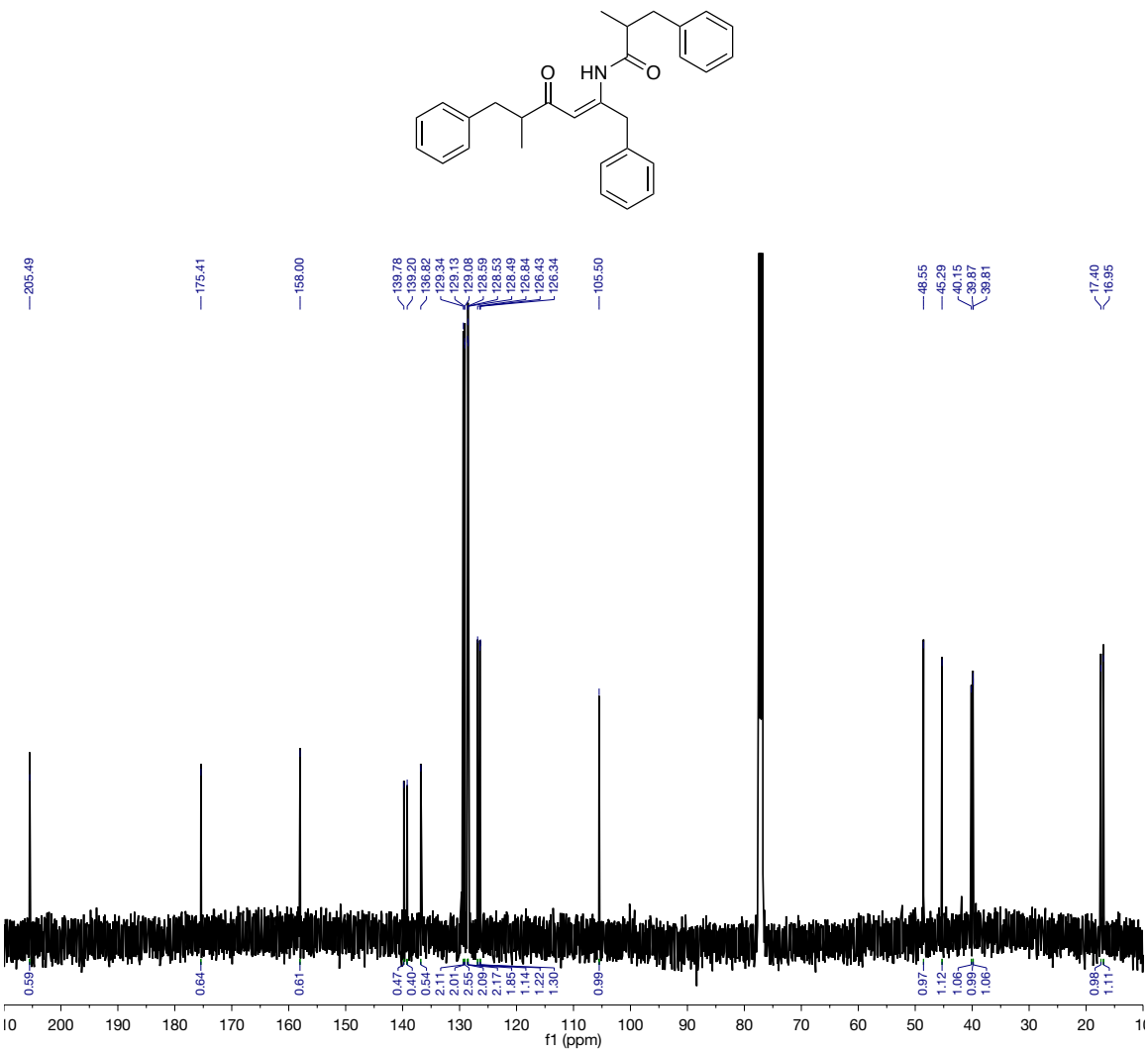


Figure S116. ^{13}C NMR spectrum ($CDCl_3$, 25 °C) of backbone decomposition product.

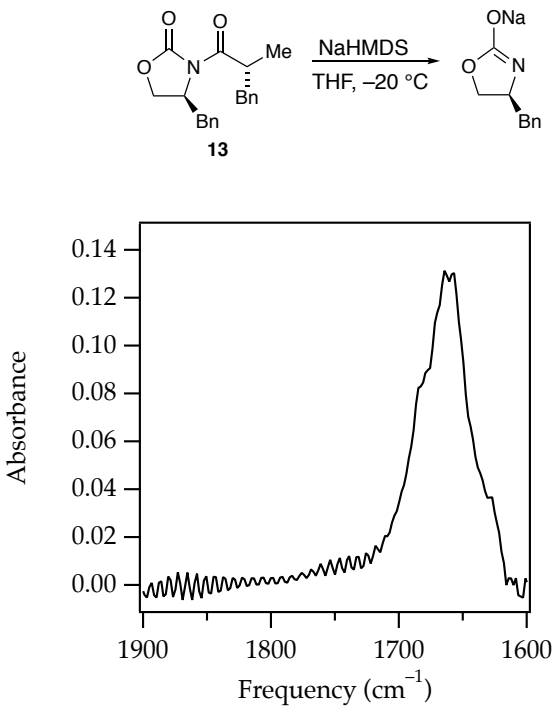


Figure S117. IR spectrum of 0.010 M **13** and 0.015 M NaHMDS in THF recorded at –20 °C. Switching the solvent to THF produces decomposition product only.

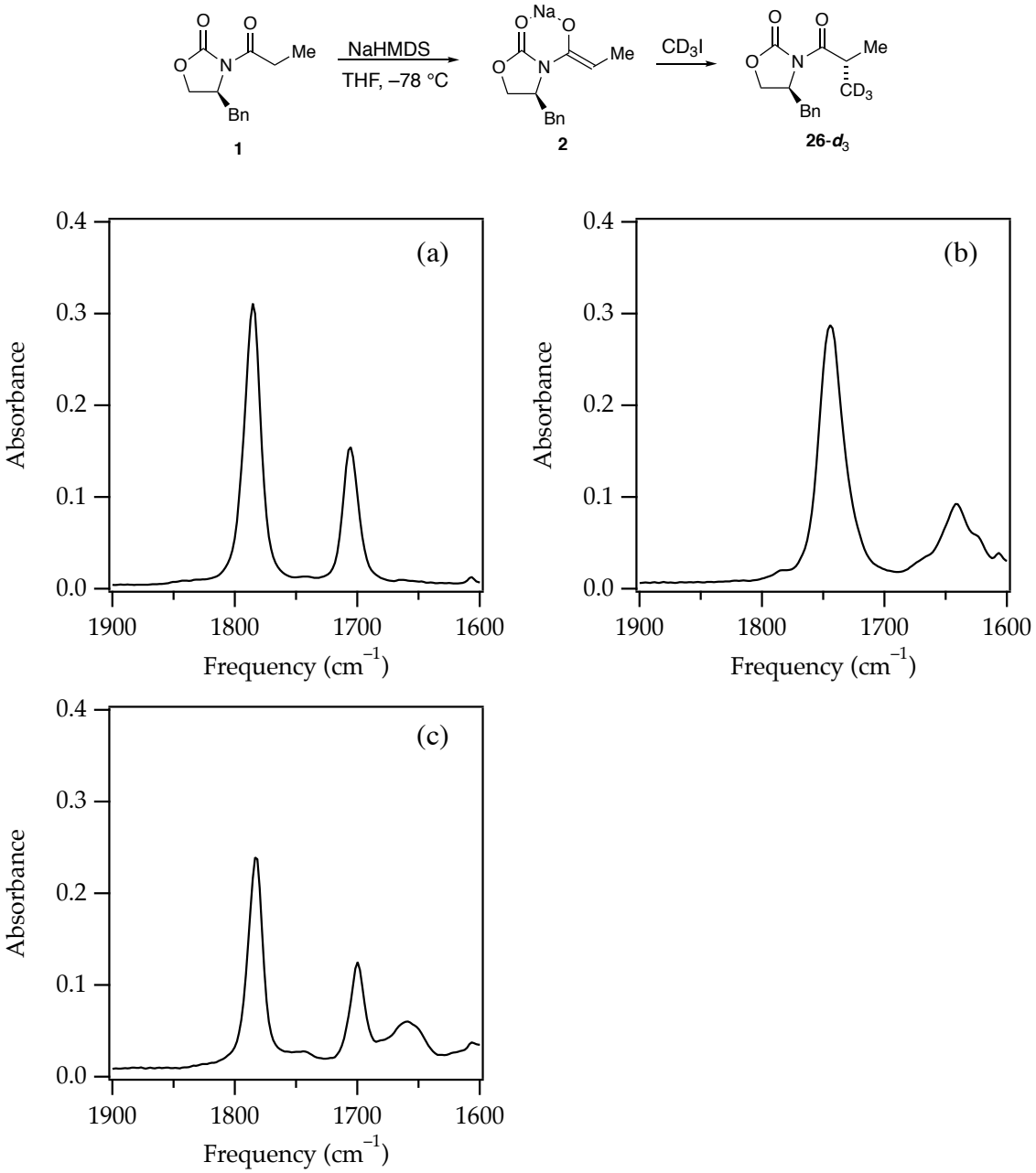


Figure S118. IR spectra in THF recorded at –78 °C of (a) 0.10 M **1**; (b) 0.11 M **2**; (c) and 0.20 M **26**-d_3.

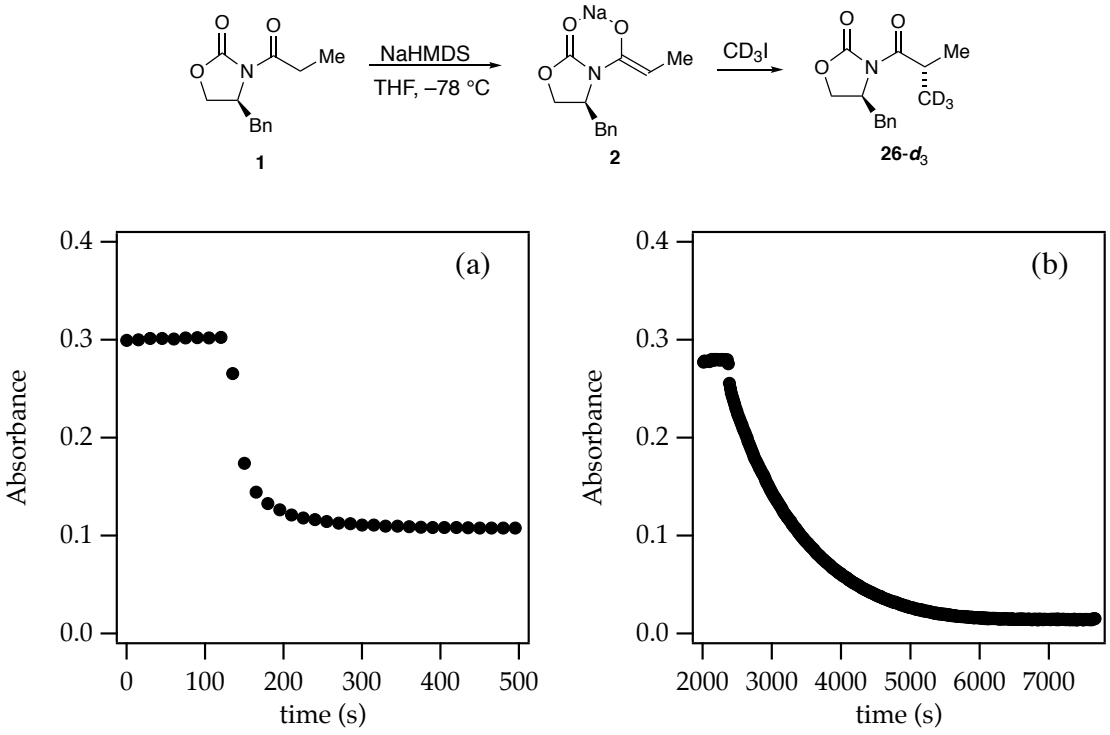


Figure S119. IR spectrum in a solution of 0.10 M **1**, 0.11 M NaHMDS and 0.20 M CD_3I in THF recorded at –78 °C following (a) loss of **1**; (b) loss of **2**.

(4S)- 4-benzyl-3-((2R)-2-methylpropanoyl)-2-oxazolidinone-d_3 (26-d_3). To a solution of NaHMDS (0.55 mmol, 100.7 mg) in THF (5.0 mL), **1** (0.50 mmol, 116.5 mg) was added and reaction was stirred under Ar for 40 minutes at –78 °C. After injection of CD_3I (1.0 mmol, 62 μL), the mixture was stirred at –78 °C for 1.5 hours. The reaction was quenched by saturated NH_4Cl and extracted with three times EtOAc. The organic extracts were dried over $MgSO_4$, concentrated in vacuo, and purified by flash chromatography (20% EtOAc/hexanes). The desired product was obtained. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.36 – 7.31 (m, 2H), 7.30 – 7.27 (m, 1H), 7.23 – 7.19 (m, 2H), 4.68 (ddt, *J* = 9.5, 7.5, 3.2 Hz, 1H), 4.21 (t, *J* = 9.1 Hz, 1H), 4.17 (dd, *J* = 9.1, 3.0 Hz, 1H), 3.74 (q, *J* = 6.8 Hz, 1H), 3.27 (dd, *J* = 13.4, 3.3 Hz, 1H), 2.77 (dd, *J* = 13.4, 9.6 Hz, 1H), 1.19 (d, *J* = 6.8 Hz, 3H).

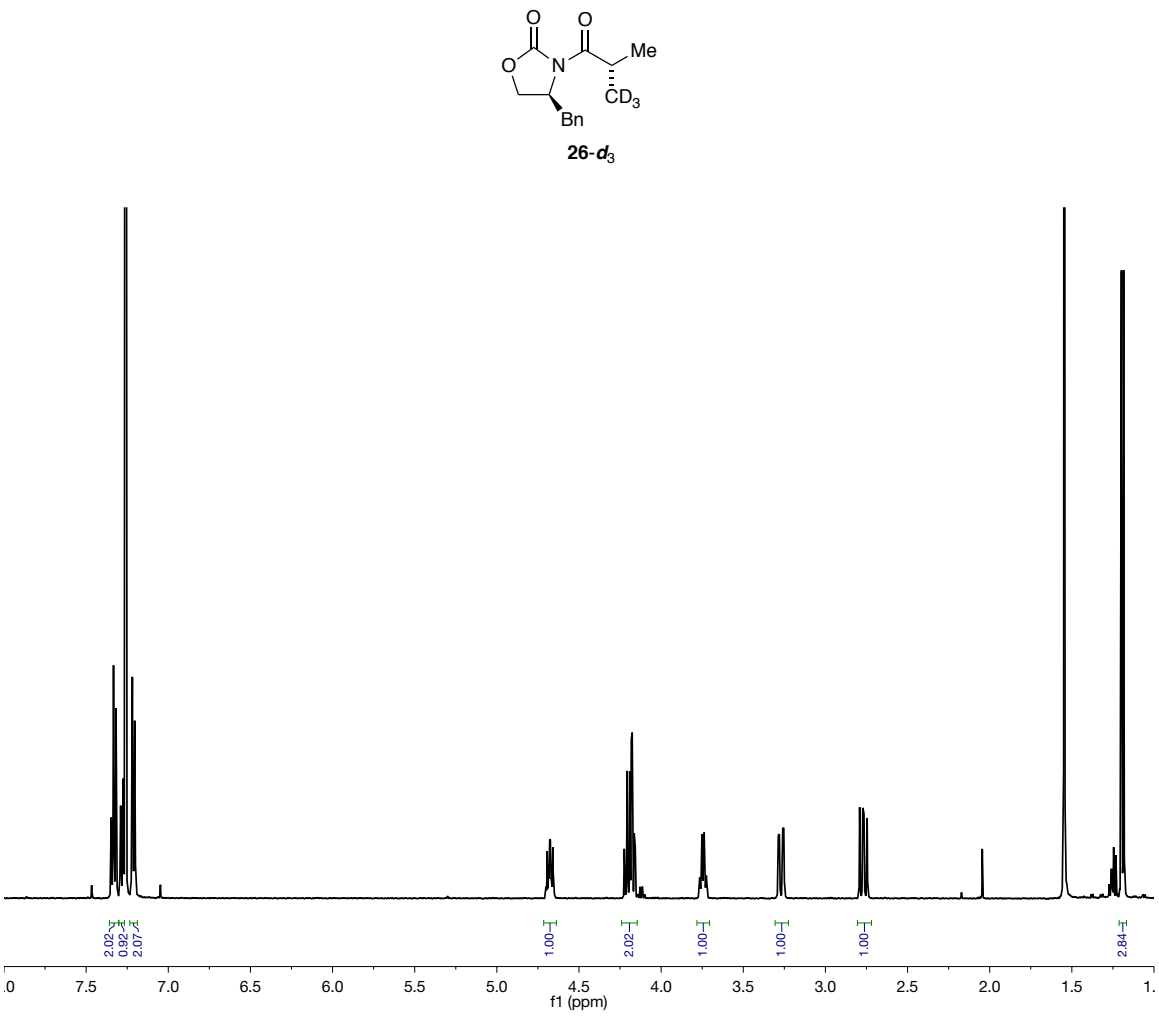


Figure S120. ^{1}H NMR spectrum ($CDCl_3$, 25 °C) of **26**-d_3.

(4S)- 4-benzyl-3-(2,2-dimethylpent-4-enoyl)-2-oxazolidinone (**31**). To a solution of NaHMDS (0.12 mmol, 22 mg) and TMEDA (0.30 mmol, 45 μL) in toluene (2 mL), **26**-d_3 (0.060 mmol, 15 mg) was added and reaction was stirred under Ar for 0.5 hour at –20 °C. After injection of allyl bromide (1 mmol, 86 μL), the mixture was warmed to 0 °C over 2 hours. The reaction was quenched by saturated NH_4Cl and extracted three times with EtOAc. The organic extracts were dried over $MgSO_4$, concentrated in vacuo, and purified by flash chromatography (15% EtOAc/hexanes). The desired product was obtained in 57% yield (10 mg). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.36 – 7.30 (m, 2H), 7.29 – 7.26 (m, 1H), 7.25 – 7.20 (m, 2H), 5.77 (ddt, *J* = 17.4, 10.1, 7.4 Hz, 1H), 5.13 – 5.03 (m, 2H), 4.68 (ddt, *J* = 10.2, 7.3, 3.1 Hz, 1H), 4.17 (t, *J* = 9.0 Hz, 1H), 4.13 (dd, *J* = 9.0, 2.8 Hz, 1H), 3.26 (dd, *J* = 13.3, 3.3 Hz, 1H), 2.73 – 2.65 (m, 2H), 2.61 (dddd, *J* = 13.9, 7.3, 2.9, 1.5 Hz, 1H), 1.39 (s, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 177.59, 152.50, 135.82, 134.53, 129.57, 129.05, 127.40, 118.13, 66.36, 57.85, 45.27, 42.30, 38.19, 24.74.

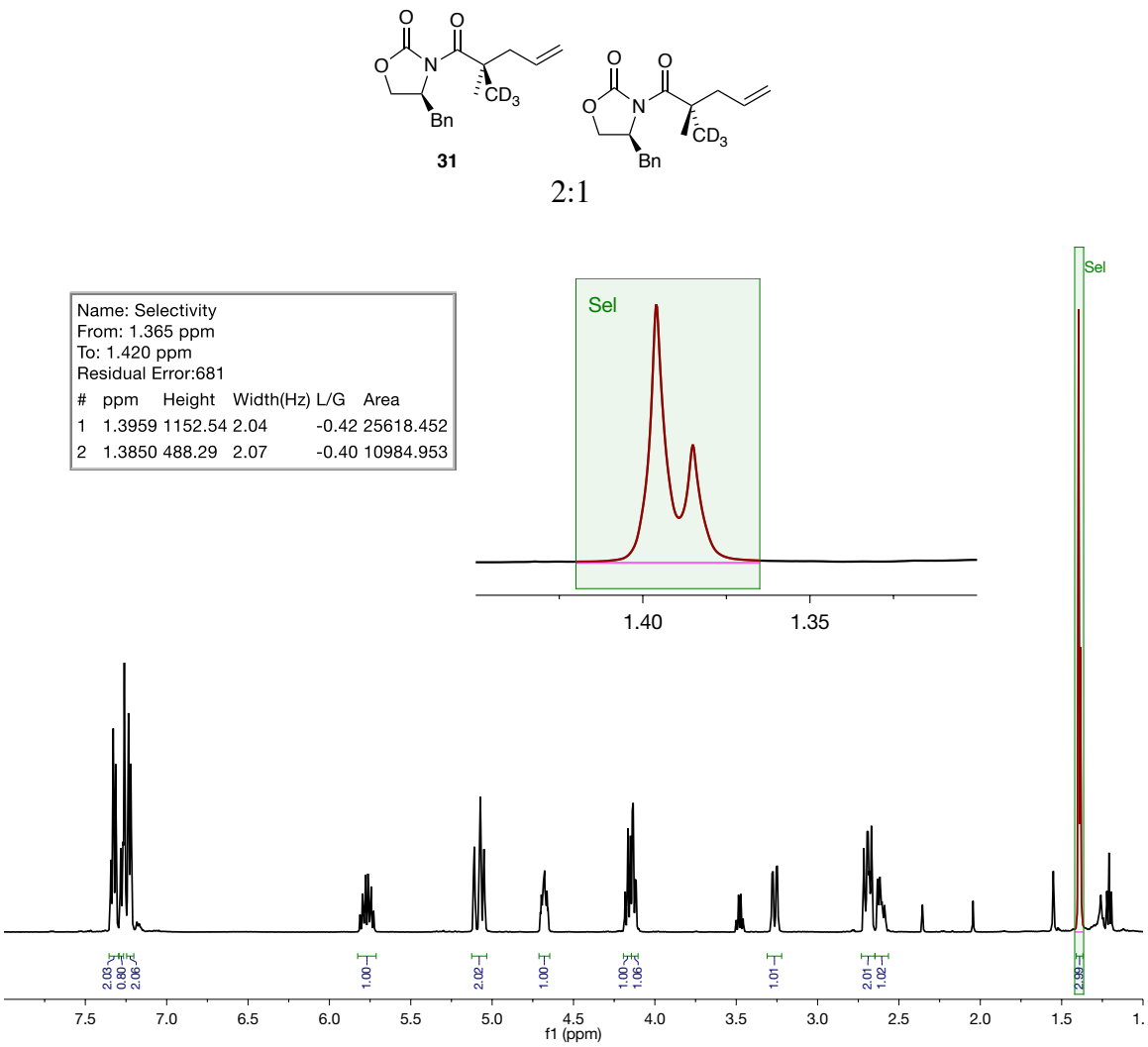


Figure S121. ^{1}H NMR spectrum ($CDCl_3$, 25 °C) of **31** prepared from **26**-d_3. The integration shows a 2:1 selectivity.

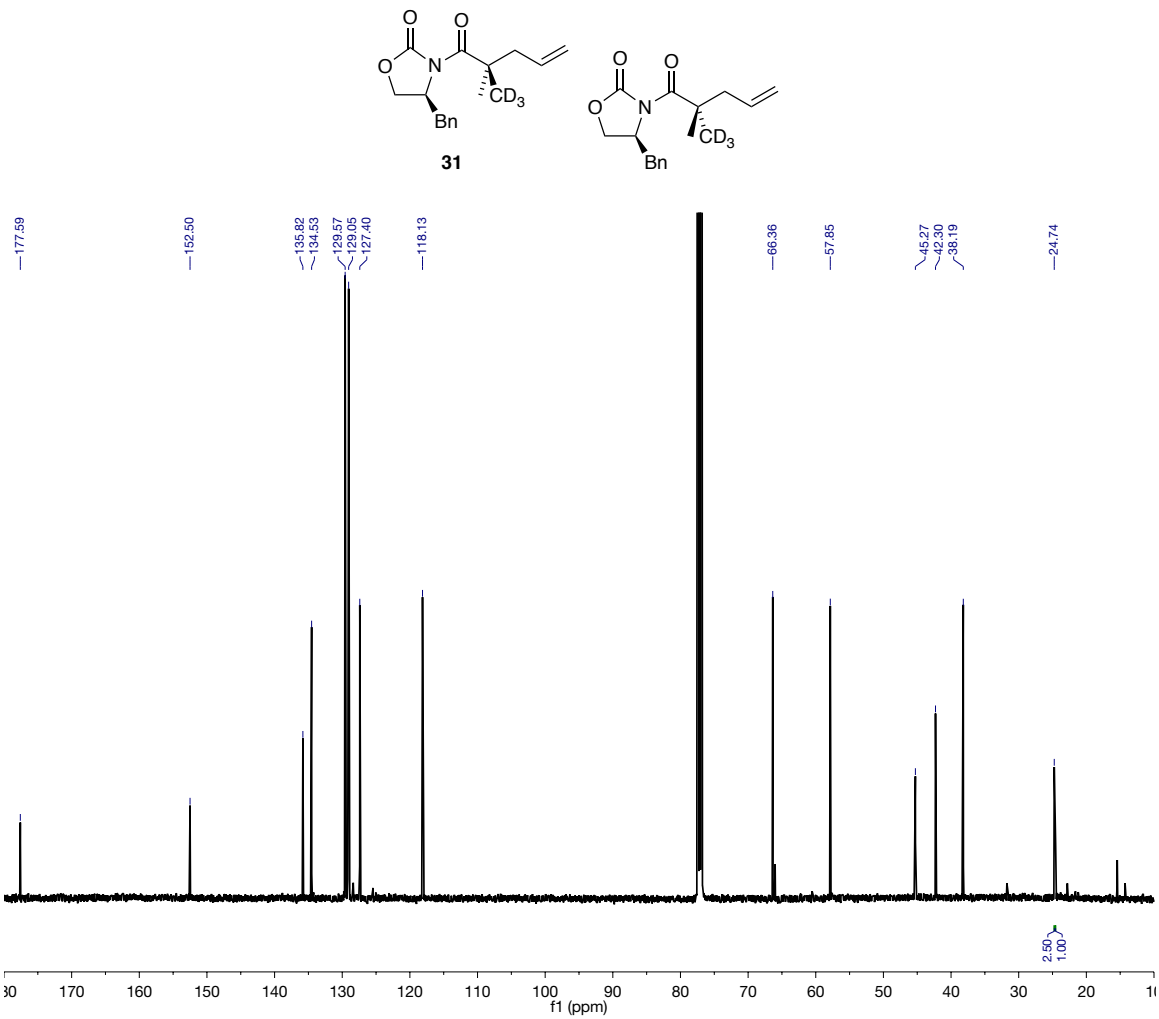


Figure S122. ^{13}C NMR spectrum ($CDCl_3$, 25 °C) of **31**.

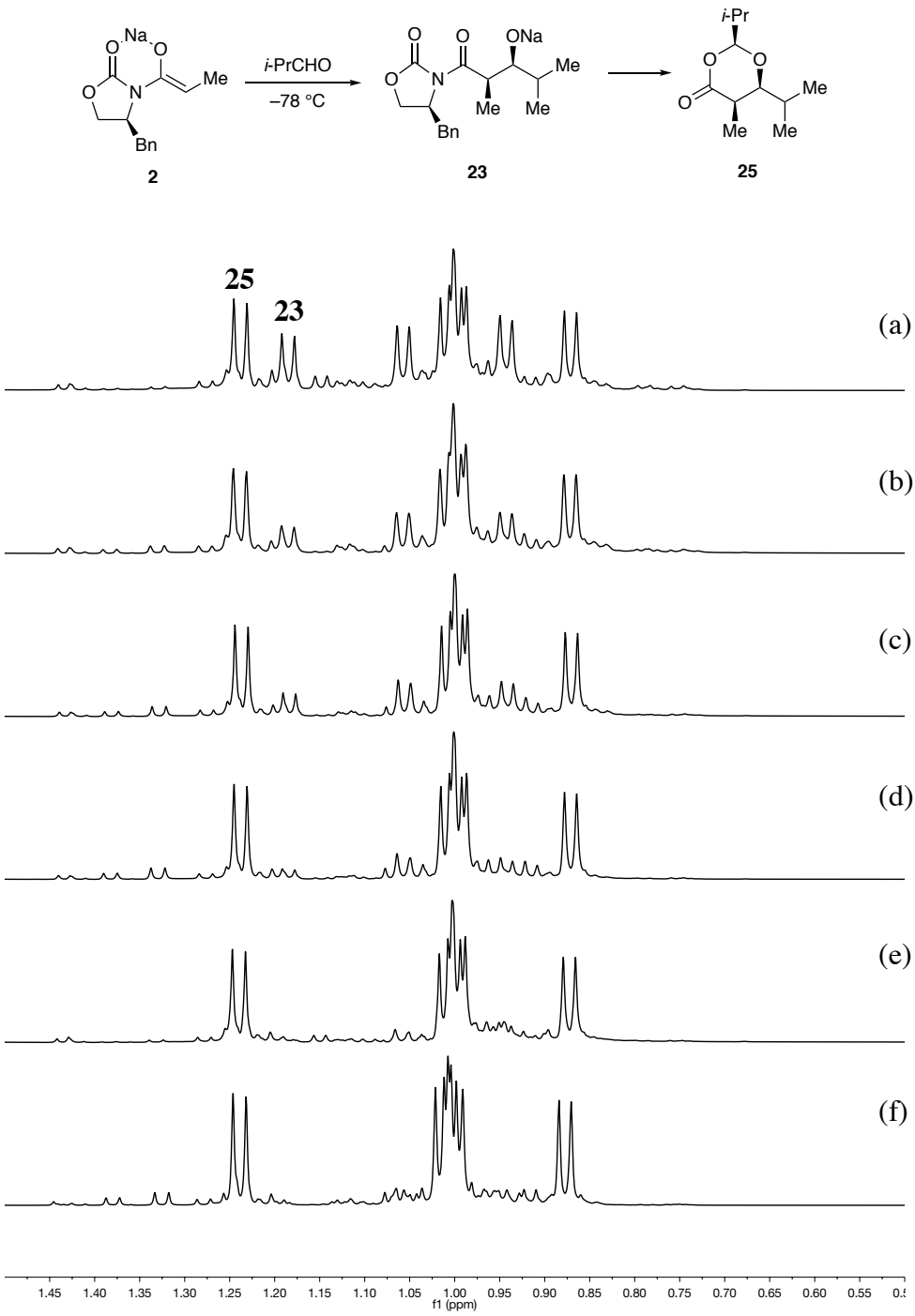


Figure S123. ^{1}H NMR spectra recorded in $CDCl_3$ at rt of 0.10 M **2** and 0.30 M isobutyraldehyde in 0.30 M TMEDA/toluene, quenched with NH_4Cl after (a) 1 min; (b) 3 min; (c) 10 min; (d) 25 min; (e) 1 h; (f) 2 h at –78 °C. The regular aldol product is detected as the minor species and disappears as the reaction proceeds. Another major product is observed and isolated.

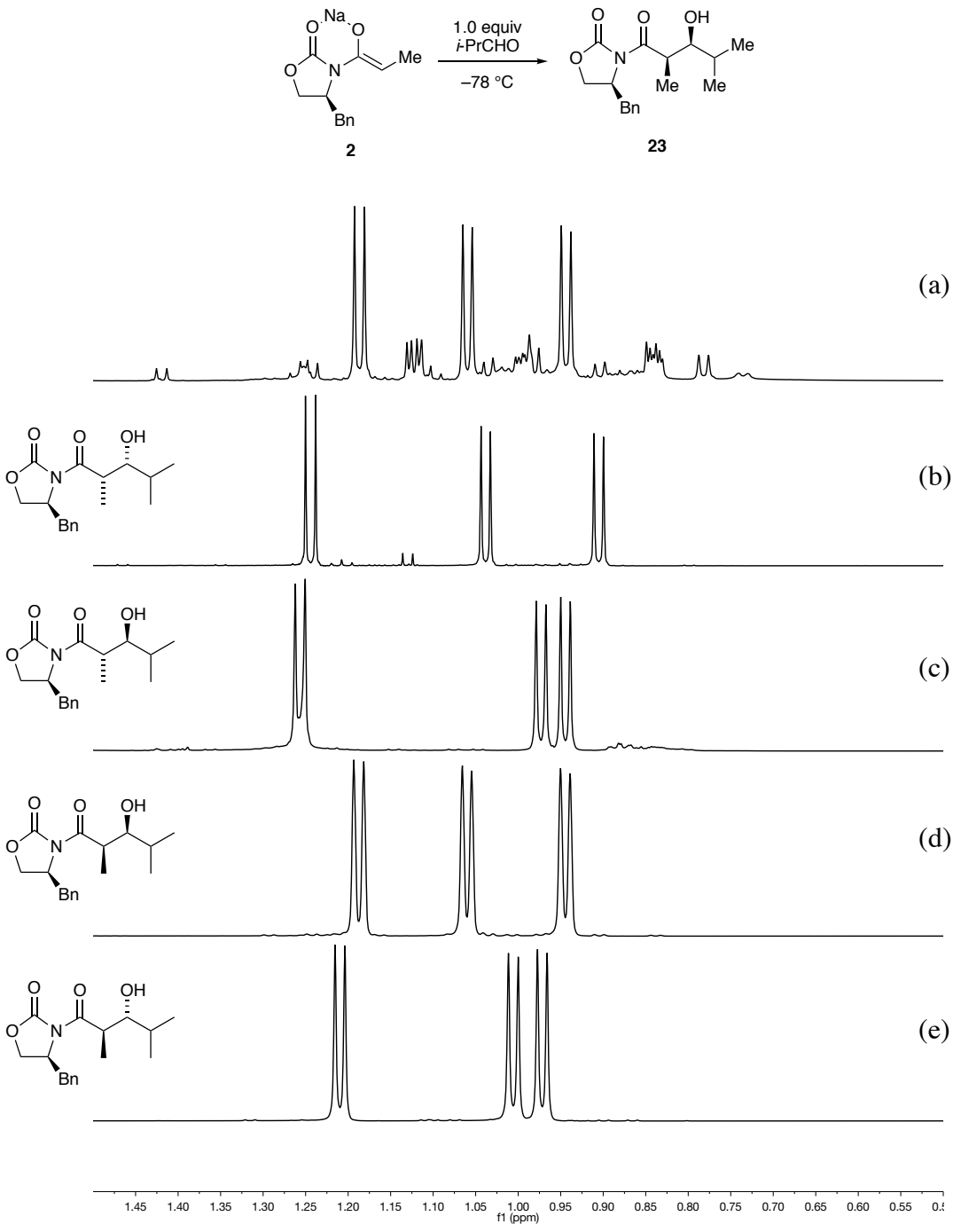


Figure S124. ^{1}H NMR spectrum in $CDCl_3$ recorded at rt of (a) **23** prepared from adding 1 equivalent of isobutyraldehyde to **1**; (b) non-Evans syn; (c) Evans anti; (d) Evans syn; (e) non-Evans anti. The yield is only 15%. The majority of the products are starting material **2** and deacylated product.

Synthesis of 25.

To a solution of NaHMDS (0.3 mmol, 54.9 mg) and TMEDA (0.90 mmol, 144 μL) in toluene (3.0 mL) was added **1** (0.30 mmol, 69.9 mg) in 0.10 mL of toluene. After stirring under Ar for 30 min at –78 °C isobutyraldehyde (0.90 mmol, 82 μL) was injected and the mixture was stirred for 1 hr at –78 °C. After quenching with 1.0 mL saturated NH_4Cl and extracting three times with EtOAc, the organic extracts were dried over $MgSO_4$ and concentrated in vacuo. Flash chromatography with 10% ethyl acetate in hexanes afforded 36.4 mg of **25** (61% combined yield). ^{1}H NMR showed a 17:1:0.7:0.4 mixture of **25** and three minor stereoisomers. ^{1}H NMR (599 MHz, $CDCl_3$) δ 5.06 (d, *J* = 4.2 Hz, 1H), 3.39 (dd, *J* = 9.0, 3.7 Hz, 1H), 2.73 (qd, *J* = 7.2, 3.7 Hz, 1H), 1.98 (hd, *J* = 6.9, 4.2 Hz, 1H), 1.84 (dh, *J* = 9.0, 6.6 Hz, 1H), 1.23 (d, *J* = 7.2 Hz, 3H), 1.01 – 0.97 (m, 9H), 0.86 (d, *J* = 6.8 Hz, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 172.94, 106.45, 82.07, 38.20, 32.71, 28.45, 18.67, 17.60, 16.17, 15.83, 11.74. m/z calculated for $(M+H)^+$ 201.14852, found 201.14824.

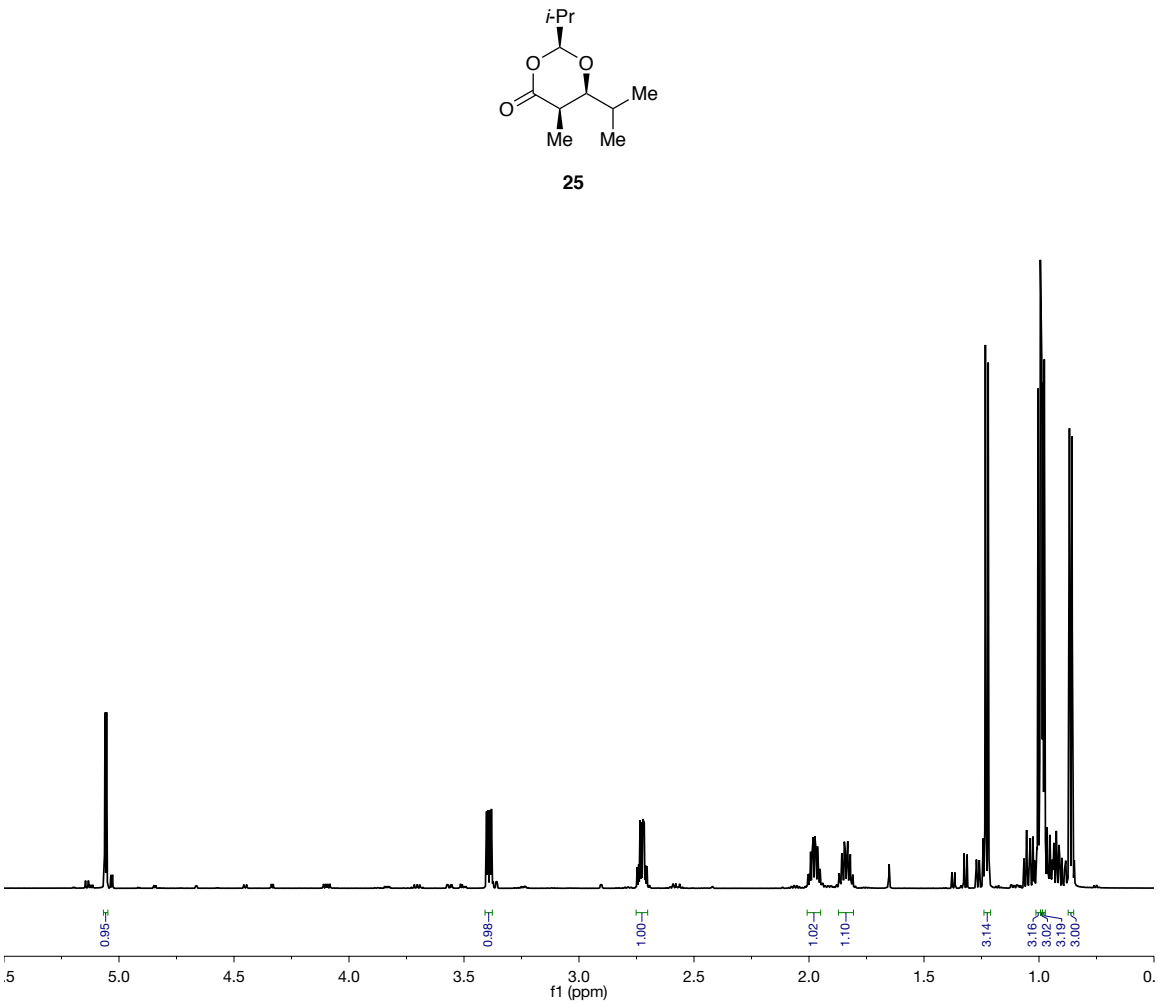


Figure S125. ^{1}H NMR spectrum ($CDCl_3$, 25 °C) of **25** prepared from (*S*)-**2** in TMEDA reacting with 3 equivalents of isobutyraldehyde. An isolated yield of 61% is obtained. Integration provides a diastereo selectivity of 17:1:0.7:0.4.

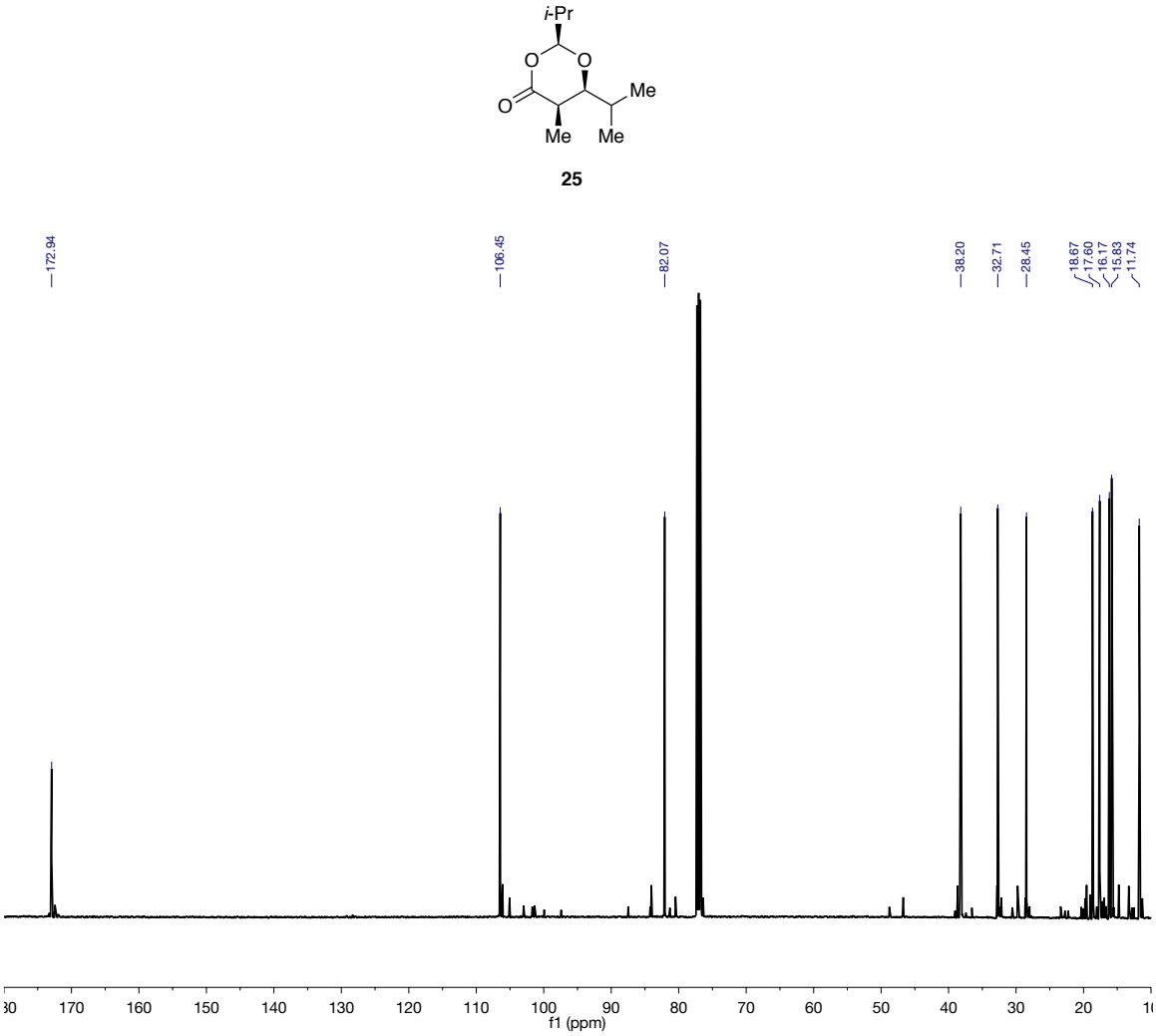
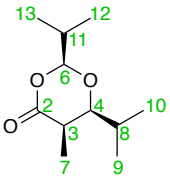


Figure S126. ^{13}C NMR spectrum ($CDCl_3$, 25 °C) of **25**.

Parameter	Value
1 Solvent	cdcl3
2 Temperature	23.0
3 Pulse Sequence	ROESYAD
4 Number of Scans	8
5 Receiver Gain	32
6 Relaxation Delay	1.5000
7 Pulse Width	8.2500
8 Acquisition Time	0.1500



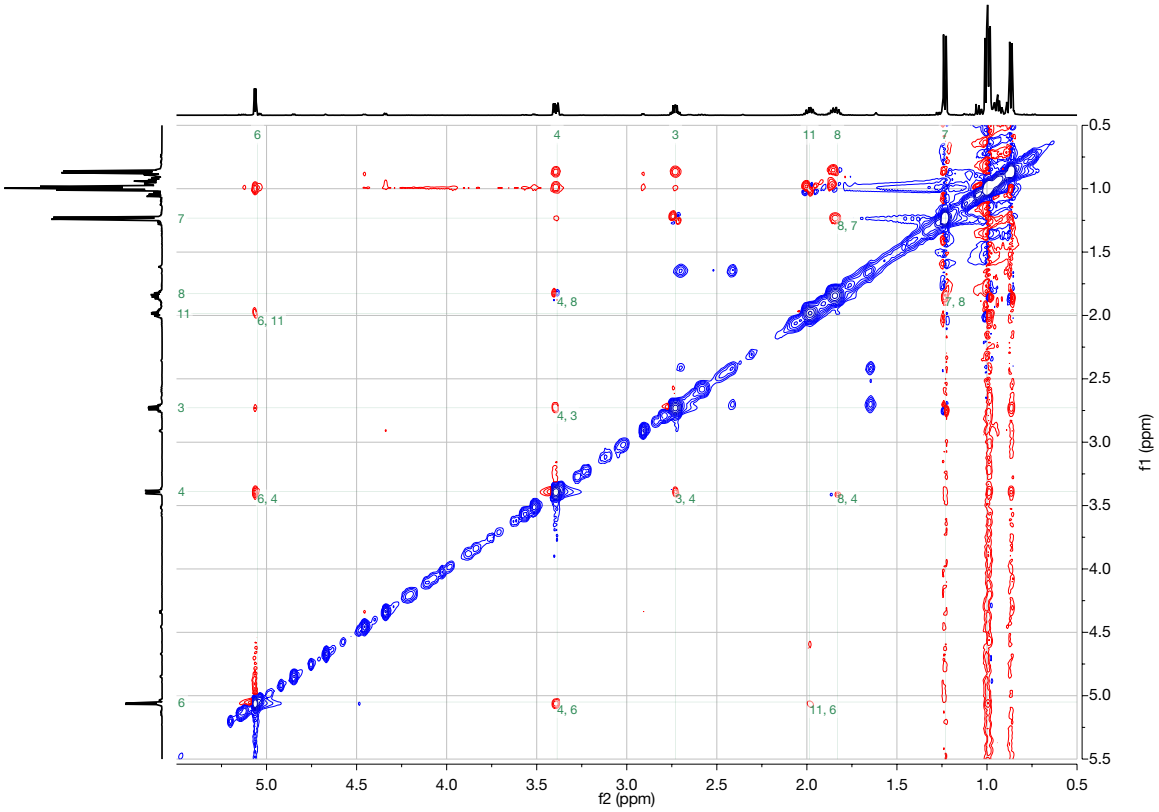
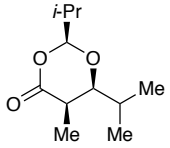


Figure S127. ROESY spectrum of **25** in $CDCl_3$ recorded at rt.

Table S3. ^{1}H and ^{13}C chemical shift assignments for **25**.

Atom #	δC, ppm	δH, ppm	ROESY
2	172.94		
3	38.20	2.73	4, 7, 9
4	82.07	3.39	3, 6, 8, 9, 10
6	106.45	5.05	4, 11, 12
7	18.67	1.23	3, 8
8	28.45	1.83	4, 7, 9, 10
9	11.74	0.84	3, 4, 8
10	15.83	0.96	4, 8
11	32.71	1.98	6, 12
12	16.17	0.98	6, 11
13	17.60	0.99	

The strong correlation between H#4 and H#6 through space is only viable by a 1, 3 diaxial interaction and thus sets the stereo center of C#6.



25

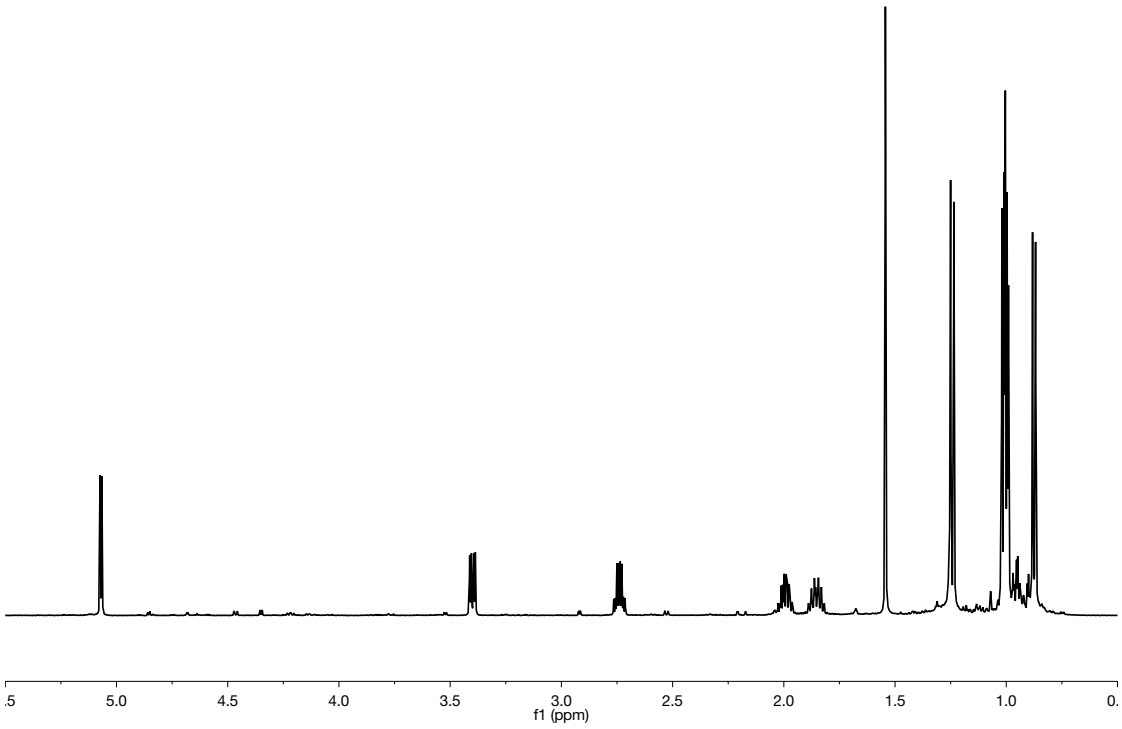


Figure S128. ^{1}H NMR spectrum ($CDCl_3$, 25 °C) of 0.10 M **25** prepared from **23** reacting with 1 equivalent of isobutyraldehyde. An isolated yield of 59% is obtained. The minor isomers are not observed in ^{1}H NMR.

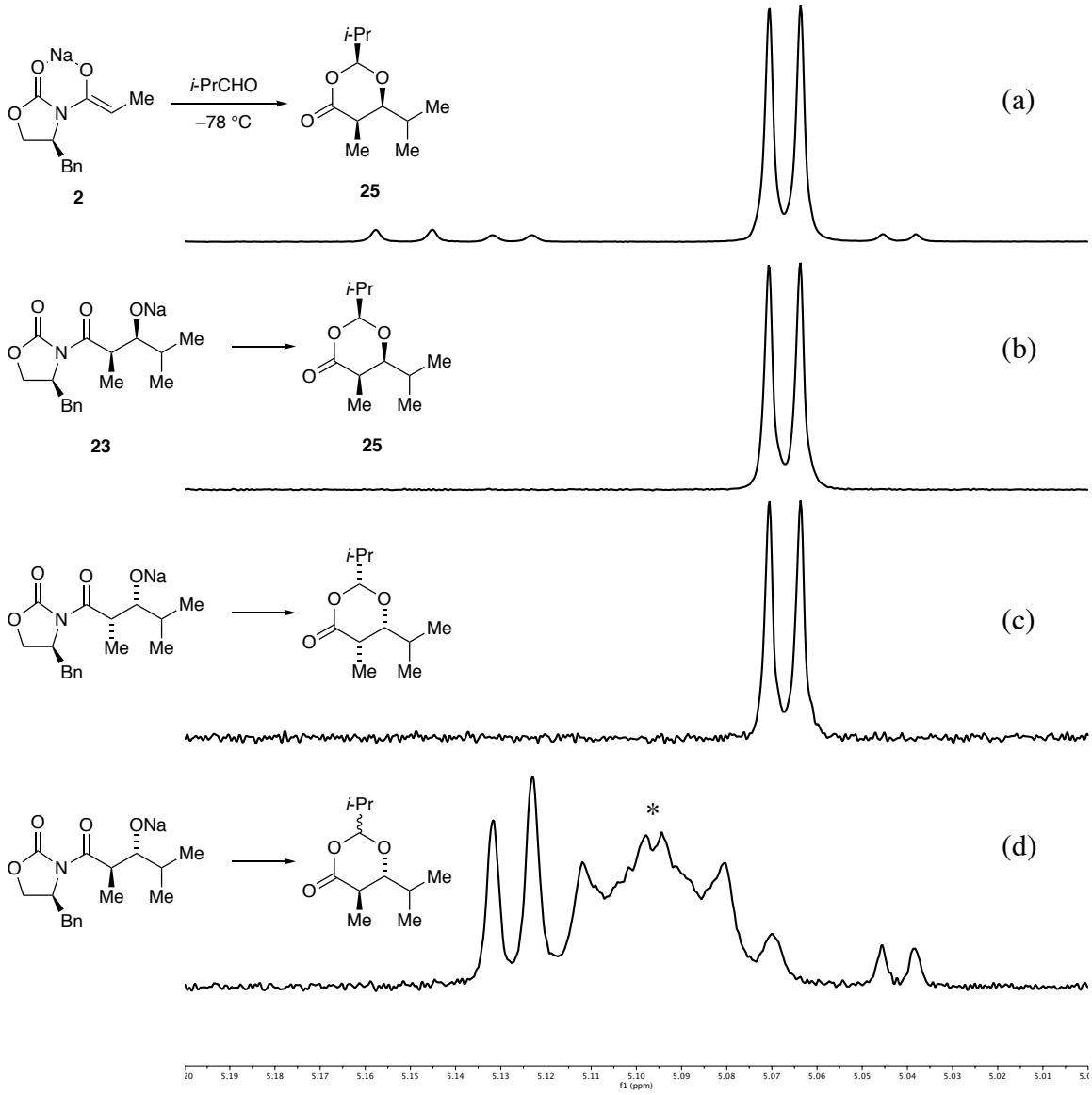


Figure S129. ^{1}H NMR spectrum ($CDCl_3$, 25 °C) of **25** prepared from isobutyraldehyde in TMEDA reacting with (a) (*S*)-**2**; (b) **23**; (c) Evans syn aldolate; (d) Evans anti aldolate. * Side product

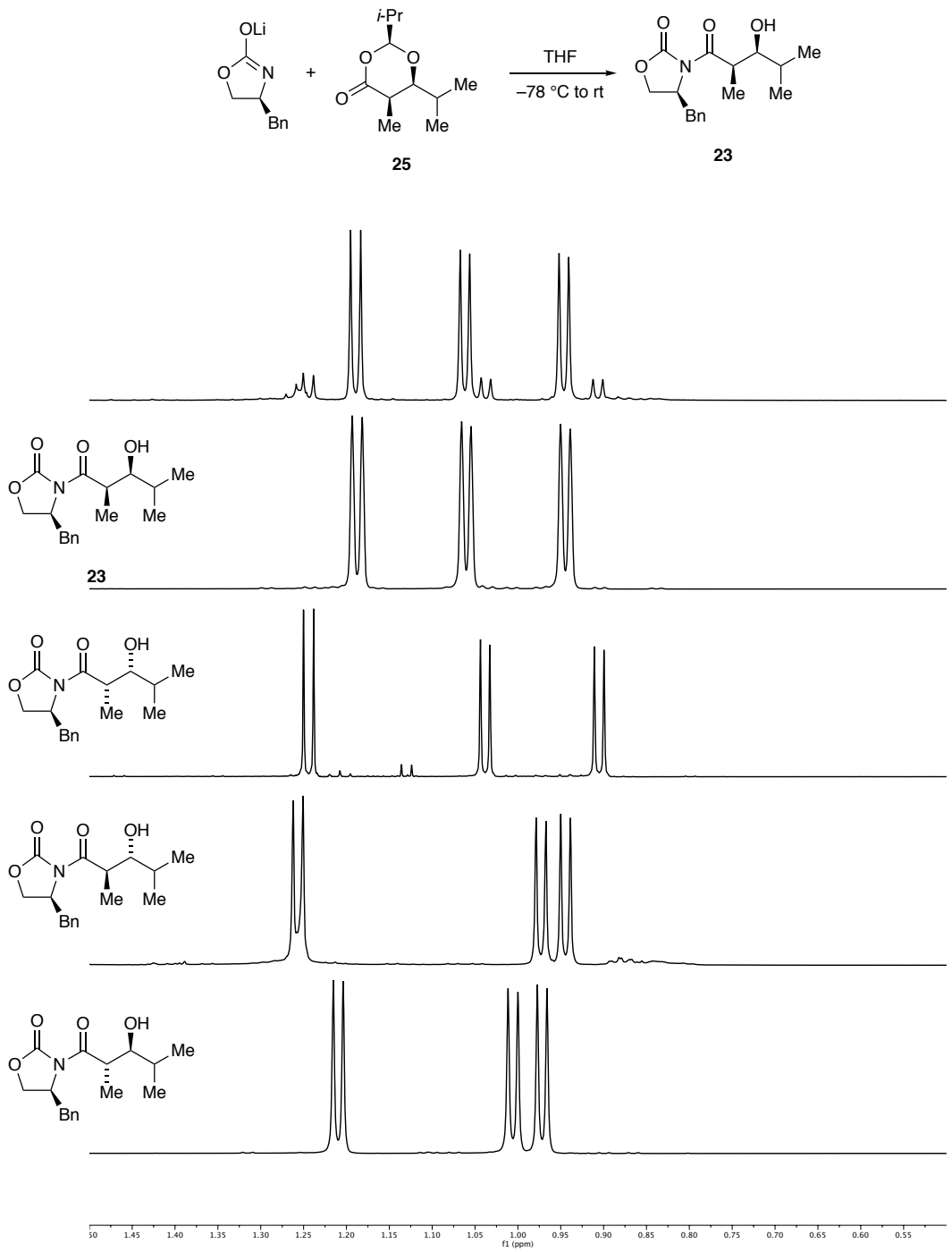


Figure S130. ^{1}H NMR spectrum in $CDCl_3$ recorded at rt of (a) **23** prepared from adding lithiated auxilliary to **25**; (b) non-Evans syn; (c) Evans syn; (d) non-Evans anti; (e) Evans anti.

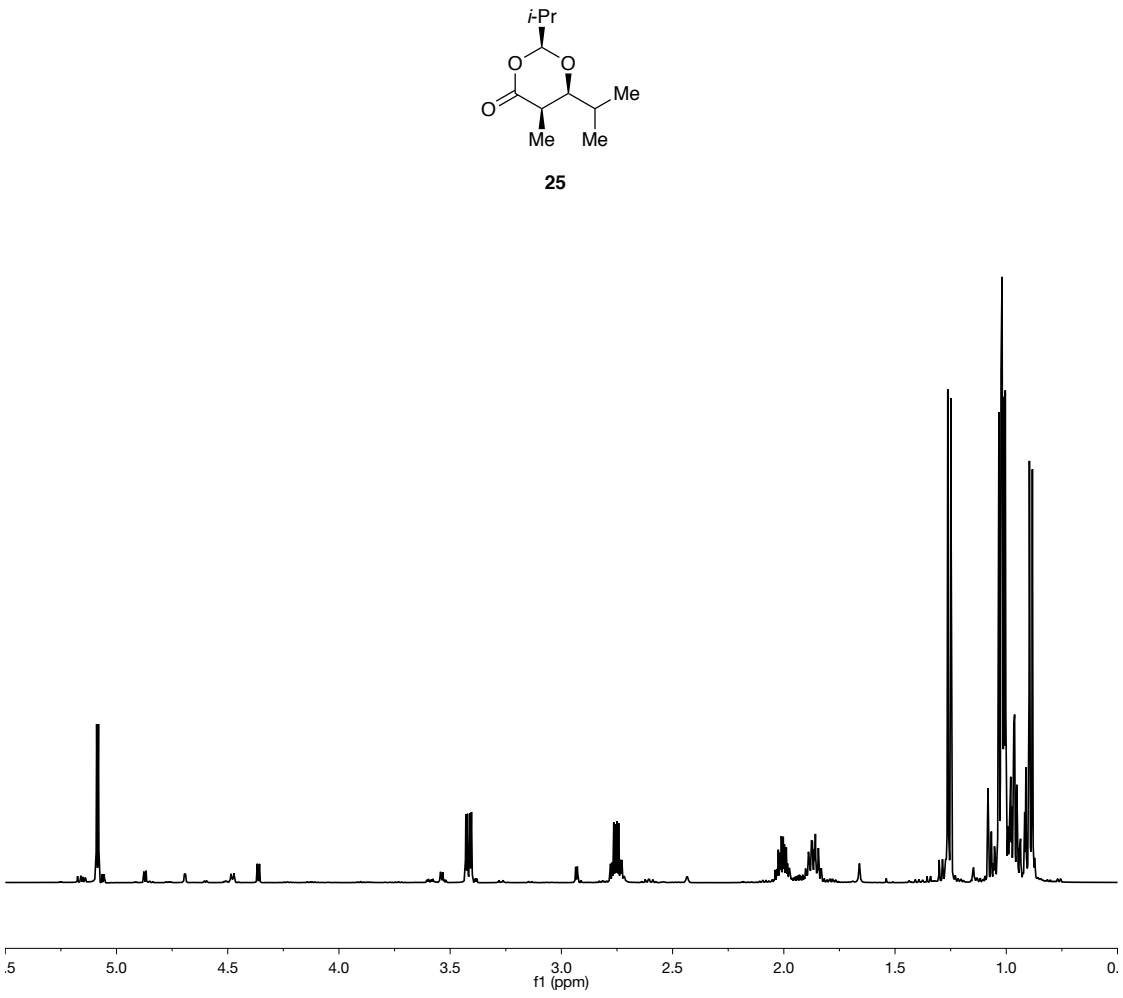


Figure S131. ^{1}H NMR spectrum ($CDCl_3$, 25 °C) of 0.10 M **25** prepared from **6** reacting with 3 equiv of isobutyraldehyde. An isolated yield of 58% is obtained. Integration provides a selectivity of 16:1:0.7:0.6.

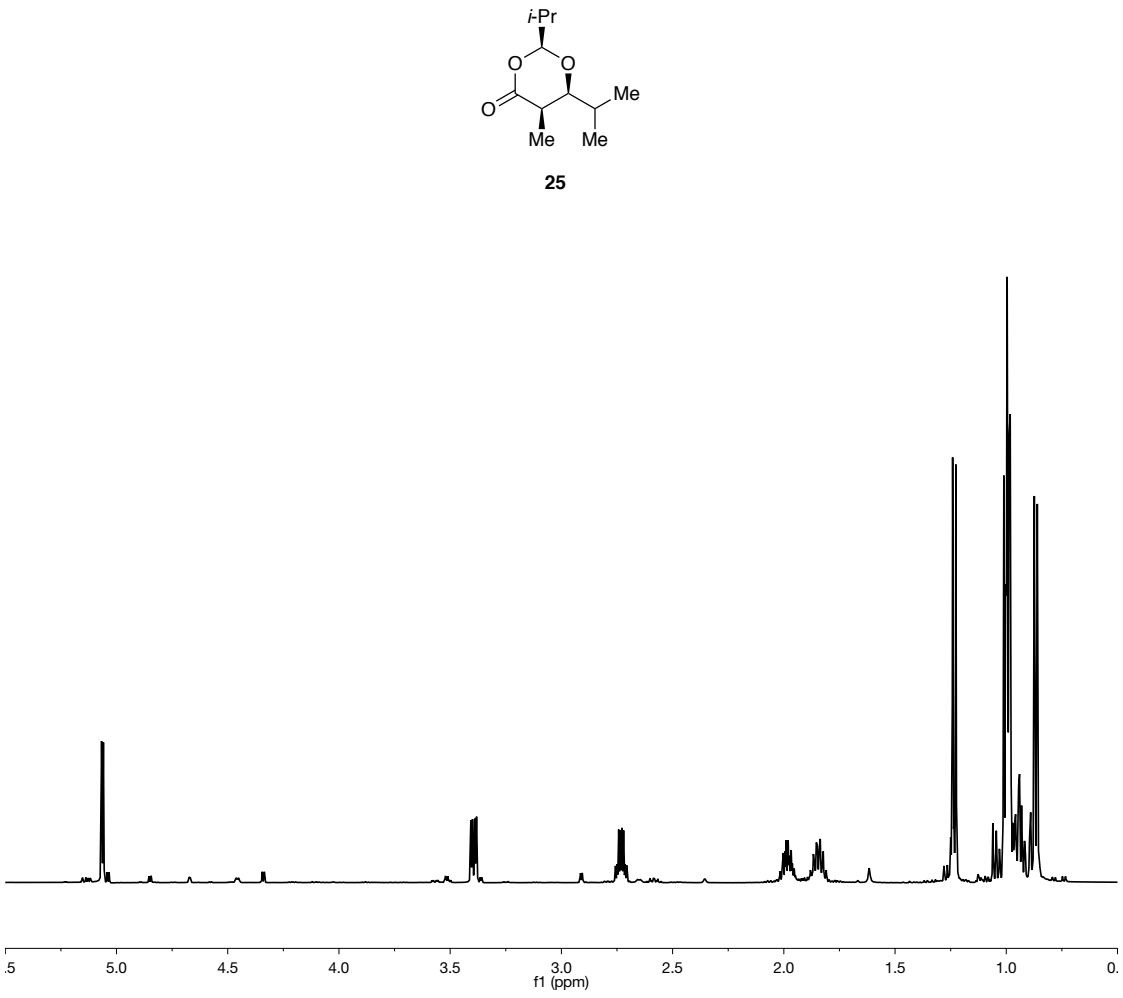


Figure S132. ^{1}H NMR spectrum ($CDCl_3$, 25 °C) of 0.10 M **25** prepared from **7** in TMEDA reacting with 3 equivalent of isobutyraldehyde. An isolated yield of 57% is obtained. Integration provides a selectivity of 13:1:0.5:0.5.

(4*S*)-4-benzyl-3-(2-methyl-3-(phenylamino)-3-(4-(trifluoromethyl)phenyl)propanoyl) oxazolidinone (**32**). To a solution of NaHMDS (0.11 mmol, 20.2 mg) and TMEDA (0.22 mmol, 33 μL) in toluene (5.0 mL), **1** (0.10 mmol, 23.3 mg) was added. After stirring for 1.5 hr under Ar at –78 °C, complex **38** formed from imine **37** (0.10 mmol, 24.9 mg) and BF_3 (0.10 mmol, 19 μL) was injected as a slush. The reaction was stirred for 1 hour at –78 °C, quenched with saturated NH_4Cl, and extracted three times with EtOAc. The organic extracts were dried over $MgSO_4$, concentrated in vacuo, and purified by flash chromatography (10% EtOAc/hexanes/3% Et_3N). Adduct **32** (38 mgs) was obtained 79% yield. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.56 –6.61 (m, 14H), 5.03 (t, *J* = 5.1 Hz, 1H), 4.72 (tt, *J* = 8.4, 3.2 Hz, 1H), 4.32 (qd, *J* = 6.9, 4.6 Hz, 1H), 4.24 (t, *J* = 8.7 Hz, 1H), 4.15 (dd, *J* = 9.1, 3.0 Hz, 1H), 2.91 (dd, *J* = 13.7, 3.3 Hz, 1H), 2.49 (dd, *J* = 13.7, 8.9 Hz, 1H), 1.13 (d, *J* = 7.0 Hz, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 174.26, 153.38, 146.65, 134.62, 129.31, 129.28, 128.96, 127.46, 127.35, 125.56, 118.19, 113.64, 66.22, 58.08, 54.99, 43.95, 37.34, 10.51. ^{19}F NMR (470 MHz, $CDCl_3$) δ -62.36 (major), -62.47 (minor).

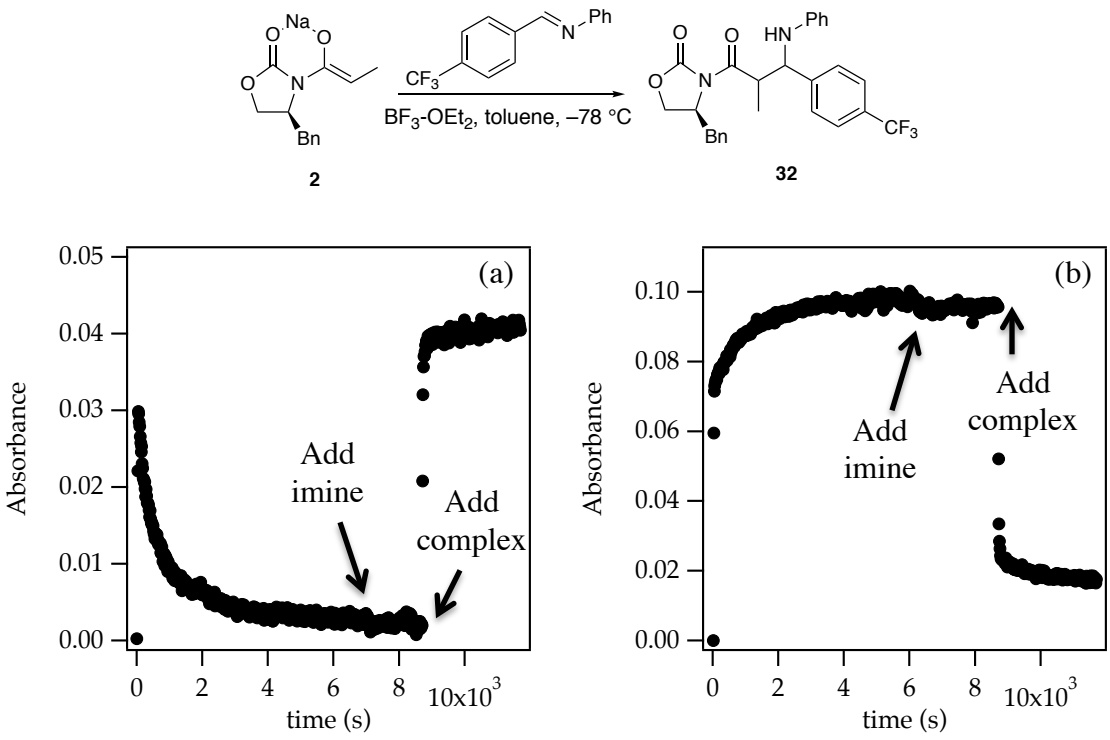


Figure S133. IR spectra from a solution of 0.020 M **2** in toluene at –78 °C with first 0.020 M imine and then 0.020 M imine-BF_3 complex added, following (a) auxiliary C=O peak; (b) enolate peak. Adding only imine to enolate **2** shows no reactivity. Aza-aldol reaction occurs after imine-BF_3 complex addition.

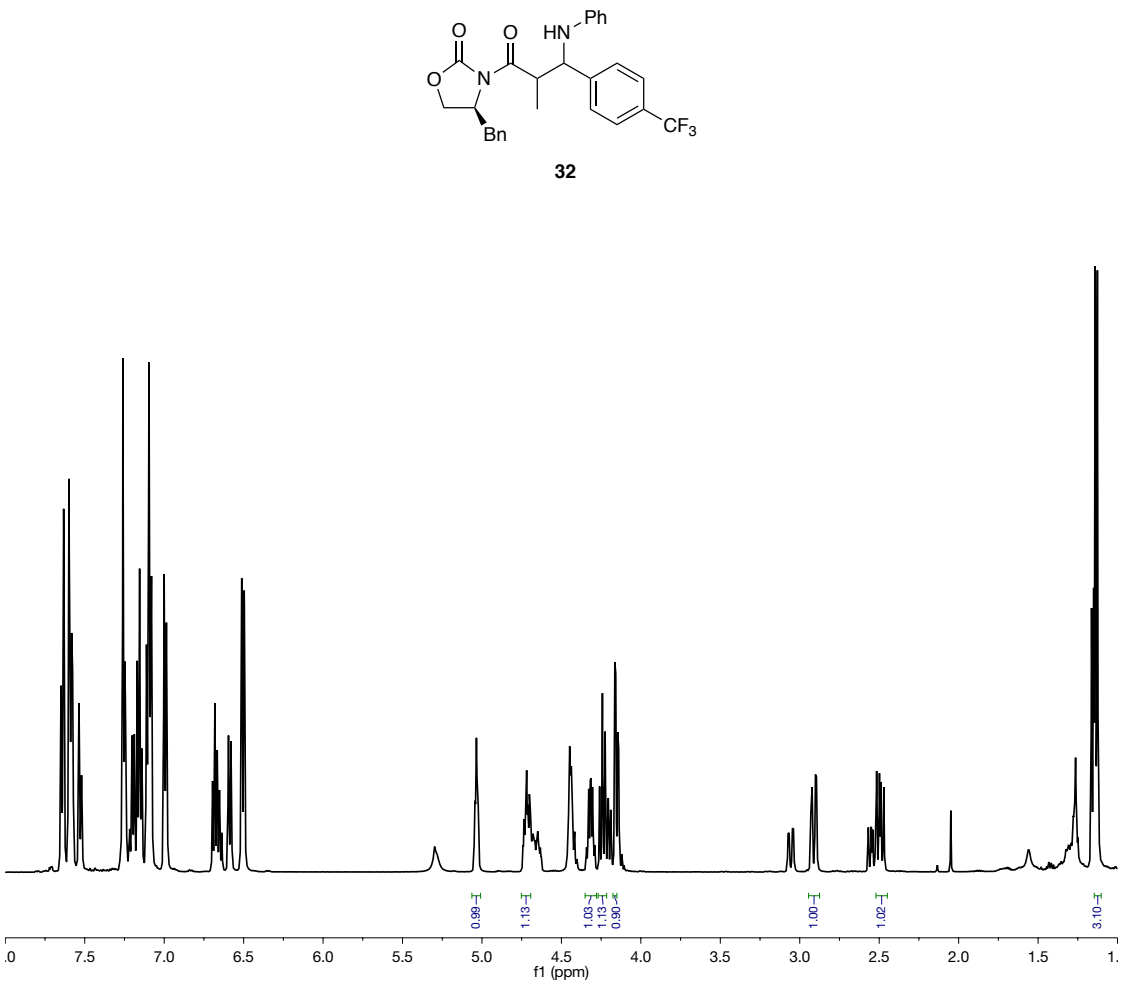


Figure S134. ^{1}H NMR spectrum ($CDCl_3$, 25 °C) of **32**.

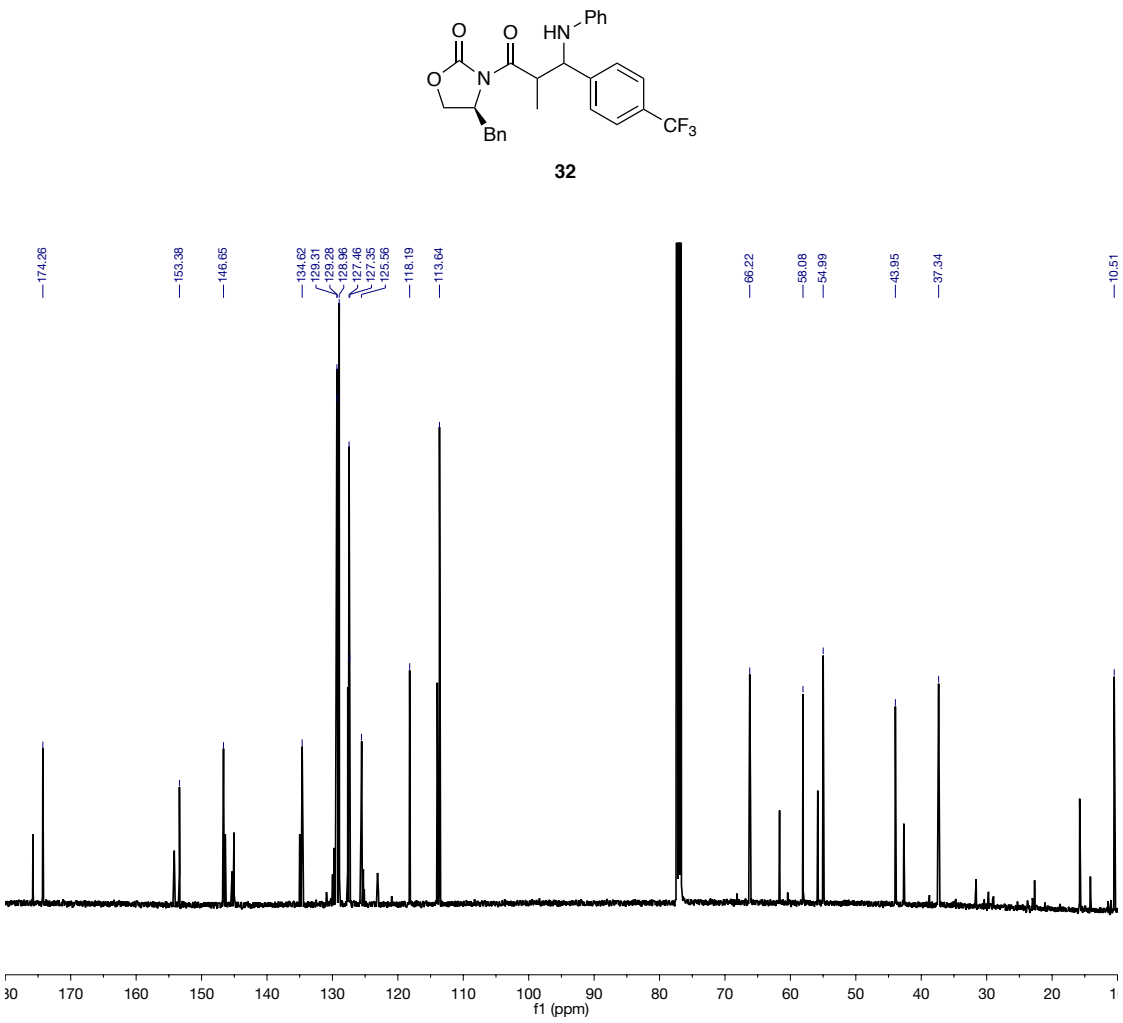


Figure S135. ^{13}C NMR spectrum ($CDCl_3$, 25 °C) of **32**.

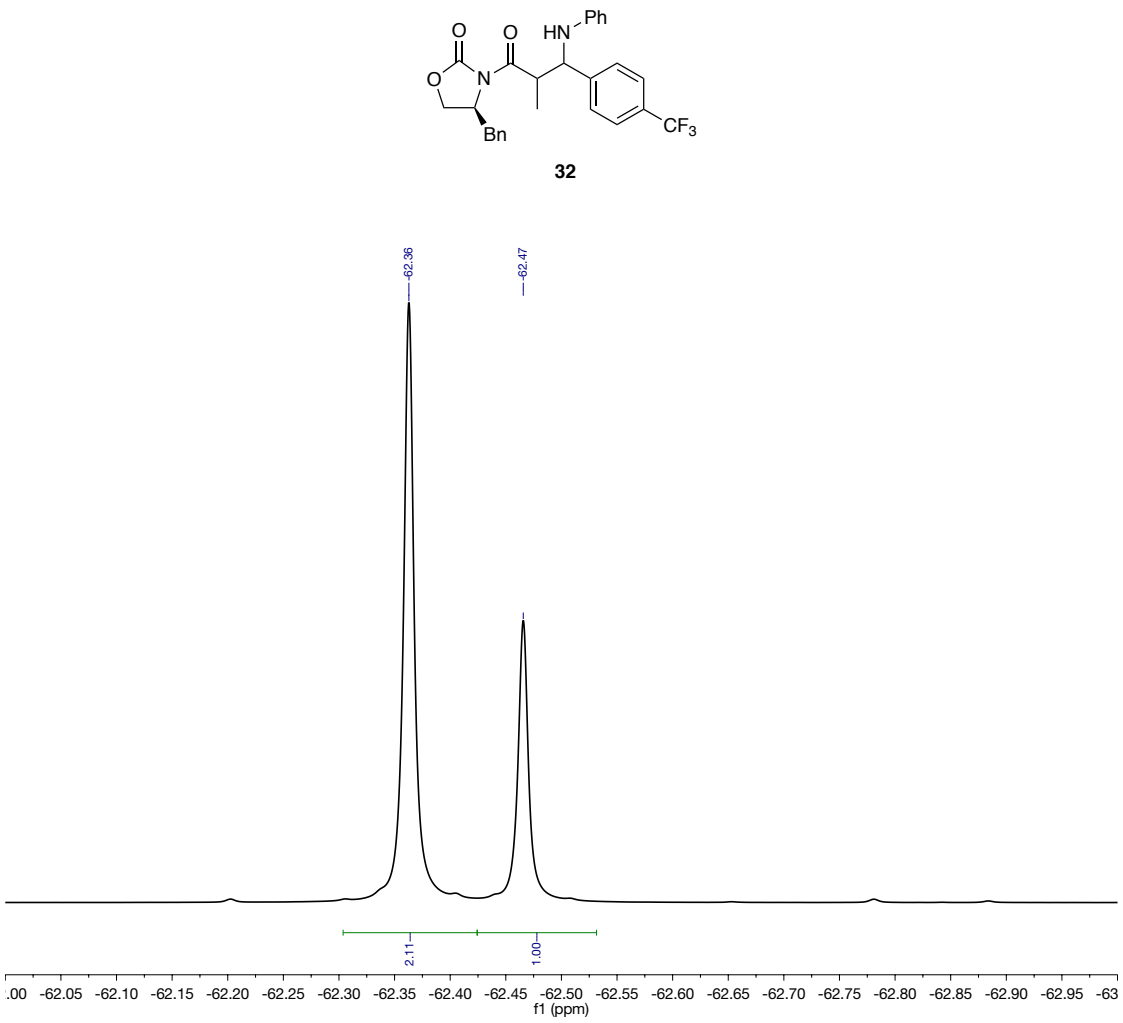


Figure S136. ^{19}F NMR spectrum ($CDCl_3$, 25 °C) of **32**. Integration provides a selectivity of 2:1.

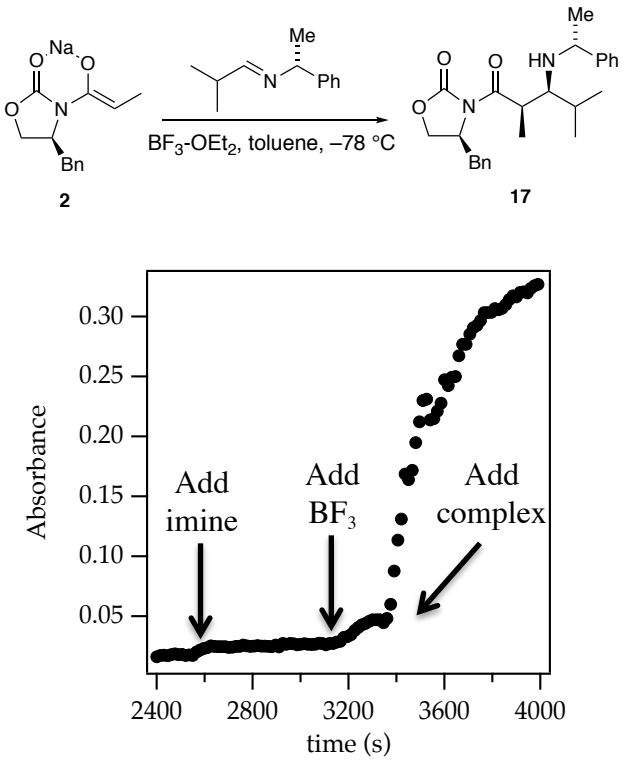


Figure S137. IR spectra following auxiliary C=O peak in a solution of 0.20 M **2** in 0.40 M TMEDA/toluene with sequential addition of 0.20 M imine, 0.20 M BF_3•OEt_2 and 0.20 M **20** recorded at –78 °C.
Aza-aldol reaction requires the imine and BF_3 to be precomplexed. Adding imine and BF_3 separately does not work. Only adding the pre-formed complex works.

(4*S*)-4-benzyl-3-(2,4-dimethyl-3-(((*R*)-1-phenylethyl)amino)pentanoyl)oxazolidin-2-one (**17**). To a solution of NaHMDS (0.11 mmol, 20.2 mg) and TMEDA (0.22 mmol, 33 μL) in toluene (2.0 mL), **1** (0.10 mmol, 23.3 mg) was added. The reaction was stirred under Ar for 30 minutes at –78 °C. A solution of imine-BF_3 complex **20** (0.10 mmol) in toluene (0.20 mL) was injected and the mixture was stirred for 30 minutes. The reaction was quenched by 1.0 mL saturated NH_4Cl and extracted three times with EtOAc. The organic extracts dried over $MgSO_4$ and concentrated in vacuo. Flash chromatography (10% ethyl acetate/hexanes/3% Et_3N) afforded **17** in >30:1 selectivity and 82% yield. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.37 – 7.30 (m, 4H), 7.30 – 7.24 (m, 3H), 7.22 – 7.16 (m, 3H), 4.63 (ddt, *J* = 10.8, 7.3, 3.4 Hz, 1H), 4.16 – 4.10 (m, 1H), 4.09 (dd, *J* = 9.1, 3.4 Hz, 1H), 3.96 – 3.86 (m, 2H), 3.25 (dd, *J* = 13.2, 3.4 Hz, 1H), 2.87 (dd, *J* = 6.7, 4.2 Hz, 1H), 2.52 (dd, *J* = 13.2, 10.3 Hz, 1H), 1.80 (pd, *J* = 6.9, 4.2 Hz, 1H), 1.34 (d, *J* = 6.5 Hz, 3H), 1.12 (d, *J* = 6.9 Hz, 3H), 1.07 (d, *J* = 6.9 Hz, 3H), 0.96 (d, *J* = 6.9 Hz, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 177.23, 153.22, 146.33, 135.63, 129.48, 129.09, 128.42, 127.43, 127.16, 127.00, 66.04, 60.80, 56.84, 55.53, 40.84, 38.16, 31.84, 24.32, 20.67, 18.09, 14.15. m/z calculated for $(M+H)^+$ 409.24857, found 409.24796.

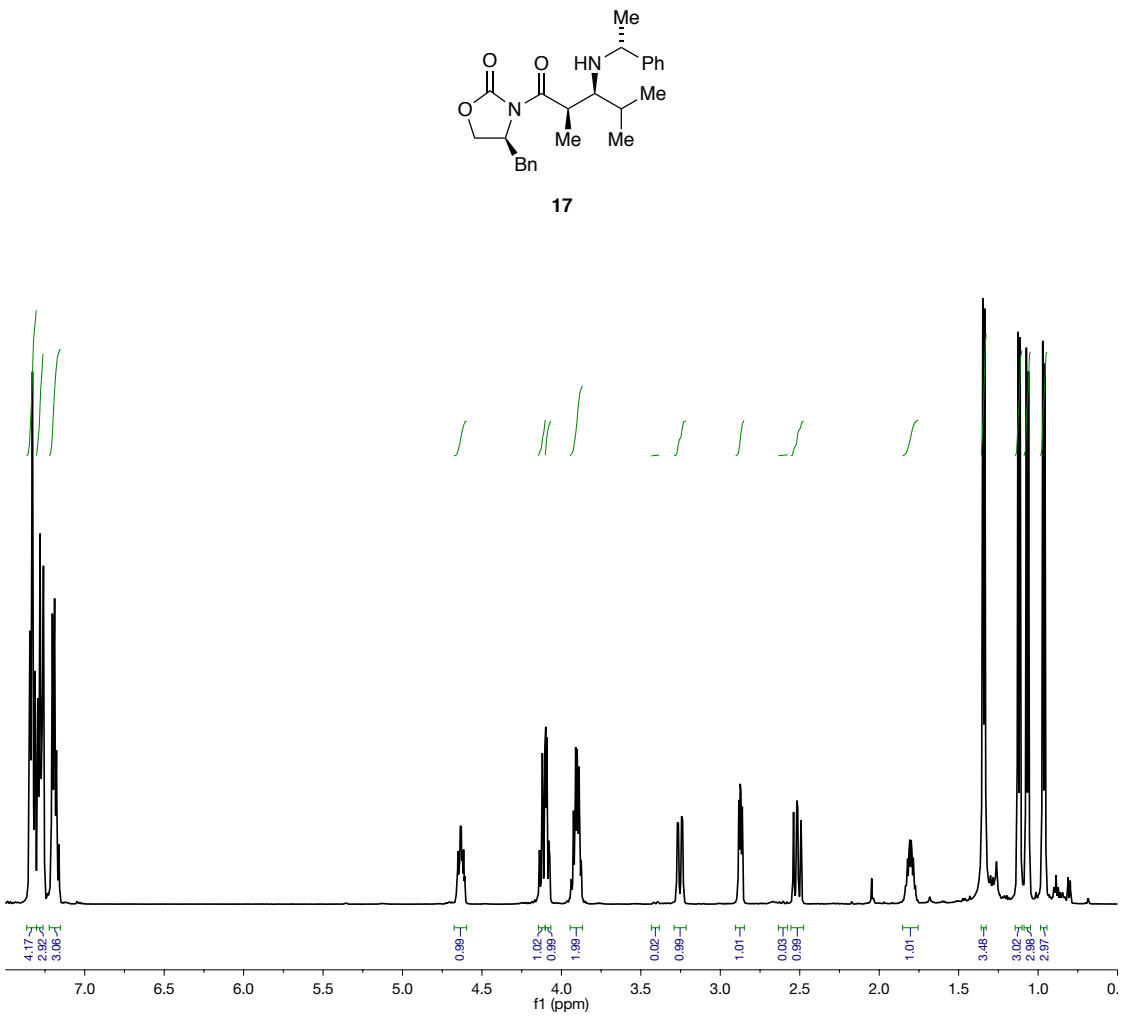


Figure S138. ^{1}H NMR spectrum ($CDCl_3$, 25 °C) of **17**.

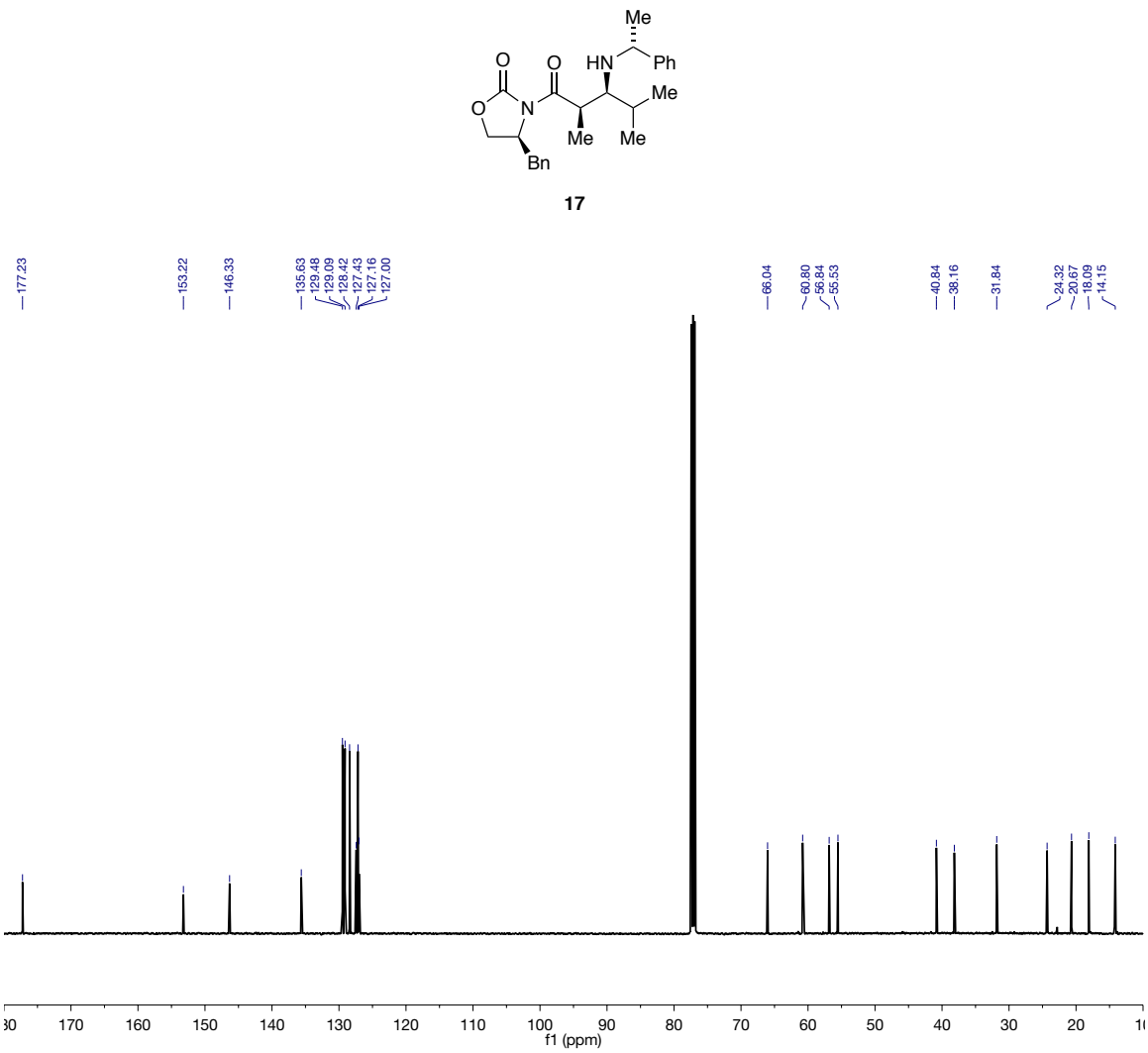
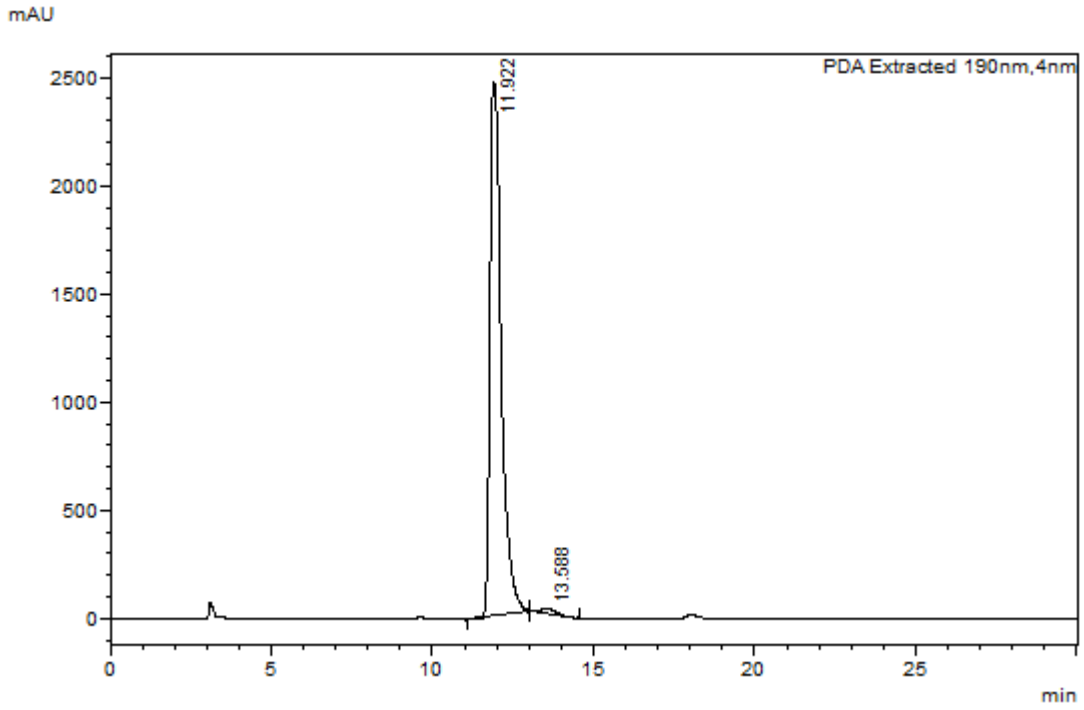


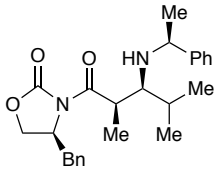
Figure S139. ^{13}C NMR spectrum ($CDCl_3$, 25 °C) of **17**.



Peak#	Ref. Time	Area	Height	Area%
1	11.922	60192867	2465748	98.89
2	13.588	675348	20705	1.11
Total		60868215	2486453	100

Figure S140. HPLC spectrum of **17** in *i*-PrOH using OD column and 5% *i*-PrOH/hexane.

(4*S*)-4-benzyl-3-(2,4-dimethyl-3-(((*S*)-1-phenylethyl)amino)pentanoyl)oxazolidin-2-one (**16**). To a solution of NaHMDS (1.0 mmol, 183 mg) and TMEDA (2.0 mmol, 300 μL) in toluene (4.5 mL) was added **1** (1.0 mmol, 233 mg) followed by stirring under argon for 30 minutes at –78 °C. A solution of imine-BF_3 complex **19** (1.0 mmol) in toluene (0.20 mL) was injected. After stirring for 30 m, the reaction was quenched by 5.0 mL saturated NH_4Cl and extracted three times with EtOAc. The organic extracts were dried over $MgSO_4$ and concentrated in vacuo. The crude product showed **16** in >30:1 selectivity using ^{1}H NMR spectroscopy. Flash chromatography (10% ethyl acetate/hexanes/3% Et_3N) afforded **16** (380 mg, 93% yield). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.33 (dt, *J* = 7.6, 2.8 Hz, 4H), 7.31 – 7.25 (m, 3H), 7.25 – 7.19 (m, 3H), 4.70 (ddt, *J* = 10.9, 7.2, 3.4 Hz, 1H), 4.20 – 4.15 (m, 1H), 4.15 – 4.11 (m, 1H), 3.95 (p, *J* = 6.8 Hz, 1H), 3.86 (q, *J* = 6.5 Hz, 1H), 3.40 (dd, *J* = 13.2, 3.4 Hz, 1H), 2.88 (dd, *J* = 6.2, 4.8 Hz, 1H), 2.60 (dd, *J* = 13.1, 10.4 Hz, 1H), 1.67 (pd, *J* = 6.9, 4.9 Hz, 1H), 1.33 (d, *J* = 6.6 Hz, 3H), 1.29 (d, *J* = 6.9 Hz, 3H), 0.80 (d, *J* = 6.8 Hz, 6H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 177.35, 153.32, 146.49, 135.64, 129.48, 129.13, 128.37, 127.46, 127.27, 127.02, 66.17, 61.44, 57.74, 55.71, 41.64, 38.38, 32.49, 24.25, 20.74, 17.86, 13.82. m/z calculated for $(M+H)^+$ 409.24857, found 409.24889.



16

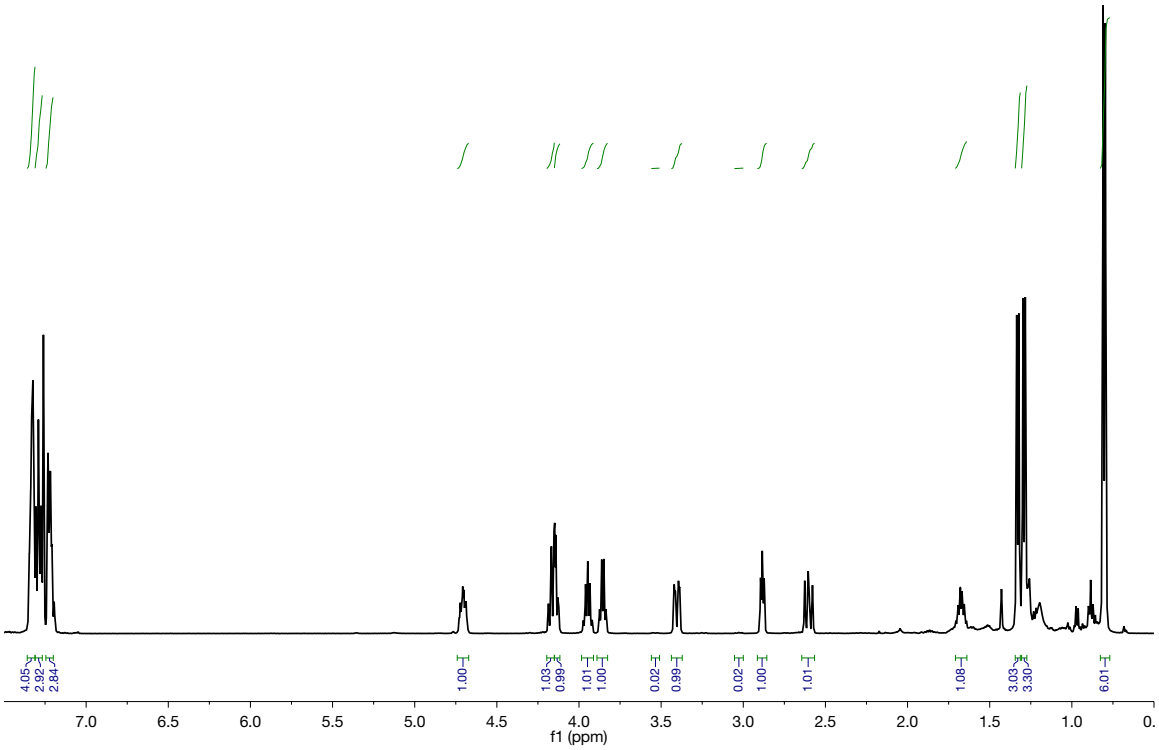


Figure S141. ^{1}H NMR spectrum ($CDCl_3$, 25 °C) of **16**.

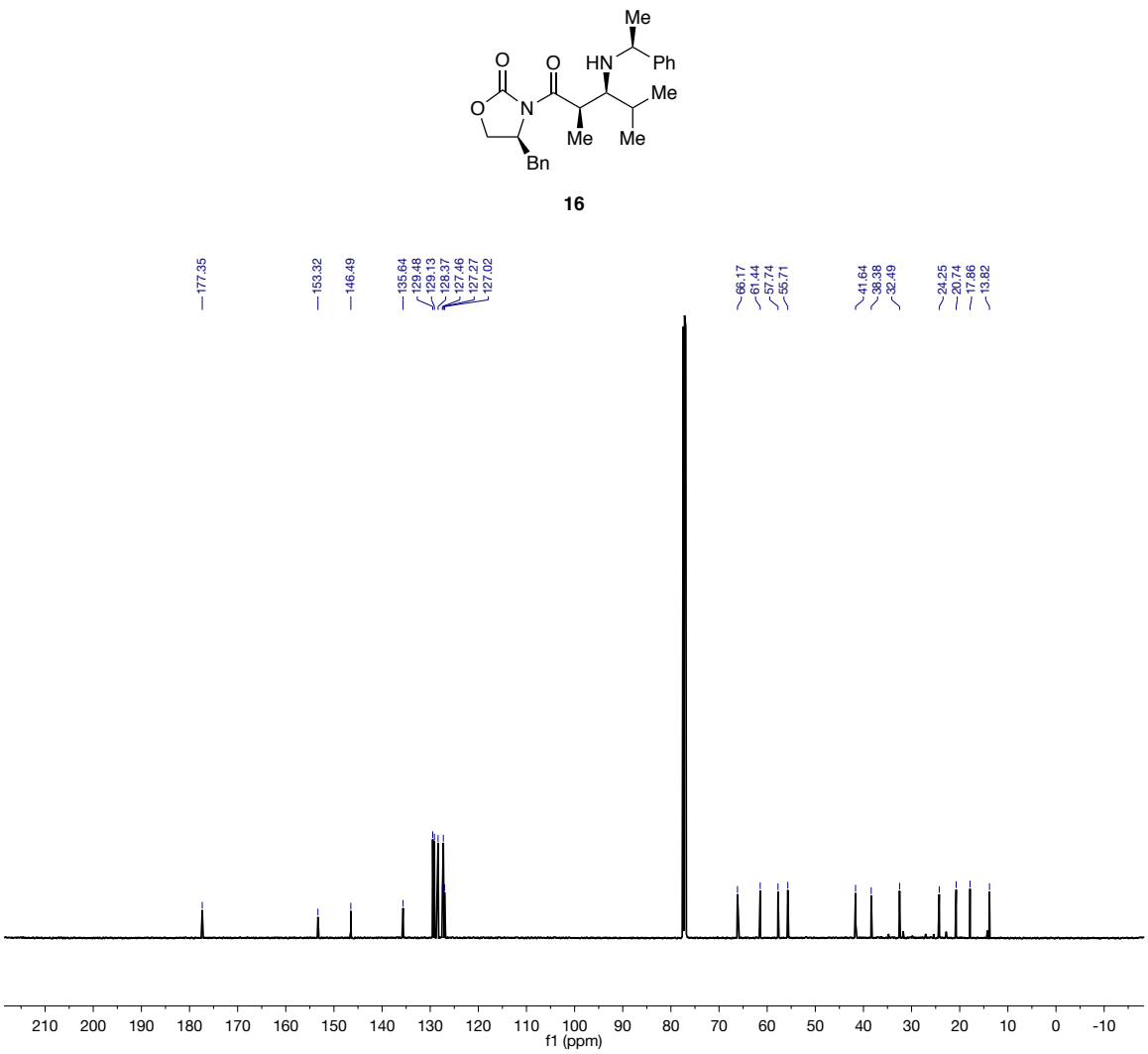


Figure S142. ^{13}C NMR spectrum ($CDCl_3$, 25 °C) of **16**.

(4*S*)-3-(3-amino-2,4-dimethylpentanoyl)-4-benzyloxazolidin-2-one (**22**). To a solution of **17** (0.08 mmol, 33.3 mg) in methanol (2 mL) was added palladium on carbon (0.008 mmol, 8.5 mg). Reaction was stirred under 1.0 atm of H_2 for 24 hr at room temperature. After filtering through Celite and concentrating in vacuo, flash chromatography with 3% triethylamine in ethyl acetate afforded **22** (14.5 mg, 60% yield). ^{1}H NMR (599 MHz, $CDCl_3$) δ 7.26 – 7.25 (m, 1H), 7.25 – 7.20 (m, 3H), 7.20 – 7.16 (m, 1H), 5.17 – 5.05 (m, 2H), 4.02 – 3.95 (m, 1H), 3.83 (dd, *J* = 12.0, 3.0 Hz, 1H), 3.24 (dd, *J* = 13.7, 9.7 Hz, 1H), 3.12 (dd, *J* = 13.7, 6.9 Hz, 1H), 2.66 (p, *J* = 7.0 Hz, 1H), 1.64 (pd, *J* = 14.0, 6.9 Hz, 1H), 0.97 – 0.87 (m, 3H), 0.86 (d, *J* = 6.7 Hz, 3H), 0.83 (d, *J* = 6.6 Hz, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 171.32, 155.43, 138.18, 129.51, 128.49, 126.62, 63.85, 60.55, 55.92, 34.67, 27.90, 18.77, 18.18, 9.89. m/z calculated for $(M+H)^+$ 305.18597, found 305.18521.

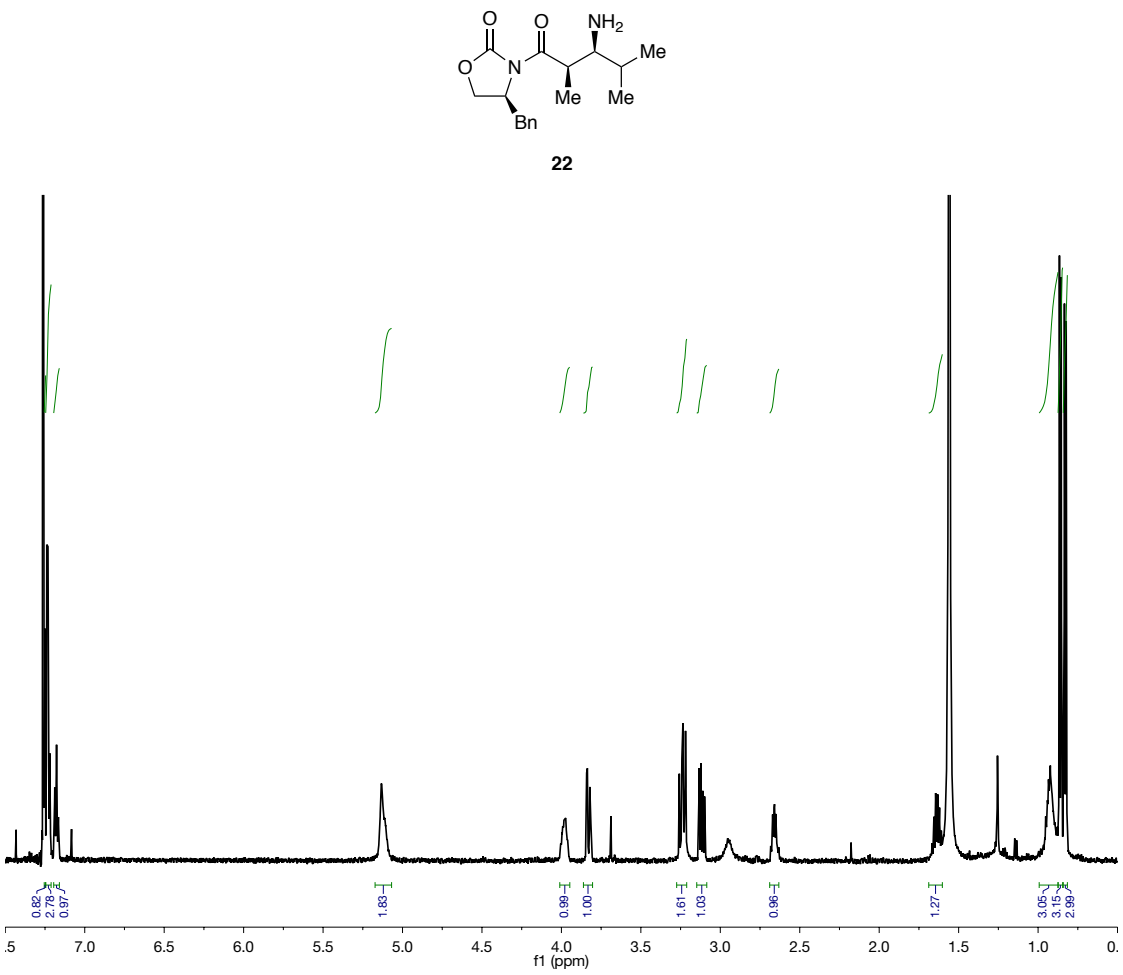


Figure S143. ^{1}H NMR spectrum ($CDCl_3$, 25 °C) of **22**.

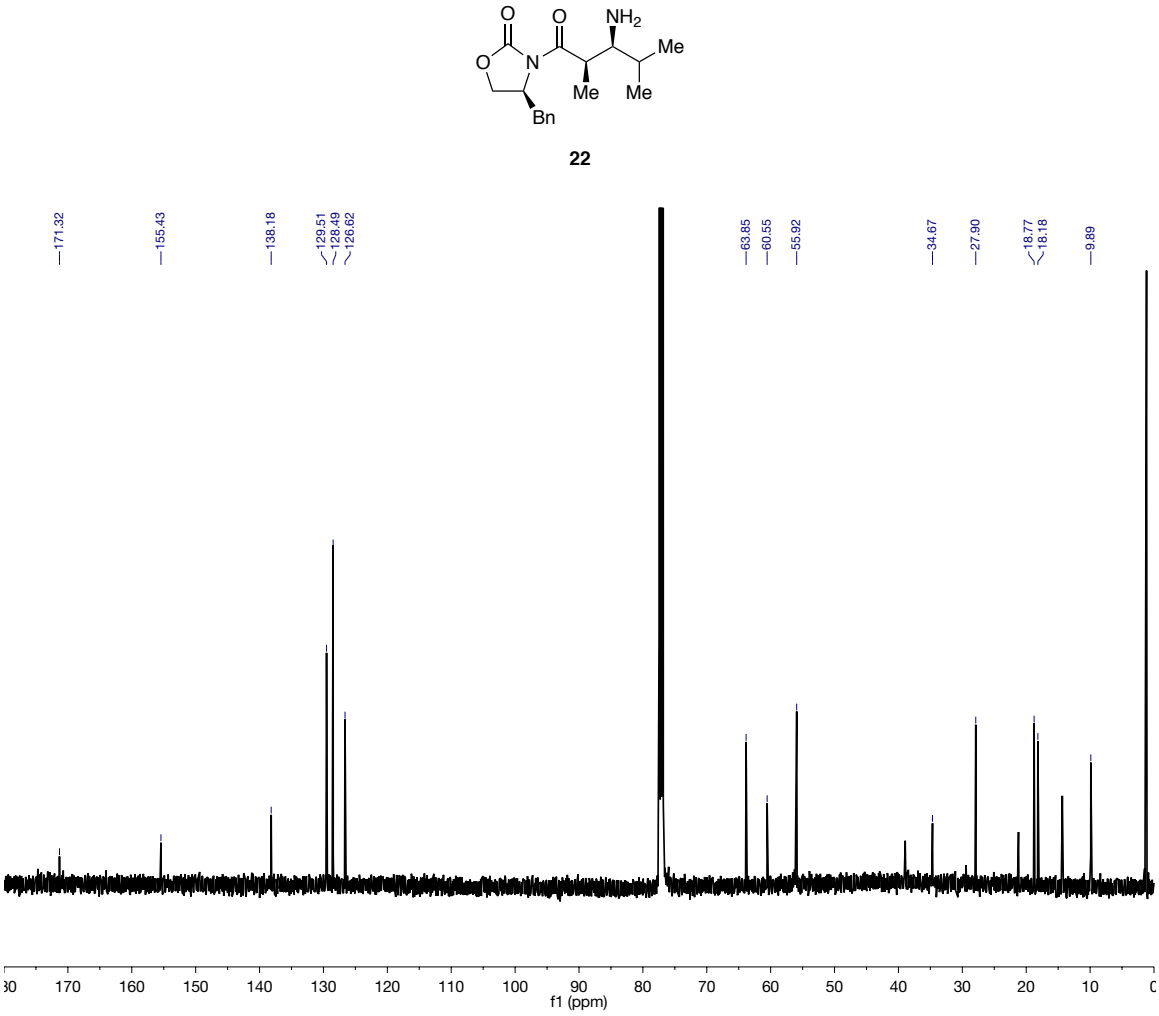


Figure S144. ^{13}C NMR spectrum ($CDCl_3$, 25 °C) of **22**.

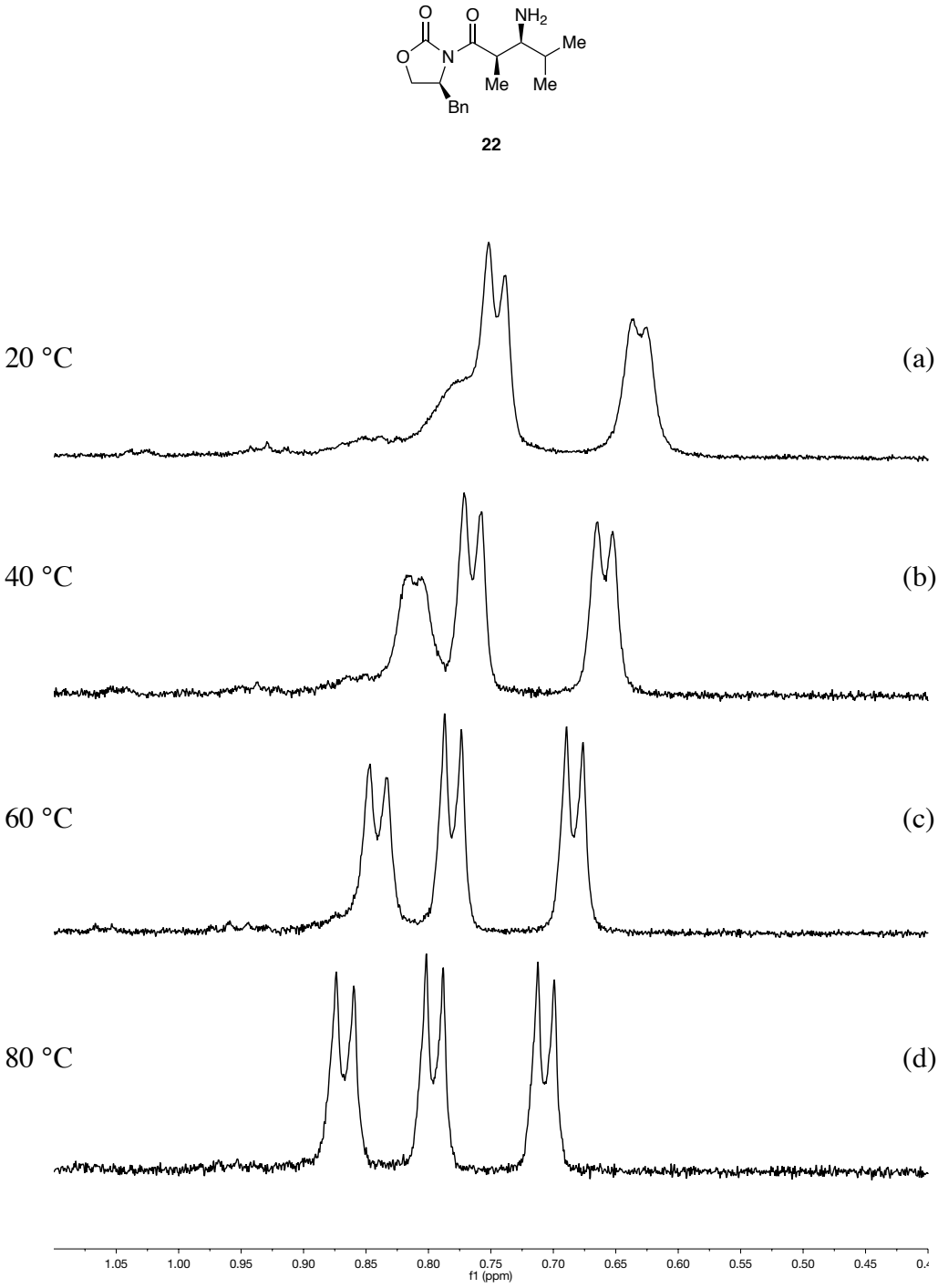


Figure S145. ^{1}H NMR spectrum of **22** in DMSO-d_6 recorded at (a) 20 °C; (b) 40 °C; (c) 60°C; (d) 80 °C.

(4*S*)-4-benzyl-3-(3-(benzylamino)-2,4-dimethylpentanoyl)oxazolidin-2-one (**18**). To a solution of NaHMDS (0.11 mmol, 20.2 mg) and TMEDA (0.22 mmol, 33 μL) in toluene (2.0 mL), **1** (0.10 mmol, 23.3 mg) was added. Reaction was stirred under argon for 30 minutes at –78 °C. A solution of imine-BF_3 complex **21** (0.10 mmol) in toluene (0.20 mL) was injected and the mixture was stirred for 30 minutes. The reaction was quenched by 1.0 mL saturated NH_4Cl and extracted three times with EtOAc. The organic extracts dried over $MgSO_4$ and concentrated in vacuo. Flash chromatography (10% ethyl acetate/hexanes/3% Et_3N afforded **18** (34.3 mg, 87% yield), shown by ^1H NMR to be **18** and its minor diastereomer in 17:1 selectivity. ^1H NMR (500 MHz, $CDCl_3$) δ 7.39 – 7.34 (m, 2H), 7.34 – 7.30 (m, 2H), 7.30 – 7.24 (m, 3H), 7.24 – 7.21 (m, 3H), 4.73 (ddt, *J* = 11.0, 7.3, 3.5 Hz, 1H), 4.20 – 4.15 (m, 1H), 4.14 (dd, *J* = 9.1, 3.6 Hz, 1H), 4.06 – 3.99 (m, 1H), 3.86 (d, *J* = 12.5 Hz, 1H), 3.81 (d, *J* = 12.5 Hz, 1H), 3.40 (dd, *J* = 13.2, 3.4 Hz, 1H), 2.90 (t, *J* = 6.0 Hz, 1H), 2.60 (dd, *J* = 13.1, 10.4 Hz, 1H), 1.81 (pd, *J* = 13.3, 6.7 Hz, 1H), 1.25 (d, *J* = 6.9 Hz, 3H), 1.04 (d, *J* = 6.8 Hz, 3H), 1.03 (d, *J* = 6.8 Hz, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 176.99, 153.30, 141.05, 135.60, 129.43, 129.09, 128.46, 128.28, 127.42, 127.06, 66.20, 64.67, 55.57, 55.30, 41.14, 38.33, 32.33, 20.42, 18.83, 12.57. m/z calculated for $(M+H)^+$ 395.23292, found 395.23215.

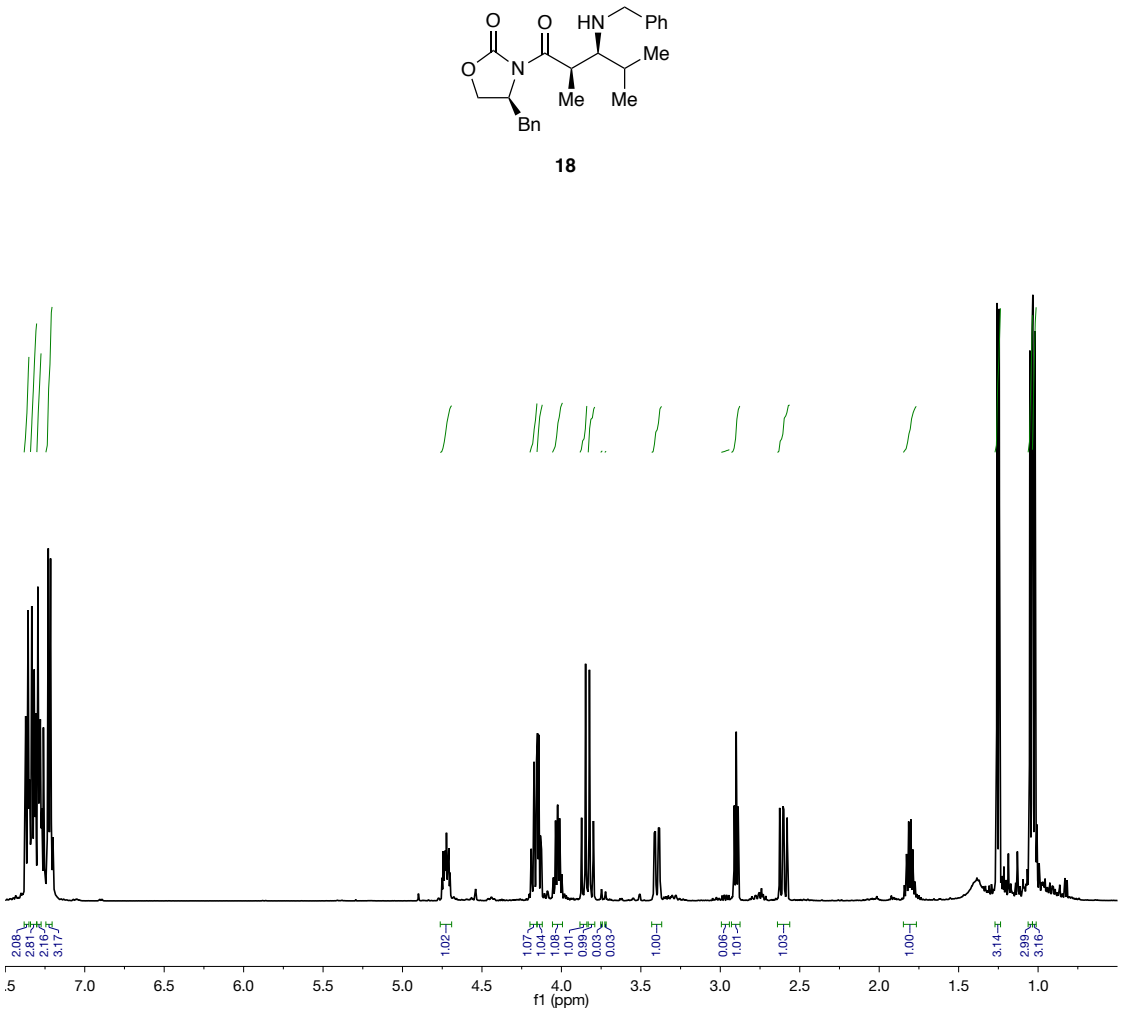
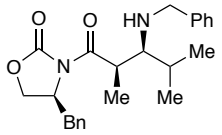


Figure S146. ^{1}H NMR spectrum ($CDCl_3$, 25 °C) of **18**.



18

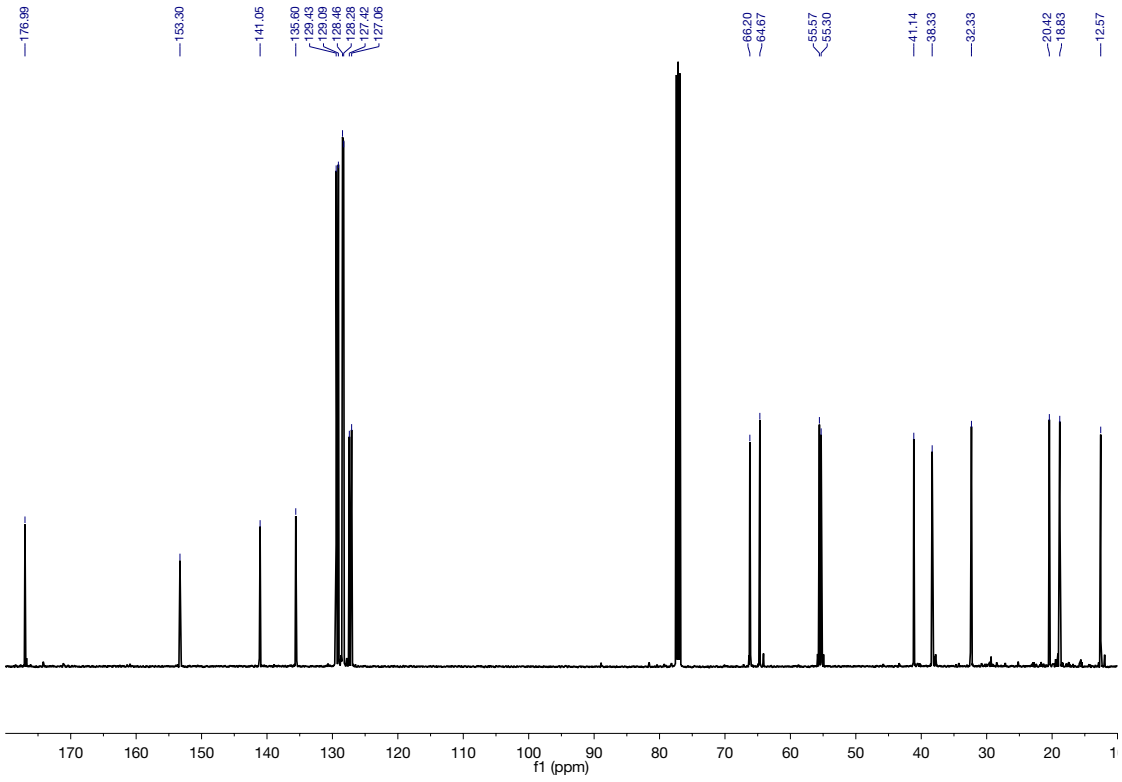


Figure S147. ^{13}C NMR spectrum ($CDCl_3$, 25 °C) of **18**.

(2*R*, 3*S*)-3-((*tert*-butoxycarbonyl)amino)-2,4-dimethylpentanoate (**37**). To a solution of **18** (1.3 mmol, 500 mg) in methanol (5.0 mL), sodium methoxide (1.3 mmol, 70 mg) was added. The mixture was stirred for 30 minutes at 0 °C. The reaction was quenched by 1.0 mL saturated NH_4Cl and extracted three times with EtOAc. The organic extracts dried over $MgSO_4$ and concentrated in vacuo. Flash chromatography (10% ethyl acetate/hexanes afforded the methyl ester (57.8 mg, 18% yield). The methyl ester in THF (1.0 mL) was added to palladium on carbon (6.0 mg) and stirred under H_2 (1.0 atm) for 24 hrs. The mixture was filtered through celite and used in the next step without further purification. To the primary amine in THF, di-tert-butyl dicarbonate (0.30 mmol, 218 mg), triethyl amine (1.0 mmol, 139 μL), and 4-dimethylaminopyridine (0.020 mmol, 2.4 mg) were added. The reaction was stirred at room temperature for 8 hrs and concentrated in vacuo. Flash chromatography (15% ethyl acetate/hexanes) afforded the product (8.8 mg, 15%) shown by ^{1}H NMR. ^{1}H NMR (500 MHz, $CDCl_3$) δ 4.38 (d, *J* = 10.6 Hz, 1H), 3.78 (dt, *J* = 10.7, 6.6 Hz, 1H), 3.67 (s, 3H), 2.62 (p, *J* = 7.0 Hz, 1H), 1.66 (dp, *J* = 13.4, 6.7 Hz, 1H), 1.46 (s, 1H), 1.42 (s, 8H), 1.12 (d, *J* = 7.0 Hz, 3H), 0.93 (d, *J* = 6.7 Hz, 3H), 0.88 (d, *J* = 6.7 Hz, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 175.47, 155.97, 79.29, 57.53, 51.90, 42.36, 30.51, 28.48, 20.32, 17.67, 12.31. m/z calculated for $(M+H)^+$ 260.18563, found 260.18518. $[\alpha]^{22} = -11$, c 0.40, $CDCl_3$. Literature reported $[\alpha]^{22} = -16.3$, c 1.0, $CHCl_3$.

Seebach, D.; Abele, S.; Gademann, K.; Guichard, G.; Hintermann, T.; Jaun, B.; Matthews, J. L.; Schreiber, J. V. *Helvetica Chimica Acta,* **1998**, *81*, 932.

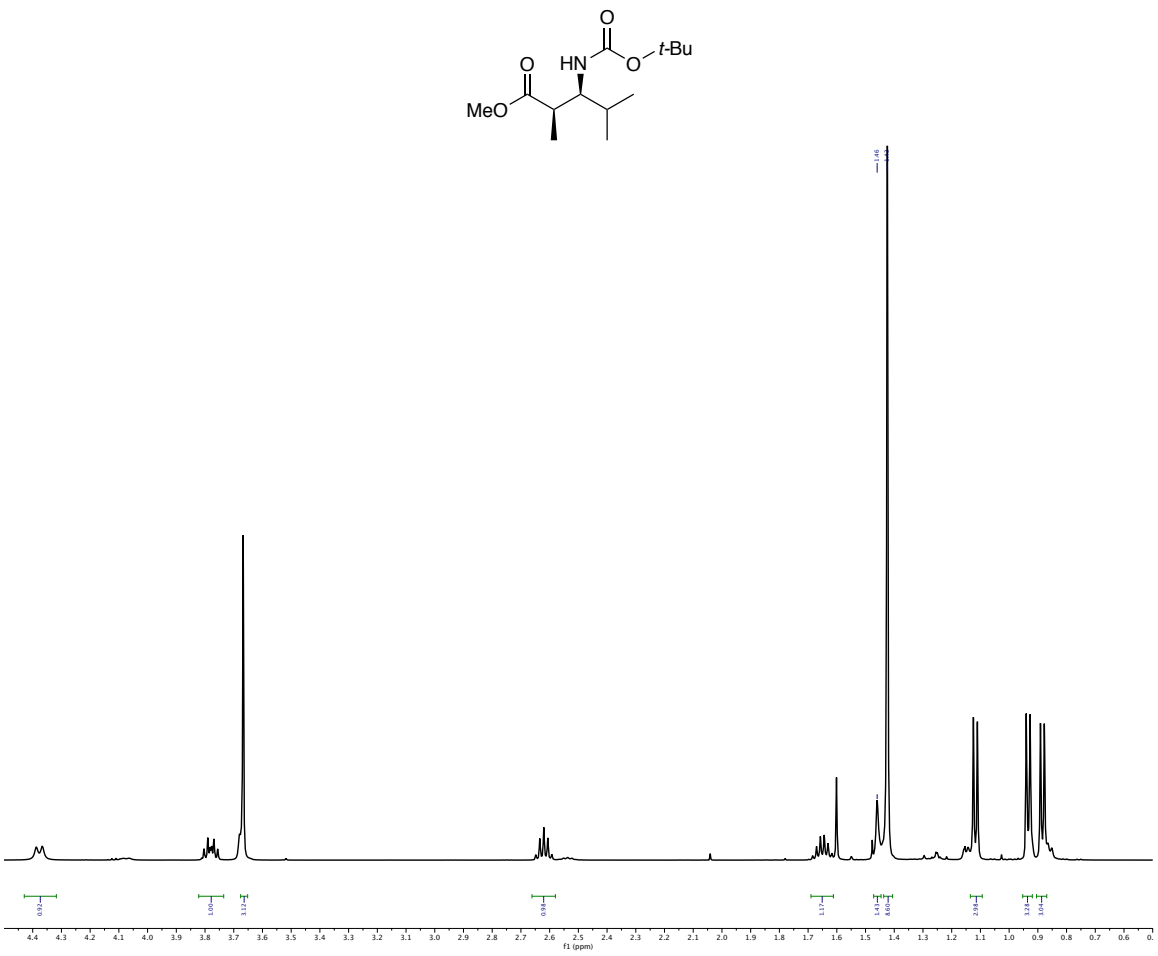


Figure S148. ^{1}H NMR spectrum ($CDCl_3$, 25 °C) of **37**.

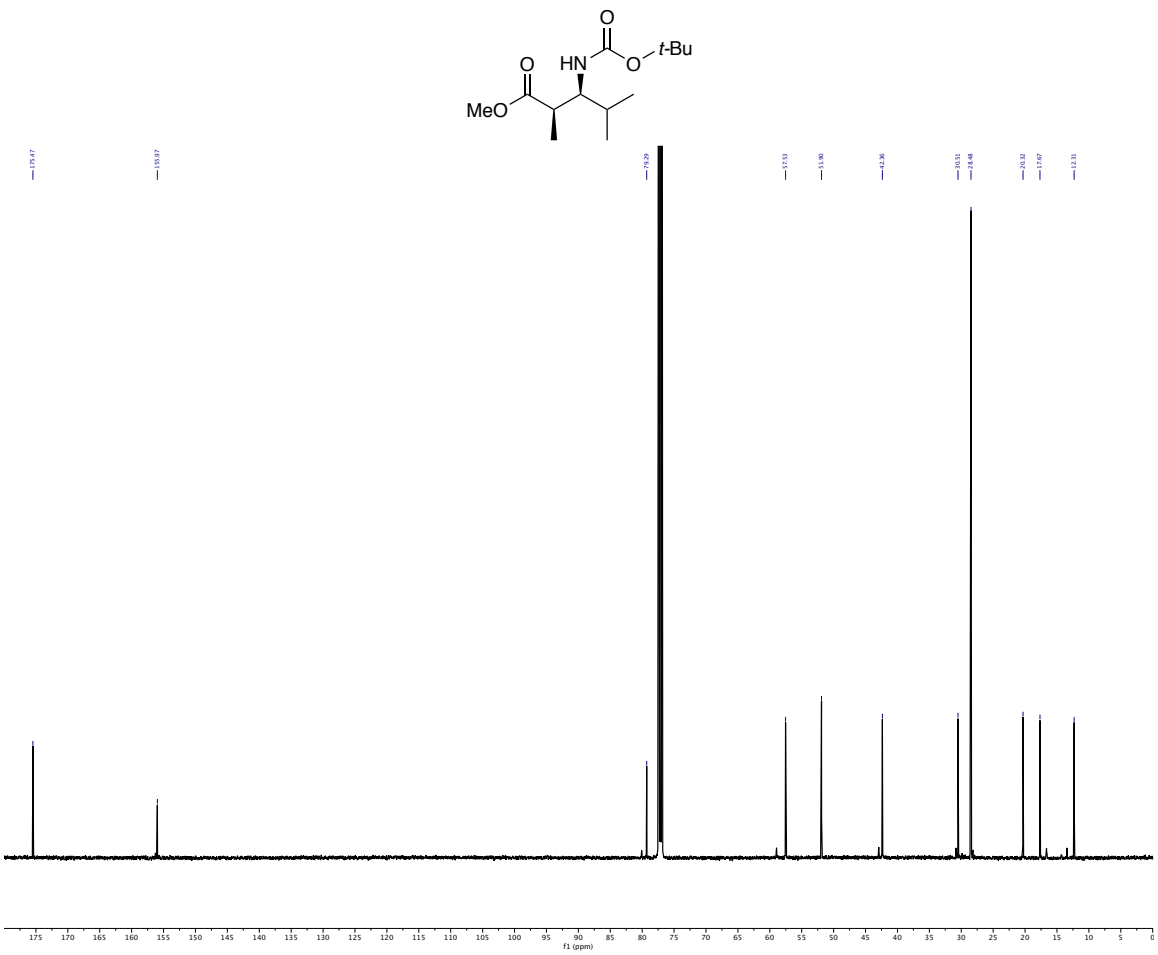


Figure S149. ^{13}C NMR spectrum ($CDCl_3$, 25 °C) of **37**.

(4*S*)-4-benzyl-3-(4-methyl-3-(((*R*)-1-phenylethyl)amino)pentanoyl)oxazolidin-2-one (**33**). To a solution of NaHMDS (0.11 mmol, 20.2 mg) and TMEDA (0.22 mmol, 33 μL) in toluene (2.0 mL) was added **1** (0.10 mmol, 23.3 mg). The reaction was stirred under argon for 30 minutes at –78 °C. A solution of imine-BF_3 complex **20** (0.10 mmol) in toluene (0.20 mL) was injecte, and the mixture was stirred for 30 minutes. The reaction was quenched by 1.0 mL saturated NH_4Cl and extracted three times with EtOAc. The organic extracts dried over $MgSO_4$ and concentrated in vacuo. Flash chromatography (10% ethyl acetate/hexanes/3% Et_3N) afforded the product (33 mg, 84% yield), shown by ^{1}H NMR to be **33** in 1.2:1 selectivity. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.37 – 7.31 (m, 2H), 7.31 – 7.26 (m, 5H), 7.23 – 7.16 (m, 3H), 4.61 (ddt, *J* = 10.4, 7.0, 3.5 Hz, 1H), 4.15 – 4.11 (m, 1H), 4.11 – 4.08 (m, 1H), 3.87 (q, *J* = 6.6 Hz, 1H), 3.27 (dd, *J* = 13.4, 3.4 Hz, 1H), 3.03 – 2.96 (m, 1H), 2.96 – 2.92 (m, 1H), 2.83 (dd, *J* = 13.8, 2.7 Hz, 1H), 2.64 (dd, *J* = 13.4, 9.9 Hz, 1H), 2.01 (dtt, *J* = 10.3, 6.9, 3.5 Hz, 1H), 1.29 (d, *J* = 6.6 Hz, 3H), 0.93 (d, *J* = 6.8 Hz, 3H), 0.88 (d, *J* = 6.9 Hz, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 173.10, 153.70, 146.13, 135.61, 129.56, 129.09, 128.40, 127.44, 126.88, 126.83, 66.14, 56.96, 55.38, 54.98, 38.16, 36.23, 29.35, 25.50, 19.19, 16.47.

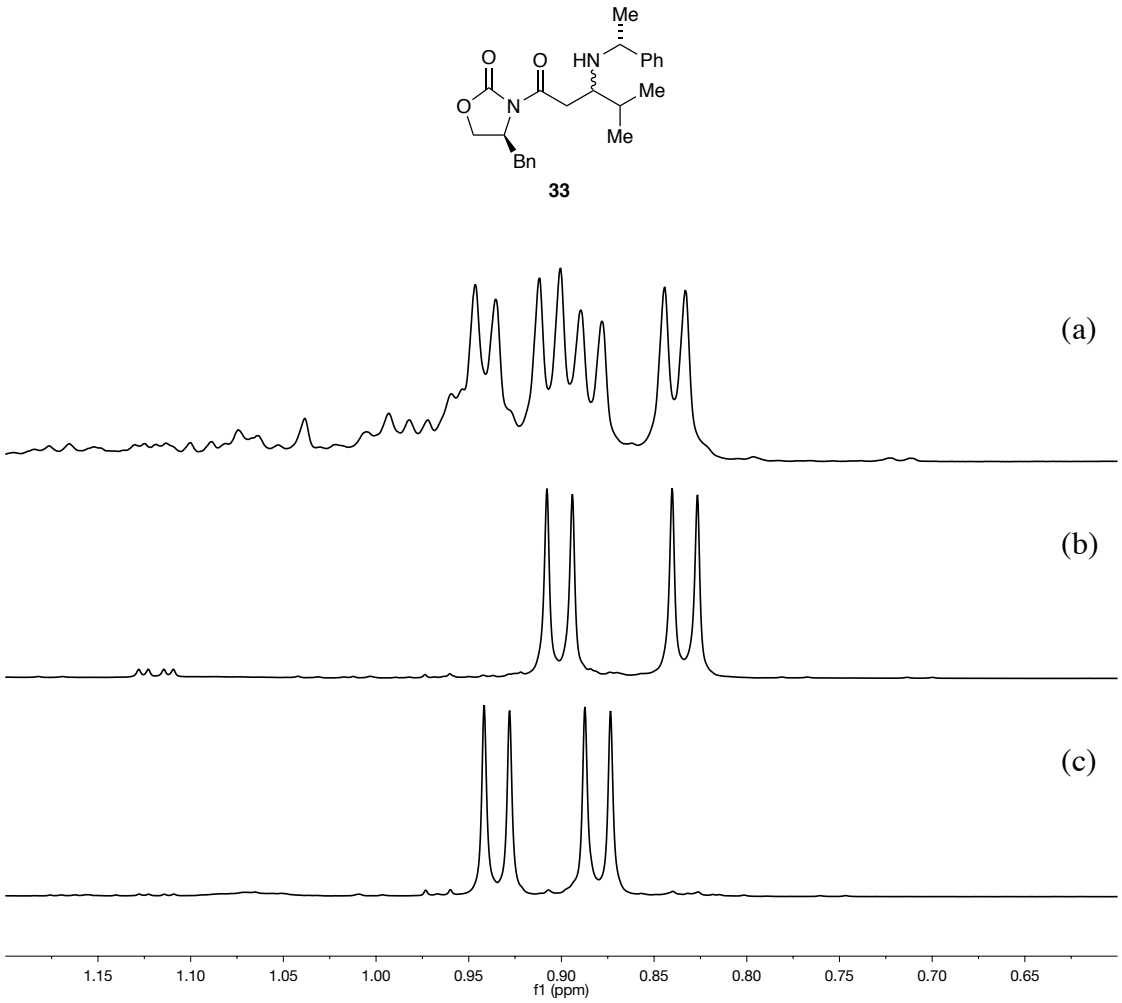


Figure S150. ^{1}H NMR spectrum ($CDCl_3$, 25 °C) of (a) **33**; (b) isomer A, and (c) isomer B.

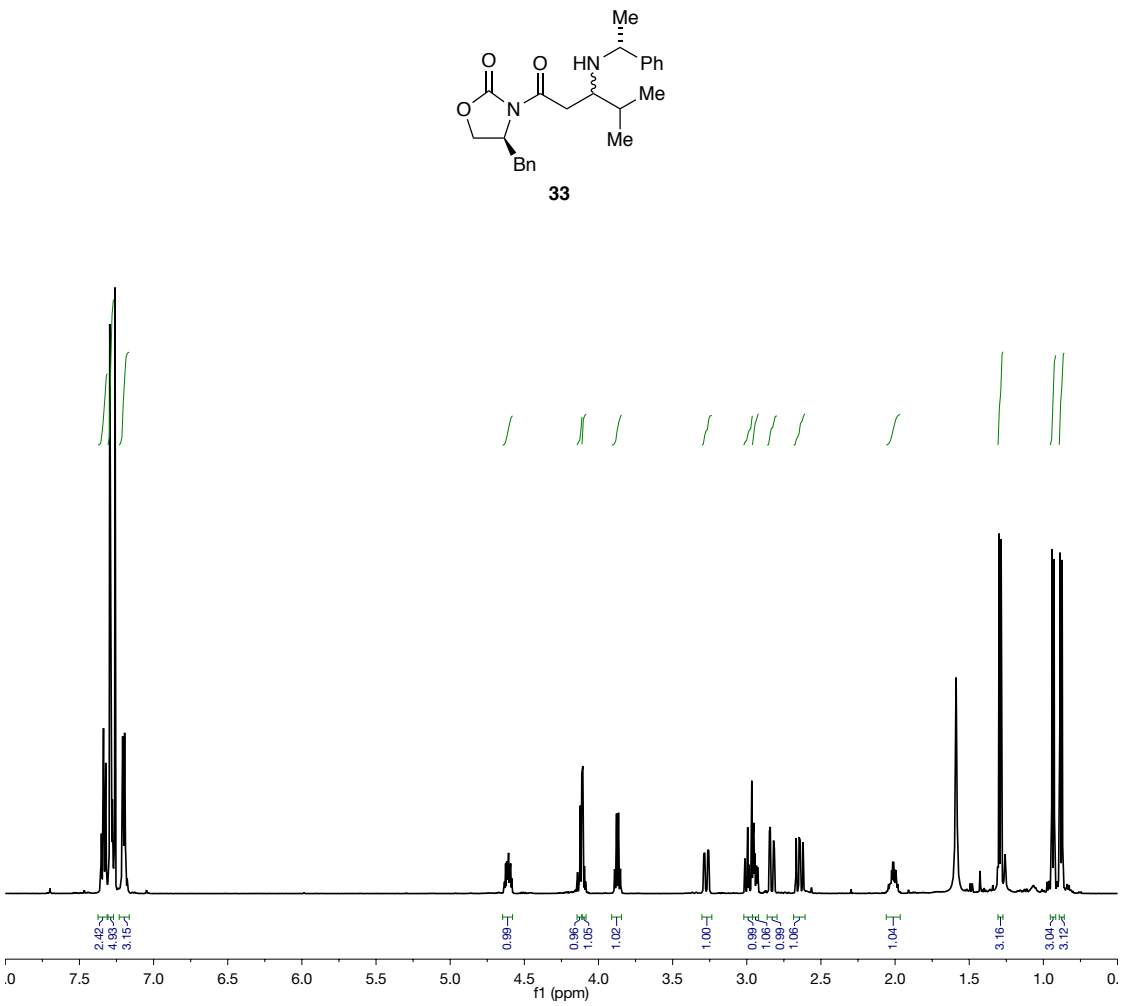


Figure S151. ^{1}H NMR spectrum ($CDCl_3$, 25 °C) of **33**.

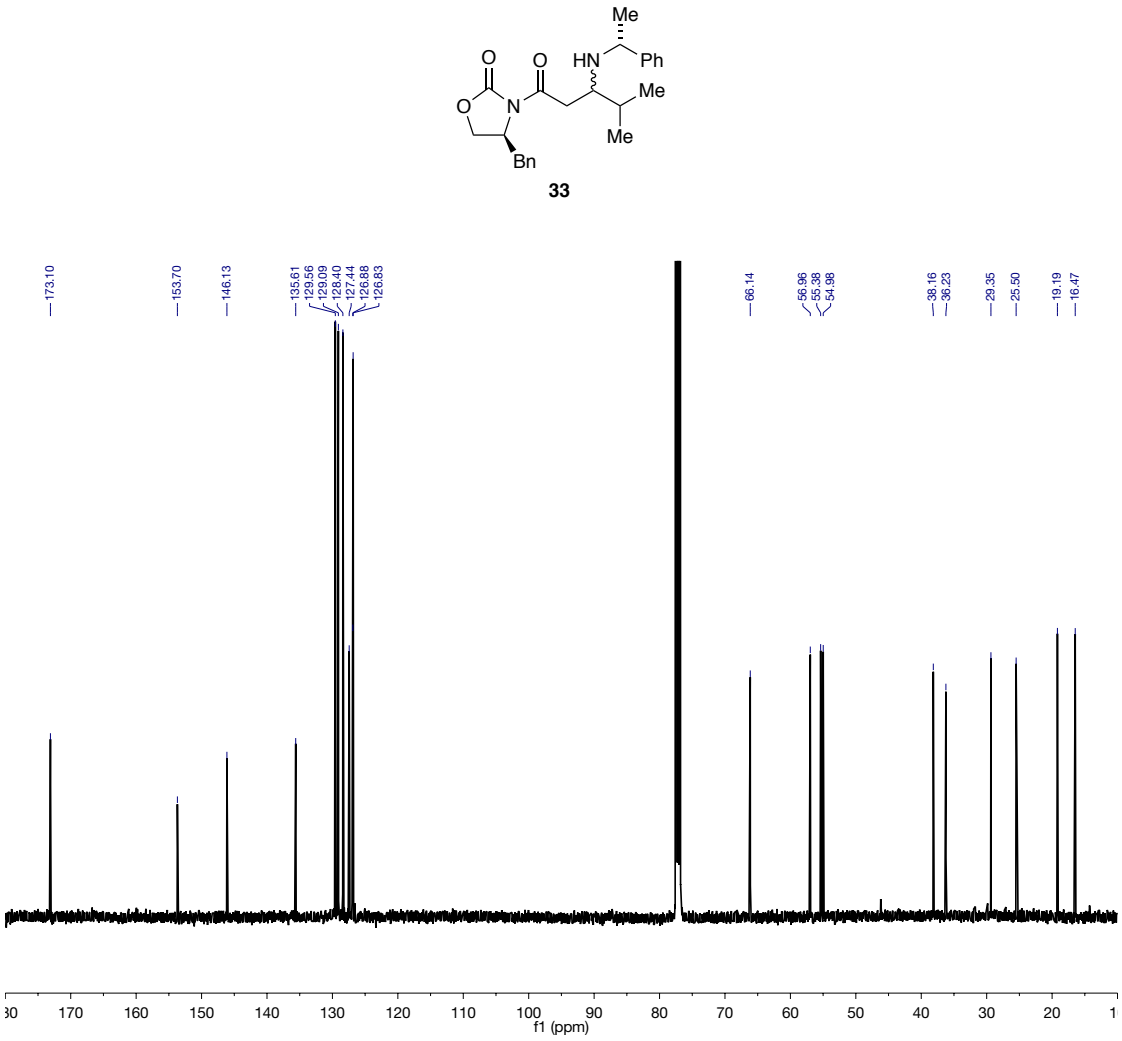


Figure S152. ^{13}C NMR spectrum ($CDCl_3$, 25 °C) of **33**.

(4*S*)-4-benzyl-3-(4-methyl-3-(((*S*)-1-phenylethyl)amino)pentanoyl)oxazolidin-2-one (**34**). To a solution of NaHMDS (0.11 mmol, 20.2 mg) and TMEDA (0.22 mmol, 33 μL) in toluene (2.0 mL) was added **1** (0.10 mmol, 23.3 mg). The reaction was stirred under argon for 30 minutes at –78 °C. A solution of imine-BF_3 complex **19** (0.10 mmol) in toluene (0.20 mL) was injected, and the mixture was stirred for 30 minutes. The reaction was quenched by 1.0 mL saturated NH_4Cl and extracted three times with EtOAc. The organic extracts dried over $MgSO_4$ and concentrated in vacuo. Flash chromatography (10% ethyl acetate/hexanes/3% Et_3N) afforded **34** (33.4 mg, 85% yield) as a 1:1 mixture of diastereomers. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.37 – 7.32 (m, 2H), 7.32 – 7.26 (m, 5H), 7.26 – 7.23 (m, 2H), 7.20 – 7.15 (m, 1H), 4.53 (dddd, *J* = 9.8, 7.6, 3.4, 2.3 Hz, 1H), 4.07 (dd, *J* = 9.0, 2.3 Hz, 1H), 3.97 (ddd, *J* = 8.7, 7.6, 0.8 Hz, 1H), 3.86 (q, *J* = 6.6 Hz, 1H), 3.34 (dd, *J* = 13.4, 3.4 Hz, 1H), 2.95 – 2.91 (m, 1H), 2.87 – 2.77 (m, 2H), 2.74 (dd, *J* = 13.4, 9.7 Hz, 1H), 2.04 (ddh, *J* = 10.1, 6.9, 3.1 Hz, 1H), 1.31 (d, *J* = 6.6 Hz, 3H), 0.93 (d, *J* = 6.9 Hz, 3H), 0.87 (d, *J* = 6.9 Hz, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 173.02, 153.53, 146.14, 135.68, 129.62, 129.10, 128.31, 127.43, 126.99, 126.88, 65.99, 56.91, 55.56, 54.88, 37.87, 36.47, 29.19, 25.36, 19.25, 16.31.

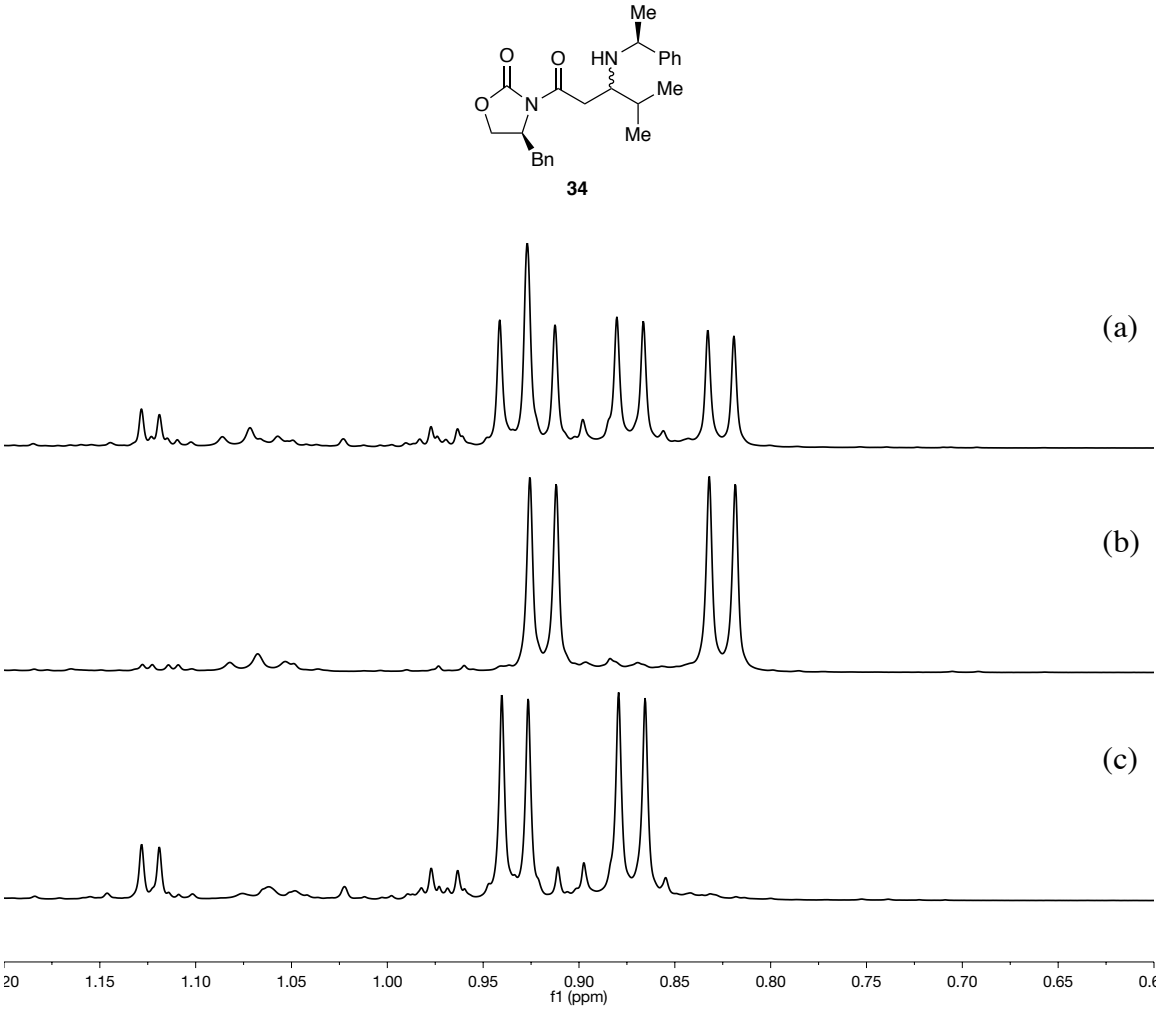


Figure S153. ^{1}H NMR spectrum ($CDCl_3$, 25 °C) of (a) **34**; (b) isomer A, and (c) isomer B.

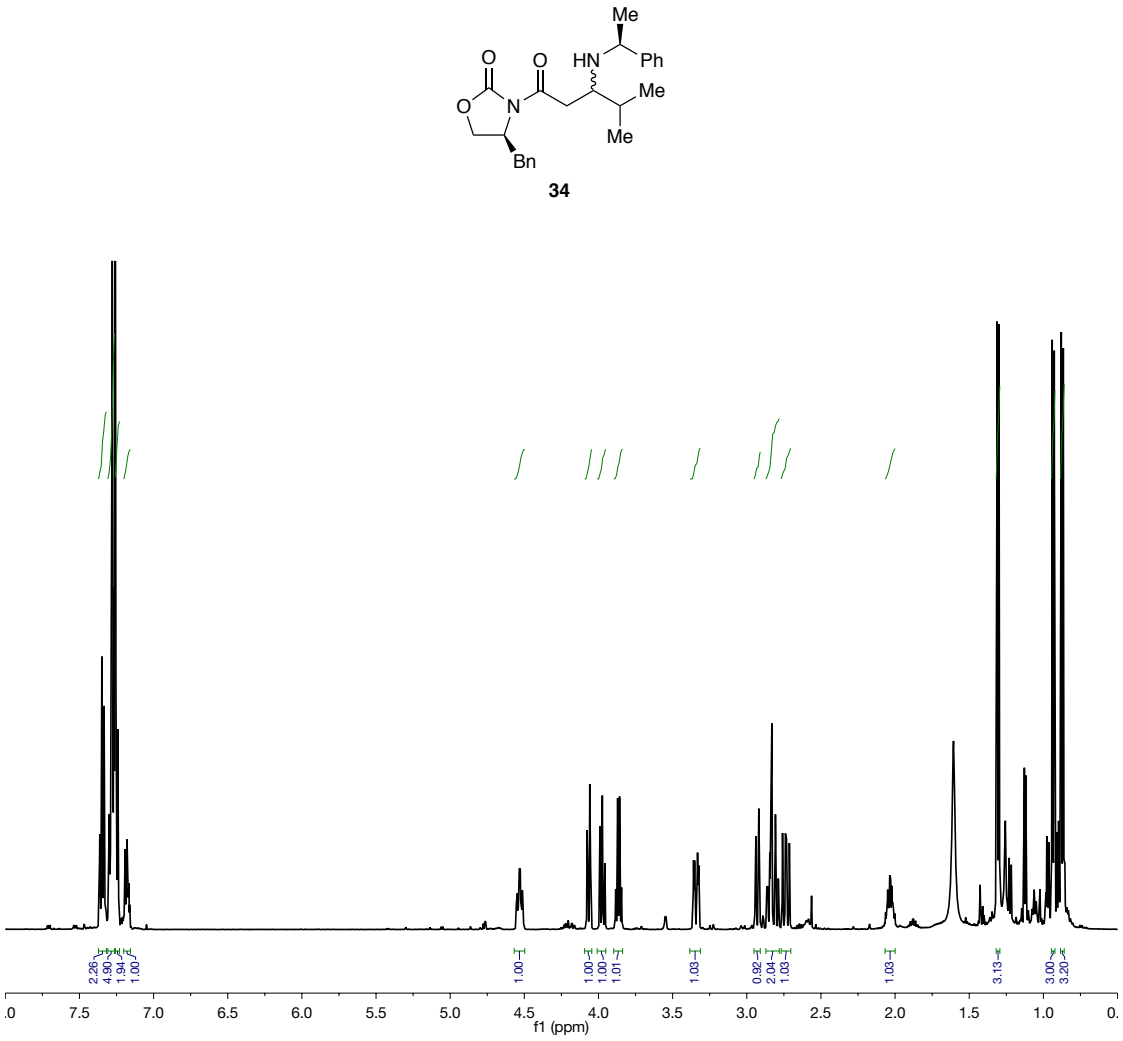


Figure S154. ^{1}H NMR spectrum ($CDCl_3$, 25 °C) of **34**.

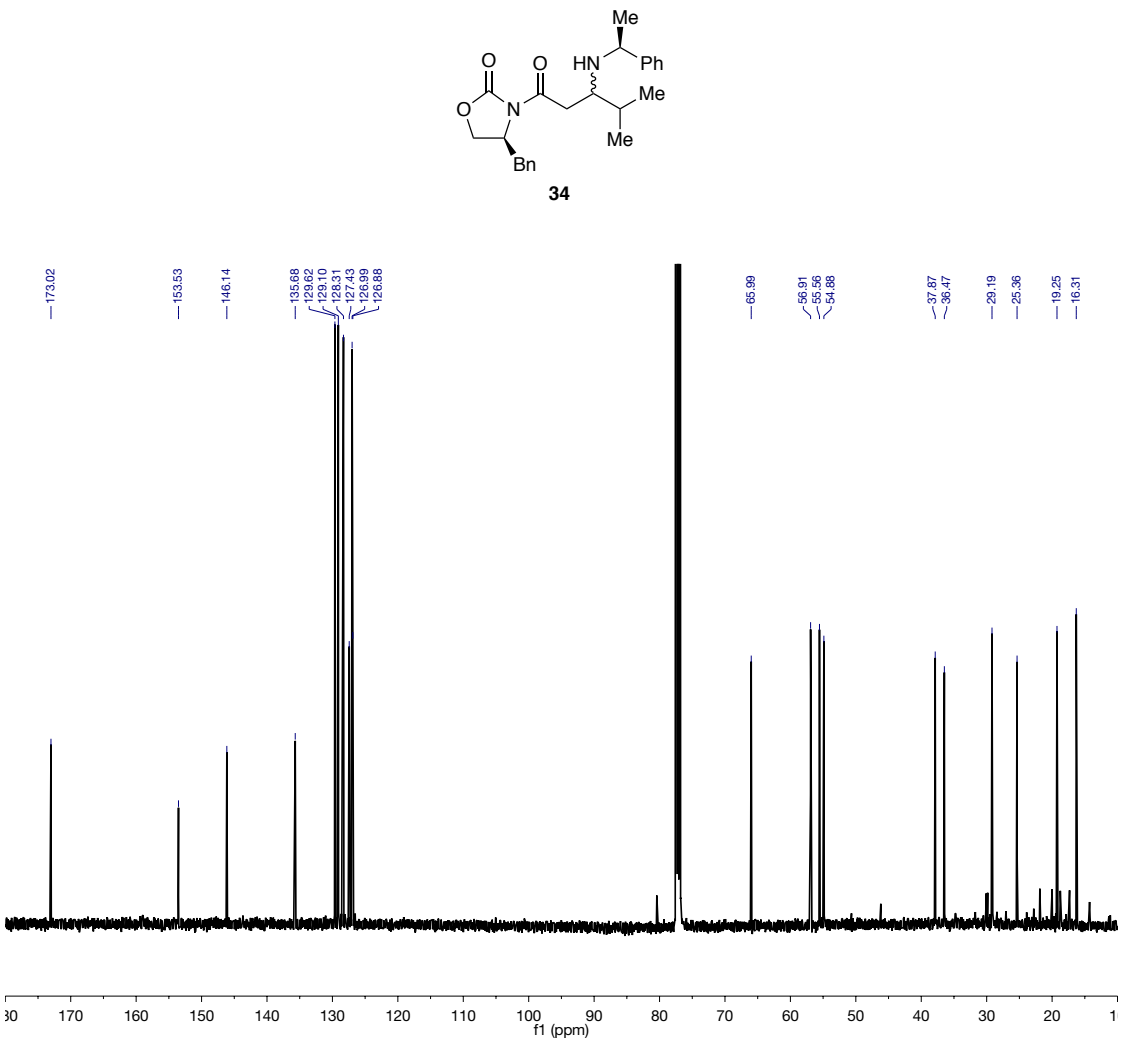


Figure S155. ^{13}C NMR spectrum ($CDCl_3$, 25 °C) of **34**.

$$K_{eq}(1) = \frac{[LL'][L]}{[L_2][L']}$$
$$K_{eq}(2) = \frac{[L'_2][L]}{[LL'][L']}$$

The distributions of homo- and heterosolvated enolate disolvated monomers are assumed to track as power functions of the L and L' mole fractions. While the fit is superficially similar to that described previously for two subunits aggregating to form one or more ensembles, we substitute the measured mole fraction for the total mole fraction of solvent and consequently obviate parametric fitting. Accordingly,

$$[L_2] = c\Phi_0(1-\chi_{L'})^2$$
$$[LL'] = 2c\Phi_1(1-\chi_{L'})\chi_{L'}$$
$$[L'_2] = c\Phi_2{\chi_{L'}}^2$$

The c prefactor subsumes the concentration units and normalization such that $[enolate]_{total} = [L_2] + [LL'] + [L'_2]$. Therefore,

$$c = \frac{[enolate]}{\Phi_0(1-\chi_{L'})^2 + 2\Phi_1(1-\chi_{L'})\chi_{L'} + \Phi_2{\chi_{L'}}^2}$$

We wish to compute each of the equilibrium constants defined above and do so by substituting in the fitting functions for each homo- and heterosolvate,

$$K_{eq}(1) = \frac{[LL'][L]}{[L_2][L']} = \frac{2c\Phi_1(1-\chi_{L'})\chi_{L'}[L]}{c\Phi_0(1-\chi_{L'})^2[L']} = \frac{2\Phi_1\chi_{L'}[L]}{\Phi_0(1-\chi_{L'})[L']}$$
$$K_{eq}(2) = \frac{\Phi_2\chi_{L'}[L]}{2\Phi_1(1-\chi_{L'})[L']}$$

Assuming the absence of unsolvated enolate tetramers, one can compute the normalities of all species and thereby extract the equilibrium constants point-wise from the data employing the equations described above.

L = TMEDA, L’ = (*S*,*S*)-TMCDA

Normalities of homo- and heterosolvated enolate tetramers corresponding to computed molarities of free solvent

$[L_2]$	[LL']	$[L'_2]$	[L]	[L']
0.200	0	0	0.600	0
0.166	0.034	0	0.434	0.166
0.106	0.089	0.005	0.299	0.301
0.058	0.095	0.047	0.189	0.411
0.037	0.101	0.062	0.125	0.475
0.017	0.079	0.104	0.087	0.513
0	0.050	0.150	0.050	0.550
0	0	0.200	0	0.600

Computed equilibrium constants

K(1)	*K*(2)
-	-
0.525	-
0.831	0.060
0.756	0.225
0.729	0.161
0.812	0.224
-	0.268
-	-

Averaging the computed equilibrium constants gives $K(1) = 0.782$, $K(2) = 0.220$.

The data from the Job plot experiments can be fit parametrically to a mathematical model for a specific ensemble. The programs for performing these fits were written for use in MATLAB_R2018a.

Data1.m

```
XA = [1
0.8
0.6
0.4
0.3
0.2
0.1
0];

Expt_Populations =[0    0   1
0   0.16    0.84
0.04    0.34    0.62
0.23    0.44    0.33
0.32    0.46    0.21
0.58    0.37    0.06
0.81    0.19    0
1   0   0;];

peak_assignment = [3  2  1];

phi = [ 1  1  1 ];

%To see your plot:  try_fit(XA, phi, peak_assignment, Expt_Populations)

%To fit your plot:  [phi_new, error] = refine_fit(XA, phi, peak_assignment,
Expt_Populations)

%or for symmetric plots:  [phi_new, error] = refine_fit_s(XA,phi,peak_assignment,
Expt_Populations)
```

Error of Model.m

```
function [mean_error, pop_error] = Error_of_Model(XA,phi, peak_assignment,
Expt_Populations, Expt_weights)

   if (nargin<5) % If no info on data given assume all points equally precise.
            Expt_weights=ones(size(Expt_Populations));
   end

   Concentrations = multimers(XA,phi);
   PP = Populations(Concentrations, peak_assignment);
```

```
    % Compute the mean error.
    diff = PP - Expt_Populations;
    mean_error = sqrt(sum(sum(diff.*diff.*Expt_weights)) / sum(sum(Expt_weights)));

    % Compute the error for each population independently.
    pop_error = sum(diff.*Expt_weights,1) ./ sum(Expt_weights,1);
    pop_error(2,:) = sqrt(sum(diff.*diff.*Expt_weights,1) ./ sum(Expt_weights,1));
```

multimers.m

```
function Concentration = multimer(XA, phi)

if (nargin<2)
    phi = [ 1 1 20 400 20 1 1];
end

for j=1:length(XA)
   % Use the function bisect to find Cconc
   Concentration(j,:) = bisect(XA(j),phi);
end

function Conc = bisect(XA, phi)

tolerance = 1e-6; % Amount XA may differ by an end of bisection..
    Amax = 1; Amin = 0;
    [Xmin, Conc]=Cparametric(Amin, phi);
    [Xmax, Conc]=Cparametric(Amax, phi);

    while ((Xmax-XA)>tolerance) % While not close enough, continue to bisect
difference of rmin and rmax.
        Atest = (Amin+Amax)/2;
        [Xtest, Conc]=Cparametric(Atest,phi);

        if (Xtest>XA)
           Amax = Atest; Xmax=Xtest;
       else
           Amin = Atest; Xmin=Xtest;
       end
   end

function [XA, Concs] = Cparametric( A, phi)

N = length(phi)-1;
B = 1-A;
```

```
Concs(1)= B^N*phi(1);
Concs(N+1)=A^N*phi(N+1);
Mn=1;

for k=2:N
   idx=k-1;
   Mn = Mn * (N+1-idx)/idx;
   Concs(k) = phi(k)*A^idx*B^(N-idx)*Mn;
end

Concs = Concs / sum(Concs);
XA = sum(Concs.*[0:N]/N);
```

Populations.m

```
function result = Populations(Concentrations, peak_assignment)

   result = zeros(size(Concentrations,1),max(peak_assignment));
   N = size(Concentrations,2);

   for j=1:N % Go through each type of aggregate and add to correct NMR peak.
      idx = peak_assignment(j);
      result(:,idx) = result(:,idx) + Concentrations(:,j);
   end
```

refine fit.m

```
function [phi_new, error] = refine_fit(XA,phi, peak_assignment, Expt_Populations)

if (nargin<5)
    Expt_weight = ones(size(Expt_Populations));
 end

N = length(phi)-1;
param = [ 2:(N+1)];

step_size = 0.1*phi(param),

N_no_progress = 0;
N_max_trials = 30;

[error_best, temp] = Error_of_Model(XA,phi, peak_assignment, Expt_Populations) ;
```

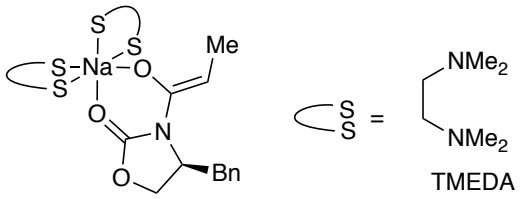
```
fprintf(1,'\n Initial Error of Fit = %f percent.\n', error_best * 100);

while (N_no_progress < N_max_trials)

   flag = 0;

   for k=1:length(param)

         phi_testr = phi;
         phi_testr(param(k))=abs(phi(param(k)) + step_size(k));
         [error_testr, temp] = Error_of_Model(XA,phi_testr, peak_assignment,
Expt_Populations, Expt_weight);

         phi_testl = phi;
         phi_testl(param(k))=abs(phi(param(k)) - step_size(k));
         [error_testl, temp] = Error_of_Model(XA,phi_testl,
peak_assignment,Expt_Populations, Expt_weight);
.
       if (error_testr<error_best)
            error_best=error_testr; phi=phi_testr; step_size(k) = step_size(k) * 1.5;
            N_no_progress=0;
      elseif     (error_testl <error_best)
            error_best=error_testl; phi=phi_testl; step_size(k) = step_size(k) * 1.5;
            N_no_progress=0;
      else
         flag = flag + 1;
      end
   end

   if (flag>2)
      step_size = step_size * (0.75 + 0.25*rand);
      N_no_progress=N_no_progress+1;
   end

   fprintf(1,'\nError - %f , Last Good Step - %d , Mean Step Size - %f \n ',error_best,
N_no_progress, 100*mean(step_size./phi(param)));
   fprintf(1,' Phi - %f',phi);

   end

   error=error_best;
   phi_new = phi;
```

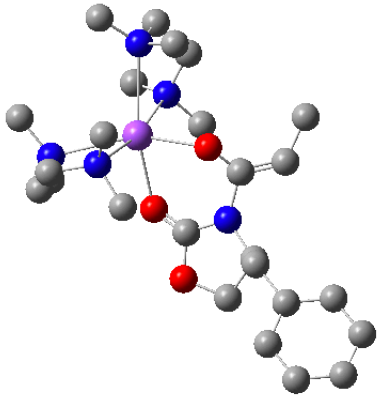
Try fit.m

```
function try_fit(XA, phi, peak_assignment, Expt_Populations)

if (nargin<5)
            Expt_weights=ones(size(Expt_Populations));
   else
            Expt_weights = 1./( Expt_Errors + mean(mean(Expt_Errors)));
   end

hold on ; cscheme='bgrmkcybgrmkcy'; axis([0 1 0 1]); xlabel('X_A'); ylabel('Mole
Fractions');
     for j=1:size(Expt_Populations,2)
          if (nargin<5)
             plot(XA, Expt_Populations(:,j),sprintf('%so',cscheme(j)));
          else
             errorbar(XA, Expt_Populations(:,j),
Expt_Errors(:,j),sprintf('%so',cscheme(j)));
          end
     end

XAc = [0:0.01:1]; TP=Populations(multimers(XAc,phi), peak_assignment);
     for j=1:size(TP,2)
        plot(XAc,TP(:,j),sprintf('%c',cscheme(j)) );
     end

[mean_error, pop_error] = Error_of_Model(XA,phi, peak_assignment,
Expt_Populations, Expt_weights);
   N = length(phi)-1;
          fprintf(1,'\nThe Mean mismatch is %f peAcent.\n', mean_error*100);
          for j=1:size(pop_error,2)
          fprintf(1,'Predicted value of species A%dB%d +A%dB%d exceeds
measurement by %f percent and mean square error of %f percent.\n ',j-1,N-j+1,N-
j+1,j-1,pop_error(1,j)*100,pop_error(2,j)*100);
          end
```

Geometries are optimized at the B3LYP level of theory using the 6-31G(d) basis set. Energies are defined as follows: G is the sum of electronic and thermal free energies calculated at the B3LYP level of theory (T = 195 K). GMP2 is derived from an MP2 SP calculation corresponding to the DFT-optimized geometry and includes a thermal correction from the DFT calculation.

Table S4. 4a with TMEDA at –78 °C.



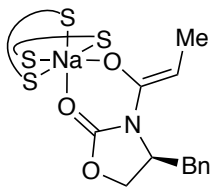


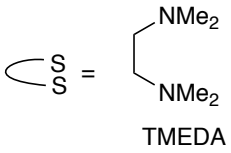
G = –1636.832111
G_{MP2} = –1636.168318

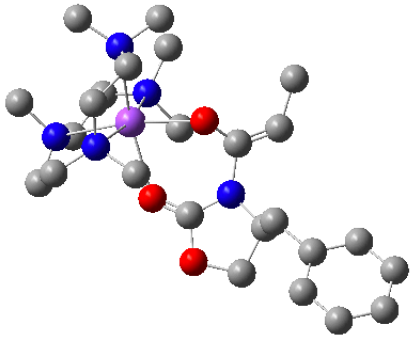
Na	0.00000000	0.00000000	0.00000000	O	1.78018700	-1.17246100	-0.75407000
C	2.76311500	-1.64992600	-0.08949200	N	3.44164200	-0.70334500	0.84316900
C	2.81971900	0.30784100	1.50056700	O	3.74600300	1.10964100	2.12062900
C	5.03144600	0.46944800	2.04322600	H	5.79154200	1.23418200	1.87085500
H	5.23104600	-0.02665800	3.00028200	C	4.89799500	-0.53923500	0.88875000
H	5.38191500	-1.48382500	1.14895200	C	5.46425500	-0.04505900	-0.46345300
H	5.10102700	-0.74008500	-1.22897200	H	5.03745400	0.94094500	-0.68428000
C	6.97499600	0.01707300	-0.48027100	C	7.65619000	1.23887300	-0.39625800
C	9.05205000	1.28495700	-0.38281900	C	9.79175800	0.10424300	-0.45216600
C	9.12626600	-1.12109100	-0.53960500	C	7.73256800	-1.16218700	-0.55450000
H	7.22065300	-2.11897800	-0.63496600	H	9.69417900	-2.04585600	-0.60238200
H	10.8779750	0.13742900	-0.44354300	H	9.55975000	2.24423200	-0.32166600
H	7.08651300	2.16500100	-0.35254600	O	1.62489100	0.56753600	1.59914000
C	3.31946000	-2.89598100	-0.13358200	H	4.11429400	-3.15053000	0.56173300
C	2.86012600	-3.95380100	-1.09695500	H	3.70766000	-4.49470200	-1.54290000
H	2.21671300	-4.72087000	-0.63368400	H	2.28739700	-3.50370200	-1.91549900
N	0.51543500	2.04241100	-1.62128200	C	0.33882700	1.77644800	-3.04805600
H	0.69055300	2.61117200	-3.68451900	H	0.90273800	0.87885600	-3.31860500
H	-0.71957300	1.60239000	-3.26950500	C	1.94395500	2.20953500	-1.33209100
H	2.09316400	2.43098800	-0.27375400	H	2.45515300	1.26748900	-1.54653900
H	2.39256600	3.02462000	-1.93184600	C	-0.27551500	3.20175500	-1.19488200
C	-0.49334400	3.27601900	0.31991700	H	0.47511100	3.26742900	0.82857600
H	-0.96405400	4.25223500	0.55121700	N	-1.28621400	2.17047200	0.88010500

C	-2.69448100	2.25820500	0.49403900	H	-2.80308100	2.19068000	-0.59163800
H	-3.24418500	1.42093900	0.93605800	H	-3.16879300	3.19934300	0.83323100
C	-1.16387700	2.16986300	2.34266400	H	-1.76410900	1.35401000	2.75711300
H	-0.11993500	2.00285000	2.61755300	H	-1.51600400	3.11663500	2.79433100
H	-1.24420500	3.15315900	-1.70449300	H	0.19379100	4.15145500	-1.51877400
N	-0.96813600	-1.96436900	1.43949300	C	-2.10952500	-1.69904700	2.31457900
H	-2.48704600	-2.61676300	2.80609100	H	-1.80591700	-0.99715500	3.09701200
H	-2.93555700	-1.24470200	1.75991200	C	0.16356100	-2.44058600	2.24619800
H	0.45016100	-1.66408000	2.96131500	H	-0.08719700	-3.36250000	2.80492500
H	1.02223500	-2.64273300	1.60141200	C	-1.28645500	-2.94954400	0.39521900
H	-0.34567500	-3.21334900	-0.09698900	H	-1.68818000	-3.88055500	0.84325300
C	-2.29597100	-2.46470900	-0.64876600	H	-3.20263800	-2.11019000	-0.14721800
H	-2.60331900	-3.33985900	-1.25419200	N	-1.81134000	-1.38233600	-1.51911400
C	-2.94327300	-0.74380300	-2.19268200	H	-2.58249700	0.07476100	-2.82359300
H	-3.51036300	-1.44354200	-2.83584800	H	-3.63291300	-0.32602200	-1.45143500
C	-0.85346300	-1.89008800	-2.51329400	H	-0.60587200	-1.08707000	-3.21320800
H	0.07791100	-2.19035000	-2.02858200	H	-1.27188500	-2.73536700	-3.09208500

Table S5. 4b with TMEDA at –78 °C.





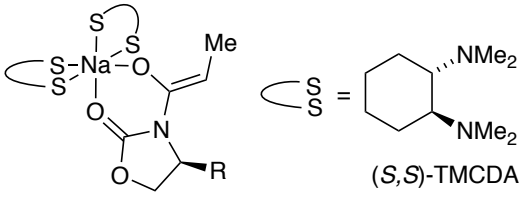


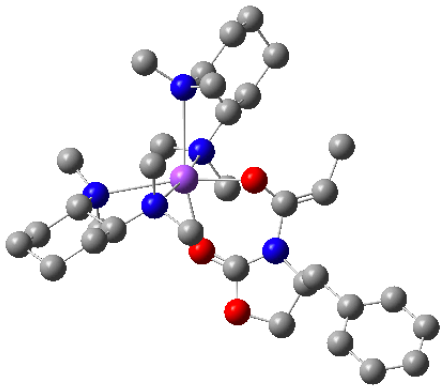
G = –1636.83276
G_{MP2} = –1636.168975

Na	0.00000000	0.00000000	0.00000000	O	1.86394300	-0.43183800	-1.21911200
C	2.77458100	-1.26434700	-0.87641800	N	3.41348800	-1.01648700	0.44810700
C	2.76317700	-0.52109300	1.53106700	O	3.66180900	-0.20332100	2.51838400
C	4.95530900	-0.70792400	2.14159700	H	5.71327800	0.02142200	2.43465800
H	5.13244500	-1.64623800	2.67999600	C	4.86583900	-0.92479400	0.62012700
H	5.34320200	-1.86709300	0.33920000	C	5.47770200	0.21568000	-0.22751900
H	5.14027500	0.05920800	-1.25824100	H	5.06054400	1.17116500	0.11335700
C	6.98844500	0.24591900	-0.16814000	C	7.67035200	1.20388500	0.59414700
C	9.06519200	1.20626100	0.66627200	C	9.80316800	0.24578100	-0.02574200
C	9.13714600	-0.71312600	-0.79312100	C	7.74450700	-0.71086500	-0.86320400
H	7.23288400	-1.45310900	-1.47261200	H	9.70398200	-1.46029900	-1.34276000

H	10.8886510	0.24662300	0.02690900	H	9.57355500	1.96175900	1.25995000
H	7.10272100	1.96421800	1.12680200	O	1.56262300	-0.34783700	1.71440700
C	3.28742700	-2.32879900	-1.55907000	H	4.02295400	-2.96459700	-1.07384700
C	2.86612200	-2.67825200	-2.95838100	H	3.72816300	-2.92300500	-3.59627100
H	2.19167600	-3.54980000	-3.00662500	H	2.33960100	-1.83688500	-3.42155600
N	-0.93335900	-2.50568400	0.09357300	C	0.18844100	-3.22216300	0.71491500
H	0.49090800	-2.72897300	1.64044800	H	-0.07220800	-4.27539900	0.93550000
H	1.04845800	-3.20260800	0.03934100	C	-1.23562000	-3.11160800	-1.20428400
H	-2.06594700	-2.57957600	-1.68087600	H	-0.35762900	-3.03384100	-1.85128400
H	-1.51601000	-4.17912800	-1.12051700	C	-2.12121200	-2.50070500	0.95370000
H	-2.97768000	-2.19639600	0.34121400	H	-2.35285700	-3.51970400	1.32285900
C	-2.00420200	-1.57649400	2.16925800	H	-1.11221500	-1.84254900	2.74390200
H	-2.87153500	-1.76564500	2.83182700	N	-1.90364600	-0.14542500	1.84056200
C	-3.18753600	0.39944700	1.39808500	H	-3.06678400	1.45856400	1.14928500
H	-3.53629900	-0.11592100	0.49893800	H	-3.97345500	0.31328900	2.17297200
C	-1.41537300	0.59853200	3.00758300	H	-0.40517300	0.26324200	3.25543500
H	-1.37171300	1.66435200	2.76650500	H	-2.07085900	0.47284900	3.88996900
N	0.46537900	2.72576300	0.03322400	C	-0.03199400	3.20545600	-1.26353100
H	0.55146500	4.08349200	-1.60429700	H	-1.05720200	3.56255300	-1.11775200
C	-0.00214000	2.16204600	-2.38350700	N	-0.95760900	1.05179900	-2.22324100
C	-2.34461600	1.49250100	-2.36818700	H	-2.60884800	2.21576200	-1.59196200
H	-2.54116900	1.95626400	-3.35415300	H	-3.01140900	0.63070900	-2.25964300
C	-0.65434700	0.01622000	-3.22074700	H	0.34684000	-0.37640000	-3.02656800
H	-1.37653400	-0.80091100	-3.12907300	H	-0.71019900	0.40664000	-4.25466000
H	0.99437800	1.71584600	-2.44559900	H	-0.18411300	2.68968400	-3.34109100
C	1.93095200	2.61912200	0.03938900	H	2.25896700	2.32706500	1.04079100
H	2.25551900	1.83772300	-0.65171400	H	2.41257100	3.58102600	-0.22320800
C	0.03229200	3.62375100	1.10388100	H	-1.06203100	3.66969600	1.13669500
H	0.39077800	3.24428100	2.06542200	H	0.41416600	4.65529800	0.97862800

Table S6. 4a with (*S*,*S*)-TMCDA at –78 °C.





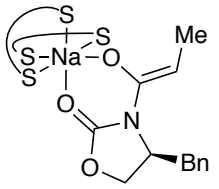
G = –1947.826475

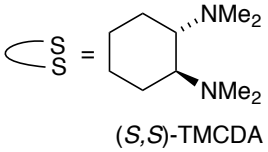
$G_{MP2} = -1946.976178$

Na	0.00000000	0.00000000	0.00000000	O	1.69134300	-1.24928600	-0.82692500
C	2.63232600	-1.81976700	-0.17394100	N	3.39020200	-0.95054100	0.77066000
C	2.85688600	0.10072600	1.44373000	O	3.85105100	0.82265500	2.05764400
C	5.08117700	0.08379800	1.96057600	H	5.89743600	0.78635200	1.78063900
H	5.25340900	-0.43113400	2.91290000	C	4.85520300	-0.90496600	0.80304400
H	5.26329300	-1.88678000	1.05600500	C	5.44942900	-0.45127100	-0.55135300
H	5.01256500	-1.09815800	-1.32035700	H	5.11701200	0.57378300	-0.75538800
C	6.95877400	-0.53586400	-0.58817600	C	7.75783000	0.61157100	-0.49563300
C	9.15155200	0.52064000	-0.50362500	C	9.77071800	-0.72540600	-0.60370000
C	8.98694000	-1.87797600	-0.69991900	C	7.59590100	-1.78223500	-0.69301400
H	6.99152600	-2.68284300	-0.78037200	H	9.46040100	-2.85264700	-0.78676900
H	10.8549570	-0.79896300	-0.61215600	H	9.75172200	1.42444800	-0.43565000
H	7.28283400	1.58825800	-0.42871200	O	1.68766100	0.45005600	1.56224100
C	3.08301200	-3.10695900	-0.24340600	H	3.85881700	-3.43709300	0.44158400
C	2.54845700	-4.10349400	-1.23237700	H	3.35661000	-4.66485400	-1.72462900
H	1.88435400	-4.85949000	-0.77953600	H	1.97474300	-3.59506300	-2.01489300
N	0.75456100	2.25085900	-1.27134700	C	0.36833500	3.49673000	-0.56889100
C	-1.11268400	3.49267600	-0.10456500	N	-1.47632600	2.27078100	0.65880000
C	-2.92014000	2.03517200	0.65127600	H	-3.28742900	2.00652400	-0.37959500
H	-3.12971300	1.06461200	1.11159500	H	-3.50031900	2.79709300	1.20361900
C	-0.96488500	2.24451400	2.03501300	H	-1.16390400	1.25880800	2.46720500
H	0.11780800	2.38080500	2.04522900	H	-1.43574500	2.99443700	2.69329200
C	-1.44194700	4.81000600	0.64342600	C	-1.13526200	6.06360500	-0.18405300
C	0.33582200	6.06970600	-0.60921300	C	0.67155000	4.78528000	-1.37585300
H	1.72732300	4.78648800	-1.67113400	H	0.08749500	4.77781800	-2.30623600
H	0.55804100	6.94668800	-1.23043600	H	0.97360500	6.14808100	0.28344100
H	-1.37753000	6.96296700	0.39627400	H	-1.77478200	6.08686700	-1.07897100
H	-2.49613600	4.80587500	0.94598300	H	-0.85191400	4.85640600	1.56804600
H	-1.73947900	3.46693800	-1.00668000	H	0.99257100	3.51858800	0.33392900
C	2.20988300	2.07200800	-1.33648300	H	2.64258400	2.25790000	-0.34982600
H	2.42091300	1.03331800	-1.60810000	H	2.69946100	2.74335600	-2.06533600
C	0.17977900	2.09298400	-2.60713300	H	0.46484200	1.10908200	-2.99130700
H	-0.91343700	2.14044300	-2.56796100	H	0.53234100	2.84282600	-3.33720700
N	-1.98919800	-1.49488500	-1.40745700	C	-2.28183900	-2.77978700	-0.71658500
C	-1.24829200	-3.12861600	0.38862100	N	-1.04970500	-2.02021200	1.36323600
C	-2.24174700	-1.64964200	2.12498200	H	-2.62250400	-2.45222300	2.78126400
H	-1.99529300	-0.79896500	2.76941100	H	-3.05017600	-1.33951200	1.45731100
C	0.06091700	-2.29737000	2.28597900	H	0.34361000	-1.37154300	2.79576200
H	-0.19117100	-3.05058200	3.05297000	H	0.92978900	-2.64753000	1.72160000
H	-0.27089600	-3.25188100	-0.09412400	C	-1.62955100	-4.47169200	1.06575200
H	-2.56669200	-4.34428200	1.62572900	H	-0.86165300	-4.73693700	1.80015000
C	-1.81422000	-5.62753100	0.07575600	C	-2.86653700	-5.26715100	-0.97566700
C	-2.46476100	-3.97194700	-1.68855000	H	-3.21132100	-3.70741400	-2.44827000
H	-1.52395200	-4.15402600	-2.22274900	H	-2.98236000	-6.07703100	-1.70726500

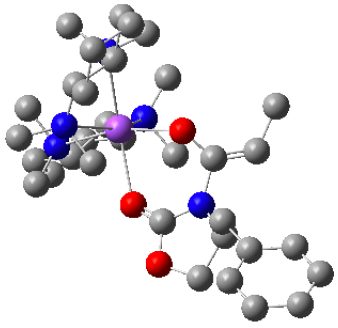
H	-3.84533700	-5.14098300	-0.48888400	H	-2.09742700	-6.53991100	0.61620400
H	-0.85870300	-5.84229800	-0.42433200	H	-3.24993700	-2.63187600	-0.22027600
C	-3.21121600	-0.84822900	-1.88304100	H	-2.96055700	0.13204900	-2.30400500
H	-3.74241500	-1.41851100	-2.66831500	H	-3.90388000	-0.69008300	-1.04962200
C	-1.01859700	-1.60559200	-2.50531000	H	-0.81937800	-0.60055600	-2.88923600
H	-0.06974600	-2.00534300	-2.13971500	H	-1.38159200	-2.20983600	-3.35417700

Table S7. 4b with (*S*,*S*)-TMCDA at –78 °C.





(*S*,*S*)-TMCDA

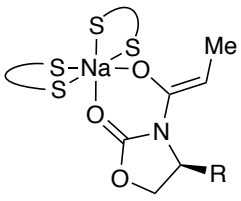


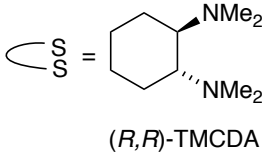
G = –1947.825997
G_{MP2} = –1946.976005

Na	0.00000000	0.00000000	0.00000000	O	-1.90030700	-0.14397300	1.18271400
C	-2.58834600	-1.20126500	1.41318700	N	-3.01793100	-1.96578000	0.20998000
C	-4.40579600	-2.37198600	-0.02414100	C	-4.24935400	-3.15839600	-1.33842400
O	-3.01924000	-2.67919900	-1.91058600	C	-2.27970800	-2.08199900	-0.92189500
O	-1.11972100	-1.74564200	-1.13801500	H	-5.05692700	-2.98187900	-2.05182100
H	-4.15432200	-4.23626800	-1.16277400	H	-4.75194000	-3.03041400	0.77688600
C	-5.35288700	-1.15203600	-0.11357200	H	-5.19284100	-0.56241400	0.79622600
H	-5.04715600	-0.53178000	-0.96517000	C	-6.80810200	-1.54341300	-0.23891100
C	-7.48577000	-1.45172900	-1.46214500	C	-8.82190000	-1.84248500	-1.57531800
C	-9.50390200	-2.33400900	-0.46203200	C	-8.84224700	-2.42770700	0.76487900
C	-7.50863700	-2.03514200	0.87351300	H	-7.00302900	-2.09926900	1.83489100
H	-9.36786300	-2.80157500	1.63986000	H	-10.5441280	-2.63690400	-0.54708600
H	-9.32941100	-1.75852800	-2.53295400	H	-6.96426700	-1.05851900	-2.33245200
C	-3.02323000	-1.71626600	2.59828300	H	-3.54486100	-2.66953800	2.60229900
C	-2.79105600	-1.03384200	3.91623500	H	-3.70136200	-1.01382100	4.53383300
H	-2.01519000	-1.52286600	4.52829400	H	-2.47409100	0.00264400	3.75887900
N	0.11459000	2.51434600	0.93913700	C	-1.19908900	3.14878400	0.63437300
C	-1.38010400	3.47072600	-0.87479000	N	-1.09259000	2.31758200	-1.76232500
C	-2.19235400	1.35287000	-1.87825400	H	-1.83100800	0.46899300	-2.41293200
H	-2.51301200	1.02565100	-0.88503900	H	-3.06347300	1.74706000	-2.43184800
C	-0.65714600	2.74776400	-3.08854400	H	0.22519000	3.39254900	-3.00660200

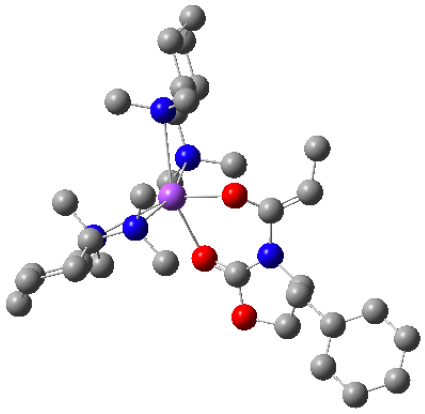
H	-0.38114100	1.86939200	-3.68215300	H	-1.43034100	3.29692200	-3.65897100
H	-0.63260800	4.23239800	-1.13564200	C	-2.76892100	4.10909100	-1.12589600
C	-3.00177100	5.37366700	-0.29262800	C	-2.84332600	5.05383000	1.19577200
C	-1.47011800	4.42829900	1.47055200	H	-1.38444900	4.19472400	2.53707100
H	-0.69668000	5.17825200	1.25177600	H	-2.97032600	5.95783000	1.80519800
H	-3.63457400	4.35473300	1.50328800	H	-3.99879600	5.78310500	-0.49997900
H	-2.27736200	6.15016800	-0.58080000	H	-2.87699400	4.33249900	-2.19469200
H	-3.55252100	3.38203200	-0.87690700	H	-1.94115400	2.39061800	0.91420400
C	1.28188500	3.33870600	0.62721200	H	1.28907100	3.61445300	-0.43062900
H	1.35153700	4.26240500	1.22838100	H	2.18747300	2.75428100	0.82280900
C	0.18124800	2.04816200	2.32940400	H	-0.66348300	1.38105500	2.52188800
H	1.10769000	1.48025100	2.46503100	H	0.18902100	2.86350300	3.07369000
N	2.07130400	-0.58658800	-1.41576600	C	2.75153400	-1.82851400	-0.96227100
C	2.95079400	-1.88434300	0.57737500	N	1.69641700	-1.63174900	1.33035700
C	0.75448800	-2.76201500	1.34423400	H	0.52977500	-3.08233700	0.32488000
H	1.12715700	-3.62566800	1.92114900	H	-0.18573400	-2.43478700	1.79792300
C	1.95973500	-1.20297500	2.70556900	H	2.63580100	-0.34069100	2.70773500
H	1.01644300	-0.90308500	3.17209900	H	2.40933400	-1.99083200	3.33658200
H	3.62408900	-1.05908200	0.84925200	C	3.66253300	-3.20299500	0.97743400
H	3.82342700	-3.21519500	2.06214300	H	3.00387500	-4.05144300	0.75114300
C	4.99176100	-3.41839400	0.24496600	H	5.44239700	-4.36804300	0.56013300
H	5.70448100	-2.62699500	0.52100900	C	4.76912700	-3.39786300	-1.26959600
C	4.09643600	-2.08502800	-1.68747500	H	4.78900200	-1.26089400	-1.46841400
H	3.93344700	-2.07422600	-2.77145400	H	5.71896200	-3.51889200	-1.80578800
H	4.13568400	-4.24979500	-1.55697300	H	2.06668100	-2.64199800	-1.23397700
C	2.90442100	0.61807100	-1.37473300	H	2.26772100	1.49084800	-1.55068400
H	3.36412300	0.73282300	-0.38861800	H	3.70676200	0.62997000	-2.13272600
C	1.47852400	-0.74569800	-2.74870500	H	0.77417400	-1.58022600	-2.73960000
H	0.91735200	0.16131000	-2.99476900	H	2.22559300	-0.90129600	-3.54732200

Table S8. 4a with (*R*,*R*)-TMCDA at –78 °C.





(*R*,*R*)-TMCDA



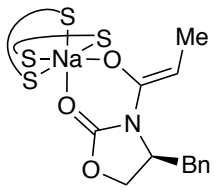
G = –1947.826729

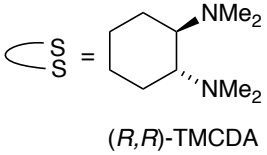
G_{MP2} = –1946.976863

Na	0.00000000	0.00000000	0.00000000	O	1.63823800	-1.16363400	-1.01249900
C	2.53732400	-1.91123100	-0.49312000	N	3.29417400	-1.32011700	0.65124800
C	2.78315700	-0.42287400	1.53241100	O	3.77878200	0.07287100	2.33614900
C	4.97418200	-0.69516600	2.11367300	H	5.83150100	-0.01921800	2.13074300
H	5.07524900	-1.42351200	2.92677100	C	4.75588600	-1.37778400	0.75140800
H	5.09532900	-2.41599600	0.78739900	C	5.44456400	-0.66853600	-0.43852400
H	5.02374700	-1.10613100	-1.35076500	H	5.16788600	0.39291800	-0.42385700
C	6.94855600	-0.82334700	-0.42283200	C	7.78737700	0.23059100	-0.03617600
C	9.17412200	0.06898800	0.00445300	C	9.74618900	-1.15533800	-0.34175500
C	8.92267500	-2.21405000	-0.73271500	C	7.53883600	-2.04773500	-0.77316300
H	6.90413900	-2.87266900	-1.09023600	H	9.35983400	-3.16924000	-1.01239100
H	10.8250000	-1.28339300	-0.31273200	H	9.80599500	0.90163300	0.30304200
H	7.34964700	1.19212400	0.22451800	O	1.62669500	-0.04227200	1.68883800
C	2.94377800	-3.16108500	-0.85813500	H	3.67863300	-3.68378900	-0.25268800
C	2.38123500	-3.87236800	-2.05620200	H	3.16379400	-4.39471400	-2.62577500
H	1.62658700	-4.63548300	-1.80017600	H	1.89989200	-3.15719400	-2.73241700
N	-1.40089900	-1.83101700	1.35480800	C	-1.64701400	-1.35958000	2.71851300
H	-1.91953300	-2.16332800	3.42640200	H	-0.73784100	-0.88008500	3.09408100
H	-2.45752200	-0.62152200	2.71986700	C	-0.29557900	-2.80112000	1.36365700
H	0.58860700	-2.30569800	1.76816200	H	-0.50274000	-3.69192200	1.98081900
H	-0.04576600	-3.11815300	0.34971500	C	-2.63888700	-2.30967800	0.69113400
H	-3.39173100	-1.53002600	0.88078300	C	-2.47379400	-2.43300200	-0.84711600
N	-1.96612100	-1.18538300	-1.47712400	C	-2.99065400	-0.16679000	-1.71274100
H	-2.49905000	0.77193700	-1.99098500	H	-3.69921800	-0.42215200	-2.51968400
H	-3.56499600	0.01683900	-0.79978000	C	-1.23326800	-1.47761800	-2.71526100
H	-0.91149800	-0.53736100	-3.17058000	H	-0.33319200	-2.04955700	-2.47860700
H	-1.83890800	-2.01960900	-3.46399300	H	-1.69483800	-3.18337600	-1.02916500
C	-3.77783200	-2.95990500	-1.49753200	H	-4.57503000	-2.21466100	-1.37265600
H	-3.62434300	-3.07267700	-2.57762500	C	-4.26380800	-4.28080200	-0.89055400
C	-4.47542800	-4.11845900	0.61695200	C	-3.18267800	-3.63492000	1.28434600
H	-2.42299200	-4.41861800	1.16775200	H	-3.33950900	-3.51326300	2.36253200
H	-5.28421300	-3.39412100	0.79579500	H	-4.79819600	-5.06440400	1.07007200
H	-5.19130500	-4.59952200	-1.38309000	H	-3.52301900	-5.07278400	-1.07368600
N	-0.85405300	2.45981000	1.08413000	C	-0.15024100	3.62382200	0.48687700
C	0.10543600	3.46051400	-1.03607900	N	0.76540500	2.17554200	-1.36109200
C	0.65327500	1.82442600	-2.77764700	H	1.23241700	2.48641600	-3.44716200
H	1.02301800	0.80339700	-2.91165400	H	-0.39654600	1.86431300	-3.09097900
C	2.17320400	2.08090200	-0.94989300	H	2.27895800	2.32081700	0.11093600
H	2.48813500	1.04393400	-1.09388100	H	2.83961200	2.74218700	-1.53101800
H	-0.87538800	3.41956000	-1.53311000	C	0.85108300	4.70198300	-1.59081600
C	0.13884000	6.02465400	-1.28483000	C	-0.06571100	6.18031100	0.22463500
C	-0.84113900	4.97992400	0.77925700	H	-1.84351700	4.98150400	0.33012500
H	-0.98487900	5.08975500	1.86102900	H	-0.60207300	7.11037200	0.45214400
H	0.91332300	6.25359700	0.72057200	H	-0.83836600	6.04893300	-1.78971400
H	0.71899500	6.86440300	-1.68809900	H	1.85703100	4.74204400	-1.15281500

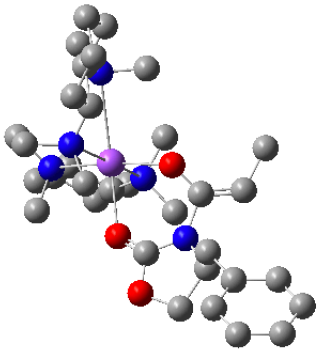
H	0.98850900	4.58999900	-2.67284700	H	0.83019000	3.64774900	0.97876000
C	-2.29841600	2.44130300	0.85117900	H	-2.51649000	2.58402300	-0.21109600
H	-2.69234200	1.46153800	1.14318700	H	-2.85372000	3.20653200	1.42173700
C	-0.56483600	2.33314400	2.51548300	H	-1.07938200	1.45220300	2.90854300
H	0.50681300	2.17962000	2.66272500	H	-0.89635500	3.20443800	3.10949000

Table S9. 4b with (*R*,*R*)-TMCDA at –78 °C.





(*R*,*R*)-TMCDA

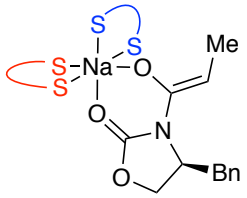


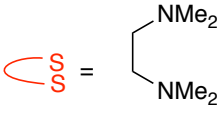
G = –1947.82383
G_{MP2} = –1946.975166

Na	0.00000000	0.00000000	0.00000000	O	-1.86724800	0.10961300	1.23277800
C	-2.70513400	-0.82533400	1.48007200	N	-3.24279900	-1.54364500	0.28909400
C	-2.56148300	-1.73640200	-0.87103200	O	-3.38850900	-2.29055400	-1.81652300
C	-4.61880700	-2.67863200	-1.18329200	H	-5.44561600	-2.45804200	-1.86162700
H	-4.58836600	-3.75824900	-0.99470200	C	-4.66274300	-1.86645700	0.12346000
H	-5.01184500	-2.49343200	0.94774200	C	-5.53955500	-0.59383900	0.05713400
H	-5.29704200	0.00271400	0.94375400	H	-5.24545300	-0.01012200	-0.82394200
C	-7.01942900	-0.90218800	0.01766600	C	-7.75596700	-0.79755100	-1.16989500
C	-9.11589100	-1.11428100	-1.20340400	C	-9.76303200	-1.54350300	-0.04447900
C	-9.04236000	-1.64911100	1.14773000	C	-7.68516000	-1.33047500	1.17682100
H	-7.13249700	-1.40356500	2.11127600	H	-9.53989500	-1.97481500	2.05771800
H	-10.8214590	-1.78903400	-0.06733100	H	-9.66879100	-1.02162700	-2.13473800
H	-7.26090800	-0.45293400	-2.07553800	O	-1.39059300	-1.50166000	-1.14886000
C	-3.20612500	-1.24712300	2.67809300	H	-3.87097300	-2.10546000	2.70949900
C	-2.85499900	-0.58509800	3.98013700	H	-3.74821900	-0.30208400	4.55835100
H	-2.25330600	-1.22973600	4.64154400	H	-2.27613100	0.32591100	3.79729700
N	2.33084900	-0.78572600	-1.13625500	C	3.13428000	0.37342600	-1.52866500
H	2.48228700	1.13203400	-1.97158300	H	3.61081500	0.80997800	-0.64577600
H	3.92238200	0.14016100	-2.26690400	C	1.68045900	-1.37021400	-2.31600200
H	1.02513600	-2.19326900	-2.02710200	H	1.04474300	-0.61004300	-2.78179200
H	2.39269900	-1.72147700	-3.08207500	C	3.11822700	-1.74914300	-0.32282300

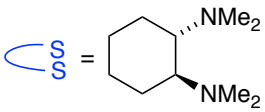
H	3.61295800	-1.13568900	0.44408600	C	2.23293500	-2.79120800	0.41171900
N	1.11008900	-2.18100500	1.16041600	C	0.00566100	-3.12803600	1.35080900
H	-0.33968800	-3.48313300	0.37629100	H	0.28334000	-3.99992400	1.97145300
H	-0.83040500	-2.61914100	1.83895700	C	1.47997100	-1.58182300	2.44413800
H	2.30769600	-0.87602800	2.31416200	H	0.61566600	-1.03204900	2.82935800
H	1.77620600	-2.31858800	3.21137300	H	1.75963200	-3.41287300	-0.35943300
C	3.11762800	-3.72939400	1.27110900	H	3.60215000	-3.14554200	2.06541200
H	2.48038200	-4.46760700	1.77211300	C	4.20679800	-4.43619200	0.45659900
H	4.81025300	-5.07788400	1.11115700	H	3.74242200	-5.09763200	-0.28947400
C	5.08767200	-3.40532400	-0.25472900	H	5.63492400	-2.81451100	0.49492000
H	5.84558800	-3.90084100	-0.87466100	C	4.23116000	-2.47529300	-1.12301400
H	3.76978000	-3.07312500	-1.92041400	H	4.87110700	-1.73647500	-1.61938000
N	-0.83321800	2.20803900	-1.27409300	C	-2.10536500	1.63743000	-1.73400300
H	-1.89996400	0.75161600	-2.34218400	H	-2.68139900	1.31891900	-0.86212700
H	-2.70553100	2.33659600	-2.34272200	C	-0.01063500	2.58190600	-2.42422600
H	0.95158300	2.98707900	-2.09855500	H	0.18783900	1.68479400	-3.02161800
H	-0.48547800	3.31963700	-3.09498800	C	-1.04824800	3.29116000	-0.27683600
C	0.25049400	3.69194700	0.47548000	N	0.95180600	2.53732700	1.09506700
C	2.38366300	2.79182100	1.24102200	H	2.81912500	3.06021800	0.27279500
H	2.62517900	3.59627600	1.96089200	H	2.87910300	1.88002000	1.59392800
C	0.38625700	2.10094700	2.37903400	H	-0.66254100	1.81842200	2.26327900
H	0.92457500	1.20610700	2.70463300	H	0.48827900	2.85087500	3.18223900
H	0.94902500	4.08923400	-0.27307300	C	-0.03305900	4.84120000	1.47679300
H	0.90039100	5.11926500	1.98194700	H	-0.71497300	4.48084500	2.25726400
C	-0.66885800	6.07020100	0.82039500	H	-0.84667600	6.84818700	1.57383400
H	0.02117400	6.50144100	0.07977900	C	-1.97434600	5.66921300	0.13017300
H	-2.69510000	5.32456500	0.88582800	H	-2.43363900	6.53130600	-0.37039700
C	-1.71546000	4.55267700	-0.88793600	H	-1.06866600	4.95528900	-1.67986400
H	-2.65696500	4.26912800	-1.37113500	H	-1.73766700	2.85795800	0.45857900

Table S10. 4a with TMEDA and (*S*,*S*)-TMCDA at –78 °C.

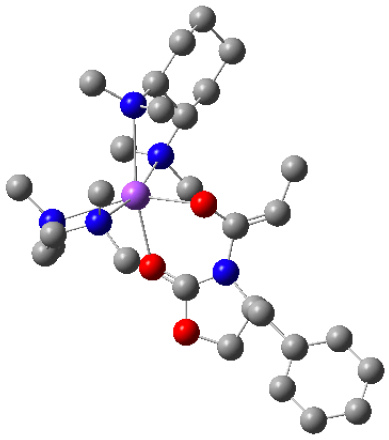




TMEDA



(*S*,*S*)-TMCDA

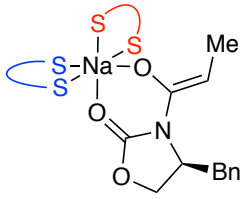


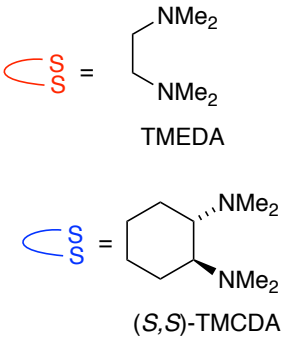
G = –1792.329366
G_{MP2} = –1791.572685

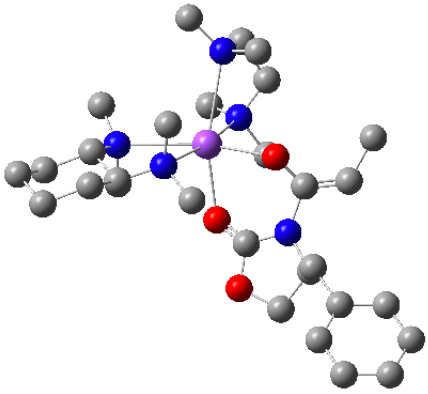
Na	0.00000000	0.00000000	0.00000000	O	-1.55419200	-1.42334400	0.81177000
C	-2.42062400	-2.08710800	0.14783700	N	-3.28563600	-1.29184800	-0.77202400
C	-2.90174500	-0.14856600	-1.39342300	O	-3.97836000	0.44346600	-2.00504600
C	-5.08888200	-0.46960100	-1.96215300	H	-6.00218900	0.10021500	-1.77963700
H	-5.16527000	-0.96966200	-2.93476600	C	-4.74162800	-1.45510100	-0.83286700
H	-4.99981400	-2.47588300	-1.12539700	C	-5.41459000	-1.13698700	0.52343000
H	-4.90114700	-1.74151700	1.27936100	H	-5.23539200	-0.08246900	0.76692300
C	-6.89679300	-1.43666200	0.52612700	C	-7.85026200	-0.41286900	0.44568400
C	-9.21636200	-0.70265900	0.41683700	C	-9.65183200	-2.02697400	0.46722800
C	-8.71270000	-3.05794100	0.55143100	C	-7.35001800	-2.76391600	0.58141800
H	-6.62415100	-3.57082900	0.65875300	H	-9.04281300	-4.09253300	0.59970200
H	-10.7141860	-2.25509300	0.44665100	H	-9.93875800	0.10757500	0.35890400
H	-7.51903000	0.62326400	0.41745700	O	-1.79378200	0.37411900	-1.47277300
C	-2.70503200	-3.42261800	0.18422500	H	-3.43526800	-3.83549200	-0.50556700
C	-2.02225700	-4.36262200	1.13726300	H	-2.72656800	-5.08847800	1.56901100
H	-1.21765200	-4.95657200	0.67015700	H	-1.57081400	-3.80443400	1.96509100
N	1.22636900	-1.78365400	-1.46717200	C	2.26793200	-1.15948300	-2.28193800
H	2.76176500	-1.85154200	-2.98693900	H	1.80978700	-0.36411200	-2.87797100
H	3.03642700	-0.70293700	-1.65137400	C	0.12605000	-2.24064200	-2.32675600
H	-0.34912800	-1.36962400	-2.78832000	H	0.45625800	-2.92027000	-3.13212300
H	-0.62821500	-2.75182400	-1.72160500	C	1.70005700	-2.85288000	-0.54963200
H	0.79795800	-3.18946800	-0.02278300	C	2.69951600	-2.32789100	0.51449100
H	3.59005200	-1.97489700	-0.02204600	N	2.18652400	-1.14368500	1.25439100
C	3.27180000	-0.29016300	1.73479100	H	2.84751300	0.61438000	2.18513400
H	3.91325200	-0.76968100	2.49753200	H	3.90861700	0.01689400	0.89811500
C	1.27022100	-1.46891300	2.35631700	H	0.87207800	-0.53401800	2.76010800
H	0.41654300	-2.04354500	1.98982800	H	1.75614100	-2.00634000	3.18836600
C	3.16672800	-3.47857600	1.44010600	H	3.88764000	-3.08731900	2.16917700
H	2.31069500	-3.85273000	2.01557400	C	3.77562500	-4.65425600	0.66738700
H	4.08578500	-5.44134500	1.36648800	H	4.68404200	-4.32682800	0.13974800
C	2.76249600	-5.19272100	-0.34515400	H	1.89434400	-5.60222500	0.19151200
H	3.19145300	-6.02021600	-0.92464500	C	2.30424400	-4.07548600	-1.29014300
H	1.56699200	-4.46998400	-1.99772300	H	3.16765800	-3.75062700	-1.88757700
N	-0.76349500	1.97313100	1.74554500	C	-0.46914000	1.83469400	3.17203100
H	-0.94438000	2.62697500	3.78172200	H	-0.83719900	0.86769100	3.52729900
H	0.61240800	1.87869500	3.34061600	C	-2.21034700	1.82781100	1.53810400
H	-2.45840600	1.97541800	0.48586900	H	-2.50309800	0.80822700	1.80130200
H	-2.78564200	2.55397200	2.14392500	C	-0.26278900	3.25751800	1.24146600
C	-0.16650100	3.34087300	-0.28431500	H	-1.14062900	3.11242700	-0.72600600
H	0.06480100	4.39159000	-0.55104400	N	0.80977600	2.42719100	-0.89973500
C	2.18751300	2.80146400	-0.57681000	H	2.36537000	2.73655400	0.49975000
H	2.87638200	2.10797600	-1.06927400	H	2.43597000	3.82814400	-0.90823500

C	0.61806900	2.43602900	-2.35528600	H	1.36076000	1.78466400	-2.82568400
H	-0.37804500	2.05452100	-2.59083900	H	0.73392900	3.44859800	-2.78618400
H	0.72472700	3.42868700	1.68418100	H	-0.90028100	4.09611500	1.58483900

Table S11. 4a with (*S*,*S*)-TMCDA and TMEDA at –78 °C.





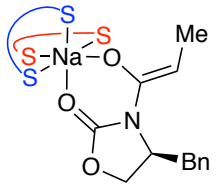


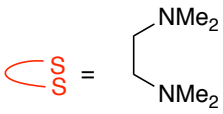
G = –1792.329831
G_{MP2} = –1791.572979

Na	0.00000000	0.00000000	0.00000000	O	1.96176100	-0.74005200	-0.85056800
C	3.03978900	-1.05129200	-0.23320700	N	3.52717000	-0.06038700	0.76626800
C	2.72040400	0.74519900	1.50389900	O	3.47175600	1.68246900	2.17062800
C	4.86106000	1.33737600	2.03591200	H	5.43848900	2.25506600	1.90681400
H	5.18560900	0.83538200	2.95490700	C	4.91776900	0.39987500	0.81642900
H	5.59181000	-0.43803300	1.01185500	C	5.34715400	1.08782000	-0.50095000
H	5.11871000	0.38688500	-1.31176200	H	4.72509300	1.97853100	-0.65090000
C	6.81337700	1.45686100	-0.52061200	C	7.23473500	2.78385100	-0.36155700
C	8.59239100	3.11186700	-0.35437300	C	9.55436500	2.11297400	-0.50547900
C	9.14917000	0.78584900	-0.66818500	C	7.79264600	0.46328000	-0.67637000
H	7.48388900	-0.57073600	-0.81595300	H	9.89116900	0.00158300	-0.79487500
H	10.6113390	2.36568800	-0.50191000	H	8.89646400	4.14860600	-0.23431100
H	6.49050600	3.57045400	-0.25444700	O	1.50238200	0.73106700	1.63661200
C	3.84107300	-2.14670900	-0.38145600	H	4.68770200	-2.28049100	0.28582300
C	3.59654400	-3.19971200	-1.42508300	H	4.52469800	-3.48632100	-1.94143600
H	3.17295700	-4.13234200	-1.01626000	H	2.89729600	-2.83152400	-2.18350100
N	-0.50198800	-2.26979600	1.25981400	C	-1.68575500	-2.42778900	2.10490900
H	-1.77053200	-3.44945500	2.52342700	H	-1.62931700	-1.72429500	2.94190000
H	-2.60090100	-2.21233900	1.54716700	C	0.70065700	-2.47935800	2.07928600
H	0.75000500	-1.71191300	2.85698200	H	0.69801000	-3.47532600	2.56190600
H	1.59490000	-2.39540700	1.45791600	C	-0.49806600	-3.21384800	0.13010100
H	0.48377200	-3.13985300	-0.34579300	H	-0.60567600	-4.25504800	0.49462800

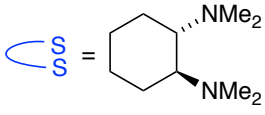
C	-1.59423800	-2.97321600	-0.91203400	H	-2.56851700	-2.91282800	-0.41595700
H	-1.63953100	-3.86686800	-1.56485900	N	-1.42594200	-1.75619200	-1.72215500
C	-2.68976400	-1.41685400	-2.37758200	H	-2.56685800	-0.49751300	-2.95918900
H	-3.04334000	-2.20917100	-3.06501700	H	-3.46775000	-1.24614700	-1.62614600
C	-0.37196100	-1.93640500	-2.73146500	H	-0.35221300	-1.06126100	-3.38799700
H	0.60678400	-2.00301800	-2.25240100	H	-0.55309500	-2.83011000	-3.35868400
N	-2.02814400	1.66136200	0.76383800	C	-3.32445100	0.98442900	0.76638300
H	-3.66437200	0.82913600	-0.26278000	H	-3.21785300	0.00412900	1.24115500
H	-4.11438900	1.53203000	1.31223200	C	-1.52277600	1.79694400	2.13592700
H	-1.39484800	0.79762200	2.56431400	H	-0.53860400	2.26845100	2.13807200
H	-2.19995900	2.36124600	2.79986100	C	-2.07274200	2.93043400	-0.00727900
C	-0.67054100	3.40532500	-0.47455300	N	0.09727600	2.33990400	-1.15855000
C	1.53684200	2.61845000	-1.19468900	H	1.87942300	2.88966300	-0.19212400
H	2.05910100	1.70557600	-1.49626400	H	1.80618500	3.43346700	-1.89102800
C	-0.37473400	2.00054700	-2.50165400	H	0.17162100	1.11741200	-2.84708900
H	-1.44160000	1.75660400	-2.48602500	H	-0.21382500	2.80158300	-3.24459700
H	-0.08984600	3.64232700	0.42661700	C	-0.79730500	4.71105000	-1.30027700
H	0.20227100	5.04870200	-1.59854300	H	-1.34530600	4.50146000	-2.22902800
C	-1.52983300	5.82904400	-0.54937500	H	-1.60346100	6.72194600	-1.18309800
H	-0.95070100	6.12180900	0.33869400	C	-2.91984800	5.35521200	-0.11473600
C	-2.80657300	4.07967900	0.72898300	H	-3.80360300	3.74121300	1.03608100
H	-2.26248700	4.32360500	1.65102900	H	-3.43679900	6.13662700	0.45663200
H	-3.53519100	5.16003800	-1.00561000	H	-2.65628300	2.69796400	-0.90900800

Table S12. 4b with TMEDA and (*S*,*S*)-TMCDA at –78 °C.

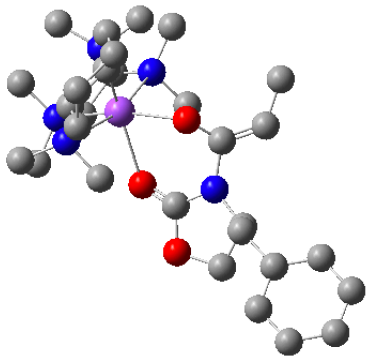




TMEDA



(*S*,*S*)-TMCDA

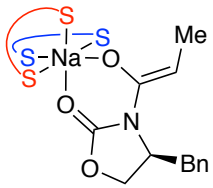


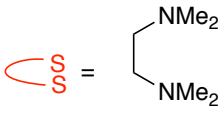
G = –1792.328649
G_{MP2} = –1791.572442

Na	0.00000000	0.00000000	0.00000000	O	-1.81054800	0.53010300	1.24295700
C	-2.80192100	-0.24554500	1.47514900	N	-3.50178300	-0.77932500	0.27040100
C	-2.88527200	-1.09732900	-0.89421600	O	-3.81420200	-1.36439800	-1.86647100
C	-5.11678300	-1.41360300	-1.25637800	H	-5.83453100	-0.94058200	-1.92970000

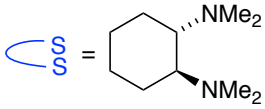
H	-5.39467400	-2.46460500	-1.11586000	C	-4.95161100	-0.67559200	0.08471200
H	-5.47684600	-1.20766000	0.88216800	C	-5.42614100	0.79655400	0.06945500
H	-5.04148300	1.26137800	0.98428100	H	-4.95856500	1.30816300	-0.78074000
C	-6.93126600	0.92802400	0.00405000	C	-7.58063200	1.30270800	-1.17987100
C	-8.97309800	1.39426100	-1.23874400	C	-9.74131200	1.10990700	-0.10955200
C	-9.10745700	0.73803500	1.07870000	C	-7.71694800	0.64940600	1.13329200
H	-7.22922900	0.37080300	2.06522700	H	-9.69723900	0.52252100	1.96604500
H	-10.8248260	1.18221300	-0.15204700	H	-9.45552700	1.69149100	-2.16641300
H	-6.98811400	1.53714200	-2.06189100	O	-1.68672900	-1.17566500	-1.15160400
C	-3.34992800	-0.63100800	2.66356200	H	-4.16055400	-1.35467700	2.66498200
C	-2.86436500	-0.11013100	3.98664200	H	-3.69813100	0.15776000	4.65219600
H	-2.24840800	-0.83656100	4.54300500	H	-2.25304300	0.78726600	3.84218100
N	-0.14589500	2.47035900	-1.53956000	C	0.17946700	3.60810700	-0.64244100
H	1.18198200	3.94080800	-0.94337600	C	0.26205400	3.20541000	0.85562200
N	1.15429800	2.03614400	1.09186900	C	2.55932900	2.24474700	0.74472400
H	2.65844200	2.54999900	-0.30034100	H	3.07229100	2.99242300	1.37515900
H	3.09441600	1.29581400	0.86348900	C	1.03562800	1.53188000	2.46519600
H	-0.01361800	1.30272000	2.66945100	H	1.61147500	0.60456500	2.55051900
H	1.42223200	2.22758100	3.23034400	H	-0.73117700	2.85991300	1.16875600
C	0.64268400	4.44487500	1.70831500	C	-0.29880500	5.63760000	1.50201100
C	-0.34837700	6.03205100	0.02405400	C	-0.76169100	4.82500900	-0.82449500
H	-0.79610900	5.09989700	-1.88634500	H	-1.78278000	4.53858400	-0.54216800
H	-1.04980100	6.86106100	-0.13542500	H	0.64135300	6.39318200	-0.29351600
H	0.02777200	6.48296200	2.12124800	H	-1.31052200	5.37210700	1.84157200
H	0.65726100	4.17006000	2.76848100	H	1.66427600	4.76230600	1.45469600
C	-1.57844200	2.16163800	-1.64281800	H	-1.69132000	1.23548000	-2.21435100
H	-1.99656600	1.98194300	-0.64867400	H	-2.15953600	2.94817900	-2.15552300
C	0.42522100	2.65215900	-2.87186800	H	1.51266500	2.77078500	-2.80473800
H	0.21596500	1.76423800	-3.47750300	H	0.01899700	3.52484500	-3.41775600
N	0.77784000	-2.29741000	1.31778800	C	-0.48939100	-3.04126000	1.29715400
H	-0.89094200	-3.08088200	0.28374400	H	-0.36047200	-4.07384600	1.67558100
H	-1.22633600	-2.52350500	1.91791100	C	1.25467500	-2.20474200	2.69897800
H	2.19195600	-1.63925400	2.73657100	H	0.50999900	-1.68227200	3.30619000
H	1.43673200	-3.19818100	3.15171800	C	1.79253500	-2.93384000	0.46922600
H	2.76703400	-2.51135500	0.73808700	H	1.86040600	-4.02001300	0.67822300
C	1.55457600	-2.76169100	-1.03360500	H	0.54964700	-3.11072100	-1.28713000
H	2.26421700	-3.42259800	-1.56947500	N	1.67059600	-1.37760300	-1.52249500
C	3.05896100	-0.91339900	-1.51572600	H	3.09918000	0.11699700	-1.88178400
H	3.46595100	-0.92126100	-0.50085200	H	3.71430100	-1.53521800	-2.15540300
C	1.12407200	-1.29218800	-2.88255900	H	0.06012300	-1.53914900	-2.86169900
H	1.23496300	-0.26898800	-3.25347000	H	1.64436200	-1.96936300	-3.58595600

Table S13. 4b with (*S*,*S*)-TMCDA and TMEDA at –78 °C.

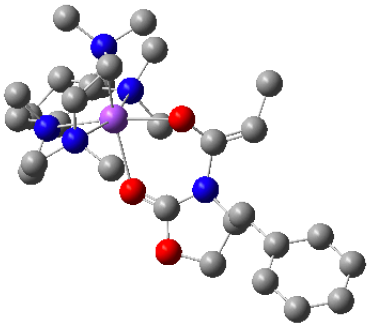




TMEDA



(*S*,*S*)-TMCDA

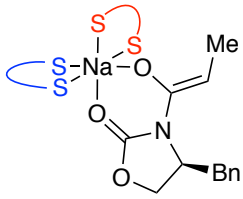


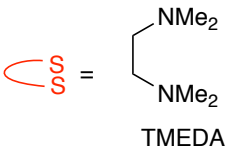
G = –1792.330877
G_{MP2} = –1791.573569

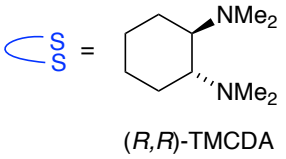
Na	0.00000000	0.00000000	0.00000000	O	-1.88224800	-0.25973800	1.22135900
C	-2.65450300	-1.28294200	1.20379200	N	-3.18242800	-1.67292200	-0.13252900
C	-2.50083700	-1.52576500	-1.29791300	O	-3.32692300	-1.78630900	-2.36321700
C	-4.55654900	-2.34126400	-1.86552300	H	-5.38374200	-1.94238400	-2.45622600
H	-4.52098100	-3.43029300	-1.98654200	C	-4.60332700	-1.92855300	-0.38313100
H	-4.95728500	-2.75915800	0.23294000	C	-5.47363600	-0.68342900	-0.09112700
H	-5.22798600	-0.35874100	0.92623300	H	-5.17614900	0.12127900	-0.77459200
C	-6.95515200	-0.96088600	-0.21180400	C	-7.69267600	-0.52334200	-1.32012900
C	-9.05473000	-0.80990600	-1.43664600	C	-9.70315900	-1.54272300	-0.44235200
C	-8.98152100	-1.98240700	0.67021200	C	-7.62221300	-1.69276300	0.78300400
H	-7.06881300	-2.02826000	1.65777500	H	-9.47993500	-2.54675300	1.45429300
H	-10.7632540	-1.76550400	-0.52964700	H	-9.60830900	-0.45644800	-2.30283700
H	-7.19716600	0.05870300	-2.09454000	O	-1.33017500	-1.21805800	-1.49008100
C	-3.10013100	-2.05290800	2.23798400	H	-3.70155600	-2.93243300	2.02539100
C	-2.77353200	-1.75469600	3.67378100	H	-3.65781900	-1.84396200	4.32197800
H	-2.01277300	-2.43160500	4.09717500	H	-2.39014400	-0.73383700	3.77514300
N	-0.87965100	2.41845600	-1.20481600	C	-0.66783900	3.45689900	-0.18694400
H	-1.43384000	4.25223500	-0.27937500	H	0.29339300	3.93935700	-0.39544400
C	-0.69188700	2.95326800	1.25829700	N	0.45329000	2.11057500	1.64363500
C	1.70115300	2.87260000	1.69398600	H	1.95620100	3.27492900	0.71006800
H	1.65200600	3.71591200	2.40962500	H	2.51726700	2.21182400	2.00419300
C	0.18234100	1.52085600	2.96236600	H	-0.69350000	0.87209700	2.88552000
H	1.04074300	0.91896700	3.27538800	H	0.00879000	2.29461600	3.73438600
H	-1.59410100	2.35942900	1.42902600	H	-0.75528700	3.83902300	1.92176400
C	-2.28530600	1.99217800	-1.24792900	H	-2.41026400	1.26917500	-2.05810200
H	-2.55772300	1.49096100	-0.31612200	H	-2.96661900	2.84657200	-1.42705600
C	-0.47914200	2.92002700	-2.52017200	H	0.58420100	3.18430900	-2.51494200
H	-0.63781200	2.14165100	-3.27277600	H	-1.05323100	3.81461900	-2.82940700
N	2.12144100	-0.49514300	-1.45052800	C	2.74898700	-1.81211000	-1.16889400
C	2.76025200	-2.16189100	0.34431900	N	1.42233700	-2.02592300	0.96733800
C	0.46835900	-3.08669300	0.61253800	H	0.35143200	-3.15022200	-0.47183400
H	0.75905600	-4.07780100	1.00138300	H	-0.50847300	-2.83594000	1.03516800
C	1.49675500	-1.90289300	2.42445300	H	2.19182100	-1.10035300	2.69492700

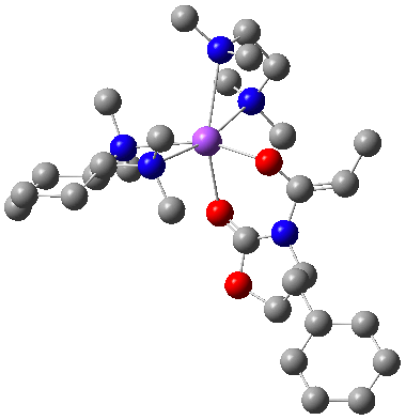
H	0.50522000	-1.64527000	2.80819400	H	1.82779000	-2.82762100	2.93131700
H	3.39261800	-1.41619800	0.84776000	C	3.41772400	-3.54739000	0.56883800
C	4.82464500	-3.65191000	-0.03097700	C	4.78564500	-3.34102100	-1.53039800
C	4.16976100	-1.95730000	-1.76881500	H	4.83240000	-1.20590800	-1.31834200
H	4.13638500	-1.73834600	-2.84298500	H	5.79300200	-3.38167200	-1.96392200
H	4.19075000	-4.10850700	-2.04699000	H	5.49949000	-2.94293500	0.47146800
H	5.23482400	-4.65383100	0.14830600	H	3.44756300	-3.76643100	1.64292200
H	2.79034800	-4.32289900	0.11067300	H	2.10534100	-2.54797700	-1.66770700
C	2.96938000	0.66012600	-1.14867700	H	2.36323000	1.56982600	-1.21577300
H	3.35636400	0.59338600	-0.12738800	H	3.82506000	0.77737500	-1.83625000
C	1.61448900	-0.41539400	-2.82388800	H	0.88023500	-1.20718200	-2.99114800
H	1.10249900	0.54168400	-2.95901900	H	2.40707600	-0.48347800	-3.59107800

Table S14. 4a with TMEDA and (*R*,*R*)-TMCDA at –78 °C.







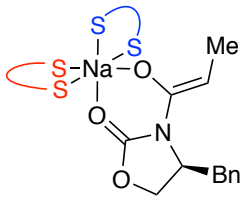


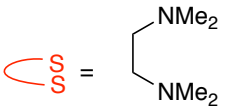
G = –1792.331233
G_{MP2} = –1791.574674

Na	0.00000000	0.00000000	0.00000000	O	-1.95531400	-0.73205900	0.86321000
C	-3.01451900	-1.09029900	0.23823700	N	-3.52292700	-0.13118300	-0.78184900
C	-2.73232000	0.67018500	-1.54076100	O	-3.50080700	1.57583900	-2.22961100
C	-4.88483100	1.21717700	-2.07317400	H	-5.47216500	2.13111000	-1.96322600
H	-5.21102000	0.68690300	-2.97553100	C	-4.91884500	0.31202200	-0.82851300
H	-5.58590800	-0.53812000	-0.99253800	C	-5.33809000	1.03074700	0.47581300
H	-5.08786000	0.35565500	1.30203500	H	-4.72570100	1.93326200	0.59174600
C	-6.80873900	1.38059100	0.50974000	C	-7.25131900	2.69652800	0.31990800
C	-8.61337600	3.00579200	0.32795100	C	-9.55837500	1.99882000	0.52544900
C	-9.13178200	0.68256800	0.71898200	C	-7.77095400	0.37875200	0.71182600
H	-7.44511000	-0.64644600	0.87557600	H	-9.86032400	-0.10759900	0.88191400
H	-10.6186750	2.23704500	0.53409600	H	-8.93407500	4.03441200	0.18377200
H	-6.52016600	3.48965000	0.17680700	O	-1.51367200	0.67355600	-1.67179500

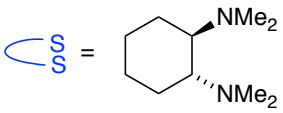
C	-3.78159000	-2.20853200	0.39376400	H	-4.61546600	-2.37806100	-0.28161200
C	-3.51687800	-3.23730100	1.45630000	H	-4.43934000	-3.53454500	1.97703100
H	-3.07344300	-4.16769800	1.06397900	H	-2.82639400	-2.84056600	2.20830300
N	0.55843600	-2.27252700	-1.26270900	C	1.74511900	-2.39131500	-2.11044000
H	1.89159600	-3.42181100	-2.48822200	H	1.63802900	-1.72886200	-2.97474900
H	2.64922900	-2.09396600	-1.57137200	C	-0.64047700	-2.52957400	-2.07380100
H	-0.72188000	-1.76779700	-2.85419300	H	-0.60653400	-3.52747000	-2.55129500
H	-1.53353800	-2.47326700	-1.44693500	C	0.59497400	-3.20855000	-0.12817900
H	-0.38354000	-3.16314100	0.35857700	H	0.73120100	-4.24862500	-0.48684000
C	1.69536900	-2.92591300	0.89832400	H	2.66309300	-2.85369700	0.39075900
H	1.76708600	-3.80566500	1.56735300	N	1.50576600	-1.69738400	1.68541200
C	2.76690500	-1.31547700	2.32252000	H	2.62561700	-0.39207700	2.89345900
H	3.14909400	-2.08865800	3.01627500	H	3.53196500	-1.13259600	1.56062900
C	0.46409800	-1.88218900	2.70697400	H	0.42830400	-0.99491200	3.34501100
H	-0.51725700	-1.98136600	2.23860500	H	0.67072000	-2.75985800	3.34870200
N	1.69416800	1.77957400	-0.95697300	C	1.35234700	3.15647500	-0.51418100
C	1.01514800	3.23667200	1.00021700	N	-0.00977000	2.24668100	1.40539400
C	0.05267800	1.92728900	2.83143000	H	-0.20983100	2.77725500	3.48844400
H	-0.64913400	1.11391700	3.03985500	H	1.06157300	1.59228600	3.09736400
C	-1.38932600	2.60129400	1.04423000	H	-1.44712800	2.87493400	-0.01184400
H	-2.01310900	1.71548100	1.19500000	H	-1.79437400	3.43136000	1.64902100
H	1.92430600	2.96008500	1.55265400	C	0.66372400	4.69237400	1.39863500
C	1.75521300	5.70153300	1.02421200	C	2.04394300	5.63463400	-0.47815600
C	2.43154600	4.20703400	-0.88106900	H	3.37323100	3.95212700	-0.37564000
H	2.63451800	4.16237400	-1.95760800	H	2.84589100	6.33174000	-0.75257300
H	1.15025800	5.94945800	-1.03661200	H	2.67683000	5.48185500	1.58353100
H	1.44636700	6.71316100	1.31678600	H	-0.26629000	4.98785600	0.89541100
H	0.46069600	4.73398300	2.47578700	H	0.43924700	3.41354000	-1.06661600
C	3.01803300	1.31558100	-0.53977400	H	3.15043800	1.45472800	0.53687200
H	3.09889900	0.24290900	-0.74690900	H	3.85208800	1.81849000	-1.05973800
C	1.52210700	1.61419900	-2.40365700	H	1.70595100	0.56745700	-2.66633600
H	0.49046200	1.84703500	-2.67710700	H	2.21246700	2.23332200	-3.00417700

Table S15. 4a with (*R*,*R*)-TMCDA and TMEDA at –78 °C.

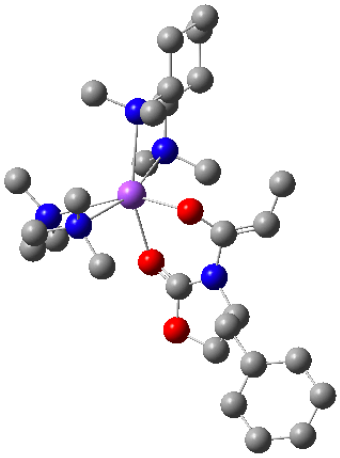




TMEDA



(*R*,*R*)-TMCDA

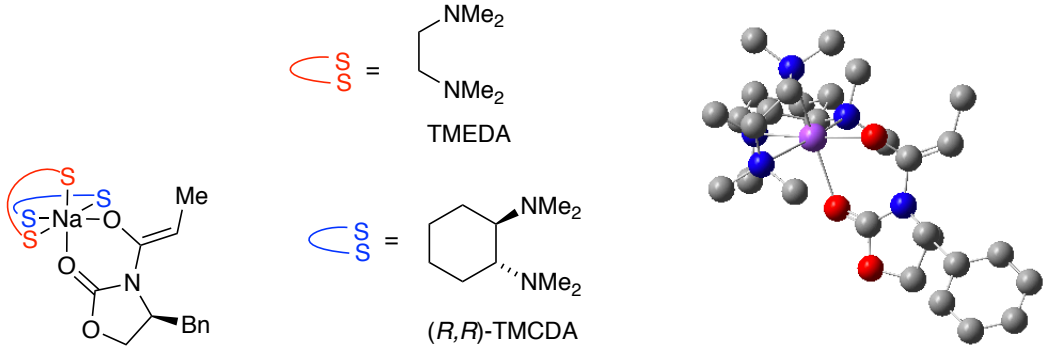


G = –1792.328352
G_{MP2} = –1791.572251

Na	0.00000000	0.00000000	0.00000000	O	-1.55576500	-1.42783300	0.78802400
C	-2.39925300	-2.12462900	0.12709100	N	-3.21783000	-1.37489000	-0.87387800
C	-2.78719700	-0.28613500	-1.55695300	O	-3.82996100	0.29369500	-2.23510500
C	-4.96740600	-0.58436300	-2.16407200	H	-5.86754800	0.02019500	-2.03570900
H	-5.03790600	-1.13753800	-3.10783600	C	-4.67415800	-1.51211800	-0.97121000
H	-4.94380800	-2.54292400	-1.21469800	C	-5.38171400	-1.10776000	0.34366000
H	-4.90470400	-1.68102400	1.14645600	H	-5.18767300	-0.04540600	0.53649900
C	-6.86940700	-1.37715000	0.31619300	C	-7.79824000	-0.33899600	0.16363400
C	-9.16900700	-0.60199200	0.11038400	C	-9.63423600	-1.91342400	0.20864400
C	-8.72006000	-2.95831000	0.36506600	C	-7.35263700	-2.69096300	0.41909600
H	-6.64681100	-3.50806000	0.55350500	H	-9.07347500	-3.98269300	0.45115600
H	-10.7003640	-2.12051900	0.16936300	H	-9.87195300	0.21932400	-0.00377800
H	-7.44438800	0.68796900	0.09802900	O	-1.66136800	0.19844800	-1.64085400
C	-2.70042400	-3.45173600	0.22501300	H	-3.40214800	-3.89521200	-0.47569800
C	-2.06117500	-4.34773800	1.24795700	H	-2.79105300	-5.02941800	1.70896500
H	-1.26289700	-4.98726200	0.83417600	H	-1.61224800	-3.75046200	2.04921900
N	0.73718400	2.58849000	-0.88429400	C	2.08821700	3.03957500	-0.54991700
H	2.25424400	3.00203700	0.53012900	H	2.82092900	2.37733400	-1.02220000
H	2.28595600	4.07347500	-0.89332200	C	0.55452900	2.59535800	-2.34042800
H	1.34131000	1.99779000	-2.80898700	H	-0.41085800	2.14624700	-2.58585500
H	0.60339200	3.61639800	-2.76458600	C	-0.28866600	3.43840200	-0.26132900
C	-0.43948200	3.25867000	1.25159700	N	-0.93155400	1.93550400	1.65148800
C	-0.71965700	1.72027400	3.08314500	H	-1.25813100	2.45929900	3.70709800
H	-1.07410100	0.72177800	3.35403200	H	0.34751100	1.78897800	3.32136200
C	-2.35798100	1.76111800	1.34927000	H	-2.54736200	1.94518300	0.29008800
H	-2.63174900	0.72352300	1.55583700	H	-2.99040000	2.44667500	1.94543900
H	0.52917400	3.41642900	1.73960700	H	-1.10547200	4.06195600	1.62466300
H	-1.23936300	3.21131200	-0.75226000	H	-0.08154600	4.50902500	-0.45904300
N	1.55448600	-1.53772100	-1.56877300	C	1.91716200	-0.87045200	-2.81822900

H	2.29911400	-1.55679100	-3.59643100	H	1.03215300	-0.37012300	-3.22296900
H	2.68581900	-0.11271400	-2.62783900	C	0.46866200	-2.49779200	-1.81455200
H	-0.39969700	-1.94769800	-2.18413600	H	0.73055600	-3.26873500	-2.55936100
H	0.16466300	-2.98574900	-0.88656500	C	2.73555000	-2.10446100	-0.87442300
H	3.51933500	-1.33757000	-0.95764300	C	2.48023200	-2.34236500	0.63811800
N	1.95065900	-1.13998200	1.33266900	C	2.94857400	-0.10477000	1.60487800
H	2.43435600	0.80332600	1.93934500	H	3.67917400	-0.37890200	2.38565000
H	3.49918300	0.14395200	0.69243800	C	1.22682900	-1.50558200	2.55619500
H	0.86121600	-0.59492600	3.03826800	H	0.35539100	-2.10957700	2.29177300
H	1.85068900	-2.04270300	3.29275300	H	1.68284900	-3.09153400	0.72091400
C	3.74660600	-2.92888000	1.31178700	H	4.55217400	-2.18240200	1.28078300
H	3.54122500	-3.12065700	2.37155900	C	4.25482200	-4.20686400	0.63410200
C	4.53819700	-3.94256000	-0.84739500	C	3.28288500	-3.39506200	-1.53618900
H	2.50751800	-4.17140900	-1.50434200	H	3.48665200	-3.20268400	-2.59652400
H	5.36212900	-3.21905800	-0.93890500	H	4.87080000	-4.85953400	-1.35025000
H	5.15612300	-4.56829300	1.14545800	H	3.50154700	-5.00287900	0.72579700

Table S16. 4b with TMEDA and (*R*,*R*)-TMCDA at –78 °C.

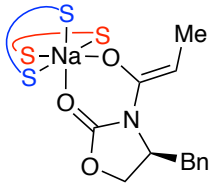


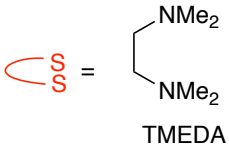
G = –1792.330851
G_{MP2} = –1791.573696

Na	0.00000000	0.00000000	0.00000000	O	-1.86926100	-0.24195900	1.24414300
C	-2.68148500	-1.23374500	1.23376100	N	-3.21443600	-1.62212400	-0.10057900
C	-2.53204700	-1.49551400	-1.26910000	O	-3.36305900	-1.76015700	-2.33009300
C	-4.59521300	-2.30080200	-1.82433400	H	-5.42046900	-1.90691000	-2.42098700
H	-4.56555200	-3.39189100	-1.92800200	C	-4.63853700	-1.86461000	-0.34923300
H	-5.00391600	-2.68100600	0.27868300	C	-5.49406100	-0.60430300	-0.07912000
H	-5.24992000	-0.26907600	0.93515700	H	-5.18211100	0.18676400	-0.77201200
C	-6.97828400	-0.86390200	-0.20608800	C	-7.70193500	-0.43174300	-1.32567100
C	-9.06655200	-0.70272300	-1.44893600	C	-9.73160500	-1.41413700	-0.45009300
C	-9.02396500	-1.84805100	0.67368100	C	-7.66192200	-1.57413100	0.79311100
H	-7.11925400	-1.90529900	1.67621500	H	-9.53537100	-2.39581700	1.46114200
H	-10.7937080	-1.62489500	-0.54268400	H	-9.60903800	-0.35399700	-2.32402300

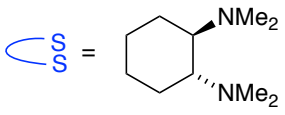
H	-7.19319300	0.13353900	-2.10390200	O	-1.35948800	-1.20237300	-1.46972700
C	-3.16348700	-1.96869000	2.27741600	H	-3.79607200	-2.82877800	2.07666800
C	-2.83160000	-1.66049900	3.71014100	H	-3.71780600	-1.72789200	4.35806200
H	-2.08203900	-2.34487600	4.14141700	H	-2.43107800	-0.64524800	3.80143000
N	-0.86606900	2.39613400	-1.16428400	C	-0.63249000	3.43207400	-0.14740600
H	-1.38425600	4.24070400	-0.23981300	H	0.33694200	3.89652900	-0.35846200
C	-0.66308900	2.93071700	1.29966300	N	0.48077800	2.08879400	1.69180800
C	1.72513900	2.85525300	1.75712800	H	1.98901100	3.26121500	0.77726600
H	1.66485300	3.69568700	2.47545400	H	2.54053000	2.19686400	2.07483100
C	0.20293000	1.49032400	3.00516400	H	-0.67599100	0.84682600	2.92049100
H	1.05850700	0.88211900	3.31634800	H	0.03070200	2.25827900	3.78324500
H	-1.56569000	2.33668100	1.46664100	H	-0.72927500	3.81768600	1.96119400
C	-2.28064200	1.99882300	-1.20381700	H	-2.42308300	1.28129300	-2.01589800
H	-2.55942100	1.50113900	-0.27227600	H	-2.94392500	2.86794200	-1.37895600
C	-0.46222500	2.88591700	-2.48351400	H	0.59993600	3.15356100	-2.47874800
H	-0.61618600	2.09908100	-3.22871700	H	-1.03723700	3.77621800	-2.80276600
N	2.31791100	-0.28163600	-1.20956000	C	2.98570800	1.01780000	-1.28323400
H	2.25010300	1.78300200	-1.55095600	H	3.40335100	1.27698400	-0.30528200
H	3.79965700	1.06034000	-2.02940500	C	1.74618000	-0.63036400	-2.51643300
H	1.20251100	-1.57490500	-2.45788000	H	1.02007400	0.13757800	-2.79976000
H	2.49886700	-0.69451400	-3.32086800	C	3.19347100	-1.32493800	-0.61743800
H	3.62512600	-0.85967800	0.28064600	C	2.40592500	-2.58109900	-0.15703100
N	1.22941700	-2.24997700	0.67713600	C	0.21245800	-3.30601000	0.63804700
H	-0.09423400	-3.47756500	-0.39770700	H	0.56102100	-4.26238000	1.06965600
H	-0.66886500	-2.98263400	1.19960900	C	1.53462800	-1.89278400	2.06418000
H	2.29331400	-1.10353100	2.09718200	H	0.62218000	-1.50840400	2.53005000
H	1.89429800	-2.74052000	2.67367200	H	1.99493000	-3.05386700	-1.05875500
C	3.37151100	-3.60501700	0.49126200	H	3.79433700	-3.17618600	1.40995300
H	2.80599000	-4.49408800	0.79464000	C	4.52699400	-4.00267700	-0.43496300
H	5.18657100	-4.71791400	0.07270800	H	4.13117900	-4.51743600	-1.32283800
C	5.30958100	-2.76126100	-0.87370500	H	5.79356300	-2.30697000	0.00372100
H	6.11462800	-3.03329400	-1.56804800	C	4.37226600	-1.74196400	-1.53305800
H	3.97425300	-2.18323600	-2.45659100	H	4.93900900	-0.85228400	-1.83253600

Table S17. 4b with (*R*,*R*)-TMCDA and TMEDA at –78 °C.

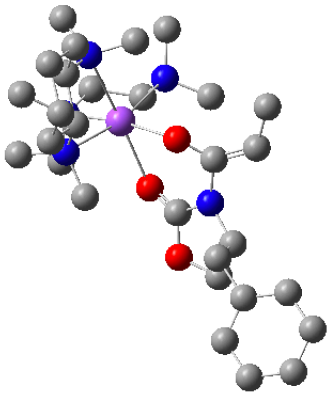




TMEDA



(*R,R*)-TMCDA

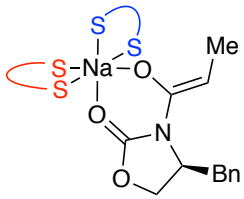


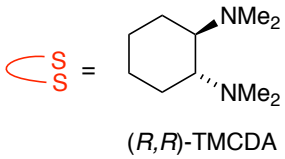
G = –1792.328122
G_{MP2} = –1791.571598

Na	0.00000000	0.00000000	0.00000000	O	-1.77738200	0.77415000	1.18363600
C	-2.82825100	0.15328000	1.56760900	N	-3.56061300	-0.59191200	0.49999300
C	-2.96725300	-1.15678600	-0.58098200	O	-3.91598800	-1.58674100	-1.47381200
C	-5.20931200	-1.48273000	-0.85251300	H	-5.93001200	-1.14538600	-1.60010500
H	-5.50272000	-2.47582700	-0.49254400	C	-5.00963900	-0.48672500	0.30345100
H	-5.54296800	-0.82485600	1.19540600	C	-5.44239700	0.96322700	-0.01932600
H	-5.03431700	1.59754700	0.77557400	H	-4.96939700	1.26854500	-0.96076500
C	-6.94344800	1.12399700	-0.10434600	C	-7.59655200	1.24234700	-1.33858000
C	-8.98651100	1.36067000	-1.40858500	C	-9.74845900	1.36151900	-0.24003100
C	-9.11079200	1.24795300	0.99785600	C	-7.72278000	1.13120200	1.06306200
H	-7.23161400	1.05428900	2.03099000	H	-9.69534900	1.25605500	1.91432200
H	-10.8299460	1.45524400	-0.29169900	H	-9.47188100	1.45608900	-2.37658100
H	-7.00852400	1.25434800	-2.25409400	O	-1.77571400	-1.32629500	-0.82462200
C	-3.41143000	0.09696600	2.79902800	H	-4.27584700	-0.54358600	2.95048700
C	-2.88512700	0.85741600	3.98264100	H	-3.67908500	1.41307800	4.50466000
H	-2.41603500	0.20849800	4.74074600	H	-2.12845600	1.58162700	3.66320600
N	-0.20694100	2.15154900	-1.43294200	C	-1.60056100	1.96118900	-1.85245500
H	-1.67290800	1.03824300	-2.43809100	H	-2.21896700	1.84368000	-0.95964100
H	-1.99061900	2.78697100	-2.47367700	C	0.66270100	2.24503800	-2.60451900
H	1.71068800	2.33777800	-2.30551900	H	0.56243200	1.32386500	-3.18913800
H	0.41965300	3.08643300	-3.27729000	C	-0.06896800	3.26108900	-0.45129300
C	1.31148300	3.26079100	0.26192200	N	1.64805000	1.94933700	0.88080400
C	3.09037300	1.71238800	0.89675900	H	3.49465600	1.78185300	-0.11859900
H	3.65076500	2.41704700	1.53966300	H	3.28615000	0.70129500	1.27114000
C	1.08697300	1.74452100	2.22421000	H	0.00157700	1.86461900	2.20665400
H	1.28713700	0.71087200	2.52444400	H	1.52974700	2.40367700	2.99020200
H	2.07516000	3.42418700	-0.51004300	C	1.41728100	4.44727700	1.25182000
H	2.40937400	4.44000400	1.72105300	H	0.68781300	4.30951600	2.05989600
C	1.15025300	5.80503300	0.59396600	H	1.23013000	6.60478300	1.34132600
H	1.91586200	6.01105200	-0.16898400	C	-0.23452500	5.80465600	-0.05823500
H	-1.00359100	5.69191900	0.71961400	H	-0.43129600	6.76231700	-0.55711200

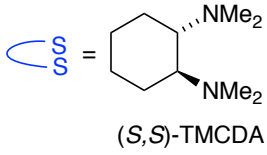
C	-0.34688000	4.65666400	-1.06814200	H	0.36940800	4.84323400	-1.88068000
H	-1.34286800	4.66051200	-1.52507800	H	-0.83524600	3.05540400	0.30649600
N	0.72186400	-2.19221100	1.40165200	C	-0.52485400	-2.56100500	2.08527300
H	-1.33959200	-2.58764800	1.36050700	H	-0.45072300	-3.54755300	2.58102600
H	-0.77298100	-1.80622400	2.83605400	C	1.81367900	-2.14865200	2.37539200
H	2.73664300	-1.78223800	1.91640800	H	1.54962000	-1.46516300	3.18804000
H	2.02024000	-3.14177000	2.81912500	C	1.00123000	-3.14192700	0.31353800
H	0.06698100	-3.29378200	-0.23415900	H	1.29857600	-4.12839500	0.72183300
C	2.09323000	-2.68361300	-0.65728700	N	1.70913300	-1.55332300	-1.51802700
C	2.90651800	-0.92036200	-2.07535000	H	2.61591600	-0.07045500	-2.69948500
H	3.54238000	-0.54852600	-1.26601900	H	3.50514600	-1.61316800	-2.69717600
C	0.82906500	-1.99284600	-2.60883400	H	-0.11257200	-2.37480600	-2.21329800
H	0.58737700	-1.13588700	-3.24535100	H	1.30822400	-2.76676900	-3.23827200
H	2.98325800	-2.38684700	-0.09261800	H	2.39631300	-3.55376100	-1.27137700

Table S18. 4a with (*S*,*S*)-TMCDA and (*R*,*R*)-TMCDA at –78 °C.

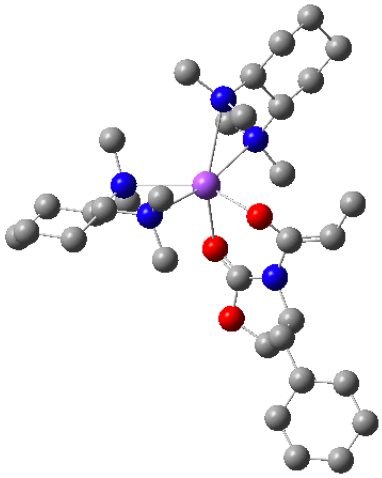




(*R*,*R*)-TMCDA



(*S*,*S*)-TMCDA

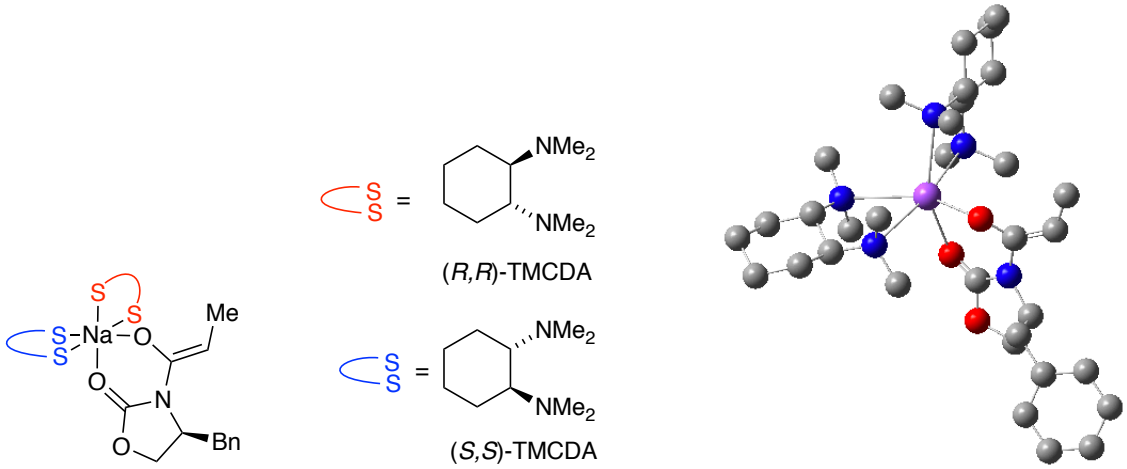


G = –1947.826333
G_{MP2} = –1946.976201

Na	0.00000000	0.00000000	0.00000000	O	1.64695400	-1.15654000	-1.00285300
C	2.54052600	-1.87041700	-0.43009600	N	3.33702700	-1.18733400	0.62996300
C	2.85890900	-0.20865600	1.44012000	O	3.88363700	0.35164900	2.16087600
C	5.06783400	-0.44150800	1.96860100	H	5.92803200	0.22730000	1.89742200
H	5.19314100	-1.09584300	2.83926400	C	4.80110200	-1.24060000	0.68039400
H	5.14233700	-2.27272400	0.79363800	C	5.44401100	-0.63901200	-0.59160600
H	4.98687800	-1.14899000	-1.44695800	H	5.17066800	0.42140000	-0.65612700
C	6.94690200	-0.80243700	-0.62304400	C	7.80497300	0.27319000	-0.35774400
C	9.19153600	0.10496500	-0.36048100	C	9.74383200	-1.14762400	-0.62893400
C	8.90072400	-2.22858000	-0.89850200	C	7.51714400	-2.05569700	-0.89592000
H	6.86620800	-2.89889900	-1.11801900	H	9.32211500	-3.20656500	-1.11685600
H	10.8224010	-1.28080700	-0.63362900	H	9.83864200	0.95433300	-0.15671500
H	7.38220000	1.25598900	-0.15915500	O	1.71040000	0.19343800	1.59630000
C	2.90935500	-3.16221300	-0.67386100	H	3.65400100	-3.63399500	-0.03891200
C	2.31173700	-3.97519000	-1.78711700	H	3.07953900	-4.52423700	-2.35230300
H	1.58850700	-4.73229600	-1.43917300	H	1.78455200	-3.32248500	-2.49132400
N	-1.15658500	-2.08295700	1.27535600	C	-2.11937400	-1.56238600	2.24630600
H	-2.48693500	-2.31885900	2.96185500	H	-1.63314800	-0.77580100	2.83200600
H	-2.98419900	-1.12238900	1.74062500	C	0.01845100	-2.61379400	1.98015100
H	0.50019200	-1.79760100	2.52551900	H	-0.23191000	-3.41173000	2.70184800
H	0.74150700	-3.00258500	1.25715100	C	-1.71813700	-3.06512000	0.31316800
H	-0.85643600	-3.41432400	-0.2699120	C	-2.72946100	-2.42934800	-0.67848000
H	-3.58490700	-2.07187300	-0.08887700	N	-2.19415500	-1.22459500	-1.36544000
C	-3.26691000	-0.35743800	-1.85163300	H	-2.83223700	0.56880100	-2.24377300
H	-3.87348600	-0.80517900	-2.66016800	H	-3.93954100	-0.09290700	-1.02877000
C	-1.25358900	-1.52125500	-2.45483600	H	-0.86467000	-0.57707000	-2.84360100
H	-0.39468300	-2.08344500	-2.08325600	H	-1.71580800	-2.05872500	-3.30006100
C	-3.27324700	-3.50376300	-1.65535000	H	-3.99819200	-3.04202200	-2.33696900
H	-2.45013100	-3.87460700	-2.27906800	C	-3.90681000	-4.70082300	-0.93850700
H	-4.27014200	-5.42909700	-1.67473700	H	-4.78477500	-4.37205200	-0.36248000
C	-2.88731000	-5.34218500	0.00621100	C	-2.35529200	-4.30228900	0.99913800
H	-1.61937700	-4.76556900	1.66563500	H	-3.18999000	-3.97595100	1.63470900
H	-3.33436200	-6.18412300	0.55011100	H	-2.05501700	-5.75513200	-0.58210700
N	-0.97851800	2.35421700	0.97597400	C	-0.30297300	3.54870600	0.40378800
C	-0.04701000	3.42955500	-1.12342000	N	0.64284500	2.17023800	-1.48554800
C	0.49575800	1.83826500	-2.90281300	H	1.01408600	2.54127900	-3.58043200
H	0.91477500	0.84184100	-3.07281200	H	-0.56528800	1.82536700	-3.17771400
C	2.06643600	2.11794500	-1.12171600	H	2.20046500	2.37409400	-0.06820800
H	2.40561000	1.08774100	-1.26080000	H	2.69362900	2.78958600	-1.73369400
H	-1.02823600	3.37879900	-1.61802000	C	0.66617100	4.70237500	-1.64894600
C	-0.08042200	5.99842000	-1.31320300	C	-0.28865200	6.11291700	0.19929700
C	-1.03053600	4.87913500	0.72573900	H	-2.03243900	4.86291600	0.27562900

H	-1.17808200	4.96211900	1.80912300	H	-0.85035400	7.02225600	0.44836900
H	0.68818100	6.20147100	0.69705400	H	-1.05785300	6.00888600	-1.81814400
H	0.47772300	6.86217000	-1.69637700	H	1.67070600	4.75820400	-1.20961400
H	0.80650600	4.61840700	-2.73329700	H	0.67681700	3.58406700	0.89658900
C	-2.41245300	2.27619000	0.69122600	H	-2.59425700	2.39697900	-0.38029300
H	-2.77837900	1.28503200	0.97910200	H	-3.01738500	3.02544800	1.23123800
C	-0.73071300	2.23864800	2.41666900	H	-1.22039700	1.33534300	2.79308700
H	0.34156100	2.13239100	2.59616200	H	-1.12081600	3.09087300	3.00159200

Table S19. 4a with (*R*,*R*)-TMCDA and (*S*,*S*)-TMCDA at –78 °C.

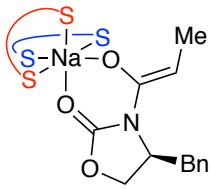


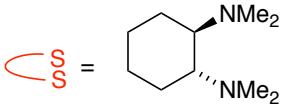
G = –1947.826796
G_{MP2} = –1946.977177

Na	0.00000000	0.00000000	0.00000000	O	1.69945200	-1.00390700	-1.07507100
C	2.63693200	-1.72665200	-0.58944900	N	3.36786100	-1.14743600	0.57661800
C	2.81772300	-0.30837600	1.49143000	O	3.79188300	0.20250500	2.31223000
C	5.02003400	-0.50284700	2.06280400	H	5.84625800	0.20998700	2.10230300
H	5.15576600	-1.25308600	2.85052200	C	4.83065000	-1.14756600	0.67765500
H	5.21251100	-2.17160600	0.67990700	C	5.49156400	-0.37045000	-0.48522800
H	5.08270700	-0.78563700	-1.41320200	H	5.18042600	0.67976700	-0.42816100
C	6.99989100	-0.47558100	-0.47926400	C	7.80502200	0.58903000	-0.05232400
C	9.19656900	0.47246500	-0.02344000	C	9.80747900	-0.71654400	-0.42232400
C	9.01779500	-1.78520900	-0.85392600	C	7.62898600	-1.66387800	-0.88231800
H	7.02056300	-2.49561000	-1.23152000	H	9.48515000	-2.71269400	-1.17495100
H	10.8901170	-0.80924800	-0.40280000	H	9.80175900	1.31284900	0.30705500
H	7.33694300	1.52384800	0.24961700	O	1.64539500	0.01035800	1.66518900
C	3.10187800	-2.93834100	-1.00972000	H	3.86244000	-3.45233300	-0.42924100
C	2.56381700	-3.62286600	-2.23469300	H	3.35944900	-4.12757100	-2.80125000
H	1.80724300	-4.39484000	-2.01183800	H	2.09080300	-2.89447500	-2.90308400
N	0.88404400	2.35513000	-1.01477800	C	0.32194400	3.62516500	-0.50980400

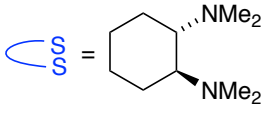
C	-1.16009400	3.49336200	-0.06928600	N	-1.39125500	2.33124500	0.82743900
C	-2.81623400	2.09837100	1.06225700	H	-3.35581600	2.10485200	0.10999600
H	-2.95032400	1.11358400	1.52258600	H	-3.28891600	2.84200700	1.72815100
C	-0.67368500	2.39167900	2.10641800	H	-0.89153900	1.48124800	2.67223500
H	0.40502100	2.41098200	1.94444200	H	-0.96378000	3.25147800	2.73498400
C	-1.65867100	4.84374900	0.50870100	C	-1.47052800	6.01648600	-0.46262000
C	-0.00311400	6.14259000	-0.88194100	C	0.49229400	4.82090600	-1.47933100
H	1.54782700	4.90417400	-1.76532300	H	-0.06693800	4.62507700	-2.40423200
H	0.12494000	6.95634000	-1.60704400	H	0.60597400	6.40597800	-0.00461700
H	-1.82429600	6.94564200	0.00198800	H	-2.09204900	5.85851400	-1.35664200
H	-2.71643700	4.76022100	0.78354100	H	-1.11290100	5.06600900	1.43571000
H	-1.75732600	3.28341900	-0.96939200	H	0.90422200	3.86203100	0.39012800
C	2.33921100	2.28283400	-0.86300900	H	2.61039800	2.46841500	0.18109900
H	2.65465600	1.26990100	-1.12570800	H	2.88233700	3.00488900	-1.50120100
C	0.51479200	2.01321400	-2.39004600	H	0.85568300	0.99286200	-2.58966700
H	-0.57280400	2.05113900	-2.51669600	H	0.96817800	2.67593000	-3.14862100
N	-1.86997100	-1.24976200	-1.51915800	C	-2.97821400	-0.31273700	-1.71266800
H	-2.57032900	0.67884400	-1.93796600	H	-3.65691000	-0.58763200	-2.53866900
H	-3.57066800	-0.22777900	-0.79757400	C	-1.12673200	-1.43271000	-2.77200100
H	-0.88616300	-0.45073200	-3.18964600	H	-0.18161300	-1.93907300	-2.56422400
H	-1.69439000	-1.98894400	-3.53959500	C	-2.26958900	-2.55721500	-0.93196900
C	-2.44193800	-2.49919200	0.61063700	N	-1.24125100	-1.95408900	1.29196700
C	-0.08173500	-2.85862800	1.30371700	H	0.18600500	-3.16360800	0.29047200
H	0.77190500	-2.31361200	1.70984100	H	-0.24073500	-3.75852000	1.92177200
C	-1.52520900	-1.50937700	2.65759700	H	-0.64891800	-0.97928900	3.04470300
H	-2.37771100	-0.82094000	2.65855100	H	-1.75410000	-2.33427100	3.35666400
H	-3.25013100	-1.78454800	0.82571200	C	-2.88672100	-3.88020100	1.15865000
H	-2.07198000	-4.60175800	1.01615000	H	-3.05010300	-3.80631300	2.24044000
C	-4.14042000	-4.43415400	0.47252700	C	-3.91306800	-4.53671700	-1.03804000
C	-3.52650200	-3.16538400	-1.60324400	H	-4.37882700	-2.48795700	-1.45969300
H	-3.36219200	-3.23343700	-2.68542000	H	-4.81258600	-4.90951800	-1.54432300
H	-3.11431700	-5.26521800	-1.23996300	H	-4.39660900	-5.41326900	0.89674600
H	-4.99848900	-3.77363500	0.66791600	H	-1.43068700	-3.23306900	-1.13818800

Table S20. 4b with (*S*,*S*)-TMCDA and (*R*,*R*)-TMCDA at –78 °C.

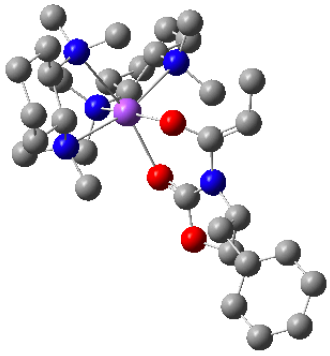




(*R,R*)-TMCDA



(*S,S*)-TMCDA

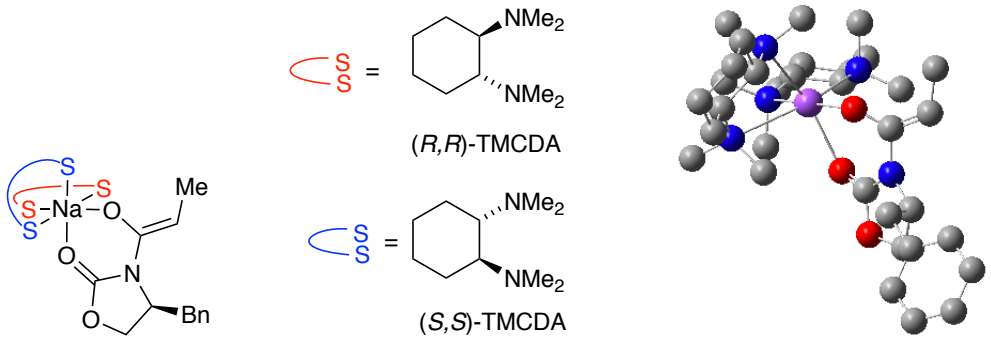


G = –1947.825274
G_{MP2} = –1946.975833

Na	0.00000000	0.00000000	0.00000000	O	-1.90357100	0.15445500	1.18586500
C	-2.69249500	-0.80929100	1.48135900	N	-3.22219000	-1.58657700	0.32447200
C	-2.53922900	-1.80679100	-0.82813000	O	-3.35846600	-2.39625000	-1.75780700
C	-4.58911800	-2.77129800	-1.11618300	H	-5.41509800	-2.57140400	-1.80187600
H	-4.55526700	-3.84540300	-0.89935400	C	-4.63920300	-1.92499200	0.16943500
H	-4.98150500	-2.53252800	1.01127100	C	-5.52655300	-0.66180300	0.07196200
H	-5.29049300	-0.04272000	0.94481500	H	-5.23573200	-0.09571000	-0.82161200
C	-7.00367400	-0.98355700	0.03716600	C	-7.73910200	-0.90932500	-1.15339100
C	-9.09627600	-1.23799100	-1.18257900	C	-9.74182100	-1.64890800	-0.01616000
C	-9.02231700	-1.72413500	1.17904300	C	-7.66785800	-1.39362200	1.20378100
H	-7.11648200	-1.44295400	2.14055700	H	-9.51869600	-2.03531200	2.09472800
H	-10.7981240	-1.90369900	-0.03560900	H	-9.64829300	-1.16890000	-2.11647900
H	-7.24544200	-0.57897700	-2.06509400	O	-1.36886400	-1.56828000	-1.10668800
C	-3.15083000	-1.21779400	2.70028200	H	-3.77541500	-2.10429900	2.76642800
C	-2.80730300	-0.50275900	3.97589500	H	-3.70072400	-0.26719200	4.57436400
H	-2.14403700	-1.08890400	4.63325700	H	-2.29726400	0.44059400	3.75526900
N	2.04249100	-1.05987300	-1.30737500	C	2.53733500	-2.33676700	-0.72853000
C	2.62412400	-2.30912300	0.82177900	N	1.35833900	-1.86960300	1.46037300
C	0.27587200	-2.86462500	1.41690800	H	0.07748000	-3.16814700	0.38706300
H	0.48912700	-3.76151400	2.02331200	H	-0.63848700	-2.40859700	1.80688700
C	1.56236600	-1.43892400	2.84504200	H	2.35120500	-0.67950100	2.88993300
H	0.63358300	-0.99811500	3.21963400	H	1.84137900	-2.26029400	3.52972600
H	3.36762800	-1.54662000	1.09559400	C	3.14474000	-3.66939500	1.35284800
C	4.48296400	-4.09089400	0.73524600	C	4.36288900	-4.15185800	-0.78975700
C	3.88697600	-2.80089700	-1.33537500	H	4.66013500	-2.05251700	-1.11460500
H	3.80012700	-2.84500500	-2.42755500	H	5.32307400	-4.42223200	-1.24724600
H	3.64901400	-4.94057500	-1.06906300	H	5.26753300	-3.37056400	1.01131000
H	4.79350400	-5.06185900	1.14155600	H	3.23115100	-3.62398900	2.44479900
H	2.40473900	-4.44933900	1.13168400	H	1.78086500	-3.08439400	-0.99869000
C	3.03161500	0.02073900	-1.32362900	H	2.52841600	0.95959700	-1.57661500
H	3.47825300	0.14262300	-0.33297700	H	3.84550500	-0.13131900	-2.05387500
C	1.47844700	-1.26002100	-2.64657000	H	0.64607600	-1.96504900	-2.59237500

H	1.08116800	-0.30819500	-3.01296800	H	2.21714200	-1.61549900	-3.38709300
N	0.97217700	2.54426700	0.98558900	C	2.40443900	2.80892200	1.10654700
H	2.82492200	3.06466700	0.12812300	H	2.65109100	3.62583100	1.81028500
H	2.90992500	1.90533600	1.46542900	C	0.42864600	2.11566500	2.28154900
H	-0.62375300	1.83771300	2.18720700	H	0.96855100	1.22050900	2.60125100
H	0.54701700	2.86964600	3.07884500	C	0.25131500	3.68737400	0.36725100
C	-1.04897300	3.26136700	-0.36749200	N	-0.82113800	2.17615200	-1.35941300
C	-2.08491300	1.58344900	-1.81447500	H	-1.86631100	0.69164100	-2.40974000
H	-2.65758000	1.26914300	-0.93868500	H	-2.69363200	2.26591500	-2.43384600
C	-0.00136500	2.55584500	-2.50946300	H	0.97235300	2.93543200	-2.18592300
H	0.17407000	1.66677700	-3.12406600	H	-0.46722400	3.31380500	-3.16357300
H	-1.72329300	2.81997100	0.37695800	C	-1.74603500	4.50660800	-0.97832800
H	-1.11846600	4.91544500	-1.78228500	H	-2.68931100	4.20269700	-1.44547600
C	-2.00885900	5.62527300	0.03658000	H	-2.48967600	6.47645900	-0.46246200
H	-2.71261500	5.27354700	0.80488600	C	-0.70030800	6.05255200	0.70527100
C	-0.03587200	4.83965000	1.36351600	H	-0.70098700	4.47562500	2.15662600
H	0.90022400	5.13680600	1.85280500	H	-0.88008800	6.83424900	1.45439800
H	-0.02737200	6.48805200	-0.04848600	H	0.93624400	4.08864800	-0.39152600

Table S21. 4b with (*R*,*R*)-TMCDA and (*S*,*S*)-TMCDA at –78 °C.

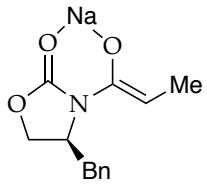


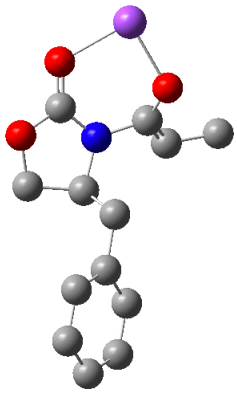
G = –1947.825101
G_{MP2} = –1946.975146

Na	0.00000000	0.00000000	0.00000000	O	-1.92415900	-0.10640600	1.16071600
C	-2.66552900	-1.12883300	1.38047300	N	-3.07815500	-1.89652400	0.17297200
C	-2.31335700	-2.04140100	-0.93847100	O	-3.04071700	-2.63516600	-1.93915400
C	-4.29267600	-3.08553100	-1.39247800	H	-5.07931700	-2.90376200	-2.12760400
H	-4.22148500	-4.16270200	-1.20158600	C	-4.46719500	-2.28044400	-0.09229400
H	-4.84587900	-2.92311200	0.70664500	C	-5.38952500	-1.04511500	-0.22017000
H	-5.23747200	-0.44483600	0.68393200	H	-5.05516800	-0.44402900	-1.07484200
C	-6.84865200	-1.41247500	-0.36968400	C	-7.49893000	-1.33206900	-1.60849000
C	-8.83914200	-1.70168300	-1.74269400	C	-9.55291900	-2.16004100	-0.63520300
C	-8.91884300	-2.24185400	0.60704800	C	-7.58100100	-1.87069500	0.73659200
H	-7.09653500	-1.92568800	1.70936600	H	-9.46921100	-2.58981100	1.47749000
H	-10.5963450	-2.44642200	-0.73673100	H	-9.32494200	-1.62712200	-2.71230100
H	-6.95276900	-0.96419400	-2.47475100	O	-1.14160900	-1.73360800	-1.13159400

C	-3.16962300	-1.60219600	2.55568500	H	-3.72965900	-2.53332000	2.55637900
C	-2.95745000	-0.90820700	3.87103500	H	-3.89089400	-0.82561800	4.44774000
H	-2.23710400	-1.42743200	4.52465900	H	-2.57615000	0.10570000	3.71043400
N	2.27651900	-0.36356800	-1.30008500	C	2.90566700	0.92016400	-1.61480500
H	2.13507800	1.62406800	-1.94367300	H	3.38061600	1.33239700	-0.71911100
H	3.66915000	0.85692700	-2.41170500	C	1.62258200	-0.90292000	-2.50053900
H	1.13540200	-1.85390300	-2.28068500	H	0.83718900	-0.20894600	-2.81539100
H	2.31274600	-1.03374300	-3.35122100	C	3.22427600	-1.30272300	-0.64423600
H	3.78612000	-0.69129700	0.07570900	C	2.50412300	-2.41875700	0.16075900
N	1.50472100	-1.88167900	1.11703600	C	0.50744600	-2.89041100	1.49624900
H	0.05491000	-3.30766900	0.59380100	H	0.92971000	-3.71302000	2.10134700
H	-0.29028400	-2.41507000	2.07488800	C	2.07189800	-1.26707800	2.31859200
H	2.79896100	-0.49316100	2.05117000	H	1.26237800	-0.79289100	2.88162400
H	2.56707200	-1.98481300	2.99545100	H	1.92218500	-3.01265800	-0.55595800
C	3.54309600	-3.36644500	0.81331600	H	4.11224200	-2.81388800	1.57318900
H	3.01772100	-4.17020200	1.34259800	C	4.53896400	-3.95852300	-0.19078800
H	5.25314800	-4.60867900	0.33031000	H	4.00768200	-4.59346100	-0.91492100
C	5.26810100	-2.83726000	-0.93660600	H	5.87545400	-2.25915200	-0.22420400
H	5.96379000	-3.24924300	-1.67856400	C	4.25405300	-1.91715400	-1.62500600
H	3.72311900	-2.50276800	-2.38694900	H	4.77447000	-1.11227600	-2.15839600
N	-0.99347400	2.27385200	-1.75383100	C	-1.25521600	3.46132400	-0.90214000
H	-0.46290000	4.17973700	-1.15266400	C	-1.14283800	3.16627900	0.61982300
N	0.13708700	2.49705000	0.98930600	C	1.34044800	3.28820800	0.73410600
H	1.40352300	3.56931300	-0.32000600	H	1.41148400	4.20551400	1.34480300
H	2.21835300	2.67502700	0.96501500	C	0.12388900	2.03583700	2.38325700
H	-0.73815000	1.38027400	2.53276900	H	1.03566100	1.45764600	2.56990200
H	0.10541300	2.85424000	3.12385700	H	-1.91892300	2.43741000	0.88445900
C	-1.40213300	4.46950600	1.42242700	H	-1.37015600	4.25132200	2.49511200
H	-0.59290200	5.18699600	1.22579900	C	-2.73671000	5.14255600	1.07905900
C	-2.81465500	5.44532200	-0.41896300	C	-2.60175600	4.15787300	-1.22162900
H	-2.65439700	4.36759800	-2.29741200	H	-3.42760600	3.47146200	-0.99572300
H	-3.78254500	5.89369100	-0.67746000	H	-2.04482800	6.18507200	-0.68528400
H	-2.85492000	6.05986200	1.67006900	H	-3.56791000	4.47929600	1.35937500
C	-2.13731400	1.36406500	-1.89300300	H	-1.80340300	0.45501100	-2.40257800
H	-2.50471200	1.06880800	-0.90633200	H	-2.96767300	1.79236500	-2.48204000
C	-0.49126000	2.64993900	-3.07340600	H	0.41114500	3.26384000	-2.97482300
H	-0.22681600	1.74499500	-3.63162500	H	-1.22058100	3.21109600	-3.68767100

Table S22. 2 at –78 °C.

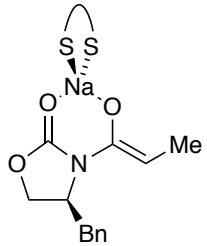


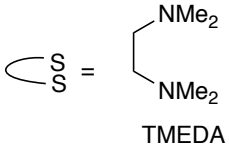


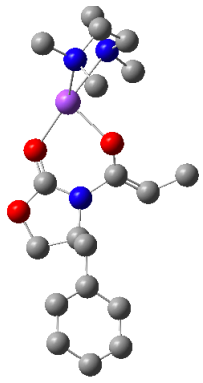
G = –943.7474627
G_{MP2} = –943.5222257

C	0.00000000	0.00000000	0.00000000	O	1.18017500	-0.70637600	-0.43182600
C	2.14058700	0.20809700	-0.74752200	N	1.62996000	1.46102200	-0.73748800
C	2.35042600	2.68299700	-1.19767700	C	2.08244800	3.80758500	-0.48290500
H	1.45745400	3.73747300	0.40319200	C	2.64361500	5.15001700	-0.85455000
H	1.85643800	5.90649700	-0.99623000	H	3.32307800	5.55074500	-0.08636900
H	3.20692700	5.07310400	-1.78963300	O	3.09829700	2.53515500	-2.23617200
Na	4.54213000	1.03633300	-2.27962100	O	3.29221700	-0.17053600	-0.98427300
C	0.17521500	1.42664500	-0.55066600	H	-0.12857500	2.16689700	0.19347000
C	-0.57780900	1.70256100	-1.87271600	H	-0.18341700	2.64261000	-2.27449100
H	-0.32954800	0.91133300	-2.59078200	C	-2.07549300	1.79717800	-1.68366300
C	-2.92540300	0.74616100	-2.05323600	C	-4.30426500	0.83014000	-1.84701300
C	-4.85632200	1.97136100	-1.26490200	C	-4.02148400	3.02871900	-0.89497000
C	-2.64556500	2.94109800	-1.10371700	H	-2.00268300	3.77330500	-0.82388600
H	-4.44358800	3.92550700	-0.44873800	H	-5.92908800	2.04015300	-1.10555600
H	-4.94582400	0.00518200	-2.14598000	H	-2.50416500	-0.14208800	-2.51971300
H	-0.87632200	-0.51785600	-0.39406300	H	-0.03024700	-0.01905900	1.09509300

Table S23. 11 at –78 °C.



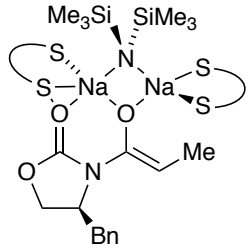


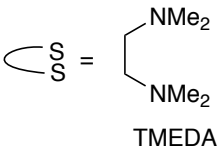


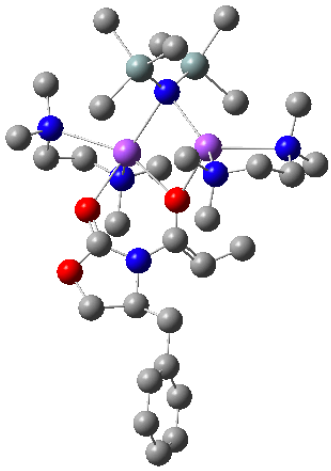
G = –1290.294396
G_{MP2} = –1289.850469

Na	0.00000000	0.00000000	0.00000000	O	1.41962900	-1.10296800	-1.20598700
C	2.43912000	-1.75050200	-0.76959900	N	3.26313100	-1.05607500	0.25846400
C	2.78783300	-0.19054200	1.18990500	O	3.82311900	0.40395000	1.85839900
C	5.04700900	-0.25482300	1.48675500	H	5.83613400	0.49553500	1.40878800
H	5.30748900	-0.97237400	2.27349500	C	4.72302400	-0.95181700	0.15536900
H	5.17618500	-1.94538400	0.12219300	C	5.14985900	-0.15986600	-1.10308000
H	4.65075100	-0.63148800	-1.95695200	H	4.76377600	0.86372000	-1.02078000
C	6.64771200	-0.14620800	-1.31005800	C	7.41624000	0.98696500	-1.01143900
C	8.80290200	0.98019900	-1.17866000	C	9.44542500	-0.16561300	-1.64819500
C	8.69170300	-1.30180700	-1.95298900	C	7.30740300	-1.29011000	-1.78583000
H	6.72503600	-2.17465700	-2.03575700	H	9.18259600	-2.19665400	-2.32706300
H	10.5240150	-0.17293800	-1.78096500	H	9.37890800	1.87208600	-0.94537900
H	6.92152700	1.88860100	-0.65590900	O	1.62851300	0.09448500	1.48592400
C	2.90791800	-2.97159300	-1.15037100	H	3.75411200	-3.40736700	-0.62727400
C	2.27919700	-3.76408800	-2.26087100	H	3.02623900	-4.12930900	-2.98186500
H	1.73534600	-4.65391300	-1.90422600	H	1.56432600	-3.14068000	-2.80855000
N	-1.98775300	-1.39354800	-0.39006700	C	-3.23550800	-1.31188600	0.37290800
H	-4.01434100	-1.98906300	-0.02377900	H	-3.04187600	-1.58597900	1.41462400
H	-3.63193600	-0.29261500	0.36473000	C	-1.42220100	-2.74995000	-0.29775700
H	-1.28300200	-3.01303100	0.75599700	H	-2.08118100	-3.50790300	-0.75821700
H	-0.44615100	-2.76534400	-0.79020300	C	-2.17298300	-1.01941300	-1.80449000
H	-1.27770700	-1.34337500	-2.34432600	H	-3.02873900	-1.56524800	-2.24528200
C	-2.39549900	0.48136300	-2.03058300	H	-3.22130300	0.82893400	-1.40109300
H	-2.72096300	0.62854300	-3.07713000	N	-1.21879000	1.31902900	-1.73103800
C	-1.62098400	2.71382000	-1.51914000	H	-0.74080300	3.31387400	-1.26744800
H	-2.09592700	3.15995300	-2.41173100	H	-2.32852500	2.77619100	-0.68572100
C	-0.21617900	1.24173400	-2.80844000	H	0.61291900	1.91655600	-2.57469900
H	0.20128200	0.23488600	-2.87669400	H	-0.64253300	1.53750500	-3.78420200

Table S24. 6a with TMEDA at –78 °C.





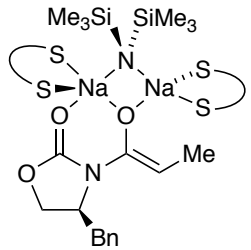


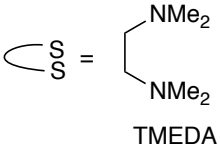
G = –2669.984607
G_{MP2} = –2669.100098

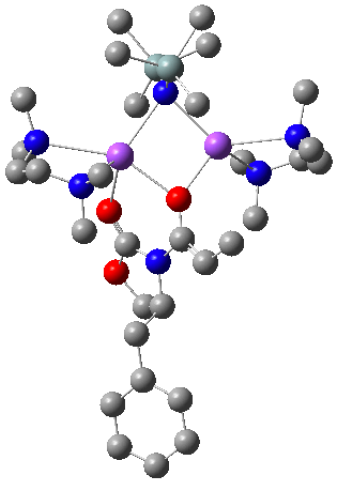
Na	0.00000000	0.00000000	0.00000000	O	-1.94008200	-0.80476400	-1.04180900
C	-3.10723600	-0.46569600	-0.91851400	O	-4.07451800	-1.04083700	-1.69302900
C	-5.33286300	-0.40496500	-1.42522300	C	-5.13186900	0.33756600	-0.09218700
N	-3.66653800	0.44112500	-0.05925100	C	-2.88622100	1.08323200	1.01841500
C	-3.48506100	1.18287600	2.23957200	H	-4.46610400	0.74488200	2.39676700
C	-2.82817800	1.84919700	3.41579600	H	-2.73829600	1.17469400	4.28079100
H	-1.81838100	2.17799900	3.15169500	H	-3.38731200	2.72923500	3.77371100
O	-1.71481200	1.48858100	0.66526500	Na	-0.39627000	3.19372900	0.20684400
N	1.59133100	1.93211600	-0.27569300	Si	2.69845400	2.01640800	1.02471400
C	3.98504700	3.43065200	0.93612700	H	4.60199600	3.46476700	1.84417600
H	4.66605300	3.31085400	0.08403900	H	3.50230500	4.41061000	0.82709800
C	1.76074900	2.30059100	2.66768400	H	2.41933900	2.16881600	3.53628000
H	1.36115300	3.32203600	2.72231600	H	0.91281000	1.61442200	2.78512100
C	3.73034200	0.42909800	1.29287500	H	3.08446200	-0.44059800	1.47068800
H	4.34689400	0.20203300	0.41428000	H	4.40257400	0.52358000	2.15628300
Si	1.99700500	2.19344200	-1.91703200	C	3.60038000	1.36409200	-2.54442500
H	3.76078700	1.56837500	-3.61148600	H	4.48324700	1.73057800	-2.00539500
H	3.57309600	0.27476600	-2.41819300	C	0.59463200	1.54863600	-3.04274200
H	0.52774200	0.45356200	-3.01677100	H	-0.38742600	1.92987300	-2.73290700
H	0.74831000	1.84101400	-4.08992700	C	2.21747400	4.04765400	-2.35325400
H	1.35183200	4.64216800	-2.03012600	H	3.10031300	4.46341400	-1.85161100
H	2.34320900	4.20641700	-3.43294200	N	-1.86692800	4.74867800	-1.29340400
C	-1.65793200	4.78031900	-2.74557100	H	-1.70213900	3.76411100	-3.14576400
H	-2.42043900	5.39222100	-3.26233400	H	-0.67063000	5.19110200	-2.97303200
C	-3.16946000	4.13820000	-1.00244800	H	-4.00527800	4.72427200	-1.42993700
H	-3.19207500	3.12875000	-1.41962700	H	-3.32469200	4.04026000	0.07421100
C	-1.76705900	6.11086500	-0.74963300	H	-2.61091600	6.73752500	-1.09966000
H	-0.85795600	6.56388200	-1.15939100	C	-1.74225700	6.18980900	0.77848100
N	-0.61557700	5.49215300	1.41976500	C	0.65822100	6.17837900	1.16654200

H	0.64436700	7.22469400	1.52459400	H	1.46480700	5.64826300	1.68020800
H	0.89240500	6.17997900	0.09888900	C	-0.85454300	5.40966200	2.86677600
H	-0.02479800	4.88600800	3.34857100	H	-0.95060300	6.40827800	3.33135700
H	-1.77081800	4.84443700	3.06044600	H	-1.74645900	7.26126900	1.05780800
H	-2.66564100	5.76337100	1.18329600	H	-5.47763600	-0.28782700	0.74381200
C	-5.86623900	1.68923300	-0.03788700	H	-5.54419600	2.21096600	0.86891900
H	-5.54317000	2.29541000	-0.89248700	C	-7.37187800	1.52499800	-0.05444500
C	-8.05272100	1.07149200	1.08584300	C	-9.43565600	0.89226600	1.07118800
C	-10.1668210	1.16719900	-0.08677400	C	-9.50422700	1.62460200	-1.22609600
C	-8.11910700	1.80086200	-1.20738700	H	-7.61205000	2.16692200	-2.09770700
H	-10.0642750	1.84842000	-2.13031300	H	-11.2448180	1.03101900	-0.09808200
H	-9.94392800	0.54357300	1.96642000	H	-7.49368900	0.86654000	1.99646000
H	-5.55399500	0.28959800	-2.24484100	H	-6.10951900	-1.17038200	-1.38763200
N	-0.11132300	-1.83810200	1.89965200	C	0.39688100	-1.37258000	3.19353000
H	1.44269600	-1.06612800	3.09835200	H	-0.18621600	-0.50740900	3.52213400
H	0.33082700	-2.15110000	3.97716900	C	-1.53518000	-2.17207500	2.03075000
H	-2.09047300	-1.28598400	2.35179200	H	-1.94214600	-2.48392200	1.06705700
H	-1.69882700	-2.98476800	2.76443000	C	0.66754100	-2.99481600	1.43083500
H	0.41874800	-3.89663400	2.02393700	H	1.72493800	-2.78387800	1.62078600
C	0.46874500	-3.32719700	-0.05158400	N	1.06135600	-2.35043300	-0.97736700
C	2.52101700	-2.46996600	-1.01604300	H	2.92822200	-1.72581300	-1.70522200
H	2.95588700	-2.27764400	-0.03311700	H	2.84644500	-3.47330000	-1.35286900
C	0.51780800	-2.55311800	-2.32642800	H	-0.55916200	-2.37245100	-2.31781800
H	0.98171400	-1.84053900	-3.01537300	H	0.71666400	-3.57321300	-2.70675700
H	0.88254400	-4.33860100	-0.23535500	H	-0.60060800	-3.38337900	-0.27429000

Table S25. 6b with TMEDA at –78 °C.







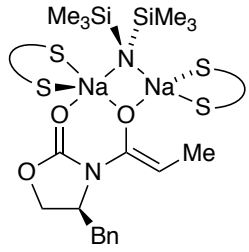
G = –2669.985141

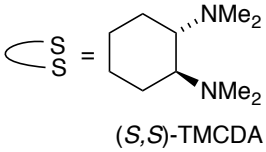
G_{MP2} = –2669.100814

Na	0.00000000	0.00000000	0.00000000	O	1.85936200	0.12450500	-1.40781900
C	2.86876500	0.80407000	-1.30523900	O	3.83482100	0.74729900	-2.27805000
C	4.83085500	1.74667600	-1.99494100	C	4.69491800	1.97787100	-0.48608300
N	3.27312100	1.65555900	-0.31112000	C	2.43189800	2.12116100	0.80116500
C	3.06005900	2.73979900	1.84420700	H	4.13733200	2.85516800	1.84846400
C	2.31223700	3.26740400	3.03597100	H	2.71762800	2.87776800	3.98190600
H	2.35409700	4.36649600	3.11936800	H	1.25829800	2.97725600	2.98615000
O	1.16835700	1.91536100	0.65049500	Na	-0.63050800	3.11944900	0.14835200
N	-2.16392600	1.28471200	-0.10859700	Si	-2.86409300	1.28842900	-1.66961700
C	-4.20696700	-0.03169300	-2.00301500	H	-4.55727300	0.01622000	-3.04279900
H	-3.82953800	-1.04758700	-1.82989500	H	-5.08376500	0.10164000	-1.35703400
C	-3.69825500	2.95634700	-2.11466600	H	-4.08159200	2.96640800	-3.14392700
H	-4.54158700	3.16419100	-1.44385800	H	-2.99275500	3.79376200	-2.01871800
C	-1.52443800	1.00358900	-2.99916600	H	-0.66629200	1.67564100	-2.87332200
H	-1.12923800	-0.01897400	-2.95626700	H	-1.92047200	1.15736100	-4.01175300
Si	-3.02499600	1.04118500	1.34839800	C	-3.35395500	-0.79718600	1.75968600
H	-3.87624300	-0.91596300	2.71850000	H	-3.96860600	-1.26995400	0.98368700
H	-2.41546400	-1.36334600	1.82101000	C	-4.73914400	1.88395900	1.47372100
H	-4.67676600	2.96527400	1.29364200	H	-5.45079500	1.47662800	0.74481300
H	-5.17597200	1.73999200	2.47115700	C	-2.01899800	1.73335900	2.82081600
H	-2.40931000	1.37748900	3.78329900	H	-0.95974800	1.45307400	2.76301200
H	-2.06282200	2.83066800	2.84611200	N	-1.20077100	5.47081000	1.14067000
C	-2.64390300	5.63478400	0.91993200	H	-2.90293500	5.44314500	-0.12421300
H	-3.18926100	4.91117100	1.53190700	H	-2.99044500	6.65073900	1.18681100
C	-0.89865600	5.64418000	2.56745600	H	0.98483200	-1.91221600	3.99365400
H	0.16339600	5.45580300	2.74761300	H	-1.14420600	6.66126900	2.92474200
H	-1.47563200	4.92629700	3.15634900	C	-0.42118900	6.44065300	0.35389400
H	0.60255100	6.43278800	0.74179100	H	-0.80503700	7.46735400	0.51082900
C	-0.40085500	6.17830700	-1.15373600	N	0.21420900	4.90162100	-1.54657400
C	-0.02266800	4.65775600	-2.97453600	H	0.41635500	3.69832800	-3.26115200
H	-1.09691400	4.61257400	-3.17384600	H	0.41961600	5.44645600	-3.61105500
C	1.65829400	4.88850000	-1.28181400	H	2.07413000	3.93764700	-1.62393600
H	2.18172800	5.71301200	-1.80205200	H	1.86440600	4.95979600	-0.21142500
H	-1.42379300	6.18609600	-1.54465700	H	0.12255300	7.02905900	-1.63272700
H	4.87141700	3.02271800	-0.21910600	C	5.61974000	1.04815300	0.34349900
H	5.27765800	1.07000200	1.38264800	H	5.48070700	0.02130900	-0.01713000
C	7.07958600	1.43691900	0.25675700	C	7.98339100	0.69819100	-0.51884000
C	9.32457700	1.07545600	-0.61557800	C	9.78486100	2.20313100	0.06442600
C	8.89633200	2.94756200	0.84405500	C	7.55831500	2.56637500	0.93862200
H	6.87724300	3.14672000	1.55794900	H	9.24742400	3.82307400	1.38410700
H	10.8283760	2.49762200	-0.00718200	H	10.0087470	0.48475300	-1.21915300
H	7.63519000	-0.18944900	-1.04300300	H	5.80560800	1.35847900	-2.29437600
H	4.60261700	2.64868400	-2.57579400	N	0.97013100	-1.56648100	1.87515600
C	0.64055000	-2.95426100	1.51902800	H	-0.39284500	-3.13997100	1.83001500
H	1.27066400	-3.66464500	2.08999400	C	0.79434400	-3.27859700	0.03001300

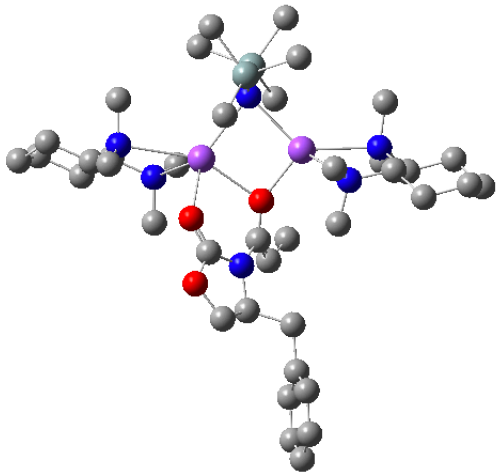
H	1.80162300	-3.00851500	-0.30177600	H	0.71198200	-4.37699000	-0.08963900
N	-0.16225600	-2.58794300	-0.84723500	C	-1.50113100	-3.17495700	-0.74473000
H	-2.18793800	-2.62691400	-1.39524200	H	-1.51160500	-4.24112400	-1.04299100
H	-1.88344000	-3.09817700	0.27533400	C	0.30144900	-2.65676500	-2.23864100
H	-0.43231600	-2.17452200	-2.89106100	H	1.24659100	-2.11851100	-2.33753500
H	0.43192300	-3.69995500	-2.58406300	C	2.41329300	-1.31391700	1.79075100
H	2.76378300	-1.44174300	0.76422300	H	2.61881800	-0.28122700	2.08484000
H	2.98917500	-1.99283200	2.44875100	C	0.50455500	-1.26776700	3.23312800
H	0.73130200	-0.22532400	3.47312600	H	-0.57849500	-1.40664900	3.29755300

Table S26. 6a with (*S*,*S*)-TMCDA at –78 °C.





(*S*,*S*)-TMCDA



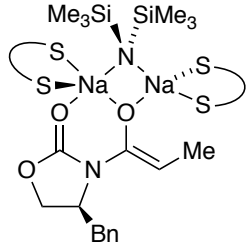
G = –2980.980268
G_{MP2} = –2979.909959

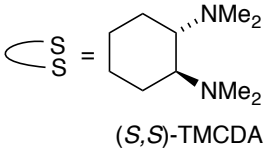
Na	0.00000000	0.00000000	0.00000000	O	0.99869200	1.69982000	-1.25352100
C	1.99820600	2.36713900	-1.04201100	O	2.33905500	3.38160900	-1.89228500
C	3.59752100	3.93729400	-1.48606400	C	3.80784200	3.44556100	-0.04265600
N	2.90234000	2.28900300	-0.01430100	C	2.67680800	1.42289700	1.16056400
C	3.00028900	1.93872700	2.38050400	H	3.33266900	2.96909300	2.45834200
C	2.86806300	1.15789300	3.65781700	H	2.08575400	1.55961900	4.32103600
H	2.60819200	0.11685800	3.44392800	H	3.79817600	1.16025200	4.24656800
O	2.19614600	0.25723600	0.88628300	Na	2.63732200	-1.86178200	0.46729200
N	0.35311400	-2.52500400	-0.03373100	Si	-0.38347700	-3.25871300	1.32791200
C	-0.22136500	-5.16334200	1.45275500	H	-0.63643300	-5.52808300	2.40216500
H	-0.75719400	-5.67816700	0.64555200	H	0.82539300	-5.49118200	1.40479600

C	0.39831200	-2.59548000	2.94449400	H	-0.26221700	-2.75362500	3.80719200
H	1.33938200	-3.11429300	3.17146400	H	0.62140200	-1.52339200	2.88571500
C	-2.26030500	-2.92861300	1.48726300	H	-2.47482100	-1.85452200	1.55839200
H	-2.80685700	-3.31554100	0.61825600	H	-2.67770700	-3.40820200	2.38281100
Si	0.32141500	-3.21005400	-1.60352400	C	-1.31735300	-4.02442700	-2.16080600
H	-1.24729700	-4.36324900	-3.20326400	H	-1.56014600	-4.90240800	-1.54928500
H	-2.17054100	-3.33851700	-2.09532500	C	0.69807200	-1.87252000	-2.91686800
H	-0.18559800	-1.25029100	-3.10962200	H	1.49895200	-1.18910200	-2.60587600
H	0.99147200	-2.31636400	-3.87725100	C	1.62446600	-4.59661900	-1.83973600
H	2.62955200	-4.26607600	-1.54673100	H	1.37520800	-5.46467200	-1.21655600
H	1.67929600	-4.94042900	-2.88160400	N	4.85367600	-1.94374000	-0.93712900
C	4.59654800	-2.15710900	-2.36575900	H	3.74786400	-1.54031700	-2.67585400
H	5.45359500	-1.89500700	-3.01036800	H	4.33519700	-3.20329300	-2.54774200
C	5.19481200	-0.53501700	-0.70510400	H	6.07327700	-0.19974000	-1.28349300
H	4.34171600	0.08778600	-0.98703500	H	5.38649600	-0.35284900	0.35512300
C	5.84192400	-2.91322000	-0.39737000	H	5.49824300	-3.89648800	-0.74820600
C	5.86259600	-2.94857600	1.15489400	N	4.50890800	-3.09085300	1.75509000
C	3.95860600	-4.45129500	1.67828400	H	4.48887600	-5.17581000	2.31820200
H	2.91235400	-4.43426300	1.99737700	H	3.98274500	-4.81528900	0.64724700
C	4.48098900	-2.60876400	3.14150300	H	3.45260800	-2.63116000	3.51344200
H	5.09870100	-3.21216100	3.82937900	H	4.82786800	-1.57169400	3.17997900
H	6.22546500	-1.97058700	1.49747800	C	6.87738400	-4.00811500	1.65180300
H	6.89307600	-4.01269000	2.74815500	H	6.54379500	-5.00669000	1.33993700
C	8.29088000	-3.77757200	1.10543800	H	8.96696300	-4.55826400	1.47578600
H	8.68334000	-2.82031800	1.47920200	C	8.27110600	-3.75828300	-0.42549200
C	7.28027300	-2.70552200	-0.93707000	H	7.26443200	-2.71079900	-2.03288400
H	7.63994000	-1.71263600	-0.63473500	H	9.27223100	-3.55350100	-0.82501300
H	7.98264700	-4.75173700	-0.79927400	H	3.45760000	4.20655500	0.66979800
C	5.27838300	3.11143900	0.26914200	H	5.31385600	2.62109600	1.24708100
H	5.63433300	2.38485100	-0.47081200	C	6.15897300	4.34375500	0.25760300
C	6.10493400	5.26736600	1.31297100	C	6.89205000	6.41839500	1.29964000
C	7.75342900	6.66724900	0.22861000	C	7.82227000	5.75509500	-0.82470300
C	7.03074000	4.60472800	-0.80799400	H	7.09740000	3.89486500	-1.62979700
H	8.49405000	5.93543800	-1.65990800	H	8.36941400	7.56237400	0.21878700
H	6.83754500	7.11886100	2.12896700	H	5.44626200	5.07664600	2.15772800
H	4.37831600	3.56093600	-2.15836800	H	3.54493800	5.02356100	-1.57450200
N	-1.48099100	1.45942000	1.62962600	C	-1.35113900	0.86737200	2.96454400
H	-1.89913300	-0.07880900	3.00895300	H	-0.29481200	0.66038000	3.16023700
H	-1.71802800	1.51955300	3.77692900	C	-0.70624800	2.70620700	1.56451900
H	0.33841300	2.48616100	1.80382500	H	-0.73636500	3.12055800	0.55400100
H	-1.05576400	3.47541200	2.27455800	C	-2.90133900	1.59652400	1.21199900
H	-3.35865800	0.61798900	1.41684200	C	-3.05043100	1.87179000	-0.30914900
N	-2.32283800	0.88435100	-1.14649800	C	-3.02683200	-0.38935400	-1.32474800
H	-2.34284400	-1.11131500	-1.77859900	H	-3.33871000	-0.79687600	-0.36024000
H	-3.91509000	-0.31391600	-1.97596700	C	-1.95986600	1.44269500	-2.45282500
H	-1.34302700	2.33375100	-2.31837500	H	-1.35829400	0.71222500	-3.00193600

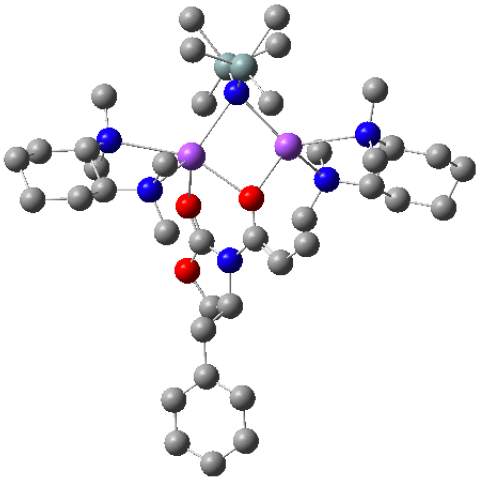
H	-2.83595700	1.69499500	-3.07798400	H	-2.56774900	2.83631200	-0.51284000
C	-4.54406400	2.02430000	-0.69283000	C	-5.27232000	3.09156000	0.13112100
C	-5.15917500	2.76917000	1.62317200	C	-3.68592000	2.65492300	2.03075400
H	-3.61055600	2.41903300	3.09849000	H	-3.21559400	3.63805100	1.89600800
H	-5.65505800	3.53885100	2.22828200	H	-5.67976100	1.82289500	1.83247100
H	-6.32396900	3.14983200	-0.17719200	H	-4.83276400	4.08109200	-0.06387900
H	-4.61964700	2.25355600	-1.76268000	H	-5.05879600	1.06604600	-0.54302000

Table S27. 6b with (*S*,*S*)-TMCDA at –78 °C.





(*S*,*S*)-TMCDA



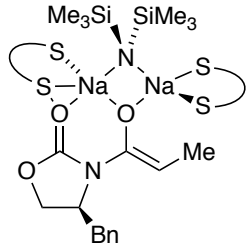
G = –2980.979634
G_{MP2} = –2979.908533

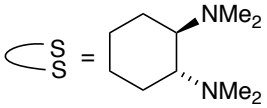
Na	0.00000000	0.00000000	0.00000000	O	0.24428000	1.71372100	-1.56017600
C	0.38268400	2.90550200	-1.33073100	O	0.89118100	3.72979200	-2.30296400
C	0.76024600	5.09346900	-1.86854700	C	0.66971300	4.99113000	-0.34101600
N	0.12662500	3.63396200	-0.19985100	C	-0.56911100	3.13394000	0.99689600
C	-0.68604900	3.99262700	2.05323100	H	-0.27853700	4.99503600	1.99861100
C	-1.31299200	3.58589500	3.35728100	H	-0.62244100	3.72154300	4.20389100
H	-2.21397800	4.16991000	3.60382700	H	-1.59779000	2.53014100	3.33097100
O	-1.00437200	1.92177700	0.91625800	Na	-3.01042800	1.04901500	0.36845800
N	-2.22953800	-1.21323000	0.04163700	Si	-2.79193900	-1.78854800	-1.47215800
C	-2.43259200	-3.62110400	-1.89099500	H	-2.77426000	-3.85819900	-2.90771800
H	-1.36414100	-3.86179300	-1.83938000	H	-2.95277400	-4.30413700	-1.20766600
C	-4.69397800	-1.64643200	-1.67083600	H	-5.02363900	-1.93921300	-2.67703400
H	-5.20261800	-2.30181200	-0.95248200	H	-5.05546400	-0.62574400	-1.49105800
C	-2.02436100	-0.77974400	-2.90341800	H	-2.01340500	0.29979400	-2.70607500
H	-0.97935400	-1.06650300	-3.08066200	H	-2.56524500	-0.94493100	-3.84476100
Si	-2.31058200	-2.13461000	1.48344700	C	-0.90227400	-3.41822400	1.65865300
H	-0.93597100	-3.93268600	2.62852500	H	-0.97577000	-4.18252900	0.87497600

H	0.08573000	-2.95062400	1.56543200	C	-3.90631400	-3.15624800	1.75647300
H	-4.80988100	-2.53589200	1.70468800	H	-4.01513800	-3.94833300	1.00504500
H	-3.89497900	-3.64176700	2.74180600	C	-2.18346400	-0.98512800	3.01119400
H	-1.83983100	-1.53072800	3.89986500	H	-1.49761600	-0.14475500	2.84356900
H	-3.16217300	-0.55534100	3.26660300	N	-5.29201400	1.65379600	1.43511800
C	-6.00054200	0.40866900	1.75159000	H	-6.29633600	-0.09619000	0.82711200
H	-5.32934100	-0.26056400	2.29723500	H	-6.89947300	0.56249700	2.37434700
C	-4.77440200	2.26699400	2.66577700	H	-4.27117300	3.21090100	2.44142000
H	-5.55308000	2.45712200	3.42339800	H	-4.03331800	1.59881700	3.11503100
C	-6.12201000	2.56446300	0.59995300	H	-6.64455500	1.90945000	-0.10953000
C	-5.26131000	3.55217200	-0.23300800	N	-4.22494700	2.85755900	-1.04311300
C	-4.74112100	2.19857600	-2.25042000	H	-3.95987700	1.55830300	-2.67032900
H	-5.59532100	1.56176800	-2.00770200	H	-5.04950100	2.90878800	-3.03582500
C	-3.12351800	3.75560500	-1.40603100	H	-2.34618700	3.17427800	-1.91071800
H	-3.42992900	4.56948400	-2.08767400	H	-2.69043600	4.19351600	-0.50196100
H	-4.70145400	4.17745000	0.47572500	C	-6.16508600	4.49124700	-1.06983100
H	-5.53930300	5.20598300	-1.61743100	H	-6.69785000	3.90017300	-1.82627400
C	-7.20663100	5.23591600	-0.22742200	H	-7.82075200	5.87599200	-0.87318100
H	-6.70315900	5.90284900	0.48790200	C	-8.07940700	4.23509200	0.53531000
C	-7.20337900	3.32665300	1.40608500	H	-7.82681100	2.60667500	1.94988000
H	-6.71507500	3.95170600	2.16502100	H	-8.81326300	4.75603800	1.16287900
H	-8.65369800	3.62986000	-0.18150300	H	-0.04066200	5.71936200	0.05789100
C	2.04173500	5.15353000	0.36134300	H	1.92881700	4.81039200	1.39453800
H	2.75755600	4.48041600	-0.12684400	C	2.55738800	6.57549400	0.32632300
C	3.59115800	6.95367900	-0.54109100	C	4.04512500	8.27366000	-0.58732200
C	3.46923400	9.24089600	0.23653000	C	2.44045300	8.87808000	1.10909100
C	1.99127900	7.55868100	1.15259000	H	1.19784200	7.28425600	1.84491600
H	1.99116600	9.62270500	1.76110400	H	3.82191000	10.2681940	0.20397500
H	4.85129700	8.54320900	-1.26465500	H	4.05414200	6.20350400	-1.17899900
H	1.62819900	5.65486700	-2.21834500	H	-0.14870700	5.51907000	-2.31039000
N	2.22609700	0.06684500	1.51072500	C	3.43643700	-0.47404100	0.84040300
C	3.13053500	-1.71331700	-0.04296800	N	2.02535400	-1.47024900	-1.00619100
C	1.43863300	-2.72344000	-1.48867800	H	0.55912900	-2.49728200	-2.09746000
H	2.12885900	-3.32247600	-2.10984200	H	1.11151300	-3.33362000	-0.64224900
C	2.39037400	-0.62240700	-2.14907900	H	1.48385300	-0.33383900	-2.68698400
H	2.86308600	0.30122800	-1.80660400	H	3.06903900	-1.12247000	-2.86124500
H	2.76332500	-2.50714400	0.62228300	C	4.42987500	-2.23244000	-0.71029400
C	5.55109800	-2.52774300	0.29304600	C	5.86591500	-1.27719300	1.11821600
C	4.59851500	-0.77730800	1.81984300	H	4.82025100	0.12044000	2.40930600
H	4.27697500	-1.54689900	2.53408800	H	6.64676400	-1.48570300	1.86057200
H	6.26351000	-0.49271800	0.45728400	H	6.44425600	-2.88012500	-0.23831100
H	5.24561400	-3.34200800	0.96661600	H	4.20450700	-3.13054300	-1.29728000
H	4.79629500	-1.48000400	-1.42118900	H	3.77622900	0.32672200	0.16989700
C	2.38217900	1.48029800	1.86372200	H	2.62462500	2.05898400	0.96702400
H	1.43927700	1.86254200	2.26261000	H	3.17074400	1.66051900	2.61724700
C	1.79546600	-0.69133100	2.69032700	H	0.80191300	-0.34672300	2.99238300

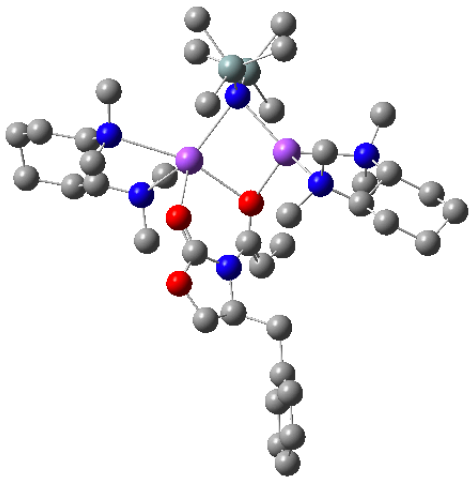
H	1.72255900	-1.75639600	2.45731200	H	2.46761900	-0.57234100	3.55760800

Table S28. 6a with (*R*,*R*)-TMCDA at –78 °C.





(*R*,*R*)-TMCDA

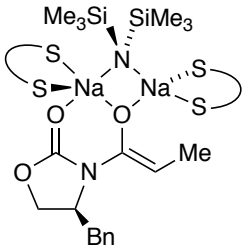


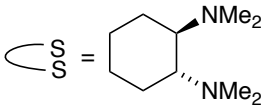
G = –2980.979251
G_{MP2} = –2979.910704

Na	0.00000000	0.00000000	0.00000000	O	1.30966000	1.37728800	-1.34241900
C	2.36201700	1.94891700	-1.10689400	O	2.85403400	2.86521600	-1.99436800
C	4.14224800	3.31484700	-1.55404500	C	4.24996400	2.86694000	-0.08371000
N	3.20078700	1.84024500	-0.02759900	C	2.83178200	1.08119800	1.18661600
C	3.20982300	1.61449100	2.38421900	H	3.69882000	2.58319800	2.41039500
C	2.92462500	0.95643200	3.70535300	H	2.26435400	1.56644900	4.34116100
H	2.43224400	-0.00780500	3.55514500	H	3.83829200	0.77999600	4.29383800
O	2.18669600	-0.01321300	0.96463800	Na	2.36165600	-2.15100800	0.39655000
N	0.00688900	-2.58303600	0.12385100	Si	-0.74218700	-3.06240400	1.58935400
C	-0.79104400	-4.94459200	1.93238800	H	-1.20508700	-5.15005500	2.92887200
H	-1.41064800	-5.48360700	1.20495900	H	0.21319500	-5.38646100	1.89395400
C	0.18059600	-2.31770500	3.09001600	H	-0.44994600	-2.30775100	3.98866200
H	1.07245900	-2.91072500	3.33606200	H	0.51812200	-1.29231300	2.89932800
C	-2.56146800	-2.49205100	1.75198800	H	-2.65371200	-1.40401000	1.63820100
H	-3.18939500	-2.95416300	0.97979800	H	-2.98734000	-2.75892500	2.72860400
Si	-0.17787000	-3.44464000	-1.34510500	C	-1.93482800	-4.05631200	-1.79009800
H	-1.93633900	-4.54432900	-2.77419500	H	-2.29579600	-4.79511000	-1.06328800
H	-2.67245800	-3.24674000	-1.82286400	C	0.39559400	-2.36305600	-2.81494600
H	-0.25917000	-1.49499400	-2.96713700	H	1.40728600	-1.96416500	-2.66140900
H	0.40563000	-2.92995800	-3.75523600	C	0.88391700	-5.04027900	-1.42256000
H	1.92965400	-4.85388000	-1.14565100	H	0.49613300	-5.79283200	-0.72468000
H	0.88267500	-5.48850600	-2.42562500	N	4.44912400	-2.37779800	-1.13020100
C	4.28701600	-3.45278000	-2.11767300	H	3.31126300	-3.34859500	-2.59940600

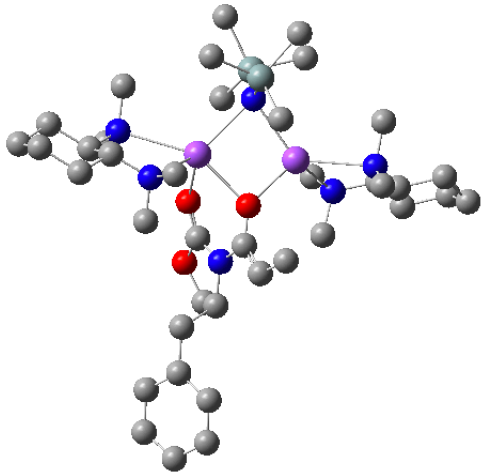
H	5.05529100	-3.43655400	-2.90866100	H	4.31227500	-4.43173500	-1.63249700
C	4.44548600	-1.07999700	-1.81362200	H	5.27388700	-0.96036600	-2.53447800
H	3.50774900	-0.96652800	-2.36742300	H	4.49265600	-0.27420600	-1.07754100
C	5.62959400	-2.53718100	-0.23573200	C	5.41710000	-3.65242300	0.82392600
N	4.17259500	-3.45451400	1.61757100	C	3.63901700	-4.72560100	2.12035400
H	4.30677700	-5.22622800	2.84394400	H	2.68278600	-4.54500800	2.62109400
H	3.45610600	-5.40908700	1.28523200	C	4.30274500	-2.48872000	2.71925900
H	3.31134900	-2.28432800	3.13288300	H	4.94024600	-2.84867000	3.54352100
H	4.70328500	-1.53913200	2.35386200	H	5.26685800	-4.59326900	0.27875400
C	6.68023700	-3.83263300	1.70208800	H	6.83318500	-2.93070500	2.30855200
H	6.51615400	-4.65731600	2.40638700	C	7.95473600	-4.07382200	0.88592400
H	8.81313500	-4.18502400	1.56008500	H	7.87191200	-5.01650500	0.32518000
C	8.17545600	-2.91609600	-0.09054800	C	6.95615700	-2.75924200	-1.00636700
H	6.87083400	-3.66776500	-1.61693600	H	7.11354400	-1.92984300	-1.70588400
H	9.07586300	-3.08131800	-0.69537100	H	8.34384900	-1.98776800	0.47506100
H	5.71363000	-1.58348100	0.30367100	H	3.98885500	3.69917900	0.58509900
C	5.65654700	2.35620000	0.28365100	H	5.60435100	1.90898900	1.28133800
H	5.92977300	1.55684700	-0.41579800	C	6.69501600	3.45805200	0.24459200
C	6.73402400	4.43641900	1.25012000	C	7.67035000	5.46905200	1.20971600
C	8.59050400	5.54147100	0.16122800	C	8.56732200	4.57267500	-0.84230200
C	7.62653300	3.54156900	-0.79887800	H	7.62142600	2.78539100	-1.58114200
H	9.28301600	4.61580600	-1.65917400	H	9.32249000	6.34396000	0.13050300
H	7.68574800	6.21453600	2.00050900	H	6.02961200	4.38123100	2.07742300
H	4.90850300	2.84112500	-2.17925800	H	4.19869800	4.39685800	-1.68482600
N	-1.08515100	2.13381000	1.28717600	C	-1.26615100	1.42559100	2.55854400
H	-2.03514300	0.65354900	2.46166400	H	-0.32551400	0.93364800	2.82569800
H	-1.54524300	2.08620700	3.39773700	C	-0.07617600	3.18636700	1.43694800
H	0.85444900	2.75008400	1.81207600	H	0.12786000	3.63922500	0.46112900
H	-0.38227300	3.98739400	2.13524000	C	-2.33600200	2.66502600	0.69108900
H	-2.00838400	3.40907200	-0.04625000	C	-3.15037900	1.59303800	-0.07963900
H	-3.49570700	0.84670600	0.65034100	N	-2.32137400	0.83056300	-1.04888400
C	-3.01821900	-0.36035900	-1.54148200	H	-2.32114500	-0.96595800	-2.12589400
H	-3.36382000	-0.96546300	-0.69909300	H	-3.88308200	-0.13150200	-2.18918900
C	-1.82370600	1.61899800	-2.18345000	H	-1.26327100	2.48734200	-1.83333300
H	-1.12683600	1.00548300	-2.76186800	H	-2.62358900	1.95661500	-2.86489100
C	-4.40869400	2.24307700	-0.71225900	H	-4.09466500	2.96004500	-1.48311600
H	-5.00026900	1.47563700	-1.22389900	C	-5.28570100	2.98160500	0.30646800
H	-6.14706900	3.43358800	-0.20165800	H	-5.69380300	2.26535600	1.03491800
C	-4.46960800	4.04657500	1.04388700	C	-3.24281000	3.40817000	1.70400600
H	-3.59105400	2.70282100	2.47047200	H	-2.65396500	4.17150600	2.22723300
H	-5.08282200	4.55277200	1.80025100	H	-4.14849000	4.82046500	0.33093400

Table S29. 6b with (*R*,*R*)-TMCDA at –78 °C.





(*R*,*R*)-TMCDA

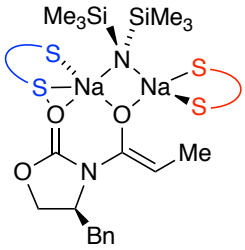


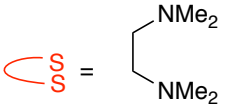
G = –2980.981718
G_{MP2} = –2979.911493

Na	0.00000000	0.00000000	0.00000000	O	0.42304000	1.75527000	-1.47830700
C	0.53297500	2.94475200	-1.22683200	O	0.97061700	3.81119500	-2.19684500
C	0.84444400	5.15690700	-1.70462800	C	0.85920000	4.99367200	-0.18032300
N	0.30952200	3.63717800	-0.06459600	C	-0.33315600	3.08918100	1.14010700
C	-0.30903300	3.85603300	2.26864100	H	0.18877000	4.81859800	2.27175100
C	-0.95113400	3.41699800	3.55445600	H	-0.22953200	3.36690200	4.38448900
H	-1.74865800	4.10161900	3.88544300	H	-1.39250800	2.42234300	3.44240200
O	-0.88185000	1.93113500	0.98464000	Na	-2.93328700	1.17533600	0.54275500
N	-2.28872700	-1.11662300	0.08488800	Si	-2.86126300	-1.63906900	-1.44378300
C	-2.63906100	-3.49511700	-1.85420900	H	-2.95202700	-3.70281700	-2.88643900
H	-1.59392100	-3.81582100	-1.75916800	H	-3.23664800	-4.13962000	-1.19803000
C	-4.73541100	-1.32087400	-1.69281400	H	-5.07127800	-1.61713100	-2.69569900
H	-5.32637300	-1.88925100	-0.96332300	H	-4.98832800	-0.25980700	-1.56151400
C	-1.97485300	-0.71432700	-2.86216600	H	-1.81656500	0.34896100	-2.64656700
H	-0.98411500	-1.14592100	-3.05563900	H	-2.54066900	-0.78580600	-3.80063200
Si	-2.39824500	-2.06356400	1.50830700	C	-1.00189000	-3.35788300	1.69474200
H	-1.09739400	-3.92504400	2.63046300	H	-1.01909100	-4.07708900	0.86662000
H	-0.01191800	-2.88396800	1.69567300	C	-4.01169300	-3.06657900	1.74693000
H	-4.90539700	-2.43250300	1.68306200	H	-4.12220800	-3.85611600	0.99362700
H	-4.02368900	-3.55247200	2.73202100	C	-2.28363600	-0.94850400	3.06028400
H	-2.00649800	-1.52880700	3.95020200	H	-1.54620800	-0.14555400	2.94100900
H	-3.25007400	-0.47590200	3.28305200	N	-5.12551300	1.98151100	1.71156300
C	-5.84964200	0.70562500	1.62175600	H	-6.07615700	0.46624600	0.57929700
H	-5.21464800	-0.09463300	2.01189500	H	-6.79050200	0.69483300	2.19682400
C	-4.84447300	2.30477900	3.11529500	H	-4.23184000	3.20957000	3.17357500
H	-5.75502100	2.45695500	3.72175500	H	-4.27631600	1.48742600	3.56923900
C	-5.79803500	3.11081200	1.01407000	H	-5.31925800	4.01743100	1.40608400

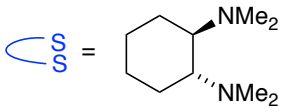
C	-5.56665600	3.09865500	-0.52159300	N	-4.13139900	2.96211600	-0.88160900
C	-3.94274000	2.64317200	-2.30170400	H	-2.89180000	2.39319600	-2.47698300
H	-4.54667500	1.77247200	-2.57315300	H	-4.20510600	3.47421700	-2.97891700
C	-3.30201000	4.11854100	-0.52013500	H	-2.25883700	3.88122200	-0.74087400
H	-3.56579800	5.03671800	-1.07234500	H	-3.36566700	4.32325400	0.55129200
H	-6.05095600	2.19778800	-0.92419000	C	-6.25796700	4.32583600	-1.16986700
H	-5.76725100	5.24454400	-0.82116700	H	-6.11907100	4.29184100	-2.25633300
C	-7.75172600	4.41907800	-0.83812000	C	-7.96168000	4.45108400	0.67846200
C	-7.30985700	3.22570300	1.32946300	H	-7.82724000	2.32752100	0.96790000
H	-7.45392900	3.25333900	2.41632900	H	-9.03085000	4.47934700	0.92310900
H	-7.52151400	5.37115800	1.09041800	H	-8.18375300	5.31053400	-1.30982200
H	-8.28168200	3.55331700	-1.26176000	H	0.18789300	5.70703200	0.30402900
C	2.28384000	5.10805800	0.42219500	H	2.24648400	4.72942300	1.44829200
H	2.94702700	4.44080900	-0.14223800	C	2.82307400	6.52163500	0.39696300
C	3.80103900	6.91016300	-0.52868900	C	4.27787100	8.22238700	-0.56368600
C	3.78100200	9.17137200	0.32995100	C	2.80808100	8.79814700	1.26027300
C	2.33600900	7.48640600	1.29242300	H	1.58676900	7.20353000	2.02917300
H	2.42068400	9.52846100	1.96597100	H	4.15170600	10.1925550	0.30622300
H	5.04005200	8.50009400	-1.28708400	H	4.20184200	6.17359100	-1.22203700
H	1.67691400	5.74687300	-2.09136200	H	-0.10072600	5.57891400	-2.06693900
N	2.08921900	-0.25274500	1.58299700	C	3.01831000	-1.33931800	1.17891400
H	2.49512500	-2.27318000	1.42907200	C	3.28782200	-1.35040100	-0.35030200
H	3.78925100	-0.40536300	-0.59679500	N	2.03857500	-1.35282400	-1.15414400
C	1.40615900	-2.67075800	-1.27876700	H	0.41208600	-2.54909800	-1.71754000
H	1.97112500	-3.36992300	-1.91943300	H	1.27551400	-3.13001700	-0.29591000
C	2.24539000	-0.76858000	-2.48328100	H	1.28474600	-0.69491700	-3.00036900
H	2.63882500	0.24645000	-2.38675700	H	2.93025700	-1.36053900	-3.11778600
C	4.26825800	-2.49073700	-0.72390200	H	3.79249900	-3.46018800	-0.52588900
H	4.46748700	-2.45639400	-1.80192300	C	5.58252400	-2.43421400	0.06191600
H	6.23306900	-3.26618200	-0.23631200	H	6.12575600	-1.50883200	-0.18097700
C	5.29746000	-2.47811400	1.56523800	H	6.22921800	-2.41172200	2.14125300
H	4.83962700	-3.44497100	1.82176100	C	4.35705700	-1.33424200	1.96212100
H	4.87870900	-0.38431800	1.78386800	H	4.15027800	-1.37723100	3.03760500
C	2.62760500	1.10338500	1.42575800	H	2.89438300	1.29106200	0.38196100
H	1.85283000	1.82070000	1.70824400	H	3.51127700	1.30231500	2.05620700
C	1.58315600	-0.42702400	2.94821500	H	0.78533000	0.30068200	3.12341400
H	1.16315500	-1.43054500	3.06500400	H	2.35084900	-0.27948400	3.72822100

Table S30. 6a with TMEDA and (*R*,*R*)-TMCDA at –78 °C.

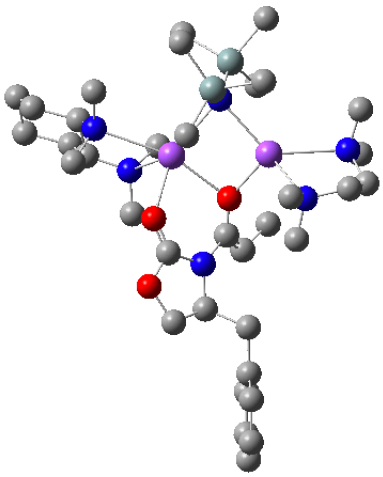




TMEDA



(*R*,*R*)-TMCDA

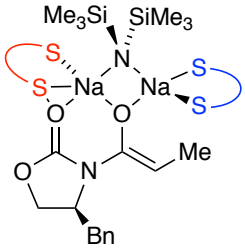


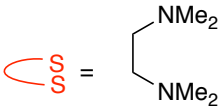
G = –2825.480621
G_{MP2} = –2824.50266

Na	0.00000000	0.00000000	0.00000000	O	-1.70657400	-0.93229300	-1.25519600
C	-2.89506700	-1.05738800	-1.01213700	O	-3.68616200	-1.80254900	-1.84144700
C	-5.05015800	-1.71204400	-1.41175700	C	-4.99083800	-1.13619700	0.01590600
N	-3.63896800	-0.56056200	0.02906700	C	-3.02060900	0.09423600	1.19892600
C	-3.58373500	-0.14604900	2.41838800	H	-4.41092100	-0.84248600	2.50715300
C	-3.07724200	0.48592800	3.68488200	H	-2.76932600	-0.26240900	4.43084500
H	-2.20726200	1.11587800	3.47578500	H	-3.83668000	1.11338500	4.17926200
O	-2.00271500	0.83859400	0.92900200	Na	-1.29530000	2.90396900	0.65182400
N	0.97546800	2.37355300	0.03867400	Si	2.03248300	2.65857600	1.35416200
C	2.79391300	4.41269600	1.45580800	H	3.40450700	4.52480300	2.36189200
H	3.44176600	4.63117200	0.59780100	H	2.02005000	5.19105500	1.48184400
C	1.10620400	2.43799900	3.01289600	H	1.79882400	2.45198800	3.86467700
H	0.38595800	3.25153300	3.17302100	H	0.54478500	1.49721800	3.05513900
C	3.53377600	1.47749300	1.43670800	H	3.21940700	0.42676700	1.48463000
H	4.16955200	1.58849800	0.54913200	H	4.15877300	1.67479800	2.31800200
Si	1.21621200	3.00137400	-1.53615400	C	2.99783600	2.96037500	-2.22984600
H	3.02362300	3.34800400	-3.25726400	H	3.67719300	3.58116900	-1.63220300
H	3.41739600	1.94803500	-2.24986800	C	0.13485600	2.05241100	-2.79506200
H	0.50709000	1.03378100	-2.96750100	H	-0.90365600	1.95012600	-2.45346500
H	0.11610000	2.55619500	-3.77050700	C	0.71042200	4.84585900	-1.68813200
H	-0.30756500	5.02003300	-1.31464400	H	1.38471100	5.47995400	-1.09874400
H	0.74581900	5.20039800	-2.72729300	N	-3.23868300	4.05210300	-0.68511400
C	-3.10703100	4.25885800	-2.13202900	H	-2.85347000	3.31189200	-2.61645200
H	-4.04048100	4.64283300	-2.58394900	H	-2.30361900	4.97068300	-2.33824400
C	-4.29294500	3.06363300	-0.43199700	H	-5.28185700	3.41505400	-0.78367600
H	-4.04258900	2.13412500	-0.94795200	H	-4.36290600	2.82709300	0.63193600
C	-3.51883400	5.33396700	-0.02207600	H	-4.51580200	5.71868000	-0.31446900
H	-2.78776700	6.06241000	-0.38914800	C	-3.47873700	5.28349700	1.50735200
N	-2.17978100	4.89656900	2.08237700	C	-1.18375500	5.96418300	1.92171000
H	-1.50628100	6.90722700	2.40108200	H	-0.23894200	5.65195800	2.37472300

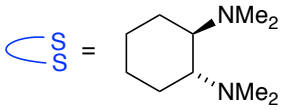
H	-0.99387100	6.15994200	0.86342800	C	-2.34923800	4.58747400	3.50847200
H	-1.38694500	4.30168000	3.94152100	H	-2.74264000	5.44918900	4.07845700
H	-3.03840700	3.74606000	3.62661800	H	-3.79135000	6.27667700	1.88388500
H	-4.22517200	4.56974200	1.87012500	H	-5.05384400	-1.94752700	0.75487800
C	-6.11846100	-0.12275800	0.29171700	H	-5.91937600	0.35478400	1.25598300
H	-6.07446800	0.66113400	-0.47332900	C	-7.48608100	-0.77397800	0.29150400
C	-7.88381100	-1.59685300	1.35669900	C	-9.13116300	-2.22031700	1.35446700
C	-10.0089740	-2.03000900	0.28469300	C	-9.62967700	-1.21025300	-0.77840200
C	-8.37876800	-0.58938700	-0.77278500	H	-8.09593000	0.05564200	-1.60202100
H	-10.3075420	-1.04969200	-1.61271900	H	-10.9823550	-2.51300100	0.28332500
H	-9.42074500	-2.85058900	2.19129300	H	-7.21231100	-1.74196900	2.20038900
H	-5.58727100	-1.04384600	-2.09567100	H	-5.49998300	-2.70510100	-1.46205100
N	0.29117800	-2.26662000	1.49173600	C	0.70060800	-1.51652900	2.68203000
H	1.66999600	-1.03532800	2.51957500	H	-0.03944800	-0.73241100	2.87198900
H	0.77207400	-2.13350000	3.59505800	C	-1.00636800	-2.90761800	1.72063900
H	-1.73884200	-2.15270400	2.02319500	H	-1.35706600	-3.36854700	0.79132700
H	-0.97606800	-3.68652900	2.50533300	C	1.29647700	-3.23287900	0.98481500
H	0.73475300	-3.91760600	0.33681200	C	2.38769300	-2.57152400	0.10134000
H	2.97210100	-1.89542000	0.74179300	N	1.81760900	-1.70272700	-0.96121400
C	2.84767700	-0.88741500	-1.61072800	H	2.36490800	-0.15539100	-2.26354500
H	3.42018600	-0.34018100	-0.85760000	H	3.54858200	-1.47280000	-2.23175600
C	1.03686300	-2.41417500	-1.98084800	H	0.22850300	-2.98499900	-1.52113000
H	0.56680600	-1.68042500	-2.64119000	H	1.64699900	-3.09146800	-2.60339900
C	3.35765700	-3.65667100	-0.43462600	H	2.81286300	-4.32218500	-1.11807100
H	4.14835500	-3.18275500	-1.02668800	C	3.98477100	-4.50518300	0.67788200
H	4.64850800	-5.26248700	0.24166800	H	4.61433700	-3.86907700	1.31761000
C	2.89721600	-5.16319600	1.53130900	H	2.33264900	-5.87956800	0.91644300
H	3.34215400	-5.73894200	2.35290100	C	1.94694100	-4.09874300	2.09220800
H	2.51472700	-3.45319800	2.77544200	H	1.15966100	-4.57174800	2.69230000

Table S31. 6a with (*R*,*R*)-TMCDA and TMEDA at –78 °C.

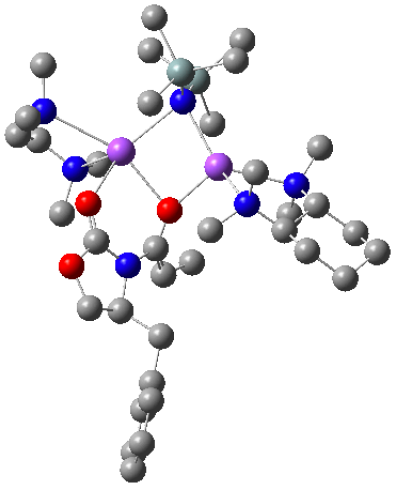




TMEDA



(*R*,*R*)-TMCDA

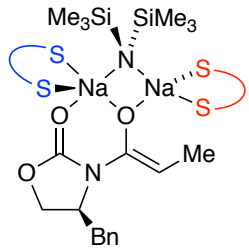


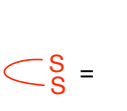
G = –2825.482535
G_{MP2} = –2824.505237

Na	0.00000000	0.00000000	0.00000000	O	-1.73894900	-0.98833900	-1.21645000
C	-2.94850800	-0.95366300	-1.04547500	O	-3.77849200	-1.64788800	-1.88014100
C	-5.14153900	-1.36547900	-1.53081800	C	-5.07612800	-0.75800300	-0.11820200
N	-3.67629000	-0.31356400	-0.07971300	C	-3.03195700	0.35971600	1.06977200
C	-3.59897800	0.15500500	2.29310200	H	-4.44623500	-0.51799500	2.38431600
C	-3.08373800	0.78666600	3.55595600	H	-2.82250100	0.03618500	4.31749900
H	-2.18362200	1.37217400	3.35014000	H	-3.81909500	1.45708500	4.02882100
O	-1.99931200	1.06921400	0.76625900	Na	-1.11051100	3.01396500	0.18890300
N	1.14980100	2.25265500	-0.07747800	Si	2.09812400	2.40255600	1.34074900
C	3.07967900	4.03402400	1.52991900	H	3.58757700	4.07585000	2.50293600
H	3.85013600	4.14159900	0.75586500	H	2.42569600	4.91301700	1.46048900
C	0.99577100	2.29613800	2.90045700	H	1.59240200	2.08206800	3.79698500
H	0.47166400	3.24300300	3.08886000	H	0.23122700	1.51483600	2.81105600
C	3.40272600	1.01867500	1.54579400	H	2.92983700	0.02818700	1.57017000
H	4.11414900	1.01746500	0.71107000	H	3.97735300	1.13404600	2.47472300
Si	1.68060100	2.74633900	-1.62812700	C	3.47058800	2.28592900	-2.11706200
H	3.69101500	2.60761300	-3.14382700	H	4.20709900	2.76678700	-1.46093400
H	3.64808500	1.20501200	-2.06534300	C	0.56603100	1.96893300	-2.97276200
H	0.69649800	0.88005400	-3.01510600	H	-0.50199700	2.14611600	-2.78685600
H	0.79582700	2.36498500	-3.97080200	C	1.60260500	4.64319000	-1.89213200
H	0.61416100	5.05457100	-1.64951700	H	2.32955300	5.15021000	-1.24546500
H	1.83062600	4.92278200	-2.92977900	N	-2.87393300	4.16146200	-1.31875900
C	-2.21706300	4.88376500	-2.41590900	H	-1.45966000	4.23651100	-2.86584200
H	-2.91205700	5.19158800	-3.21505400	H	-1.70818500	5.77550100	-2.04088600
C	-3.58860700	2.99592000	-1.84919200	H	-4.40993400	3.26102700	-2.53889500
H	-2.88574200	2.36236000	-2.40017200	H	-3.98955400	2.40152000	-1.02500200
C	-3.74482500	5.00859400	-0.45844500	H	-4.31400100	4.30155200	0.16074700
C	-2.92126000	5.90941300	0.50231000	N	-1.94411600	5.13603600	1.31564700
C	-0.80556600	5.96359600	1.73070200	H	-1.08573800	6.78523600	2.41365200

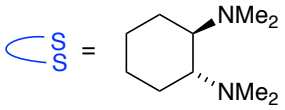
H	-0.07088300	5.33840300	2.24682300	H	-0.31842900	6.39377400	0.85003600
C	-2.53034500	4.45706600	2.48056400	H	-1.78455400	3.78550800	2.91544600
H	-2.85729200	5.14909600	3.27404400	H	-3.38366200	3.84406700	2.17766500
H	-2.31393000	6.57795100	-0.12212100	C	-3.85482000	6.80346300	1.35521800
C	-4.82489700	7.63668000	0.51138200	C	-5.67134100	6.71875200	-0.37520700
C	-4.76406400	5.85587100	-1.26071900	H	-4.21975000	6.52382000	-1.94103300
H	-5.36964000	5.19524700	-1.89258700	H	-6.35456300	7.30424900	-1.00310400
H	-6.30105200	6.07662500	0.25804600	H	-4.26381200	8.34074700	-0.12076300
H	-5.46288400	8.24343400	1.16593800	H	-4.44678200	6.17134700	2.03010100
H	-3.24775200	7.45704300	1.99341800	H	-5.23658600	-1.54148400	0.63671600
C	-6.10574300	0.36420200	0.10560200	H	-5.87355800	0.84782300	1.06002200
H	-5.97645900	1.11798600	-0.68023000	C	-7.52836100	-0.15555600	0.10097400
C	-8.03175100	-0.86148400	1.20441100	C	-9.33029200	-1.37001400	1.19856900
C	-10.1537100	-1.17899900	0.08657700	C	-9.66878700	-0.47399100	-1.01529900
C	-8.36733700	0.03210100	-1.00565700	H	-8.00109800	0.58837500	-1.86607300
H	-10.3034040	-0.31370600	-1.88301500	H	-11.1666630	-1.57225700	0.08217700
H	-9.70180800	-1.91071700	2.06514900	H	-7.40192600	-1.00472600	2.07993500
H	-5.54698100	-0.65213200	-2.25872200	H	-5.71459200	-2.29250000	-1.58290000
N	1.52409100	-1.99490000	-1.14934000	C	1.15707000	-3.16486900	-0.33793200
C	1.23738500	-2.93553700	1.17450400	N	0.20645900	-2.02818100	1.70144500
C	0.54629400	-1.61135700	3.06588600	H	1.50749900	-1.08931600	3.07091300
H	-0.21938500	-0.92464900	3.43751200	H	0.61082000	-2.46852100	3.76271300
C	-1.11491000	-2.66897400	1.70742600	H	-1.85968200	-1.96275400	2.08554900
H	-1.40801500	-2.94658300	0.69292900	H	-1.12645200	-3.57774800	2.33956800
H	1.18104000	-3.92158800	1.67646100	H	2.21536700	-2.51487100	1.43080100
H	1.80137900	-4.03040500	-0.58913500	H	0.13708000	-3.44975200	-0.61144000
C	2.97474900	-1.78929000	-1.15573500	H	3.21513100	-0.91370600	-1.76378600
H	3.51579600	-2.66161900	-1.57084400	H	3.34688700	-1.60014400	-0.14650900
C	1.04578900	-2.17506500	-2.52577200	H	-0.04498000	-2.22900900	-2.52937600
H	1.34858500	-1.31503200	-3.13075800	H	1.46124300	-3.08613200	-2.99702800

Table S32. 6b with TMEDA and (*R*,*R*)-TMCDA at –78 °C.

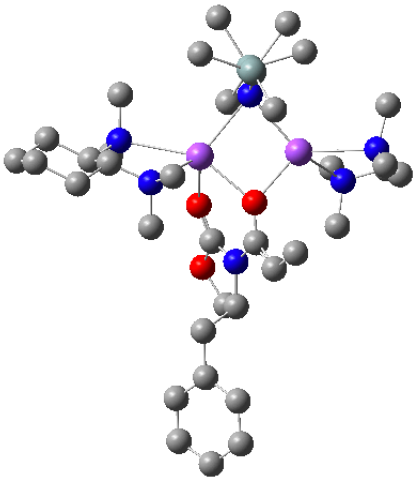




TMEDA



(*R*,*R*)-TMCDA

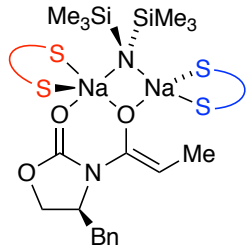


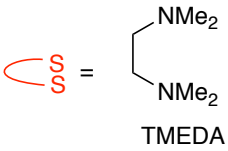
G = –2825.483369
G_{MP2} = –2824.505837

Na	0.00000000	0.00000000	0.00000000	O	-1.67123700	-0.63969300	-1.49333100
C	-2.69791800	-1.25965400	-1.26822200	O	-3.66457400	-1.35407800	-2.23841900
C	-4.67839600	-2.27110400	-1.79343100	C	-4.54265200	-2.25781100	-0.26668200
N	-3.12081400	-1.91366200	-0.13932000	C	-2.30392500	-2.15906700	1.05814300
C	-2.93329900	-2.68094000	2.15212600	H	-3.99650200	-2.88873800	2.13268800
C	-2.20406000	-2.97231900	3.43337300	H	-2.66415300	-2.46643200	4.29580500
H	-2.19083900	-4.04610500	3.68368000	H	-1.16568600	-2.63341700	3.36785000
O	-1.05271600	-1.86816400	0.93728300	Na	0.78542300	-3.04900900	0.50647000
N	2.24944100	-1.19252600	0.03761400	Si	2.97276600	-1.35964900	-1.50640200
C	4.34011600	-0.09765200	-1.95153200	H	4.68051900	-0.24083200	-2.98595800
H	3.99083300	0.93863800	-1.86220400	H	5.21909700	-0.19939400	-1.30301300
C	3.80721700	-3.06667500	-1.76667000	H	4.19137900	-3.18539800	-2.78886700
H	4.65168200	-3.19728900	-1.07832800	H	3.10640600	-3.89215800	-1.58116000
C	1.66418400	-1.19589500	-2.88811500	H	0.73318100	-1.72604700	-2.65304000
H	1.39223300	-0.14527700	-3.05479400	H	2.03972700	-1.58272900	-3.84469000
Si	3.11416700	-0.79548600	1.46074700	C	3.37200800	1.08156500	1.72227300
H	3.90718700	1.29220800	2.65791600	H	3.95321500	1.51927700	0.90104700
H	2.41277300	1.61376500	1.76462000	C	4.86280000	-1.55416200	1.64177500
H	4.84758000	-2.64832300	1.55256800	H	5.55884500	-1.17780400	0.88230900
H	5.29100200	-1.31078200	2.62363700	C	2.15863600	-1.40678900	3.00071100
H	2.55930000	-0.97047800	3.92519200	H	1.09076400	-1.16278600	2.94934800
H	2.23760300	-2.49740500	3.10338600	N	1.43947500	-5.27170100	1.72450700
C	2.89498400	-5.37445900	1.55347400	H	3.17093200	-5.27633100	0.50081400
H	3.38326900	-4.56219000	2.09858000	H	3.28944300	-6.33627000	1.93136300
C	1.10660800	-5.32680700	3.15400700	H	0.03098000	-5.18418100	3.29122200
H	1.39806500	-6.28958500	3.61274800	H	1.62552000	-4.52417400	3.68454400
C	0.73710800	-6.35319100	1.01395000	H	-0.29154900	-6.38057000	1.38720200

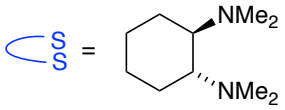
H	1.18313800	-7.33580200	1.26122400	C	0.72427800	-6.21736600	-0.51044600
N	0.02763400	-5.02300600	-1.01120200	C	0.25342000	-4.88504000	-2.45546800
H	-0.23168900	-3.97450300	-2.81779300	H	1.32395500	-4.80348200	-2.66086300
H	-0.14799600	-5.74455200	-3.02374700	C	-1.41542000	-5.08645200	-0.74827500
H	-1.89583800	-4.21141900	-1.19165100	H	-1.87425200	-5.99729600	-1.17753500
H	-1.62559700	-5.05685000	0.32342300	H	1.75152000	-6.18472100	-0.88884100
H	0.26857500	-7.13885000	-0.92338200	H	-4.72416500	-3.24899400	0.15621600
C	-5.46620000	-1.21227100	0.41106700	H	-5.12220800	-1.07953100	1.44157100
H	-5.32769700	-0.25196000	-0.10103900	C	-6.92581000	-1.61037600	0.38596400
C	-7.83103600	-1.00167400	-0.49398200	C	-9.17170300	-1.39136500	-0.53047200
C	-9.63027000	-2.40087200	0.31608100	C	-8.74065700	-3.01393300	1.20152300
C	-7.40323300	-2.62075500	1.23516100	H	-6.72151800	-3.09646700	1.93737300
H	-9.09035500	-3.79544600	1.87114400	H	-10.6733490	-2.70446500	0.29119100
H	-9.85692900	-0.90219600	-1.21787700	H	-7.48460500	-0.20520300	-1.14943800
H	-5.64721000	-1.91825900	-2.15060100	H	-4.47206500	-3.26076400	-2.21876800
N	-1.01049500	1.77823100	1.64288000	C	-0.66973200	3.18064000	1.29071700
H	0.39163000	3.29306400	1.55415900	C	-0.80698900	3.46131200	-0.23013300
H	-1.86688600	3.33742700	-0.48750500	N	-0.08144300	2.47040600	-1.06575500
C	1.36032100	2.71920900	-1.17778700	H	1.83716100	1.84952000	-1.63805300
H	1.60634200	3.60124600	-1.79396700	H	1.80661500	2.85232700	-0.18925700
C	-0.67404000	2.34679100	-2.40151100	H	-0.17006600	1.54529900	-2.94879700
H	-1.72751300	2.06825800	-2.31750300	H	-0.59231300	3.27180300	-3.00103000
C	-0.43645100	4.93205000	-0.54749000	H	0.62789100	5.09410800	-0.33294500
H	-0.56932700	5.11463700	-1.62078000	C	-1.24980000	5.94361400	0.26782000
H	-0.94122500	6.96525700	0.01235000	H	-2.31574000	5.86360500	0.00748800
C	-1.07008600	5.67925800	1.76508200	H	-1.67066200	6.37921700	2.35978100
H	-0.02008900	5.85355000	2.04285500	C	-1.46353800	4.23632800	2.10316800
H	-2.53664900	4.11562800	1.90324300	H	-1.32446100	4.05291300	3.17474800
C	-2.42679800	1.43072800	1.47646600	H	-2.74259700	1.59246200	0.44220100
H	-2.55253000	0.36938800	1.70490500	H	-3.10057400	1.99724900	2.14194400
C	-0.57204800	1.42013800	2.99536300	H	-0.70655900	0.34338300	3.13441200
H	0.49036000	1.65201800	3.11772300	H	-1.13371600	1.93567300	3.79436600

Table S33. 6b with (*R*,*R*)-TMCDA and TMEDA at –78 °C.

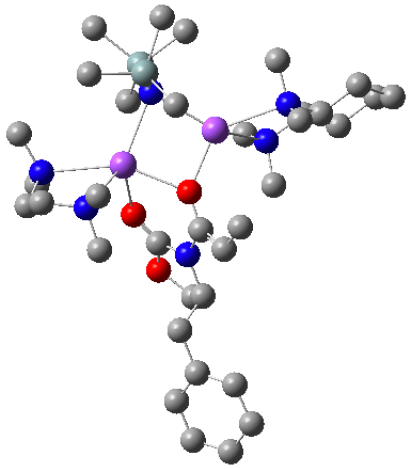




TMEDA



(*R*,*R*)-TMCDA

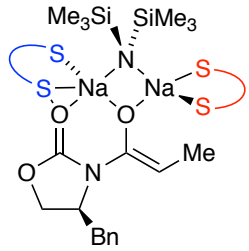


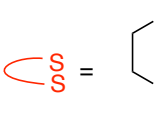
G = –2825.483544
G_{MP2} = –2824.506824

Na	0.00000000	0.00000000	0.00000000	O	1.64778700	0.80309600	-1.45045100
C	2.48876600	1.66564200	-1.24889800	O	3.40746400	1.96797300	-2.22218200
C	4.16492700	3.11561000	-1.79718300	C	4.03683800	3.09121100	-0.27004900
N	2.73244200	2.43003900	-0.13855400	C	1.83994700	2.54119500	1.02585200
C	2.34565900	3.13328200	2.14678200	H	3.37211600	3.47990900	2.16920000
C	1.53053400	3.33314700	3.39328300	H	2.02519300	2.91061300	4.28094200
H	1.35127300	4.39650900	3.62268300	H	0.55549200	2.84644900	3.29726300
O	0.64876200	2.08299300	0.84010300	Na	-1.39755000	2.84033900	0.41935700
N	-2.43167400	0.67465400	0.07999700	Si	-3.21648200	0.56194900	-1.43840400
C	-4.27075900	-1.00602500	-1.74217200	H	-4.66826700	-1.01412500	-2.76605900
H	-3.68427000	-1.92439900	-1.61082200	H	-5.12805700	-1.06943600	-1.06061600
C	-4.41611500	2.01925900	-1.77117100	H	-4.86209300	1.96593400	-2.77345600
H	-5.23658600	2.02125400	-1.04197700	H	-3.90552100	2.98872500	-1.68965900
C	-1.94544600	0.57802500	-2.86300300	H	-1.17678100	1.35093400	-2.74156400
H	-1.41801100	-0.38242700	-2.92020100	H	-2.42939700	0.73892600	-3.83542800
Si	-3.11004800	0.09792400	1.54217000	C	-2.93454100	-1.79180100	1.79012000
H	-3.32450500	-2.11425800	2.76502200	H	-3.48215400	-2.34223400	1.01504900
H	-1.88490800	-2.10782200	1.73282800	C	-4.97429600	0.44126300	1.81078400
H	-5.21392800	1.50959400	1.73300800	H	-5.59580700	-0.08183200	1.07374400
H	-5.29484800	0.10389100	2.80571100	C	-2.23222600	0.90360500	3.03931200
H	-2.43747600	0.35625800	3.96859900	H	-1.14443100	0.94344700	2.90450000
H	-2.57897400	1.93400500	3.19892400	N	-2.48576300	4.94509300	1.49083600
C	-3.87395400	4.46670700	1.41953300	H	-4.19759600	4.38109900	0.37868900
H	-3.93193200	3.46907400	1.86417400	H	-4.58795800	5.11285400	1.95674400
C	-2.06923500	5.07232200	2.89236400	H	-1.01307800	5.35366800	2.94325400
H	-2.65861200	5.81424600	3.45962700	H	-2.18191500	4.10649800	3.39383500
C	-2.23565900	6.19995900	0.73105600	H	-1.27066200	6.57122700	1.09968800
C	-2.08325700	5.96567700	-0.79623500	N	-1.11333800	4.88569500	-1.11558100
C	-1.19776500	4.46095800	-2.51752000	H	-0.59026300	3.56148500	-2.65703600

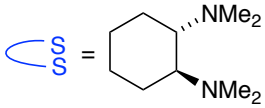
H	-2.23229500	4.21299200	-2.77235300	H	-0.83518700	5.22051400	-3.23138800
C	0.28136800	5.19501200	-0.77616200	H	0.88871900	4.30541200	-0.96058500
H	0.70238000	6.02507900	-1.36859400	H	0.37948000	5.43569700	0.28521700
H	-3.04951500	5.60347000	-1.17516800	C	-1.77959100	7.30910700	-1.50839000
C	-2.82262800	8.39460900	-1.21607800	C	-2.94578300	8.62681700	0.29213200
C	-3.28014600	7.31066400	1.00344300	H	-4.26804100	6.97575400	0.66077800
H	-3.36344000	7.47512100	2.08441100	H	-3.71751500	9.37580400	0.50926400
H	-1.99878300	9.03076900	0.67960600	H	-2.54826100	9.32321200	-1.73208700
H	-3.79953600	8.08992300	-1.61948600	H	-0.79669500	7.67694000	-1.18411800
H	-1.70907700	7.14257600	-2.58917400	H	3.98219100	4.09971100	0.14698000
C	5.17829200	2.29091100	0.41122000	H	4.88371600	2.09528500	1.44674900
H	5.25592100	1.31712500	-0.08834700	C	6.51098700	3.00610900	0.36567400
C	7.52299900	2.60048500	-0.51494300	C	8.74323000	3.27760800	-0.56953900
C	8.97113700	4.37648500	0.25896400	C	7.97291700	4.79052800	1.14415800
C	6.75648500	4.11061200	1.19604200	H	5.98977200	4.43420000	1.89723600
H	8.14430900	5.64068600	1.79933600	H	9.92050900	4.90371600	0.22006700
H	9.51574300	2.94245200	-1.25673000	H	7.35780400	1.73700500	-1.15600000
H	5.18990100	3.00583600	-2.15465600	H	3.71885900	4.01617000	-2.23615700
N	1.39294800	-1.45403500	1.70276300	C	1.37762900	-2.84285300	1.22054600
H	0.41408000	-3.28107600	1.50159600	H	2.15515900	-3.44376600	1.73305900
C	1.59035400	-2.99022900	-0.28844400	H	2.52179700	-2.49275400	-0.57524900
H	1.73475500	-4.06626700	-0.50867000	N	0.51313400	-2.43025600	-1.11743400
C	-0.67022300	-3.29503900	-1.11075400	H	-1.45800500	-2.83734700	-1.71527100
H	-0.45309000	-4.30039200	-1.52036600	H	-1.05992800	-3.41205400	-0.09705600
C	0.99034200	-2.25168500	-2.49431500	H	0.17739100	-1.86741000	-3.11630600
H	1.79785100	-1.51652600	-2.51046600	H	1.34488200	-3.20067100	-2.93942700
C	2.73456800	-0.86500200	1.62321000	H	3.06808500	-0.80662800	0.58433500
H	2.70605700	0.15359200	2.01948400	H	3.47713400	-1.45054500	2.19883600
C	0.92121500	-1.39587000	3.08994100	H	0.91000200	-0.35548100	3.42587100
H	-0.09724100	-1.78834700	3.15636800	H	1.56534500	-1.97696700	3.77677900

Table S34. 6a with TMEDA and (*S*,*S*)-TMCDA at –78 °C.

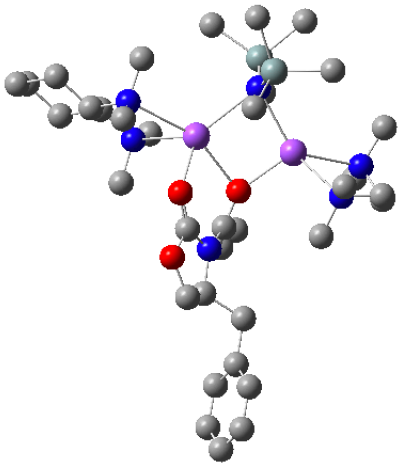




TMEDA



(*S,S*)-TMCDA

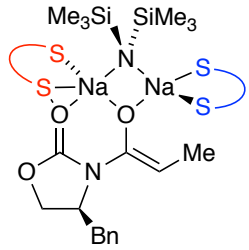


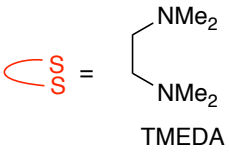
G = –2825.482008
G_{MP2} = –2824.504717

Na	0.00000000	0.00000000	0.00000000	O	-1.69597700	-1.02269000	-1.24150300
C	-2.89116300	-1.13117900	-1.02154800	O	-3.67974600	-1.86651300	-1.86213100
C	-5.04882600	-1.74990000	-1.45173700	C	-4.99519600	-1.19703800	-0.01561300
N	-3.64274500	-0.62356900	0.00655100	C	-3.02794400	0.03998300	1.17419200
C	-3.56330000	-0.23840900	2.39725800	H	-4.35655800	-0.97414400	2.48396200
C	-3.07452100	0.40204800	3.66618900	H	-2.64602900	-0.32886600	4.36940500
H	-2.29468400	1.13774100	3.44696900	H	-3.87989600	0.91594300	4.21433500
O	-2.04410200	0.82526700	0.89328400	Na	-1.35438400	2.88182800	0.54369300
N	0.94227800	2.37783400	-0.01663300	Si	1.94268200	2.68945600	1.33763500
C	2.70252800	4.44437200	1.43629100	H	3.26036000	4.57773200	2.37303800
H	3.39950000	4.64069700	0.61206200	H	1.93014600	5.22379900	1.39869400
C	0.94086800	2.50489700	2.95631300	H	1.59658000	2.47726400	3.83653700
H	0.25929300	3.35513000	3.09405600	H	0.33021400	1.59426100	2.96519300
C	3.43362400	1.50552200	1.51006700	H	3.10939900	0.46156800	1.61102400
H	4.08474800	1.56284300	0.62875800	H	4.04335800	1.74756100	2.39085900
Si	1.22646300	3.00796700	-1.58286900	C	3.02767200	2.97054200	-2.22650300
H	3.08217600	3.37426900	-3.24661200	H	3.69551400	3.57653600	-1.60142100
H	3.44356200	1.95600600	-2.25432300	C	0.19866500	2.04500100	-2.87496000
H	0.62558400	1.05088200	-3.06151600	H	-0.83768300	1.88570200	-2.54922900
H	0.16862500	2.56684200	-3.84051700	C	0.71708400	4.84962400	-1.75102500
H	-0.31168600	5.01882600	-1.40575300	H	1.37120100	5.48752000	-1.14351700
H	0.77971400	5.20386100	-2.78895400	N	-3.25433500	3.97367200	-0.88821900
C	-3.06890900	4.15178200	-2.33308000	H	-2.79486000	3.19638500	-2.78868800
H	-3.98571300	4.52369100	-2.82721000	H	-2.26001900	4.86196900	-2.52287400
C	-4.30925300	2.98153600	-0.65381100	H	-5.28708500	3.31549200	-1.05066600
H	-4.03131700	2.04276300	-1.13816000	H	-4.41712500	2.76909700	0.41193500
C	-3.56881900	5.26714800	-0.26420000	H	-4.55349700	5.64125900	-0.60783500
H	-2.82489600	5.99115900	-0.61378100	C	-3.59535700	5.24789900	1.26617400
N	-2.31990400	4.88127100	1.90379200	C	-1.33106500	5.96073700	1.78275500

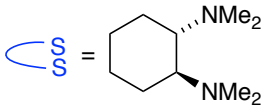
H	-1.68345800	6.89940200	2.24950700	H	-0.40060700	5.65988500	2.27199100
H	-1.10278800	6.16005100	0.73272500	C	-2.54964000	4.57545200	3.32202500
H	-1.60486400	4.29965300	3.79784800	H	-2.97592800	5.43498200	3.87132300
H	-3.23524600	3.72767600	3.41245900	H	-3.93055400	6.24570800	1.60918800
H	-4.35230100	4.53612800	1.61032900	H	-5.06002500	-2.02146200	0.70901700
C	-6.11962600	-0.18682900	0.27905200	H	-5.91682900	0.27029400	1.25269000
H	-6.07364200	0.61201900	-0.47024900	C	-7.48937600	-0.83324100	0.26790900
C	-7.89332000	-1.66514900	1.32361900	C	-9.14298700	-2.28389700	1.31129300
C	-10.0167250	-2.07962000	0.24078200	C	-9.63108200	-1.25080600	-0.81300800
C	-8.37795200	-0.63467500	-0.79730300	H	-8.09015300	0.01765600	-1.61910900
H	-10.3058370	-1.07933200	-1.64767900	H	-10.9919730	-2.55874600	0.23170300
H	-9.43761700	-2.92126300	2.14094700	H	-7.22479300	-1.82073600	2.16779200
H	-5.55916900	-1.05745500	-2.13237700	H	-5.52079500	-2.73105900	-1.52425100
N	0.56715300	-1.99837800	1.61772600	C	0.68509600	-1.41929700	2.95917200
H	1.60074900	-0.82399000	3.03012100	H	-0.16858900	-0.75787100	3.13594300
H	0.69735700	-2.17172200	3.76792300	C	-0.68054600	-2.76731800	1.51851500
H	-1.52073500	-2.10601900	1.75089200	H	-0.81991800	-3.13925500	0.50070700
H	-0.72509900	-3.62043100	2.21742800	C	1.78689300	-2.74826300	1.21827100
H	2.62617300	-2.07647700	1.44843600	C	1.82998700	-3.04366500	-0.30614600
N	1.63650300	-1.82418000	-1.13268500	C	2.84487700	-1.00984300	-1.29727600
H	2.56565400	-0.04009100	-1.71728800	H	3.31658300	-0.82125100	-0.33033900
H	3.59374200	-1.46499000	-1.96872800	C	1.06302000	-2.14268100	-2.44398500
H	0.10122200	-2.64453800	-2.31763800	H	0.87503700	-1.21329200	-2.98997400
H	1.72505300	-2.77055700	-3.06808800	H	0.97259500	-3.68889300	-0.53539500
C	3.10715900	-3.83860100	-0.67489800	C	3.27334300	-5.12654500	0.13943300
C	3.28378900	-4.80253700	1.63576500	C	2.00386200	-4.05441100	2.02638000
H	2.01807600	-3.82286800	3.09772300	H	1.15103100	-4.72697600	1.86443900
H	3.37784400	-5.71808900	2.23352300	H	4.16358200	-4.18457000	1.86867200
H	4.19784600	-5.63920700	-0.15530900	H	2.44705200	-5.81913400	-0.07942300
H	3.09331300	-4.06652900	-1.74767100	H	3.98969800	-3.20922600	-0.50162300

Table S35. 6a with (*S*,*S*)-TMCDA and TMEDA at –78 °C.

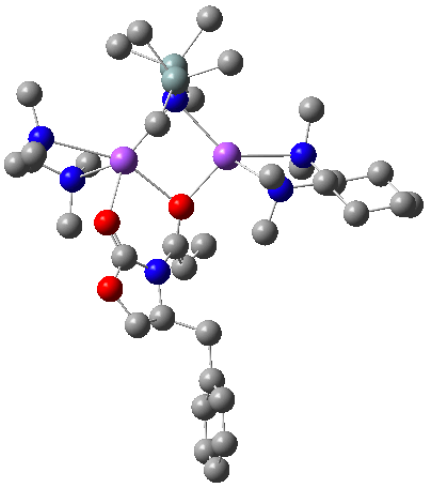




TMEDA



(*S,S*)-TMCDA

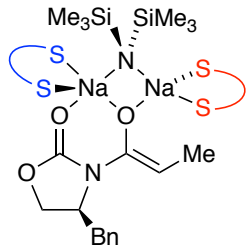


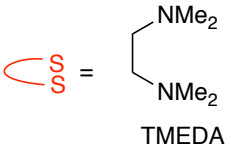
G = –2825.482974
G_{MP2} = –2824.506031

Na	0.00000000	0.00000000	0.00000000	O	-1.68560400	-1.21874700	-1.07344800
C	-2.89879900	-1.17643000	-0.93585600	O	-3.70754900	-1.94318200	-1.72570900
C	-5.07894700	-1.63307500	-1.43640300	C	-5.04863500	-0.91015800	-0.07813500
N	-3.65080900	-0.45844000	-0.04567700	C	-3.03648300	0.32044500	1.04868700
C	-3.61999200	0.22289800	2.27704900	H	-4.45395800	-0.45703700	2.42312600
C	-3.13352700	0.98901800	3.47493200	H	-2.80197700	0.32712800	4.28989200
H	-2.28331300	1.62154300	3.20270100	H	-3.91179100	1.63780000	3.90764900
O	-2.00982900	1.01805600	0.69936200	Na	-1.19643000	3.02140500	0.24381100
N	1.06098700	2.28421800	-0.21163200	Si	2.13348100	2.57041400	1.09092300
C	3.07520800	4.23633400	1.05227600	H	3.67850300	4.37119900	1.96020900
H	3.75788800	4.30011700	0.19567400	H	2.39014300	5.09151200	0.98198100
C	1.17757500	2.57525200	2.74876600	H	1.85103800	2.42810300	3.60329800
H	0.66875100	3.53491100	2.91116200	H	0.41416300	1.78794700	2.78585900
C	3.49524900	1.24237200	1.28616000	H	3.05829600	0.24507400	1.42526000
H	4.13343400	1.19519000	0.39531100	H	4.14256900	1.44406200	2.15026200
Si	1.42810600	2.64093300	-1.84540600	C	3.20747000	2.26114200	-2.43233200
H	3.32414500	2.48339600	-3.50162200	H	3.95179500	2.86002700	-1.89267700
H	3.47193700	1.20669200	-2.28565400	C	0.28553500	1.63488800	-3.00099800
H	0.56366600	0.57311600	-3.00104100	H	-0.76757700	1.67956000	-2.69351600
H	0.34282800	1.98520700	-4.03992300	C	1.17062300	4.48859500	-2.28477000
H	0.17564000	4.84192100	-1.98342100	H	1.90571700	5.11414000	-1.76256600
H	1.27856800	4.67834900	-3.36131500	N	-3.01270000	4.23214100	-1.20987800
C	-2.69865000	4.23392600	-2.64306200	H	-2.30979800	3.25248700	-2.92905600
H	-3.57252500	4.44640300	-3.28343500	H	-1.92488500	4.97680900	-2.85637000
C	-4.03020300	3.21050500	-0.93075900	H	-4.95937400	3.35451600	-1.50847300
H	-3.62171600	2.22682400	-1.17696300	H	-4.28007700	3.19413200	0.13314000
C	-3.35897100	5.59132700	-0.71940900	H	-2.58064400	6.25023900	-1.12865600
C	-3.30570300	5.70983200	0.82761200	N	-2.05348900	5.16451400	1.41475500
C	-0.86802000	6.00431000	1.19529300	H	-0.90095400	6.96245600	1.74022600

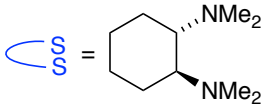
H	0.02104400	5.46305400	1.53317000	H	-0.74044800	6.21469600	0.12982200
C	-2.21058900	4.87250300	2.84468400	H	-1.31446600	4.36398700	3.21190800
H	-2.36000600	5.77345200	3.46480100	H	-3.06173600	4.20154700	2.99471700
H	-4.10734400	5.07752500	1.23231600	C	-3.61532800	7.16745600	1.25426000
H	-3.58961500	7.24314100	2.34756100	H	-2.82760500	7.83277600	0.87599300
C	-4.96656900	7.66486400	0.72682000	C	-5.01919300	7.55139000	-0.79931200
C	-4.72278400	6.11244700	-1.23877800	H	-4.74883700	6.04306600	-2.33225600
H	-5.52483500	5.46174300	-0.86502600	H	-5.99993300	7.86406100	-1.17901700
H	-4.27981300	8.23470000	-1.24241700	H	-5.13348100	8.70117600	1.04608200
H	-5.77887100	7.06724200	1.16606300	H	-5.22518700	-1.62916600	0.73517900
C	-6.08335800	0.22390400	0.02818600	H	-5.88186500	0.77515400	0.95225000
H	-5.92462100	0.91878700	-0.80502200	C	-7.50705300	-0.29254100	0.01503700
C	-8.04723100	-0.92340800	1.14628300	C	-9.34938700	-1.42260100	1.13574600
C	-10.1399280	-1.29727800	-0.00896400	C	-9.61816600	-0.66775600	-1.13932600
C	-8.31323200	-0.17085800	-1.12476700	H	-7.91836300	0.32705400	-2.00792800
H	-10.2267720	-0.55884000	-2.03325500	H	-11.1558530	-1.68275000	-0.01690000
H	-9.74963000	-1.90424700	2.02412000	H	-7.44392200	-1.01454500	2.04714400
H	-5.46454100	-0.98266100	-2.23105500	H	-5.65148900	-2.56178300	-1.42626300
N	0.34500900	-1.84856300	1.85834800	C	0.70915100	-1.27644900	3.15840800
H	1.64415500	-0.71536800	3.07359300	H	-0.07584600	-0.58836900	3.48491100
H	0.83569700	-2.05144200	3.93814200	C	-0.94598900	-2.53782100	1.98018000
H	-1.71204900	-1.82414300	2.29686400	H	-1.25378800	-2.94409000	1.01490500
H	-0.89968400	-3.36525800	2.71403100	C	1.39793000	-2.76348000	1.39064000
H	1.39396100	-3.69733900	1.98655800	H	2.36422200	-2.28352300	1.57694900
C	1.28958400	-3.14085000	-0.09020900	N	1.60573100	-2.04754300	-1.02135800
C	3.04892800	-1.80399000	-1.08510900	H	3.24858300	-0.97974700	-1.77494500
H	3.44022000	-1.51509500	-0.10740400	H	3.60526600	-2.69490700	-1.43576700
C	1.10374600	-2.37645800	-2.36134600	H	0.01528900	-2.46029100	-2.33378100
H	1.36878800	-1.57359400	-3.05613200	H	1.53584500	-3.31849700	-2.75003000
H	1.95112900	-4.01074500	-0.27264100	H	0.27142100	-3.47498900	-0.30873000

Table S36. 6b with TMEDA and (*S*,*S*)-TMCDA at –78 °C.

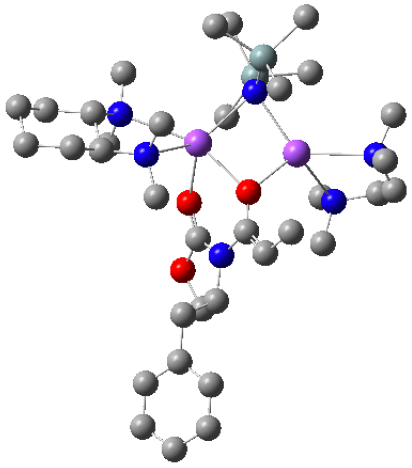




TMEDA



(*S,S*)-TMCDA

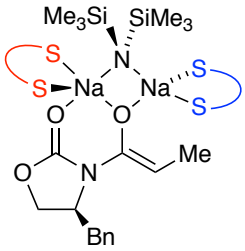


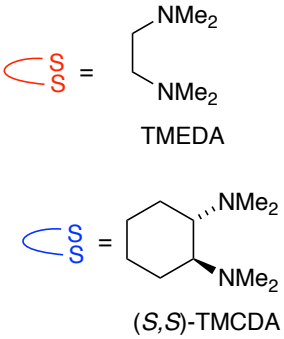
G = –2825.481536
G_{MP2} = –2824.503779

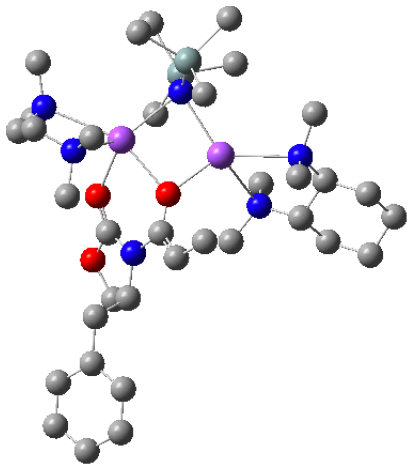
Na	0.00000000	0.00000000	0.00000000	O	-1.60889000	-0.71545200	-1.52068100
C	-2.61829700	-1.37197100	-1.32143900	O	-3.57236900	-1.46786200	-2.30361900
C	-4.55861200	-2.43195700	-1.89899700	C	-4.43403400	-2.47087100	-0.37147300
N	-3.02975300	-2.07051300	-0.21569700	C	-2.21632000	-2.32263300	0.98302700
C	-2.82723400	-2.94245400	2.03580700	H	-3.87346600	-3.21915600	1.98380500
C	-2.10898800	-3.23335700	3.32341700	H	-2.60171600	-2.76393100	4.18894700
H	-2.06025100	-4.31077700	3.55140700	H	-1.08399800	-2.85276700	3.28365100
O	-0.98711300	-1.93939800	0.90237900	Na	0.88787400	-3.04700300	0.41194800
N	2.27608800	-1.12425300	0.00413000	Si	3.01635900	-1.24925000	-1.53592200
C	4.35404600	0.05330600	-1.95178800	H	4.71874300	-0.07582800	-2.97976300
H	3.97388700	1.07826600	-1.86382800	H	5.22260600	-0.02811800	-1.28621500
C	3.90312900	-2.92870500	-1.80536800	H	4.30296600	-3.02481600	-2.82393600
H	4.74237900	-3.04151800	-1.10750500	H	3.22512800	-3.77659700	-1.63735000
C	1.71468100	-1.11614700	-2.92756800	H	0.81036100	-1.69822700	-2.71173700
H	1.38818500	-0.07832500	-3.07550600	H	2.11796400	-1.46366400	-3.88799600
Si	3.11741000	-0.70878100	1.43590200	C	3.41911700	1.16742000	1.65265400
H	3.88663400	1.39555800	2.62004100	H	4.08218300	1.54930100	0.86619200
H	2.48273000	1.73617700	1.59512300	C	4.85020500	-1.49076900	1.66469900
H	4.82357400	-2.58534200	1.58773700	H	5.56311300	-1.13224200	0.91185200
H	5.26565400	-1.24012100	2.65027700	C	2.11339100	-1.27418500	2.96541300
H	2.43368800	-0.75347600	3.87734300	H	1.03552500	-1.10908800	2.84175500
H	2.25136600	-2.34867700	3.14881100	N	1.61963400	-5.25565300	1.59562400
C	3.07647400	-5.33537100	1.42559500	H	3.35313900	-5.22737900	0.37427200
H	3.55048700	-4.51862900	1.97607600	H	3.48485400	-6.29291800	1.79961100
C	1.28951800	-5.31744300	3.02533400	H	0.21185600	-5.19633500	3.16457300
H	1.60132400	-6.27398200	3.48384900	H	1.79394600	-4.50438600	3.55441400
C	0.93462900	-6.34692600	0.88314200	H	-0.09579600	-6.38623000	1.25043900
H	1.39184900	-7.32338600	1.13463900	C	0.93023400	-6.21277800	-0.64160400
N	0.20791000	-5.03626100	-1.14900700	C	0.45904400	-4.88052800	-2.58740500

H	-0.04722100	-3.98310000	-2.95357600	H	1.53032600	-4.76350700	-2.77025000
H	0.09647900	-5.74791900	-3.16957300	C	-1.23775100	-5.15110300	-0.91896500
H	-1.73815900	-4.28840900	-1.36466400	H	-1.65505500	-6.07206300	-1.36864800
H	-1.47323600	-5.14056600	0.14782200	H	1.95937100	-6.15532100	-1.01139500
H	0.50100300	-7.14517100	-1.05815800	H	-4.57598300	-3.48532600	0.00916900
C	-5.40637100	-1.49539300	0.34053700	H	-5.07676000	-1.39537700	1.37949600
H	-5.30279000	-0.50840300	-0.12742500	C	-6.84825600	-1.95025300	0.28095000
C	-7.76974100	-1.33502400	-0.57729600	C	-9.09310900	-1.77580300	-0.64742600
C	-9.51746700	-2.84418100	0.14282500	C	-8.61131500	-3.46474300	1.00603600
C	-7.29132600	-3.02028000	1.07371200	H	-6.59689600	-3.50246600	1.75881700
H	-8.93474500	-4.29240000	1.63198400	H	-10.5470380	-3.18790600	0.09162200
H	-9.79164000	-1.28076700	-1.31700800	H	-7.44994600	-0.49381500	-1.18899100
H	-5.53625900	-2.09798600	-2.25030700	H	-4.31800300	-3.39821400	-2.35869600
N	0.05316300	2.53004300	-0.95743800	C	-0.44201600	3.54977200	0.00334600
C	-1.61352200	3.02811400	0.87861700	N	-1.30000900	1.73966900	1.54742000
C	-2.51151800	1.00920300	1.93075600	H	-3.14698200	0.86330900	1.05153300
H	-2.23476800	0.02194000	2.30856300	H	-3.10535500	1.52235100	2.70878200
C	-0.40865900	1.85875800	2.70623400	H	-0.08913900	0.85872400	3.01432700
H	0.48699100	2.42907500	2.44703400	H	-0.88454500	2.33903100	3.57871300
H	-2.44989500	2.80509700	0.20250600	C	-2.09178900	4.13110100	1.85684100
H	-2.94118900	3.75691900	2.44084000	H	-1.29070300	4.34782000	2.57593100
C	-2.46882400	5.44032200	1.15434600	H	-2.78718300	6.18396900	1.89593600
H	-3.32833500	5.27453400	0.48805200	C	-1.28311000	5.95980400	0.33675700
C	-0.82573300	4.89428200	-0.66584600	H	0.02432800	5.26558000	-1.25036400
H	-1.64254600	4.72179100	-1.37902100	H	-1.54882600	6.88304700	-0.19359900
H	-0.45595200	6.21499200	1.01559500	H	0.40442200	3.74973400	0.67435300
C	1.41946800	2.81886000	-1.40194900	H	1.78193300	1.98728600	-2.01235800
H	1.50011800	3.73909800	-2.00866400	H	2.08276800	2.91299300	-0.53749400
C	-0.81567300	2.32632100	-2.12476400	H	-0.48525300	1.43750700	-2.66814500
H	-1.84472400	2.13975100	-1.80926900	H	-0.80814200	3.17890600	-2.82521700

Table S37. 6b with (*S*,*S*)-TMCDA and TMEDA at –78 °C.





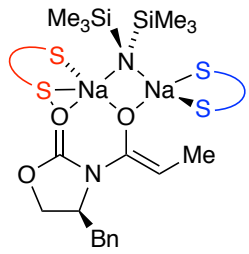


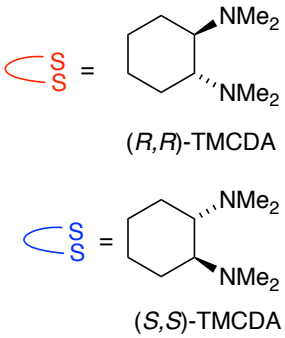
G = –2825.48261
G_{MP2} = –2824.506047

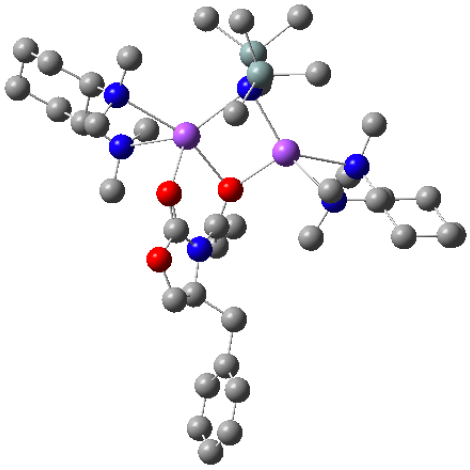
Na	0.00000000	0.00000000	0.00000000	O	1.85919400	0.37922400	-1.34735700
C	2.73430400	1.22535400	-1.24294900	O	3.68126200	1.35666300	-2.22618500
C	4.48965300	2.51090700	-1.93181100	C	4.33706600	2.68219100	-0.41624900
N	2.99583000	2.11271700	-0.23447300	C	2.08204400	2.43083600	0.87377800
C	2.61140000	3.09398600	1.94410100	H	3.66659800	3.33887500	1.97003700
C	1.79348200	3.47437000	3.14591100	H	2.25266600	3.11947300	4.08063400
H	1.67210600	4.56405300	3.26175900	H	0.79362000	3.03423500	3.08355800
O	0.85820600	2.06708800	0.69349500	Na	-1.08932400	3.05296700	0.19675600
N	-2.28957400	0.98896300	-0.15862200	Si	-2.89619600	0.94686200	-1.75819100
C	-3.89277000	-0.61025300	-2.24455900	H	-4.19177900	-0.57591300	-3.30074500
H	-3.30598800	-1.52566100	-2.09720800	H	-4.80864400	-0.71243600	-1.64907400
C	-4.06064700	2.41173700	-2.17179500	H	-4.35057100	2.42047000	-3.23125800
H	-4.98126000	2.35388300	-1.57748500	H	-3.59190200	3.37999300	-1.95040500
C	-1.45508200	1.03498800	-3.01008800	H	-0.74202300	1.83747400	-2.77948500
H	-0.87415400	0.10416100	-3.01659100	H	-1.81924800	1.19937300	-4.03291000
Si	-3.17083000	0.51255700	1.22798800	C	-3.19596900	-1.37740000	1.52206600
H	-3.72668200	-1.63687900	2.44808100	H	-3.69124700	-1.90148700	0.69544200
H	-2.17795600	-1.78087100	1.59873500	C	-5.00997100	1.03629300	1.28219100
H	-5.13107800	2.11742600	1.13936400	H	-5.59617200	0.53942700	0.49858700
H	-5.46814600	0.77561000	2.24583700	C	-2.37541500	1.25413400	2.80404600
H	-2.72625400	0.74240700	3.70988600	H	-1.28057100	1.18003500	2.78040100
H	-2.62846000	2.31608400	2.92465400	N	-2.21785900	5.21712600	1.12166900
C	-3.64641000	4.93840100	1.31073200	H	-4.12789900	4.79043900	0.33928500
H	-3.76258500	4.01545300	1.88522000	H	-4.18157800	5.73881200	1.85149500
C	-1.53907900	5.28439900	2.42320800	H	-0.48158500	5.52761800	2.29130900
H	-1.98387600	6.02035800	3.11333100	H	-1.59347400	4.30456500	2.90740100
C	-2.00108800	6.41188000	0.25964400	H	-2.75838900	6.33693100	-0.53182300
C	-0.61025900	6.40167300	-0.42973800	N	-0.35975400	5.14021000	-1.17605000

C	-1.07634300	5.04188500	-2.45404100	H	-0.98534800	4.02210500	-2.83859300
H	-2.14089500	5.24784500	-2.31588000	H	-0.68774600	5.72540700	-3.22764200
C	1.07181000	4.90223500	-1.38835000	H	1.20570100	3.91258600	-1.83512800
H	1.54333300	5.64319700	-2.05882200	H	1.59622100	4.90649200	-0.42804900
H	0.14931300	6.42269600	0.36362500	C	-0.41620500	7.67545900	-1.29064800
H	0.58995100	7.66891300	-1.72625500	H	-1.12000900	7.65423400	-2.13307000
C	-0.64718000	8.97497100	-0.51160300	H	-0.50614300	9.83740800	-1.17500000
H	0.09980900	9.07054800	0.29030300	C	-2.05127600	8.97998700	0.09847300
C	-2.23746700	7.75301100	0.99813900	H	-3.24215000	7.75403400	1.43730900
H	-1.53151400	7.83505200	1.83490700	H	-2.22177900	9.89575900	0.67818500
H	-2.80109900	8.97430500	-0.70631400	H	4.33318300	3.73532000	-0.12462800
C	5.42359400	1.90994800	0.37842300	H	5.10349000	1.84988100	1.42306400
H	5.45836000	0.88233400	-0.00405000	C	6.79234900	2.54778700	0.27923900
C	7.79737100	1.98953400	-0.52230900	C	9.05141600	2.59470200	-0.62995900
C	9.32095000	3.77384000	0.06494900	C	8.33024700	4.34021100	0.87065300
C	7.07998000	3.73168800	0.97608400	H	6.31930900	4.17541600	1.61538200
H	8.53366100	5.25430100	1.42247900	H	10.2964690	4.24579500	-0.01522200
H	9.81725400	2.14132800	-1.25386100	H	7.59931200	1.06396000	-1.05881400
H	5.51271400	2.30680800	-2.25135300	H	4.09629200	3.36976000	-2.48874900
N	0.22305600	-2.57996300	-0.94401700	C	1.34004600	-3.06777100	-0.12179000
C	1.14521100	-2.88119500	1.38650700	N	1.18368300	-1.47948000	1.83118100
C	2.55510700	-0.95684700	1.83004800	H	2.97044900	-0.98039600	0.82028000
H	2.55074800	0.08485500	2.16141300	H	3.21684900	-1.54095100	2.49819000
C	0.61813100	-1.35286200	3.17783900	H	0.63295100	-0.30170900	3.47954700
H	-0.42056800	-1.69567300	3.18168300	H	1.18240200	-1.93727000	3.92901000
H	0.17958400	-3.30065500	1.68623900	H	1.91800900	-3.47749800	1.90993800
H	2.24102500	-2.53664800	-0.44355400	H	1.52413700	-4.14385800	-0.31259600
C	-0.94425400	-3.45904500	-0.83605900	H	-1.75376100	-3.06512300	-1.45613900
H	-0.71941400	-4.49049400	-1.17009900	H	-1.31033000	-3.49998600	0.19186500
C	0.64125400	-2.49274400	-2.34893000	H	-0.20172700	-2.15165700	-2.95758800
H	1.44974300	-1.76524700	-2.44705100	H	0.97565500	-3.47016900	-2.74615100

Table S38. 6a with (*S*,*S*)-TMCDA and (*R*,*R*)-TMCDA at –78 °C.





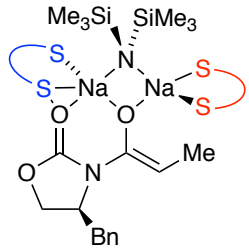


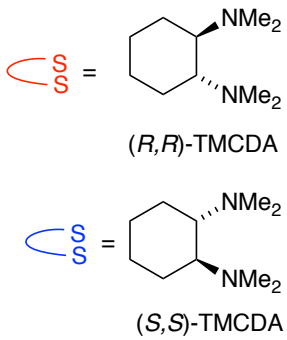
G = –2980.979088
G_{MP2} = –2979.90941

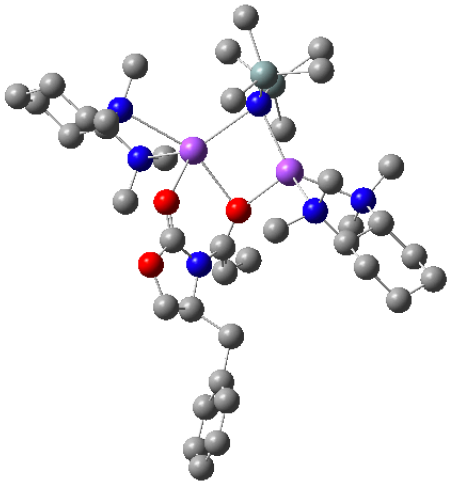
Na	0.00000000	0.00000000	0.00000000	O	1.11116300	1.59101300	-1.25982000
C	2.12807800	2.22140600	-1.02220000	O	2.52969400	3.21589600	-1.86925700
C	3.79820200	3.72650500	-1.43883400	C	3.97007500	3.22213500	0.00622000
N	3.00369900	2.11553300	0.02923800	C	2.72454400	1.27104500	1.20708500
C	3.08906900	1.76348800	2.42582800	H	3.49726500	2.76612200	2.50314800
C	2.90840100	0.99242400	3.70352500	H	2.20648800	1.48254700	4.39597000
H	2.51409500	-0.00621600	3.49335100	H	3.85175000	0.87276800	4.25906300
O	2.16647800	0.13850800	0.94082200	Na	2.50724800	-2.01274500	0.59348400
N	0.21273500	-2.54812900	0.00701800	Si	-0.62037600	-3.30398800	1.29861400
C	-0.51819400	-5.21581500	1.36149800	H	-1.00117800	-5.60416300	2.26840100
H	-1.01760900	-5.68236300	0.50321900	H	0.51974100	-5.57332000	1.36310000
C	0.06677800	-2.72807800	2.98874500	H	-0.59650800	-3.03572000	3.80796600
H	1.05046800	-3.16938100	3.19773900	H	0.18077400	-1.63933600	3.04492900
C	-2.49460200	-2.92765500	1.36191500	H	-2.68899400	-1.84933500	1.43050200
H	-3.00164700	-3.29543100	0.46102900	H	-2.97268700	-3.40419400	2.22822500
Si	0.23806100	-3.17776700	-1.58692400	C	-1.39603100	-3.90775900	-2.26152100
H	-1.27867100	-4.21615500	-3.30926300	H	-1.70831200	-4.79505500	-1.69646900
H	-2.22238400	-3.18886200	-2.22089400	C	0.74520000	-1.81362600	-2.82791000
H	-0.07003800	-1.09769600	-2.99738000	H	1.60388200	-1.22522000	-2.47929700
H	1.00709900	-2.23727400	-3.80646500	C	1.49795000	-4.60736700	-1.80173000
H	2.49382400	-4.33368200	-1.43003000	H	1.17259000	-5.48910200	-1.23520500
H	1.60741000	-4.90968700	-2.85214700	N	4.78546200	-2.22513300	-0.70709800
C	4.60387400	-2.40890300	-2.15163000	H	3.79545200	-1.75925600	-2.49975900
H	5.50490400	-2.16643100	-2.74116300	H	4.31957700	-3.44286000	-2.36545800
C	5.17966200	-0.83729900	-0.43707600	H	6.11204900	-0.54307000	-0.94944200
H	4.38073900	-0.17142800	-0.77318800	H	5.30471900	-0.67081400	0.63567000
C	5.69441500	-3.24690600	-0.12605100	H	5.31579900	-4.21015100	-0.49626600
C	5.64338900	-3.28615000	1.42489700	N	4.25796200	-3.35582400	1.96327000
C	3.63573500	-4.68189900	1.84685300	H	4.09764300	-5.44229300	2.49813200

H	2.58005000	-4.60842600	2.12385900	H	3.68107100	-5.03580500	0.81305100
C	4.19602100	-2.88497300	3.35227200	H	3.15236400	-2.84962300	3.67840900
H	4.74470600	-3.52978500	4.06075800	H	4.60154400	-1.87079100	3.41781100
H	6.04263500	-2.33002100	1.78807100	C	6.57756500	-4.39986400	1.96120700
H	6.54429400	-4.40857300	3.05703500	H	6.20732600	-5.37880900	1.62909600
C	8.02510800	-4.24270700	1.48016200	C	8.07552700	-4.21909200	-0.04951700
C	7.16532200	-3.11451500	-0.59936400	H	7.19899500	-3.11631000	-1.69471200
H	7.56214000	-2.14269600	-0.27607300	H	9.10296200	-4.06605700	-0.40278700
H	7.75287900	-5.19512100	-0.44087800	H	8.64143600	-5.05869500	1.87767400
H	8.44966400	-3.30814600	1.87556600	H	3.65767700	3.99957200	0.71807100
C	5.41928800	2.80734800	0.32303300	H	5.42565800	2.31468900	1.30029400
H	5.73602900	2.06290500	-0.41678100	C	6.36942600	3.98699300	0.31505300
C	6.35055500	4.92399600	1.35981200	C	7.20675400	6.02462800	1.35169200
C	8.10355500	6.20832800	0.29665700	C	8.13748000	5.28222700	-0.74610600
C	7.27653700	4.18270100	-0.73490100	H	7.31588400	3.46093200	-1.54806400
H	8.83582800	5.41192900	-1.56883200	H	8.77361500	7.06376100	0.29103000
H	7.17851800	6.73626600	2.17277400	H	5.66482800	4.78302400	2.19269500
H	4.57685700	3.32833700	-2.10074000	H	3.78395400	4.81448600	-1.52226000
N	-2.41632700	0.76654300	-0.91335700	C	-3.30072500	1.19679300	0.19986100
C	-2.63495000	2.25636300	1.11785700	N	-1.26637300	1.87927900	1.54605900
C	-1.20867600	0.97600400	2.69815700	H	-1.84093700	0.09874500	2.52964500
H	-0.17633900	0.63316400	2.82109800	H	-1.51923500	1.44501900	3.64839700
C	-0.42806700	3.05680300	1.78256200	H	0.58847100	2.73649200	2.03127500
H	-0.38046100	3.66382500	0.87218300	H	-0.79503000	3.69683600	2.60707100
H	-2.50910600	3.16492300	0.51559200	C	-3.57843000	2.62779100	2.28811700
C	-4.94349800	3.13268400	1.80673400	C	-5.60875600	2.08396200	0.91045700
C	-4.69059500	1.70982900	-0.26003700	H	-4.55801900	2.59449700	-0.89781900
H	-5.17727900	0.94897500	-0.88015500	H	-6.56941100	2.45207400	0.52829500
H	-5.83271200	1.18639900	1.50559100	H	-4.81513200	4.06815000	1.24220600
H	-5.58174400	3.37109800	2.66707100	H	-3.73730700	1.74735400	2.92497400
H	-3.09348000	3.38471400	2.91712000	H	-3.46772100	0.29009000	0.79908100
C	-2.97150100	-0.37822800	-1.64044400	H	-2.21065700	-0.77683600	-2.31720100
H	-3.24470000	-1.16920800	-0.93690100	H	-3.85796500	-0.12825200	-2.24983100
C	-2.05955200	1.82980800	-1.86010100	H	-1.57130100	2.65767400	-1.34369500
H	-1.33478400	1.43482800	-2.57714400	H	-2.92413400	2.21821300	-2.42621800

Table S39. 6a with (*R*,*R*)-TMCDA and (*S*,*S*)-TMCDA at –78 °C.





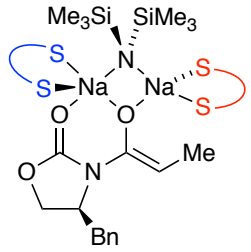


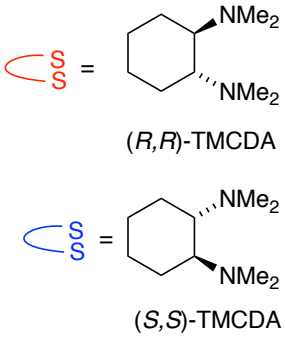
G = –2980.981237
G_{MP2} = –2979.912354

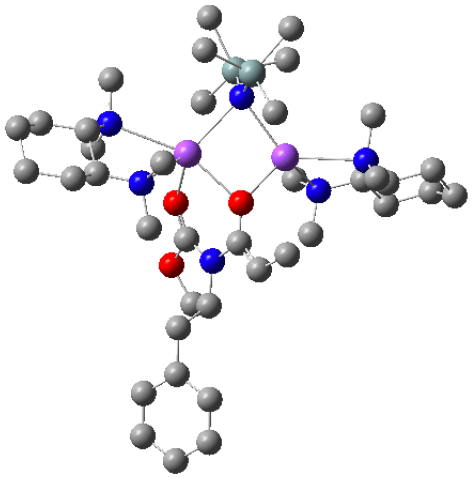
Na	0.00000000	0.00000000	0.00000000	O	1.28110900	1.46211700	-1.30869400
C	2.35181300	2.00458400	-1.08529400	O	2.86432700	2.90651800	-1.97566500
C	4.16985900	3.31304400	-1.54093700	C	4.25919100	2.87919500	-0.06570000
N	3.19181800	1.87173300	-0.01210800	C	2.81103000	1.10278800	1.19264600
C	3.14803600	1.64817400	2.39603900	H	3.60772500	2.63141700	2.42624200
C	2.87480000	0.97821600	3.71328600	H	2.16547000	1.54694100	4.33447400
H	2.44735200	-0.01584500	3.55736100	H	3.78605400	0.86133300	4.31982800
O	2.20153900	-0.00843900	0.95210400	Na	2.35392300	-2.14237400	0.35922300
N	0.00193300	-2.57877200	0.07459000	Si	-0.73110300	-3.06558200	1.54742000
C	-0.80505300	-4.95074600	1.86758000	H	-1.20502900	-5.16087500	2.86882500
H	-1.44485700	-5.47258700	1.14525600	H	0.19199100	-5.40627400	1.80744300
C	0.23293500	-2.35941600	3.04036400	H	-0.37767700	-2.35957400	3.95273700
H	1.12185200	-2.96884800	3.25516300	H	0.57752300	-1.33434000	2.86181300
C	-2.53489900	-2.46086800	1.74587900	H	-2.59990900	-1.36856800	1.66009100
H	-3.18196800	-2.88720900	0.96916100	H	-2.95578500	-2.74197900	2.72065700
Si	-0.21985100	-3.43442500	-1.39331200	C	-1.99707900	-4.01221200	-1.80524500
H	-2.03016100	-4.48498000	-2.79623000	H	-2.35643900	-4.75418200	-1.08102200
H	-2.72147400	-3.18901800	-1.80995400	C	0.32531100	-2.35513800	-2.87529900
H	-0.38703400	-1.54159700	-3.06437100	H	1.30237800	-1.88240000	-2.70879700
H	0.39588200	-2.94243600	-3.80035500	C	0.81676700	-5.04423800	-1.49719400
H	1.87037600	-4.87175700	-1.24178800	H	0.43439800	-5.79448800	-0.79402100
H	0.78831200	-5.48840000	-2.50158400	N	4.39406600	-2.34185500	-1.20911500
C	4.21349400	-3.41052200	-2.20008600	H	3.22527700	-3.30820600	-2.65619400
H	4.96129400	-3.38453100	-3.01024800	H	4.25658800	-4.39285200	-1.72291100
C	4.36314400	-1.03824000	-1.88085900	H	5.17486700	-0.90349900	-2.61775200
H	3.41309600	-0.92969000	-2.41424900	H	4.41634900	-0.23884300	-1.13816600
C	5.59682900	-2.49886200	-0.34482400	H	5.68624900	-1.54884200	0.20023600
C	5.41911200	-3.62393500	0.71084700	N	4.19328000	-3.44149100	1.53721800
C	3.68155300	-4.72104000	2.04146400	H	4.37112700	-5.22344200	2.74299400

H	2.73716400	-4.55229000	2.56816500	H	3.48232900	-5.39810300	1.20479100
C	4.34379400	-2.48452100	2.64414600	H	3.36103300	-2.29012800	3.08265400
H	5.00326200	-2.84777200	3.44940300	H	4.72933100	-1.52917900	2.27772100
H	5.26160700	-4.56136700	0.16194800	C	6.70531300	-3.80187400	1.55521100
C	7.96060000	-4.02684800	0.70518300	C	8.14860100	-2.85953000	-0.26656300
C	6.90559700	-2.70403300	-1.14996400	H	6.81143000	-3.60780000	-1.76632600
H	7.03934800	-1.86744400	-1.84579400	H	9.03467100	-3.01322800	-0.89512700
H	8.32473900	-1.93475800	0.30252800	H	7.87047100	-4.96541000	0.13870800
H	8.83634300	-4.13742500	1.35675900	H	6.86683000	-2.90379600	2.16515700
H	6.56514200	-4.63354300	2.25645300	H	4.00633500	3.72358200	0.59146300
C	5.65031000	2.34556100	0.32332300	H	5.57879200	1.92336800	1.33086700
H	5.90864700	1.52308500	-0.35481200	C	6.71563000	3.42049600	0.26640000
C	6.77571500	4.41887800	1.25096900	C	7.73788800	5.42666000	1.19198200
C	8.66326200	5.45344700	0.14592900	C	8.61928100	4.46414500	-0.83666400
C	7.65273000	3.45822500	-0.77476700	H	7.63156500	2.68572300	-1.54060700
H	9.33878300	4.47159700	-1.65129000	H	9.41529100	6.23650100	0.10109900
H	7.76926300	6.18836600	1.96667400	H	6.06741100	4.39917400	2.07655900
H	4.91756400	2.80180700	-2.15927000	H	4.26681100	4.39023900	-1.68562800
N	-1.28649900	1.76442600	1.47580800	C	-2.67311700	2.02982900	1.00846500
C	-2.75994100	2.18634400	-0.53439500	N	-2.13736700	1.05156400	-1.26307900
C	-2.98814700	-0.13881600	-1.36438700	H	-2.38626400	-0.97395100	-1.73083900
H	-3.84187300	-0.01140300	-2.05235100	H	-3.37390600	-0.42165000	-0.38191200
C	-1.67283900	1.45174600	-2.59518200	H	-0.95149000	2.26719500	-2.50784800
H	-1.15527600	0.60946800	-3.06424400	H	-2.49282200	1.75982900	-3.26946400
H	-2.16334600	3.06682100	-0.80508200	C	-4.21740500	2.47649300	-0.97281500
H	-4.24643900	2.61584300	-2.06035400	H	-4.84456600	1.60233000	-0.75397100
C	-4.82805900	3.69088200	-0.26518000	C	-4.78110500	3.49211000	1.25200300
C	-3.34003700	3.24096600	1.71083200	H	-3.31400200	3.09295700	2.79656100
H	-2.75266800	4.14596300	1.50617500	H	-5.19166600	4.36614100	1.77346600
H	-5.41570600	2.63677900	1.52746100	H	-5.85978900	3.84323700	-0.60685000
H	-4.27149100	4.60120500	-0.53327300	H	-3.24619100	1.13266600	1.28257900
C	-1.25147500	1.28268700	2.86074400	H	-1.91559100	0.42052100	2.97395400
H	-0.23338600	0.96303800	3.10152600	H	-1.54508600	2.04652900	3.60247300
C	-0.36806200	2.90163800	1.32594900	H	0.63792700	2.58161800	1.61351000
H	-0.32987600	3.22707200	0.28360600	H	-0.63688800	3.76539400	1.95807500

Table S40. 6b with (*S*,*S*)-TMCDA and (*R*,*R*)-TMCDA at –78 °C.





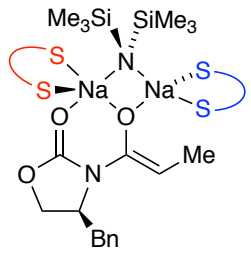


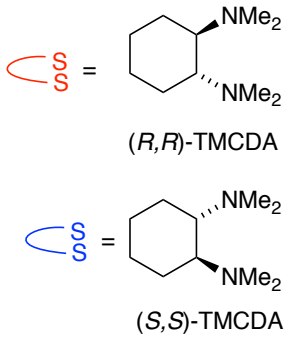
G = –2980.980203
G_{MP2} = –2979.910211

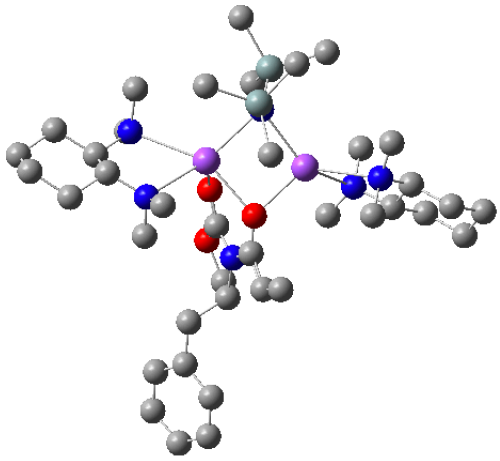
Na	0.00000000	0.00000000	0.00000000	O	0.31374200	1.75013400	-1.50306600
C	0.36107100	2.94801500	-1.27169700	O	0.75344300	3.81841400	-2.25739800
C	0.55020100	5.16440100	-1.79293500	C	0.56759500	5.03361100	-0.26581300
N	0.10011600	3.64899600	-0.12223800	C	-0.51915900	3.09330600	1.09081700
C	-0.55853900	3.89080200	2.19776200	H	-0.12431700	4.88355000	2.17886400
C	-1.17594900	3.44115900	3.49222200	H	-0.45575700	3.45802200	4.32492900
H	-2.01778600	4.07939300	3.80544700	H	-1.54986200	2.41708300	3.40290700
O	-0.98801900	1.89770400	0.96265600	Na	-3.00664900	1.06813800	0.50127400
N	-2.26140000	-1.19254200	0.06264100	Si	-2.82499300	-1.72364100	-1.46614700
C	-2.58056900	-3.57517000	-1.88256200	H	-2.89712500	-3.78385900	-2.91351700
H	-1.53283000	-3.88640900	-1.79245300	H	-3.17057400	-4.22523900	-1.22477800
C	-4.70690800	-1.44079900	-1.70554800	H	-5.04153600	-1.73535000	-2.70941300
H	-5.28194600	-2.02810800	-0.97817900	H	-4.98196200	-0.38680400	-1.56356500
C	-1.96856500	-0.77058300	-2.88403500	H	-1.86934200	0.30086700	-2.67346700
H	-0.95346000	-1.14726500	-3.06563300	H	-2.52117300	-0.87772900	-3.82698700
Si	-2.33236100	-2.14325700	1.48494800	C	-0.92063900	-3.42509400	1.64212900
H	-0.95994100	-3.95634500	2.60265300	H	-0.98564800	-4.17613300	0.84501000
H	0.06634200	-2.95194600	1.56506000	C	-3.92450500	-3.17378000	1.75068300
H	-4.83255900	-2.55919500	1.70462100	H	-4.03070600	-3.96179400	0.99499000
H	-3.90973600	-3.66497400	2.73314000	C	-2.20347900	-1.02200100	3.03268700
H	-1.88685600	-1.59047100	3.91697200	H	-1.49507300	-0.19605700	2.89091100
H	-3.17592000	-0.57365300	3.27996000	N	-5.22935000	1.78425700	1.67999200
C	-5.89079800	0.47373600	1.60987100	H	-6.11442600	0.21178800	0.57235900
H	-5.21379400	-0.28960000	2.00315200	H	-6.82458200	0.42329000	2.19423800
C	-4.95340500	2.13361700	3.07841900	H	-4.38351300	3.06641900	3.12456500
H	-5.86571400	2.24816200	3.69050000	H	-4.34419700	1.34782600	3.53520500
C	-5.96222900	2.87272700	0.97782500	H	-5.53161700	3.80563300	1.36366900
C	-5.73355000	2.86466100	-0.55852400	N	-4.29327600	2.80434700	-0.92134200

C	-4.09014900	2.50826900	-2.34444000	H	-3.02958600	2.30338100	-2.52081200
H	-4.65718200	1.61658500	-2.62656200	H	-4.38570300	3.33513100	-3.01296700
C	-3.52212600	3.99756000	-0.55146100	H	-2.46960500	3.81523200	-0.78037000
H	-3.83425800	4.90641100	-1.09374700	H	-3.58930900	4.18901800	0.52204000
H	-6.16869300	1.93623200	-0.95504900	C	-6.49112900	4.04939700	-1.21165900
H	-6.04746000	4.99481800	-0.87135900	H	-6.35571200	4.01528600	-2.29850400
C	-7.98649500	4.06670500	-0.87498900	H	-8.46576700	4.93175500	-1.35022200
H	-8.47168600	3.17216700	-1.29243100	C	-8.19398300	4.09572600	0.64190700
C	-7.47691200	2.90940000	1.29674600	H	-7.94775900	1.98349500	0.94123600
H	-7.61911400	2.93461800	2.38391300	H	-9.26257000	4.06869500	0.88926900
H	-7.80218600	5.03988500	1.04830500	H	-0.14787600	5.71532800	0.20052400
C	1.97842200	5.24633700	0.34129500	H	1.95859800	4.87879200	1.37185100
H	2.68631300	4.61627100	-0.21156400	C	2.42613100	6.69121200	0.30088400
C	3.37586700	7.13279400	-0.63032600	C	3.76575700	8.47296000	-0.68017000
C	3.20896200	9.39702700	0.20415300	C	2.26367400	8.97095200	1.14025600
C	1.87829100	7.63162900	1.18703400	H	1.14985300	7.30832300	1.92804700
H	1.83020200	9.68177700	1.83902700	H	3.51215400	10.4399200	0.16891700
H	4.50742800	8.79205000	-1.40780800	H	3.82377000	6.41673800	-1.31635300
H	1.34968700	5.79249200	-2.18911600	H	-0.41563000	5.52503400	-2.16675400
N	1.96028300	-1.56500100	-1.00167800	C	3.07039700	-1.81865200	-0.04685100
C	3.44826400	-0.56332600	0.78348900	N	2.27717400	0.07901700	1.43168400
C	2.52429300	1.49487100	1.71700200	H	2.78710400	2.01601600	0.79076300
H	1.61455300	1.95325300	2.11336800	H	3.33573500	1.65945700	2.44955900
C	1.80623600	-0.59620000	2.64594800	H	0.84284500	-0.16776600	2.93915300
H	1.65602700	-1.66278900	2.45943100	H	2.49299100	-0.48902500	3.50339800
H	3.83313200	0.18575300	0.07877100	C	4.59709700	-0.89411700	1.76942800
H	4.86590200	0.00875900	2.33071700	H	4.24182800	-1.62567800	2.50732000
C	5.83471700	-1.47424200	1.07615200	H	6.60977800	-1.69942900	1.81969900
H	6.26443000	-0.72773300	0.39179400	C	5.45588200	-2.73054800	0.28756800
C	4.33745400	-2.41472200	-0.71302100	H	4.06662400	-3.31923300	-1.26966000
H	4.72665400	-1.70006200	-1.45059400	H	6.32715500	-3.13634000	-0.24205600
H	5.12185900	-3.51228500	0.98568900	H	2.68050000	-2.57176300	0.65214500
C	1.35472900	-2.81378400	-1.47313000	H	0.45796200	-2.58229400	-2.05360300
H	2.02394300	-3.41214400	-2.11717900	H	1.05197800	-3.42704600	-0.62010900
C	2.32485600	-0.72583200	-2.15092000	H	1.41814600	-0.45149900	-2.69659400
H	2.78669000	0.20566800	-1.81611500	H	3.00916100	-1.22767400	-2.85648400

Table S41. 6b with (*R*,*R*)-TMCDA and (*S*,*S*)-TMCDA at –78 °C.





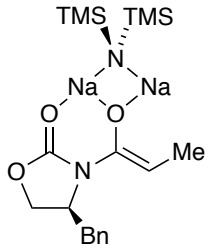


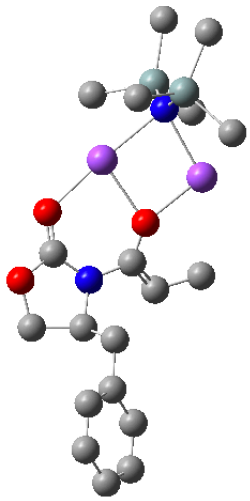
G = –2980.981324
G_{MP2} = –2979.910697

Na	0.00000000	0.00000000	0.00000000	O	0.31656300	1.73190400	-1.52871500
C	0.47625300	2.91614900	-1.27656900	O	0.99524000	3.75165500	-2.23395400
C	0.89745200	5.10712100	-1.76572600	C	0.82437800	4.96803900	-0.24054100
N	0.23884600	3.62584400	-0.12967900	C	-0.45566200	3.11215100	1.06231100
C	-0.51995600	3.93738100	2.14906100	H	-0.07187100	4.92340400	2.12179700
C	-1.16013400	3.51987200	3.44303400	H	-0.45930100	3.58840800	4.28918500
H	-2.02670200	4.14377900	3.71426000	H	-1.50338000	2.48313000	3.38291600
O	-0.94432100	1.92312100	0.94706300	Na	-2.96945900	1.08187400	0.42454600
N	-2.23386800	-1.19578900	0.07716100	Si	-2.80094600	-1.77026400	-1.43512200
C	-2.44174400	-3.60381300	-1.85160600	H	-2.78817200	-3.84359800	-2.86606400
H	-1.37184000	-3.84226700	-1.80687300	H	-2.95476200	-4.28778300	-1.16404700
C	-4.70098100	-1.61872900	-1.63882800	H	-5.02917500	-1.91093500	-2.64561600
H	-5.21665300	-2.26922200	-0.92117900	H	-5.05555100	-0.59500000	-1.46190900
C	-2.02076500	-0.77283900	-2.86762800	H	-1.98388700	0.30619000	-2.67051700
H	-0.98417300	-1.08637200	-3.04865000	H	-2.56841400	-0.92485900	-3.80721600
Si	-2.33190800	-2.11155800	1.52266000	C	-0.90523400	-3.36800300	1.73964000
H	-0.98330000	-3.91190700	2.69067800	H	-0.90946900	-4.10960800	0.93116100
H	0.07373800	-2.87208100	1.72206900	C	-3.92127100	-3.14957200	1.76801100
H	-4.82817300	-2.53521300	1.70055600	H	-4.01298600	-3.94498400	1.01809200
H	-3.92193000	-3.63113000	2.75530600	C	-2.25317000	-0.96131300	3.05146500
H	-1.93885200	-1.50879000	3.94980300	H	-1.55607700	-0.12716600	2.90584700
H	-3.23809200	-0.52976900	3.27633800	N	-5.23341100	1.73901600	1.49175200
C	-5.97461800	0.51265300	1.80754600	H	-6.28698000	0.01912800	0.88231500
H	-5.32088200	-0.17694300	2.34894200	H	-6.86752600	0.68888400	2.43304600
C	-4.69760800	2.33880500	2.72142300	H	-4.16408400	3.26558000	2.49455100
H	-5.47048300	2.55591500	3.47761200	H	-3.97882500	1.64874500	3.17336900
C	-6.04114600	2.67132000	0.65881400	H	-6.58495200	2.03002800	-0.04726700
C	-5.15808900	3.63415600	-0.18025900	N	-4.13923300	2.91172100	-0.98732700
C	-4.67215000	2.25452200	-2.18816000	H	-3.90378200	1.59857200	-2.60759300

H	-5.53592400	1.63370200	-1.93760700	H	-4.97200300	2.96481700	-2.97679500
C	-3.01855000	3.78226300	-1.35855200	H	-2.25427600	3.18033400	-1.85885600
H	-3.30783800	4.59781300	-2.04569500	H	-2.57487600	4.21752600	-0.45842500
H	-4.58309900	4.24990500	0.52482900	C	-6.04234400	4.58931900	-1.01956100
H	-5.40220000	5.28539200	-1.57456300	H	-6.59280400	4.00640000	-1.76977300
C	-7.06161400	5.36435900	-0.17726700	H	-7.66340800	6.01453600	-0.82452000
H	-6.53857500	6.02407600	0.53070000	C	-7.95487300	4.39070800	0.59745100
C	-7.09704600	3.46485700	1.46784800	H	-7.73550100	2.76429700	2.01958200
H	-6.58804800	4.08151300	2.22010200	H	-8.67060800	4.93444600	1.22661300
H	-8.54970900	3.79643700	-0.11171500	H	0.14419500	5.70775800	0.18876500
C	2.21216500	5.06370400	0.44415300	H	2.10165500	4.70652800	1.47280800
H	2.89304900	4.37144400	-0.06652700	C	2.78346700	6.46453100	0.42724400
C	3.82037400	6.81674700	-0.44738100	C	4.32712100	8.11787900	-0.47585800
C	3.80189600	9.09201900	0.37339100	C	2.77052500	8.75495800	1.25317300
C	2.26856400	7.45421800	1.27886900	H	1.47368700	7.19917900	1.97693300
H	2.36049600	9.50489800	1.92467400	H	4.19575200	10.1046000	0.35474600
H	5.13477800	8.36721200	-1.15914400	H	4.24386100	6.06032900	-1.10501800
H	1.77199200	5.65928500	-2.11363600	H	-0.00892700	5.56108400	-2.18417100
N	2.08264100	-0.17811300	1.61089100	C	3.05388500	-1.23053800	1.21661300
C	3.33647300	-1.23586700	-0.31029500	N	2.09513100	-1.27029000	-1.12444600
C	1.49158900	-2.60166600	-1.24683100	H	0.49840300	-2.50217600	-1.69304900
H	2.07522900	-3.29206400	-1.88021600	H	1.36308800	-3.05891400	-0.26280400
C	2.29789900	-0.68893600	-2.45525600	H	1.33885800	-0.63766100	-2.97818800
H	2.66984800	0.33457200	-2.36243500	H	2.99877800	-1.26982100	-3.08242700
H	3.81659700	-0.27900800	-0.55381700	C	4.34870800	-2.35180700	-0.67141800
H	3.89623300	-3.33214700	-0.47217700	H	4.55532600	-2.31747500	-1.74807000
C	5.65545400	-2.25594400	0.12360700	C	5.36230500	-2.29564300	1.62573000
C	4.38598900	-1.17694600	2.00851800	H	4.87941600	-0.21256300	1.82681200
H	4.17344400	-1.21901500	3.08291200	H	6.28817400	-2.19819200	2.20671300
H	4.93023200	-3.27294500	1.88714000	H	6.32917600	-3.07311800	-0.16375600
H	6.17655300	-1.31889600	-0.12312300	H	2.56277300	-2.18215900	1.46516000
C	2.57145800	1.19632000	1.45472500	H	2.85749000	1.38609600	0.41636800
H	1.76216100	1.88461400	1.71119500	H	3.43110900	1.43486000	2.10441400
C	1.57372700	-0.36668700	2.97308800	H	0.74767600	0.33071900	3.14031700
H	1.19090500	-1.38466700	3.09101000	H	2.32997700	-0.18678500	3.75740000

Table S42. 35 at –78 °C.



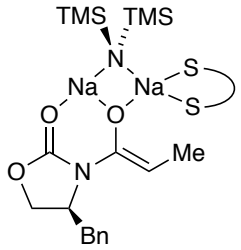


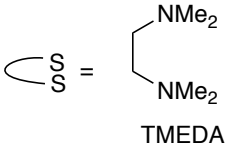
G = –1976.902878
G_{MP2} = –1976.460738

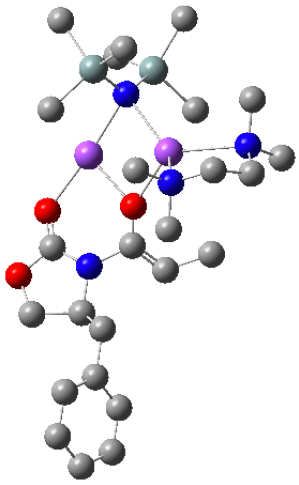
C	0.00000000	0.00000000	0.00000000	O	-1.19301100	0.43280400	0.67945400
C	-2.27134700	0.17576900	-0.11196000	O	-3.40763200	0.29462700	0.33442500
Na	-5.22947500	0.70310900	-0.84648500	N	-7.11941000	0.94599800	-2.26424700
Si	-8.08679800	-0.42591800	-1.97071400	C	-9.95895100	-0.14887500	-1.79604300
H	-10.4808410	-1.09885200	-1.62295000	H	-10.1917110	0.51285200	-0.95259400
H	-10.3884300	0.30632500	-2.69627900	C	-7.85445000	-1.70854500	-3.37933900
H	-8.45183700	-2.61495800	-3.21680400	H	-8.16116900	-1.29248300	-4.35029500
H	-6.80853400	-2.04506800	-3.46575500	C	-7.51835900	-1.32706600	-0.38026700
H	-6.47198500	-1.66482500	-0.43535200	H	-7.61848900	-0.68158900	0.50414800
H	-8.11970800	-2.22528300	-0.18954800	Si	-7.36304000	2.61169900	-2.52534100
C	-6.61806200	3.65649300	-1.10784300	H	-6.73592200	4.73374600	-1.28268400
H	-7.10728000	3.42537500	-0.15172600	H	-5.53876400	3.47906900	-0.98171700
C	-6.40877600	3.15340300	-4.10413200	H	-5.32540600	2.97163300	-4.02159400
H	-6.78217800	2.63262500	-5.00021700	H	-6.52140500	4.22718300	-4.30100100
C	-9.15396800	3.20288400	-2.76309400	H	-9.63374500	2.70543300	-3.61514100
H	-9.76803200	2.99844600	-1.87821700	H	-9.18934400	4.28426900	-2.94821200
Na	-5.54637300	0.34333400	-3.85622200	O	-3.82475500	0.26582100	-2.53977300
C	-2.73614500	-0.43847600	-2.49998100	N	-1.85887700	-0.20651700	-1.35468000
C	-0.40100900	-0.08008700	-1.48285400	H	0.02132700	-0.97698000	-1.94217800
C	-0.00355700	1.15693000	-2.32112800	H	-0.54093100	1.08529800	-3.27358500
H	-0.36380200	2.05765100	-1.80906000	C	1.48712800	1.24596600	-2.56333900
C	2.28392600	2.16209600	-1.86383300	C	3.66374600	2.21943200	-2.07207200
C	4.26966900	1.35702900	-2.98587600	C	3.48700000	0.44091700	-3.69295700
C	2.10947100	0.38798200	-3.48302900	H	1.50454700	-0.31963300	-4.04655900
H	3.94958700	-0.22885900	-4.41323200	H	5.34275000	1.40106600	-3.15112500
H	4.26264900	2.94113500	-1.52281100	H	1.81708100	2.84628000	-1.15833100
C	-2.32031900	-1.32890300	-3.43805400	H	-1.42373000	-1.91736300	-3.28061200
C	-3.11470400	-1.55944500	-4.69417000	H	-2.57962900	-2.21276100	-5.39148000

H	-4.09071000	-2.04300400	-4.50733000	H	-3.31424600 -0.61956900 -5.24000100
H	0.79328200	0.72262700	0.19814500	H	0.29081400 -0.97660400 0.40246800

Table S43. 36a at –78 °C.





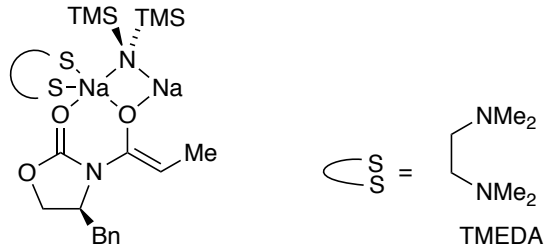


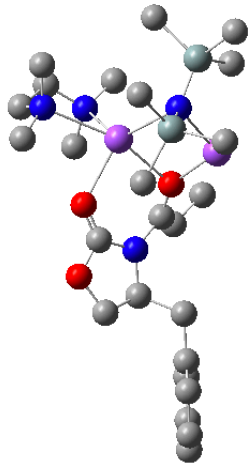
G = –2323.446494
G_{MP2} = –2322.783861

C	0.00000000	0.00000000	0.00000000	O	-1.11496100	-0.89757800	-0.13669500
C	-2.19253700	-0.20350400	-0.59377200	O	-3.28536200	-0.75090300	-0.69551800
Na	-5.19795900	0.36062700	-0.59408500	N	-7.23055900	1.46251300	-0.24165900
Si	-8.21548500	1.30541300	-1.63504000	C	-9.94826600	2.09542700	-1.49931600
H	-10.5068260	2.01527600	-2.44116700	H	-10.5508170	1.61217800	-0.71992000
H	-9.88448400	3.16119000	-1.24226300	C	-7.35907200	2.14676900	-3.12244400
H	-7.90572900	1.95812000	-4.05542900	H	-7.30690200	3.23715600	-2.99790900
H	-6.33081900	1.78783600	-3.26741800	C	-8.48995500	-0.50789900	-2.16986900
H	-7.53665400	-1.01401700	-2.38223900	H	-8.99593800	-1.08436000	-1.38582100
H	-9.10039400	-0.57761500	-3.07995200	Si	-7.69411100	1.15991000	1.37748400
C	-8.97146600	-0.23060300	1.65146600	H	-9.17087200	-0.37865500	2.72111900
H	-9.93155800	-0.01108200	1.16793800	H	-8.61466800	-1.18710700	1.24821000
C	-6.14913600	0.63012000	2.38129500	H	-5.79485200	-0.36786500	2.08080300
H	-5.30932800	1.32873800	2.25803400	H	-6.36376700	0.57055800	3.45617000
C	-8.40736100	2.70504400	2.24760900	H	-7.71371000	3.55447500	2.18122500
H	-9.34650300	3.01479800	1.77115600	H	-8.61532700	2.52942900	3.31128700
Na	-5.71454800	3.35332600	-0.42932400	O	-3.91956600	2.14407500	-0.97052500
C	-2.76160300	2.03357000	-1.54137100	N	-1.84171000	1.08021900	-0.89174000
C	-0.38561400	1.24905000	-0.81467400	H	0.05100700	1.19127400	-1.82176700
C	0.04752200	2.57212300	-0.16000600	H	-0.41220700	3.38707600	-0.72961000
H	-0.36764800	2.60909100	0.85468500	C	1.55262500	2.73375700	-0.11820100
C	2.26778900	3.04997600	-1.28343600	C	3.65628800	3.17769400	-1.25956700

C	4.35739700	2.99376900	-0.06552600	C	3.65892900	2.68397000	1.10172700
C	2.26875300	2.55531300	1.07291000	H	1.73142300	2.32368900	1.99017200
H	4.19413600	2.54539600	2.03749400	H	5.43896500	3.09636500	-0.04517800
H	4.19090600	3.42684200	-2.17248800	H	1.72884300	3.20704200	-2.21547100
C	-2.28424300	2.69359400	-2.62925300	H	-1.29467600	2.44993300	-3.00451200
C	-3.07296100	3.72411100	-3.38614700	H	-3.04567300	3.53891900	-4.46886600
H	-4.12460900	3.71009300	-3.08228300	H	-2.69464100	4.75023700	-3.23952600
N	-4.65949600	4.88732000	1.33905100	C	-4.72535500	4.46944100	2.74401300
H	-4.29506500	3.46940200	2.84964800	H	-4.17261300	5.15612000	3.41130400
H	-5.76688100	4.42879500	3.07534200	C	-3.25979600	4.87350900	0.89164400
H	-2.63801500	5.58765800	1.46306100	H	-2.85649300	3.86616800	1.01410500
H	-3.18648800	5.11673000	-0.17080200	C	-5.27407200	6.21376200	1.18079900
H	-4.65739800	6.99598300	1.66470000	H	-6.22965700	6.20182300	1.71595900
C	-5.50084900	6.63958500	-0.27237200	N	-6.38921100	5.75555500	-1.04661600
C	-7.78229400	5.84996500	-0.58806900	H	-8.17317300	6.88191100	-0.65708900
H	-8.41069400	5.19989000	-1.20317500	H	-7.87485600	5.51258000	0.44733000
C	-6.31312800	6.11189800	-2.46983200	H	-6.96595100	5.45434800	-3.05044500
H	-6.62228800	7.15669200	-2.65502000	H	-5.28861300	5.98172600	-2.83036900
H	-5.89390000	7.67437300	-0.26132600	H	-4.54088600	6.68036700	-0.79690500
H	0.12779700	0.23282000	1.06388500	H	0.89649100	-0.50224400	-0.36627400

Table S44. 36b at –78 °C.



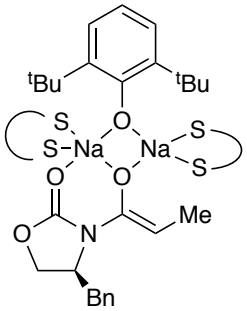


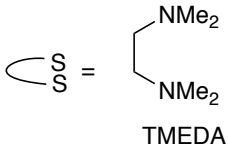
G = –2323.434659
G_{MP2} = –2322.772086

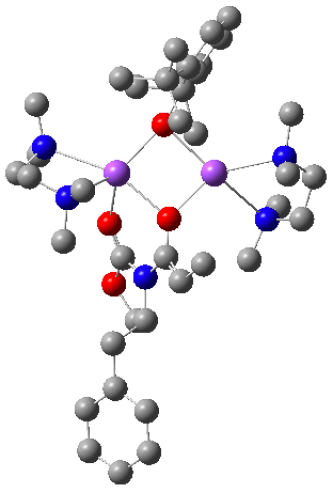
Na	0.00000000	0.00000000	0.00000000	O	1.88918300	0.68818900	-1.18477100
C	3.05625100	0.36497600	-1.00913600	O	3.96038200	0.44534600	-2.02618600
C	5.21664200	-0.09933900	-1.58696400	C	5.11674100	-0.16630400	-0.05006400
N	3.66369300	-0.08018300	0.12831300	C	2.97015000	-0.15741000	1.42009100

C	3.60929700	0.36345100	2.50049800	H	4.56021800	0.86984600	2.36015500
C	3.06369100	0.28519100	3.89854000	H	2.91861500	1.27982400	4.34588700
H	2.09147600	-0.21881100	3.90354100	H	3.73041700	-0.26476400	4.58070700
O	1.81545600	-0.74504600	1.37542300	Na	0.66184900	-2.46832600	1.75537200
N	-1.16868000	-2.26383500	0.42233500	Si	-2.45337200	-2.26409600	1.54913800
C	-3.50425900	-3.85338400	1.64578300	H	-4.29226200	-3.76239600	2.40500300
H	-3.99591400	-4.07506200	0.69042800	H	-2.89389800	-4.72715100	1.90775800
C	-1.72417500	-2.04612000	3.31877600	H	-2.51851100	-1.92812700	4.06679300
H	-1.14252500	-2.92776900	3.63788600	H	-1.07935700	-1.15860700	3.40469000
C	-3.69095400	-0.83095800	1.32751900	H	-3.18257700	0.14158800	1.34132700
H	-4.21010500	-0.91367600	0.36461000	H	-4.45342000	-0.81982200	2.11737600
Si	-1.02596700	-3.18990400	-1.01242000	C	-2.50825700	-3.07913300	-2.20805500
H	-2.34360000	-3.68119900	-3.11133600	H	-3.43582100	-3.43440200	-1.74171600
H	-2.68170100	-2.04425400	-2.52991600	C	0.51063500	-2.63153000	-1.99815600
H	0.43567700	-1.59840900	-2.36092500	H	1.42551800	-2.68885800	-1.39149800
H	0.66248000	-3.27180200	-2.87716300	C	-0.74285500	-5.05424200	-0.68484300
H	0.16307100	-5.22198300	-0.08236500	H	-1.58253200	-5.50321600	-0.14079200
H	-0.61452300	-5.61727600	-1.61882900	H	5.60301800	0.71140000	0.39917400
C	5.73633300	-1.43986300	0.55301700	H	5.47636000	-1.46199200	1.61686800
H	5.26294800	-2.31093500	0.08351000	C	7.23873500	-1.49291700	0.37122600
C	8.07986900	-0.69963400	1.16642100	C	9.46277200	-0.71873200	0.98749800
C	10.0320680	-1.53625700	0.00844700	C	9.20847200	-2.33489300	-0.78548100
C	7.82413100	-2.31174300	-0.60375900	H	7.19041600	-2.94615100	-1.21987200
H	9.64202100	-2.98065100	-1.54463400	H	11.1097460	-1.55461100	-0.12954300
H	10.0970530	-0.09991300	1.61687400	H	7.64567600	-0.06930600	1.93973400
H	5.33513000	-1.09513100	-2.02961100	H	6.01895400	0.54779100	-1.94471600
N	-1.37969400	1.48014000	-1.71592100	C	-1.08212600	2.83841800	-1.23349400
C	-1.31859800	3.03592300	0.26818000	N	-0.38059700	2.29078000	1.12219600
C	-0.88642600	2.19897900	2.49473200	H	-1.86031400	1.69954500	2.50396600
H	-0.18918800	1.60778700	3.09639800	H	-1.00047400	3.19033400	2.97213200
C	0.94859000	2.91704500	1.13338900	H	1.62815800	2.32262200	1.74991700
H	1.36584500	2.94246100	0.12520300	H	0.90936600	3.94850100	1.53204400
H	-1.27173600	4.12044900	0.48624400	H	-2.33332400	2.71415400	0.52479100
H	-1.68624800	3.58898600	-1.77964300	H	-0.03513000	3.04973400	-1.46977300
C	-2.82420000	1.24486300	-1.79400600	H	-3.00888200	0.22058400	-2.12874300
H	-3.29172500	1.35821500	-0.81359600	H	-3.31935100	1.93862400	-2.50003100
C	-0.77464500	1.26892600	-3.03790400	H	0.31127400	1.35880200	-2.96236200
H	-1.01218600	0.25888500	-3.38683500	H	-1.15144100	1.98790700	-3.78947900

Table S45. **7** at –78 °C.





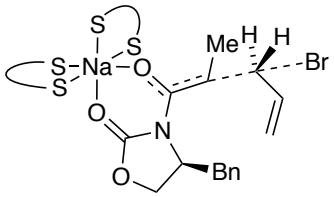


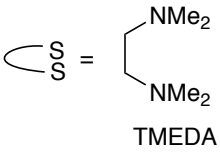
G = –2418.055192
G_{MP2} = –2417.079886

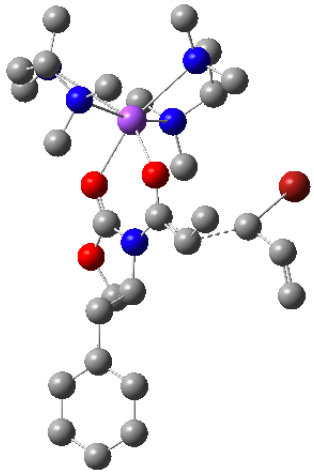
Na	0.00000000	0.00000000	0.00000000	O	-1.76405900	0.37731300	1.46863700
C	-2.75824200	1.06313300	1.28481200	O	-3.72919600	1.13464600	2.25038600
C	-4.69781300	2.12324000	1.85623000	C	-4.54844500	2.19396400	0.33193200
N	-3.13907200	1.80482600	0.19794600	C	-2.26970100	2.15654900	-0.93368900
C	-2.86523000	2.67870000	-2.04671100	H	-3.94098400	2.80081200	-2.09227900
C	-2.07310300	3.09833200	-3.25349800	H	-2.48291100	2.67347400	-4.18151600
H	-2.05611500	4.19157900	-3.40157300	H	-1.03575200	2.76073200	-3.16449600
O	-1.01179600	1.95906500	-0.73638300	Na	0.80052400	3.13248000	-0.20882000
N	1.91852900	5.13653800	-1.34711300	C	3.38185200	4.99240600	-1.28222200
H	3.70250200	4.89632000	-0.24127600	H	3.68852900	4.08124100	-1.79960000
H	3.90326800	5.85371000	-1.73827100	C	1.48638700	5.17744800	-2.75029900
H	0.39701000	5.23874100	-2.81984700	H	1.92004900	6.03974900	-3.29001900
H	1.80015200	4.26087100	-3.25590100	C	1.49414000	6.35083700	-0.63025900
H	1.70867700	7.25425500	-1.23199200	H	2.10406300	6.43237400	0.27501700
C	0.01095900	6.35740200	-0.25083400	N	-0.33293300	5.37439500	0.78927900
C	0.09522600	5.83270900	2.11504500	H	-0.14032200	5.06808700	2.86034400
H	1.17504100	5.99972200	2.14026100	H	-0.40695800	6.77403200	2.40735800
C	-1.77986600	5.13126500	0.80619700	H	-2.00891400	4.37859200	1.56670700
H	-2.35440300	6.04737200	1.04063500	H	-2.10878700	4.74258000	-0.16171100

H	-0.26786900	7.38080400	0.06577900	H	-0.59408300	6.13175500	-1.13493300
O	1.94391600	1.12734800	0.06847000	C	3.22840600	1.42484400	0.10551800
C	3.83559200	1.91841100	1.32071600	C	5.14647900	2.40704800	1.27448800
C	5.90913900	2.37644700	0.10973700	C	5.37350700	1.77678800	-1.02715800
C	4.06688500	1.27655400	-1.06326400	C	3.56717900	0.51705100	-2.31486900
C	3.19754700	-0.92874900	-1.90595900	H	2.43948700	-0.92465200	-1.12062900
H	2.81786900	-1.49270800	-2.76967300	H	4.08091200	-1.45456800	-1.52421600
C	4.64681700	0.40663400	-3.41311000	H	5.54400900	-0.11269100	-3.05862200
H	4.24655900	-0.16556800	-4.25888500	H	4.94987200	1.38825200	-3.79610100
C	2.34373000	1.20371800	-2.96538600	H	1.50900700	1.28438600	-2.26760300
H	2.61217400	2.21006000	-3.31072500	H	2.00827000	0.63802700	-3.84535000
H	6.00352300	1.69763800	-1.90658400	H	6.92314500	2.76788300	0.10273400
H	5.60191300	2.81291400	2.17157800	C	3.09381800	1.82133300	2.67581000
C	2.79310000	0.33290500	2.97381200	H	2.21770200	-0.10487800	2.15508800
H	3.72559500	-0.23270700	3.08653800	H	2.21800700	0.23041800	3.90454400
C	3.93796700	2.36157700	3.85007500	H	4.88819000	1.82721800	3.95477300
H	4.15904700	3.43082400	3.74321700	H	3.38258100	2.23202200	4.78672600
C	1.76453600	2.61260500	2.68730200	H	1.01702400	2.13751600	2.04965400
H	1.35196700	2.65756500	3.70419200	H	1.92850800	3.64509400	2.35395300
H	-4.68701000	3.21234600	-0.03964500	C	-5.50777000	1.22331300	-0.40573400
H	-5.16785800	1.13200500	-1.44205700	H	-5.40824800	0.23135300	0.05203100
C	-6.95165600	1.67474200	-0.36018900	C	-7.88703000	1.03577100	0.46485900
C	-9.21251900	1.47208900	0.52193900	C	-9.62483600	2.55962200	-0.24822700
C	-8.70443900	3.20433000	-1.07808400	C	-7.38237400	2.76434200	-1.13284500
H	-6.67635200	3.26658000	-1.79127200	H	-9.01822000	4.04757300	-1.68791600
H	-10.6559850	2.89992500	-0.20721000	H	-9.92199600	0.95865600	1.16562100
H	-7.57631900	0.17990500	1.06060300	H	-5.68380100	1.79253700	2.18629800
H	-4.44942800	3.07455200	2.34186000	N	-1.09532900	-1.64358100	-1.67037100
C	-0.74114300	-3.00131000	-1.23163400	H	0.27350700	-3.21036400	-1.58566500
H	-1.40007700	-3.75389100	-1.70729700	C	-0.80390100	-3.19898600	0.28686500
H	-1.78554500	-2.88601000	0.65638700	H	-0.72265800	-4.28318900	0.49839200
N	0.21347800	-2.44351500	1.03327900	C	1.53615300	-3.06518100	0.91383500
H	2.27379000	-2.45903400	1.44638300	H	1.55202100	-4.08856300	1.33480100
H	1.84678000	-3.11912800	-0.13234200	C	-0.16300000	-2.34917100	2.44994000
H	0.60670800	-1.79322400	2.99257200	H	-1.10385500	-1.80206900	2.54339500
H	-0.26760000	-3.34466100	2.92116000	C	-2.53823200	-1.40013900	-1.57014800
H	-2.86820200	-1.47902100	-0.53150600	H	-2.75891300	-0.38659200	-1.91620700
H	-3.12033600	-2.11761100	-2.17977200	C	-0.65518800	-1.41080300	-3.04925100
H	-0.88131100	-0.37821700	-3.33072600	H	0.42593300	-1.55703000	-3.12350100
H	-1.15092100	-2.08720600	-3.77094300				

Table S46. **4a** reacting with allyl bromide from favored face at –78 °C.





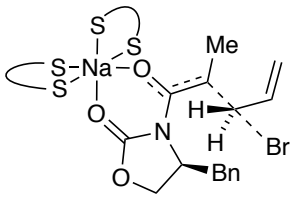


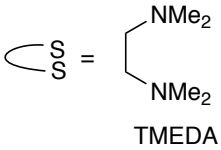
G = –4323.694916
G_{MP2} = –4322.963364

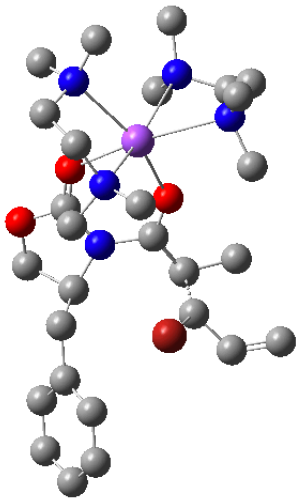
Na	0.00000000	0.00000000	0.00000000	O	1.86983900	0.55007600	1.19894700
C	3.10307500	0.68316500	1.00354200	N	3.65370200	0.13111600	-0.22705300
C	2.93822900	-0.59040300	-1.16124000	O	3.75405000	-0.90204300	-2.21157500
C	4.99607200	-0.18823400	-2.07051200	H	5.80350900	-0.82159200	-2.44037100
H	4.94327400	0.72723500	-2.67042200	C	5.08556400	0.10709700	-0.56903700
H	5.53220900	1.08806800	-0.39454000	C	5.85416700	-0.97834100	0.22460000
H	5.66226000	-0.81286900	1.29016600	H	5.42679100	-1.95595200	-0.03070400
C	7.34186200	-0.96817300	-0.05348200	C	7.93558700	-1.94937300	-0.85867600
C	9.30439100	-1.92108200	-1.13440600	C	10.1030930	-0.90604500	-0.60753900
C	9.52536300	0.07683500	0.19968800	C	8.15844500	0.04407800	0.47357400
H	7.72091600	0.80888700	1.11231000	H	10.1409300	0.86740400	0.62066000
H	11.1685390	-0.88237600	-0.81943000	H	9.74504100	-2.69470400	-1.75772200
H	7.32163700	-2.75098300	-1.26406500	O	1.77767500	-0.96140200	-1.15609000
C	3.96855800	1.43374400	1.81395400	H	5.03147400	1.44188000	1.60583700
C	3.56068000	1.77583700	3.22333800	H	2.49439000	2.01971800	3.27748200
H	3.73371000	0.94401300	3.92413900	H	4.12871400	2.63471300	3.59838200
N	-1.68924200	-2.43268000	-0.74723400	C	-1.33814000	-3.39844400	0.30441600
C	-1.28378600	-2.80906800	1.71605200	N	-0.19856200	-1.84339000	1.91706100
C	-0.35066900	-1.15365100	3.20124100	H	-0.25812500	-1.83955800	4.06481300
H	0.41797400	-0.38006800	3.27994100	H	-1.33521500	-0.67780900	3.25405100
C	1.11860900	-2.49005800	1.87501900	H	1.32233000	-2.88965900	0.87934900
H	1.87896300	-1.73757100	2.08514500	H	1.19839700	-3.30952400	2.61490100
H	-2.22922600	-2.30277000	1.94233400	H	-1.20262700	-3.65189200	2.43167800
H	-0.36255500	-3.82421600	0.05311400	H	-2.04994600	-4.24697200	0.31094100
C	-3.12814100	-2.16956300	-0.75989100	H	-3.45431200	-1.77658100	0.20728400
H	-3.36103700	-1.42020500	-1.52310400	H	-3.72326300	-3.07771600	-0.97732500
C	-1.25933400	-2.93958800	-2.05393300	H	-1.56643800	-2.24221100	-2.83778500
H	-0.16852300	-3.01681800	-2.07680900	H	-1.69534500	-3.92905800	-2.28881600
N	-0.41192500	1.53084000	-2.18123600	C	-1.16333100	0.66293900	-3.08698400

H	-1.46382200	1.18760700	-4.01457700	H	-0.54302900	-0.19500700	-3.36279500
H	-2.06898500	0.28663700	-2.60162900	C	0.82564700	1.96477400	-2.84520700
H	1.45748700	1.09133000	-3.03495200	H	0.62251400	2.46151300	-3.81251000
H	1.35617700	2.67856600	-2.20935300	C	-1.20606200	2.69853200	-1.76428500
H	-0.51514100	3.45507600	-1.38201800	H	-1.71730800	3.15714200	-2.63312900
C	-2.27621600	2.37944900	-0.71776400	H	-2.97138000	1.62774600	-1.11113100
H	-2.87255400	3.29746500	-0.55280400	N	-1.75605000	1.86375000	0.56199400
C	-2.87053400	1.37569600	1.37785200	H	-2.48915400	0.99538400	2.33029400
H	-3.60948400	2.16830400	1.60091700	H	-3.38878300	0.56115000	0.86081000
C	-1.03069000	2.90416800	1.30984900	H	-0.60104500	2.46338600	2.21524800
H	-0.21674300	3.33013600	0.71910800	H	-1.70152000	3.73139300	1.60750600
C	3.24579000	3.41025100	0.65360900	H	3.53653500	2.96749400	-0.28572000
H	2.33007000	3.08226800	1.10840900	C	4.12279400	4.37383800	1.30260800
H	3.73185200	4.84385300	2.20242300	C	5.34806600	4.70191200	0.86563300
H	5.76434200	4.27220700	-0.04307400	H	5.96341900	5.42785800	1.38822300
Br	1.75061800	4.98154900	-0.59495300				

Table S47. **4a** reacting with allyl bromide from unfavored face at –78 °C.



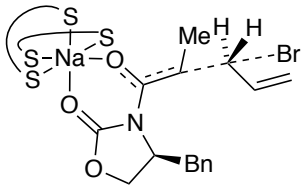


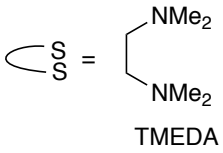


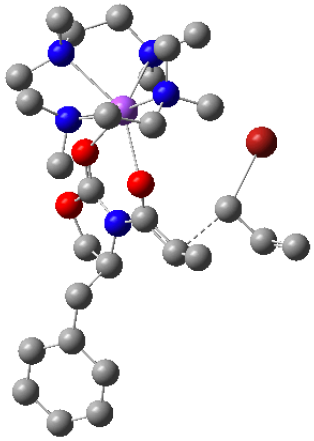
G = –4323.690428
G_{MP2} = –4322.957114

Na	0.00000000	0.00000000	0.00000000	O	1.70172400	0.20894500	-1.56082100
C	2.88196000	-0.19401300	-1.72890500	N	3.30453600	-1.32653900	-0.90793400
C	2.42301700	-2.16785900	-0.26222900	O	3.05821200	-3.33820700	0.04791800
C	4.33805800	-3.35345900	-0.61270900	H	5.03775300	-3.90241800	0.01913200
H	4.23007500	-3.86226300	-1.57826000	C	4.67291800	-1.86605500	-0.76824700
H	5.24753000	-1.68676500	-1.67676700	C	5.40785800	-1.28488100	0.47724600
H	4.92700400	-0.35174600	0.78023600	H	5.24828000	-1.97303100	1.31978400
C	6.89201400	-1.03589900	0.28637400	C	7.74431800	-2.02101700	-0.23412600
C	9.10808800	-1.77519500	-0.39717900	C	9.64437400	-0.53792800	-0.03540700
C	8.80682400	0.44749900	0.48882700	C	7.44120100	0.20298600	0.64899100
H	6.79460800	0.98060600	1.05343300	H	9.21308100	1.41388700	0.77576300
H	10.7066990	-0.34546800	-0.16041000	H	9.75159400	-2.55173500	-0.80299900
H	7.34679800	-2.99534300	-0.51241500	O	1.25618300	-2.00195900	0.04898900
C	3.81850400	0.37647300	-2.60486200	H	4.78175300	-0.10408500	-2.73741000
C	3.34944300	1.24036400	-3.74157600	H	4.06385200	2.04418200	-3.95993400
H	3.21984600	0.66151900	-4.66961700	H	2.38509600	1.70189800	-3.50917400
N	-1.14322100	2.29725900	-0.79601300	C	-1.88636700	2.00227600	-2.03373400
C	-1.33890500	0.82049900	-2.84017400	N	-1.52480400	-0.48892900	-2.19400700
C	-2.93242600	-0.88464500	-2.15601300	H	-3.38389500	-0.93392700	-3.16577900
H	-3.01883300	-1.87547400	-1.69973700	H	-3.52172900	-0.18786400	-1.55354900
C	-0.74798400	-1.51172000	-2.90533900	H	-0.85201300	-2.47199100	-2.39011500
H	-1.08402400	-1.63913800	-3.95191200	H	0.30558200	-1.22797100	-2.89540400
H	-0.26494100	0.94931100	-3.00004300	H	-1.82281800	0.83653100	-3.83717900
H	-2.92810300	1.80785900	-1.75962400	H	-1.90546300	2.89010500	-2.69375200
C	-1.98838700	3.06604000	0.12222300	H	-1.43064900	3.28874500	1.03619000
H	-2.32438500	4.02627400	-0.31199500	H	-2.87507200	2.48300200	0.39266100
C	0.08599200	3.05139500	-1.08342200	H	0.61228600	3.26080500	-0.14725500
H	0.75318300	2.45778000	-1.71085700	H	-0.13013600	4.01337800	-1.58515600
N	0.79136300	0.79470400	2.54039600	C	-0.28051600	0.25322700	3.38811900
C	-0.77645000	-1.14020500	2.99414500	N	-1.53984800	-1.19088800	1.73492800
C	-2.85924200	-0.57145000	1.88004100	H	-2.76399200	0.48769700	2.13256400
H	-3.39982700	-0.64229800	0.93149900	H	-3.46936300	-1.06101600	2.66288000
C	-1.69261700	-2.58882500	1.31189000	H	-2.26712700	-2.62728700	0.38138900
H	-0.70781700	-3.02144100	1.12374800	H	-2.22244200	-3.19839600	2.06759500
H	0.07741000	-1.81537900	2.88594800	H	-1.38695000	-1.53555200	3.82950800
H	-1.11528200	0.96244000	3.36581800	H	0.05178800	0.20462000	4.44392000
C	0.97384900	2.22251400	2.84294700	H	1.19071100	2.39449300	3.91362400
H	1.81325000	2.62080800	2.26661700	H	0.06189900	2.77449900	2.59110800
C	2.06288400	0.09196400	2.78150700	H	2.01691300	-0.92874000	2.39387400
H	2.87214600	0.63097800	2.28152700	H	2.30512200	0.04926300	3.86022900
C	4.42232200	2.01253200	-0.86798400	H	4.82449200	1.13160100	-0.42079100
H	3.35682600	2.17156900	-0.83457000	C	5.29378100	2.89683900	-1.61108200
C	4.87161800	3.96275000	-2.31279600	H	3.82220800	4.24479800	-2.34204800
H	5.56515000	4.60007300	-2.85333800	H	6.35526800	2.65781500	-1.58321000
Br	4.60519300	2.86715600	1.48930600				

Table S48. **4b** reacting with allyl bromide from favored face at –78 °C





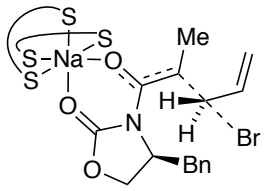


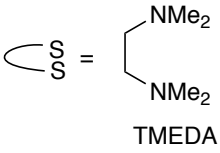
G = –4323.693275
G_{MP2} = –4322.96188

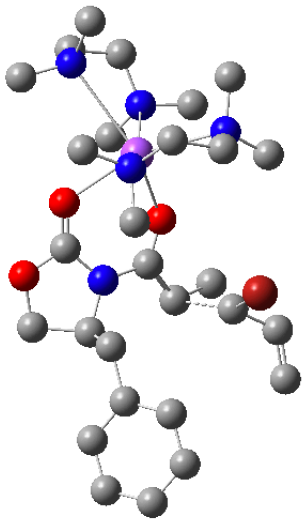
Na	0.00000000	0.00000000	0.00000000	O	1.88180400	0.26768900	1.32894600
C	3.08540000	0.59138000	1.16877700	N	3.70620100	0.27023600	-0.10655300
C	5.15910600	0.23944100	-0.34603100	C	5.18085600	0.12163200	-1.87621500
O	3.91769300	-0.48344700	-2.20514900	C	3.03647300	-0.25851100	-1.19058800
O	1.85559100	-0.52272200	-1.32827500	H	5.98036300	-0.51813800	-2.25233900
H	5.23494100	1.10029600	-2.36573000	H	5.61890900	1.17967000	-0.03526200
C	5.83803000	-0.94605800	0.38145200	H	5.56577300	-0.88462000	1.44096100
H	5.41087900	-1.87880300	-0.00712400	C	7.34288900	-0.94878800	0.22196600
C	7.97829100	-1.83633000	-0.65671400	C	9.36488000	-1.81356200	-0.82194300
C	10.1393760	-0.89874700	-0.10825300	C	9.51974800	-0.01105700	0.77453800
C	8.13517000	-0.03819400	0.93753700	H	7.66308300	0.64872200	1.63728900
H	10.1160230	0.69950200	1.34080600	H	11.2184690	-0.88015600	-0.23396700
H	9.83816300	-2.51353500	-1.50542300	H	7.38231800	-2.56080200	-1.20791600
C	3.85557000	1.34756100	2.06950700	H	4.90394700	1.51630900	1.85169000
C	3.45586400	1.46508400	3.51149200	H	3.69369900	2.46220100	3.90600900
H	2.38286500	1.29261700	3.63546000	H	3.98193800	0.73647900	4.14721800
N	-1.36117900	0.40539200	2.17813700	C	-0.83642500	-0.40056300	3.29690800
C	-1.18379200	-1.89268200	3.29454400	N	-0.65439800	-2.68002900	2.17767600
C	0.80273000	-2.81506700	2.24514600	H	1.14726200	-3.41988800	1.39933700
H	1.28677000	-1.83891500	2.17331500	H	1.13333000	-3.31315700	3.17855000
C	-1.27483700	-4.00316100	2.16592800	H	-2.36193600	-3.90898800	2.06726800
H	-0.90331400	-4.57890800	1.31162300	H	-1.06442000	-4.58540300	3.08458200
H	-0.82896500	-2.29869900	4.26460800	H	-2.27234900	-2.01578900	3.30051100
H	0.24887500	-0.26631300	3.30084000	H	-1.21464300	0.00220100	4.25795200
C	-2.81947400	0.32361200	2.07252200	H	-3.13011900	-0.68840500	1.80286500
H	-3.32838200	0.61125900	3.01217500	H	-3.16070000	1.00175400	1.28393800

C	-0.95965700	1.80492000	2.38773500	H	0.12992200	1.86008500	2.43973600
H	-1.29634300	2.42336200	1.55072300	H	-1.38118600	2.22428100	3.32030800
N	-1.30465000	-1.54794500	-1.57069100	C	-1.43364400	-0.76489100	-2.81032600
C	-1.96605700	0.65550500	-2.59920100	N	-1.05950500	1.54258200	-1.85474100
C	0.07861500	1.96544100	-2.69151900	H	0.71516100	1.11102400	-2.93268800
H	-0.26588500	2.43172700	-3.63344900	H	0.67021600	2.70225500	-2.14038300
C	-1.78982000	2.73759300	-1.40455100	H	-2.59471600	2.44479600	-0.72002800
H	-1.09956600	3.41101100	-0.88836800	H	-2.24324900	3.28937000	-2.24875800
H	-2.91692400	0.61602000	-2.05583500	H	-2.19899400	1.08325000	-3.59365100
H	-0.44322600	-0.71833700	-3.27247200	H	-2.09735700	-1.28018200	-3.53182800
C	-2.60750400	-1.94947900	-1.03637300	H	-2.45427800	-2.47506700	-0.09052100
H	-3.22951600	-1.07335900	-0.83667400	H	-3.15807200	-2.61263400	-1.73070800
C	-0.48106900	-2.73953200	-1.80368000	H	0.51197700	-2.43558500	-2.14204500
H	-0.37287100	-3.28903800	-0.86347400	H	-0.92883400	-3.41864300	-2.55352400
Br	1.35371500	4.76406000	-0.33473700	C	2.90348600	3.31270000	1.08367700
H	3.16525200	2.90606600	0.12465100	H	2.00183200	2.96374000	1.55703200
C	3.74498100	4.31313200	1.70984700	H	4.63642700	4.60567800	1.15720900
C	3.49443500	4.88332200	2.90085500	H	4.16148700	5.62759100	3.32556100
H	2.59296700	4.65525000	3.46316500				

Table S49. **4b** reacting with allyl bromide from unfavored face at –78 °C.







G = –4323.690354
G_{MP2} = –4322.956688

Na	0.00000000	0.00000000	0.00000000	O	-1.63755200	-0.19857400	1.57089800
C	-2.73676900	-0.80026200	1.66902700	N	-3.05472800	-1.76129900	0.61192000
C	-4.39602300	-2.24475200	0.23412800	C	-4.01766200	-3.63348700	-0.29632800
O	-2.68714300	-3.44607900	-0.81424700	C	-2.10284600	-2.40170700	-0.14872200
O	-0.91457500	-2.16604700	-0.29370300	H	-4.65009000	-3.98486200	-1.11292100

H	-3.98322200	-4.38863100	0.49827000	H	-5.03882900	-2.32078700	1.11154800
C	-5.04895000	-1.33880600	-0.84942600	H	-4.61875600	-0.33683300	-0.78264600
H	-4.74676800	-1.71752600	-1.83678900	C	-6.56040200	-1.22875900	-0.77783300
C	-7.38372400	-2.35844300	-0.66075400	C	-8.77218500	-2.23084300	-0.60590400
C	-9.36293700	-0.96764500	-0.67254400	C	-8.55446800	0.16353300	-0.79260800
C	-7.16463700	0.03618000	-0.84460600	H	-6.54172800	0.92557300	-0.93007600
H	-9.00213100	1.15242300	-0.84637500	H	-10.4443300	-0.86734500	-0.63165800
H	-9.39207500	-3.11919900	-0.51449700	H	-6.94425800	-3.35280500	-0.61535800
C	-3.69448900	-0.57269700	2.66585500	H	-4.57925100	-1.20048700	2.70480900
C	-3.28021700	0.06806200	3.96542300	H	-4.13158900	0.55154500	4.45775900
H	-2.86961900	-0.66725200	4.67582700	H	-2.50546200	0.82399500	3.80191500
N	-0.68273100	0.62920000	-2.49680400	C	-0.22439900	2.00508300	-2.74457900
C	-0.58078300	2.99408700	-1.63323700	N	0.04572000	2.68538500	-0.33380700
C	1.46015100	3.06229400	-0.32539600	H	2.01108200	2.51917100	-1.09893400
H	1.60505600	4.14613700	-0.49663800	H	1.90374800	2.81086500	0.64358800
C	-0.66028200	3.39384700	0.74423600	H	-1.73320500	3.19891200	0.67261300
H	-0.29368000	3.04706500	1.71574400	H	-0.51086900	4.48806800	0.68638200
H	-1.66402900	3.01831400	-1.48583900	H	-0.29173500	4.00650700	-1.97528200
H	-0.64136400	2.39553300	-3.69326900	H	0.86342500	1.96934200	-2.87886700
C	-2.14453600	0.52020400	-2.60172200	H	-2.43703000	-0.51286100	-2.39252700
H	-2.65686400	1.17587600	-1.89375500	H	-2.49892500	0.77596400	-3.61818600
C	-0.07179600	-0.28710000	-3.46243000	H	1.01869800	-0.20902600	-3.41287700
H	-0.35671300	-1.31529600	-3.21966500	H	-0.38309400	-0.07289400	-4.50237300
N	2.67065800	-1.18538700	-0.68621300	C	3.19605400	-1.61691400	0.61779300
C	2.96800900	-0.61609400	1.75295100	N	1.55565200	-0.42081200	2.09683800
C	0.96609900	-1.62456100	2.69761200	H	0.94961600	-2.44694800	1.97914200
H	1.52026800	-1.94651700	3.59975900	H	-0.06855200	-1.40579000	2.96308700
C	1.40055200	0.70224300	3.02455000	H	1.83422100	1.60900500	2.58969800
H	0.33466700	0.87242300	3.19847700	H	1.89596900	0.52092200	3.99738800
H	3.38271300	0.35994800	1.47422800	H	3.54787700	-0.96201700	2.63226700
H	2.71685900	-2.56638000	0.87209200	H	4.28090800	-1.82865600	0.55385400
C	3.57704000	-0.23466100	-1.32983400	H	3.14436100	0.10811900	-2.27540400
H	3.72730300	0.64190100	-0.69299600	H	4.56973200	-0.67490800	-1.54598900
C	2.45821500	-2.35049000	-1.55120600	H	1.68086700	-2.98849900	-1.12199900
H	2.11591000	-2.02073600	-2.53539500	H	3.37976800	-2.94624500	-1.69232200
C	-4.43140000	1.43823700	1.44412400	H	-5.02175600	0.75416900	0.86554500
H	-3.36568500	1.46664800	1.31615800	C	-5.08605500	2.22705700	2.47107500
H	-4.46788200	2.95234700	2.99586400	C	-6.38241800	2.09988500	2.79799200
H	-6.83521500	2.70546100	3.57747500	H	-7.03065300	1.39452000	2.28327900
Br	-4.43688200	2.97237800	-0.54675300				