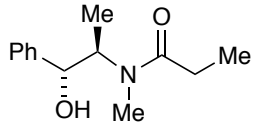
Disodium Salts of Pseudoephedrine-Derived Myers Enolates: Stereoselectivity and Mechanism of Alkylation

Yuhui Zhou, Ivan Keresztes, Samantha N. MacMillan,
and David B. Collum*

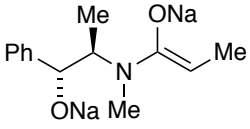
Department of Chemistry and Chemical Biology
Baker Laboratory, Cornell University
Ithaca, New York 14853–1301
E-mail: dbc6@cornell.edu

Table of contents:

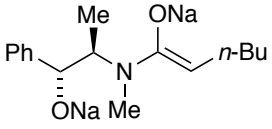
Chart 1. Substrates and aggregates



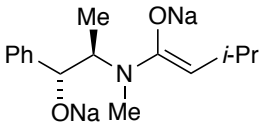
1



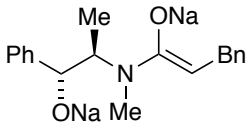
8



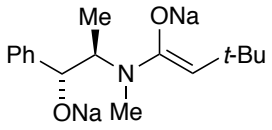
14



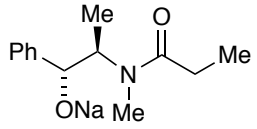
15



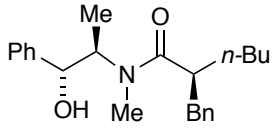
16



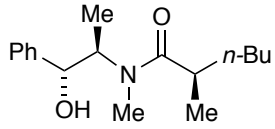
17



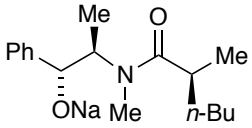
22



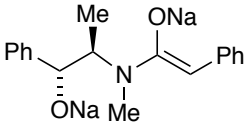
29



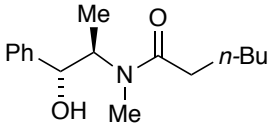
30



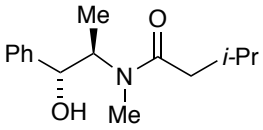
31



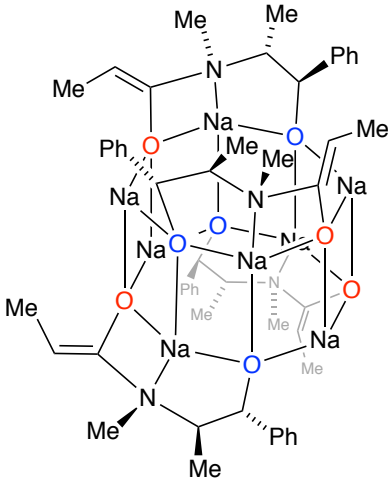
32



33



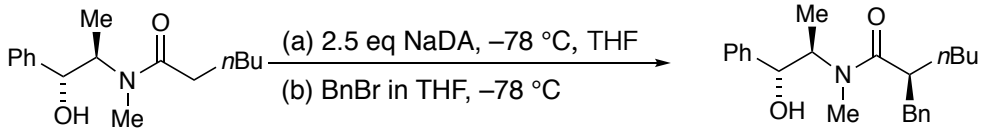
34



35

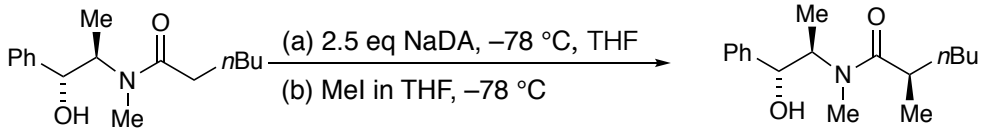
Part 1 Alkylation reactions

Synthesis of 29: alkylation with BnBr



Alkylation carried out with NaDA from glovebox:
Solid sodium diisopropylamide (NaDA, 61.6 mg, 0.25 mmol) was dissolved in 300 μL of tetrahydrofuran (THF) at 0 °C. 150 μL of the NaDA solution was added to a dry 5 mL Kimble vial equipped with a magnetic stir bar and 26.3 mg (0.10 mmol) of **33** at –78 °C in a dry ice acetone bath. The mixture was stirred at –78 °C for 20 min to dissolve. 50 μL of BnBr (0.20 mmol, 4.0 M in THF) was then added to the reaction mixture. The reaction was stirred at –78 °C for 10 min. Saturated aqueous ammonium chloride solution (0.2 mL) was added, and the resulting biphasic mixture was partitioned between water (0.2 mL) and ethyl acetate (2 mL). The aqueous layer was separated and extracted further with three 1 mL portions of ethyl acetate. The combined organic layers were dried over anhydrous magnesium sulfate and then concentrated. Purification of the residue by flash column chromatography (50 % ethyl acetate in hexanes) afforded 26 mg (73%) of product **29** as a white crystalline solid whose spectral properties were found to be in accordance with those previously reported.

Synthesis of 30: alkylation with MeI



Alkylation carried out with NaDA from glovebox:
Reaction was carried out according to synthesis of **29**. Enolization of **33** (26.3 mg) with NaDA (1.67 M, 150 μL) and addition of MeI (4 M, 50 μL, 4 equiv) followed by stirring at –78 °C for 30 min afford product. Purification of the product by flash chromatography (50 % ethyl acetate in hexanes) afforded 23.6 mg (85 %) of product **30** as a white crystalline solid whose spectral properties were found to be in accordance with those previously reported.

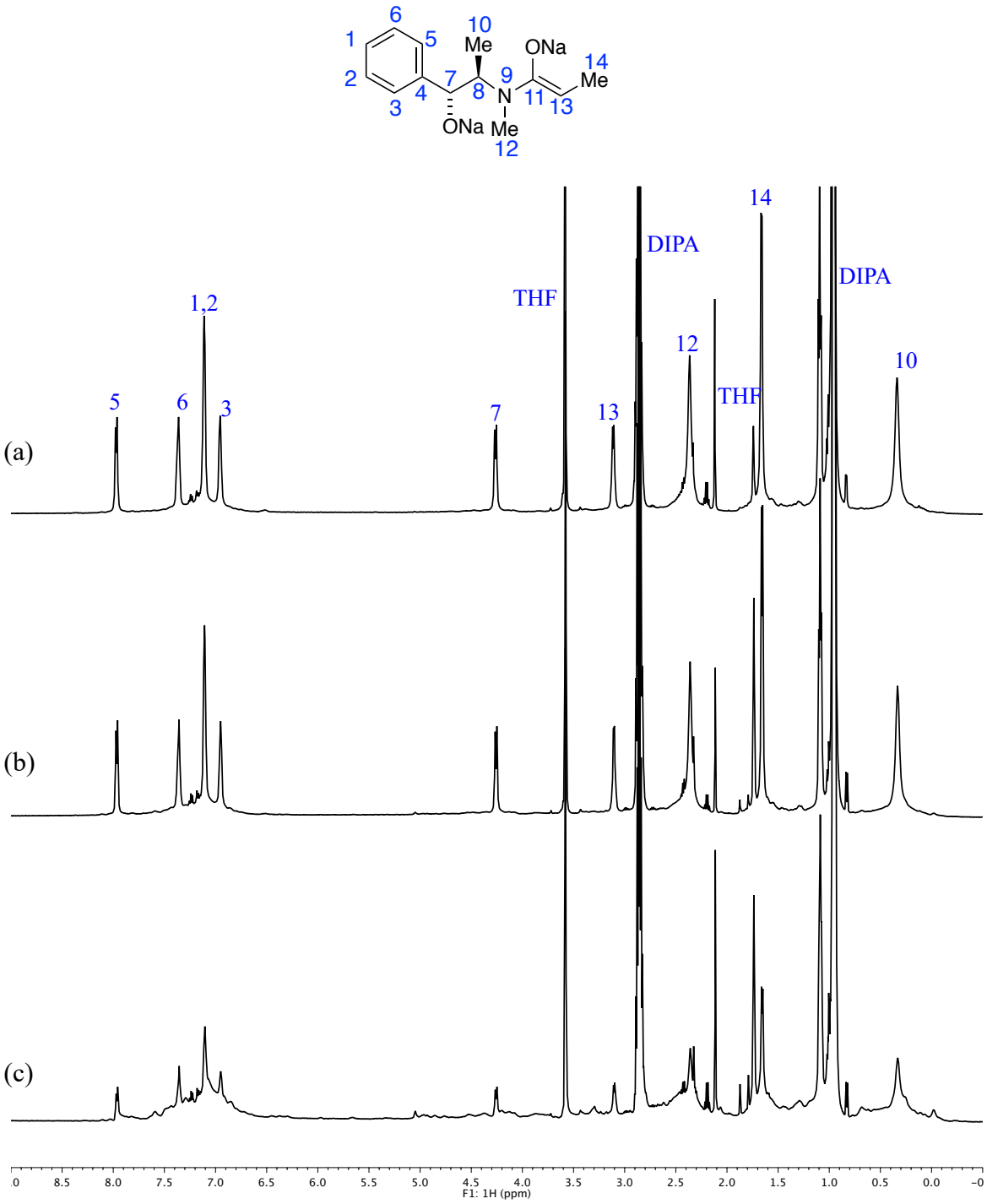


Figure 1. ^{1}H NMR spectra of a solution of 0.30 M **8** in 12.3 M THF-d_8 with varying aging time. (a) aged at –80 °C for 1 day, (b) aged at –80 °C for 7 days, and (c) aged at –80 °C for 14 days. The disodium enolates decompose even at –80 °C after 2 weeks.

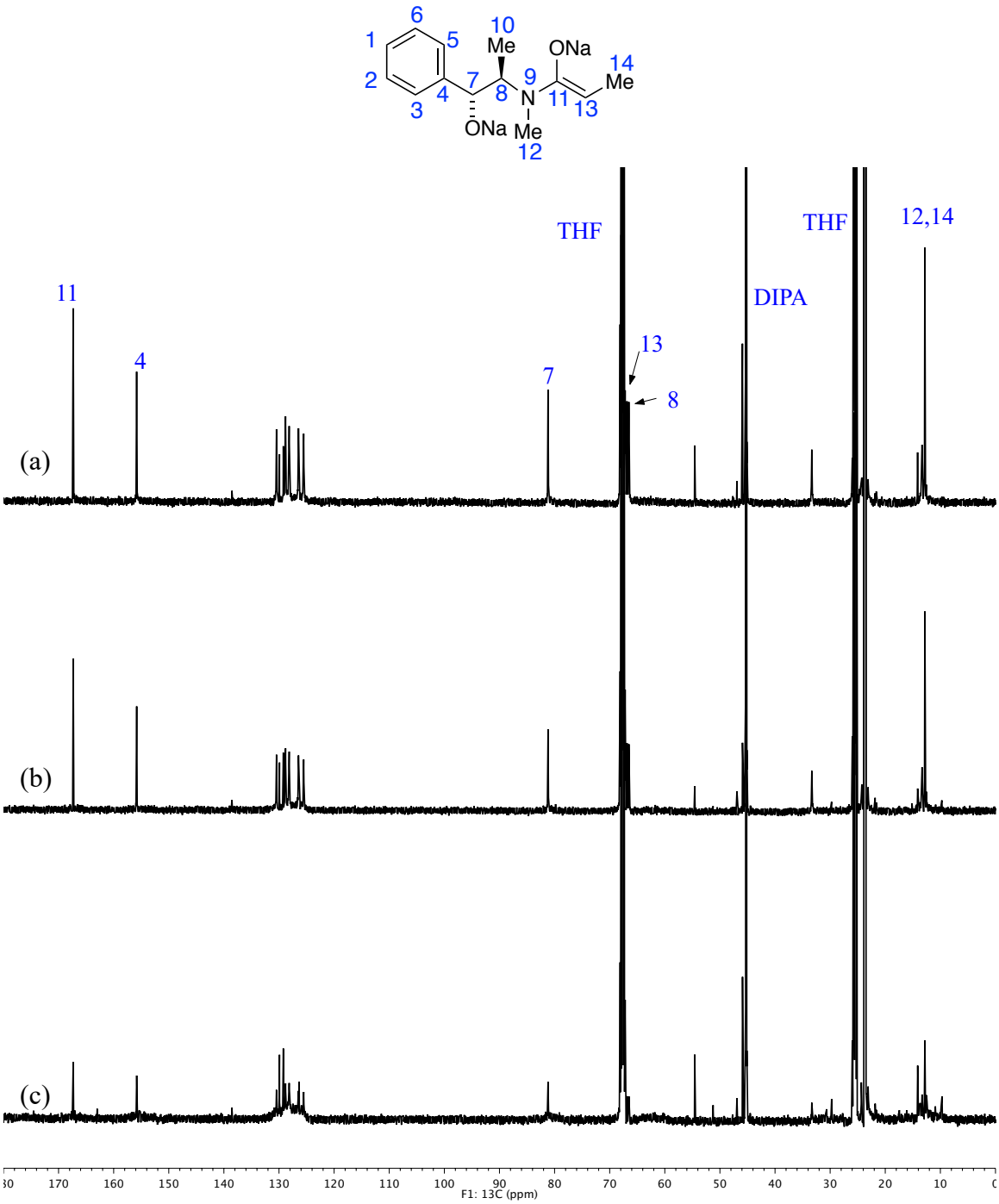


Figure 2. $^{13}C\{^{1}H\}$ NMR spectra of a solution of 0.30 M **8** in 12.3 M THF-d_8 with varying aging time. (a) aged at –80 °C for 1 day, (b) aged at –80 °C for 7 days, and (c) aged at –80 °C for 14 days. The disodium enolates decompose even at –80 °C after 2 weeks.

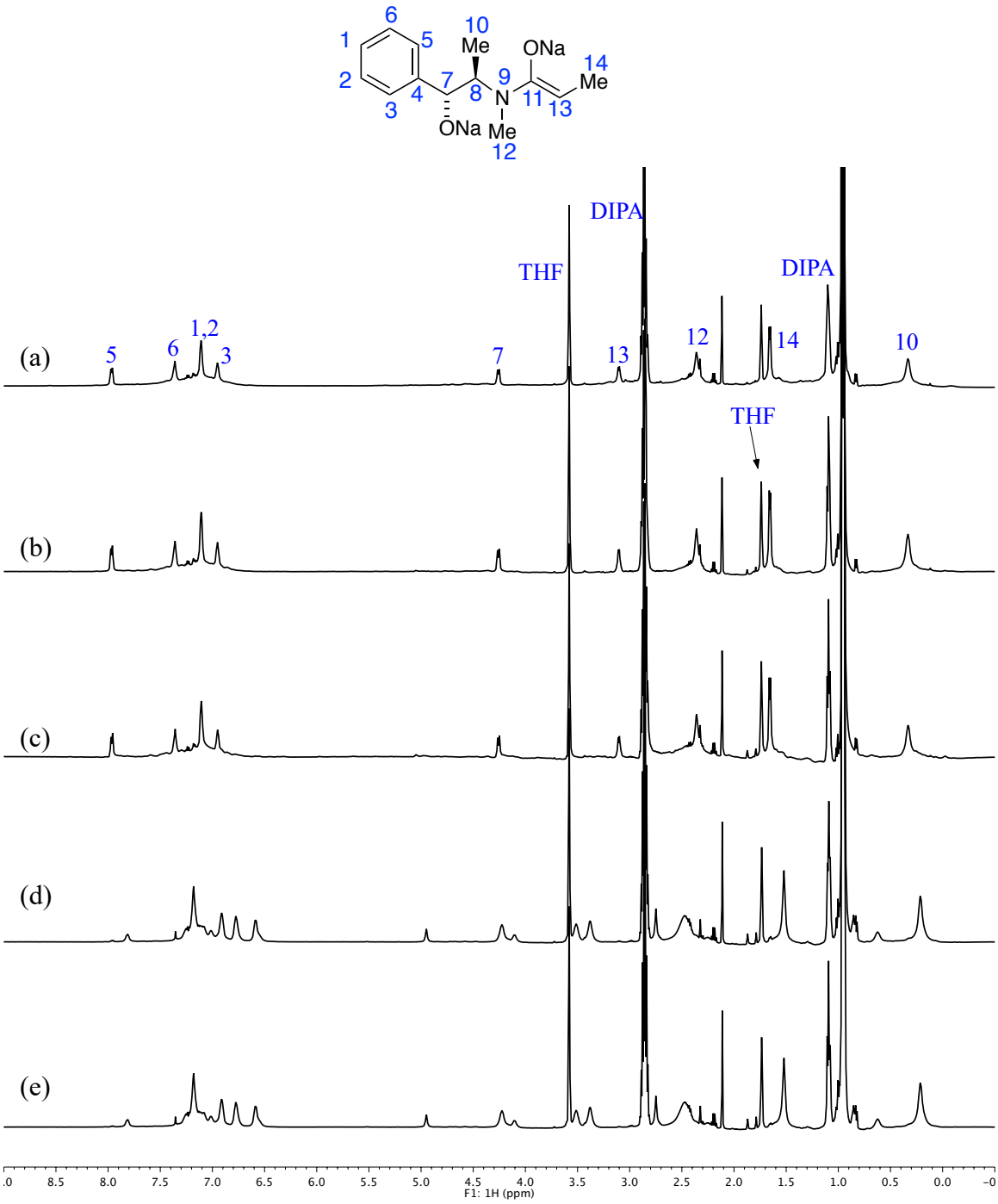


Figure 3. ^{1}H NMR spectra of a solution of 0.30 M **8** in 12.3 M THF-d_8 with varying aging temperature and time. (a) aged at –80 °C for 2 h, (b) aged at –55 °C for 30 min, (c) aged at –30 °C for 30 min, (d) aged at 0 °C for 30 min, and (e) aged at 20 °C for 30 min. The disodium enolates decompose at above –30 °C.

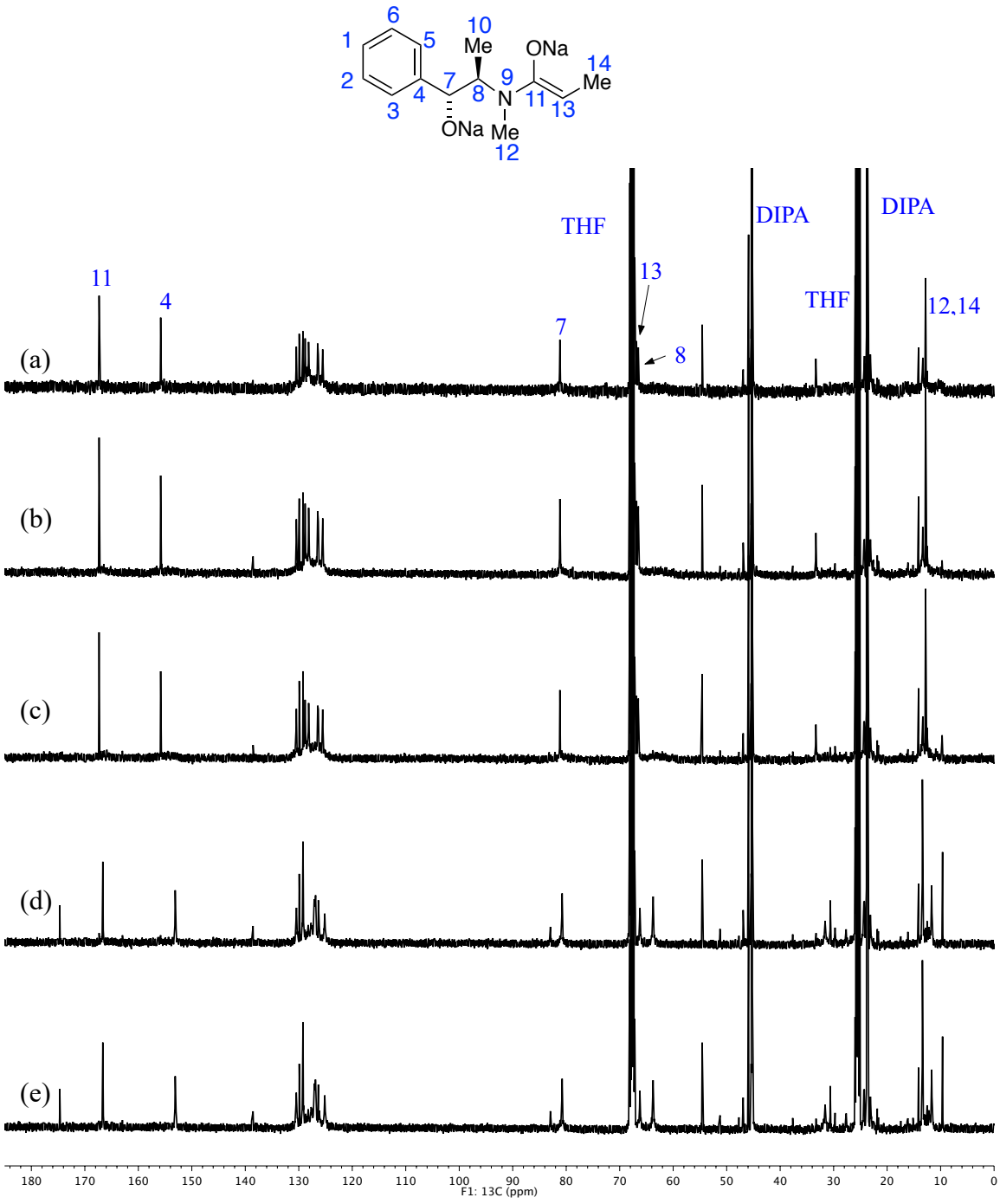


Figure 4. $^{13}C\{^{1}H\}$ NMR spectra of a solution of 0.30 M **8** in 12.3 M THF-d_8 with varying aging temperature and time. (a) aged at –80 °C for 2 h, (b) aged at –55 °C for 30 min, (c) aged at –30 °C for 30 min, (d) aged at 0 °C for 30 min, and (e) aged at 20 °C for 30 min. The disodium enolates decompose at above –30 °C.

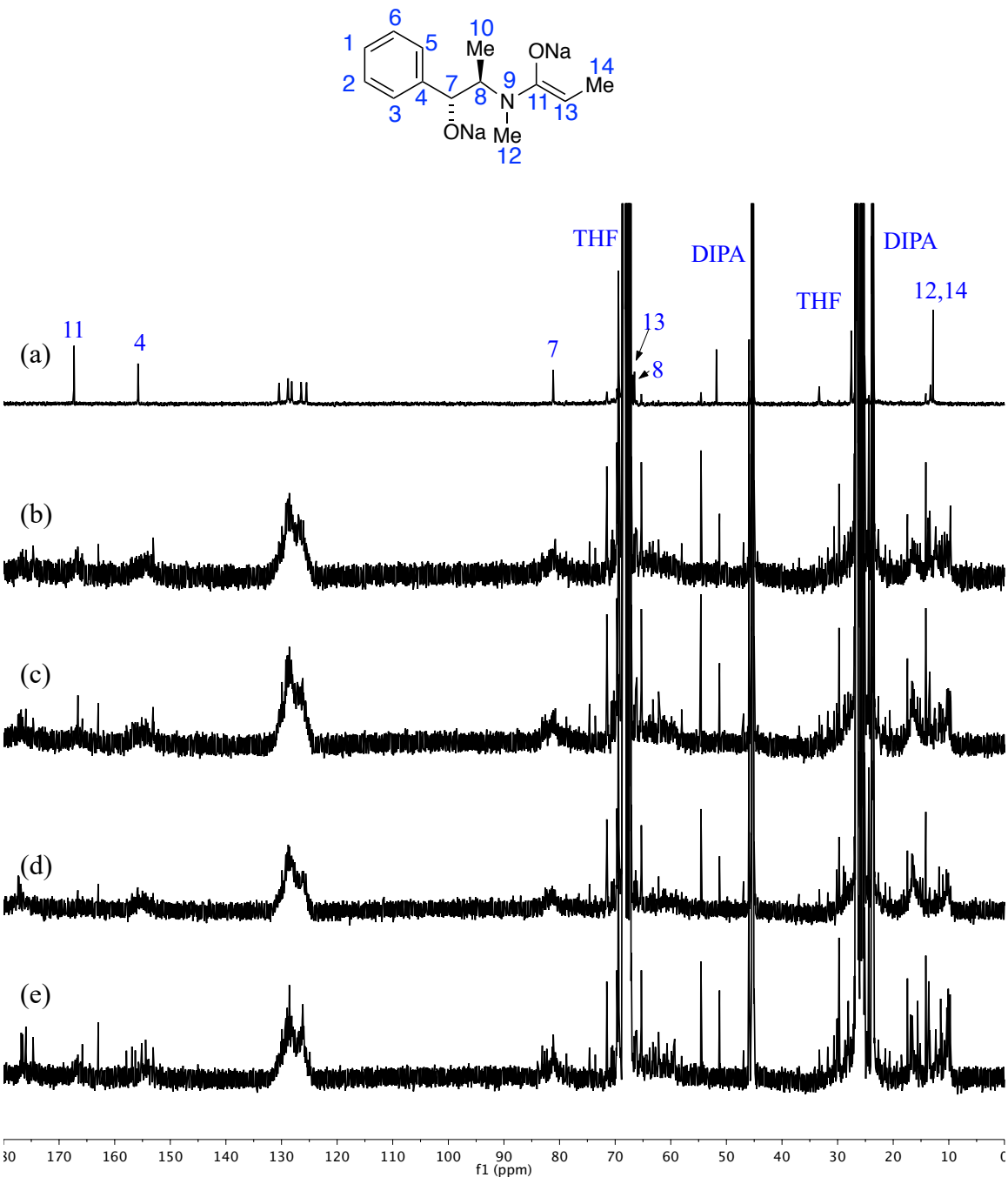


Figure 5. $^{13}C\{^{1}H\}$ NMR for a solution of 0.25 M **1** in neat THF with 0.50 M NaDA (2 equiv) at –80 °C with different aging time, (a) aged at –80 °C for 12 h; (b) aged at 0 °C for 5 min; (c) aged at 0 °C for 20 min; (d) aged at 20 °C for 10 min; and (e) aged at 20°C for 30 min.

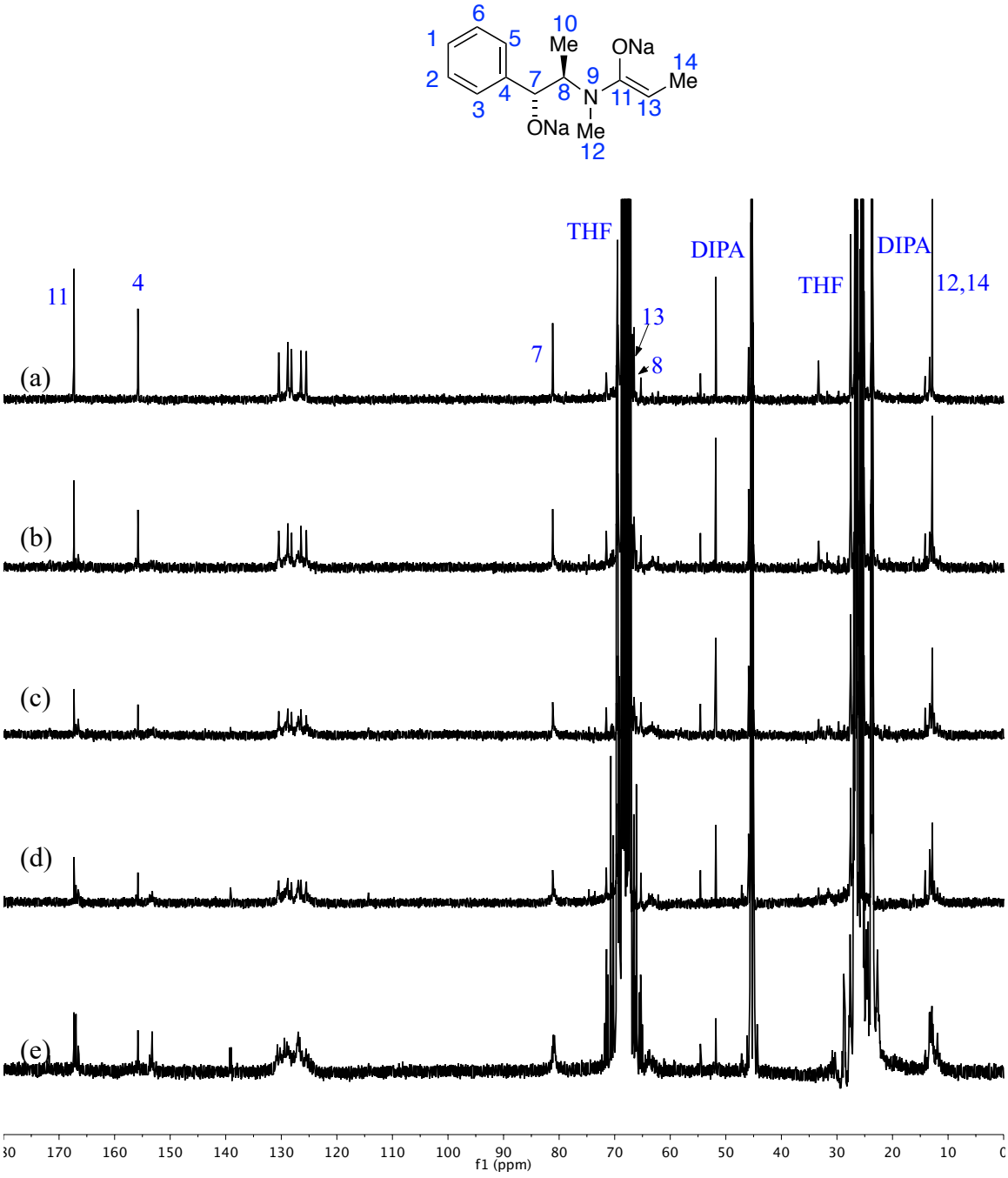


Figure 6. $^{13}C\{^{1}H\}$ NMR for a solution of 0.25 M **1** in neat THF with 0.625 M NaDA (2.5 equiv) at –80 °C with different aging time, (a) aged at –80 °C for 12 h; (b) aged at 0 °C for 10 min; (c) aged at 20 °C for 20 min; (d) aged at 20 °C for 50 min; and (e) aged at 20°C for 90 min.

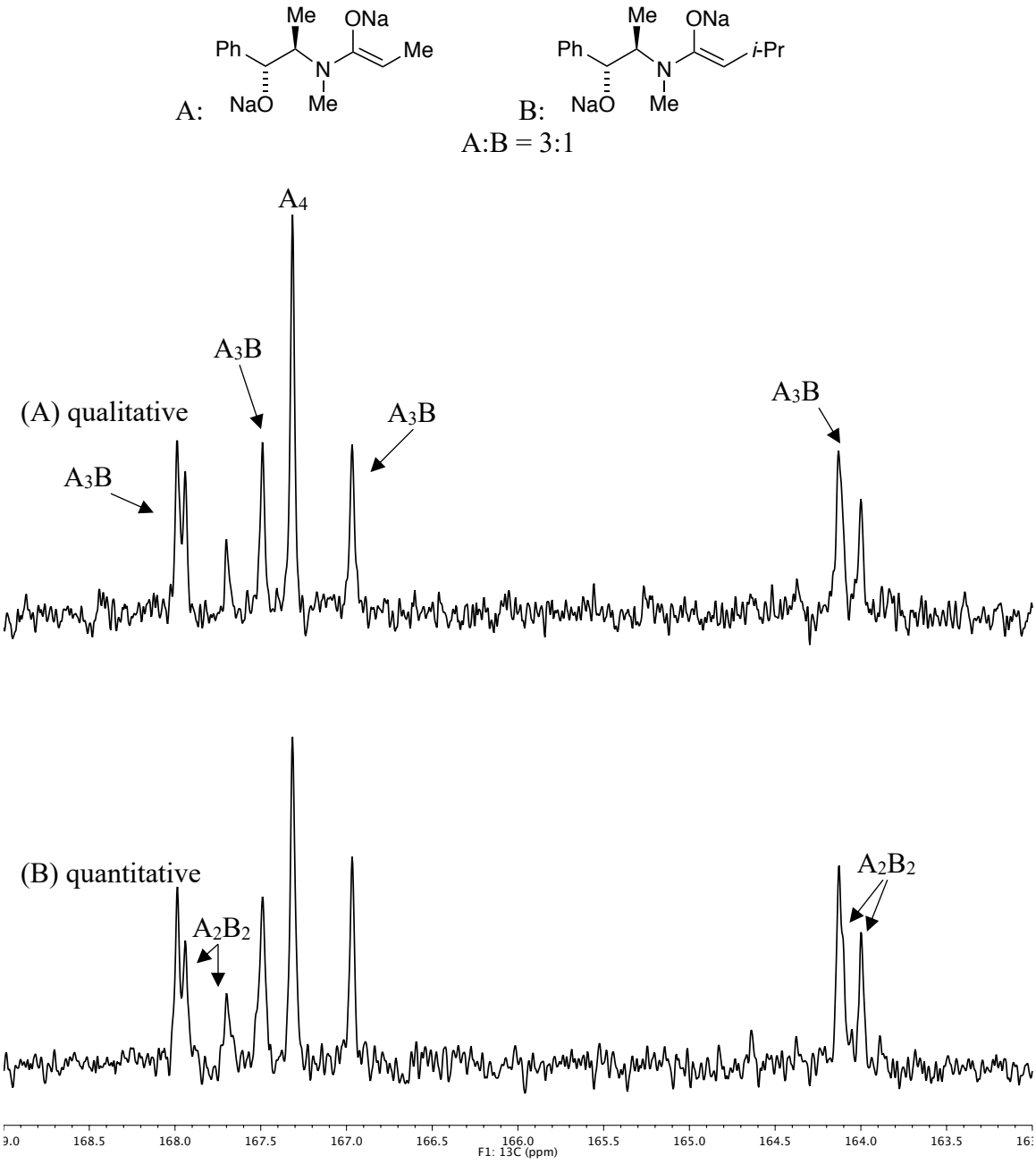


Figure 7. Partial $^{13}C\{^{1}H\}$ NMR spectra for 0.25 M solutions of 3:1 **8** (A) and **15** (B) in 12.3 M THF at −80 °C with different relaxation delay (A) 1 s, qualitative; (B) 60 s, quantitative. The region shown corresponds to quaternary enolate carbon. For the qualitative spectrum A_4:AB_3:A_2B_2=22:54:24; For the quantitative spectrum A_4:AB_3:A_2B_2=25:50:25. Longer relaxation does not improve integration of spectra obviously.

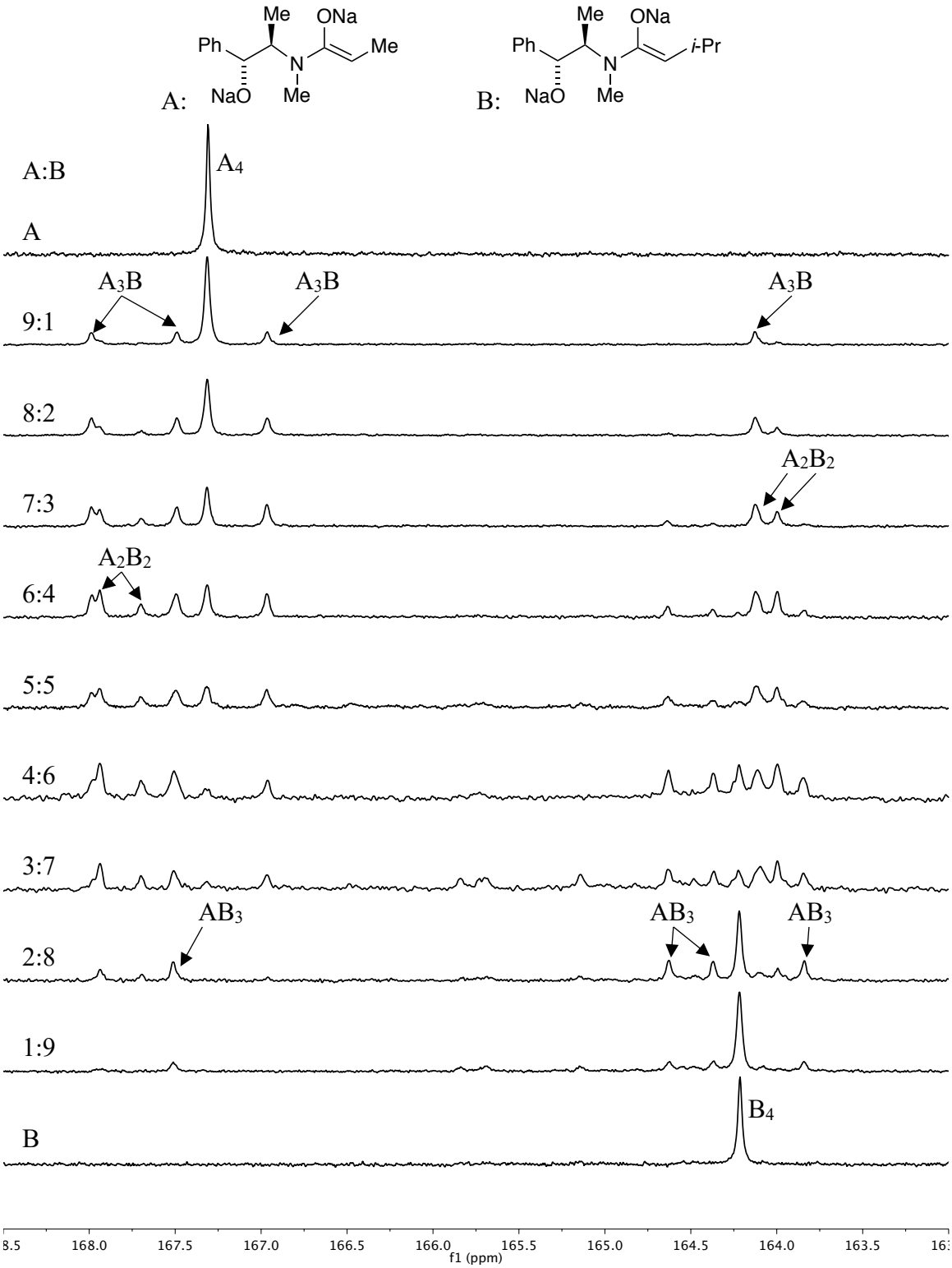


Figure 8. Partial $^{13}C\{^{1}H\}$ NMR spectra for 0.25 M solutions of **8** (A) and **15** (B) in 12.3 M THF at −80 °C. The region shown corresponds to quaternary enolate carbon. The combination of **8** vs **15** gives clear resolution. There are three heteroaggregate species corresponding to tetramer assignment. Peaks between 166.5 ppm and 165.0 ppm are resulting from decomposition of enolate **15**.

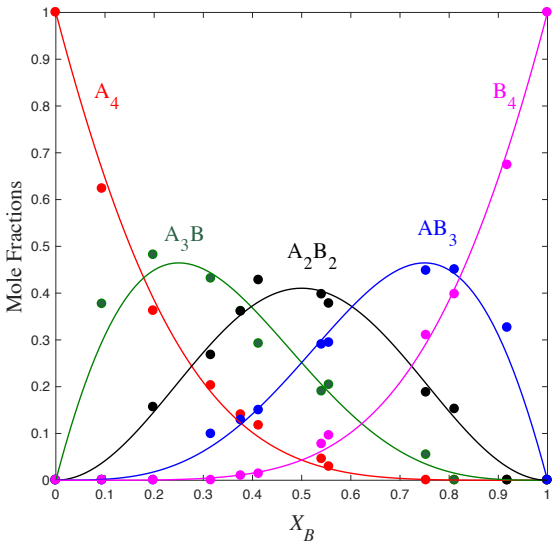


Figure 9. Job plot showing the relative integrations of octasodiated homoaggregates (**A_4**/**B_4**) and heteroaggregates (**A_3B**, **A_2B_2**, **AB_3**) versus measured mole fractions of **15** (X_B) for 0.25 M mixtures of sodium enolates **8** (**A**) and **15** (**B**) in neat THF at –80 °C. The curves result from a parametric fit to a tetramer model.

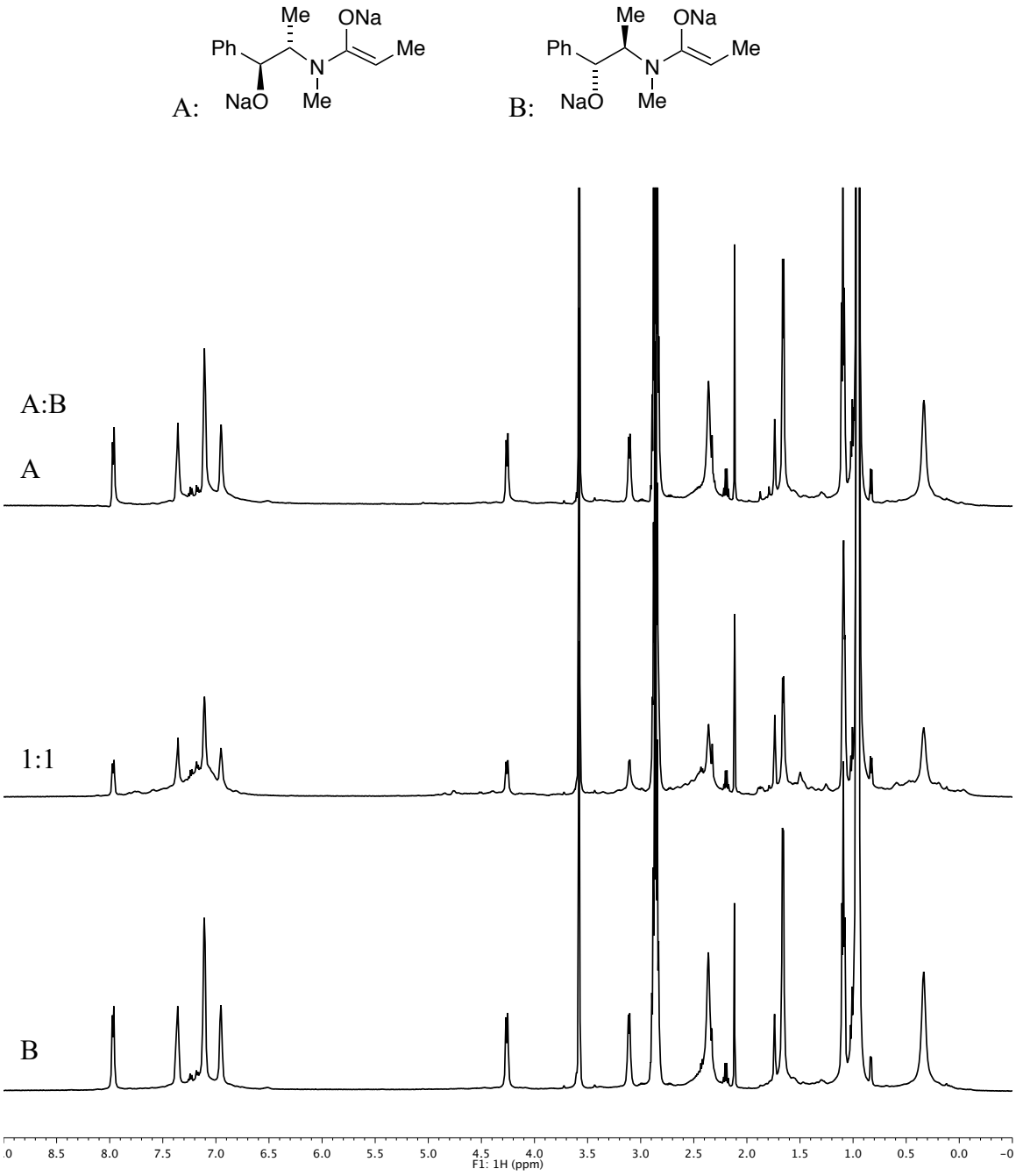


Figure 10. ^{1}H NMR spectra for 0.25 M solutions of (*S,S*)-**8** (A) and (*R,R*)-**8** (B) in 12.3 M THF at −80 °C. Mixing (*S,S*)-**8** and (*R,R*)-**8** showed no evidence of heteroaggreagtion.

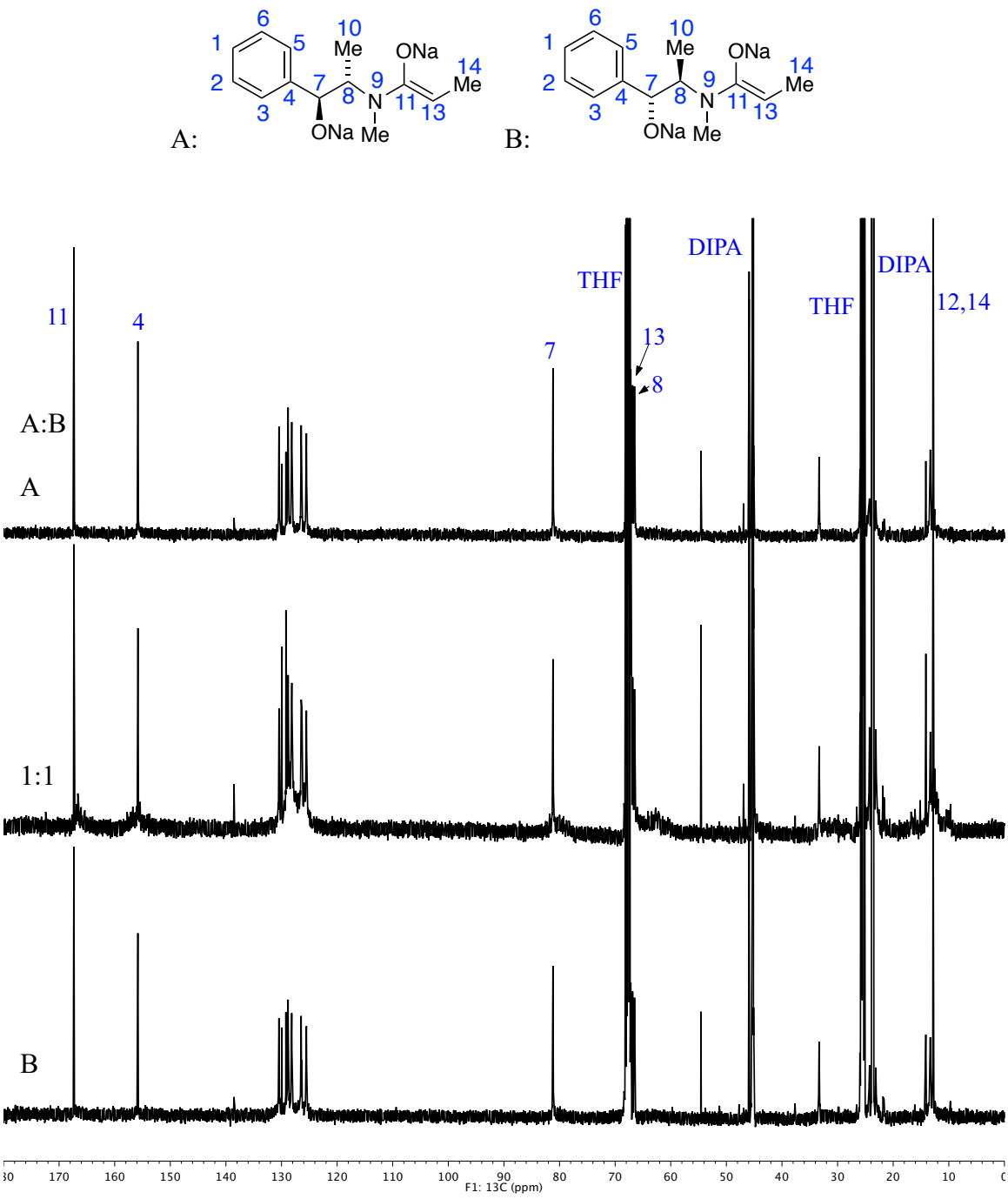


Figure 11. $^{13}C\{^{1}H\}$ NMR spectra for 0.25 M solutions of (*S,S*)-**8** (A) and (*R,R*)-**8** (B) in 12.3 M THF at −80 °C. Mixing (*S,S*)-**8** and (*R,R*)-**8** showed no evidence of heteroaggreagtion.

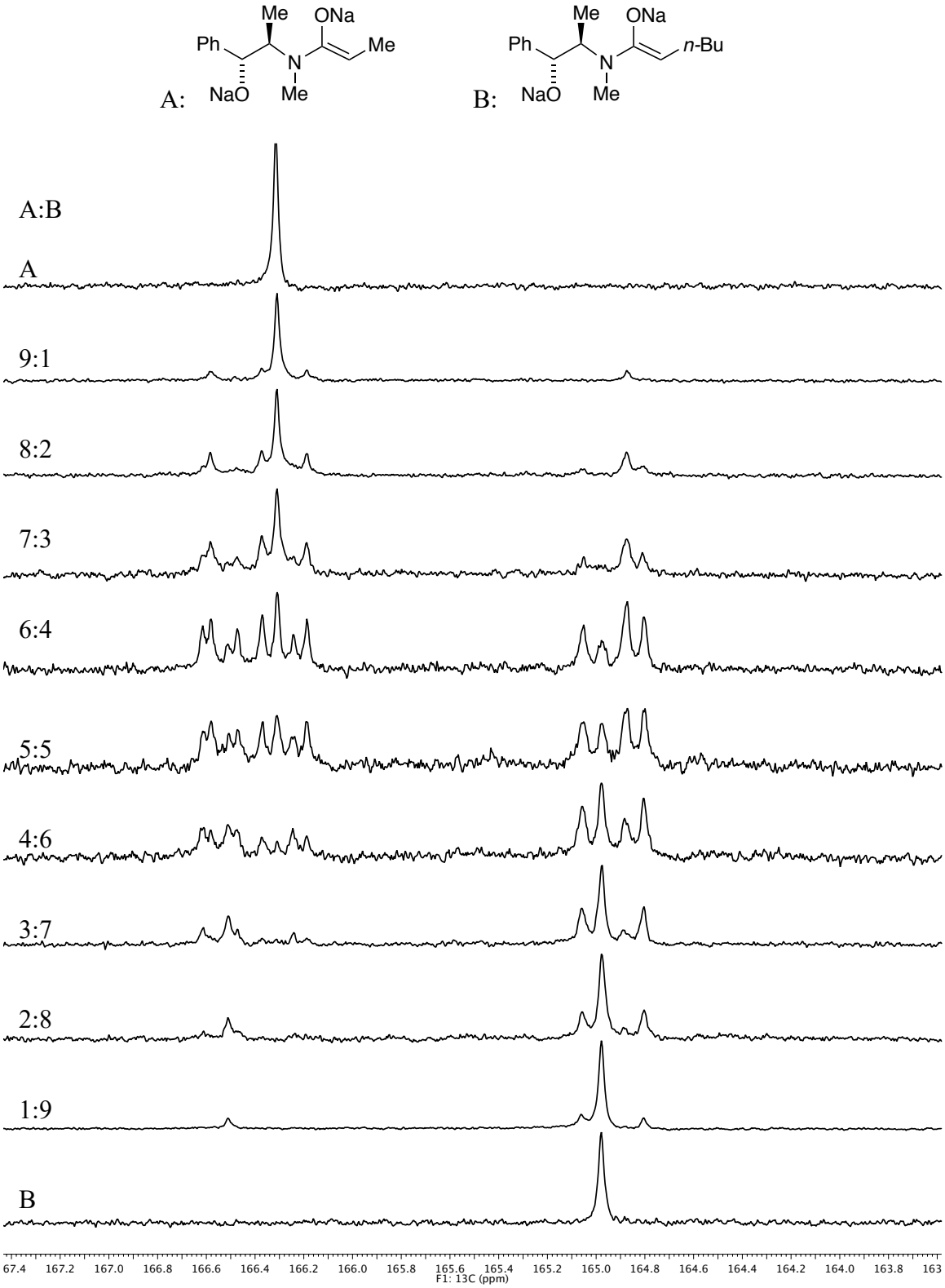


Figure 12. Partial $^{13}C\{^{1}H\}$ NMR spectra for 0.25 M solutions of **8** (A) and **14** (B) in 12.3 M THF at −80 °C. The region shown corresponds to quaternary enolate carbon. Heteroaggregates do not resolve owing to overlap between species.

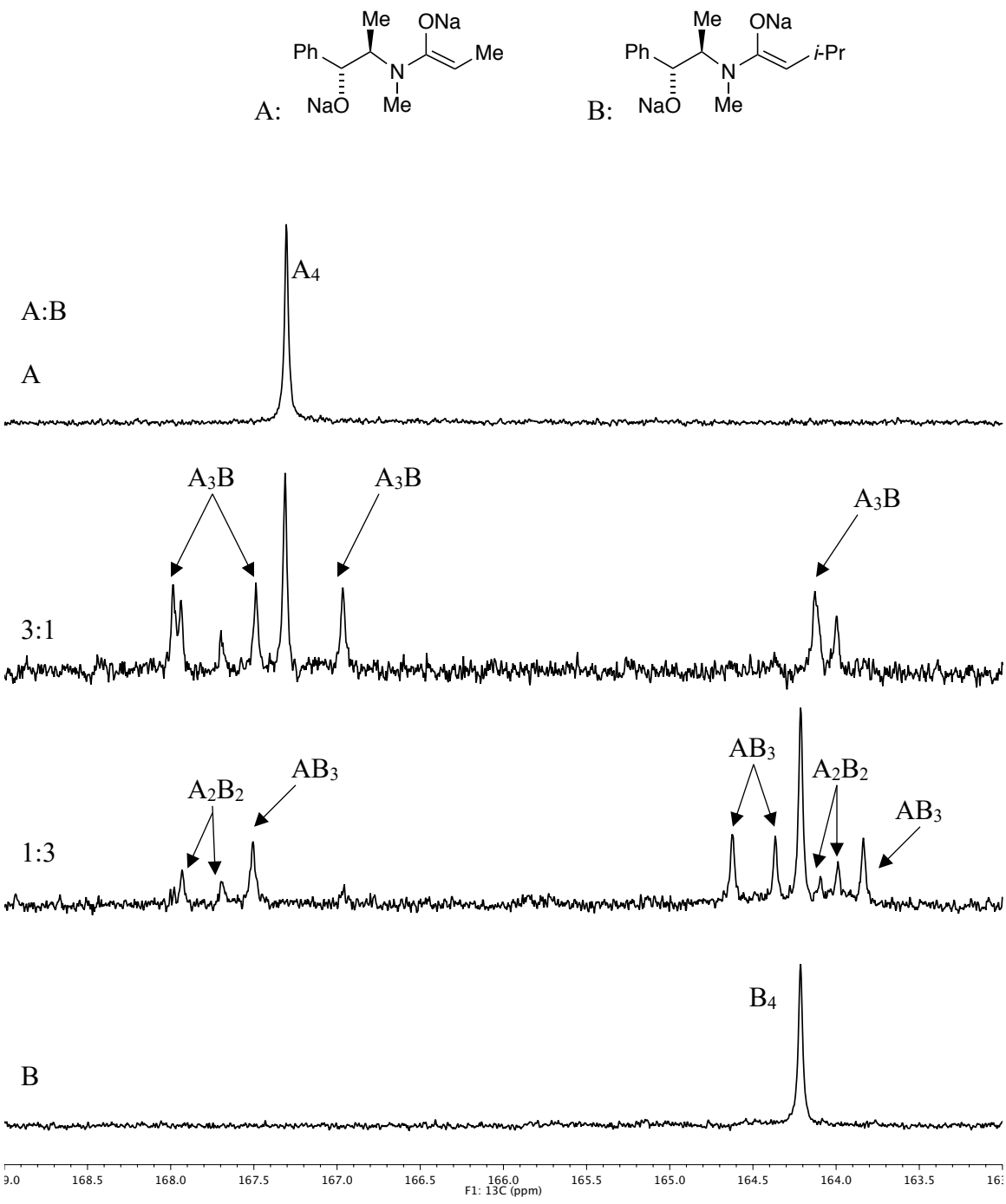


Figure 13. Partial $^{13}C\{^{1}H\}$ NMR spectra for 0.25 M solutions of **8** (A) and **15** (B) in 12.3 M THF at −80 °C. The region shown corresponds to quaternary enolate carbon. There are three heteroaggregate species corresponding to tetramer assignment.

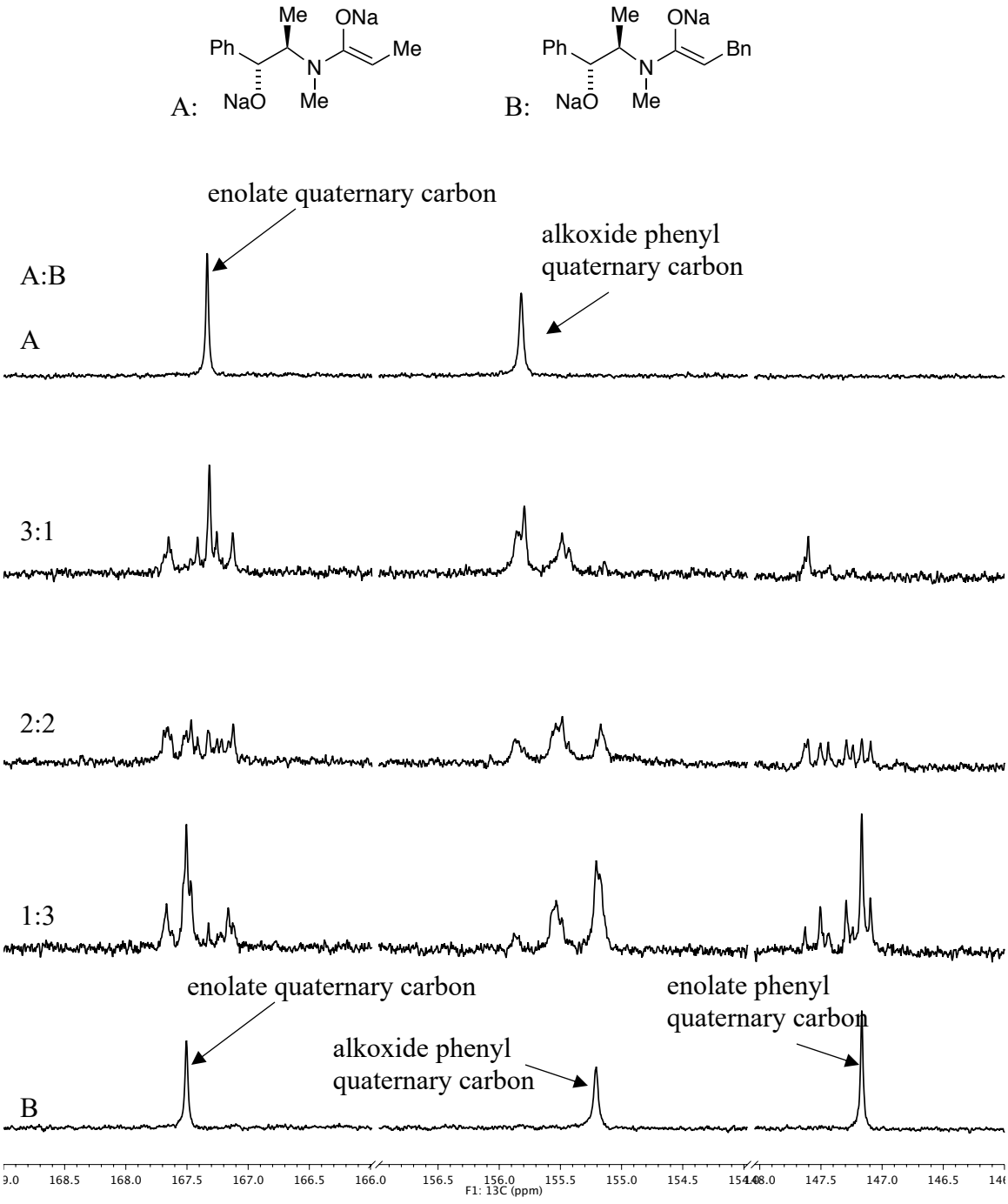


Figure 14. Partial $^{13}C\{^{1}H\}$ NMR spectra for 0.30 M solutions of **8** (A) and **16** (B) in 12.3 M THF at −80 °C. Heteroaggregates do not resolve owing to overlap between species.

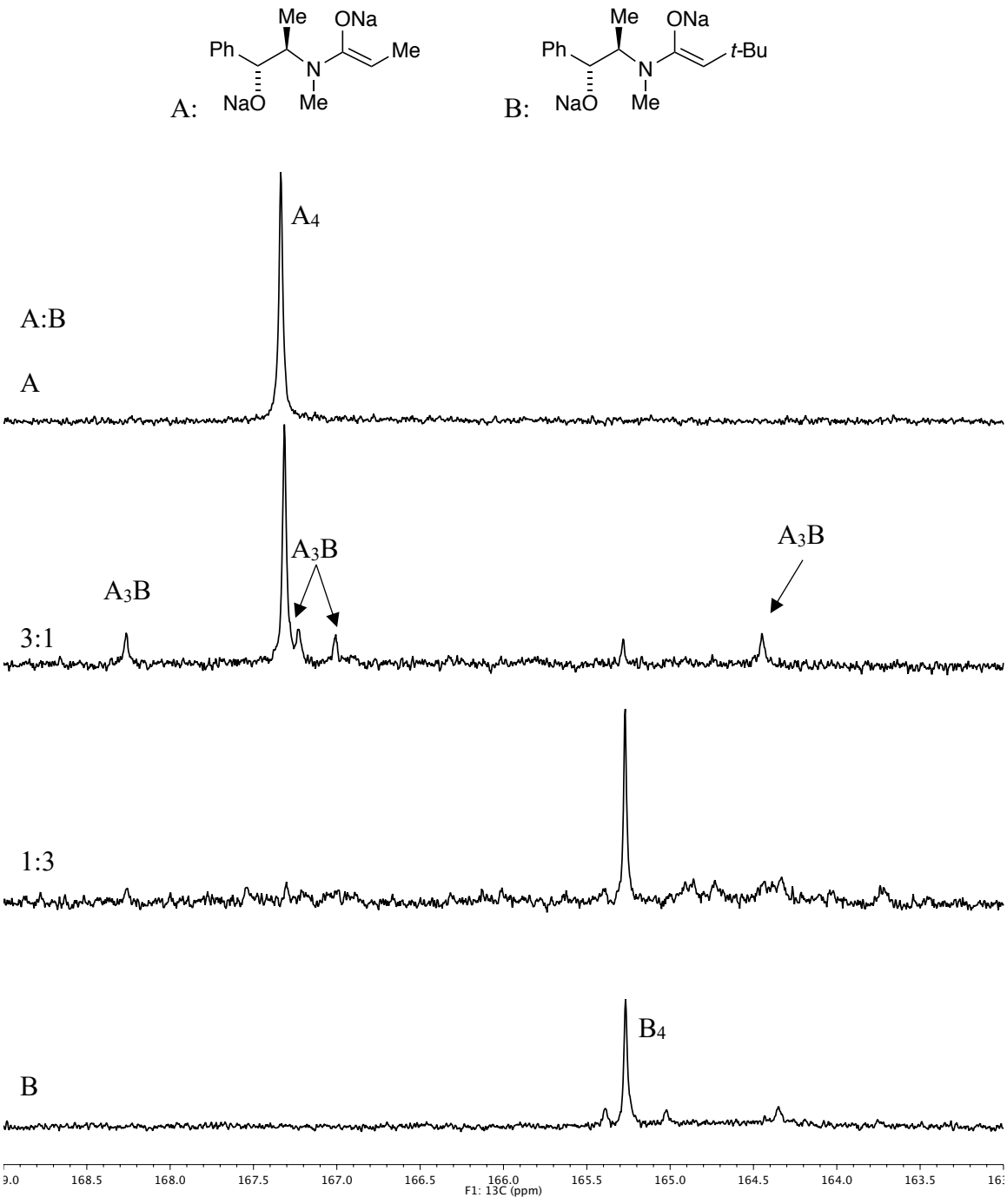


Figure 15. Partial $^{13}C\{^{1}H\}$ NMR spectra for 0.25 M solutions of **8** (A) and **17** (B) in 12.3 M THF at −80 °C. The region shown corresponds to quaternary enolate carbon. Enolate B is reluctant to mix, probably owing to different bulkiness between Me and *t*-Bu group.

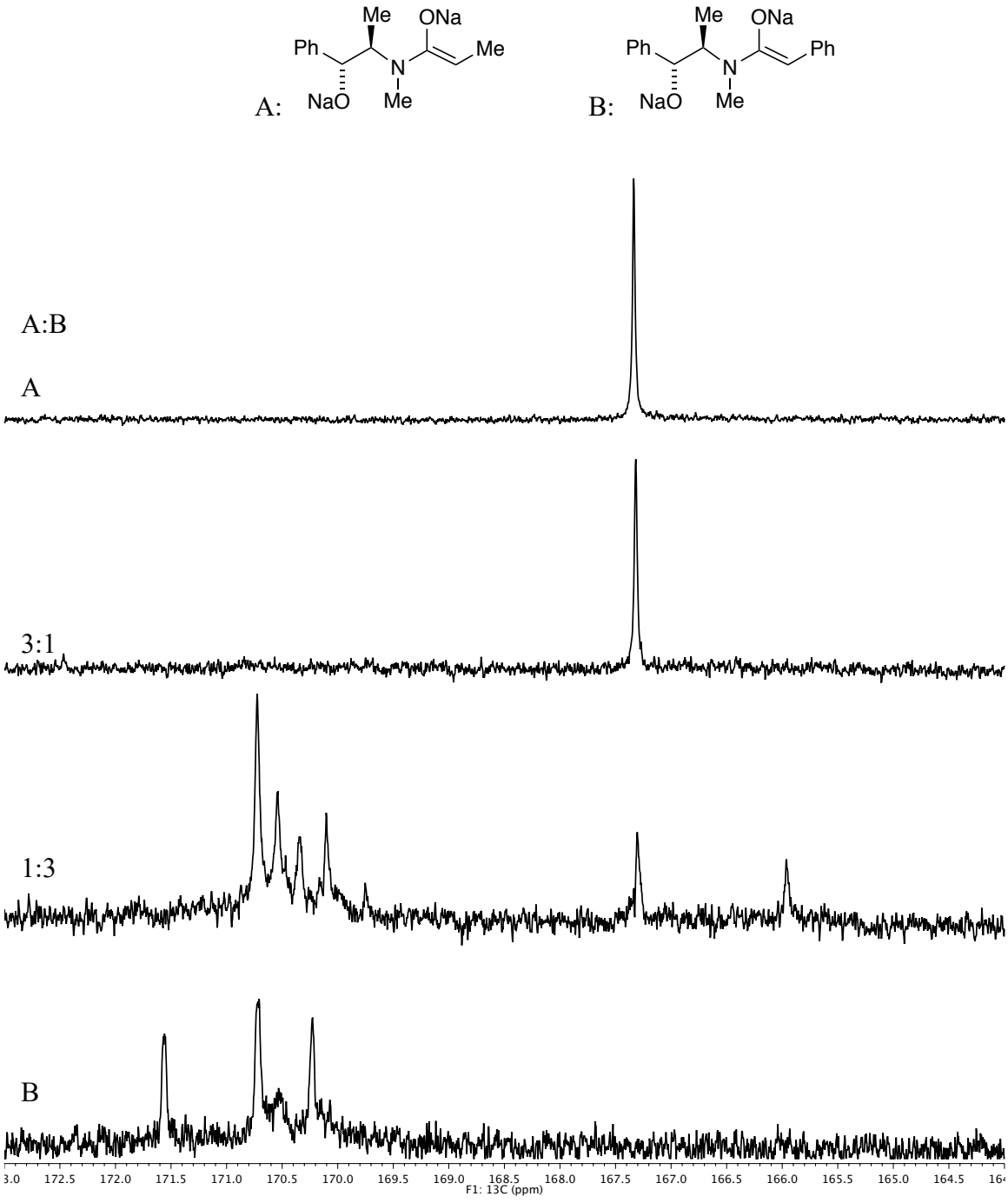


Figure 16. Partial $^{13}C\{^{1}H\}$ NMR spectra for 0.25 M solutions of **8** (A) and **32** (B) in 12.3 M THF at −80 °C. The region shown corresponds to quaternary enolate carbon. The phenyl ring on enolate B maybe metalated by NaDA.

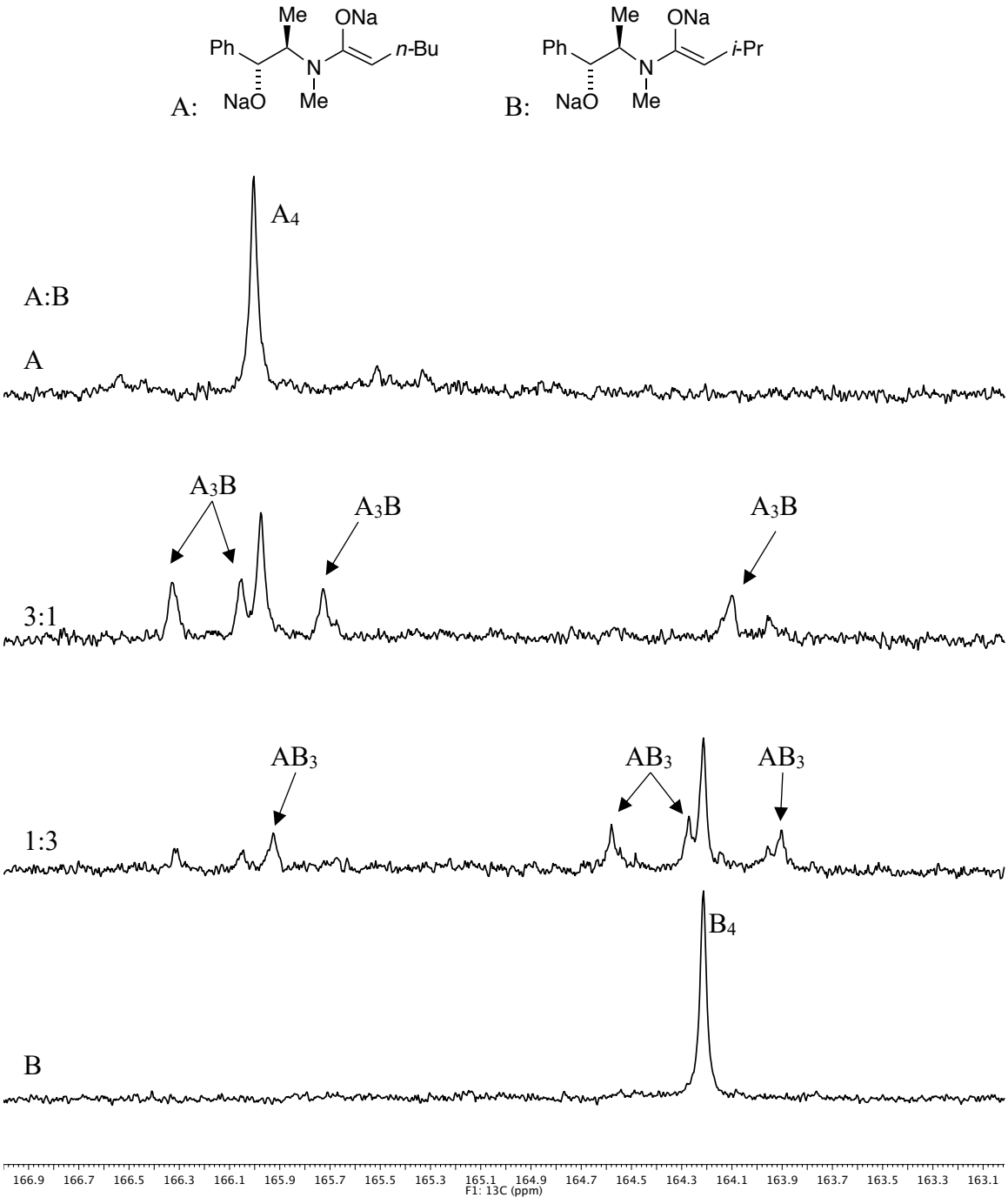


Figure 17. Partial $^{13}C\{^{1}H\}$ NMR spectra for 0.25 M solutions of **14** (A) and **15** (B) in 12.3 M THF at −80 °C. The region shown corresponds to quaternary enolate carbon. Heteroaggregate A_2B_2 are difficult to resolve. There are three heteroaggregate species corresponding to tetramer assignment.

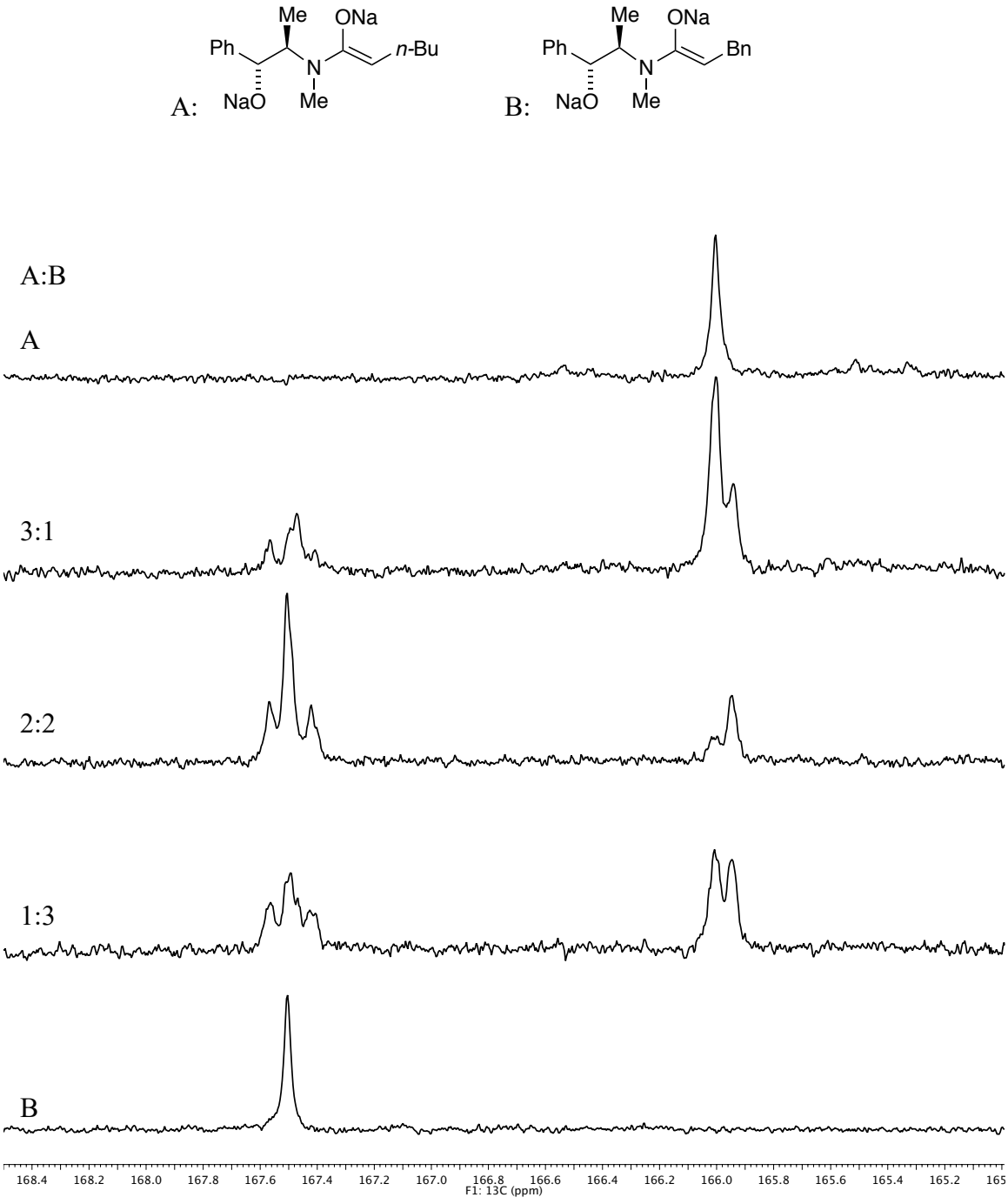


Figure 18. Partial $^{13}C\{^{1}H\}$ NMR spectra for 0.25 M solutions of **14** (A) and **16** (B) with 0.625 M NaDA in 12.3 M THF at −80 °C. The region shown corresponds to quaternary enolate carbon. Heteroaggregates do not resolve owing to overlap between species.

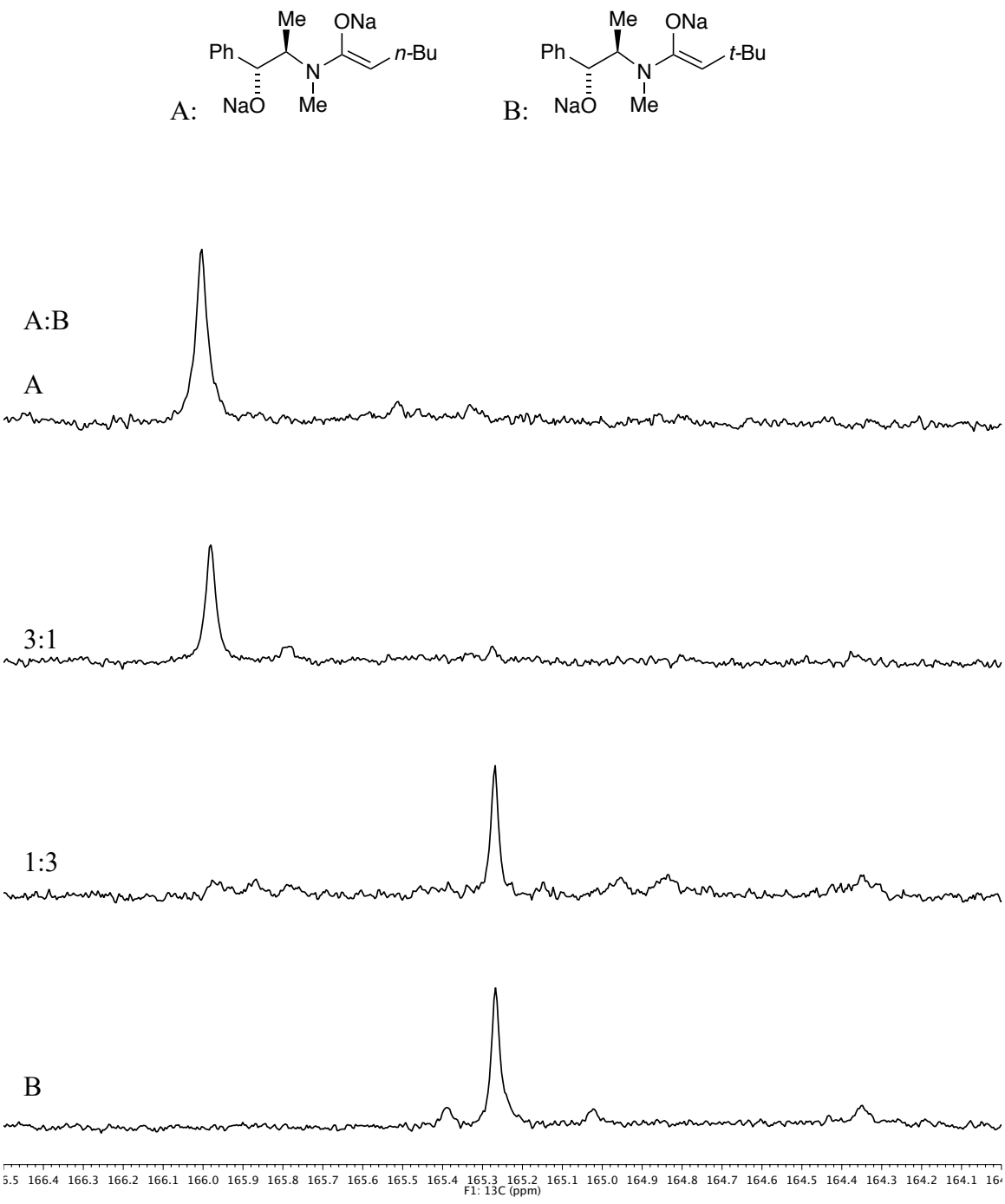


Figure 19. Partial $^{13}C\{^{1}H\}$ NMR spectra for 0.25 M solutions of **14** (A) and **17** (B) in 12.3 M THF at −80 °C. The region shown corresponds to quaternary enolate carbon. Enolate B is reluctant to mix, probably owing to different bulkiness between *n*-Bu and *t*-Bu group.

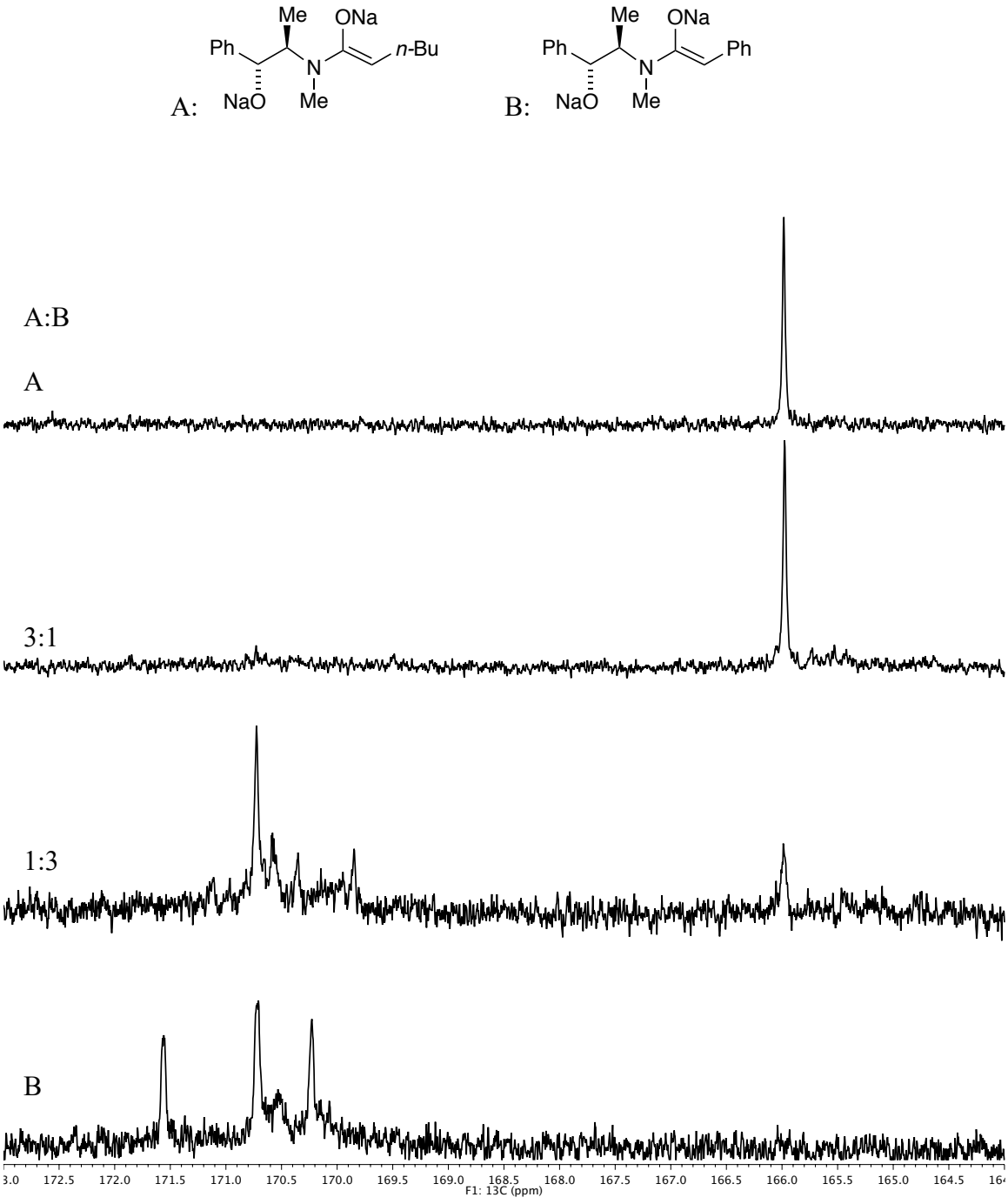


Figure 20. Partial $^{13}C\{^{1}H\}$ NMR spectra for 0.25 M solutions of **14** (A) and **32** (B) with 0.625 M NaDA in 12.3 M THF at −80 °C. The region shown corresponds to quaternary enolate carbon. The phenyl ring on enolate B maybe metalated by NaDA.

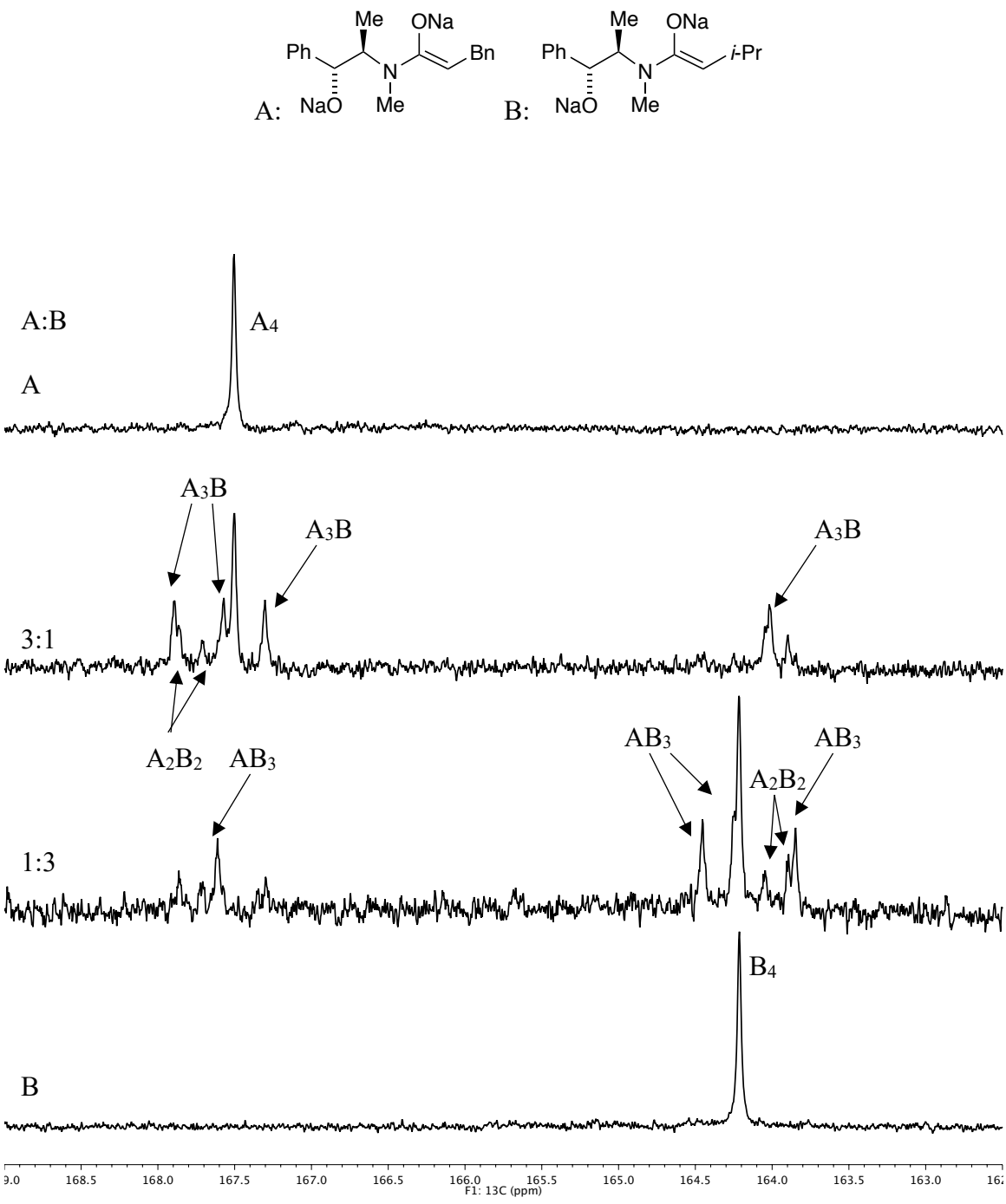


Figure 21. Partial $^{13}C\{^{1}H\}$ NMR spectra for 0.25 M solutions of **16** (A) and **15** (B) in 12.3 M THF at −80 °C. The region shown corresponds to quaternary enolate carbon. There are three heteroaggregate species corresponding to tetramer assignment.

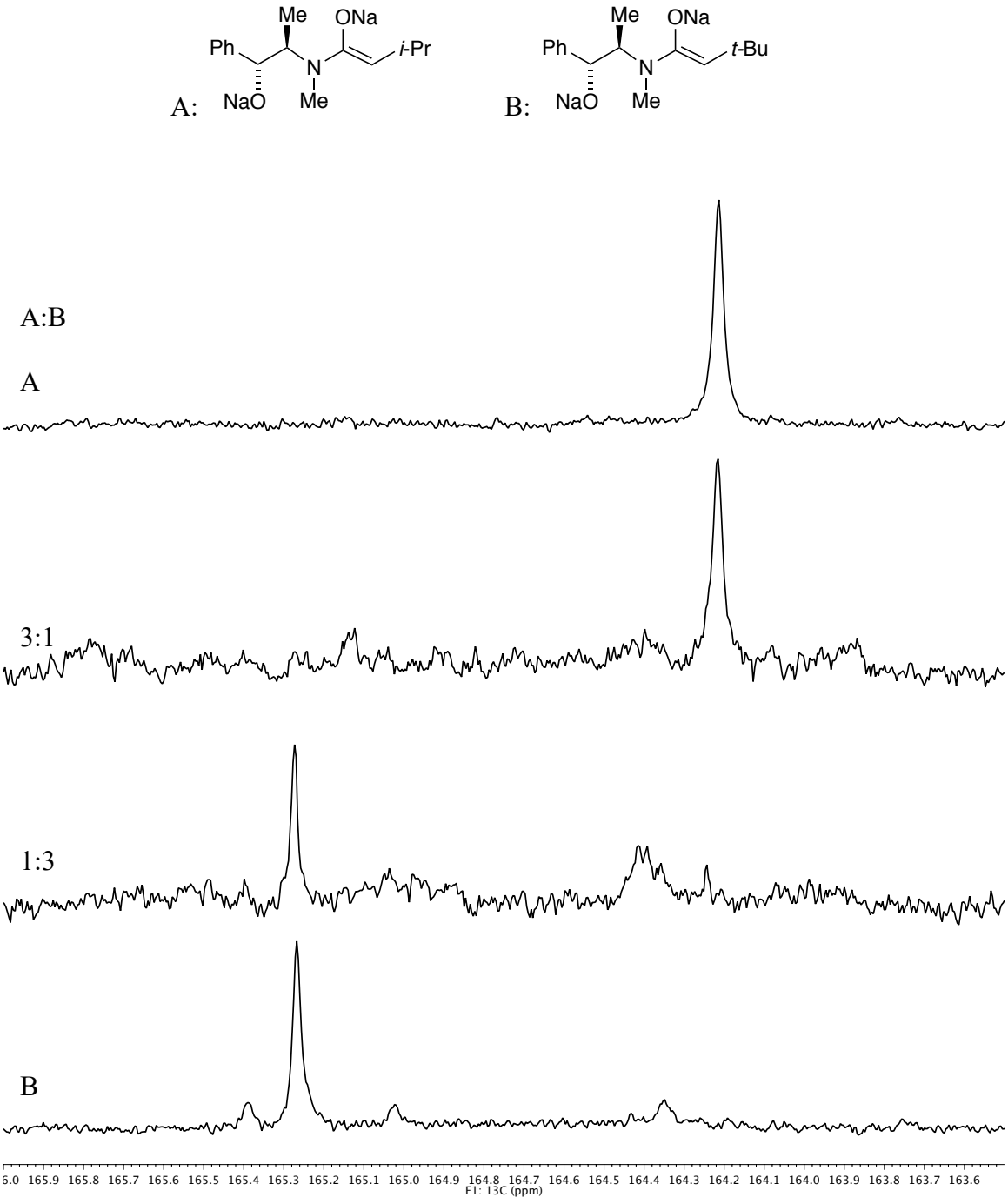


Figure 22. Partial $^{13}C\{^{1}H\}$ NMR spectra for 0.25 M solutions of **15** (A) and **17** (B) in 12.3 M THF at −80 °C. The region shown corresponds to quaternary enolate carbon. Enolate B is reluctant to mix, probably owing to different bulkiness between *i*-Pr and *t*-Bu group.

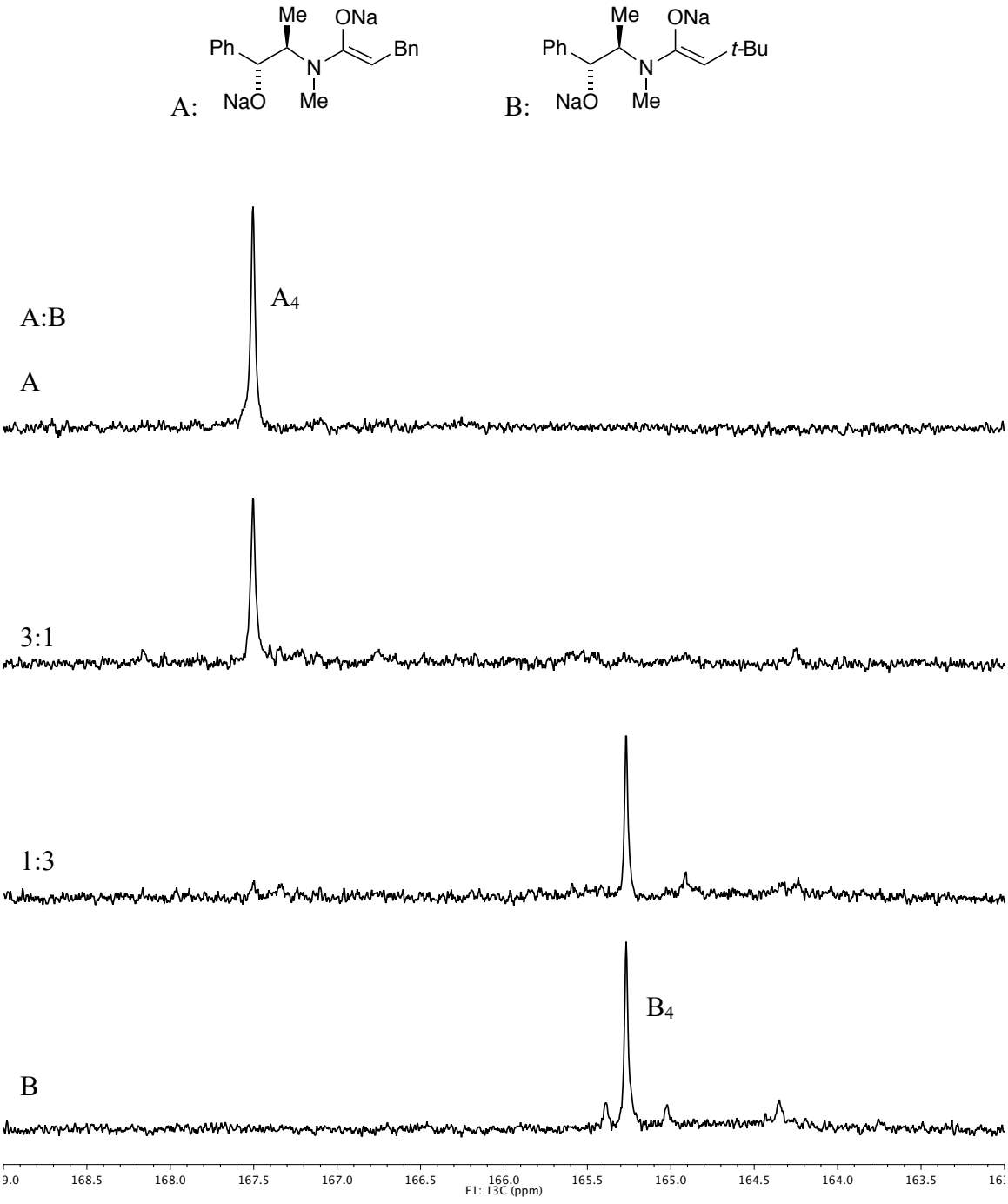


Figure 23. Partial $^{13}C\{^{1}H\}$ NMR spectra for 0.25 M solutions of **16** (A) and **17** (B) in 12.3 M THF at −80 °C. The region shown corresponds to quaternary enolate carbon. Enolate B is reluctant to mix, probably owing to different bulkiness between Bn and *t*-Bu group.

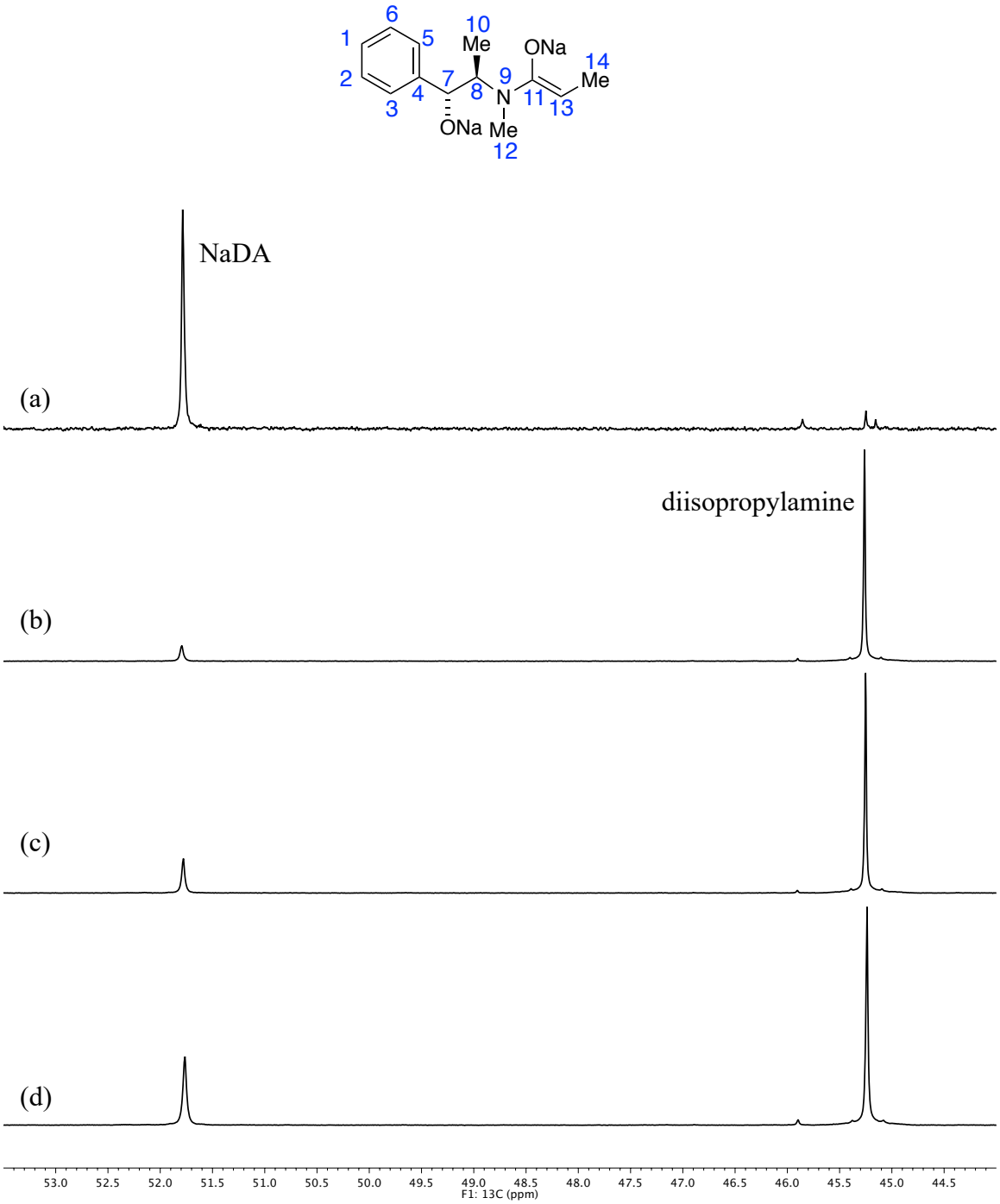


Figure 24. Partial $^{13}C\{^{1}H\}$ NMR spectra of a solution of 0.25 M **1** in 12.3 M THF at –80 °C with varying NaDA concentrations. (a) only NaDA and no substrate available, (b) 0.625 M NaDA (2.5 equiv), (c) 0.94 M NaDA (3.8 equiv), and (d) 1.25 M NaDA (5.0 equiv). No NaDA-mixed aggregate was observed.

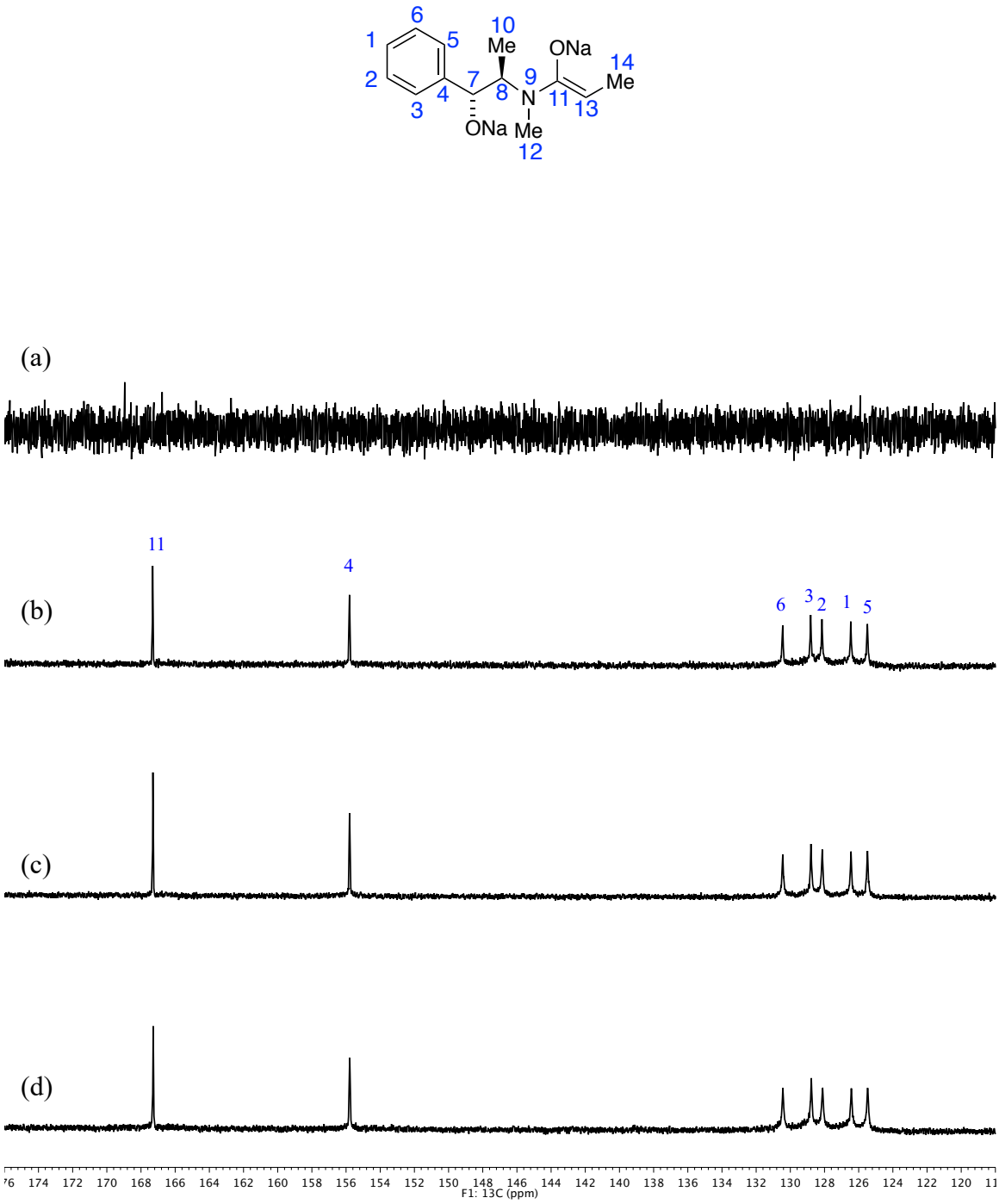


Figure 25. Partial $^{13}C\{^{1}H\}$ NMR spectra of a solution of 0.25 M **1** in 12.3 M THF at –80 °C with varying NaDA concentrations. (a) only NaDA and no substrate available, (b) 0.625 M NaDA (2.5 equiv), (c) 0.94 M NaDA (3.8 equiv), and (d) 1.25 M NaDA (5.0 equiv). No NaDA-mixed aggregate was observed.

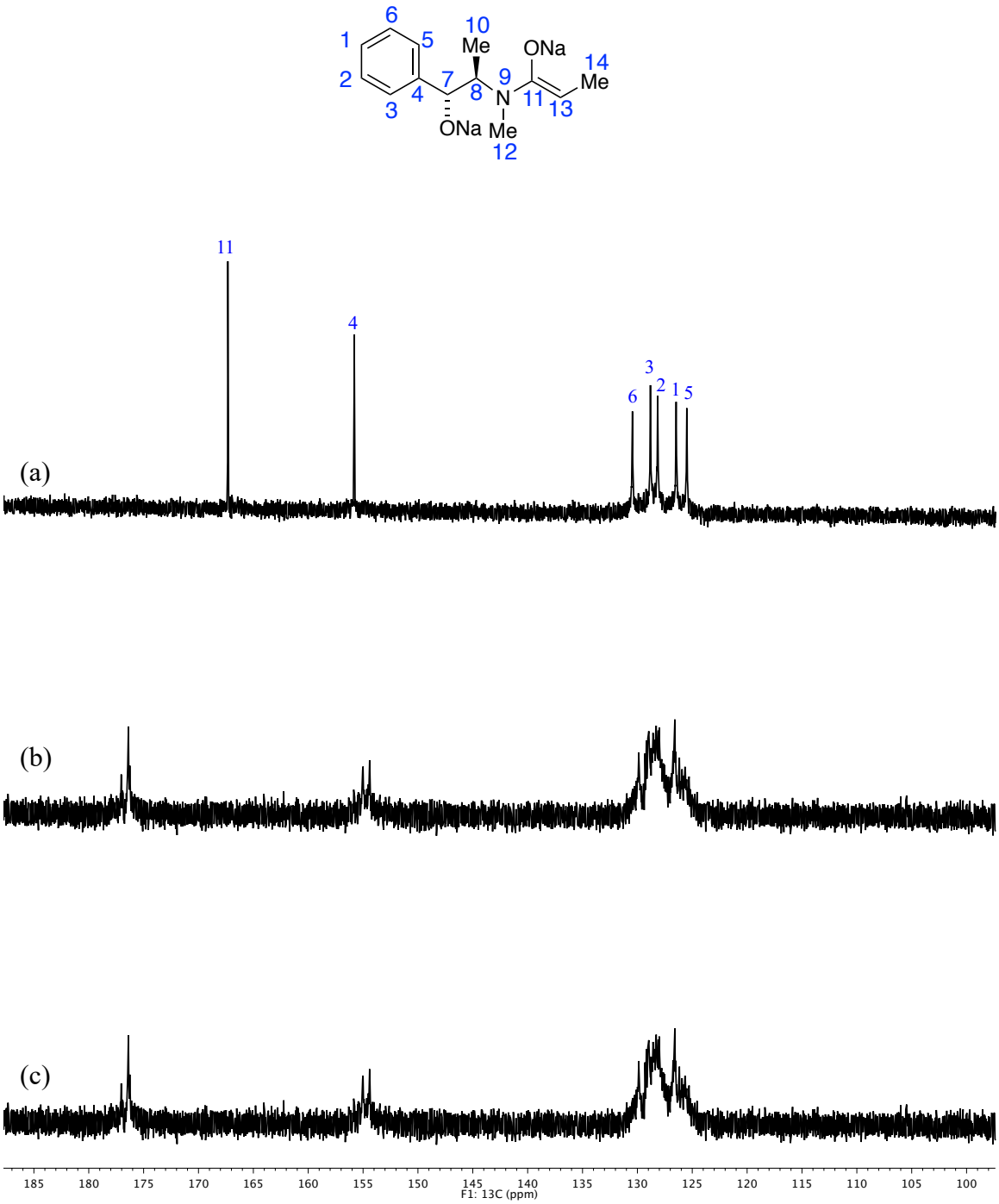


Figure 26. Partial $^{13}C\{^{1}H\}$ NMR spectra of a solution of 0.30 M **1** in 12.3 M THF at –80 °C with 0.70 M NaDA or NaHMDS. (a) 0.625 M NaDA, (b) 0.625 M NaHMDS and aged at –80 °C for 3 h, and (c) 0.625 M NaHMDS and aged at –80 °C for 29 h. NaHMDS is not basic enough to quantitatively form enolate.

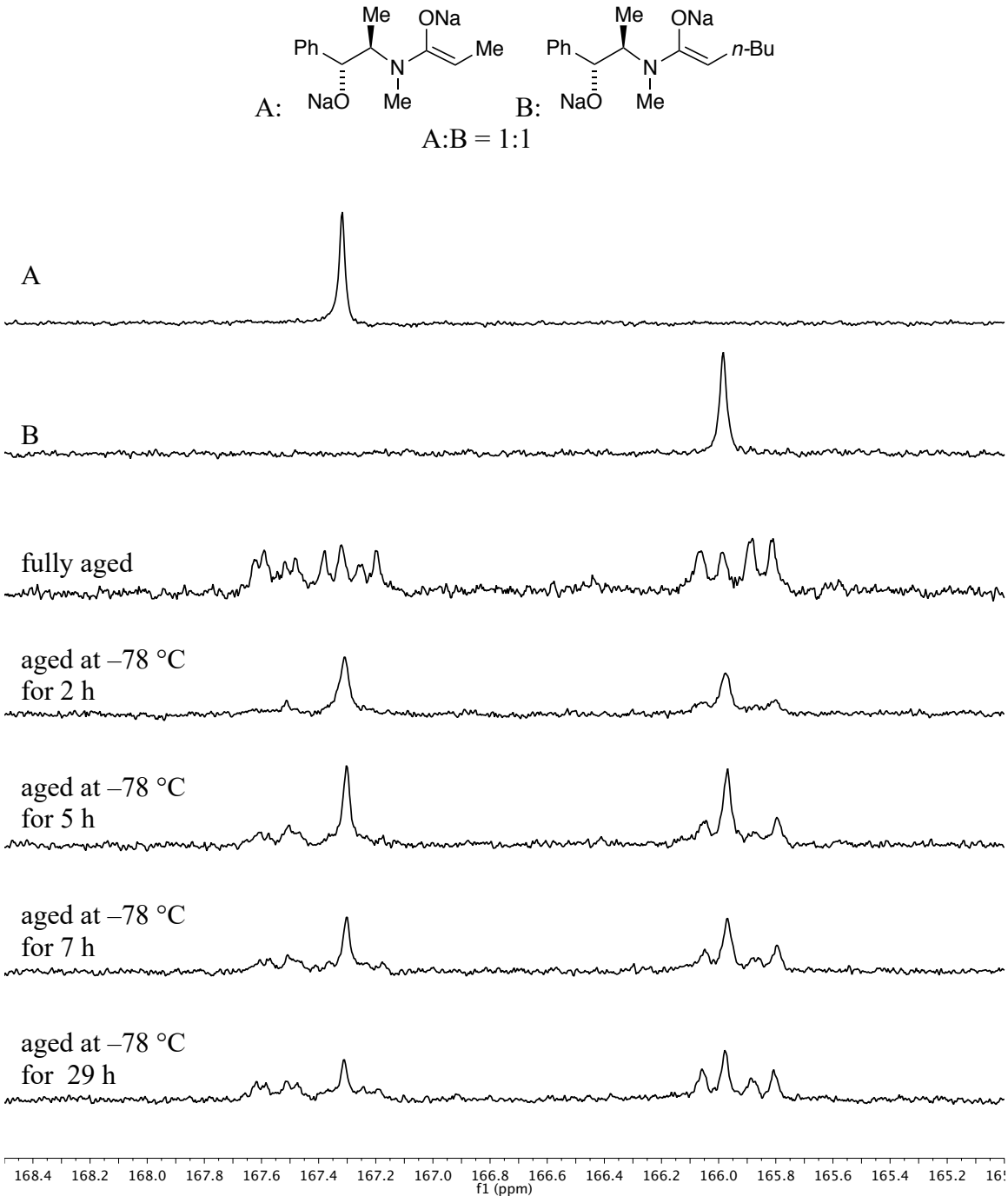


Figure 27. Partial $^{13}C\{^{1}H\}$ NMR spectra for 1:1 ratio of 0.25 M solution of **8** and **14** in 12.3 M THF at –80 °C. Formation of heteroaggregates is slow at –78 °C ($t_{1/2}$ > 5h).

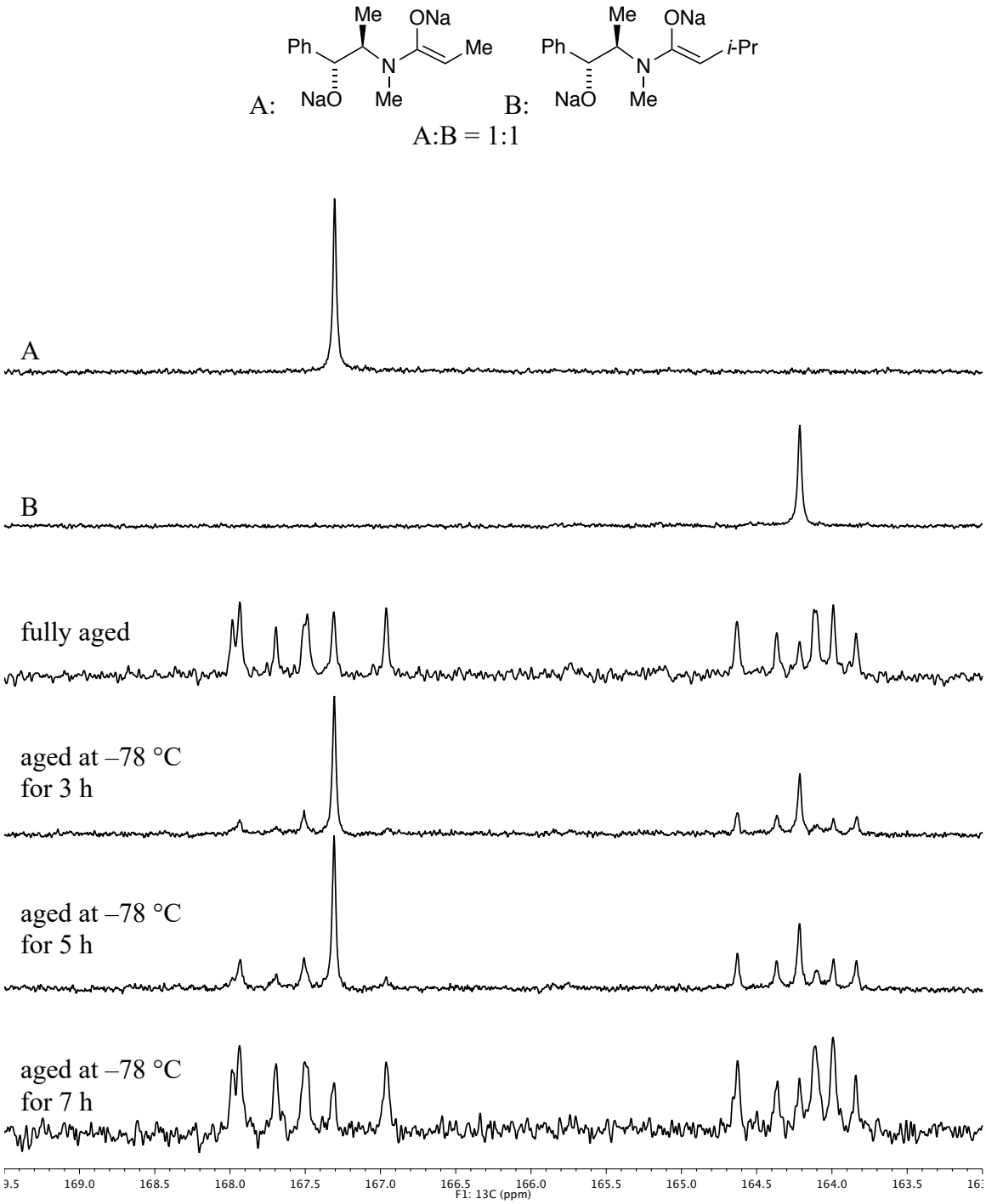


Figure 28. Partial $^{13}C\{^{1}H\}$ NMR spectra for 1:1 ratio of 0.25 M solutions of **8** and **15** in 12.3 M THF at –80 °C. Formation of heteroaggregates is slow at –78 °C ($t_{1/2}$ > 5 h).

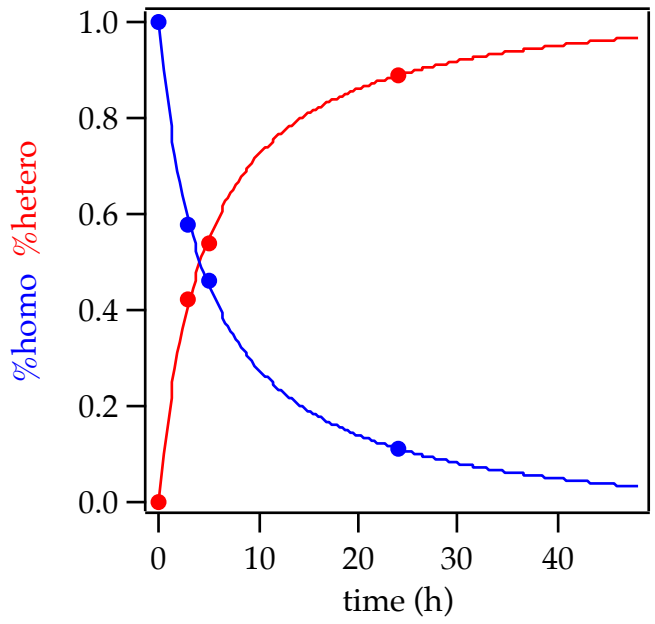


Figure 29. Plot of percent homoaggregate and percent heteroaggregate in 0.25 M solutions of **8** and **15** in neat THF at –80 °C versus time. $T_{1/2}$ is approximate 5 h.

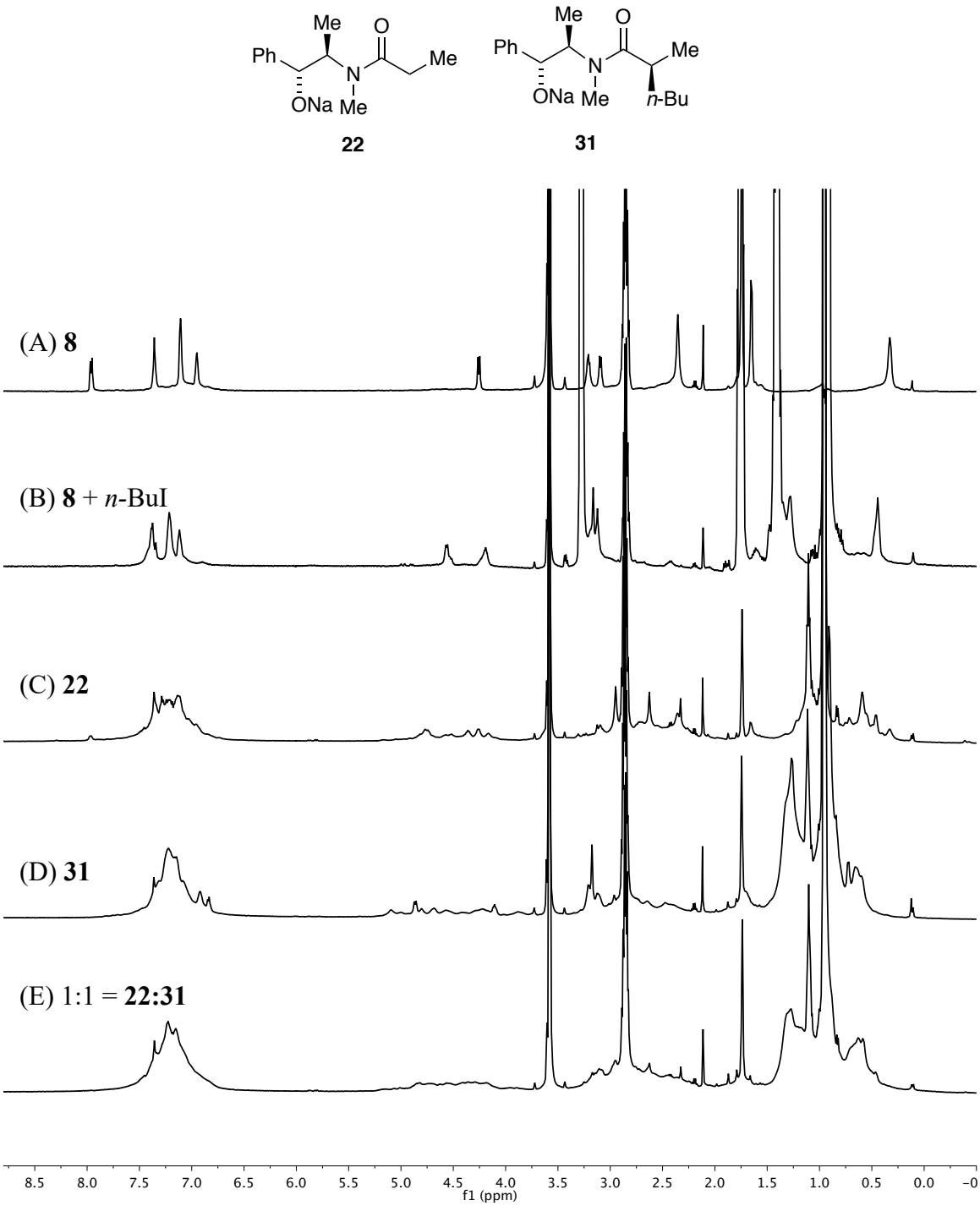


Figure 30. ^{1}H NMR spectra at –80 °C for (A) 0.25 M **8**; (B) 0.10 M **8** reacted with 10M *n*-BuI at –60 °C for 30 min; (C) 0.25 M **22**; (D) 0.25 M **31**; (E) 0.25 M solutions of 1:1 **22:31**. The ^{1}H NMR spectra of alkoxides are not simple.

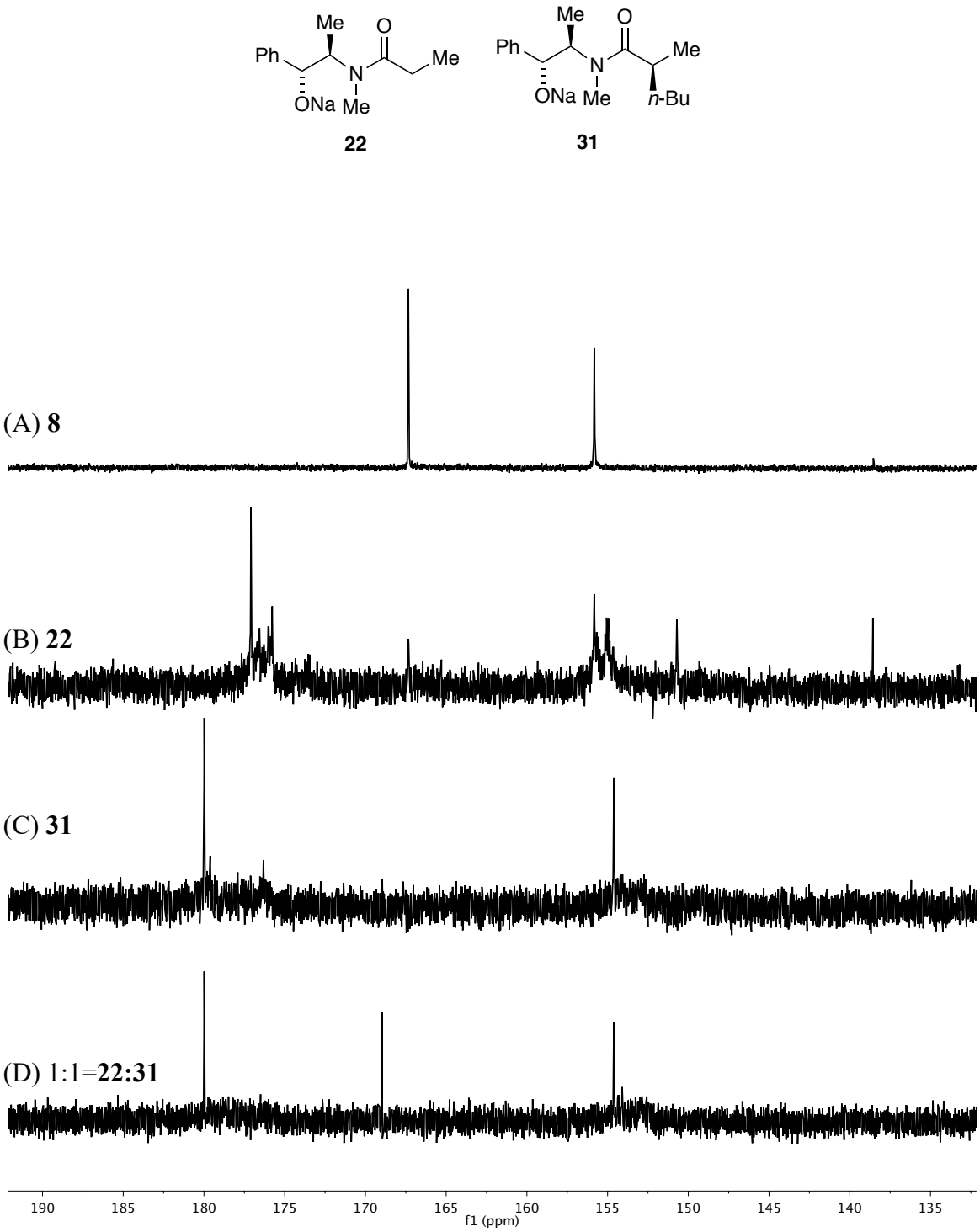


Figure 31. Partial $^{13}C\{^{1}H\}$ NMR spectra at –80 °C for (A) 0.25 M **8**; (B) 0.25 M **22**; (C) 0.25 M **31**; (D) 0.25 M solutions of 1:1 **22:31**. ^{13}C NMR spectra of alkoxides are not simple.

2D NMR analysis of 8 homoaggregates: A sample prepared from 0.70 M NaDA, 0.30 M **1** in 12.3 M THF-d_8, after aging at –80 °C for 18 h, was studied by standard 2D NMR techniques. All chemical shifts were assigned using high-field indirect-resolution 2D HSQC, COSY and HMBC experiments.

Experimental: 2D NMR spectra were acquired on a 500 MHz Varian INOVA spectrometer operating at 499.92 MHz for ^{1}H observation using a 5 mm Varian inverse-detect probe head with Z-axis pulsed field-gradient. Sample temperature was maintained at –80 °C as calibrated with a neat methanol sample. ^{1}H and ^{13}C chemical shifts were referenced to the residual downfield THF-d_7 resonance at 3.58 ppm and 67.57 ppm, respectively. 2D experiments were acquired using standard pulse sequences supplied in VnmrJ 3.2A (Agilent Inc.) and processed and analyzed in MestReNova 11.0.3 (Mestrelab Research S.L.).

Determination of the 3D aggregate structure: The 3D structure of the aggregate was derived from 2D ROESY (reported as H–H correlations). However, with only one subunit, it is hard to differentiate between inter- or intra- subunit nOe correlations. Therefore, 2D NMR of heteroaggregates was carried out.

Table 1. [1]H and [13]C chemical shifts and assignments for enolate **8** at –80 °C.

Atom	δC, ppm	δH, ppm	HMBC	COSY	ROESY[2]
1 C	126.09	7.12	5,3	6,3	
2 C	127.79	7.12	4,6	3,6	
3 C	128.41	6.96	6,7,1,5	5,1,2,7,10	7,10
4 C	155.38	–	7,2		
5 C	125.08	7.97	1,3	3,6	8,14,6,1
6 C	130.05	7.37	2	5,1,2	14,8
7 C	80.7	4.26	4,3,2	3,8	3,8,10,12,14
8 C	65.81	2.85		7,10	7,10,14,5
10 C	12.92	0.34		8,3	3,7,8,12,13
11 C	166.94	–	14,13		
12 C	32.98	2.36			7,10,13
13 C	66.54	3.10	11,14	14	10,12,14
14 C	12.47	1.66	11,13	13	6,8,13,7

[1]HSQC correlations were omitted from the table. [2]Important correlations that allowed determination of subunit arrangement are marked in red.

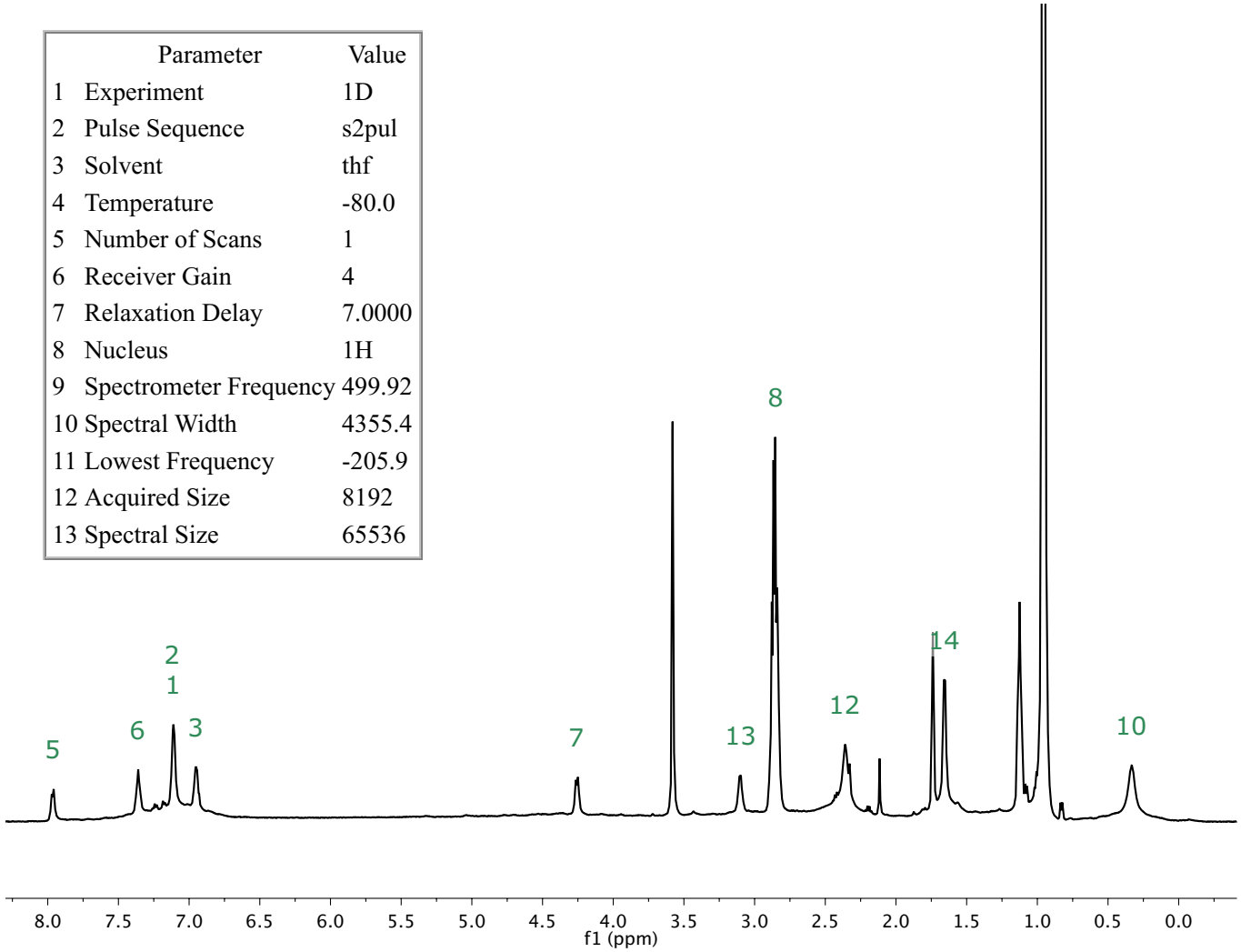


Figure 32. ^{1}H NMR spectrum of a solution of 0.30 M **8** in 12.3 M THF-d_8 at –80 °C. Labels indicate assignments by 2D NMR.

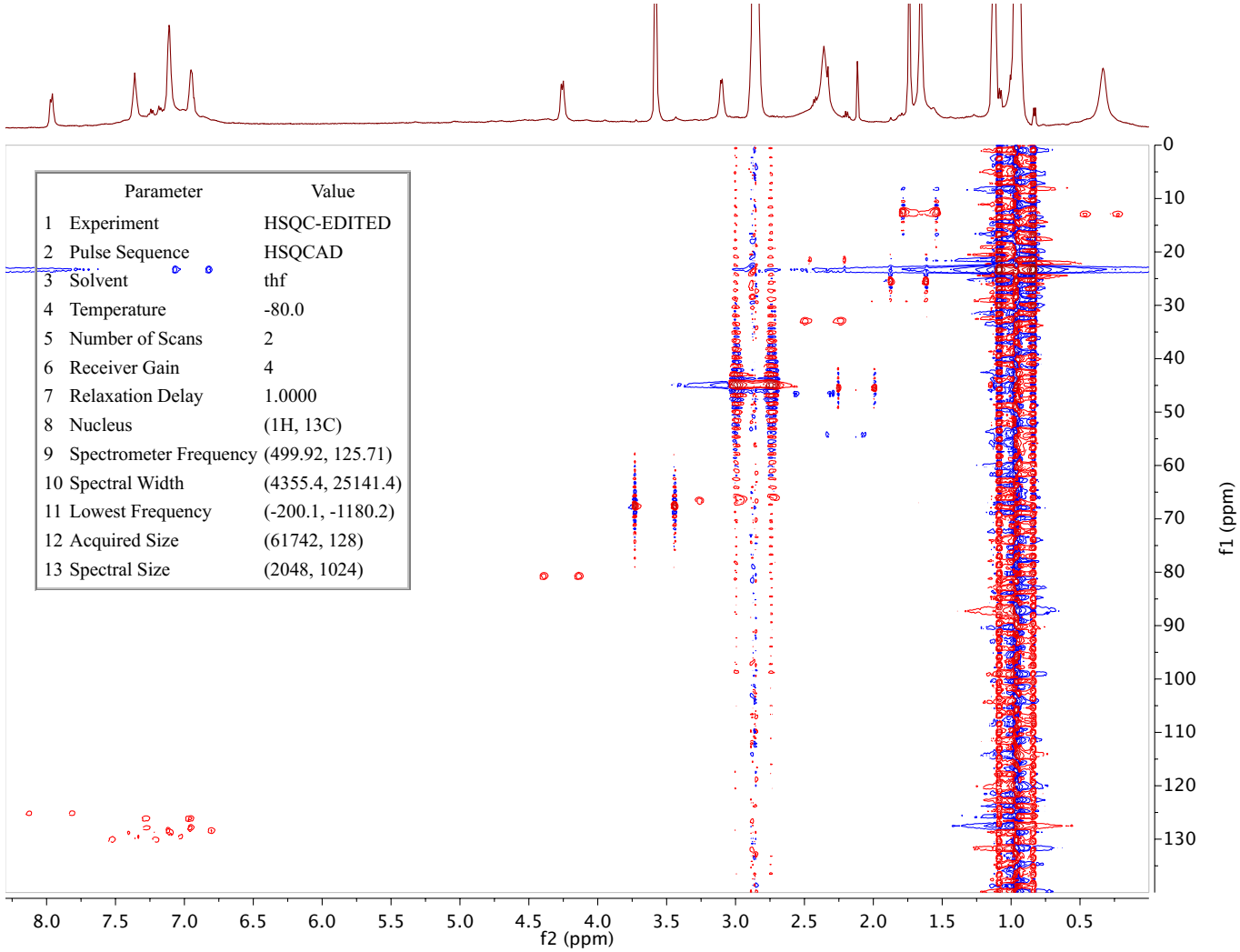


Figure 33. Full-display HSQC spectrum of a solution of 0.30 M **8** in 12.3 M THF-d_8 at –80 °C. ^{13}C decoupler was turned off.

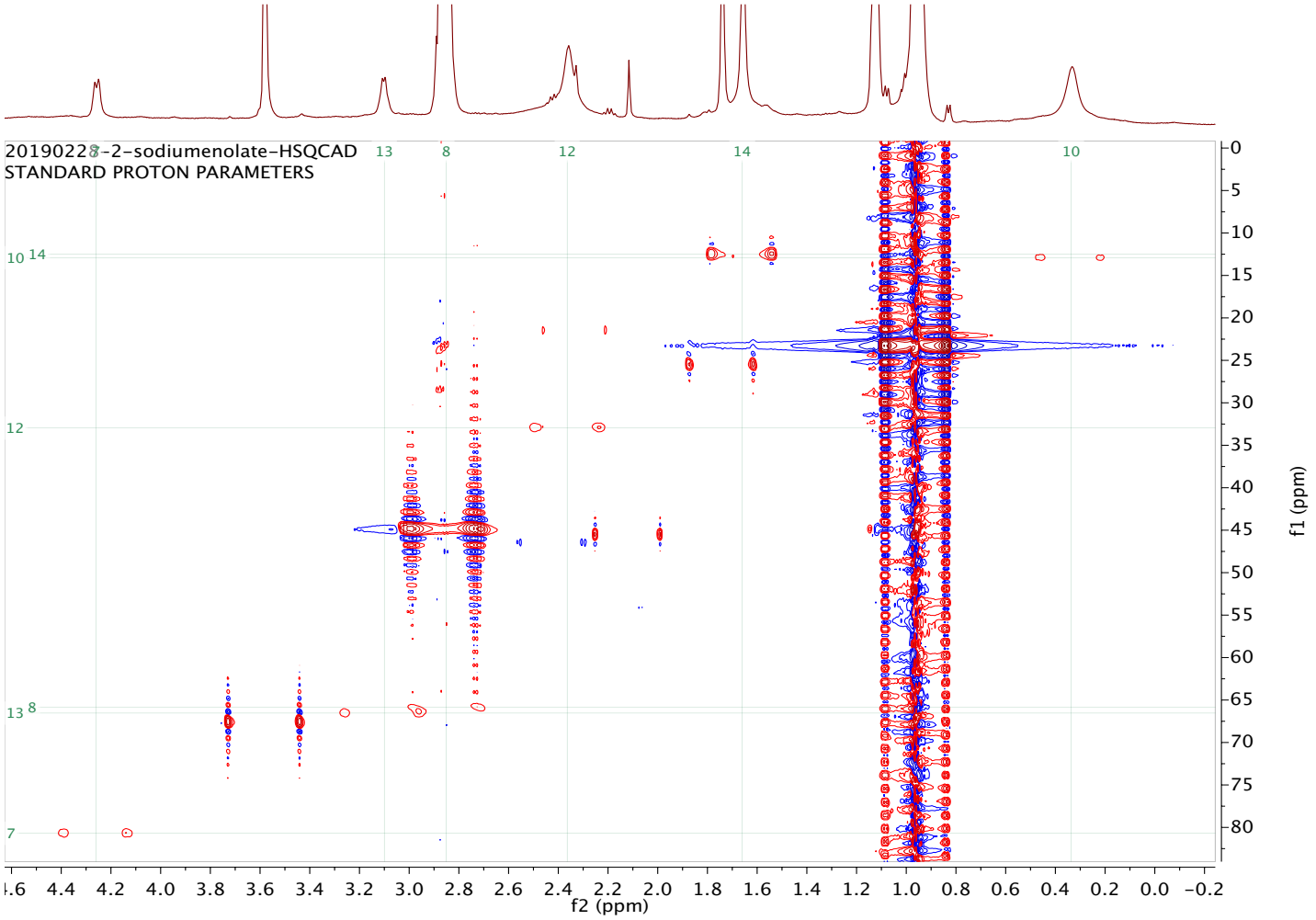


Figure 34. Expansion of the HSQC spectrum of a solution of 0.30 M **8** in 12.3 M THF-d_8 at –80 °C. ^{13}C decoupler was turned off.

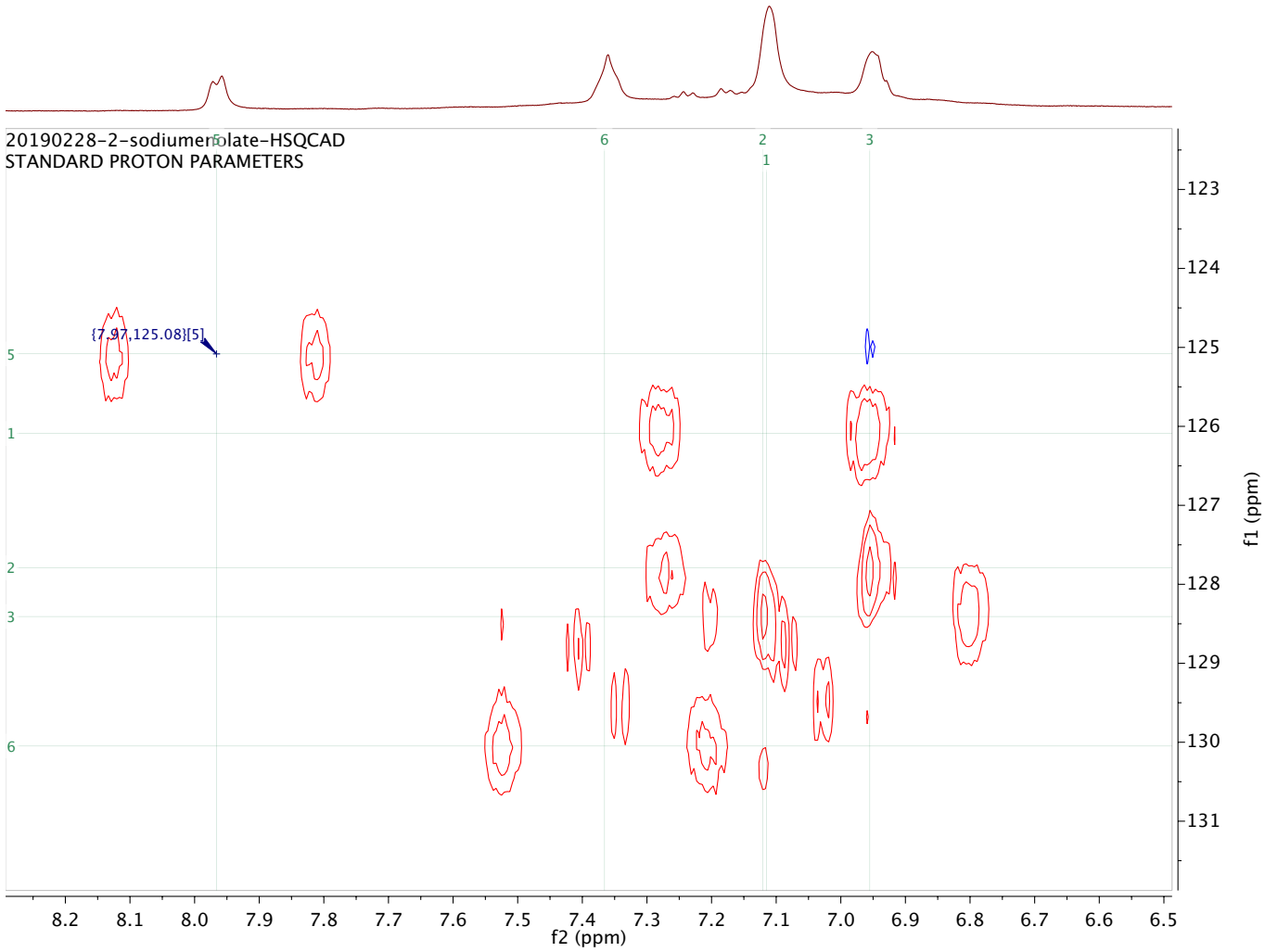


Figure 35. Expansion of the HSQC spectrum of a solution of 0.30 M **8** in 12.3 M THF-d_8 at –80 °C. ^{13}C decoupler was turned off.

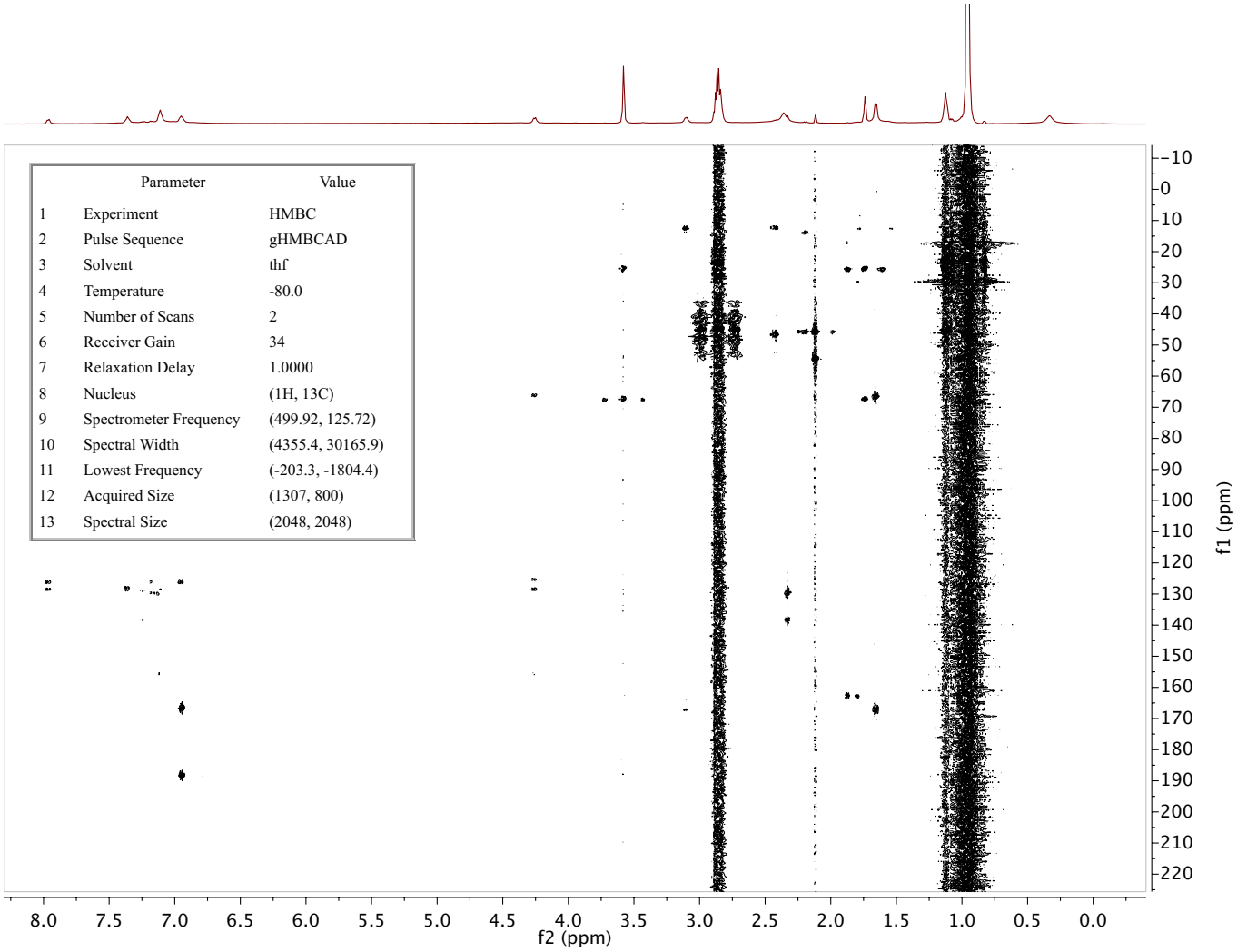


Figure 36. Full-display HMBC spectrum of a solution of 0.30 M **8** in 12.3 M THF-d_8 at –80 °C.

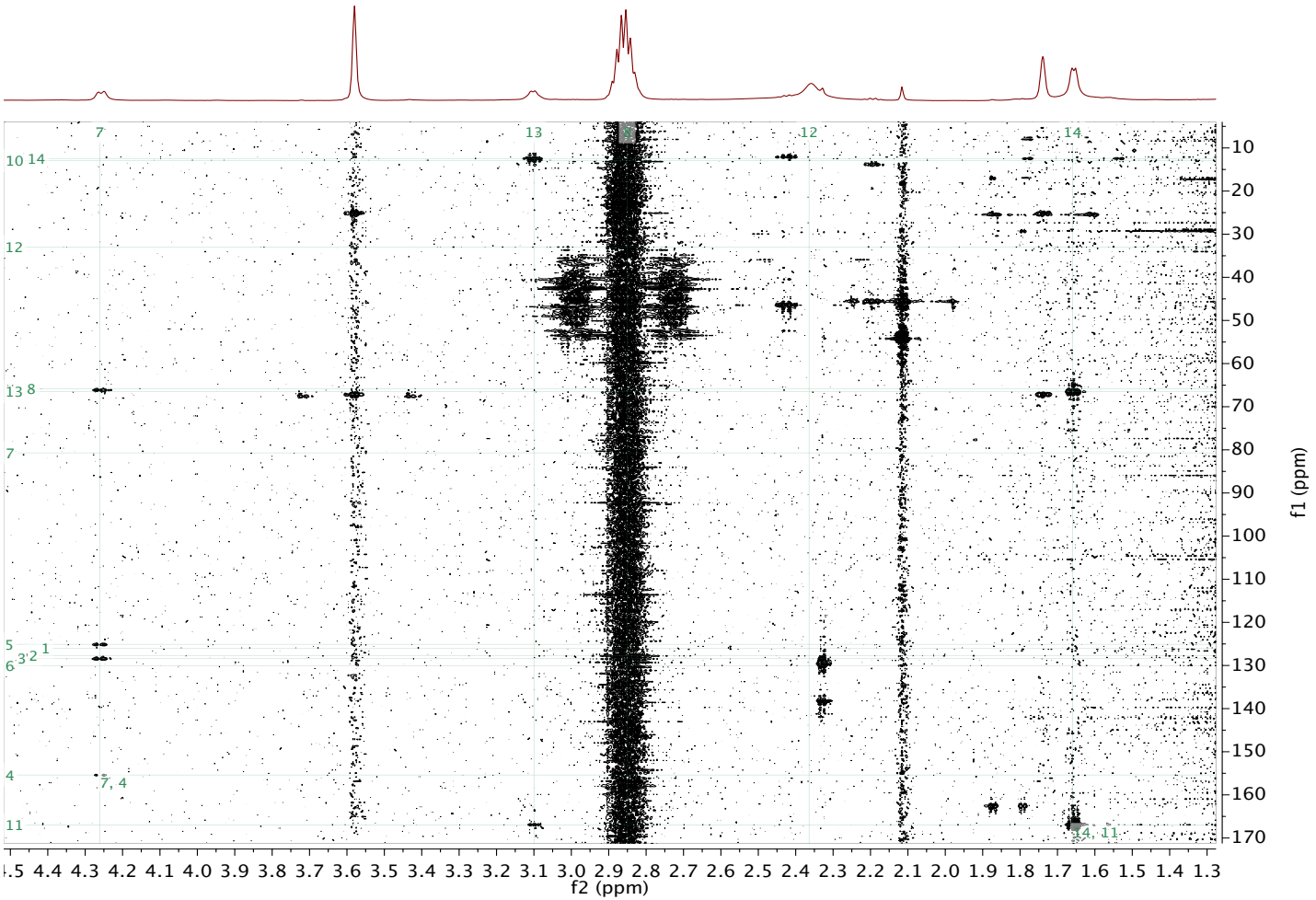


Figure 37. Expansion of the HMBC spectrum of a solution of 0.30 M **8** in 12.3 M THF-d_8 at –80 °C.

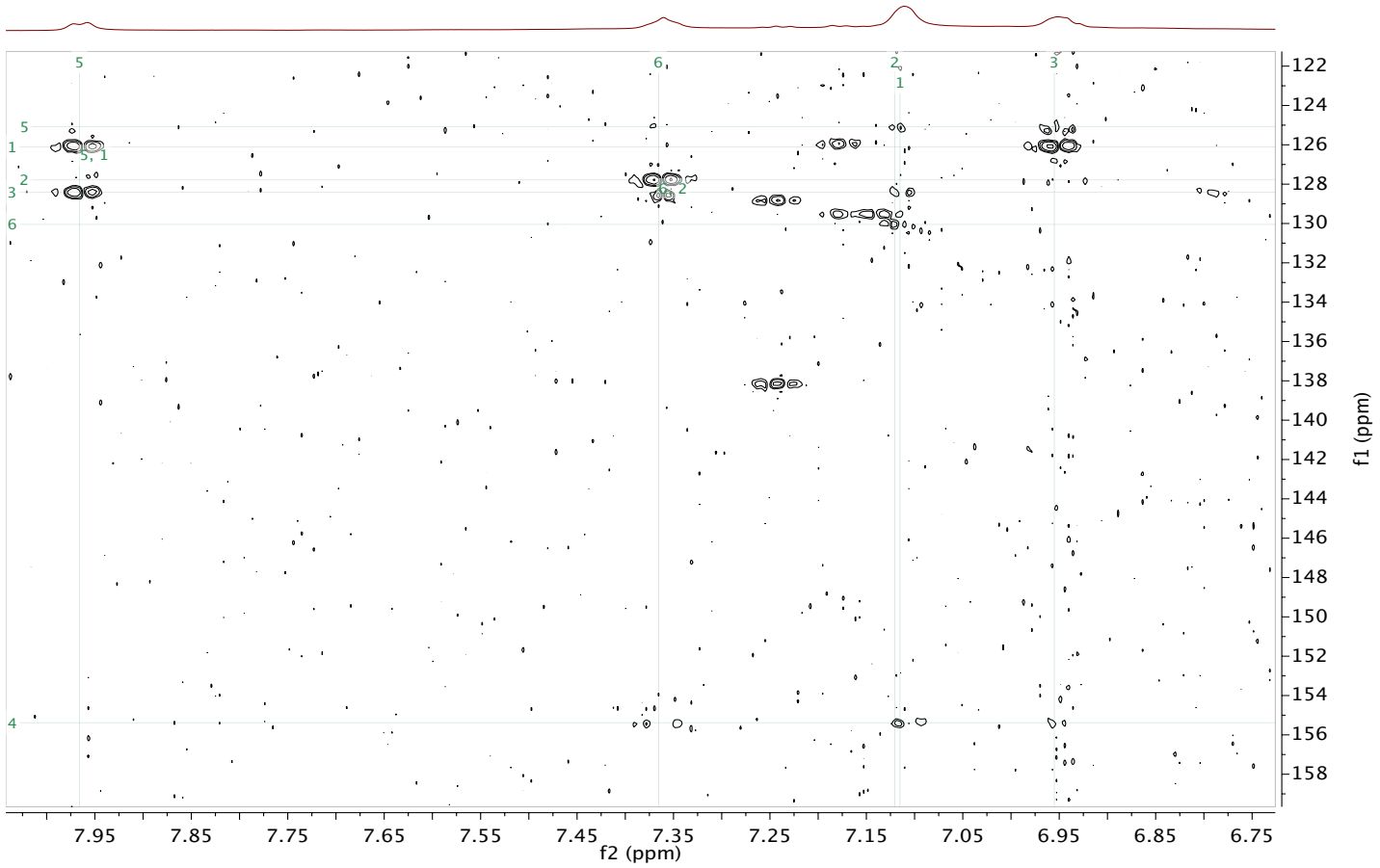


Figure 38. Expansion of the HMBC spectrum of a solution of 0.30 M **8** in 12.3 M THF-d_8 at –80 °C.

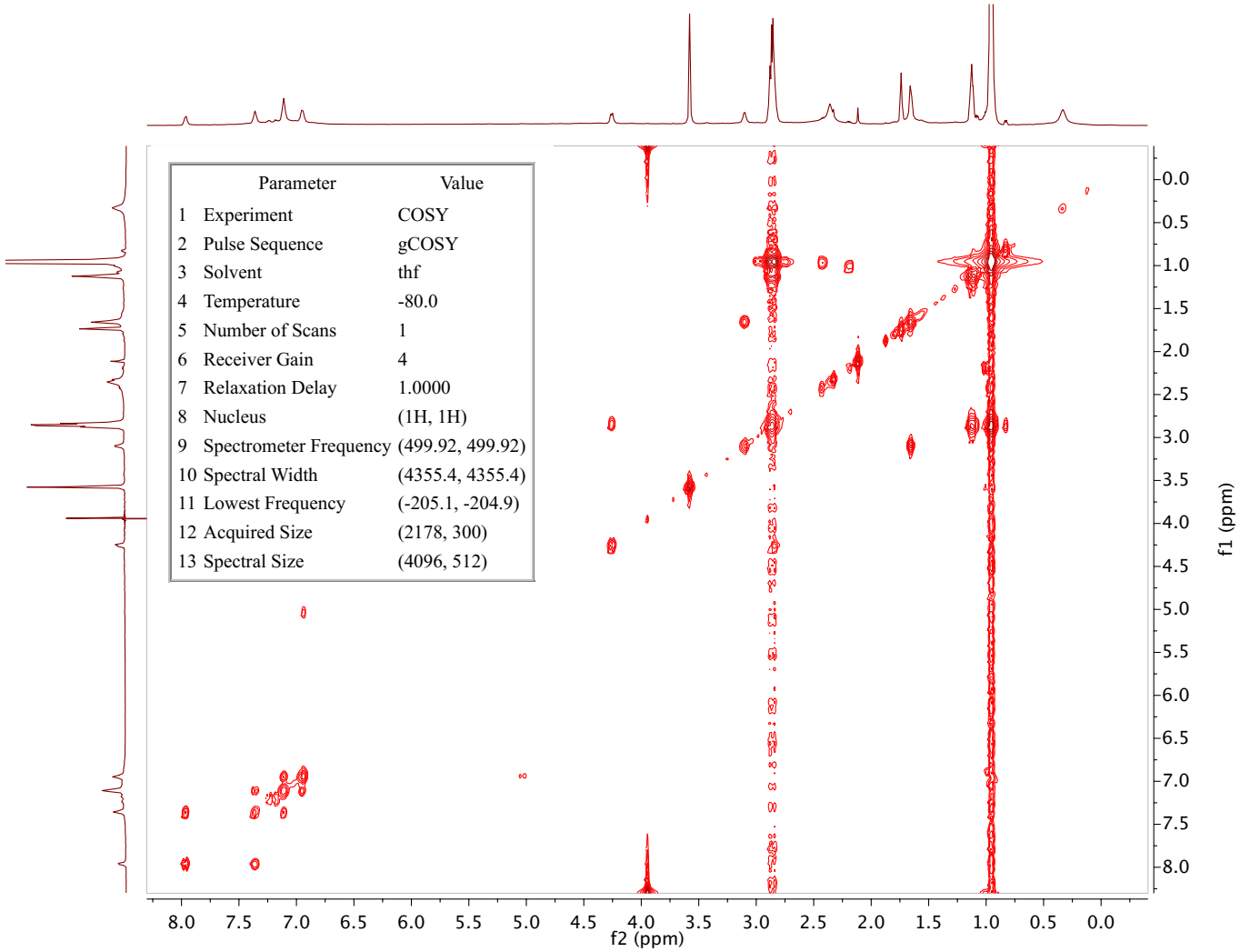


Figure 39. Full-display COSY spectrum of a solution of 0.30 M **8** in 12.3 M THF-d_8 at –80 °C.

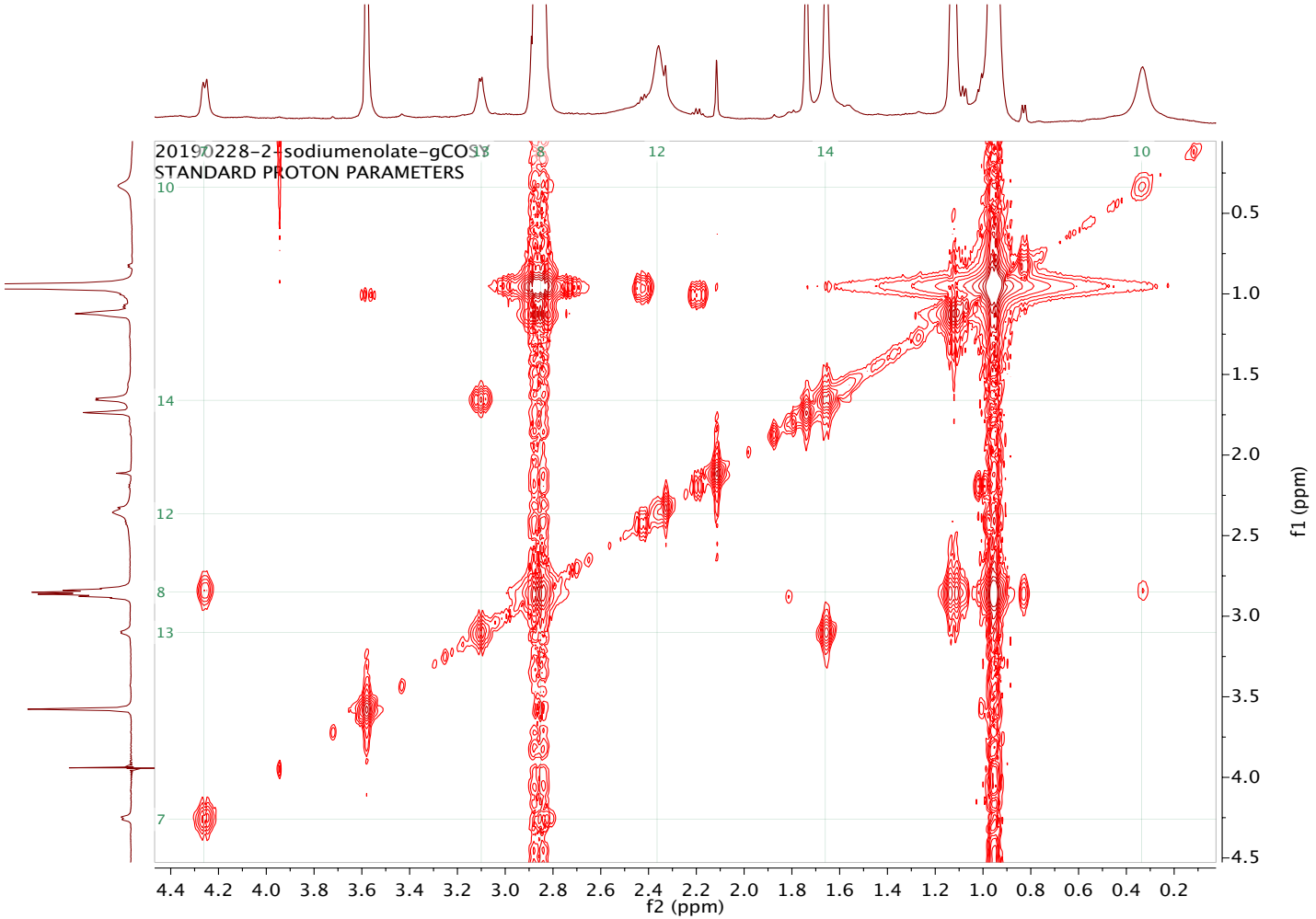


Figure 40. Expansion of the COSY spectrum of a solution of 0.30 M **8** in 12.3 M THF-d_8 at –80 °C.

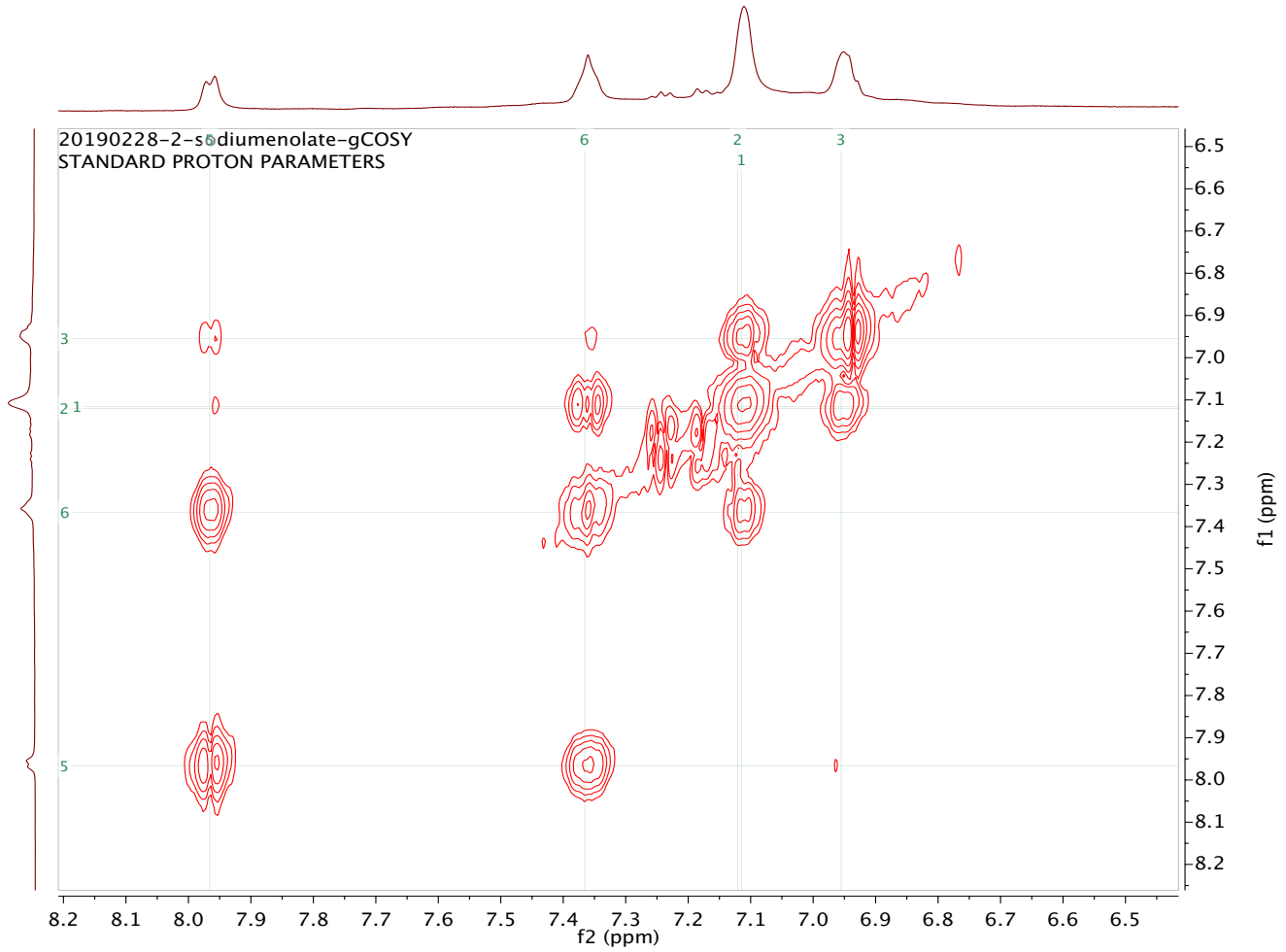


Figure 41. Expansion of the COSY spectrum of a solution of 0.30 M **8** in 12.3 M THF-d_8 at –80 °C.

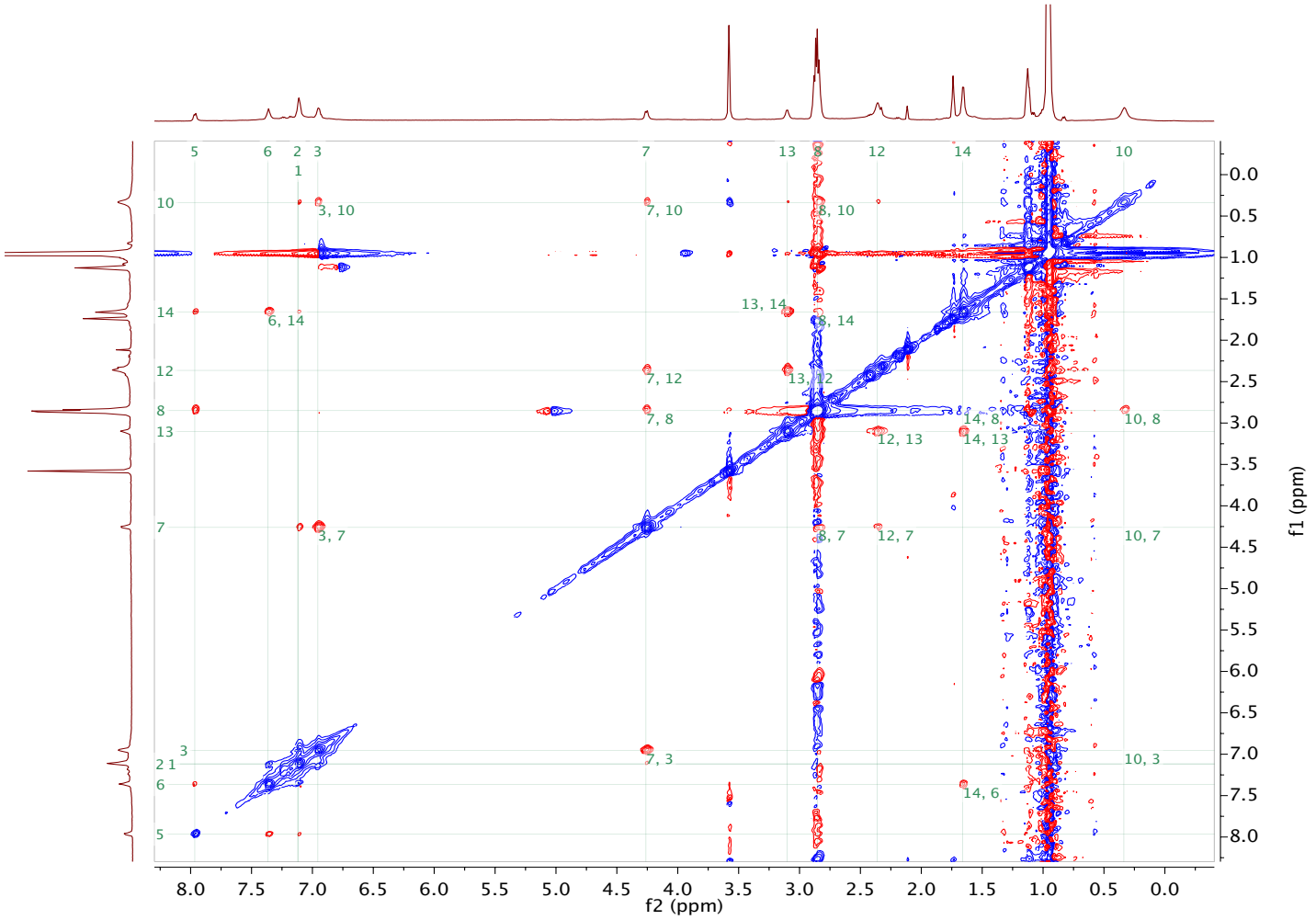


Figure 42. Full-display ROESY spectrum of a solution of 0.30 M **8** in 12.3 M THF-d_8 at –80 °C.

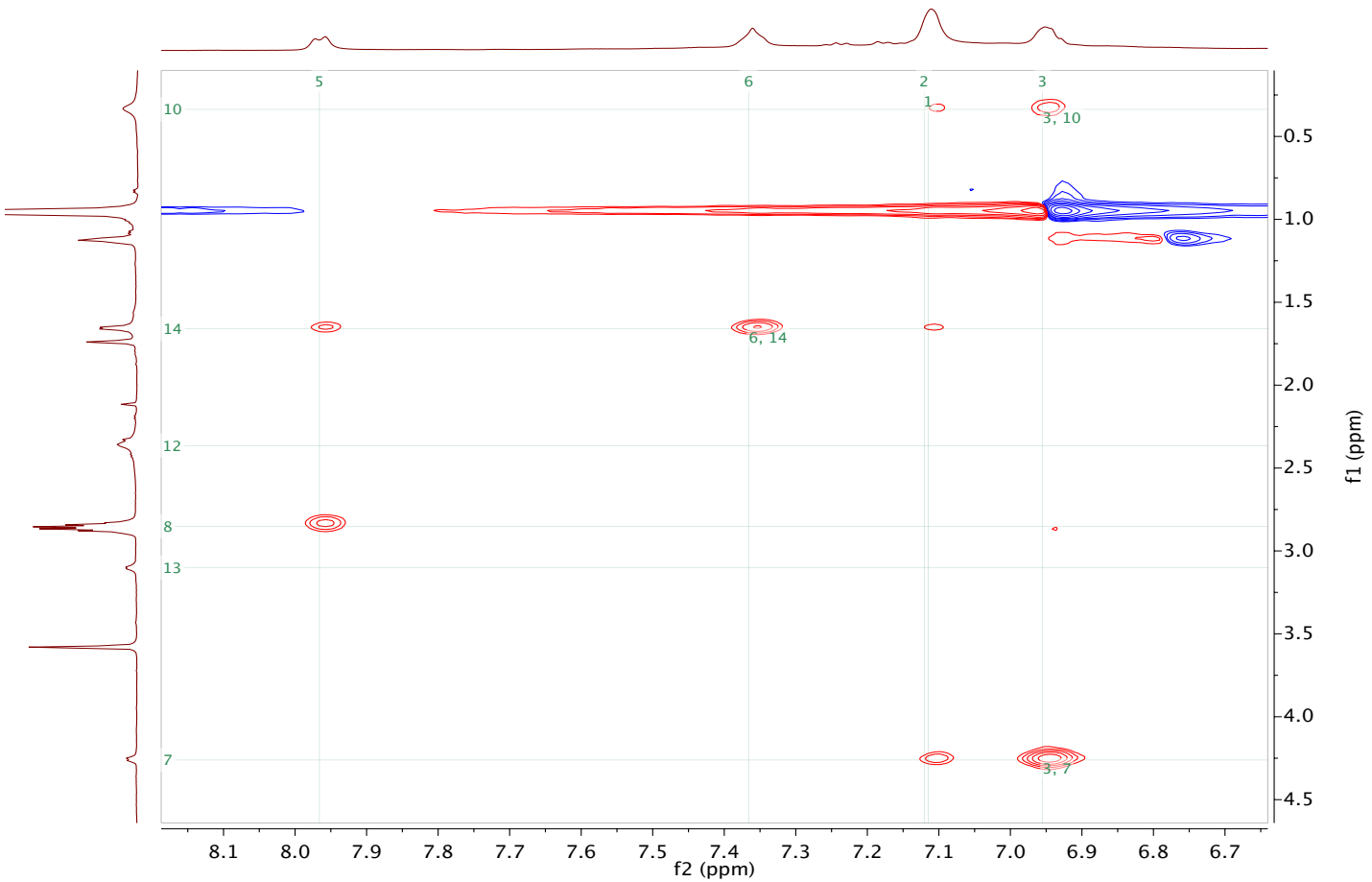


Figure 43. Expansion of the ROESY spectrum of a solution of 0.30 M **8** in 12.3 M THF-d_8 at –80 °C.

2D NMR analysis of heteroaggregate 18: A sample prepared from 0.70 M NaDA, 0.255 M **1** and 0.045 M **34** in 12.3 M THF-d_8, after aging at –80 °C for 18 h, was studied by standard 2D NMR techniques. All chemical shifts were assigned using high-field indirect-resolution 2D HSQC, COSY and HMBC experiments.

Experimental: 2D NMR spectra were acquired on a 500 MHz Varian INOVA spectrometer operating at 499.92 MHz for ^{1}H observation using a 5 mm Varian inverse-detect probe head with Z-axis pulsed field-gradient. Sample temperature was maintained at –80 °C as calibrated with a neat methanol sample. ^{1}H and ^{13}C chemical shifts were referenced to the residual downfield THF-d_7 resonance at 3.58 ppm and 67.57 ppm, respectively. 2D experiments were acquired using standard pulse sequences supplied in VnmrJ 3.2A (Agilent Inc.) and processed and analyzed in MestReNova 11.0.3 (Mestrelab Research S.L.).

Determination of the 3D aggregate structure: The 3D structure of the aggregate was derived from 2D ROESY (reported as H–H correlations) and HSQC-NOESY (reported as C–H correlations) experiments. The enolate is in the Z configuration based on the strong nOe correlation between H-12 and C-13, between H-12' and C-13', between H-12" and C-13", between H-12'" and C-13'". Reciprocal C-12 and H-13 (C-12' and H-13', C-12" and H-13", C-12'" and H-13'") correlation is also observed. The starting point for solving the structure is correlations between C-5 and H-14'" (also between C-5'" and H-15). This correlation indicates the alkoxide part (C-5) of the red subunit is close to the enolate part (H-14'") of the blue subunit. Similarly, the alkoxide part (C-5'") of the blue subunit is close to the enolate part (H-15) of the red subunit (Figure 42). The bottom face of the aggregate should me similar to the top face. There are two ways to assemble the bottom face (Figure 43-A and Figure 43-B). The right-hand structure will require close proximity of the two enolate parts from top to bottom face. However, such correlations are not available. The final structure is the left-hand structure. Black subunits are from homoaggregates **8**.

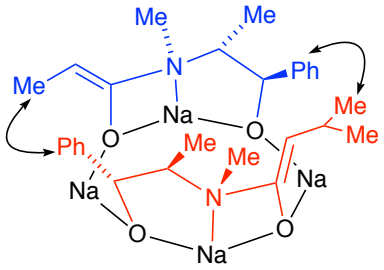


Figure 44. Illustration of blue and red subunits.

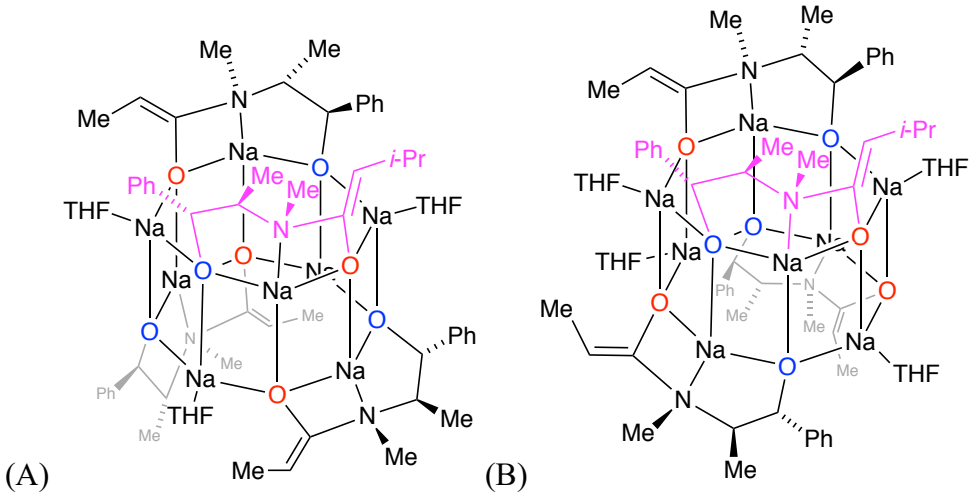


Figure 45. Two possible structures of heteroaggreagtes.

Table 2. ^{1}H and ^{13}C chemical shifts and assignments for heteroaggregate **18** at –80 °C.

Atom	δC, ppm	δH, ppm	HMBC	COSY	HSQC-NOESY[1,2]
1 C	126.50	7.12	5,6	6	
1' C	126.50	7.12	5', 6'	6'	
1''' C	126.50	7.12	5'',6''	6''	
1'' C	126.50	7.12	5''',6'''	6'''	
2 C[3]	128.18	7.12		6	
2' C	128.20	7.12		6'	
2'' C	128.20	7.12		6''	
2''' C	128.20	7.12		6'''	
3 C[3]	128.74	6.96	5,7	5,6	
3' C	128.82	6.96	5',7'	5',6'	
3'' C	128.82	6.96	5'',7''	5'',6''	
3''' C	128.82	6.96	5''',7'''	5''',6'''	
4 C[3]	155.38	–			
4' C	154.82	–			
4'' C	154.82	–			
4''' C	154.82	–			
5 C[3]	125.85	8.04	1,3,7	3,6	14'''
5' C	125.39	7.94	1',3',7'	3',6'	
5'' C	125.18	7.99	1'',3'',7''	3'',6''	
5''' C	125.47	7.84	1''',3''',7'''	3''',6'''	14,15
6 C[3]	130.48	7.37	1,3,2	1,2,3,5	
6' C	130.48	7.37	1',3',2'	1',2',3',5'	

6" C	130.48	7.37	1",3",2"	1",2",3",5"	
6"' C	130.48	7.37	1"',3"',2"'	1"',2"',3"', 5"'	
7 C	80.90	4.32	3,5,8	3,8	
7' C	81.87	4.21	3',5',8'	3',8'	12
7" C	81.87	4.21	3",5",8"	3",8"	12'
7"' C	80.81	4.35	3"',5"',8"'	3"',8"'	12"
8 C	64.49	3.05	7	7,10	12"'
8' C	67.14	2.68	7'	7',10'	
8" C	67.76	2.75	7"	7",10"	
8"' C	66.01	2.92	7"'	7"',10"'	
10 C	13.78	0.32		8	
10' C	13.35	0.35		8'	
10" C	13.35	0.34		8"	
10"' C	13.35	0.33		8"'	
11 C	164.18	–	13,14		
11' C	168.02	–	13',14'		
11" C	167.56	–	13",14"		
11"' C	166.98	–	13"',14"'		
12 C	33.34	2.40			7,13
12' C	33.56	2.36			7',13'
12" C	33.34	2.36			7",13"
12"' C	33.34	2.38			7"',13"'
13 C	64.89	2.96	11,14	14	12
13' C	67.44	3.16	11',14'	14'	12'
13" C	67.73	3.12	11",14"	14"	12"

13''' C	66.41	3.10	11''',14'''	14'''	12'''
14 C	27.05	2.60	11,13,15,16	13,15,16	5'''
14' C	12.58	1.64	11',13'	13'	
14'' C	12.85	1.64	11'',13''	13''	
14''' C	12.85	1.68	11''',13'''	13'''	5
15C	27.51	1.08	14	14	5'''
16C	27.16	1.01	14	14	

[1]HSQC correlations were omitted from the assignment table. [2]Important correlations that allowed determination of subunit arrangement are marked in red. [3]Not determined.

	Parameter	Value
1	Experiment	1D
2	Pulse Sequence	s2pul
3	Solvent	thf
4	Temperature	-80.0
5	Number of Scans	1
6	Receiver Gain	2
7	Relaxation Delay	1.0000
8	Nucleus	1H
9	Spectrometer Frequency	499.92
10	Spectral Width	7998.4
11	Lowest Frequency	-1001.1
12	Acquired Size	16384
13	Spectral Size	65536

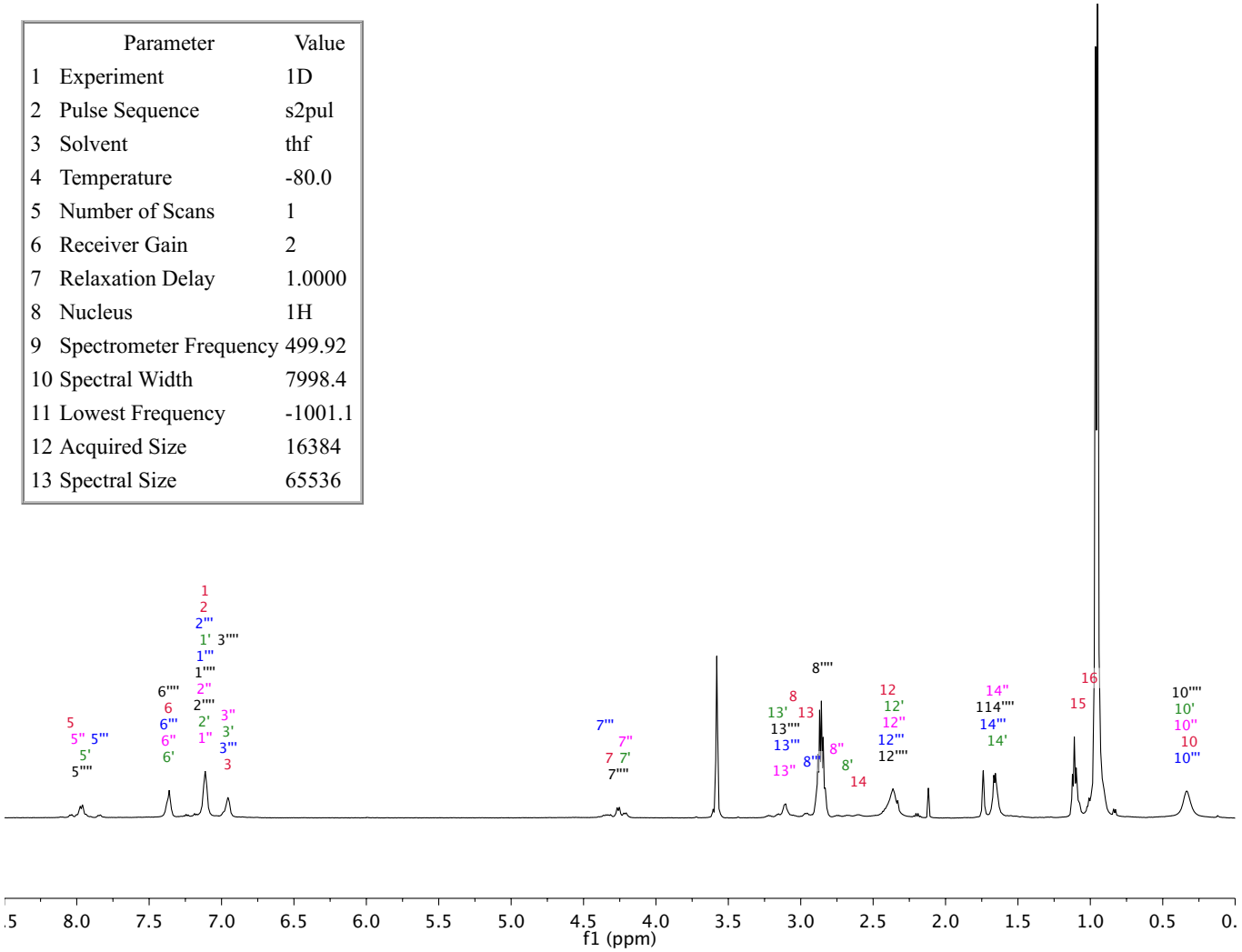


Figure 46. ^{1}H NMR spectrum for 0.30 M solutions of 85:15 **8** and **15** in 12.3 M THF-d_8 at –80 °C. Labels indicate assignments by 2D NMR.

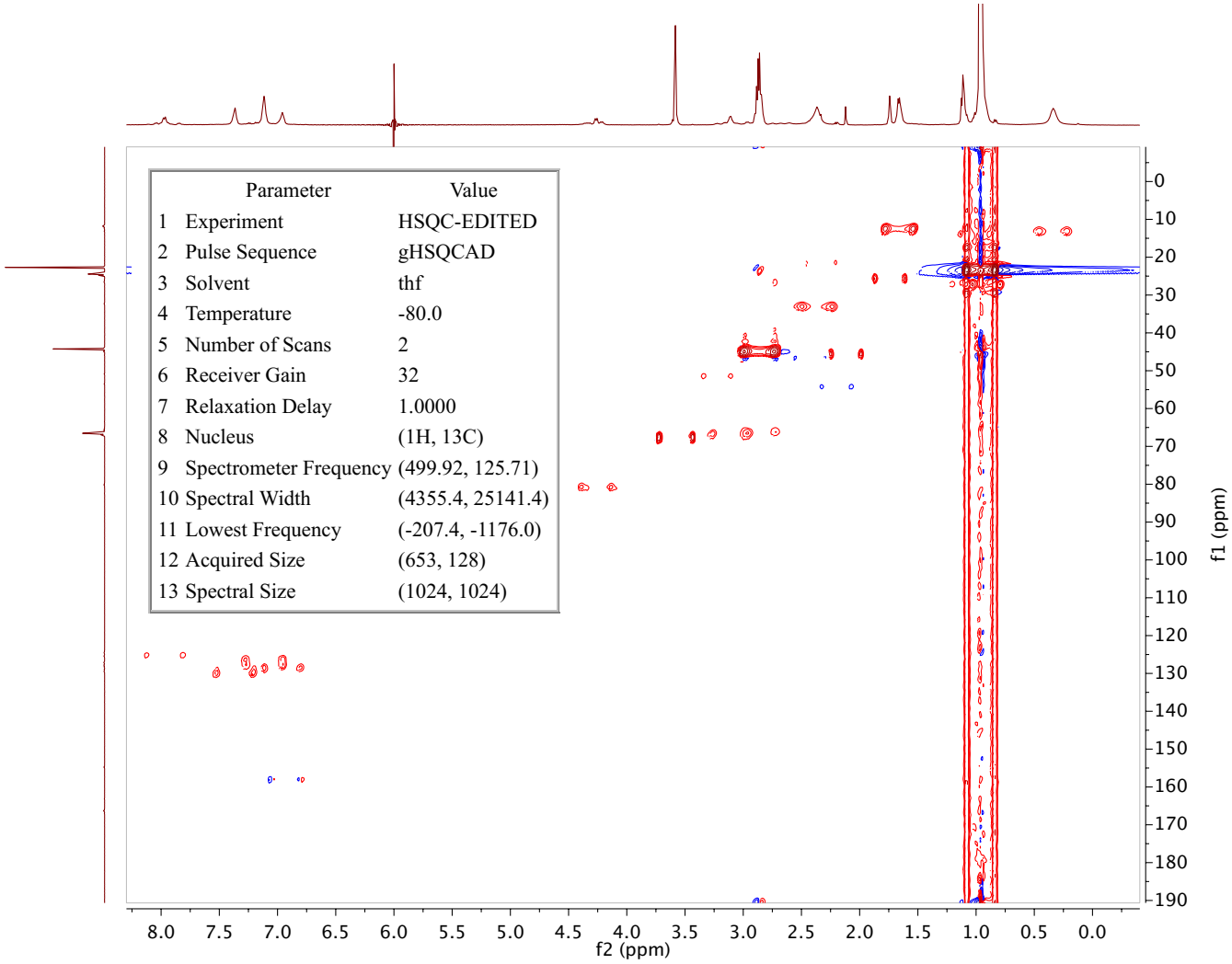


Figure 47. Full display HSQC spectrum of 0.30 M solutions of 85:15 **8** and **15** in 12.3 M THF-d_8 at –80 °C. ^{13}C decoupler was turned off.

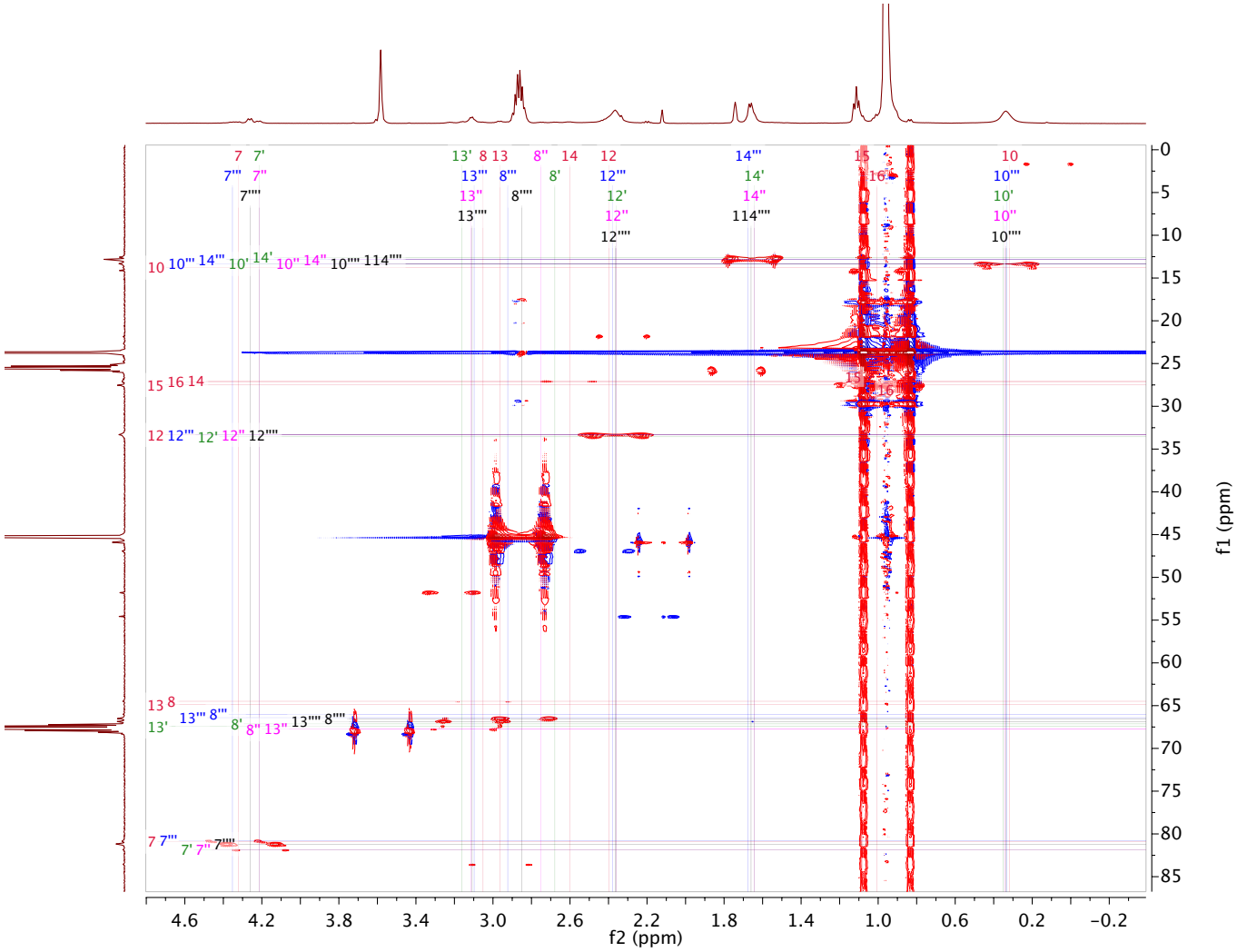


Figure 48. Expansion of the HSQC spectrum of 0.30 M solutions of 85:15 **8** and **15** in 12.3 M THF-d_8 at –80 °C. ^{13}C decoupler was turned off.

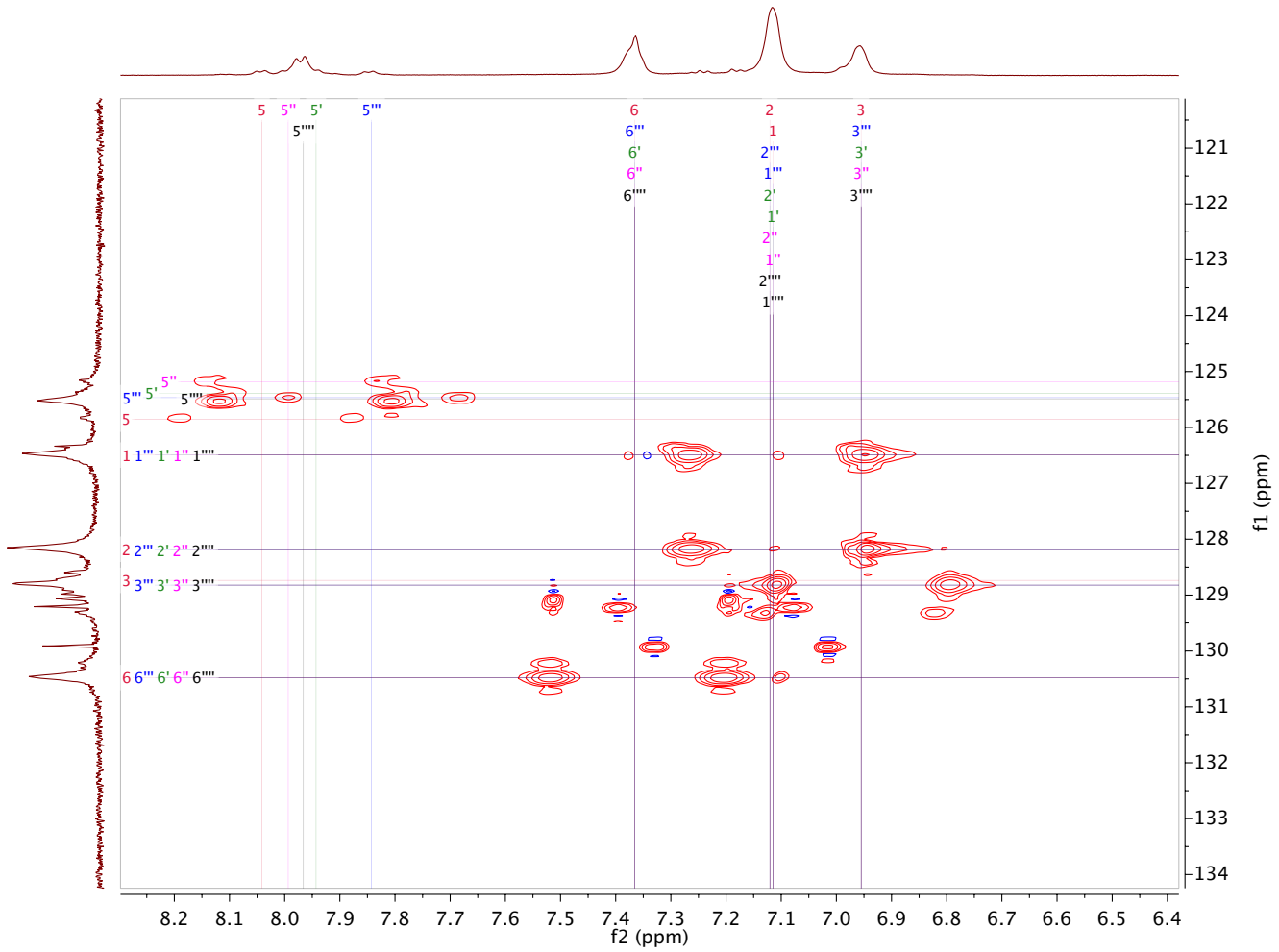


Figure 49. Expansion of the HSQC spectrum 0.30 M solutions of 85:15 **8** and **15** in 12.3 M THF-d_8 at –80 °C. ^{13}C decoupler was turned off.

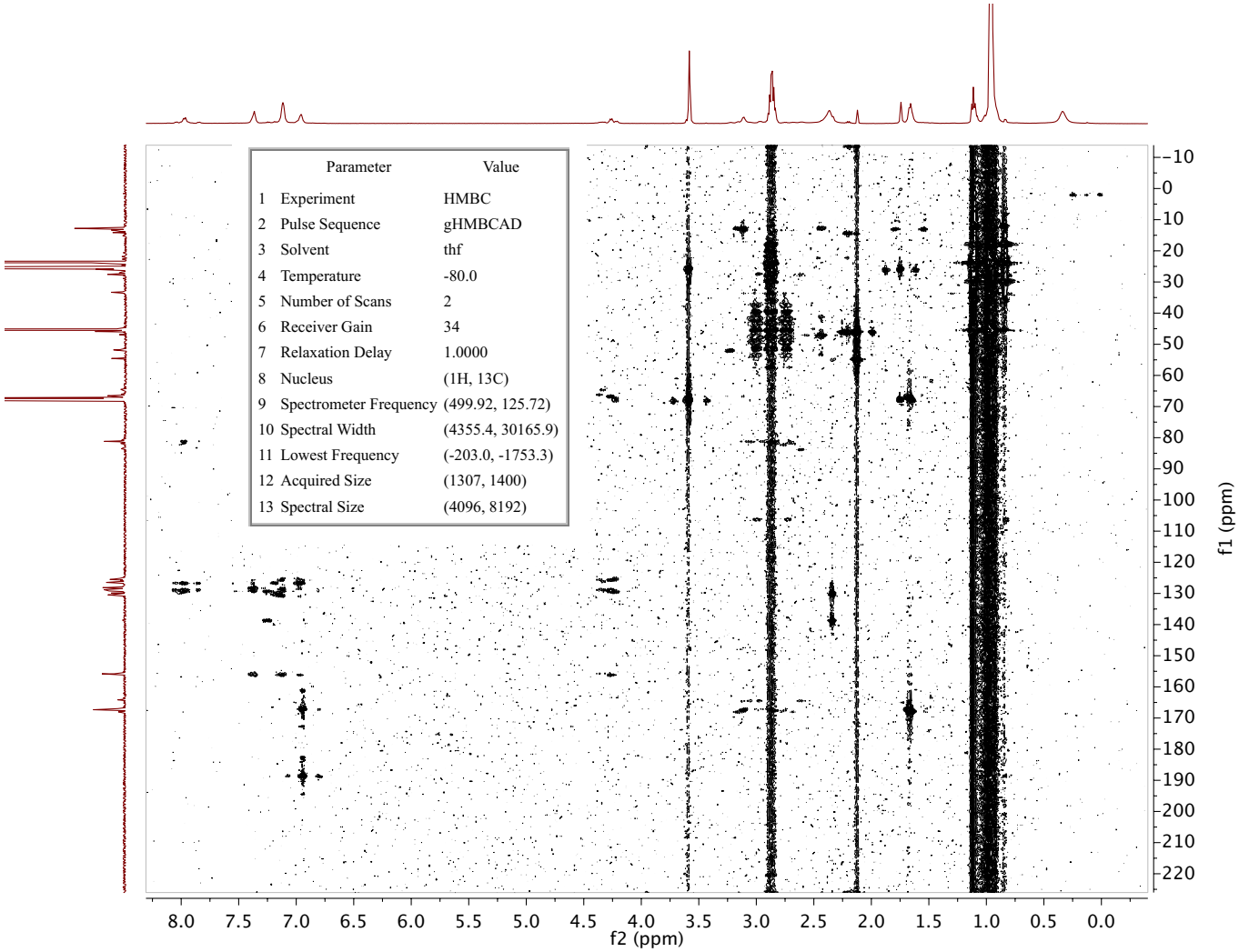


Figure 50. Full display HMBC spectrum for 0.30 M solutions of 85:15 **8** and **15** in 12.3 M THF-d_8 at –80 °C.

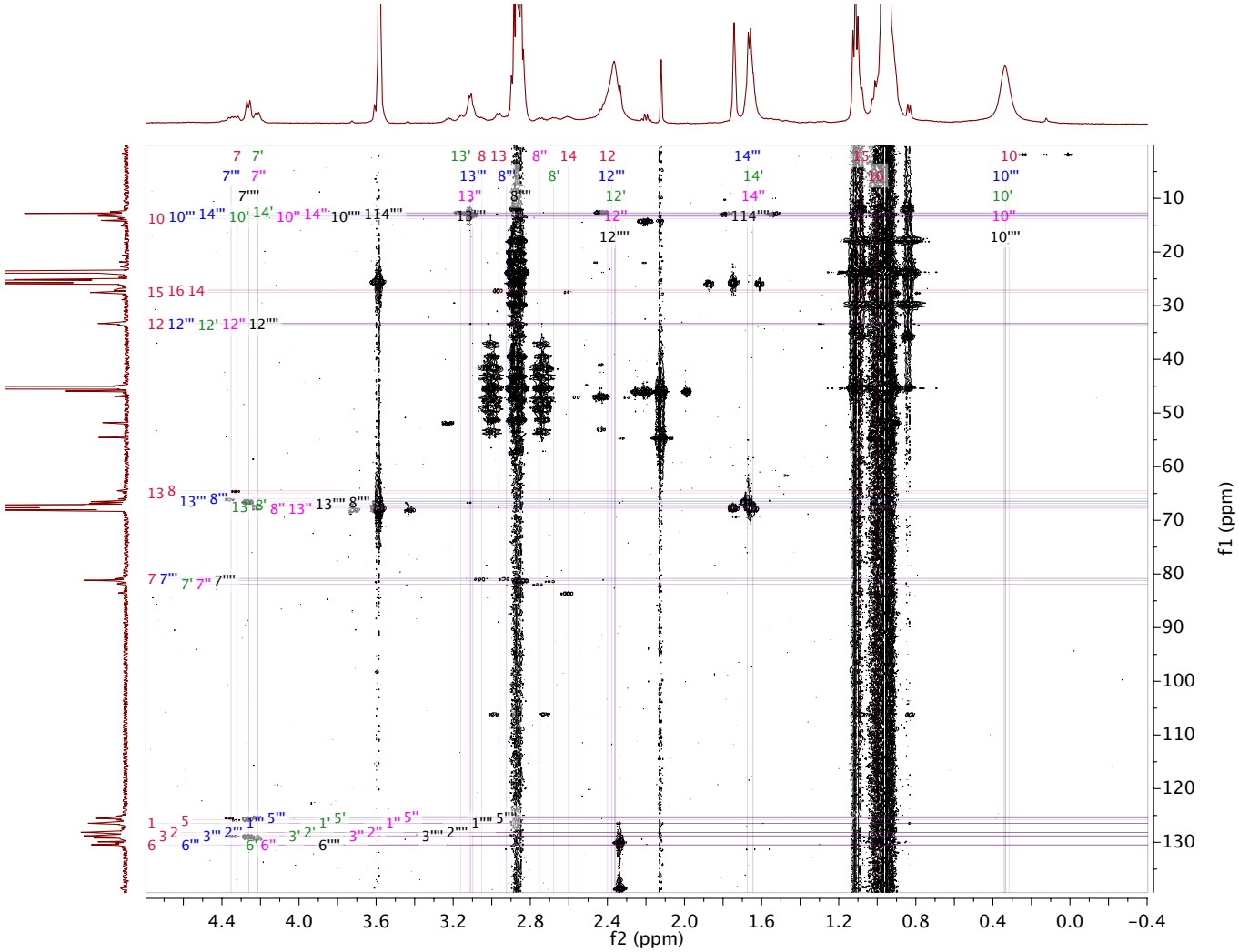


Figure 51. Expansion of the HMBC spectrum for 0.30 M solutions of 85:15 **8** and **15** in 12.3 M THF-d_8 at –80 °C.

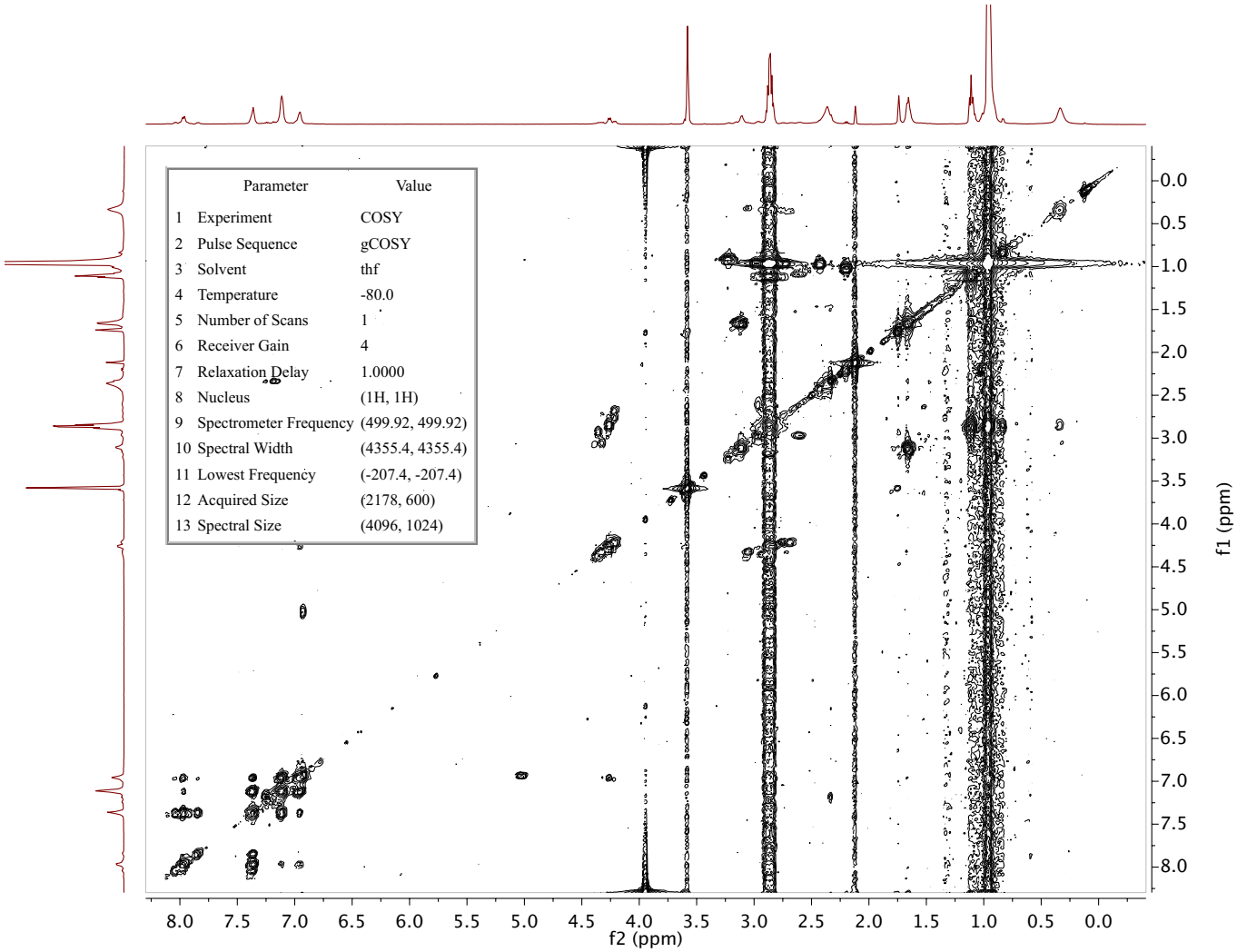


Figure 52. Full display COSY spectrum of 0.30 M solutions of 85:15 **8** and **15** in 12.3 M THF-d_8 at –80 °C.

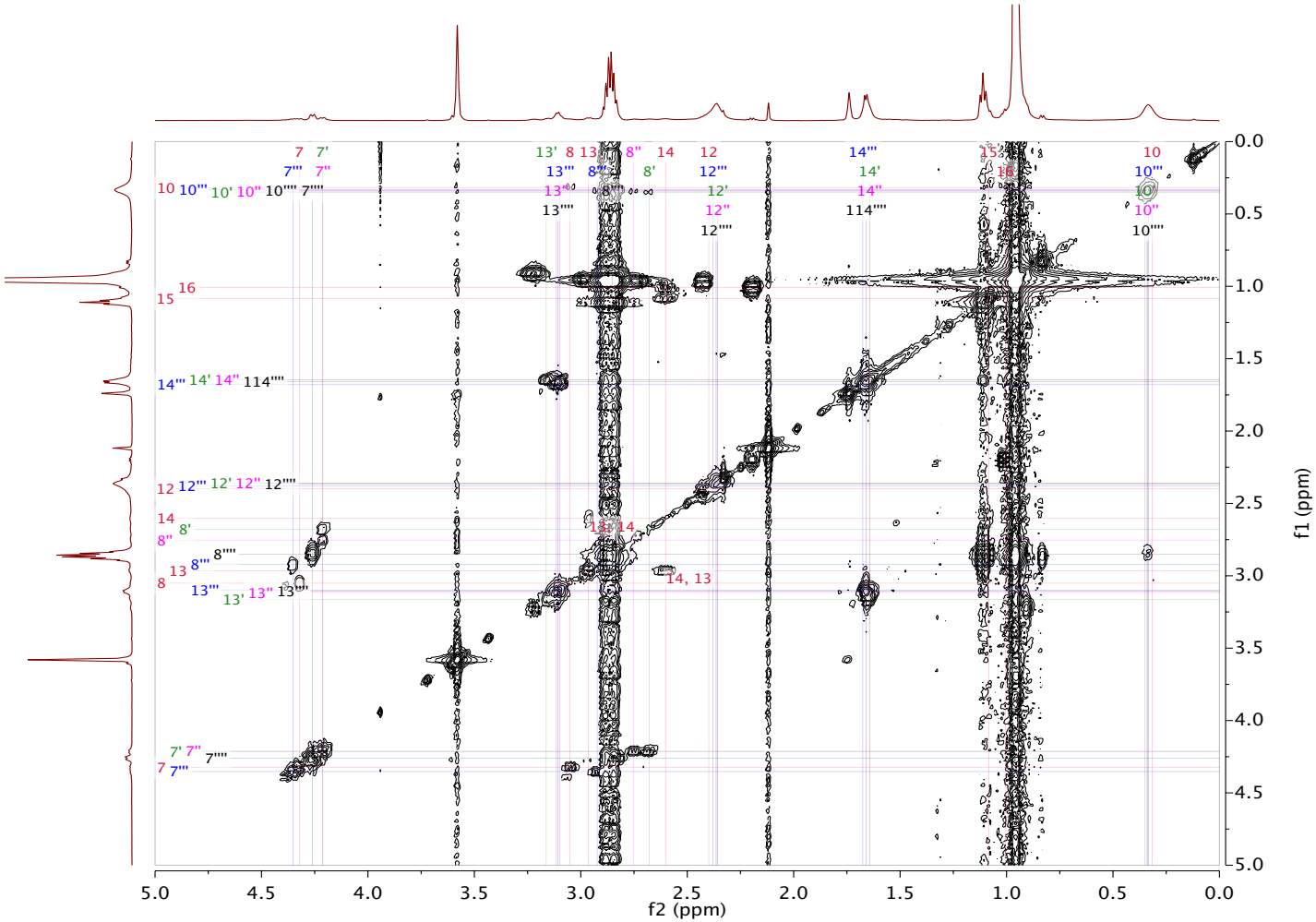


Figure 53. Expansion of the COSY spectrum of 0.30 M solutions of 85:15 **8** and **15** in 12.3 M THF-d_8 at –80 °C.

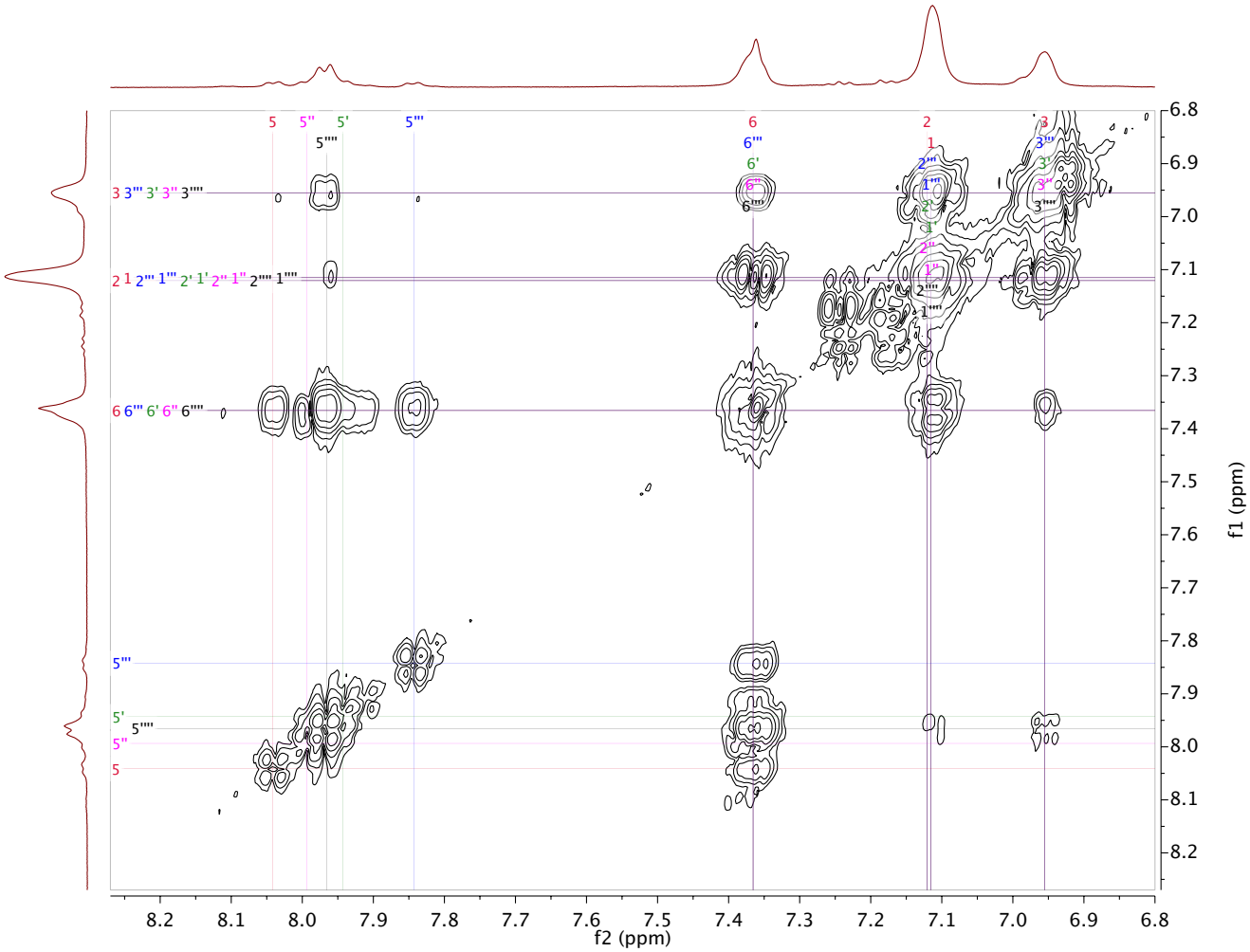


Figure 54. Expansion of the COSY spectrum of 0.30 M solutions of 85:15 **8** and **15** in 12.3 M THF-d_8 at –80 °C.

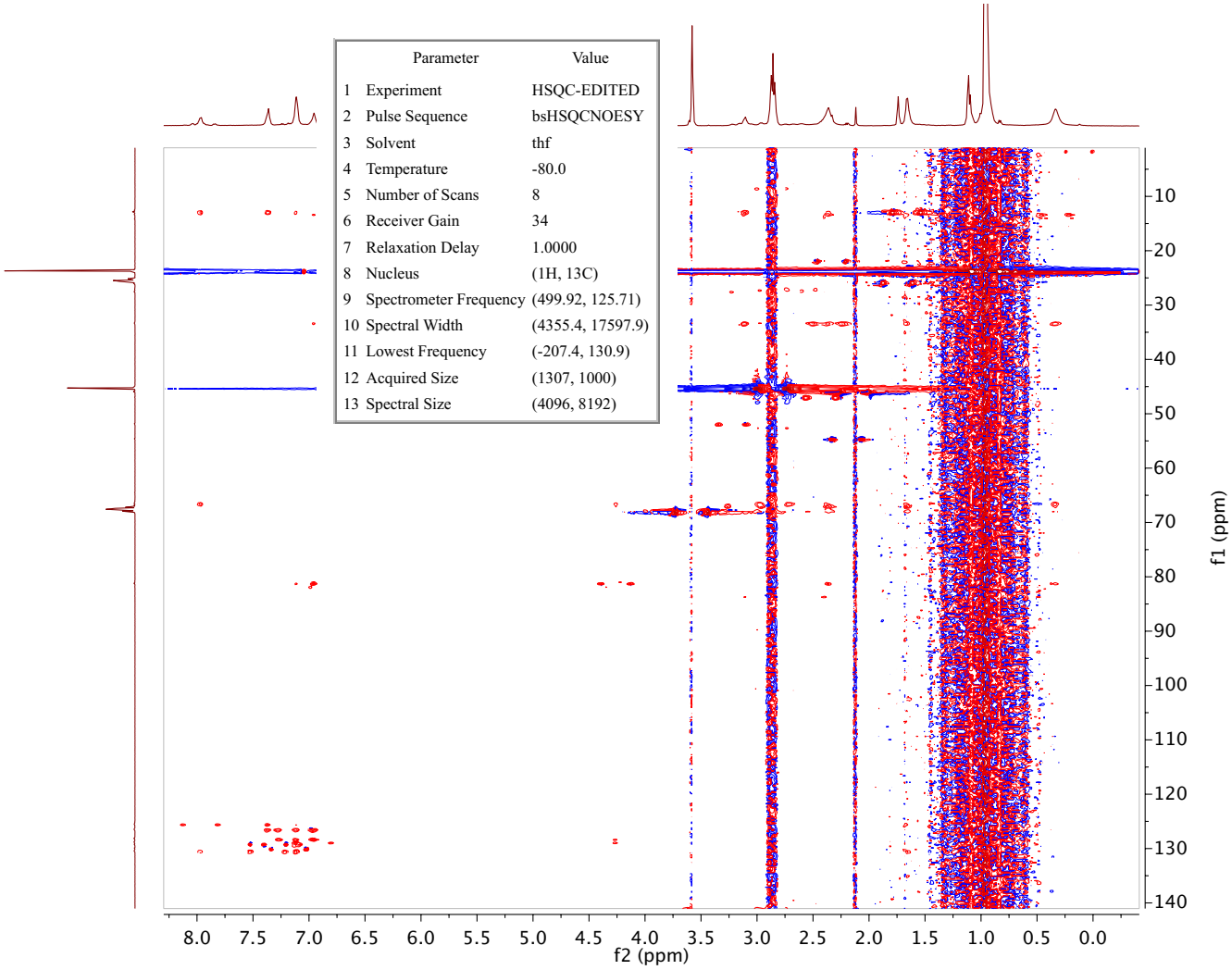


Figure 55. Full display HSQC-NOESY spectrum of 0.30 M solutions of 85:15 **8** and **15** in 12.3 M THF-d_8 at –80 °C.

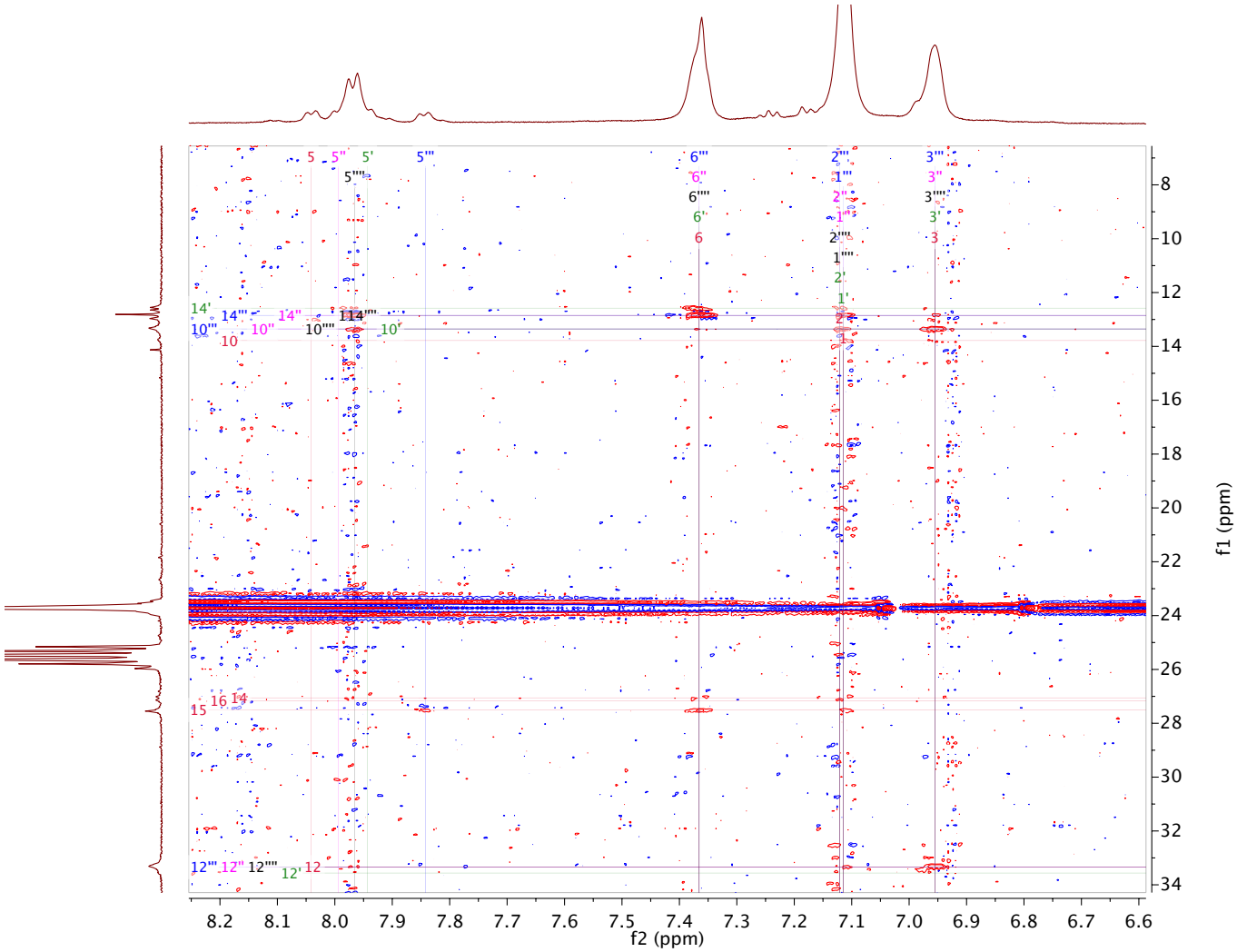


Figure 56. Expansion of the HSQC-NOESY spectrum of 0.30 M solutions of 85:15 **8** and **15** in 12.3 M THF-d_8 at –80 °C.

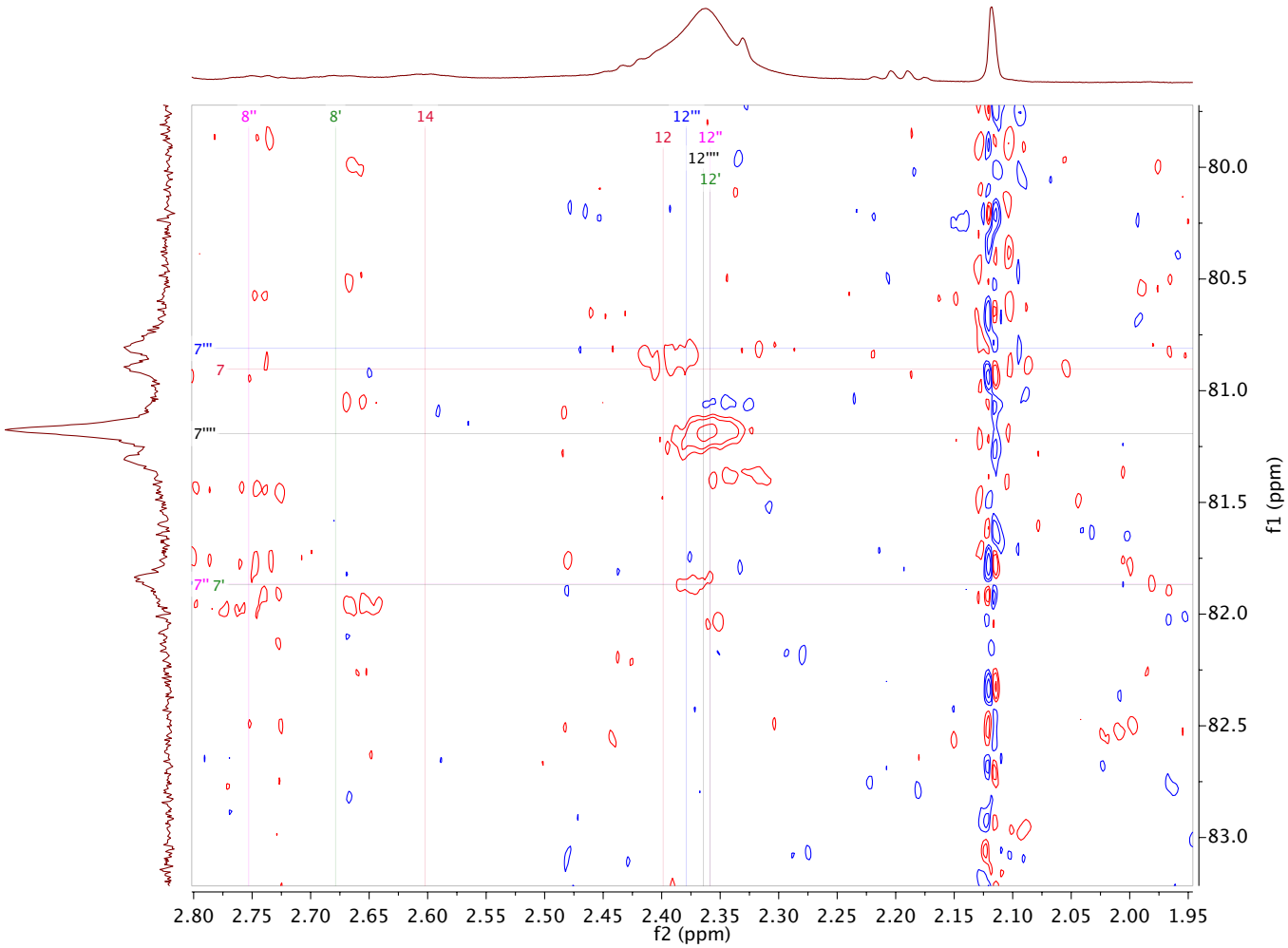


Figure 57. Expansion of the HSQC-NOESY spectrum of 0.30 M solutions of 85:15 **8** and **15** in 12.3 M THF-d_8 at –80 °C.

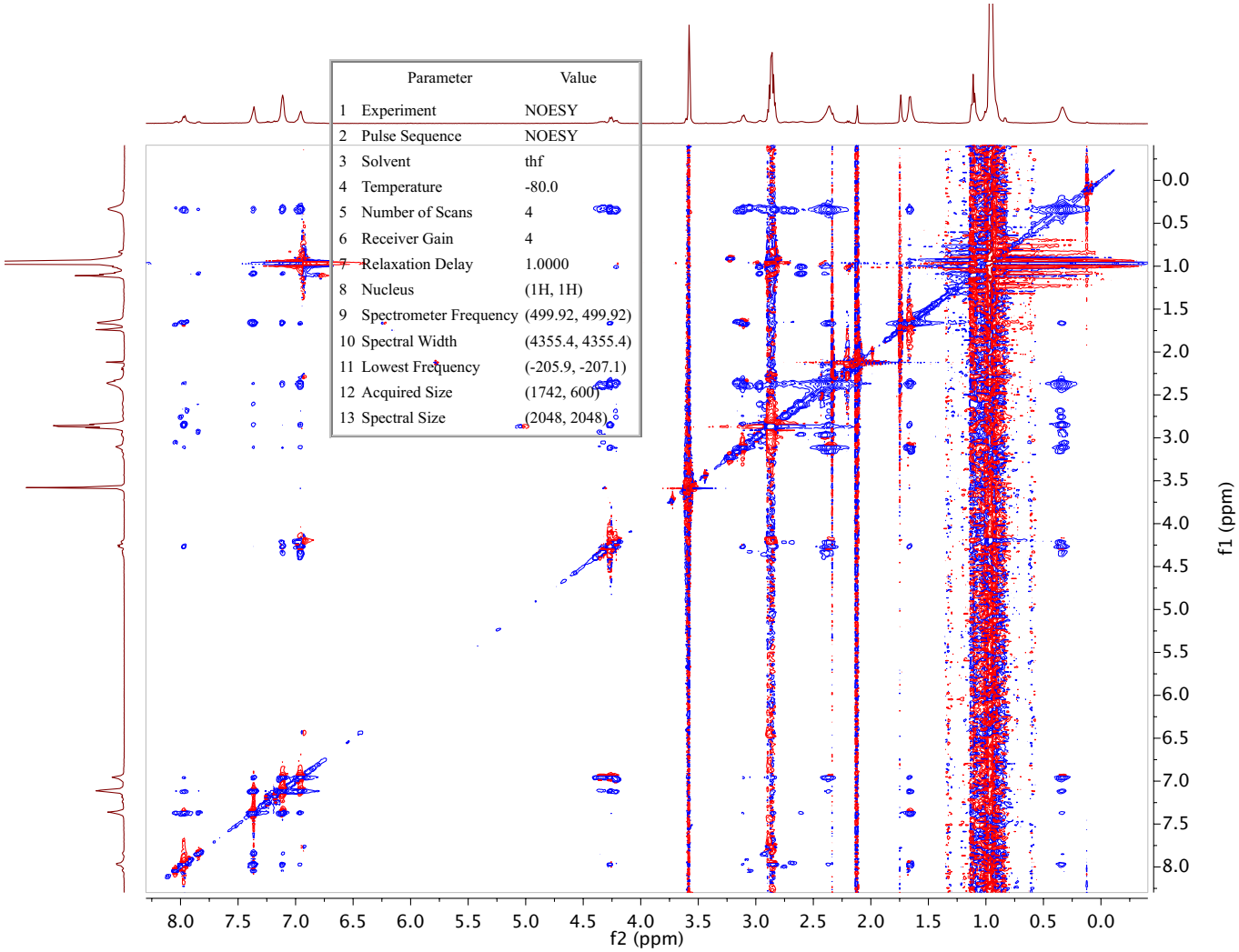


Figure 58. Full display NOESY spectrum of 0.30 M solutions of 85:15 **8** and **15** in 12.3 M THF-d_8 at –80 °C.

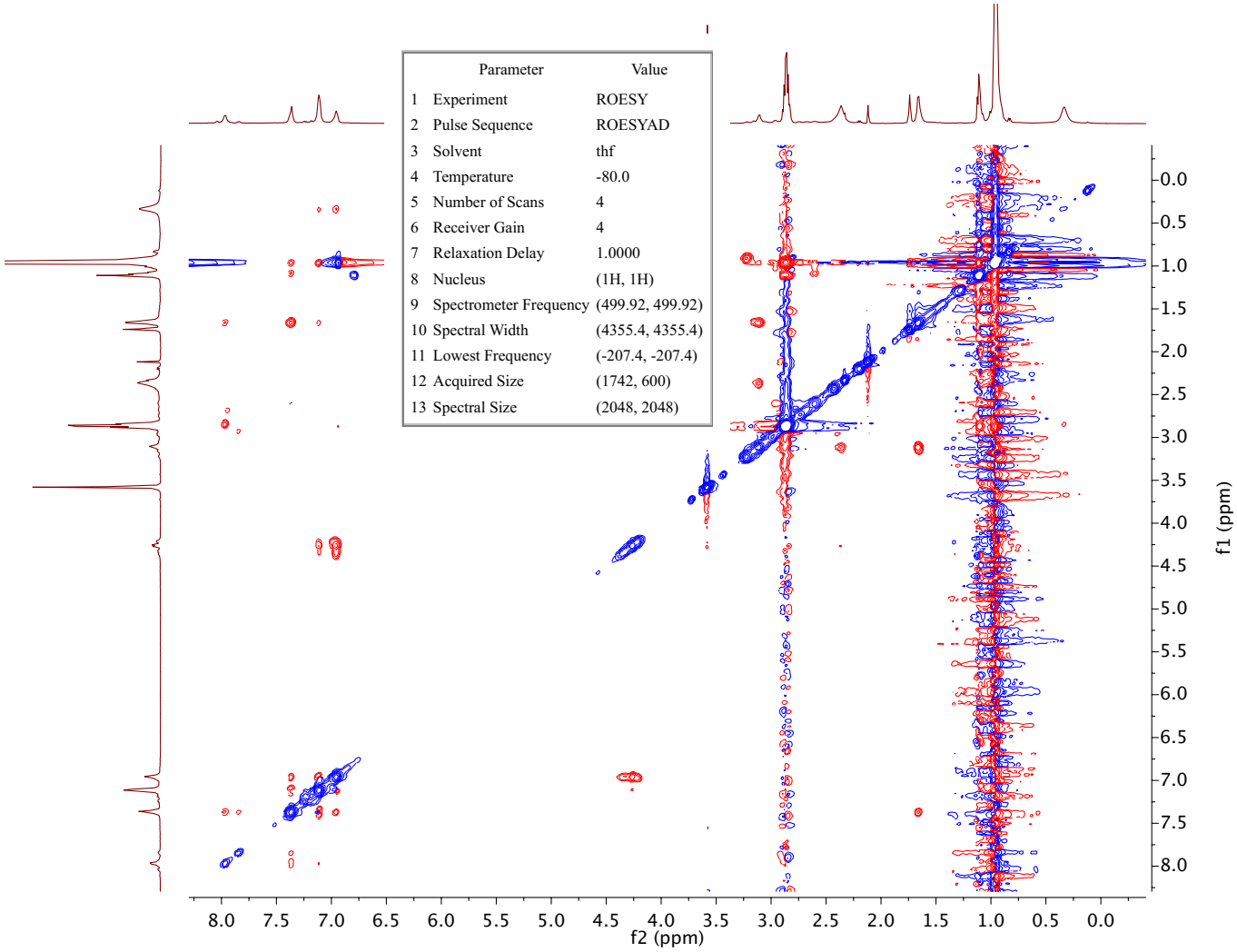


Figure 59. Full display ROESY spectrum of 0.30 M solutions of 85:15 **8** and **15** in 12.3 M THF-d_8 at –80 °C.

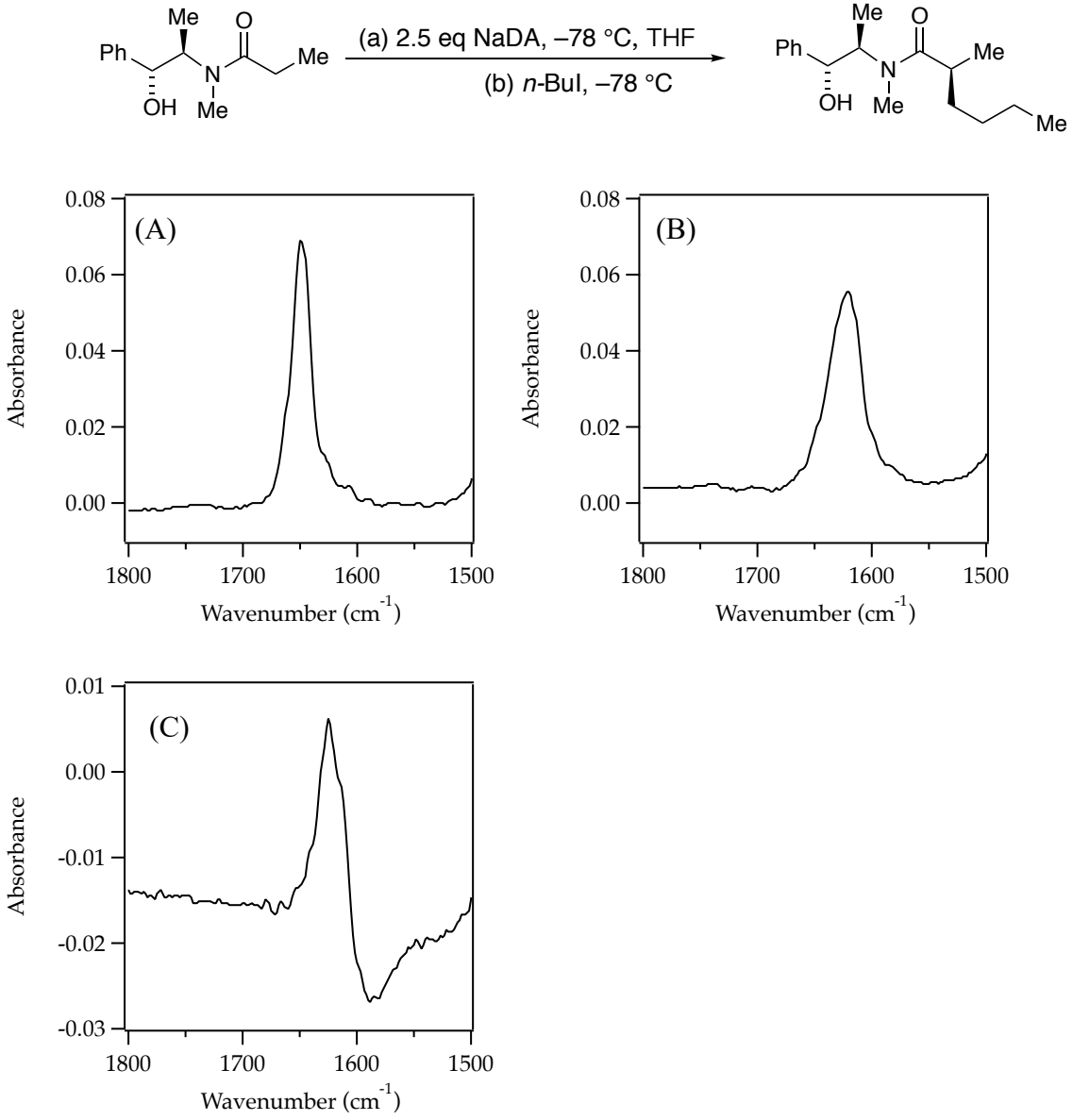


Figure 60. IR spectra in neat THF at –78 °C (A) 0.040 M substrate **1**; (B) 0.040 M enolate **8**; (C) 0.040 M product.

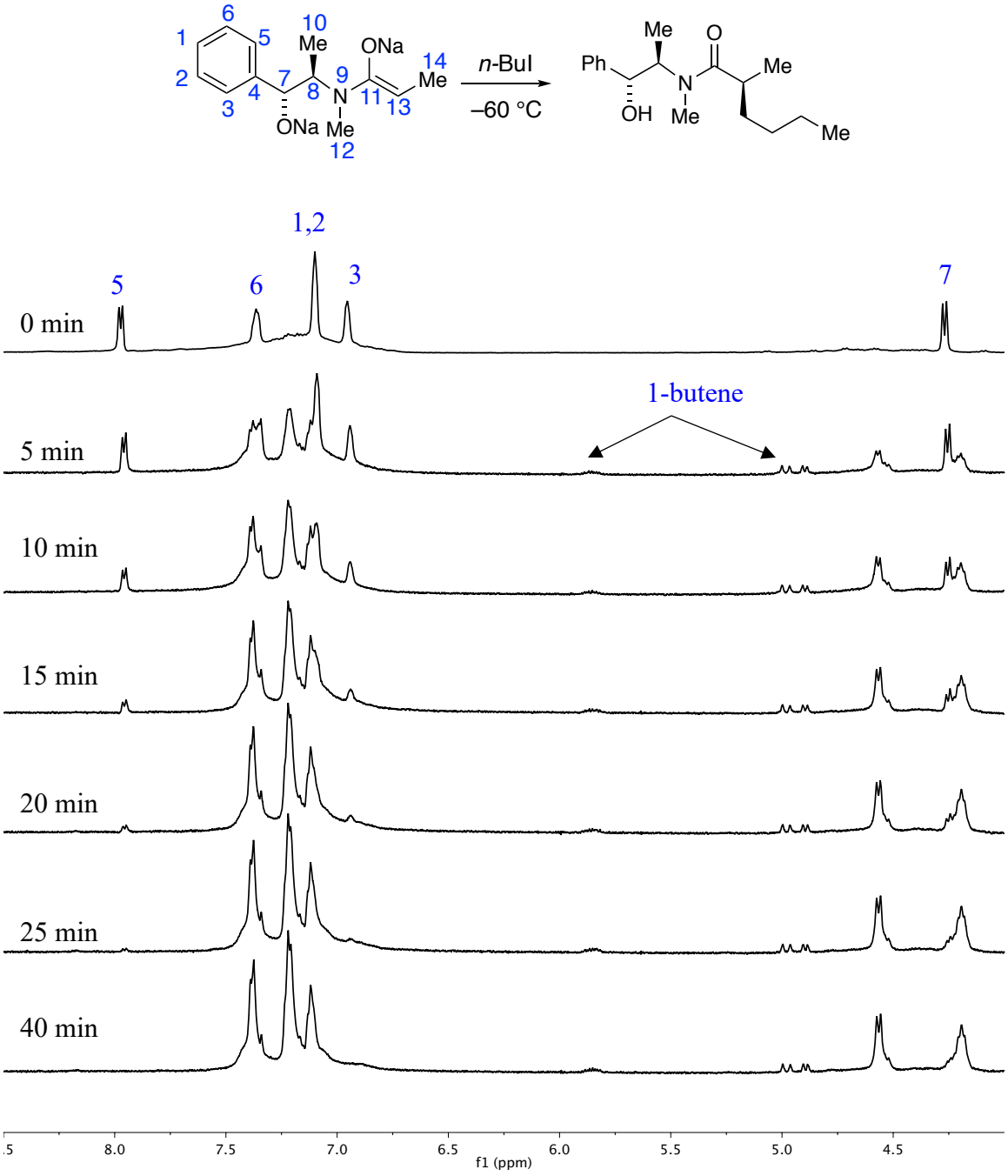


Figure 61. ^{1}H NMR spectra for reaction of 0.10 M **1** and 0.25 M NaDA in 12.3 M THF-d_8 with 0.40 M *n*-BuI at –60 °C. Reaction of enolate can be followed on NMR with clear disappearance of starting material.

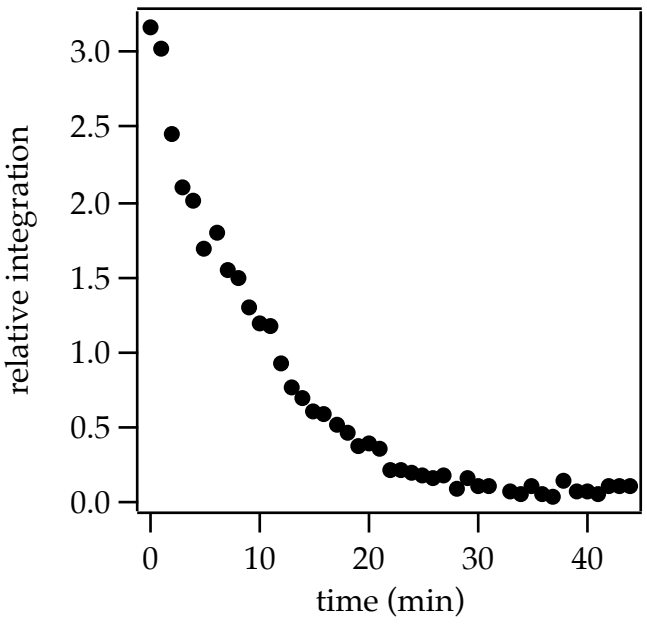


Figure 62. Plot of disappearance of enolate **8** carried out using 0.10 M **1**, 0.25 M NaDA, and 0.40 M *n*-BuI at –60 °C.

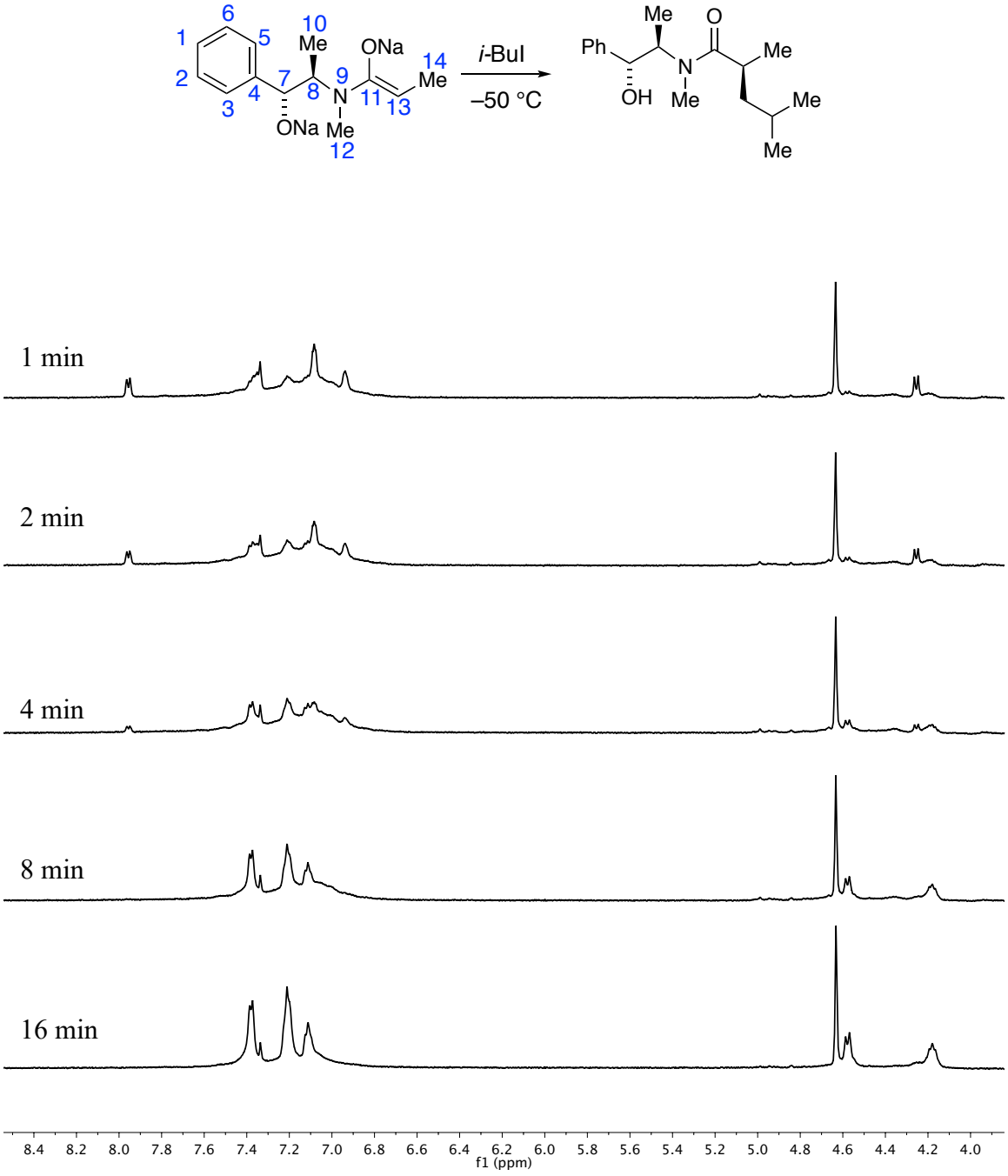


Figure 63. ^{1}H NMR spectra for reaction of 0.10 M **1** and 0.25 M NaDA in 12.3 M THF-d_8 with 1.0 M *i*-BuI at –50 °C. Reaction of enolate can be followed on NMR with clear disappearance of starting material.

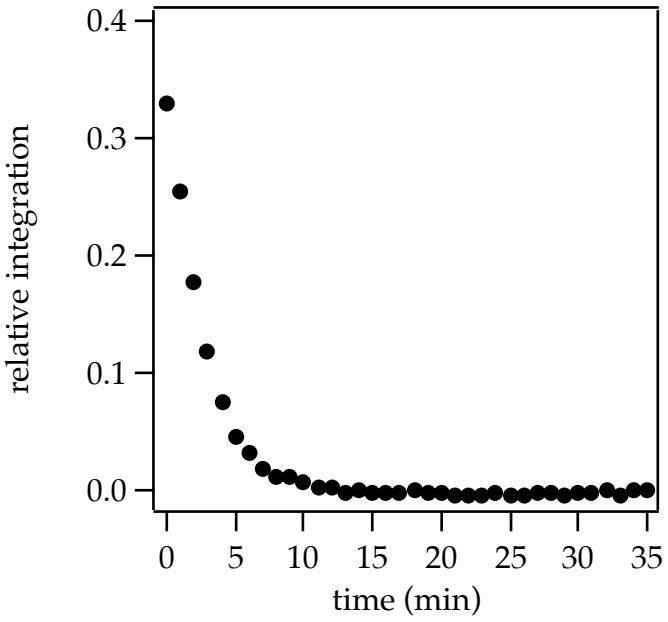


Figure 64. Plot of disappearance of enolate **8** carried out using 0.10 M **1**, 0.25 M NaDA, and 1.0 M *i*-BuI at –50 °C.

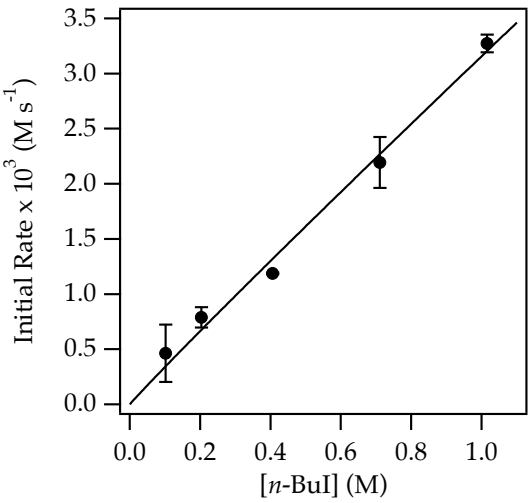


Figure 65. Plot of initial rate versus *n*-BuI concentrations for alkylation of 0.10 M **8** in neat tetrahydrofuran-d_8 (THF-d_8) at −80 °C. The curve depicts an unweighted least-squares fit to the function $f(x) = ax^n$ such that $a = (3.1 \pm 1.2) \times 10^{-3}$, $n = 0.97 \pm 0.08$.

[*n*-BuI]	Initial Rate × 10^3 (M s^{-1})	Standard Deviation × 10^3 (M s^{-1})
0.10	0.46	0.26
0.20	0.79	0.093
0.41	1.19	0.0085
0.71	2.19	0.23
1.02	3.27	0.079

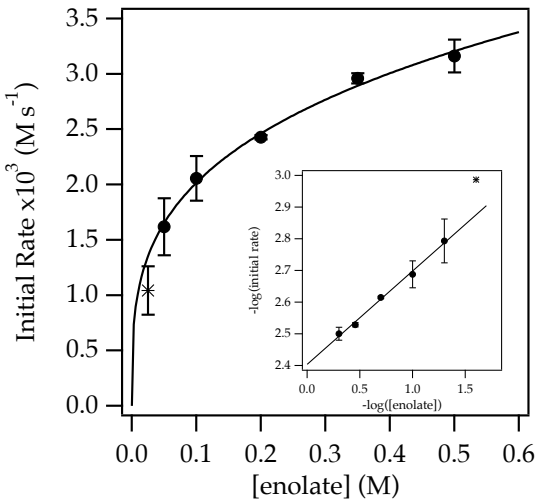


Figure 66. Plot of initial rate versus enolate **8** concentrations for alkylation of 0.493 M *n*-BuI in neat tetrahydrofuran-d_8 (THF-d_8) at −80 °C. The curve depicts an unweighted least-squares fit to the function $f(x) = ax^n$ such that $a = (3.9 \pm 0.087) \times 10^{-3}$, $n = 0.29 \pm 0.014$. Inset demonstrates plot of log(initial rate) vs log[enolate]. The curve depicts an unweighted least-squares fit to the function $f(x) = ax+b$ such that $a = 0.29 \pm 0.013$, $b = 2.4 \pm 0.011$.

[enolate] (M)	Initial Rate × 10^3 (M s^{-1})	Standard Deviation × 10^4 (M s^{-1})
0.050	1.5	2.6
0.10	2.0	2.0
0.20	2.4	0.20
0.35	2.9	0.45
0.50	3.1	1.5

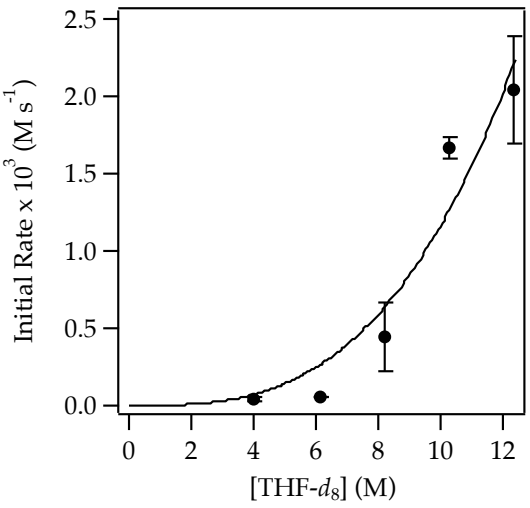


Figure 67. Plot of initial rate versus THF-d_8 concentrations for alkylation of 0.050 M **8** and 0.203 M *n*-BuI in hexanes cosolvent at −80 °C. The curve depicts an unweighted least-squares fit to the function $f(x) = ax^n$ such that $a = (1.1 \pm 2.2) \times 10^{-6}$, $n = 3.0 \pm 0.85$.

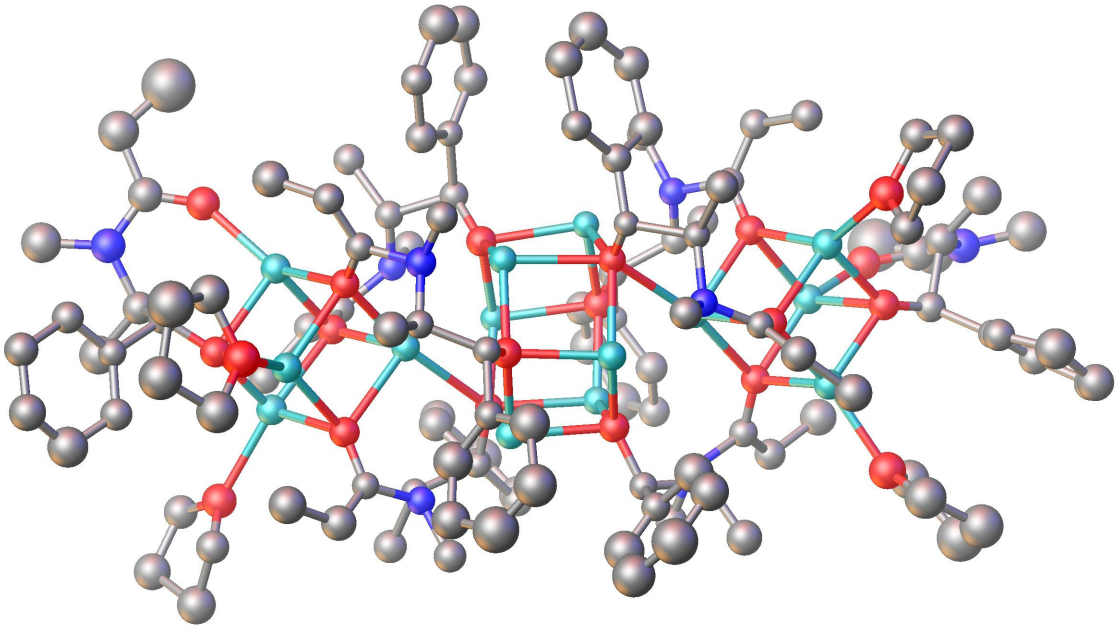
[THF] (M)	Initial Rate × 10^4 (M s^{-1})	Standard Deviation × 10^4 (M s^{-1})
4.0	0.36	0.17
6.1	0.62	0.030
8.2	4.4	2.3
10.2	16.6	0.76
12.3	20.4	3.5

Part 5 Crystal Structure Data

Owing to the low resolution of the crystal, only coordinates (xyz) are presented.

Samples for X-ray spectroscopy were prepared from 0.30 M (*R,R*)-**1** and 0.70 M NaDA in neat THF, aged at 20 °C for 20 min, cooled back down to –80 °C, crystal formed. The crystals were redissolved at 20 °C with vigorous shaking, slowly cooled back to –20 °C and left at –20 °C for 3 days until crystals grew. Owing to the low quality of the crystal, only coordinates (xyz) are presented. Samples for single crystal X-ray diffraction were prepared from 0.30 M (R,R)-1 and 0.70 M NaDA in neat THF, aged at 20 °C for 20 min, cooled back down to –80 °C, crystal formed. Unit cell parameters: a = 16.6515(6) Å, b = 15.3595(8) Å, c = 30.4861(10) Å, α = 90°, β = 92.594(3)°, γ = 90°, V = 7789.1(6) Å^3, space group = I_2.

Table 3. Geometric coordinates for crystal structure **22**



Atom	X	Y	Z	Atom	X	Y	Z
Na	0.00000000	0.00000000	0.00000000	C	2.33990600	-1.60046000	-7.68985300
Na	3.37116300	1.97830300	-0.27714000	C	0.97417300	7.90399900	-1.91257000
Na	0.91067400	1.98905500	-2.23843000	C	6.14178300	-0.86781200	-2.07398000
Na	1.68797600	3.53114900	-5.09814400	C	-0.42378900	-0.88010000	-3.25258000
Na	-0.93045800	1.87385900	-5.04332600	C	2.13162800	2.24095100	-9.81864800
Na	1.88518200	0.41931400	-5.00373400	C	2.67909900	6.38954900	-1.02633000
Na	0.21838200	4.17163900	-0.11573000	C	3.66312000	4.44657900	-2.42116000
O	-0.00856200	0.28568700	-3.59672000	C	-2.11677400	5.49869900	-1.42529000
O	2.79315800	2.02899000	-3.72768000	C	4.02480300	-1.52827000	-1.10551000
O	2.25491300	0.03993500	-0.44769000	C	-3.02204700	1.31938100	-0.29846000
O	3.07666600	4.83055900	-6.34679400	C	1.75323100	-1.48219200	-2.27498000

O	-0.76312900	2.08274800	-0.28323000	C	-0.23282800	-2.71556000	-1.55015000
O	2.41548600	3.99961900	-0.35328000	C	2.48305400	-1.25333500	-0.92583000
N	4.37042300	3.19477900	-2.30239000	C	6.79744300	-1.95680000	-1.51361000
O	-2.94293200	2.55582100	-6.12447300	C	-4.53066100	4.18699900	-6.69397900
O	2.32870900	-1.28559000	-6.45034000	C	1.54508100	6.59843900	-1.76029000
O	-0.14929100	3.57568900	-3.68808000	C	-0.76405000	0.13209200	-8.67963600
O	0.79886000	1.92300900	-6.42293100	C	3.30895900	4.95189900	-0.96237000
N	0.30861800	-1.42689800	-2.10748000	C	-3.10466600	3.91359900	-6.41379400
C	4.08620300	2.30699700	-3.52667000	C	1.32961200	1.40078600	-7.55280600
N	1.51877000	-0.86627600	-8.53040700	C	5.98627300	-2.90908900	-0.84665000
N	-1.45835400	4.38974900	-1.99175000	C	-2.87335700	0.17356200	-1.08115000
C	-2.30423100	3.10569100	-1.91866000	C	5.74315300	3.29000900	-1.94911000
C	-2.09890200	2.44523200	-0.45987000	C	3.27183500	-2.66333700	-8.22890400
C	5.09787300	1.85696300	-4.24541000	C	-4.05849100	1.41461000	0.67305000
C	2.28851100	-2.73706300	-3.06376000	O	0.32240500	-1.28559000	8.28372000
C	4.64479300	-2.62186700	-0.56646000	O	2.80040600	3.57568900	5.52147000
C	3.17759200	7.27425900	-0.26800000	O	1.85225500	1.92300900	8.25631000
C	-1.50003200	-1.53287800	-3.79163000	N	2.34249700	-1.42689800	3.94086000
C	1.25422100	2.42526500	-8.79231900	C	-1.43508400	2.30699700	5.36006000
C	-0.89586400	4.51261900	-3.27085000	N	1.13234500	-0.86627600	10.3637900
C	4.69426300	-0.63895500	-1.87907000	N	4.10947300	4.38974900	3.82513000
C	2.05127000	3.20398900	-10.9485230	C	4.95534300	3.10569100	3.75204000
C	-3.77286900	3.20859900	-2.36025000	C	4.75001300	2.44523200	2.29325000
C	-4.80131300	2.72784700	-7.48276000	C	-2.44675400	1.85696300	6.07879000
C	-3.92083100	1.76480600	-6.81275300	C	0.31120800	-1.60046000	9.52323000
C	1.38546600	-1.15810700	-9.96178600	C	1.67694200	7.90399900	3.74595000
C	0.13356800	4.26379900	-9.89478500	C	-3.49067100	-0.86781200	3.90736000
C	2.71696200	6.18373900	-7.00766400	C	3.07490400	-0.88010000	5.08596000
C	4.14482300	3.89516900	-7.02593700	C	0.51948600	2.24095100	11.6520300
C	-4.78017500	-0.91235400	0.21014000	C	-0.02798500	6.38954900	2.85971000
C	-4.91876500	0.19353000	0.88015000	C	-1.01200500	4.44657900	4.25454000
C	0.38169200	3.48199900	-8.75577300	C	4.76789300	5.49869900	3.25867000
C	-3.71697000	-1.03215900	-0.83751000	C	-1.37368300	-1.52827000	2.93889000
C	0.52845200	0.08447700	-7.87867300	C	5.67316300	1.31938100	2.13184000
C	4.40016300	5.46183900	-3.21603000	C	0.89788400	-1.48219200	4.10836000
C	3.78528300	-3.56954800	-7.06552800	C	2.88394300	-2.71556000	3.38353000
C	4.86320300	5.04712900	-8.07053900	C	0.16806100	-1.25333500	2.75921000
C	1.13476700	4.24843900	-10.8602040	C	-4.14633000	-1.95680000	3.34699000
C	-1.00192300	5.63078900	-3.98045000	C	7.18177300	4.18699900	8.52736000
C	1.53235400	8.90236900	-1.07506000	C	1.10603300	6.59843900	3.59367000
C	3.64244500	6.09157900	-8.32331400	C	3.41516500	0.13209200	10.5130200
C	2.64488200	8.73340900	-0.27105000	C	-0.65784400	4.95189900	2.79576000
C	-2.32703900	-0.82634100	-4.79664100	C	5.75578300	3.91359900	8.24718000
C	4.87541300	0.90006700	-5.39964800	C	1.32150300	1.40078600	9.38619000
C	-0.15995500	5.98405900	-5.21691800	C	-3.33515800	-2.90908900	2.68003000
Na	2.65111500	0.00000000	1.83338000	C	5.52447300	0.17356200	2.91453000

Na	-0.72004800	1.97830300	2.11052000	C	-3.09203900	3.29000900	3.78249000
Na	1.74044000	1.98905500	4.07181000	C	-0.62072000	-2.66333700	10.0622900
Na	0.96313800	3.53114900	6.93153000	C	6.70960300	1.41461000	1.16033000
Na	3.58157300	1.87385900	6.87671000	C	0.36260300	-2.73706300	4.89714000
Na	0.76593200	0.41931400	6.83712000	C	-1.99367500	-2.62186700	2.39984000
Na	2.43273300	4.17163900	1.94911000	C	-0.52647700	7.27425900	2.10139000
O	2.65967700	0.28568700	5.43010000	C	4.15114300	-1.53287800	5.62501000
O	-0.14204300	2.02899000	5.56106000	C	1.39689400	2.42526500	10.6257000
O	0.39620100	0.03993500	2.28107000	C	3.54697900	4.51261900	5.10423000
O	-0.42555100	4.83055900	8.18018000	C	-2.04315100	-0.63895500	3.71245000
O	3.41424300	2.08274800	2.11661000	C	0.59984400	3.20398900	12.7819100
O	0.23562900	3.99961900	2.18666000	C	6.42398300	3.20859900	4.19363000
N	-1.71930900	3.19477900	4.13577000	C	7.45243300	2.72784700	9.31614000
O	5.59404300	2.55582100	7.95786000	C	6.57194300	1.76480600	8.64613000
C	1.26564900	-1.15810600	11.7951700	H	4.19346577	5.02370874	-0.36454800
C	2.51754700	4.26379900	11.7281700	H	-2.85548480	4.45170892	-5.52315016
C	-0.06584700	6.18373900	8.84105000	H	-2.56920191	4.10279163	-7.32064810
C	-1.49370800	3.89516900	8.85932000	H	2.36831987	1.19630248	-7.39733110
C	7.43129300	-0.91235400	1.62324000	H	6.44150481	-3.01948658	0.11536683
C	7.56988300	0.19353000	0.95324000	H	5.94580456	-3.74124741	-1.51804756
C	2.26942300	3.48199900	10.5891600	H	-1.87577764	-0.15668099	-0.87946959
C	6.36808300	-1.03215900	2.67089000	H	-3.14310402	0.49006518	-2.06703147
C	2.12266300	0.08447700	9.71206000	H	5.89699418	2.83905555	-0.99105265
C	-1.74904500	5.46183900	5.04942000	H	6.03045085	4.31992912	-1.90880505
C	-1.13416500	-3.56954800	8.89891000	H	6.33591748	2.78276701	-2.68139126
C	-2.21208900	5.04712900	9.90392000	H	4.12691411	-2.15173057	-8.61877395
C	1.51634800	4.24843900	12.6935900	H	2.68519554	-3.28917805	-8.86849537
C	3.65303800	5.63078900	5.81383000	H	-3.55470600	1.56275011	1.60533492
C	1.11876100	8.90236900	2.90844000	H	-4.72364572	2.16477381	0.29925400
C	-0.99133000	6.09157900	10.1567000	H	3.35502762	-2.68622387	-3.13345703
C	0.00623300	8.73340900	2.10443000	H	2.00707788	-3.63030721	-2.54625620
C	4.97815300	-0.82634100	6.63002000	H	1.86687482	-2.74669705	-4.04713689
C	-2.22429700	0.90006700	7.23303000	H	4.09387197	-3.27057937	0.08204464
C	2.81106900	5.98405900	7.05030000	H	3.98135784	7.01084027	0.38734041
H	-1.93228183	2.44934991	-2.67745522	H	-1.73846319	-2.53232286	-3.49303239
H	-2.32853007	3.15641154	0.30589407	H	4.19593541	0.19378932	-2.32974340
H	6.09235826	2.17323079	-4.00903369	H	3.00906789	3.68041185	-10.9718570
H	-0.04656711	7.80910300	-1.60600129	H	1.72333195	2.62081777	-11.7835487
H	1.20662997	8.20468939	-2.91279450	H	-4.24309516	2.25264047	-2.26059740
H	6.60291703	-0.02086535	-1.61036725	H	-4.28101978	3.92185493	-1.74547462
H	6.24050003	-1.02024597	-3.12845562	H	-3.81687503	3.52294036	-3.38208804
H	2.84356474	1.44220354	-9.81167808	H	-5.81196035	2.43511950	-7.28833124
H	2.76130366	4.28707622	-2.97450089	H	-4.45979242	2.83453359	-8.49116551
H	-1.64926023	5.75551279	-0.49772461	H	-4.50223648	1.25360828	-6.07414312
H	-3.14357453	5.25317965	-1.25121839	H	-3.41167313	1.20864367	-7.57192474
H	-2.05763464	6.32978246	-2.09663403	H	2.00470875	-1.99325497	-10.2147016

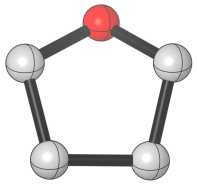
H	-2.37396790	0.89211228	0.43797392	H	0.36505365	-1.39016858	-10.1849587
H	1.99696348	-0.66595918	-2.92248170	H	1.68939941	-0.30376828	-10.5297911
H	-0.53078653	-2.56706477	-0.53325773	H	0.09033778	5.27378747	-9.54413641
H	0.52544417	-3.46926414	-1.59320097	H	-0.72158861	3.82298746	-10.3630716
H	-1.07814051	-3.02666299	-2.12769800	H	3.07641322	6.97785781	-6.38712381
H	2.09360991	-1.93598733	-0.19973145	H	1.68950505	6.16067387	-7.30548983
H	7.42961218	-1.54487922	-0.75493787	H	4.86257717	3.59417428	-6.29168150
H	7.22698899	-2.48277079	-2.34049873	H	3.63962017	3.15772428	-7.61402321
H	-5.08178465	4.21069381	-5.77713590	H	-5.42856799	-1.74013873	0.40827878
H	-4.61445584	4.99567895	-7.38961911	H	-5.68845745	0.23974966	1.62199720
H	1.07074242	5.76448062	-2.23401601	H	-0.12044550	3.71559118	-7.84024440
H	-1.45058352	0.80462419	-8.20924022	H	-3.04241998	-1.77624495	-0.46843227
H	-1.19471759	-0.84656678	-8.72028590	H	-4.24401286	-1.19535435	-1.75429411
H	-0.55592150	0.47170828	-9.67273383	H	0.13526357	-0.22099535	-6.93157770
H	3.82454117	6.36243473	-3.26589814	H	7.26556858	4.99567875	9.22300025
H	5.34137092	5.66548903	-2.74960283	H	7.73289343	4.21069544	7.61051500
H	4.56557528	5.08903143	-4.20524853	H	1.58037115	5.76448052	4.06739626
H	3.36238628	-3.23655064	-6.14077337	H	3.33468202	-0.51811514	11.3589829
H	4.85228088	-3.51033360	-7.01159118	H	3.59054538	1.13307689	10.8479394
H	3.49301557	-4.58272937	-7.24703079	H	4.22934116	-0.18519602	9.89548822
H	5.63399302	5.55585169	-7.53018360	H	-1.54235622	5.02370888	2.19794608
H	5.08954077	4.56421914	-8.99815383	H	5.22032187	4.10279314	9.15403553
H	1.73516770	5.10267990	-10.6263419	H	5.50660002	4.45170865	7.35653649
H	0.60203658	4.20652278	-11.7872107	H	0.28279521	1.19630215	9.23071495
H	-1.73407963	6.34450910	-3.66509262	H	-3.29468990	-3.74124745	3.35142753
H	0.74922579	9.10264672	-0.37399008	H	-3.79038911	-3.01948658	1.71801284
H	1.83932153	9.66024141	-1.76520516	H	5.79422154	0.49006501	3.90041112
H	4.08601190	7.05636695	-8.45496741	H	4.52689301	-0.15667982	2.71285079
H	3.03465593	5.67201803	-9.09756269	H	-3.62746684	3.78877884	4.56316002
H	2.31897480	8.93059716	0.72885066	H	-3.49401014	2.30790534	3.64540753
H	3.41849824	9.32900864	-0.70886158	H	-3.18854353	3.84506750	2.87282142
H	-1.93025517	0.15392132	-4.95957773	H	-0.03407920	-3.28917639	10.7018818
H	-3.33298391	-0.74923713	-4.44022857	H	-1.47579944	-2.15173112	10.4521599
H	-2.31540226	-1.37322413	-5.71625147	H	7.37475415	2.16478006	1.53411981
H	3.83012378	0.69174960	-5.49385152	H	6.20581650	1.56274047	0.22804435
H	5.40541501	-0.01091042	-5.21493740	H	1.18682100	-3.35592864	5.18448996
H	5.23365777	1.34385482	-6.30497284	H	-0.16112842	-2.41184461	5.77169040
H	0.52702260	5.18915178	-5.41961057	H	-0.30133150	-3.29545469	4.27080966
H	0.38374266	6.88690978	-5.03211180	H	-1.44275449	-3.27057991	1.75133544
H	-0.80450874	6.12203828	-6.05977754	H	-1.33024980	7.01084224	1.44605733
H	4.58339132	2.44934908	4.51083327	H	4.38957140	-2.53232412	5.32641438
H	4.97963814	3.15641137	1.52748489	H	-1.54482595	0.19379077	4.16312354
H	-3.44123861	2.17322818	5.84240747	H	0.92778275	2.62081660	13.6169346
H	1.44448549	8.20468956	4.74617456	H	-0.35795382	3.68041191	12.8052455
H	2.69768197	7.80910251	3.43938097	H	6.63534610	4.21231703	4.49822111
H	-3.58938819	-1.02024589	4.96183562	H	6.59742074	2.54310335	5.01334635

H	-3.95180517	-0.02086552	3.44374708	H	7.06156525	2.94201528	3.37673222
H	-0.19245161	1.44220433	11.6450586	H	7.11091740	2.83453138	10.3245474
H	-0.11018685	4.28707461	4.80787748	H	8.46307952	2.43512037	9.12170561
H	5.56883899	5.80346987	3.89937293	H	6.06278885	1.20864048	9.40530189
H	4.07452431	6.30580395	3.14588054	H	7.15334460	1.25361136	7.90751494
H	5.16046311	5.22920109	2.30046356	H	1.94971580	-0.46487152	12.2383162
H	6.32339117	1.73826313	2.87119180	H	0.31006074	-1.06795800	12.2680594
H	0.65415221	-0.66595921	4.75586200	H	1.63440659	-2.15435847	11.9232280
H	2.84265038	-3.47492983	4.13622674	H	3.37270412	3.82298825	12.1964564
H	3.89888108	-2.57273046	3.07628350	H	2.56077646	5.27378727	11.3775207
H	2.29529640	-3.01533161	2.54178647	H	0.96160995	6.16067387	9.13887583
H	0.55750566	-1.93598673	2.03311120	H	-0.42529822	6.97785781	8.22050981
H	-4.57587604	-2.48277107	4.17387853	H	-0.98850617	3.15772426	9.44740705
H	-4.77849908	-1.54487971	2.58831752	H	-2.21146084	3.59417430	8.12506320
H	8.07968455	-1.74013903	1.42509778	H	4.38519435	6.34450933	5.49847248
H	8.33958435	0.23975503	0.21140237	H	0.81179347	9.66024141	3.59858516
H	2.77156258	3.71559161	9.67363265	H	1.90188921	9.10264672	2.20737008
H	6.89512355	-1.19535708	3.58767495	H	-0.38354195	5.67201631	10.9309486
H	5.69353221	-1.77624288	2.30180950	H	-1.43489627	7.05636708	10.2883546
H	2.51585340	-0.22099596	8.76496572	H	-0.76738240	9.32901230	2.54223809
H	-2.67866375	5.04886767	5.38132913	H	0.33214074	8.93059107	1.10452832
H	-1.16183080	5.74581152	5.89761755	H	5.77328466	-1.46628298	6.95117403
H	-1.93763528	6.32227410	4.44197853	H	4.37055874	-0.56311946	7.47052202
H	-1.79161683	-4.31652703	9.29220305	H	5.38814171	0.06086215	6.19449752
H	-0.30172126	-4.04273974	8.42138828	H	-3.16489291	0.65804333	7.68203320
H	-1.66098814	-2.97034605	8.18594829	H	-1.58960547	1.36070846	7.96095590
H	-2.43843009	4.56421884	10.8315339	H	-1.76135240	0.00594270	6.87091948
H	-2.98287685	5.55585279	9.36356254	H	3.10729869	6.94291481	7.42143813
H	2.04907902	4.20652259	13.6205963	H	2.96401941	5.24515670	7.80893664
H	0.91594747	5.10268012	12.4597283	H	1.77576751	6.01002798	6.78127132

Part 6. Computations

Geometries are optimized at the M06-2X level of theory using the 6-31G(d) basis set for tetramer computation and 6-311+G(2d,p) basis set for the other computations. Energies are defined as follows: G is the sum of electronic and thermal free energies calculated at the M06-2X level of theory (T = 195 K). G_{SP} is derived from an M062X SP calculation corresponding to the DFT-optimized geometry and includes a thermal correction from the DFT calculation

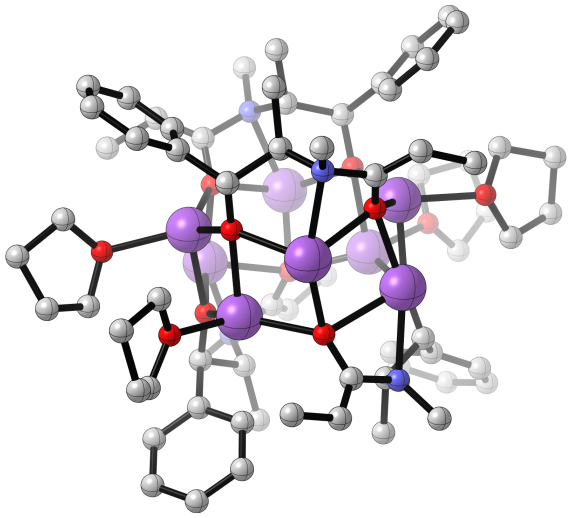
Table 4. Geometric coordinates and thermally corrected M062X energies for THF



G = –232.234012
G_{SP} = –232.3100352

Atom	X	Y	Z	Atom	X	Y	Z
C	0.00000000	0.00000000	0.00000000	H	2.01349800	2.13216900	0.74784200
O	1.14399700	-0.66754900	-0.49188300	H	2.21364000	2.16146400	-1.00354500
C	2.25059300	0.13937200	-0.12980400	H	2.58695200	-0.12086900	0.88464700
C	1.76189600	1.60800900	-0.17759100	H	3.06154200	-0.07620500	-0.82895400
C	0.23509200	1.46957700	-0.35566000	H	-0.88024700	-0.44241100	-0.47117100
H	-0.33470800	2.15678800	0.27399600	H	-0.08079300	-0.12670400	1.09241400
H	-0.04690600	1.64389100	-1.39726900				

Table 5. Geometric coordinates and thermally corrected M062X energies for **19**



G = –5068.658361

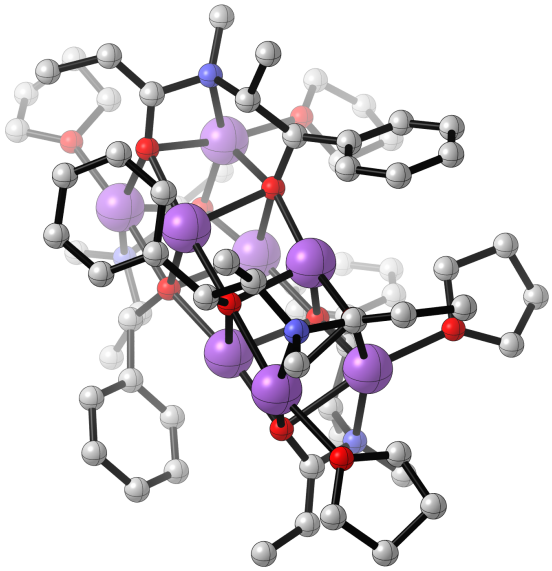
G_{SP} = –5068.658362

Atom	X	Y	Z	Atom	X	Y	Z
Na	0.00000000	0.00000000	0.00000000	H	4.80304800	-4.91689600	-2.43559200
O	1.12197700	-0.78092200	-1.72236500	H	3.60086600	-3.37872500	-0.91441800
Na	1.35056700	-0.42052900	-3.89073000	H	1.80100900	-2.17008000	-0.34808100
O	-0.02848100	-0.92364100	-5.59921500	H	-0.84731500	-2.21580800	-1.72245400
Na	-2.21530700	-0.18695800	-6.04917000	C	-0.22515700	-3.03428000	1.46278900
O	-3.36175000	-0.79778400	-4.26847600	H	-0.72465300	-4.01282500	1.50305200
Na	-3.68957300	-0.28317600	-2.13445100	H	-0.43521000	-2.50792500	2.39772900
O	-2.22489000	-0.72548800	-0.43768200	H	0.85325000	-3.20851000	1.39157400
C	-2.01673400	-1.74766800	0.36777300	C	-2.94681000	-2.27799800	1.19694300
N	-0.64710900	-2.20426800	0.34527100	H	-2.69913600	-3.12141800	1.83056300
C	-0.18788600	-2.69433100	-0.98874700	C	-4.32559000	-1.68732800	1.29682500
C	-0.33800000	-4.21399800	-1.09497200	H	-4.63404400	-1.24834800	0.33963300
H	-0.24647500	-4.54671800	-2.13059700	H	-5.06957300	-2.44737700	1.56405000
H	-1.32952000	-4.50970300	-0.72903200	H	-4.39902000	-0.89351900	2.05727300
H	0.42209200	-4.74761000	-0.51308500	Na	1.35579800	1.53572600	-1.87383200
C	1.22792600	-2.10001100	-1.30134900	O	-0.28793600	2.10749200	-0.39030300
C	1.99431200	-2.98537500	-2.28303200	Na	-2.49631900	1.39832800	-0.26541600
C	3.19730600	-3.58527100	-1.90435300	O	-3.56262300	2.04450300	-2.08687000
C	3.87266000	-4.45739200	-2.75814000	Na	-3.49450400	1.50946600	-4.25665200
C	3.34509500	-4.75251500	-4.01196200	O	-1.86244900	1.93246300	-5.76713300
C	2.15327900	-4.14893500	-4.41393000	Na	0.32154400	1.17734500	-5.90076400
C	1.49517500	-3.26486300	-3.56207300	O	1.34570200	1.89258900	-4.08086600
H	0.55238300	-2.82459500	-3.88625200	C	1.50997700	3.21240800	-4.48386900
H	1.72150000	-4.35520600	-5.38901100	C	0.14409200	3.84169500	-4.93245700
H	3.85710200	-5.44562300	-4.67322900	N	-0.17704500	3.39908000	-6.32229400
C	-1.54395000	2.97370800	-6.51224500	H	1.53615000	2.80210400	2.62525600

C	-2.36849500	3.53450500	-7.42655400	H	1.86611300	2.46488500	0.91611600
H	-2.04790800	4.39385400	-8.00335000	H	2.30763000	4.02361900	1.62067300
C	-3.72733000	2.94576800	-7.69571400	C	-2.51424200	4.56071700	1.02583600
H	-3.66912300	1.98531300	-8.23266400	H	-2.01088800	5.53822700	1.03517300
H	-4.28975000	2.75165600	-6.77275300	H	-2.43768700	4.12931900	2.02726200
H	-4.33289600	3.61681100	-8.31326500	H	-3.57071800	4.72816900	0.79452400
C	0.37886000	4.24963200	-7.36272500	C	-2.03297200	5.47201700	-1.61029200
H	-0.10066700	5.23658600	-7.42988800	H	-1.99802500	5.69023400	-2.67935900
H	0.26478800	3.75168700	-8.32921600	H	-1.07990800	5.78558600	-1.16529000
H	1.44509300	4.40438100	-7.16885600	H	-2.83556500	6.08207300	-1.18068000
C	0.01322100	5.36088500	-4.79680800	H	-1.52726200	3.40631100	-1.96017200
H	0.01362500	5.66287800	-3.74785200	H	-4.29456600	3.54460600	-0.86978000
H	-0.93375300	5.68715300	-5.24582800	C	-3.50248100	-2.13379400	-4.61897200
H	0.83434600	5.89396100	-5.28908100	C	-4.32093800	-2.93846000	-3.61038900
H	-0.60178000	3.36054900	-4.28751400	C	-3.91793300	-3.07157200	-2.27474900
C	2.19334100	4.07520200	-3.42636100	C	-4.64375800	-3.85430300	-1.37988800
C	3.41788700	4.69118400	-3.69141400	C	-5.79762900	-4.51402200	-1.80186700
C	4.03533600	5.51008500	-2.74455800	C	-6.21750600	-4.38276600	-3.12221000
C	3.42796600	5.72954400	-1.51169400	C	-5.48178700	-3.60196800	-4.01419500
C	2.20335000	5.12321600	-1.23108500	H	-5.80727200	-3.51283500	-5.04946500
C	1.59733400	4.30280800	-2.17848000	H	-7.11371900	-4.89415900	-3.46306000
H	0.62329300	3.86797600	-1.95237100	H	-6.36159700	-5.12918500	-1.10665100
H	1.70006400	5.28829100	-0.28292000	H	-4.28760400	-3.94670400	-0.35749500
H	3.89951300	6.37427300	-0.77571100	H	-2.99879700	-2.59711600	-1.92852000
H	4.98625000	5.98240800	-2.97560200	C	-2.09837300	-2.78575500	-4.87000500
H	3.88863200	4.53480400	-4.66063700	N	-1.62644700	-2.43971900	-6.24534200
H	2.17433600	3.27537800	-5.37738100	C	-0.24520600	-2.01706700	-6.30227100
C	-3.64651100	3.39616600	-1.76378400	C	0.67918500	-2.65213900	-7.06169300
C	-4.30401300	4.22814100	-2.86097100	H	0.41024800	-3.55123600	-7.60504000
C	-3.72925000	4.35772500	-4.13173300	C	2.08669800	-2.14292300	-7.19824600
C	-4.32783000	5.14528500	-5.11272800	H	2.28774500	-1.36044300	-6.45589600
C	-5.52280400	5.81218500	-4.84285500	H	2.82631700	-2.93877400	-7.03457600
C	-6.11037000	5.68569900	-3.58686200	H	2.29285800	-1.72105000	-8.19300200
C	-5.50001700	4.90234100	-2.60814500	C	-2.06132800	-3.37354000	-7.27135100
H	-5.95798700	4.81321000	-1.62422200	H	-1.58308400	-4.36111200	-7.20190800
H	-7.03996300	6.20245500	-3.36478500	H	-1.83688000	-2.95371700	-8.25553500
H	-5.98870500	6.42841500	-5.60616200	H	-3.14365400	-3.51641200	-7.18800400
H	-3.84551600	5.23253900	-6.08234100	C	-1.98237700	-4.28749100	-4.60096100
H	-2.77892300	3.87129100	-4.35712600	H	-2.09457000	-4.49784500	-3.53526000
C	-2.24651200	3.97695600	-1.36001400	H	-0.99556100	-4.64794000	-4.91799600
N	-1.95556200	3.62616200	0.06176500	H	-2.74955600	-4.86553000	-5.12838500
C	-0.59976600	3.18432800	0.30648400	H	-1.43630100	-2.24429200	-4.18488000
C	0.19273100	3.78425200	1.22681900	H	-4.05621300	-2.23901400	-5.58056400
H	-0.15571600	4.67366900	1.73891200	C	4.08677300	0.94398700	-4.94140300
C	1.53740900	3.24035800	1.61639300	O	3.59146300	-0.23567100	-4.29215200
C	4.48829100	-1.33420900	-4.49117600	H	-6.95266800	-1.74174300	-2.36191100

C	5.37306700	-0.92113900	-5.66245700	H	-6.54057500	-1.84448000	-0.63923500
C	5.48946700	0.58875700	-5.43552200	H	-9.01999000	-0.67498000	-1.72220100
H	3.41892100	1.18973300	-5.77874700	H	5.41330600	0.59547700	-2.53586100
H	4.04882500	1.77551100	-4.23072200	H	6.18890900	-0.36028700	-1.24990400
H	5.07747600	-1.48804900	-3.57558000	C	-6.31549800	0.98012700	-0.83883500
H	3.89387200	-2.23129500	-4.67813100	O	-5.92309100	-0.13597400	-1.63289500
H	6.33520900	-1.43854400	-5.66772600	C	-6.88982300	-1.17106500	-1.43041200
H	4.86104400	-1.12587100	-6.60982300	C	-8.20474700	-0.46439000	-1.02548900
H	6.23767500	0.79706500	-4.66243100	C	-7.83018100	1.02977300	-1.00302600
H	5.76559500	1.14594200	-6.33396000	H	-6.04191800	0.79954900	0.21476800
C	4.04886100	0.03299300	-0.97475700	H	-8.32671800	1.58137500	-0.20129000
O	3.35783000	1.28285000	-0.81779800	C	-6.26443900	-0.05075000	-5.02212700
C	4.29837900	2.36952400	-0.78757600	O	-5.64040800	1.24352100	-5.01481600
C	5.67985000	1.72247200	-0.70511600	C	-6.56727400	2.20962800	-4.52249800
C	5.44251600	0.41154400	-1.45584300	C	-7.92557300	1.69129400	-4.97322500
H	4.09007200	-0.47355200	0.00073500	C	-7.75759600	0.18496600	-4.74400700
H	3.47747700	-0.58045100	-1.67358200	H	-6.08772700	-0.48948700	-6.01091300
H	4.18603600	2.95441900	-1.70853900	H	-5.78833300	-0.68383300	-4.26976100
H	4.06090200	3.01253500	0.06422900	H	-6.50177400	2.26029900	-3.42565700
H	6.45799300	2.34981900	-1.14664200	H	-6.28933900	3.18264000	-4.93569900
H	5.94891200	1.51783700	0.33702800	H	-8.75684900	2.12532600	-4.41065900
H	-5.76598400	1.84505000	-1.21605500	H	-8.07247300	1.90941900	-6.03634900
H	-8.52480200	-0.79811600	-0.03466200	H	-7.98479300	-0.05909500	-3.70136400
H	-8.08021700	1.50873500	-1.95604700	H	-8.40237300	-0.42441100	-5.38181000

Table 6. Geometric coordinates and thermally corrected M062X energies for **20**



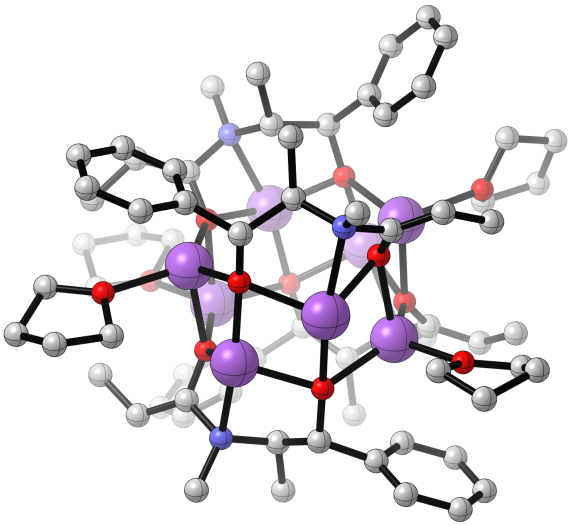
G = –5068.679769
G_{SP} = –5068.679768

Atom	X	Y	Z	Atom	X	Y	Z
Na	0.00000000	0.00000000	0.00000000	C	-3.90113200	1.45348300	1.60442700
Na	-2.20953400	1.72708900	-1.89158200	H	-4.33103500	2.37359100	1.98770700
O	-2.19517600	0.52014800	0.22470600	C	-4.52648300	0.15659200	2.02490700
Na	-2.44419100	-1.14004400	-1.14123200	H	-4.00088300	-0.68263100	1.55883200
Na	0.05047100	0.38723300	-2.97272300	H	-4.50452700	0.01272100	3.11403900
Na	2.32628400	1.55296800	-1.24204600	H	-5.58508000	0.09468500	1.72854000
O	2.39795800	-0.30599600	0.14521400	C	-3.36582800	3.90257800	0.22700600
Na	4.65241900	-0.79923500	-0.33512000	H	-3.54527300	4.34326700	1.21919900
O	4.50537600	1.55766400	-0.71533500	H	-4.32639500	3.54946400	-0.15953900
Na	4.58097900	0.74940200	-2.73723300	H	-2.99680500	4.69658700	-0.43323000
Na	2.19165100	-1.42472400	-1.80654800	C	-0.89614900	4.34063600	1.45473100
O	-0.16724500	-1.54911000	-1.65719900	H	0.12274600	4.43639100	1.83658500
C	-0.54268100	-2.83310400	-2.04893000	H	-1.56479500	4.20061100	2.31102800
C	-1.32534800	-2.83976600	-3.39716800	H	-1.15103900	5.28826700	0.96722600
N	-2.67454000	-2.23059500	-3.21750400	H	-0.58806400	2.27599200	1.01726800
C	-2.83478100	-0.92528600	-3.82952400	H	-0.91473600	3.80614300	-1.52023100
O	-2.13313500	0.01392300	-3.24993200	C	1.13393400	5.28497100	-1.53257900
C	-3.68917100	-0.73446600	-4.86645900	C	2.25624600	6.10667400	-1.43084300
H	-4.22072800	-1.57750600	-5.29538300	C	3.28156700	5.78577900	-0.54407700
C	-3.91409700	0.63263400	-5.44692800	C	3.17633000	4.64349900	0.25064300
H	-3.17735200	1.32696500	-5.02703200	H	3.97937500	4.35830600	0.92578000
H	-3.80151300	0.64178800	-6.54003000	H	4.16184200	6.41840000	-0.47384500
H	-4.91896200	1.03166900	-5.23540100	H	2.33169800	6.99722600	-2.04958400
C	-3.82021000	-3.12117100	-3.31203800	H	0.33351500	5.53797200	-2.22645200

H	-3.98404700	-3.56219200	-4.30604100	H	1.93418700	2.97332300	0.79866500
H	-4.70743200	-2.54370200	-3.04713800	C	3.77667000	3.61361300	-3.34037100
H	-3.71112300	-3.94144300	-2.59338700	O	4.91154200	2.77776600	-3.64169800
C	-1.40062000	-4.21937100	-4.05940700	C	5.83156800	3.47003500	-4.48181200
H	-0.40979500	-4.56198700	-4.35923200	C	5.01051700	4.57076800	-5.14213800
H	-2.02313600	-4.18358000	-4.95752400	C	4.07190500	4.96229000	-3.99773300
H	-1.81231800	-4.97489900	-3.38115800	H	2.88216800	3.13125300	-3.75937600
H	-0.77914300	-2.17404000	-4.07409100	H	3.67984000	3.68098400	-2.25092700
C	0.68036100	-3.74521300	-2.04501700	H	6.63958900	3.89237700	-3.86775700
C	0.97150100	-4.51194600	-0.91474800	H	6.25888700	2.74966900	-5.18511800
C	2.15227000	-5.24874000	-0.83273300	H	5.62430800	5.39759100	-5.50694100
C	3.07150800	-5.21499700	-1.87821400	H	4.44133700	4.15942200	-5.98363600
C	2.80295800	-4.44732500	-3.01059600	H	4.59115700	5.61838400	-3.29012600
C	1.61031300	-3.73144800	-3.09195000	H	3.16114200	5.46834200	-4.32723700
H	1.39851500	-3.14436400	-3.98594300	C	7.31470800	0.20793800	-1.72294500
C	3.42202800	-0.92004900	-4.93052900	O	6.95111800	-0.68556000	-0.66389300
N	4.81867900	-0.87839000	-4.41248700	C	7.99873900	-1.63698200	-0.44520900
C	5.07278900	-1.87599100	-3.39124900	C	8.98267000	-1.44494100	-1.59699200
O	4.37257500	-1.66238600	-2.30860000	C	8.82123300	0.04993400	-1.88364700
C	5.98209600	-2.86143900	-3.59652300	H	6.81435300	-0.12586900	-2.64472800
H	6.45929900	-2.94870700	-4.56779800	H	6.98921100	1.21424000	-1.44374900
C	6.30205100	-3.89895900	-2.56154800	H	8.46989200	-1.42045900	0.52327400
H	5.75657900	-3.68303100	-1.63712100	H	7.56284000	-2.63904400	-0.41272800
H	6.01001100	-4.90772700	-2.88756100	H	10.0012010	-1.73920600	-1.33375400
H	7.37500300	-3.95351500	-2.32688000	H	8.65413700	-2.02380200	-2.46759600
C	5.85210100	-0.64419600	-5.40455600	H	9.34868500	0.64944800	-1.13330200
H	5.98821700	-1.45887300	-6.13123600	H	9.17020800	0.34376900	-2.87703200
H	6.80755800	-0.49590500	-4.89120700	C	-3.12731500	4.05298600	-4.28342300
H	5.61239600	0.26799700	-5.96351300	O	-2.16998100	3.30318700	-3.52702300
C	3.35726600	-1.40926000	-6.37958700	C	-0.92143300	3.23604400	-4.23892200
H	2.32855400	-1.64524900	-6.66068000	C	-0.96905600	4.41396000	-5.20085400
H	3.95298500	-2.32189900	-6.48837000	C	-2.44322800	4.38563100	-5.61036000
H	3.72698900	-0.66392300	-7.09246300	H	-4.03270800	3.45029100	-4.40767300
C	2.71127300	0.43543100	-4.62846300	H	-3.37783400	4.96075900	-3.72058200
O	2.33442500	0.50082500	-3.28373100	H	-0.11062300	3.27167400	-3.50364800
C	1.54328400	0.70126900	-5.56959100	H	-0.87528900	2.28423500	-4.78792900
C	0.43978100	-0.15686000	-5.60066500	H	-0.73297900	5.34660900	-4.67420800
C	-0.64787100	0.07703900	-6.43634000	H	-0.27884200	4.29583300	-6.03777800
C	-0.62762200	1.17721000	-7.29629000	H	-2.80404500	5.32141700	-6.04328100
C	0.47474300	2.02841600	-7.29950600	H	-2.60676100	3.57699600	-6.33236500
C	1.54333400	1.79846400	-6.43190800	C	-5.85509100	-1.84726300	-0.70222100
H	2.39802300	2.47314000	-6.42925900	O	-4.72826300	-1.04519400	-1.04530200
H	0.50167900	2.87863700	-7.97639600	C	-5.16251400	0.24148300	-1.52341900
H	-1.46613500	1.36417000	-7.96116600	C	-6.69271700	0.22683500	-1.44641200
H	-1.50863000	-0.58638500	-6.40063200	C	-7.00793400	-1.26997700	-1.51389200
H	0.44961200	-1.04004300	-4.96313900	H	3.25270500	-1.29748600	1.75813900

H	3.46115900	1.21896100	-4.87496700	H	3.11570200	1.72454400	1.65677600
H	2.90174700	-1.65838300	-4.31261500	C	6.04681800	0.40829700	2.27479200
H	3.53283600	-4.38249400	-3.81367600	H	6.28226400	1.17733200	3.02517200
H	3.99750900	-5.77696100	-1.81042700	H	6.92411100	0.26918700	1.63957300
H	2.35694100	-5.84691900	0.05096200	H	5.84992200	-0.52924500	2.80634100
H	0.26260100	-4.52291500	-0.08908800	C	6.09025000	2.72119900	0.60085400
H	-1.24805100	-3.29320400	-1.31445500	H	6.58921500	2.79756700	1.56160900
C	5.18011000	1.73772600	0.39091600	C	6.44198300	3.71893900	-0.46658000
N	4.92479100	0.72563500	1.40240800	H	5.88433900	3.49011000	-1.38216700
C	3.56722000	0.79341700	2.01836600	H	6.19505000	4.75079200	-0.17657400
C	3.63696000	0.86375900	3.54731700	H	7.51525100	3.71495500	-0.70830100
H	2.66175500	1.09668500	3.97553100	O	0.06795300	1.98697500	-1.34048900
H	4.33487000	1.64151300	3.86825800	C	2.03908300	3.84574000	0.15462200
H	3.96016800	-0.08980100	3.97926500	C	1.00510700	4.14449400	-0.73739100
C	2.67305700	-0.37530100	1.50930000	C	-0.23006000	3.25830900	-0.83888400
C	1.34524300	-0.51456000	2.25399600	C	-1.01070800	3.14525300	0.50472000
C	0.77050500	-1.78522400	2.35810700	N	-2.42480400	2.79789800	0.21345200
C	-0.52497300	-1.95135300	2.84582600	C	-2.85563100	1.52373400	0.74322900
C	-1.27601400	-0.84203900	3.22997800	H	-5.61781300	-2.88699600	-0.94600900
C	-0.72055700	0.43110700	3.13075600	H	-6.05049500	-1.76852900	0.37618800
C	0.57863900	0.58949500	2.64906100	H	-4.72603900	1.01174000	-0.87660200
H	0.99389700	1.59271300	2.56294800	H	-4.80404000	0.34595300	-2.55615200
H	-1.31713400	1.30155900	3.38949200	H	-7.03008800	0.64013000	-0.48987000
H	-2.29247000	-0.96378800	3.58966700	H	-7.15404600	0.80214800	-2.25255300
H	-0.95096300	-2.94843400	2.92057900	H	-7.98726600	-1.52872400	-1.10469800
H	1.34496800	-2.64778300	2.02582000	H	-6.95332300	-1.62393400	-2.54965300

Table 7. Geometric coordinates and thermally corrected M062X energies for **35** (octagonal prism version of **21**)



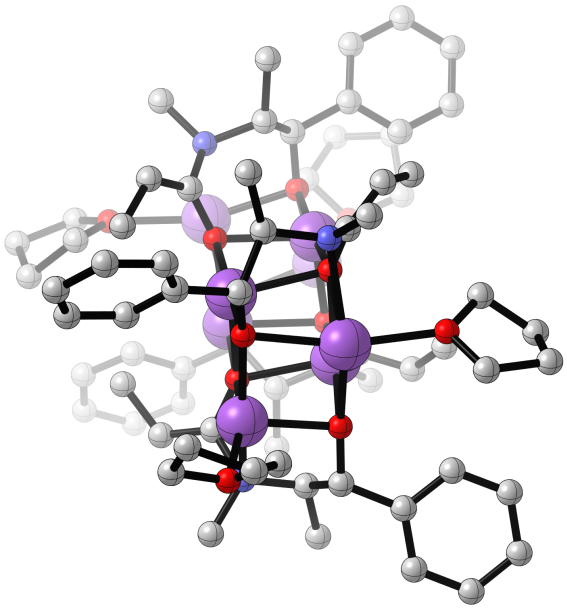
G = –5068.675275
G_{SP} = –5068.675275

Atom	X	Y	Z	Atom	X	Y	Z
Na	0.00000000	0.00000000	0.00000000	H	-6.36159700	-5.12918500	-1.10665100
O	1.12197700	-0.78092200	-1.72236500	H	-4.28760400	-3.94670400	-0.35749500
Na	1.35056700	-0.42052900	-3.89073000	H	-2.99879700	-2.59711600	-1.92852000
O	-0.02848100	-0.92364100	-5.59921500	C	-2.09837300	-2.78575500	-4.87000500
Na	-2.21530700	-0.18695800	-6.04917000	N	-1.62644700	-2.43971900	-6.24534200
O	-3.36175000	-0.79778400	-4.26847600	C	-0.24520600	-2.01706700	-6.30227100
Na	-3.68957300	-0.28317600	-2.13445100	C	0.67918500	-2.65213900	-7.06169300
O	-2.22489000	-0.72548800	-0.43768200	H	0.41024800	-3.55123600	-7.60504000
C	-2.01673400	-1.74766800	0.36777300	C	2.08669800	-2.14292300	-7.19824600
N	-0.64710900	-2.20426800	0.34527100	H	2.28774500	-1.36044300	-6.45589600
C	-0.18788600	-2.69433100	-0.98874700	H	2.82631700	-2.93877400	-7.03457600
C	-0.33800000	-4.21399800	-1.09497200	H	2.29285800	-1.72105000	-8.19300200
H	-0.24647500	-4.54671800	-2.13059700	C	-2.06132800	-3.37354000	-7.27135100
H	-1.32952000	-4.50970300	-0.72903200	H	-1.58308400	-4.36111200	-7.20190800
H	0.42209200	-4.74761000	-0.51308500	H	-1.83688000	-2.95371700	-8.25553500
C	1.22792600	-2.10001100	-1.30134900	H	-3.14365400	-3.51641200	-7.18800400
C	1.99431200	-2.98537500	-2.28303200	C	-1.98237700	-4.28749100	-4.60096100
C	3.19730600	-3.58527100	-1.90435300	H	-2.09457000	-4.49784500	-3.53526000
C	3.87266000	-4.45739200	-2.75814000	H	-0.99556100	-4.64794000	-4.91799600
C	3.34509500	-4.75251500	-4.01196200	H	-2.74955600	-4.86553000	-5.12838500
C	2.15327900	-4.14893500	-4.41393000	H	-1.43630100	-2.24429200	-4.18488000
C	1.49517500	-3.26486300	-3.56207300	H	-4.05621300	-2.23901400	-5.58056400
H	0.55238300	-2.82459500	-3.88625200	C	4.08677300	0.94398700	-4.94140300
H	1.72150000	-4.35520600	-5.38901100	O	3.59146300	-0.23567100	-4.29215200
H	3.85710200	-5.44562300	-4.67322900	C	4.48829100	-1.33420900	-4.49117600
H	4.80304800	-4.91689600	-2.43559200	C	5.37306700	-0.92113900	-5.66245700

H	3.60086600	-3.37872500	-0.91441800	C	5.48946700	0.58875700	-5.43552200
H	1.80100900	-2.17008000	-0.34808100	H	3.41892100	1.18973300	-5.77874700
H	-0.84731500	-2.21580800	-1.72245400	H	4.04882500	1.77551100	-4.23072200
C	-0.22515700	-3.03428000	1.46278900	H	5.07747600	-1.48804900	-3.57558000
H	-0.72465300	-4.01282500	1.50305200	H	3.89387200	-2.23129500	-4.67813100
H	-0.43521000	-2.50792500	2.39772900	H	6.33520900	-1.43854400	-5.66772600
H	0.85325000	-3.20851000	1.39157400	H	4.86104400	-1.12587100	-6.60982300
C	-2.94681000	-2.27799800	1.19694300	H	6.23767500	0.79706500	-4.66243100
H	-2.69913600	-3.12141800	1.83056300	H	5.76559500	1.14594200	-6.33396000
C	-4.32559000	-1.68732800	1.29682500	C	4.04886100	0.03299300	-0.97475700
H	-4.63404400	-1.24834800	0.33963300	O	3.35783000	1.28285000	-0.81779800
H	-5.06957300	-2.44737700	1.56405000	C	4.29837900	2.36952400	-0.78757600
H	-4.39902000	-0.89351900	2.05727300	C	5.67985000	1.72247200	-0.70511600
Na	1.35579800	1.53572600	-1.87383200	C	5.44251600	0.41154400	-1.45584300
O	-0.28793600	2.10749200	-0.39030300	H	4.09007200	-0.47355200	0.00073500
Na	-2.49631900	1.39832800	-0.26541600	H	3.47747700	-0.58045100	-1.67358200
O	-3.56262300	2.04450300	-2.08687000	H	4.18603600	2.95441900	-1.70853900
Na	-3.49450400	1.50946600	-4.25665200	H	4.06090200	3.01253500	0.06422900
O	-1.86244900	1.93246300	-5.76713300	H	6.45799300	2.34981900	-1.14664200
Na	0.32154400	1.17734500	-5.90076400	H	5.94891200	1.51783700	0.33702800
O	1.34570200	1.89258900	-4.08086600	H	5.41330600	0.59547700	-2.53586100
C	1.50997700	3.21240800	-4.48386900	H	6.18890900	-0.36028700	-1.24990400
C	0.14409200	3.84169500	-4.93245700	C	-6.31549800	0.98012700	-0.83883500
N	-0.17704500	3.39908000	-6.32229400	O	-5.92309100	-0.13597400	-1.63289500
C	-1.54395000	2.97370800	-6.51224500	C	-6.88982300	-1.17106500	-1.43041200
C	-2.36849500	3.53450500	-7.42655400	C	-8.20474700	-0.46439000	-1.02548900
H	-2.04790800	4.39385400	-8.00335000	C	-7.83018100	1.02977300	-1.00302600
C	-3.72733000	2.94576800	-7.69571400	H	-6.04191800	0.79954900	0.21476800
H	-3.66912300	1.98531300	-8.23266400	H	-5.76598400	1.84505000	-1.21605500
H	-4.28975000	2.75165600	-6.77275300	H	-6.95266800	-1.74174300	-2.36191100
H	-4.33289600	3.61681100	-8.31326500	H	-6.54057500	-1.84448000	-0.63923500
C	0.37886000	4.24963200	-7.36272500	H	-9.01999000	-0.67498000	-1.72220100
H	-0.10066700	5.23658600	-7.42988800	H	-8.52480200	-0.79811600	-0.03466200
H	0.26478800	3.75168700	-8.32921600	H	-8.08021700	1.50873500	-1.95604700
H	1.44509300	4.40438100	-7.16885600	H	-8.32671800	1.58137500	-0.20129000
C	0.01322100	5.36088500	-4.79680800	C	-6.26443900	-0.05075000	-5.02212700
H	0.01362500	5.66287800	-3.74785200	O	-5.64040800	1.24352100	-5.01481600
H	-0.93375300	5.68715300	-5.24582800	C	-6.56727400	2.20962800	-4.52249800
H	0.83434600	5.89396100	-5.28908100	C	-7.92557300	1.69129400	-4.97322500
H	-0.60178000	3.36054900	-4.28751400	C	-7.75759600	0.18496600	-4.74400700
C	2.19334100	4.07520200	-3.42636100	H	-6.08772700	-0.48948700	-6.01091300
C	3.41788700	4.69118400	-3.69141400	H	-5.78833300	-0.68383300	-4.26976100
C	4.03533600	5.51008500	-2.74455800	H	-6.50177400	2.26029900	-3.42565700
C	3.42796600	5.72954400	-1.51169400	H	-6.28933900	3.18264000	-4.93569900
C	2.20335000	5.12321600	-1.23108500	H	-8.75684900	2.12532600	-4.41065900
C	1.59733400	4.30280800	-2.17848000	H	-8.07247300	1.90941900	-6.03634900

H	0.62329300	3.86797600	-1.95237100	H	1.53615000	2.80210400	2.62525600
H	1.70006400	5.28829100	-0.28292000	H	1.86611300	2.46488500	0.91611600
H	3.89951300	6.37427300	-0.77571100	H	2.30763000	4.02361900	1.62067300
H	4.98625000	5.98240800	-2.97560200	C	-2.51424200	4.56071700	1.02583600
H	3.88863200	4.53480400	-4.66063700	H	-2.01088800	5.53822700	1.03517300
H	2.17433600	3.27537800	-5.37738100	H	-2.43768700	4.12931900	2.02726200
C	-3.64651100	3.39616600	-1.76378400	H	-3.57071800	4.72816900	0.79452400
C	-4.30401300	4.22814100	-2.86097100	C	-2.03297200	5.47201700	-1.61029200
C	-3.72925000	4.35772500	-4.13173300	H	-1.99802500	5.69023400	-2.67935900
C	-4.32783000	5.14528500	-5.11272800	H	-1.07990800	5.78558600	-1.16529000
C	-5.52280400	5.81218500	-4.84285500	H	-2.83556500	6.08207300	-1.18068000
C	-6.11037000	5.68569900	-3.58686200	H	-1.52726200	3.40631100	-1.96017200
C	-5.50001700	4.90234100	-2.60814500	H	-4.29456600	3.54460600	-0.86978000
H	-5.95798700	4.81321000	-1.62422200	C	-3.50248100	-2.13379400	-4.61897200
H	-7.03996300	6.20245500	-3.36478500	C	-4.32093800	-2.93846000	-3.61038900
H	-5.98870500	6.42841500	-5.60616200	C	-3.91793300	-3.07157200	-2.27474900
H	-3.84551600	5.23253900	-6.08234100	C	-4.64375800	-3.85430300	-1.37988800
H	-2.77892300	3.87129100	-4.35712600	C	-5.79762900	-4.51402200	-1.80186700
C	-2.24651200	3.97695600	-1.36001400	C	-6.21750600	-4.38276600	-3.12221000
N	-1.95556200	3.62616200	0.06176500	C	-5.48178700	-3.60196800	-4.01419500
C	-0.59976600	3.18432800	0.30648400	H	-5.80727200	-3.51283500	-5.04946500
C	0.19273100	3.78425200	1.22681900	H	-7.11371900	-4.89415900	-3.46306000
H	-0.15571600	4.67366900	1.73891200	H	-7.98479300	-0.05909500	-3.70136400
C	1.53740900	3.24035800	1.61639300	H	-8.40237300	-0.42441100	-5.38181000

Table 8. Geometric coordinates and thermally corrected M062X energies for **21**



G = –5068.684419

G_{SP} = –5068.684418

Atom	X	Y	Z	Atom	X	Y	Z
Na	0.00000000	0.00000000	0.00000000	C	-4.06617300	1.02715400	-5.79584400
Na	2.37634300	2.35628100	0.08483300	C	-5.40764000	-0.95916200	-3.92769600
O	-0.04903900	2.27514000	0.35709400	C	-6.30988300	-1.12485400	-4.98326700
Na	2.31023700	-0.00873700	-1.66654500	C	-6.68777200	-2.39334300	-5.41548700
Na	0.00038700	2.34639400	-1.88933200	C	-6.17025600	-3.52734100	-4.79096700
O	2.26862200	2.25928400	-2.05265000	C	-5.28331600	-3.37755200	-3.72765100
C	2.68554300	2.33844700	-3.35809900	C	-4.91764600	-2.10360000	-3.29575200
C	1.60454400	1.68077000	-4.27661800	O	-4.51508600	2.09994200	0.65398400
N	1.57981000	0.22673400	-3.96961900	C	-4.75955000	4.45853900	2.09636200
C	0.31875300	-0.31238100	-3.52734800	C	-4.99410700	3.24042200	2.73396900
O	-0.04223700	0.07717000	-2.31035700	C	-4.70299800	1.92633900	2.00746500
C	-0.34998700	-1.20174000	-4.29836400	C	-3.48964500	1.12282900	2.59763200
H	0.02092500	-1.40692200	-5.29663800	N	-3.57633600	-0.27097600	2.09276100
C	-1.55112000	-1.97541800	-3.84377000	C	-2.52369000	-0.76126700	1.26312900
H	-2.50121200	-1.57985900	-4.22966500	C	-1.95878000	-1.97940600	1.47784800
H	-1.50881200	-3.02185100	-4.17352300	C	-1.08366300	-2.64014900	0.45056900
H	-1.61941600	-1.99942600	-2.74710000	C	-4.22507800	-1.21467200	2.98527800
C	2.36660000	-0.60055200	-4.86982900	C	-3.26160700	1.17291200	4.10964700
H	1.96343400	-0.67868400	-5.89051500	C	-5.56454900	3.26529400	4.01078400
H	2.43747900	-1.60445200	-4.44401900	C	-5.84039800	4.46801900	4.65304600
H	3.37858800	-0.18490400	-4.94404900	C	-5.56322100	5.67868800	4.02051900
C	1.68372300	1.97190800	-5.77504700	C	-5.02996900	5.66868200	2.73540400
H	1.54851900	3.04186200	-5.95510800	C	-7.09749200	-2.36894100	-0.49862900
H	0.88443700	1.43449500	-6.29681700	O	-6.82516600	-1.02383700	-0.07584600
H	2.64043600	1.67537000	-6.21624700	C	-7.63223600	-0.10456400	-0.82763900

H	0.63148600	2.08082700	-3.96556800	C	-8.79699800	-0.93432000	-1.35137200
C	3.08405500	3.76188300	-3.75703800	C	-8.10158500	-2.26576300	-1.64853000
C	3.93011500	4.00649000	-4.84408400	C	-5.91032500	5.63472200	-1.01735000
C	4.34081300	5.29786300	-5.16053500	O	-4.79819600	4.86454700	-1.49631600
C	3.91774100	6.37564600	-4.38435700	C	-3.64941400	5.70508600	-1.64870300
C	3.08717800	6.14618500	-3.29085600	C	-3.86899200	6.84287400	-0.66172400
C	2.68199400	4.84923400	-2.97921300	C	-5.38290800	7.05624200	-0.77451900
H	2.05918900	4.65781000	-2.10924400	H	-1.31459700	-2.26009200	-0.55377400
H	2.76200300	6.97752800	-2.67091300	H	-0.00617500	-2.49206000	0.62287500
H	4.24217000	7.38364600	-4.62479200	H	-1.23428000	-3.72633600	0.42979000
H	5.00281500	5.46308500	-6.00583400	H	-2.17398400	-2.52522800	2.38833800
H	4.28910300	3.16900400	-5.43929200	H	-5.15668400	-0.77464000	3.35578500
H	3.60719000	1.72911600	-3.53831500	H	-4.47246700	-2.12092900	2.42620000
O	2.21428100	0.14096300	0.49205900	H	-3.61323500	-1.50526000	3.85263300
C	2.49164700	-2.35764600	1.68438900	H	-4.11892800	0.81800100	4.68890300
C	2.78107300	-1.20714100	2.41733500	H	-2.39829800	0.54923200	4.36795900
C	2.43778000	0.16979900	1.85103400	H	-3.04723700	2.19866900	4.42007000
C	1.22314400	0.86338500	2.56546200	H	-2.58036500	1.55619500	2.16625800
N	1.27419900	2.31254100	2.25093700	H	-5.58796200	1.28082600	2.22000800
C	0.21194700	2.89429300	1.49785800	H	-4.39745400	4.43179600	1.07237900
C	-0.36505700	4.06541300	1.87642200	H	-4.83312600	6.60951300	2.22555800
H	-0.15584600	4.47851900	2.85564800	H	-5.77816700	6.61912100	4.51911600
C	-1.23525300	4.85823700	0.94350500	H	-6.28175300	4.46131500	5.64569500
H	-0.98568100	4.62973800	-0.10155200	H	-5.80961100	2.32794200	4.50552000
H	-2.31284300	4.67730800	1.07825700	H	-2.76634100	5.09204900	-1.45291000
H	-1.09635300	5.93721300	1.08289500	H	-3.59199700	6.07201300	-2.68300800
C	1.93715900	3.14030600	3.24216000	H	-3.59313700	6.52226900	0.34833500
H	1.34620900	3.30656700	4.15562400	H	-3.28913600	7.73438200	-0.91227800
H	2.15993200	4.11489600	2.79987400	H	-5.82403700	7.50834200	0.11703300
H	2.88257000	2.66692300	3.52706700	H	-5.60842100	7.70093800	-1.62998600
C	1.03629200	0.60456900	4.06212200	H	-6.26703800	5.16728100	-0.09346200
H	0.83327500	-0.45566300	4.23375700	H	-6.71109000	5.60801600	-1.76466000
H	0.17977000	1.18170200	4.42845600	H	-0.68806400	4.63747500	-2.33720400
H	1.91026700	0.87843800	4.65994900	H	0.22479900	4.31899700	-3.82605500
H	0.31107600	0.47280000	2.09958300	H	-0.74155500	5.77019300	-3.68095400
H	3.31030300	0.81489400	2.11036000	H	-2.29126200	4.31094400	-4.95483900
C	3.43562400	-1.35277400	3.64485300	H	-5.68267600	3.12589300	-4.73186100
C	3.74729900	-2.61159200	4.14826000	H	-4.70848100	4.46551900	-4.09621600
C	3.41778800	-3.75569100	3.42354200	H	-4.26025600	3.68260800	-5.63179500
C	2.79528700	-3.62338200	2.18546700	H	-2.96839200	0.71878600	-4.03334800
H	2.55004700	-4.51142300	1.60699700	H	-5.93882700	1.05099100	-3.54906900
H	3.65843900	-4.73974100	3.81477000	H	-5.03866700	1.35949300	-6.17355500
H	4.25488300	-2.70150700	5.10451100	H	-3.28524700	1.61648700	-6.28815900
H	3.71520100	-0.46549900	4.20932900	H	-3.93613600	-0.01934700	-6.08562600
H	2.05859800	-2.22833200	0.69620800	H	-4.25621500	-1.98216200	-2.44178300
C	5.00341200	4.11964700	-0.26798100	Na	-2.30904200	2.30142200	0.14704200

O	4.58732600	2.86070300	0.28984400
C	5.22233500	1.78863800	-0.41843800
C	6.47826000	2.40603900	-1.01811300
C	5.95567400	3.78866200	-1.41907500
H	4.12205300	4.67264600	-0.61005400
H	5.49778800	4.68895400	0.52701400
H	5.39623700	0.97676000	0.29189000
H	4.54937400	1.44167000	-1.21596800
H	7.26151700	2.49028800	-0.25689100
H	6.86873900	1.83131500	-1.86165900
H	6.74213700	4.53795200	-1.53363600
H	5.39808300	3.72577700	-2.35985300
C	3.66419000	-3.00103700	-1.52663300
O	2.49563500	-2.26910800	-1.91995500
C	1.41846300	-3.17146300	-2.18365000
C	1.70489900	-4.37952700	-1.30235400
C	3.23409300	-4.46985600	-1.38510200
H	4.44207000	-2.86944700	-2.28754900
H	4.01393000	-2.57888100	-0.57890200
H	0.48825200	-2.64570800	-1.95447900
H	1.40955400	-3.44106700	-3.24950300
H	1.37786900	-4.18039100	-0.27664600
H	1.20385400	-5.28456700	-1.65429700
H	3.68483700	-4.94209700	-0.50910200
H	3.52860700	-5.04293800	-2.26973500
Na	-4.74723500	-0.04005900	-0.02900700
O	-2.25190500	0.00562000	0.22060200
Na	-4.63222400	2.57387200	-1.46167400
Na	-2.32620900	0.21125400	-2.00673800
O	-4.59524000	0.39773900	-2.11458900
C	-5.01746700	0.42920100	-3.41774900
C	-3.94202200	1.16264400	-4.27863600
N	-3.89117600	2.57463800	-3.81663000
C	-2.62416100	3.03938300	-3.31390300
O	-2.27654200	2.51791400	-2.14335800
C	-1.93290000	3.99327300	-3.98168900
C	-0.72853300	4.70080300	-3.43406100
C	-4.66126200	3.50875000	-4.62198900
H	-4.88591200	-4.25415400	-3.22241000
H	-6.46696900	-4.51768600	-5.12294500
H	-7.39562300	-2.49788800	-6.23274800
H	-6.73240800	-0.24438000	-5.46405600
H	-7.51036200	-2.91471500	0.35788400
H	-6.15999100	-2.84520400	-0.80447400
H	-8.78580700	-3.11711700	-1.67507500
H	-7.57794200	-2.21003400	-2.60834300
H	-9.26379800	-0.48943900	-2.23346500
H	-9.55895800	-1.05656100	-0.57385400
H	-7.02827100	0.30158400	-1.64989400
H	-7.92553600	0.70570400	-0.15410200

Figure 68. Computation overview for resting state of tetrasolvated monomers.

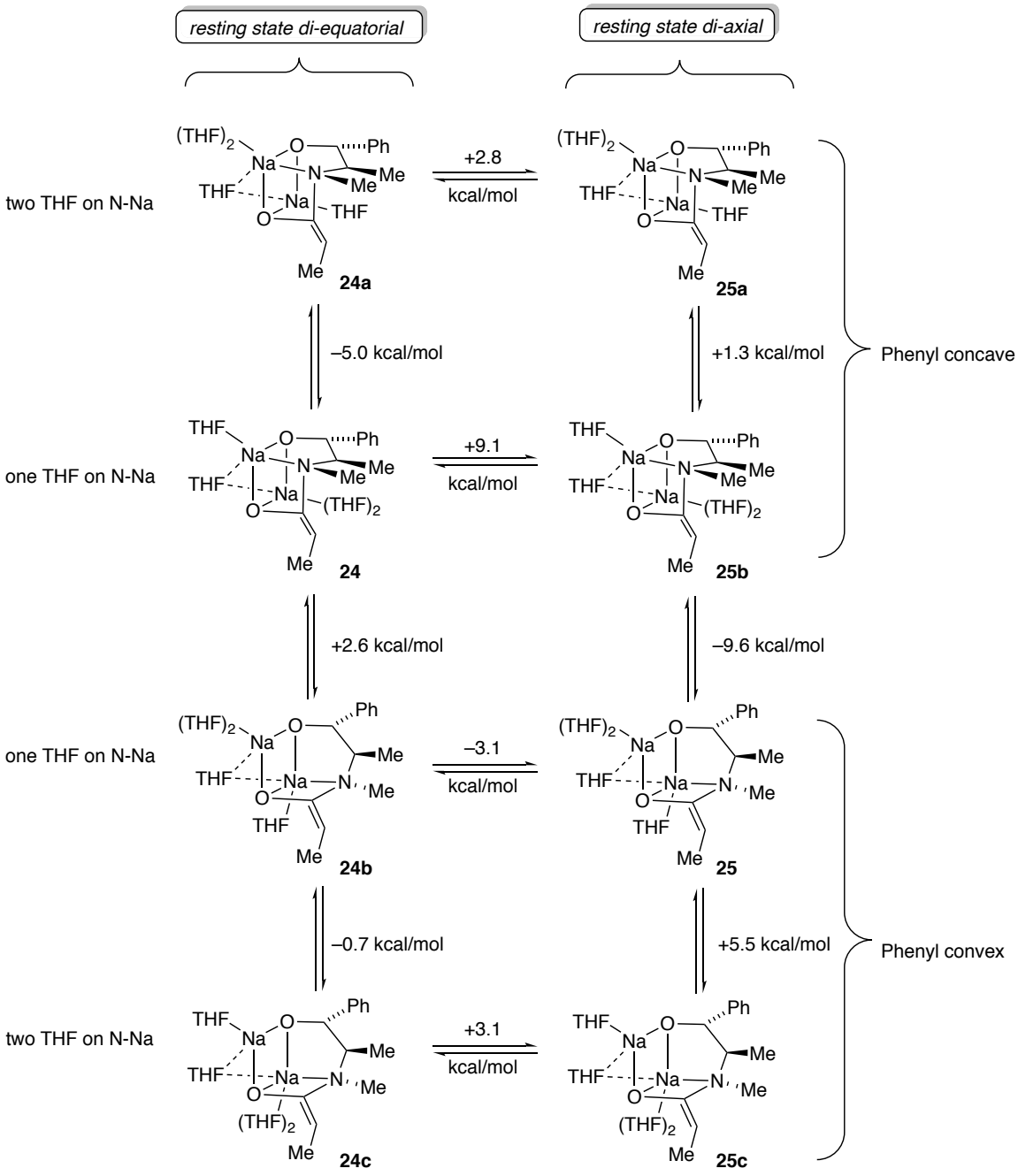
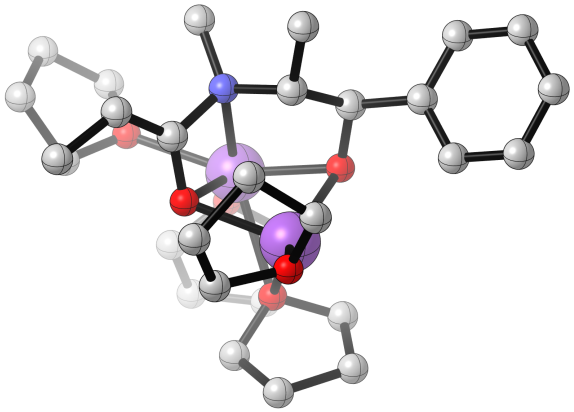


Table 9. Geometric coordinates and thermally corrected M062X energies for resting state **24a**



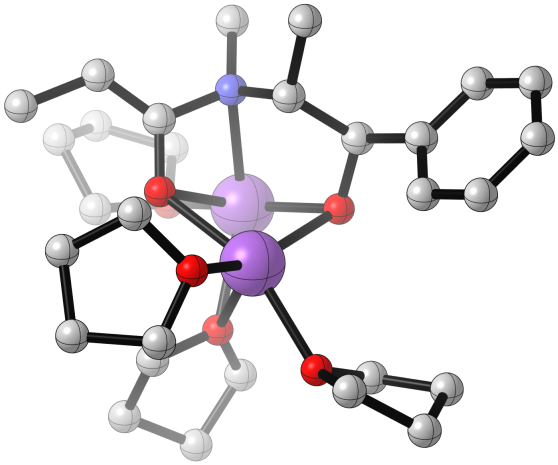
G = –1963.852597

G_{SP} = –1964.367172

Atom	X	Y	Z	Atom	X	Y	Z
Na	0.00000000	0.00000000	0.00000000	H	3.09589600	1.33255900	0.57342800
O	0.72393600	1.42004300	1.71549100	C	3.77507900	2.45989700	-1.07676000
C	0.97584400	2.40979200	0.89911800	H	3.65455400	2.55926600	-2.16146700
N	1.39848600	1.98218200	-0.42437000	H	3.63128100	3.44844000	-0.62522800
C	2.78526700	1.46013100	-0.47298700	H	4.80379400	2.14058400	-0.88856500
C	2.78996600	0.01713700	-1.08266800	C	1.02307200	2.83152800	-1.53862800
O	2.05109900	-0.82949200	-0.29729600	H	1.18526900	2.28838700	-2.47786300
Na	2.12755900	-0.24638900	1.81247900	H	-0.04124200	3.06277700	-1.44505800
O	0.22381300	-1.73342500	1.82668100	H	1.57429400	3.78267200	-1.60353400
C	1.07390700	-2.87932900	1.70853900	C	0.84286300	3.73254400	1.18372500
C	1.89806700	-2.90173300	3.01214600	C	0.29547300	4.22907900	2.49045100
C	1.08149400	-2.01877900	3.99175800	H	0.17919000	3.39341300	3.18825800
C	-0.17867000	-1.65836400	3.18943400	H	0.94955700	4.97515500	2.96173500
H	-0.54514200	-0.64328900	3.36259500	H	-0.69060200	4.71031200	2.38619600
H	-0.98781300	-2.38108000	3.37698800	H	1.09853300	4.46686100	0.42542400
H	1.63791500	-1.11392500	4.26127900	O	-1.80997700	-1.37235800	-0.50904400
H	0.84003900	-2.53608100	4.92270600	C	-2.80822200	-1.17345900	0.49422000
H	2.90332000	-2.49335000	2.85675700	C	-3.44936900	-2.54072500	0.70665400
H	2.02758300	-3.92027200	3.38378600	C	-2.25020300	-3.46834400	0.50335000
H	0.45604000	-3.78498400	1.62711600	C	-1.49955400	-2.76706300	-0.62917000
H	1.65908500	-2.73003900	0.79650300	H	-1.84468300	-3.11442000	-1.61032000
O	3.60846800	0.68891300	3.25493700	H	-0.41274400	-2.88571600	-0.57601500
C	2.85707000	1.60198600	4.09186000	H	-2.52493700	-4.49542800	0.25239300
C	3.58150100	2.95000800	4.01990500	H	-1.63899200	-3.48163800	1.41096000
C	4.35264700	2.83699600	2.70215500	H	-4.21083000	-2.72469400	-0.05887600
C	4.75353200	1.36944600	2.72090000	H	-3.91580300	-2.64020500	1.68982700
H	5.61640800	1.19956800	3.37971800	H	-2.33135000	-0.80789500	1.41596900
H	4.97148600	0.94299900	1.73639700	H	-3.50511700	-0.40958500	0.14192000
H	5.21168400	3.50942500	2.64124900	O	-1.77365800	1.52608500	-0.22623200

H	3.67481300	3.03968100	1.86461800
H	4.27462700	3.06615200	4.85998000
H	2.87836100	3.78537900	4.02886800
H	1.84741400	1.66990300	3.67122300
H	2.82369900	1.19262800	5.10736600
H	2.37158300	0.12852600	-2.11038100
C	4.23325100	-0.45611200	-1.26281400
C	4.95709100	-0.18652300	-2.42715300
C	6.28674000	-0.57734500	-2.55710000
C	6.92213800	-1.25154300	-1.51612000
C	6.20947900	-1.54191400	-0.35539900
C	4.87591000	-1.15536100	-0.23895800
H	4.30376700	-1.42363800	0.64642600
H	6.69040700	-2.08353000	0.45508000
H	7.95891600	-1.55945000	-1.61444200
H	6.82750300	-0.36036600	-3.47414500
H	4.46494400	0.33612400	-3.24533600
C	-2.27018200	2.33609600	0.83349100
C	-2.51113600	3.69402900	0.17831400
C	-2.94576500	3.31519900	-1.25463500
C	-2.54956900	1.82618000	-1.37714600
H	-1.93961700	1.59901400	-2.25499300
H	-3.44153800	1.18239600	-1.39973300
H	-2.43706900	3.92946000	-2.00169900
H	-4.02173800	3.44155000	-1.40098200
H	-1.56525200	4.24221800	0.16350000
H	-3.25918300	4.29071200	0.70582300
H	-3.21348000	1.90465600	1.21105800
H	-1.51424900	2.33416300	1.62192000

Table 10. Geometric coordinates and thermally corrected M062X energies for resting state **24**



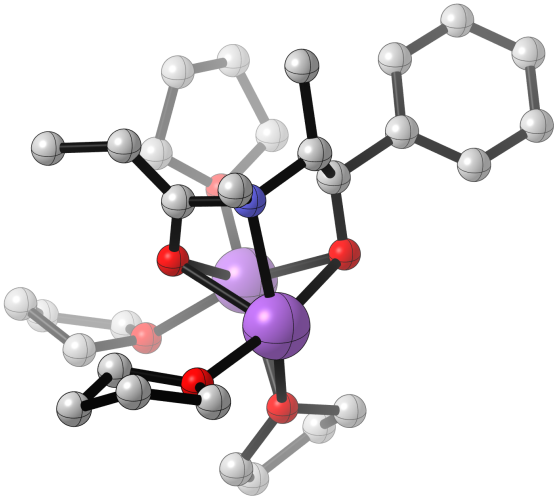
G = –1963.860043

G_{SP} = –1964.375154

Atom	X	Y	Z	Atom	X	Y	Z
Na	0.00000000	0.00000000	0.00000000	H	1.36162200	-2.90948200	1.18954500
O	0.08689400	0.43387500	2.27308400	H	0.28104600	-3.71151000	2.34047100
C	0.39638700	-0.81336500	2.51292200	C	1.32771100	-1.24203100	3.40558500
N	-0.29954000	-1.75105400	1.65427300	C	2.18093300	-0.28519800	4.18798300
C	-1.77392500	-1.77189400	1.84333100	H	2.22833000	0.68496900	3.67890500
C	-2.48994200	-1.50457800	0.47960700	H	1.80346400	-0.09131000	5.20324200
O	-2.15873300	-0.26512900	-0.00824800	H	3.20817500	-0.65549900	4.30182400
Na	-1.87135500	1.28151500	1.56554700	H	1.46935200	-2.30506600	3.56917000
O	-3.41223900	2.82533700	0.86918900	O	-0.30054400	2.34465300	0.00641000
C	-3.55053400	2.54992600	-0.54295100	C	0.13619100	3.27791000	1.00942900
C	-5.05163100	2.44397100	-0.79396200	C	0.99060600	4.29697400	0.26548300
C	-5.62154600	3.39812000	0.25840700	C	0.28152800	4.34975600	-1.09053600
C	-4.68442100	3.15506800	1.43894700	C	-0.06991900	2.88015000	-1.30461500
H	-5.02572800	2.31628600	2.06014600	H	0.76734300	2.33438400	-1.75978600
H	-4.56299900	4.03262800	2.08147000	H	-0.96923500	2.72030800	-1.90535000
H	-6.66581800	3.19672000	0.50903800	H	0.89984300	4.75470000	-1.89471200
H	-5.54146600	4.43642400	-0.08182700	H	-0.63142400	4.95120700	-1.01556700
H	-5.38803300	1.41942600	-0.60584200	H	2.01198900	3.91939300	0.14511700
H	-5.32269500	2.71616300	-1.81671000	H	1.03413400	5.26221300	0.77521300
H	-3.10969800	3.39194200	-1.09571600	H	-0.75377700	3.75929500	1.44277000
H	-3.01331200	1.61846300	-0.75680500	H	0.65331900	2.70741700	1.78572600
O	-2.33138800	1.97344400	3.69411800	O	2.18981100	0.10721300	-0.58292400
C	-1.55482500	1.35027100	4.72196900	C	2.88626600	0.66798800	0.54902900
C	-0.34852100	2.26868600	4.87244300	C	3.86261900	-0.41458100	0.99158500
C	-0.95067500	3.66921300	4.63633400	C	4.23816500	-1.05547200	-0.34659500
C	-2.31247400	3.37163300	3.96873800	C	2.90187100	-1.03269000	-1.08608400
H	-2.46444200	3.89125300	3.01872400	H	2.31475300	-1.93517500	-0.87177300
H	-3.14548900	3.61987800	4.64118400	H	3.00456200	-0.92891900	-2.17015100

H	-0.30992500	4.28226900	3.99603600
H	-1.09421400	4.21307100	5.57373600
H	0.36177800	1.99982400	4.08693600
H	0.13984500	2.17166500	5.84514800
H	-2.15494700	1.29962400	5.64267700
H	-1.28957800	0.34606500	4.38677600
H	-2.16872100	-2.33537300	-0.19282500
C	-3.99868200	-1.66771500	0.66170400
C	-4.65602300	-2.87130900	0.40238300
C	-6.02734600	-3.00305900	0.61133300
C	-6.76972100	-1.92471400	1.08542300
C	-6.12792900	-0.71414800	1.34116700
C	-4.75798700	-0.59126800	1.12557800
H	-4.26180100	0.36202300	1.29109600
H	-6.69949200	0.13872100	1.70184600
H	-7.83906800	-2.02411300	1.24681000
H	-6.51871200	-3.94851800	0.39857500
H	-4.08208600	-3.71710500	0.02780700
H	-2.01083100	-0.90509300	2.47540300
C	-2.24796400	-3.00771400	2.61236900
H	-2.19252200	-3.91968700	2.00679900
H	-1.63493500	-3.15100200	3.50927500
H	-3.28788000	-2.88317000	2.92373200
C	0.31041900	-3.05295600	1.45875600
H	-0.19773100	-3.56936600	0.63653800
H	4.64061500	-2.06618900	-0.24916300
H	4.97508800	-0.43957400	-0.87359000
H	3.33482300	-1.12648000	1.63609600
H	4.71821900	-0.01008600	1.53747000
H	3.41157100	1.57501500	0.21845900
H	2.13968200	0.91760800	1.31053200

Table 11. Geometric coordinates and thermally corrected M062X energies for resting state **24b**



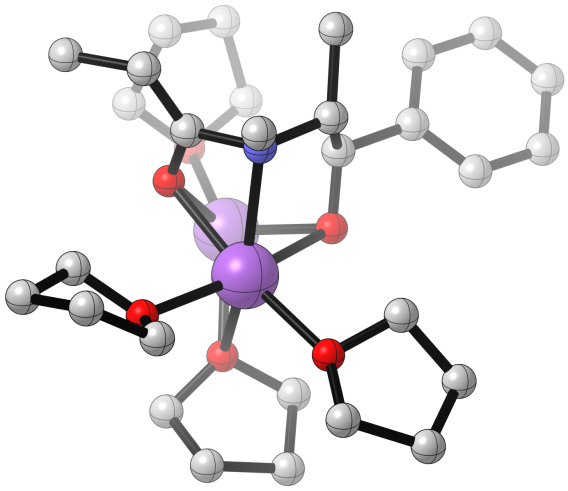
G = –1963.85727

G_{SP} = –1964.371067

Atom	X	Y	Z	Atom	X	Y	Z
Na	0.00000000	0.00000000	0.00000000	C	2.63956000	-2.09719100	-0.27838900
O	-0.02794300	1.17995900	-1.97065100	O	2.09896600	-0.78998300	-0.49530700
C	-0.49192700	0.19628400	-2.69176000	C	2.71815700	-0.17937700	-1.64160400
N	-0.93305700	-0.97579400	-1.91603700	C	4.02239900	-0.94405100	-1.82904100
C	-2.38091200	-1.07263800	-1.60935800	C	3.59582100	-2.36268700	-1.44305500
C	-2.87552300	0.23611700	-0.91307700	H	3.06249000	-2.83304100	-2.27581300
O	-2.11930500	0.58978800	0.17118300	H	4.42813200	-3.01050700	-1.15893200
Na	-1.20754600	2.44631300	-0.60996200	H	4.40904100	-0.87125300	-2.84792500
O	-2.68000200	3.67479900	-1.85573800	H	4.78726700	-0.57451500	-1.13706900
C	-2.21166200	3.46795600	-3.19725200	H	2.05381000	-0.27419900	-2.50950700
C	-3.37764000	2.82696500	-3.93988200	H	2.84658000	0.88330200	-1.42358500
C	-4.58371500	3.48626300	-3.26206800	H	3.16830500	-2.10089200	0.68274600
C	-4.11485900	3.63065800	-1.81184500	H	1.81629400	-2.81825100	-0.22996000
H	-4.41384400	2.77356700	-1.19948400	C	-0.52490300	0.15763400	-4.04821300
H	-4.47698900	4.54948700	-1.33924600	C	0.04674400	1.25434200	-4.90019900
H	-5.50140400	2.89732700	-3.33578900	H	0.67631200	0.86069000	-5.70858800
H	-4.77239100	4.47028100	-3.70469800	H	-0.72091200	1.87968800	-5.38293100
H	-3.36483800	1.74514800	-3.77084200	H	0.66656800	1.91271300	-4.28071700
H	-3.33576900	3.00828400	-5.01664700	H	-0.94910900	-0.71194300	-4.54118800
H	-1.94703800	4.44371000	-3.63504700	O	0.26199600	1.91135500	1.30805400
H	-1.32163800	2.82999000	-3.15268400	C	-0.70371600	2.23198200	2.31488300
O	0.18889000	4.25207500	-1.03576000	C	-0.68935000	3.76011500	2.33295300
C	1.34265800	3.96597200	-1.83328600	C	0.79644900	4.09389400	2.07378000
C	1.15966800	4.81802700	-3.08127300	C	1.37765500	2.77149200	1.52798600
C	0.55200300	6.10165100	-2.50035400	H	2.05336000	2.30282000	2.25613200
C	-0.22996900	5.60182700	-1.27063100	H	1.89812900	2.87843300	0.57463300
H	-1.31069900	5.57629100	-1.43255700	H	1.30572600	4.39090900	2.99412000

H	-0.01745900	6.20811200	-0.38042800
H	-0.09151500	6.62667000	-3.21035400
H	1.34576400	6.79060500	-2.19561700
H	0.46136100	4.32396900	-3.76310800
H	2.09676600	4.99401700	-3.61493800
H	2.25106000	4.26714800	-1.28591200
H	1.33841900	2.88817300	-2.01961800
H	-2.84510800	1.00314900	-1.73017400
C	-4.35835400	0.09524800	-0.54508100
C	-5.39053900	0.34746200	-1.45399400
C	-6.72655200	0.22062400	-1.08184400
C	-7.05262900	-0.16407600	0.21672300
C	-6.03304900	-0.41164300	1.13370000
C	-4.69943000	-0.27527400	0.75601000
H	-3.88945800	-0.42958500	1.46215300
H	-6.28046400	-0.70370500	2.15099200
H	-8.09298300	-0.26262400	0.51299700
H	-7.51260100	0.42371300	-1.80437700
H	-5.13917800	0.64431400	-2.47225400
C	-3.22283600	-1.46728700	-2.82752500
H	-4.24509300	-1.71660800	-2.53534600
H	-3.25569200	-0.65080700	-3.55787800
H	-2.80202500	-2.34302700	-3.33160400
H	-2.46611400	-1.86831700	-0.85146300
C	-0.36305400	-2.23319600	-2.36975400
H	-0.61869900	-3.02072300	-1.64785800
H	-0.69757800	-2.56906500	-3.36265400
H	0.72702400	-2.13549800	-2.40809600
H	0.90322100	4.89971700	1.34544400
H	-1.06357600	4.17346100	3.27232200
H	-1.31750800	4.15014400	1.52296000
H	-1.64188900	1.76138400	2.00840500
H	-0.36943800	1.82496900	3.28099500

Table 12. Geometric coordinates and thermally corrected M062X energies for resting state **24c**

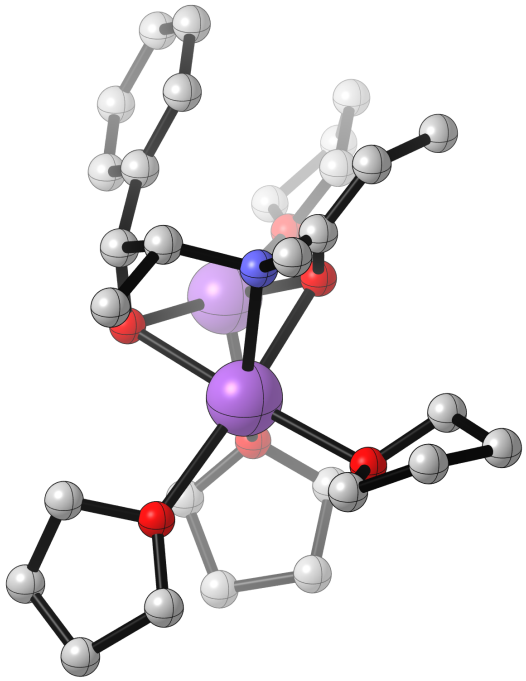


G = –1963.857962
G_{SP} = –1964.372211

Atom	X	Y	Z	Atom	X	Y	Z
Na	0.00000000	0.00000000	0.00000000	H	0.23269100	0.23881600	-3.42309400
O	1.31794400	-1.88122000	0.13080200	H	1.11654100	-1.21104600	-3.94115500
C	1.50969900	-1.92761800	-1.15536100	H	-0.33926500	-1.38252700	-2.95075100
N	1.27469500	-0.65362600	-1.85334000	C	-2.83858000	-0.94974700	-1.16157300
C	2.43366100	0.26709500	-1.93765300	O	-1.83968000	-1.34482200	-0.21461100
C	2.95395400	0.63400300	-0.50997000	C	-1.59628100	-2.75743800	-0.33741400
O	1.96190000	1.07475600	0.32811800	C	-2.92533100	-3.31628100	-0.82395000
Na	2.04577600	-0.60914000	1.74177500	C	-3.34044700	-2.23813400	-1.82973400
O	3.85888900	-1.82004200	2.31292300	H	-2.82233900	-2.40029800	-2.78069700
C	3.78299400	-3.13288500	1.73297500	H	-4.41437800	-2.21240600	-2.02815500
C	4.66200700	-3.05073800	0.49572300	H	-2.82905100	-4.30760900	-1.27221100
C	5.81583600	-2.17431100	0.99591100	H	-3.64329100	-3.37094100	0.00201100
C	5.13128800	-1.22876300	1.99469400	H	-0.79137600	-2.93615900	-1.06213100
H	4.94616700	-0.23791600	1.56275200	H	-1.26793500	-3.12021100	0.63803900
H	5.70770200	-1.10673900	2.91779200	H	-3.63770800	-0.43483900	-0.61322500
H	6.32128700	-1.62902700	0.19561500	H	-2.40023800	-0.24302000	-1.87570500
H	6.56348600	-2.78983800	1.50667600	C	1.80758600	-3.04153100	-1.87408000
H	4.09751200	-2.56685100	-0.31030700	C	1.89580200	-4.39899800	-1.24012700
H	4.99460100	-4.03211900	0.14879800	H	1.37427700	-5.16299800	-1.83157300
H	4.16340100	-3.86765400	2.45641500	H	2.92893900	-4.75647100	-1.11451400
H	2.73531500	-3.33051000	1.49713800	H	1.43741000	-4.36866300	-0.24567000
O	-0.04834100	0.21733900	2.38589300	H	1.97535900	-2.95693600	-2.94352800
C	-0.06360000	1.64716800	2.56594400	O	-1.28629400	1.85062300	-0.58472200
C	-1.55122600	2.05588500	2.62468100	C	-2.53997200	2.50212300	-0.74384100
C	-2.30798500	0.72792500	2.44246900	C	-2.25757900	4.01933800	-0.64435000
C	-1.27749000	-0.30015700	2.89067500	C	-0.71614300	4.10131200	-0.63049600

H	-1.42130700	-1.29074500	2.45425500
H	-1.22773700	-0.37710600	3.98682800
H	-2.53209300	0.54808900	1.38616300
H	-3.23763600	0.68090700	3.01488100
H	-1.80065500	2.77785700	1.84365000
H	-1.78806200	2.50828000	3.59172600
H	0.45320700	1.88721600	3.50351800
H	0.50219200	2.06521600	1.72879200
H	3.43946200	-0.31287100	-0.15582300
C	4.09451000	1.65436200	-0.61131200
C	5.42210200	1.27679300	-0.83037900
C	6.43790000	2.22597100	-0.91678300
C	6.13852100	3.57899500	-0.77978900
C	4.82123700	3.96813900	-0.54568300
C	3.81294000	3.01247900	-0.45389000
H	2.78949700	3.29585800	-0.22652000
H	4.58248500	5.02141700	-0.42353000
H	6.92684000	4.32322200	-0.84625800
H	7.46318600	1.90885400	-1.08695700
H	5.65800100	0.21968400	-0.94436100
C	3.53736900	-0.26980700	-2.85458900
H	4.29356200	0.49319600	-3.05239300
H	4.02409100	-1.13940600	-2.39773900
H	3.13148900	-0.59206600	-3.81861900
H	2.03831900	1.20003700	-2.37088000
C	0.55117100	-0.76425600	-3.10870000
C	-0.30095900	2.72767100	-1.14722600
H	0.67609600	2.37265200	-0.80211400
H	-0.35981500	2.68077200	-2.24611400
H	-0.34243000	4.23239200	0.39038400
H	-0.32733000	4.91841800	-1.24203600
H	-2.69676700	4.45752200	0.25550800
H	-2.67832300	4.54509900	-1.50515300
H	-2.96412400	2.24380400	-1.72462200
H	-3.21360000	2.13014100	0.03347900

Table 13. Geometric coordinates and thermally corrected M062X energies for resting state **25a**

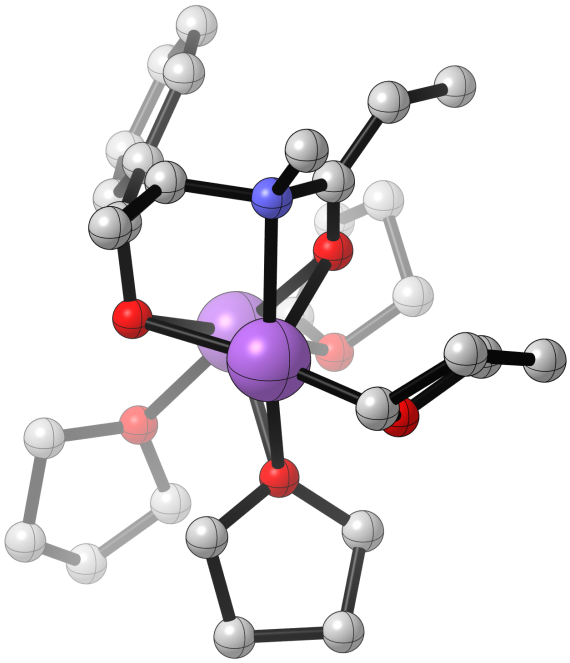


G = –1963.848449
G_{SP} = –1964.362667

Atom	X	Y	Z	Atom	X	Y	Z
Na	0.00000000	0.00000000	0.00000000	H	-1.84363100	2.04211000	2.92328000
O	-2.01525900	0.81683200	-0.69690300	C	0.14553500	1.26538200	3.06894800
C	-2.00104800	1.92420600	-0.02395800	H	0.48313000	2.22909700	3.45985500
N	-0.94477900	1.99975800	1.00223300	H	0.05862100	0.57678700	3.91468300
C	-1.19636600	1.37246500	2.32536400	H	0.92057100	0.88057200	2.39518400
C	-1.86198900	-0.03880800	2.33711200	C	-0.39373600	3.33792300	1.18151500
O	-1.21133400	-0.99322900	1.59452400	H	0.62551500	3.28712700	1.57981500
Na	-2.52487700	-1.23253400	-0.19036000	H	-0.99104200	3.96090900	1.87131500
O	-4.39575400	-1.57479500	-1.43091900	H	-0.36859000	3.84386600	0.21452400
C	-4.91540100	-0.22558600	-1.50267000	C	-2.78035500	3.01113800	-0.26512700
C	-6.42084300	-0.36504800	-1.73799700	C	-3.77363500	3.03602600	-1.38881000
C	-6.53829900	-1.76559200	-2.34678400	H	-3.87670800	4.03919400	-1.82005300
C	-5.46044200	-2.50971400	-1.56802200	H	-4.78445300	2.71865500	-1.08318400
H	-5.83085000	-2.80255800	-0.57519700	H	-3.44888200	2.35479800	-2.18321900
H	-5.07123700	-3.39465500	-2.07904300	H	-2.71801500	3.87733200	0.38638100
H	-7.52932200	-2.21062300	-2.23012100	O	1.21824700	1.20188400	-1.56205900
H	-6.28515300	-1.74731000	-3.41227500	C	2.25806900	1.88514700	-0.85025300
H	-6.95482300	-0.32310900	-0.78367100	C	2.27452200	3.33222400	-1.36803000
H	-6.81001200	0.42417700	-2.38541000	C	1.48425300	3.23362000	-2.67803900
H	-4.40334800	0.27631800	-2.32732000	C	0.46863500	2.15360400	-2.33282200
H	-4.66888800	0.30434900	-0.57644200	H	-0.36596200	2.54824700	-1.74033400

O	-0.62677600	-1.95060100	-1.26863400
C	0.06369300	-3.09230400	-0.75022800
C	1.38976100	-3.18616200	-1.53539800
C	1.32288600	-1.99915100	-2.51506000
C	-0.17567500	-1.73390300	-2.60279400
H	-0.44552300	-0.70966100	-2.86940500
H	-0.67633000	-2.43761500	-3.28443000
H	1.80476500	-1.11080800	-2.09456000
H	1.77531100	-2.22031100	-3.48489400
H	2.25734700	-3.12176700	-0.87536100
H	1.44929700	-4.13533900	-2.07534000
H	-0.55531800	-3.98546500	-0.90715200
H	0.18050900	-2.92025100	0.32226300
C	-3.39368900	-0.02761600	2.11100000
C	-4.02246100	-1.27931900	2.03703800
C	-5.40545100	-1.39996900	1.92121100
C	-6.20243600	-0.25760900	1.87950800
C	-5.59639700	0.99388500	1.95454500
C	-4.21167600	1.10798600	2.07722900
H	-3.77283800	2.09748100	2.11697400
H	-6.20361800	1.89441900	1.92044800
H	-7.28298300	-0.34230700	1.80073800
H	-5.86206600	-2.38637000	1.88873700
H	-3.39632700	-2.16857900	2.09745300
H	-1.81025800	-0.28342600	3.42523700
H	0.06418700	1.62636100	-3.20014000
H	1.01548900	4.17720700	-2.96650000
H	2.13211300	2.89892200	-3.49538900
H	1.75788200	3.99245300	-0.66604200
H	3.29039900	3.71042000	-1.50408900
H	3.19920200	1.36393600	-1.05831100
H	2.05719900	1.82917400	0.22795200
O	1.97853500	-0.99483400	0.82327600
C	3.36469300	-1.09758600	0.52037000
C	3.86766600	-2.39459600	1.19914800
C	2.64029800	-2.88810500	1.99216600
C	1.79270700	-1.62515000	2.09853100
H	0.71244500	-1.74419100	2.23596600
H	2.18937700	-0.96659100	2.88704700
H	2.09936700	-3.65914200	1.43387900
H	2.90504900	-3.30074700	2.96835600
H	4.21376100	-3.13287400	0.47116500
H	4.70488700	-2.17561800	1.86687800
H	3.89186000	-0.21747900	0.91491200
H	3.46901800	-1.10462700	-0.56886100

Table 14. Geometric coordinates and thermally corrected M062X energies for resting state **25b**



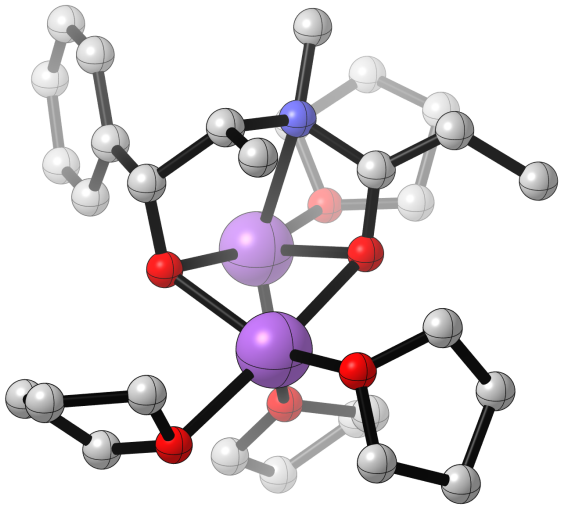
G = –1963.846487

G_{SP} = –1964.360672

Atom	X	Y	Z	Atom	X	Y	Z
Na	0.00000000	0.00000000	0.00000000	C	-2.08403200	-3.10741400	-0.99170200
O	-0.52051300	-1.76292300	1.25156400	C	-1.61061200	-4.35963900	-0.58375800
C	0.41460800	-2.53520400	0.78947400	C	-2.45807700	-5.29405800	0.01042800
N	1.03139400	-2.06072600	-0.46723500	C	-3.81027900	-5.01542800	0.19051200
C	0.28454000	-2.30382400	-1.73365800	C	-4.30713100	-3.78602900	-0.23576200
C	-1.25191200	-2.02014100	-1.71551800	C	-3.45198600	-2.85401300	-0.82057200
O	-1.58652300	-0.73398500	-1.36347100	H	-3.84568500	-1.90625600	-1.17636800
Na	-2.48424100	-0.87388000	0.68577300	H	-5.36522700	-3.55556600	-0.12821000
O	-4.43796000	0.21788000	0.06116300	H	-4.46902900	-5.74911100	0.64705800
C	-5.05040600	1.21811900	0.87253600	H	-2.05287000	-6.24893900	0.33441500
C	-5.91216700	2.05598100	-0.07243200	H	-0.56268500	-4.61047300	-0.69255300
C	-5.14392300	1.93817000	-1.39244200	H	-1.51184300	-2.21340000	-2.78349100
C	-4.64618700	0.49543100	-1.33352100	C	0.88546200	-1.44131900	-2.85128200
H	-5.41379500	-0.19071700	-1.71780000	H	1.91889400	-1.70624100	-3.08716800
H	-3.69695400	0.29647300	-1.84423900	H	0.29714000	-1.56387200	-3.76513200
H	-5.76311700	2.12949800	-2.27185800	H	0.84639800	-0.37975900	-2.57840100
H	-4.30555700	2.64326600	-1.40919000	H	0.42622900	-3.36017100	-2.02917600
H	-6.90614500	1.60791300	-0.17513000	C	2.42891700	-2.44726900	-0.62040400
H	-6.03555800	3.08578500	0.27277400	H	2.95014300	-1.75986100	-1.29425400
H	-4.25994400	1.81522800	1.34585700	H	2.55010800	-3.46761300	-1.02459400
H	-5.62599800	0.72960900	1.66419800	H	2.91429100	-2.41620200	0.35714200
O	-3.50067900	-0.93372300	2.75894200	C	0.90914800	-3.63927000	1.40556600

C	-2.57635900	-1.67552200	3.56984900
C	-2.90870600	-3.12528200	3.25356000
C	-4.44013800	-3.08526500	3.21589500
C	-4.73681300	-1.66304000	2.70486700
H	-5.07383400	-1.64961600	1.66264900
H	-5.48404900	-1.15161700	3.32512100
H	-4.86332600	-3.85116800	2.56270800
H	-4.85182900	-3.22348900	4.22088500
H	-2.48673200	-3.37509000	2.27132900
H	-2.51330900	-3.83046200	3.98869300
H	-2.74796200	-1.43798700	4.63067400
H	-1.56679500	-1.39037100	3.26481600
O	-1.61097400	1.34619100	0.95648400
C	-1.69459900	2.27399100	-0.13106500
C	-2.09497600	3.59804800	0.50538000
C	-1.33796700	3.52598900	1.83732500
C	-1.45281700	2.04371000	2.20162700
H	-0.56228200	1.65642600	2.70416300
H	-2.33283600	1.82816000	2.81791600
H	-0.28730600	3.79313900	1.68221100
H	-1.74994000	4.17983400	2.60893300
H	-1.81471200	4.45978700	-0.10467500
H	-3.17705300	3.63199300	0.67536000
H	-2.38810300	1.85625600	-0.86189100
H	-0.70746500	2.37076300	-0.61174100
C	0.37181500	-4.11111100	2.72310100
H	1.15091300	-4.57315100	3.34164600
H	-0.43314900	-4.85479200	2.61118400
H	-0.05030800	-3.26691300	3.27980700
H	1.65712600	-4.24929200	0.90979600
O	1.71410400	0.97769000	1.15728600
C	2.83285300	1.12210900	0.26938200
C	4.05123400	0.51327300	0.98362400
C	3.57491300	0.39342200	2.43603700
C	2.09177100	0.11236500	2.24238300
H	1.90590400	-0.93657000	1.97574500
H	1.46739600	0.37310000	3.09990900
H	4.08557200	-0.39902100	2.98736000
H	3.71412700	1.34008800	2.96841500
H	4.27046100	-0.47778200	0.57738900
H	4.94521700	1.13119800	0.87387000
H	2.95536100	2.19075600	0.06645900
H	2.61842900	0.60377300	-0.67520700

Table 15. Geometric coordinates and thermally corrected M062X energies for resting state **25**

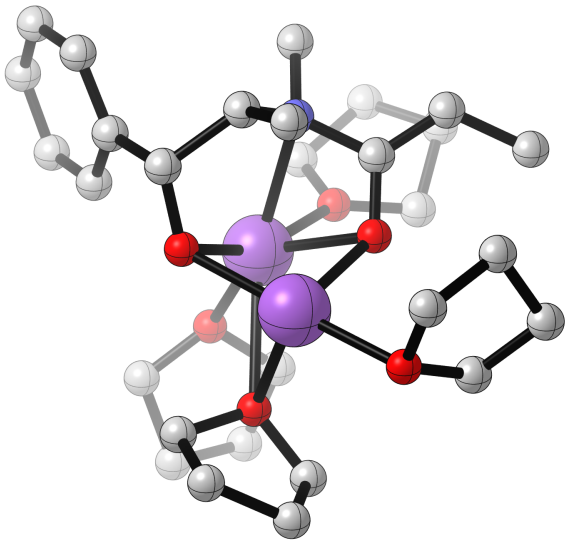


G = –1963.86228
G_{SP} = –1964.37606

Atom	X	Y	Z	Atom	X	Y	Z
Na	0.00000000	0.00000000	0.00000000	C	-4.17411800	-2.89472100	0.96946100
Na	-2.75401900	-0.12037000	0.56826800	C	-5.26805200	-3.33288100	-0.00443300
O	-1.49129200	-1.54394700	-0.57397800	C	-6.38918100	-2.32295700	0.26244900
C	-2.27510600	-1.68805100	-1.60772800	C	-5.61096700	-1.05442600	0.59556200
N	-3.12127700	-0.53424800	-1.89487800	H	-5.32963500	-0.49750200	-0.30928300
C	-2.44156800	0.71725600	-2.36266700	H	-6.13761500	-0.37698200	1.27275700
C	-2.34111600	1.83867900	-1.28003700	H	-7.05748400	-2.18689500	-0.59152800
O	-1.49745400	1.54946100	-0.25139100	H	-6.98849400	-2.63459300	1.12459200
C	-3.75701500	2.20624700	-0.77157100	H	-4.88839900	-3.24987600	-1.02672600
C	-3.95812400	2.37395900	0.60201800	H	-5.57763200	-4.36727500	0.16332400
C	-5.21821100	2.66550900	1.12646000	H	-4.21907300	-3.44671000	1.91657600
C	-6.30954300	2.81317000	0.27736300	H	-3.17539300	-2.98857300	0.53071900
C	-6.11829000	2.69747700	-1.09972300	O	1.52001500	1.66765000	0.47805500
C	-4.85796000	2.40833100	-1.61417300	C	0.82020100	2.61344700	1.30834700
H	-4.73342100	2.34669700	-2.69261500	C	0.55874400	3.84382700	0.44011500
H	-6.95563000	2.83974800	-1.77754800	C	1.65907300	3.73814200	-0.61921500
H	-7.29371600	3.03845700	0.67751800	C	1.71674100	2.23110900	-0.82732200
H	-5.34268400	2.79052000	2.19935800	H	0.90659300	1.90326700	-1.49177000
H	-3.08403100	2.30301100	1.24579600	H	2.67142300	1.86058500	-1.20998500
H	-2.00224800	2.73273600	-1.86157600	H	1.42460300	4.27828100	-1.53956400
C	-1.09538700	0.44984800	-3.02851600	H	2.61490900	4.10623500	-0.22988300
H	-0.70654400	1.37760000	-3.46284600	H	-0.42503600	3.72553400	-0.02232700
H	-0.35153200	0.06714500	-2.32760300	H	0.59260700	4.77529400	1.01056000
H	-1.20650700	-0.29207500	-3.82622400	H	1.45910100	2.83193600	2.17298400
H	-3.08543200	1.11577700	-3.15756600	H	-0.12262300	2.16553300	1.63452900
C	-4.27230700	-0.81590800	-2.74498400	O	1.68960100	-0.92125000	-1.26609600
H	-4.96270200	0.03131000	-2.70385600	C	1.31842400	-2.19772100	-1.79463700

H	-4.79604700	-1.70447100	-2.38765000
H	-3.99735600	-0.98514700	-3.79988300
C	-2.39276200	-2.83639900	-2.32942600
C	-1.69032700	-4.10007900	-1.92337600
H	-1.29239400	-3.99308000	-0.90865300
H	-0.84350700	-4.36176300	-2.57649700
H	-2.36595500	-4.96630500	-1.93332000
H	-3.01882000	-2.86975000	-3.21353400
O	-0.91744600	-0.52187900	2.15615900
C	-0.97462900	-1.91982500	2.46608700
C	-1.96384800	-1.98252400	3.62087200
C	-1.54879500	-0.75460900	4.44774400
C	-0.96540300	0.20779000	3.39030000
H	-1.58813600	1.09081100	3.21805400
H	0.04506300	0.54228700	3.65274500
H	-2.38577200	-0.31135600	4.99131400
H	-0.78097000	-1.02627000	5.17774500
H	-2.98124900	-1.86090000	3.23475900
H	-1.90713000	-2.91616700	4.18544800
H	0.02180500	-2.26943800	2.77824100
H	-1.27480800	-2.42806000	1.54640400
O	-4.41941500	-1.50468200	1.26242600
C	1.50376900	-3.14040300	-0.60836700
C	2.71503200	-2.53275500	0.13673600
C	2.88542100	-1.14604300	-0.52323300
H	2.99253900	-0.31863400	0.18244100
H	3.74109300	-1.14391100	-1.21288000
H	2.52153000	-2.44434000	1.20949300
H	3.61837300	-3.13584700	0.01484300
H	0.59842900	-3.08995900	0.00386700
H	1.65932400	-4.17866300	-0.91123500
H	1.99555900	-2.45090400	-2.62444100
H	0.28800800	-2.13487500	-2.15121500

Table 16. Geometric coordinates and thermally corrected M062X energies for resting state **25c**



G = –1963.85295

G_{SP} = –1964.36724

Atom	X	Y	Z	Atom	X	Y	Z
Na	0.00000000	0.00000000	0.00000000	O	-3.54293400	1.90503200	2.25613300
Na	-2.45490300	0.01970900	1.32070200	C	-2.87924700	2.18146700	3.49427100
O	-0.58942300	-1.28394500	1.63745600	C	-3.01385800	3.68651900	3.71002700
C	-1.25968900	-2.40498700	1.60253700	C	-2.99645100	4.20613600	2.27201700
N	-2.43645100	-2.38089300	0.74779200	C	-3.78107100	3.11990600	1.54033000
C	-2.22112200	-2.38160100	-0.72378100	H	-4.85840400	3.32971000	1.55013600
C	-2.64109800	-1.02561300	-1.38437300	H	-3.46177400	2.98483100	0.50219900
O	-1.94716800	0.04732700	-0.90133800	H	-3.44091400	5.19719200	2.15570000
C	-4.16428300	-0.87070800	-1.23169000	H	-1.96773100	4.23912700	1.90004200
C	-4.70132700	0.20619600	-0.52933100	H	-3.97246400	3.91762600	4.18704500
C	-6.07594600	0.32398600	-0.31716100	H	-2.21296900	4.09485800	4.33140200
C	-6.94551300	-0.63070200	-0.83340700	H	-1.82537100	1.87927800	3.40945300
C	-6.42777600	-1.69037500	-1.57976600	H	-3.34809400	1.58305200	4.27888200
C	-5.05626700	-1.80341900	-1.77694400	O	-3.18226700	-0.75478000	3.34026800
H	-4.66873300	-2.63409800	-2.36447200	C	-2.44309200	-1.22296500	4.45832000
H	-7.09894200	-2.42917000	-2.00921100	C	-3.18428200	-2.48100600	4.90232300
H	-8.01634600	-0.54399100	-0.67448400	C	-4.65658000	-2.14870500	4.57568700
H	-6.46500900	1.17095400	0.24330100	C	-4.56438100	-0.94020000	3.61584100
H	-4.02136900	0.97536600	-0.17764200	H	-5.06786000	-1.09375500	2.65688300
H	-2.47232500	-1.18538600	-2.47460900	H	-4.97179000	-0.02962300	4.08051900
C	-0.81070800	-2.80976600	-1.12489900	H	-5.16542500	-2.99543000	4.10858300
H	-0.60404400	-3.82304300	-0.76776200	H	-5.21712900	-1.88310400	5.47589400
H	-0.71108500	-2.78629900	-2.21521200	H	-2.82823800	-3.32246600	4.30156100
H	-0.04012400	-2.16954700	-0.69010600	H	-3.02656400	-2.71116100	5.95880100
H	-2.88348300	-3.15836300	-1.13300900	H	-2.44899200	-0.45649900	5.25274900

C	-3.51804800	-3.27239000	1.13574200
H	-4.43192700	-2.97494500	0.61071100
H	-3.68356600	-3.18475800	2.21229500
H	-3.32000100	-4.33267900	0.89999900
C	-0.96321300	-3.51096500	2.33636200
C	0.12697100	-3.51555900	3.36746600
H	0.54323600	-2.50618000	3.45811600
H	0.95797700	-4.19324700	3.11965400
H	-0.23574200	-3.82170500	4.36078700
H	-1.54802500	-4.41626900	2.20930000
O	-0.70378900	2.08444200	0.95066700
C	-0.83844400	2.78006700	-0.29594400
C	0.60198200	2.92906600	-0.79749600
C	1.43957600	2.99238500	0.50394500
C	0.41531100	2.67164400	1.61152600
H	0.77041800	1.95492600	2.35608000
H	0.09414000	3.58742200	2.12967200
H	2.24224100	2.25127200	0.48272500
H	1.88751500	3.97693800	0.65697700
H	0.88803900	2.05951800	-1.40056300
H	0.72814400	3.81208700	-1.42786700
H	-1.28648500	3.76831700	-0.11224400
H	-1.48887600	2.16470900	-0.92434200
H	-1.42158900	-1.39786400	4.11483600
O	2.23410800	-0.24193200	0.41260800
C	2.38510300	-0.36560800	1.84802300
C	3.04783300	-1.72253500	2.08798600
C	2.57303700	-2.51697700	0.86932500
C	2.68636400	-1.45367900	-0.21302000
H	3.72577100	-1.32340400	-0.54382800
H	2.06213400	-1.63769100	-1.09338600
H	3.18096500	-3.40028500	0.65929200
H	1.52460300	-2.81365900	1.00137200
H	4.13968100	-1.63013100	2.08322400
H	2.73776700	-2.16755600	3.03509100
H	1.38364400	-0.34893000	2.29167300
H	2.98410700	0.48037700	2.20186500

Figure 69. Computational overview for transition state of tetrasolvated monomers with pseudo-diaxial substituents

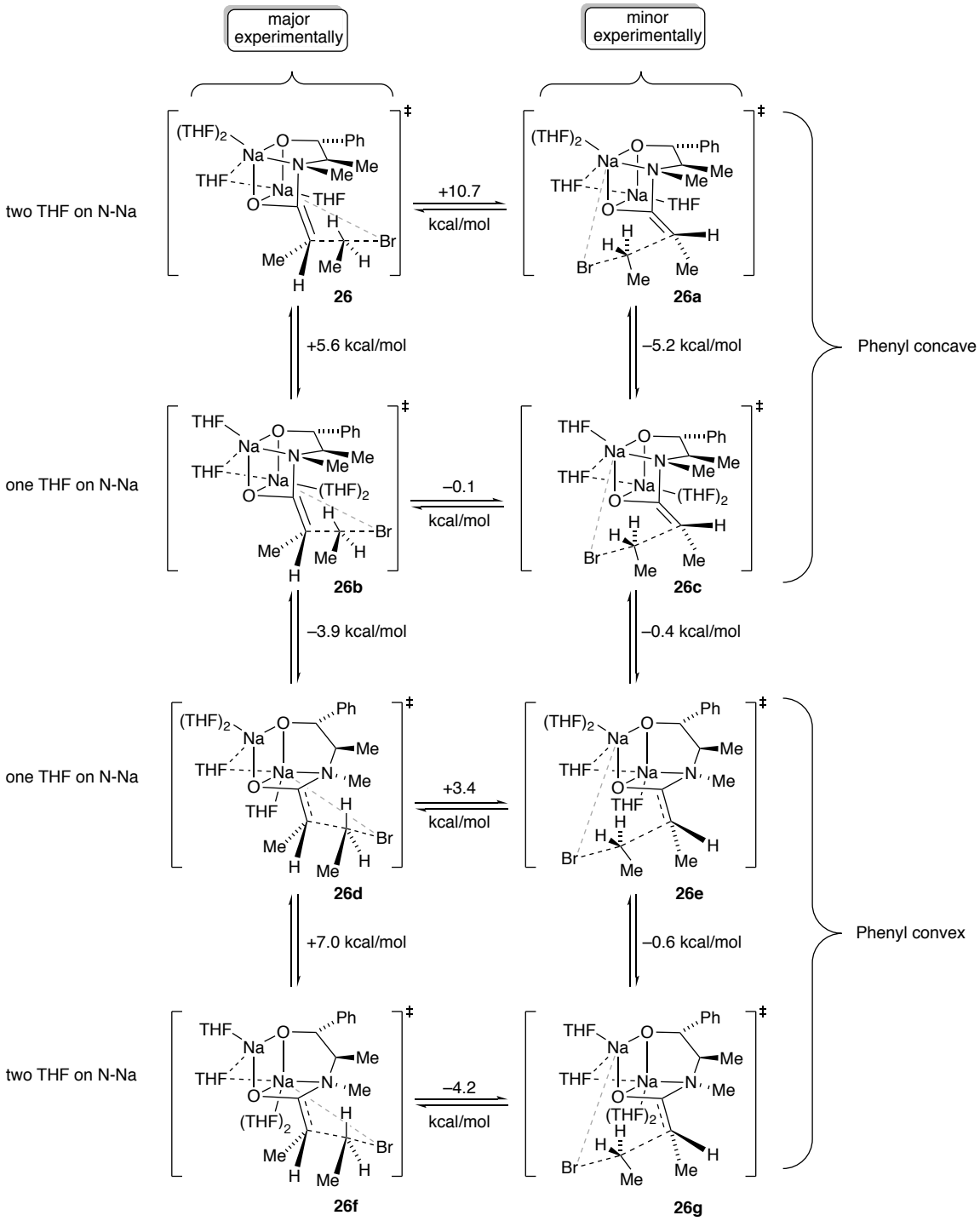
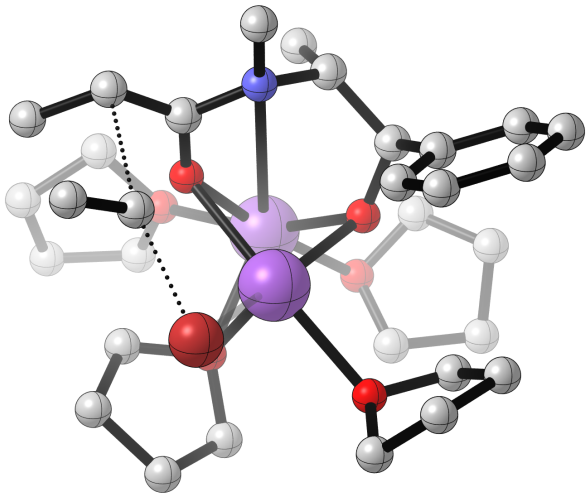


Table 17. Geometric coordinates and thermally corrected M062X energies for transition state **26**

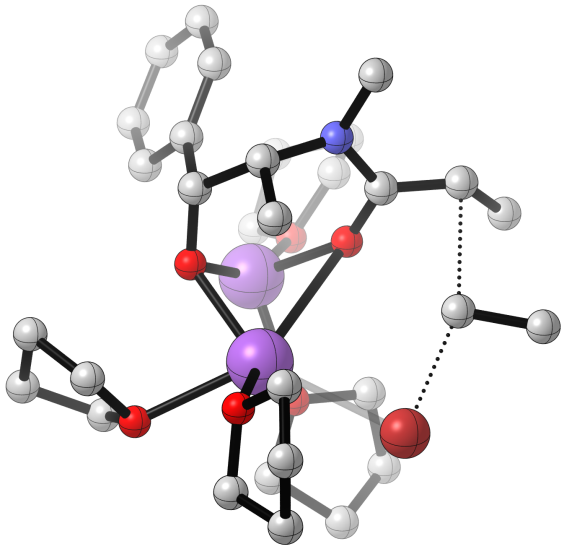


G = –4614.763936
G_{SP} = –4617.676393

Atom	X	Y	Z	Atom	X	Y	Z
Na	0.00000000	0.00000000	0.00000000	C	-5.52127200	-1.46741600	2.78516900
Na	-2.00355700	-1.74737500	0.90122000	C	-5.55562100	-0.07711100	2.11813200
O	-2.16366600	0.07628300	-0.31470900	C	-4.08129600	0.37723100	2.14887700
C	-2.79007300	0.01023100	-1.52276900	H	-3.66870900	0.66158200	1.17728400
C	-2.04998400	-0.82219300	-2.61631700	H	-3.93924400	1.19015900	2.87748000
N	-1.91663100	-2.26835800	-2.31968400	H	-5.93826300	-0.13014800	1.09597100
C	-0.72522400	-2.76511600	-1.75226200	H	-6.18468900	0.61823400	2.68115700
O	-0.21347700	-2.09439800	-0.78594100	H	-5.51456700	-2.25538900	2.02550000
C	-0.26585100	-4.04005300	-2.09244900	H	-6.35853900	-1.64372800	3.46487600
C	1.03245100	-4.56122700	-1.54420100	H	-4.21933300	-0.92093900	4.45165500
H	1.24325000	-4.12268300	-0.56154300	H	-3.74798400	-2.45602300	3.65256600
H	1.89570900	-4.33088400	-2.18593400	Br	-2.82345200	-4.28438800	1.81797700
H	1.01425500	-5.65308500	-1.42628700	O	-0.10978900	2.20038400	0.65762700
H	-0.64893600	-4.52768100	-2.98163100	C	-0.75190500	2.86313400	-0.44673900
C	-2.62976000	-3.11663500	-3.26080600	C	-2.15356700	3.24221200	0.02983200
H	-2.75594300	-4.12088800	-2.84565000	C	-1.95776900	3.34847600	1.54439000
H	-2.11794900	-3.21193500	-4.23225900	C	-0.98612000	2.20242700	1.79268700
H	-3.62434500	-2.69528400	-3.42465700	H	-0.36973900	2.32383900	2.68863500
C	-0.73149500	-0.18773000	-3.06572000	H	-1.52410200	1.24603400	1.83955200
H	-0.90819300	0.84207300	-3.39383400	H	-1.49479200	4.30480600	1.81254800
H	0.03179300	-0.18132900	-2.28557300	H	-2.88807700	3.24098000	2.10733400
H	-0.31612500	-0.74834700	-3.91094000	H	-2.51443200	4.16679400	-0.42716700
H	-2.70450100	-0.77658400	-3.49692200	H	-2.83901800	2.42103700	-0.19819600
H	-2.86730100	1.02014800	-2.00257700	H	-0.78391200	2.18089400	-1.30333400
C	-4.24430100	-0.47565700	-1.41612600	H	-0.14865700	3.74101700	-0.70583400
C	-5.28997300	0.32605700	-1.87945200	O	2.21940600	-0.22880100	-0.29574600
C	-6.61975000	-0.08755900	-1.79896400	C	2.81785800	-1.18644500	-1.16611400

C	-6.93246000	-1.32952000	-1.25476300
C	-5.90392700	-2.14240600	-0.78002700
C	-4.58118500	-1.71315500	-0.84991700
H	-3.80901100	-2.37715800	-0.47334500
H	-6.12785500	-3.11374800	-0.34575600
H	-7.96528800	-1.65955400	-1.19489200
H	-7.41044700	0.56238500	-2.16354000
H	-5.05528400	1.29736000	-2.31111400
O	-0.00685400	-1.11296400	2.09748200
C	-0.27532400	-0.91422800	3.48914700
C	-0.32090600	-2.32915000	4.08155400
C	0.52726200	-3.17084400	3.09623900
C	0.98765800	-2.14502200	2.05443300
H	1.95934600	-1.70532800	2.33034500
H	1.02389300	-2.50249000	1.02376900
H	1.37381600	-3.66605100	3.57762400
H	-0.10487000	-3.93434100	2.63390400
H	0.06507600	-2.35125200	5.10335700
H	-1.34985200	-2.70008200	4.09458900
H	-1.21708000	-0.37084600	3.56985300
H	0.54329200	-0.32137100	3.92303700
O	-3.32231000	-0.75829200	2.59251500
C	-4.17160600	-1.46346900	3.49384600
C	3.80677300	-1.92956400	-0.27184800
C	4.30166900	-0.82513500	0.68553400
C	3.24911000	0.29749600	0.53476400
H	2.78441200	0.59984200	1.47757500
H	3.68337400	1.18702900	0.06049300
H	4.37208300	-1.18440100	1.71511500
H	5.29134500	-0.46281900	0.39615900
H	3.28389200	-2.71709300	0.27830100
H	4.61689000	-2.39431600	-0.83825600
H	3.33692800	-0.66508700	-1.98439300
H	2.01078400	-1.80489300	-1.56320300
C	-1.67154400	-6.16299100	-0.26454400
H	-1.13459500	-6.59951000	0.58033700
H	-2.69100400	-6.55411900	-0.26664400
H	-1.17669000	-6.47481200	-1.18982800
C	-1.67493800	-4.66337200	-0.18039500
H	-2.41429400	-4.09940400	-0.72915900
H	-0.81138600	-4.13453800	0.19472200

Table 18. Geometric coordinates and thermally corrected M062X energies for transition state **26a**

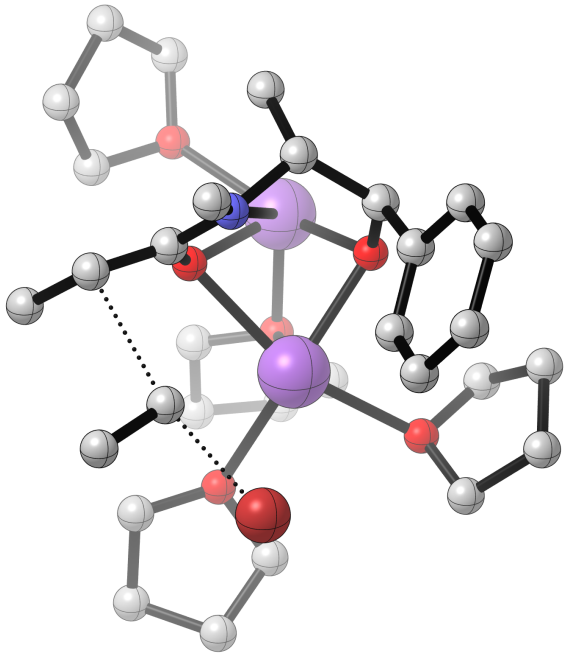


G = –4614.746531
G_{SP} = –4617.659227

Atom	X	Y	Z	Atom	X	Y	Z
Na	0.00000000	0.00000000	0.00000000	H	-2.40012500	-2.23800100	2.31803600
Na	-2.86065000	-0.16514200	0.74362500	H	-0.77096400	-2.69905900	1.74687800
O	-1.79159000	1.00568400	-0.76996000	H	-1.56609000	-1.94137900	4.60184900
C	-2.48929900	0.82334700	-1.92604600	H	-0.57874500	-3.32182800	4.07249800
C	-2.02686200	-0.33706300	-2.88179600	H	0.73794900	-1.08434500	4.88761900
N	-2.57818800	-1.69833800	-2.74295100	H	1.22574600	-1.82844500	3.34001000
C	-2.40903800	-2.45400900	-1.57747700	H	0.67561500	0.38338200	2.56282900
O	-2.27872900	-1.81794200	-0.47774700	H	-0.64649900	0.54988700	3.74539400
C	-2.30965100	-3.85549300	-1.63294400	O	-4.69465300	-1.08306400	1.68995900
C	-2.65974500	-4.68619600	-0.42667800	C	-5.21145900	-1.94362900	0.65366800
H	-3.71125700	-5.01259700	-0.42322000	C	-6.58542600	-2.36042700	1.15686600
H	-2.05479900	-5.60016500	-0.35959000	C	-7.06713600	-1.07319000	1.83242400
H	-2.49737700	-4.11380300	0.49443500	C	-5.77518300	-0.51483700	2.43837200
H	-2.36345800	-4.36280600	-2.58900100	H	-5.65313300	-0.81003800	3.48686100
C	-2.73491000	-2.40789600	-3.99785600	H	-5.72262200	0.57780200	2.37157800
H	-3.06441400	-1.70660700	-4.77035400	H	-7.84056700	-1.23728300	2.58629500
H	-1.80649500	-2.88836500	-4.34772700	H	-7.45471100	-0.38310300	1.07741900
H	-3.49814400	-3.18285200	-3.89374400	H	-6.49240400	-3.17020400	1.88876500
C	-0.50148700	-0.36804400	-2.96494200	H	-7.24251300	-2.69189200	0.34969600
H	-0.16584000	-0.94315700	-3.83641400	H	-5.27603300	-1.38061000	-0.28737300
H	-0.08516000	0.64317000	-3.02688600	H	-4.49930000	-2.75962100	0.52155300
H	-0.08090800	-0.85431200	-2.08057500	Br	1.63368200	-2.33182400	0.42194200
H	-2.39128700	-0.01604400	-3.86594000	H	2.61323100	0.54229400	0.92489700
C	-4.01549500	0.81542800	-1.71361600	C	3.04182200	0.84938100	-0.03484900
C	-4.93139700	0.19714000	-2.57515200	O	2.08541600	0.59072100	-1.07157300
C	-6.30284500	0.27696900	-2.34644000	C	2.70033400	-0.13825000	-2.13925000

C	-6.79868800	0.98216100	-1.25145400
C	-5.90469700	1.61694600	-0.39300500
C	-4.53281000	1.53519600	-0.62953000
H	-3.82837900	2.06106900	0.01404300
H	-6.27643900	2.19610700	0.44946700
H	-7.86944600	1.04896000	-1.07945700
H	-6.98969400	-0.21569000	-3.02928500
H	-4.57582100	-0.36406700	-3.43238000
H	-2.32706800	1.70477400	-2.59886800
O	0.38622900	2.25917800	0.79011300
C	0.41469700	3.03955200	-0.42277300
C	-0.82425600	3.92810100	-0.38767200
C	-1.03753400	4.11455100	1.11501800
C	-0.65870400	2.73419700	1.64037200
H	-1.51410800	2.04741600	1.57474000
H	-0.28518700	2.74900800	2.66911400
H	-2.06037900	4.39558600	1.37991800
H	-0.35453900	4.87226500	1.51531700
H	-1.65888200	3.36672300	-0.81516900
H	-0.68203800	4.86867900	-0.92562200
H	1.34356700	3.62554100	-0.42123400
H	0.41603800	2.35626300	-1.27226100
O	-1.04345100	-0.68760800	2.13653200
C	-0.11234300	-0.15788800	3.09838500
C	0.40199200	-1.35750100	3.88463600
C	-0.82189500	-2.27637700	3.87026200
C	-1.32694700	-2.07359300	2.44825700
C	4.20262700	0.02422500	-1.93336700
C	4.29322100	0.05623000	-0.40607100
H	4.21243400	-0.95937000	-0.00826600
H	5.20929200	0.51790000	-0.02997800
H	4.77554000	-0.78919600	-2.38456600
H	4.54781600	0.97267400	-2.35971000
H	2.40494200	-1.19219000	-2.06306100
H	2.33903200	0.27204800	-3.08609500
H	3.23167900	1.92961700	0.00004100
C	0.55326300	-4.89210700	-0.77330100
H	-0.04972400	-5.52055800	-1.43638500
H	0.48172100	-5.28750500	0.24233100
H	1.59490800	-4.94946800	-1.09719700
C	0.04748300	-3.48066400	-0.83900900
H	0.20907200	-2.92155800	-1.75187900
H	-0.71428000	-3.10758400	-0.18059700

Table 19. Geometric coordinates and thermally corrected M062X energies for transition state **26b**



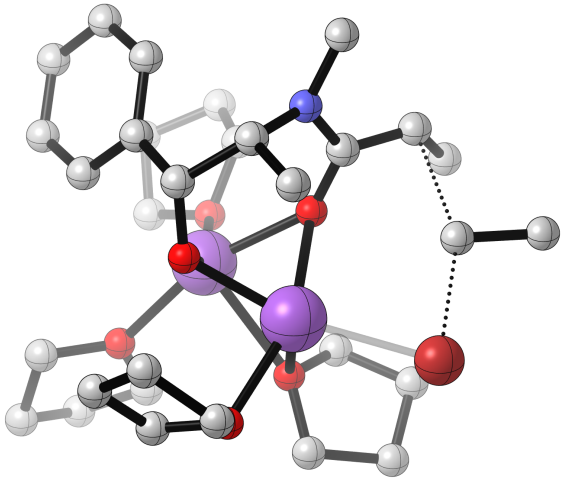
G = –4614.754017

G_{SP} = –4617.667486

Atom	X	Y	Z	Atom	X	Y	Z
Na	0.00000000	0.00000000	0.00000000	H	1.43826300	4.22227200	-2.57510600
Na	2.43341100	-0.96274900	-1.14139500	H	2.90088700	3.27287200	-2.90137600
O	0.44829800	-1.81107200	-1.29894100	H	1.62808500	3.80613100	-0.16870700
C	0.32042400	-3.12457200	-0.96686100	H	3.33478900	4.03406500	-0.62128300
C	1.28896000	-3.63803800	0.15573700	H	3.72247600	1.65665100	-0.69482300
N	1.05538000	-3.03890400	1.48250700	H	2.46286300	1.67259100	0.57224400
C	1.68675000	-1.86254600	1.90537800	O	4.68179800	-0.77487500	-0.56841000
O	1.96487000	-0.96072300	1.03123300	C	5.69748000	-1.71316200	-0.92106100
C	1.83056500	-1.61092000	3.27485000	C	6.05563100	-2.47548700	0.37198300
C	2.54016700	-0.37120000	3.73665100	C	5.36981100	-1.65581400	1.48745400
H	2.37407800	0.45033500	3.02803600	C	4.95898800	-0.36897300	0.77731000
H	3.63061800	-0.49687600	3.82492700	H	4.04618600	0.06390800	1.18500400
H	2.18150300	-0.04426600	4.72212600	H	5.77520600	0.36906800	0.76508600
H	1.74051600	-2.42208000	3.98787000	H	4.47186800	-2.16049000	1.85914200
C	0.56742300	-3.96939200	2.48566200	H	6.02950200	-1.46409500	2.33693700
H	1.37350700	-4.54843400	2.96493200	H	5.68286200	-3.50176300	0.34616600
H	-0.13515900	-4.65996100	2.01305300	H	7.13937600	-2.51845900	0.50497900
H	0.02720600	-3.43461100	3.27140200	H	6.56655300	-1.17023900	-1.31591900
C	2.77240300	-3.64436900	-0.23336300	H	5.29733900	-2.35490100	-1.71117900
H	2.88954700	-3.93215900	-1.28596700	O	-1.61156300	0.50144100	-1.62258200
H	3.26222300	-2.68579800	-0.05920900	C	-3.03353200	0.47691000	-1.48088900
H	3.31428700	-4.37609100	0.37709800	C	-3.52449500	-0.76683800	-2.24451100

H	1.02615000	-4.69547700	0.27750300
C	-1.08329400	-3.53845400	-0.50509400
C	-1.55324600	-4.83904900	-0.70673500
C	-2.78038900	-5.25097700	-0.19063200
C	-3.56184100	-4.36511600	0.54950100
C	-3.11036500	-3.06275800	0.75311300
C	-1.88934900	-2.66027800	0.21699100
H	-1.57111900	-1.63713300	0.36789600
H	-3.69356500	-2.34740800	1.32824400
Br	-2.26342300	0.36436500	2.11843300
H	-4.51524000	-4.68750700	0.95792400
H	-3.12824100	-6.26532400	-0.36691900
H	-0.94532600	-5.53965400	-1.27811300
H	0.55750100	-3.80350900	-1.82256900
O	1.80972600	1.19937700	-1.31801700
C	2.69131100	1.95073200	-0.46040300
C	2.44523300	3.42075100	-0.78370400
C	2.02095900	3.35539400	-2.25429800
C	1.20831000	2.06498600	-2.29538900
H	0.15956800	2.22367200	-2.02007700
H	1.24320300	1.55918300	-3.26421300
H	0.03932700	-0.98676700	5.14087400
H	-0.77832000	0.55117600	4.80193300
C	-0.40863500	-0.66755400	3.06618000
H	-0.63810800	-1.59132700	2.55271300
H	0.27460700	0.01600300	2.58218700
C	-2.29477100	-1.20325900	-3.06969900
C	-1.32414200	-0.03725200	-2.91263400
H	-0.28540800	-0.36855600	-2.90554500
H	-1.48972700	0.74365700	-3.67360900
H	-1.83327100	-2.08942900	-2.62801700
H	-2.53442500	-1.40747400	-4.11639100
H	-3.82846300	-1.55643400	-1.55367700
H	-4.38068100	-0.51924700	-2.87761200
H	-3.45062200	1.39867400	-1.91458700
H	-3.24777200	0.45353100	-0.41048000
O	0.00475500	2.34551300	0.79478700
C	-1.11402200	3.09370300	0.29210300
C	-1.63853500	3.91382600	1.46572200
C	-0.36118300	4.14504500	2.27430500
C	0.32996500	2.79490900	2.11486000
H	1.42100800	2.84338900	2.20371900
H	-0.06432800	2.07783600	2.84403200
H	0.24201500	4.94360100	1.82614200
H	-0.54651800	4.39538700	3.32128700
H	-2.12982700	4.83604300	1.14662000
H	-2.34068000	3.30731900	2.04464200
H	-1.84575900	2.39323000	-0.11242600
H	-0.75358200	3.74433900	-0.51964500
C	-0.72959400	-0.50632100	4.52957100
H	-1.69551500	-0.96076900	4.75924700

Table 20. Geometric coordinates and thermally corrected M062X energies for transition state **26c**



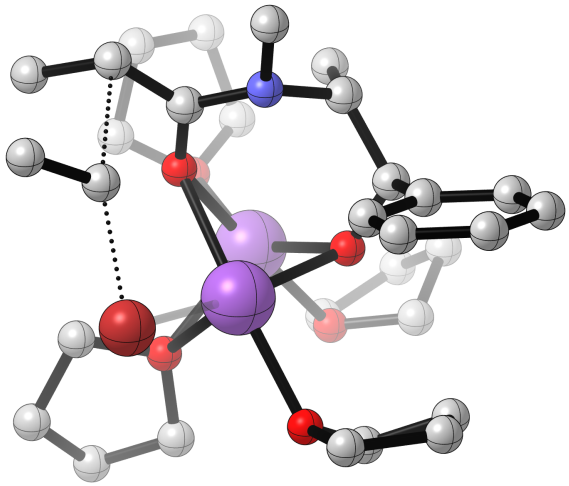
G = –4614.753942

G_{SP} = –4617.667616

Atom	X	Y	Z	Atom	X	Y	Z
Na	0.00000000	0.00000000	0.00000000	C	-2.29714900	2.02397900	3.91630500
Na	-2.63597500	0.33717600	0.65682300	C	-1.05755100	2.69786000	3.29653800
O	-0.93261200	0.00885700	2.00926100	C	-1.48049000	2.98752300	1.84235100
C	-0.63221500	-1.18714200	2.58425900	H	-0.81614700	2.52881400	1.10252100
C	-1.68427600	-2.34321700	2.46220200	H	-1.54179600	4.06905300	1.65010000
N	-1.69863900	-3.21685700	1.26902900	H	-0.21337400	2.00759900	3.31924400
C	-1.89213800	-2.74837300	-0.03256500	H	-0.79543800	3.62434000	3.81635000
O	-1.56487200	-1.53488200	-0.28907000	H	-2.14576200	0.94331000	3.90430900
C	-2.53076200	-3.55311700	-0.99053300	H	-2.50779900	2.36194700	4.93420400
C	-2.41283400	-3.26405300	-2.46169400	H	-3.83291600	3.38412900	3.16110000
H	-1.57310500	-3.78899600	-2.94183900	H	-4.22712400	1.66463800	2.88548700
H	-3.31657400	-3.56784000	-3.00644900	Br	-5.30065700	0.09877300	-0.05215100
H	-2.26784300	-2.19363900	-2.64379400	O	1.21665900	1.91233300	-0.17122300
H	-2.83947100	-4.55816900	-0.73161200	C	1.18557800	2.54740100	-1.45169900
C	-2.06497100	-4.59312300	1.54944800	C	2.45265600	3.39180300	-1.50435100
H	-1.68344200	-4.87482200	2.53478600	C	2.55430300	3.85572700	-0.04850500
H	-3.15380100	-4.76332900	1.54518600	C	2.10850400	2.60427900	0.70856200
H	-1.61622100	-5.25920900	0.80812400	H	1.58066700	2.82237100	1.64284500
C	-3.08358900	-1.84674800	2.83681900	H	2.95758800	1.94409100	0.93140400
H	-3.77677600	-2.68987900	2.93990800	H	1.85408000	4.67821600	0.13231600
H	-3.05431400	-1.31117500	3.79210100	H	3.55475000	4.18517300	0.23959600
H	-3.51483700	-1.16778600	2.09652200	H	2.38550400	4.21300400	-2.22125800
H	-1.39261900	-3.03020600	3.26647500	H	3.31409500	2.76727300	-1.76721200
C	0.78550300	-1.69078900	2.24255200	H	1.12982100	1.76181800	-2.21138100
C	1.17907100	-3.03560900	2.25468900	H	0.28594800	3.17244200	-1.52310600
C	2.49559600	-3.40420700	1.98640700	O	1.36863700	-0.81335300	-1.63580300
C	3.45718300	-2.43709100	1.70130900	C	1.27622700	-2.24390900	-1.50718200

C	3.08640800	-1.09427100	1.69468800
C	1.76831800	-0.73216500	1.96760700
H	1.47193800	0.31450200	1.99655400
H	3.83234700	-0.32652000	1.49779200
H	4.48495200	-2.72586700	1.49897200
H	2.77148500	-4.45514500	1.99925400
H	0.45310200	-3.81442600	2.46339800
H	-0.60027900	-1.07243500	3.69896000
O	-1.71419700	1.34604700	-1.27771100
C	-2.53331000	2.50508100	-1.51121900
C	-3.54114000	2.11158300	-2.61154000
C	-3.07247400	0.71271900	-3.05947900
C	-1.64720000	0.64861200	-2.52565800
H	-0.95106200	1.17797100	-3.19578600
H	-1.27311700	-0.35556600	-2.31849500
H	-3.12491200	0.56446400	-4.14071600
H	-3.68620200	-0.05027000	-2.57111700
H	-3.51100400	2.82914000	-3.43576800
H	-4.55857200	2.07282100	-2.21863300
H	-3.00120900	2.77154400	-0.56170000
H	-1.88687000	3.33082500	-1.84047700
O	-2.77919400	2.41805900	1.66370300
C	-3.41163500	2.39160600	2.94060100
C	2.47801700	-2.76863000	-2.27787200
C	3.54786900	-1.73550500	-1.90983300
C	2.73960600	-0.43537300	-1.79852700
H	2.81391600	0.17118300	-2.70969100
H	3.04544600	0.17774500	-0.94211600
H	4.35162400	-1.66064200	-2.64610000
H	3.98547500	-1.98828100	-0.94007200
H	2.27413800	-2.75159000	-3.35393500
H	2.75033500	-3.78618900	-1.98847100
H	1.32788700	-2.52131400	-0.44470400
H	0.30379700	-2.54633200	-1.90062600
C	-5.49830300	-2.60897300	-1.44925200
H	-5.24652600	-3.65115600	-1.67108900
H	-5.60956000	-2.07062200	-2.39356300
H	-6.45459400	-2.59026900	-0.92230600
C	-4.41053800	-2.00219600	-0.61177900
H	-4.31851500	-2.30036400	0.42255200
H	-3.57080000	-1.50688700	-1.06476100

Table 21. Geometric coordinates and thermally corrected M062X energies for transition state **26d**

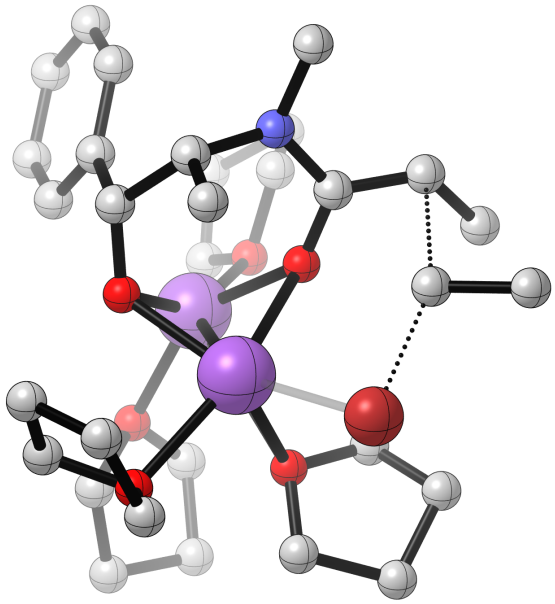


G = –4614.759838
G_{SP} = –4617.673715

Atom	X	Y	Z	Atom	X	Y	Z
Na	0.00000000	0.00000000	0.00000000	H	2.81882700	-2.71217700	2.93498000
Na	2.72451100	0.45721500	0.40386200	H	2.97854900	-3.07387200	-0.08156500
O	1.73213000	-1.09728900	-0.78230600	H	3.22346200	-4.33187100	1.16305300
C	2.11333200	-1.25509700	-2.08149900	H	5.30127800	-2.82856700	-0.07636800
C	1.65487700	-0.11571900	-3.04195600	H	5.48933000	-3.63340600	1.48825000
N	2.24541200	1.21633300	-2.76875400	H	5.38616400	-1.60851800	2.64351500
C	1.55146900	2.16582300	-1.98907100	H	5.42034600	-0.74884600	1.08488900
O	0.97467600	1.75339300	-0.92355500	Br	4.68654400	2.31487900	1.11034200
C	1.68754000	3.53216400	-2.26554400	O	-0.88615800	-1.92568800	0.90616800
C	0.89431000	4.54200000	-1.48526700	C	-0.38058500	-3.07344900	0.21218900
H	0.73180100	4.19501400	-0.45769700	C	-1.43550700	-3.32149700	-0.85797300
H	-0.09973300	4.73691100	-1.91542400	C	-2.74307400	-3.03952100	-0.09751000
H	1.40987000	5.50994900	-1.43562500	C	-2.30063200	-2.08654300	1.03762600
H	2.07686600	3.85321200	-3.22511800	H	-2.74606500	-1.09018400	0.96945900
C	3.08282500	1.70536400	-3.85178400	H	-2.52801300	-2.51005900	2.02400600
H	3.72603900	0.88999600	-4.19139500	H	-3.51379000	-2.59604800	-0.73320100
H	3.72791700	2.51486600	-3.49815900	H	-3.15111000	-3.96480900	0.31856100
H	2.50344100	2.08269300	-4.71030200	H	-1.28632100	-2.59999300	-1.67042400
C	0.13515400	-0.06496800	-3.20178100	H	-1.39458100	-4.32790000	-1.28090200
H	-0.13712600	0.67437600	-3.96526000	H	-0.31093100	-3.92192500	0.91038300
H	-0.23791900	-1.04396700	-3.52344400	H	0.60340300	-2.79282200	-0.17499100
H	-0.37042300	0.22083600	-2.27822000	O	-2.06167700	0.90809700	-0.46526900
H	2.04437000	-0.39848300	-4.02912200	C	-2.05790200	2.33197900	-0.60524900
C	3.62636800	-1.48003100	-2.23730200	C	-2.11359600	2.56395600	-2.10960300
C	4.10925200	-2.64753700	-2.83322900	C	-2.99762400	1.40238000	-2.60447100
C	5.47646200	-2.88953500	-2.96489600	C	-2.95438600	0.38146100	-1.44611600
C	6.39901900	-1.95692900	-2.49873200	H	-3.94687000	0.24098600	-0.99640100

C	5.93859200	-0.78634800	-1.89766200
C	4.57139600	-0.55650200	-1.76944200
H	4.24946100	0.38058300	-1.32536800
H	6.64221800	-0.04687400	-1.52363000
H	7.46468300	-2.14100700	-2.59768700
H	5.82023200	-3.81023800	-3.42837400
H	3.39603000	-3.38562100	-3.19510300
H	1.64641900	-2.16317800	-2.54020500
O	0.97918500	0.85542900	1.95428000
C	0.89589200	0.13888400	3.19814900
C	0.28900800	1.13504300	4.17513800
C	0.97153700	2.43231800	3.73383100
C	1.03460100	2.27700100	2.21250900
H	0.18470000	2.74078100	1.70231100
H	1.96619700	2.67276200	1.79948700
H	0.43189500	3.33310700	4.03439900
H	1.98464600	2.48391300	4.14553500
H	-0.79482000	1.19835800	4.02693300
H	0.48552700	0.87536100	5.21776900
H	1.90638900	-0.16041800	3.50201300
H	0.28721200	-0.75122400	3.01933000
O	3.55416200	-1.13573900	1.81498900
C	4.91740600	-1.53561800	1.65295800
C	4.89459300	-2.90092800	0.93530200
C	3.40056600	-3.28451900	0.90358500
C	2.77276000	-2.32170200	1.90495700
H	1.74094000	-2.05682200	1.65907900
H	-2.56697700	-0.59684600	-1.74890700
H	-4.02442500	1.73186100	-2.78379600
H	-2.61749800	0.97338000	-3.53444200
H	-2.52360400	3.54408600	-2.36523100
H	-1.09930000	2.49439000	-2.51472300
H	-1.13555100	2.70230900	-0.15543500
H	-2.93666800	2.74945500	-0.09177200
C	4.16655900	4.68070000	-0.73939600
H	3.98388200	5.23702000	0.18243800
H	5.24534200	4.59600300	-0.88511000
H	3.74549900	5.24690200	-1.57657900
C	3.52712300	3.32327100	-0.67924600
H	3.85889300	2.54651000	-1.35207800
H	2.59643100	3.17530700	-0.15653300

Table 22. Geometric coordinates and thermally corrected M062X energies for transition state **26e**

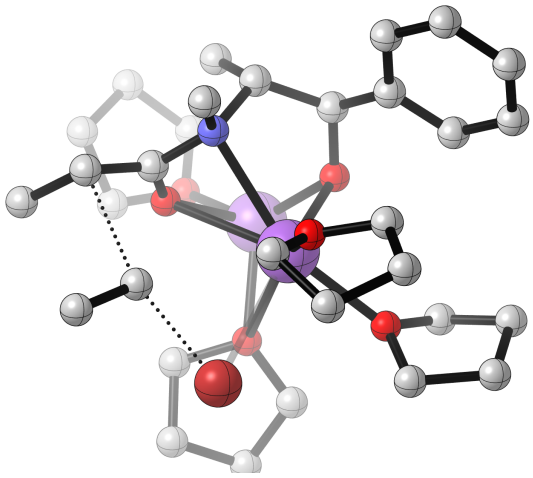


G = –4614.755276
G_{SP} = –4617.668218

Atom	X	Y	Z	Atom	X	Y	Z
Na	0.00000000	0.00000000	0.00000000	H	4.95216500	-1.06487300	-1.05616700
Na	2.70401500	0.72848900	-0.44838200	H	4.10320100	-1.21386800	-2.61277400
O	1.69759100	-0.07359500	1.38455100	H	6.83436000	-1.40721300	-2.57832600
C	2.37148300	-1.21449600	1.69974500	H	6.07732300	-0.38877700	-3.82531900
C	1.83875000	-2.57194900	1.11795600	H	7.20399800	0.49145800	-1.12389300
N	2.21047700	-2.99498400	-0.25195000	H	7.52539100	1.24177100	-2.70029200
C	1.86764700	-2.27463300	-1.39604200	H	5.40136300	2.34790300	-2.69823900
O	1.68634800	-1.01156200	-1.28270500	H	5.50137700	2.12012300	-0.93468700
C	1.63075200	-2.91336100	-2.62391100	O	-1.08562300	1.47601300	1.50175600
C	1.66529000	-2.11048300	-3.90180100	C	-2.38793400	1.05055800	1.90060500
H	2.39785600	-1.29378000	-3.85524300	C	-2.12550900	-0.05800400	2.92362300
H	1.93442000	-2.74601500	-4.75138400	C	-0.77748000	0.36292800	3.55745500
H	0.70460200	-1.63359400	-4.16357500	C	-0.34268600	1.57744700	2.72312500
H	1.74910100	-3.98509900	-2.71800400	H	0.71655700	1.53771900	2.47100700
C	2.40311300	-4.42577900	-0.40503400	H	-0.60995800	2.52514800	3.21449900
H	1.46844900	-4.96901800	-0.61946800	H	-0.02591800	-0.42331100	3.45179600
H	3.10353500	-4.62262900	-1.22095400	H	-0.87506100	0.61306500	4.61699400
H	2.82805800	-4.83490000	0.51525100	H	-2.03148300	-1.01789700	2.40500300
H	4.35213200	-3.19598700	1.27193400	H	-2.93513300	-0.14661900	3.65217500
C	4.75539500	-2.19015100	1.33120300	H	-2.91992900	1.89863800	2.35760900
C	3.89699100	-1.09584100	1.50371400	H	-2.92592800	0.71656800	1.01101900
C	4.47621400	0.17705400	1.56994800	Br	-2.37216200	-1.14788900	-1.01767900
C	5.85379600	0.35820100	1.44804600	O	0.19188300	1.69968600	-1.60182900
C	6.69039200	-0.74104500	1.27202200	C	-1.09897300	2.34647900	-1.57631200

C	6.13227000	-2.01710800	1.21869800
H	6.77347800	-2.88415600	1.08443900
H	7.76544500	-0.60762600	1.18749700
H	6.27449000	1.35912400	1.51192500
H	3.82051000	1.02771100	1.74616700
C	0.34202900	-2.74189200	1.39403000
H	0.02860000	-3.77288800	1.18873300
H	0.12311000	-2.52588000	2.44557700
H	-0.29460300	-2.09340700	0.78730400
H	2.33144800	-3.32083100	1.74943600
H	2.26961800	-1.42513200	2.79456200
O	2.81800000	2.99141200	-0.27902600
C	2.95025300	3.69580100	-1.51899900
C	1.74495200	4.62760800	-1.61270600
C	1.44152100	4.90110800	-0.13675800
C	1.74923100	3.54979700	0.50260600
H	0.88117100	2.88120800	0.45718000
H	2.09069900	3.62016900	1.53882200
H	0.41193400	5.22071100	0.04316600
H	2.11548500	5.67195700	0.25200200
H	0.90692900	4.10732200	-2.08481100
H	1.96218400	5.53183300	-2.18593000
H	3.89256400	4.25871100	-1.50113800
H	2.99770000	2.96161300	-2.33076700
O	4.38731700	0.71767300	-1.97317500
C	5.51262800	1.60308300	-1.90201600
C	6.76699200	0.73952800	-2.09510400
C	6.20669000	-0.52891400	-2.74673000
C	4.85230200	-0.64053200	-2.06369300
C	-1.68325600	2.21608100	-2.99030200
C	-0.84044500	1.09556500	-3.60898600
C	0.51025700	1.34737700	-2.95700900
H	1.02384200	2.19219300	-3.44296400
H	1.17296300	0.48072500	-2.91481300
H	-0.80154700	1.13221200	-4.70043400
H	-1.23313200	0.12457300	-3.29095100
H	-1.54698600	3.14707400	-3.55140500
H	-2.74966700	1.98083300	-2.96597000
H	-1.71178500	1.84008300	-0.82740700
H	-0.96828700	3.38988800	-1.26334100
C	-0.71038200	-2.44233800	-2.06399100
C	-1.46210900	-3.11318800	-3.17688800
H	-2.29627200	-3.70149800	-2.78912900
H	-0.78491800	-3.78138800	-3.71821300
H	-1.85439000	-2.37568800	-3.88117100
H	-0.51253700	-2.98801500	-1.15351400
H	-0.15768300	-1.53712300	-2.24506700

Table 23. Geometric coordinates and thermally corrected M062X energies for transition state **26f**

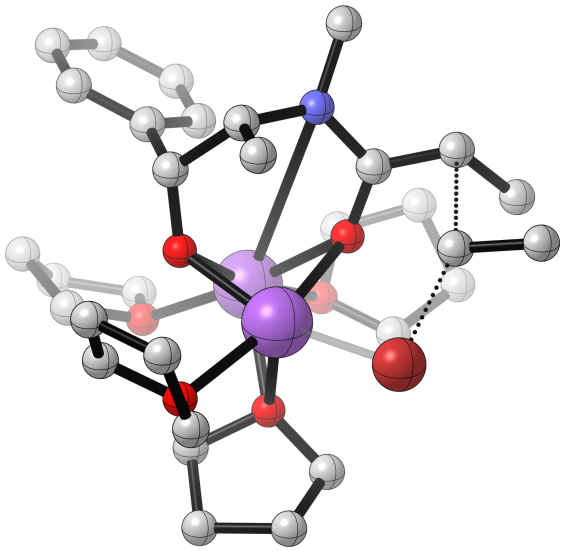


G = –4614.749488
G_{SP} = –4617.662506

Atom	X	Y	Z	Atom	X	Y	Z
Na	0.00000000	0.00000000	0.00000000	H	6.66415100	-2.25417600	4.57679300
Na	2.49239900	-0.72602800	1.48177600	H	5.75829300	-2.91151000	3.19574600
O	1.90372300	1.01215900	0.18859600	H	3.96590900	-1.92902800	4.42832400
C	2.07996300	2.18131100	0.87857000	H	4.95307500	-0.50448200	4.88990900
C	1.27797300	2.24688300	2.21619800	Br	2.58701600	-3.48681800	2.46078400
N	1.42746800	1.03939300	3.08028400	O	3.80691900	-1.58496500	-0.16977200
C	0.27476600	0.21465500	3.24996600	C	4.84888900	-2.54731000	-0.06575700
O	-0.26707800	-0.21507000	2.18096000	C	5.97453300	-2.05056500	-1.00023400
C	-0.09017000	-0.25109400	4.51473600	C	5.31647800	-0.89951700	-1.79507500
C	-1.36501700	-1.02722000	4.68769300	C	3.83003200	-1.10256500	-1.50576700
H	-1.60775300	-1.57141400	3.76797500	H	3.20518600	-0.20665400	-1.52832500
H	-2.22702400	-0.38365300	4.91414500	H	3.41223500	-1.86792500	-2.17938700
H	-1.29611600	-1.75718200	5.50533900	H	5.63943500	0.06680200	-1.39927200
H	0.32826500	0.21823900	5.39897700	H	5.54719600	-0.92994400	-2.86248200
C	2.23780800	1.31522400	4.25915300	H	6.84085700	-1.69596100	-0.43530300
H	3.20211400	1.71086600	3.93056600	H	6.31675900	-2.85409200	-1.65732900
H	2.43144300	0.39305700	4.81278600	H	4.46635800	-3.52798300	-0.38546900
H	1.76399500	2.03561600	4.94649600	H	5.12630500	-2.61556600	0.98820300
C	-0.17721400	2.63912600	1.94674800	O	-2.24038900	0.43484700	-0.13669900
H	-0.76624000	2.61576600	2.87087100	C	-3.03395800	-0.16448100	0.88992100
H	-0.19587700	3.66049200	1.55220900	C	-3.35988400	0.98557500	1.83464900
H	-0.66528200	1.97973200	1.22784600	C	-3.47656300	2.19656400	0.88560800
H	1.67017600	3.07650600	2.81686900	C	-2.83160800	1.70133000	-0.42764800
C	3.57442500	2.54723000	1.03863900	H	-3.58353200	1.57476400	-1.21724100
C	4.43746900	2.12990600	0.01998000	H	-2.03917000	2.35664200	-0.79991900
C	5.77983500	2.49610200	0.00085800	H	-4.51878200	2.47921000	0.71668800
C	6.30583500	3.28633800	1.02054200	H	-2.95475800	3.06863000	1.28686000

C	5.46228400	3.72212600	2.03810700
C	4.11270800	3.36792300	2.03731500
H	3.48546900	3.75714000	2.83375400
H	5.84998900	4.35182100	2.83436900
H	7.35376700	3.57166200	1.01434600
H	6.42061600	2.17097900	-0.81576300
H	4.01293000	1.51512700	-0.76552900
H	1.68003800	3.05313500	0.30699800
O	0.35664100	-2.24591800	-0.19778700
C	1.14380600	-3.15725800	-0.98245800
C	0.38992800	-4.48448400	-0.96813600
C	-0.29890800	-4.43841800	0.39776200
C	-0.67514100	-2.96545900	0.49758600
H	-1.63500500	-2.76742600	-0.00173700
H	-0.72003700	-2.57498900	1.51734700
H	-1.16950000	-5.09514500	0.46668900
H	0.41388200	-4.69039200	1.18674000
H	-0.35320700	-4.51706800	-1.77269200
H	1.06259600	-5.33794700	-1.08203600
H	2.12785300	-3.24747700	-0.51211100
H	1.25502500	-2.73427800	-1.98562100
O	4.35639500	-0.61687400	2.90890800
C	4.76446000	-1.25789500	4.10850300
C	6.03999700	-1.99209400	3.71932300
C	6.70909900	-0.98734500	2.76522000
C	5.53610900	-0.10810200	2.27432200
H	5.66947500	0.94682100	2.54513800
H	5.36837500	-0.16314400	1.19617000
H	7.44852700	-0.37971500	3.29428100
H	7.22422500	-1.48696500	1.94022500
H	-4.27091300	0.80759100	2.41079000
H	-2.52168700	1.10624200	2.52561400
H	-2.43124700	-0.93942600	1.36339800
H	-3.93879900	-0.59887100	0.43913500
C	1.31384800	-2.93463400	5.15511200
H	0.79616300	-3.88170400	4.99039200
H	2.32720600	-3.15555400	5.49981700
H	0.79270000	-2.38577300	5.94523700
C	1.33891200	-2.11642000	3.89453200
H	2.07024900	-1.33039300	3.79332000
H	0.51040700	-2.12611900	3.20405600

Table 24. Geometric coordinates and thermally corrected M062X energies for transition state **26g**



G = –4614.755466

G_{SP} = –4617.669147

Atom	X	Y	Z	Atom	X	Y	Z
Na	0.00000000	0.00000000	0.00000000	C	6.46986900	-1.66370700	1.48027000
Na	2.67808900	0.53006400	0.79385000	C	5.53753200	-0.51368100	1.85183900
O	1.89617000	-0.71513000	-0.85348400	H	5.76285800	0.37298000	1.24415500
C	2.31253300	-0.37816200	-2.10773400	H	5.56670900	-0.23309300	2.90823800
C	1.54165600	0.77471000	-2.84018800	H	7.47687500	-1.31886800	1.23278400
N	1.74820000	2.17668600	-2.41396300	H	6.54005500	-2.38327900	2.30368900
C	1.24691000	2.71831000	-1.22028700	H	5.87331100	-1.66283800	-0.60118900
O	1.25808400	1.97697800	-0.17193100	H	6.02364900	-3.30378000	0.06924300
C	0.68155500	4.00478900	-1.21101200	H	4.00533200	-3.02020200	1.40284700
C	0.57018200	4.81327300	0.05204000	H	3.54497700	-2.07240100	-0.05299000
H	0.61231000	4.15320600	0.92563700	O	3.62086900	2.04626400	2.23963500
H	1.37446800	5.55623800	0.16219900	C	2.51046900	2.77717300	2.79766600
H	-0.37381400	5.37276100	0.10612600	C	2.87276400	4.25708600	2.66652700
H	0.61191300	4.55568800	-2.14251100	C	3.78571900	4.24015700	1.43846100
C	2.01933200	3.08262500	-3.51668900	C	4.57309500	2.96386000	1.69532000
H	1.12868100	3.31506300	-4.12384400	H	5.38087100	3.12736000	2.42276100
H	2.42298500	4.02014200	-3.13075000	H	5.00004900	2.51519400	0.79409600
H	2.77223400	2.63237300	-4.16981500	H	4.41991300	5.12541000	1.34991500
C	0.06102700	0.42708000	-3.03973000	H	3.18941600	4.12719000	0.52469400
H	-0.42682400	1.17975800	-3.67059500	H	3.43071300	4.59726500	3.54603000
H	-0.03109500	-0.54288800	-3.54062100	H	1.99381600	4.89324000	2.54621500
H	-0.51844000	0.36195500	-2.11506700	H	1.61825800	2.53331900	2.20820500
H	1.97937700	0.75199600	-3.84607900	H	2.36867100	2.45276800	3.83306800
C	3.81851600	-0.09747600	-2.19625800	O	-0.83362500	-2.19604100	0.04629100
C	4.64342500	-0.91376600	-2.97355000	C	-2.18506800	-2.55711000	-0.22148600

C	6.01588600	-0.68428700	-3.06998900
C	6.59472600	0.37373000	-2.37607100
C	5.78664200	1.20077500	-1.59557600
C	4.41542200	0.96902300	-1.50867800
H	3.78436800	1.65988900	-0.95139500
H	6.23018600	2.04608200	-1.07396000
H	7.66213800	0.56015000	-2.44751400
H	6.63248700	-1.33517300	-3.68367200
H	4.19662300	-1.74512200	-3.51501900
H	2.14558000	-1.22277300	-2.82160500
O	0.91916400	-0.24433200	2.11744800
C	1.20040500	-1.64029200	2.34407500
C	-0.04546300	-2.22638100	3.03821300
C	-1.01197700	-1.03260200	3.13561100
C	-0.06700800	0.16044000	3.06739400
H	0.41379400	0.35899900	4.03662800
H	-0.52951300	1.07915800	2.69378500
H	-1.61810500	-1.04065800	4.04445100
H	-1.68052700	-1.00595300	2.26923600
H	0.21205100	-2.60267800	4.03235400
H	-0.47768100	-3.04382200	2.45817400
H	1.40647800	-2.07591200	1.36225500
H	2.10180500	-1.71423800	2.96279600
O	4.21674500	-0.96656700	1.53720800
C	4.27684700	-2.17396400	0.75484700
C	5.72465200	-2.27674200	0.29277100
C	-2.21944200	-2.70186000	-1.73989900
C	-0.83445100	-3.31164000	-2.04889000
C	-0.03657400	-3.08668800	-0.74586800
H	0.92926200	-2.59511600	-0.88923000
H	0.08285000	-4.03089400	-0.19275300
H	-0.35693600	-2.81490100	-2.89692600
H	-0.90569000	-4.37671100	-2.28529000
H	-2.31404200	-1.70539400	-2.18420200
H	-3.05140800	-3.31687700	-2.09100700
H	-2.41206700	-3.51252600	0.27841700
H	-2.83529600	-1.77271300	0.16759500
Br	-2.64308000	0.96668200	-0.00518500
C	-1.42222400	2.81385600	-0.80627600
C	-2.45799600	3.89521600	-0.88753700
H	-2.01128900	4.79071800	-1.33283900
H	-2.83622800	4.15267200	0.10391900
H	-3.29798000	3.58438300	-1.51213300
H	-1.15556300	2.28605200	-1.70639200
H	-0.77176700	2.71949400	0.04489000

Figure 70. Computational overview for transition state of tetrasolvated monomers with pseudo-diequatorial substituents

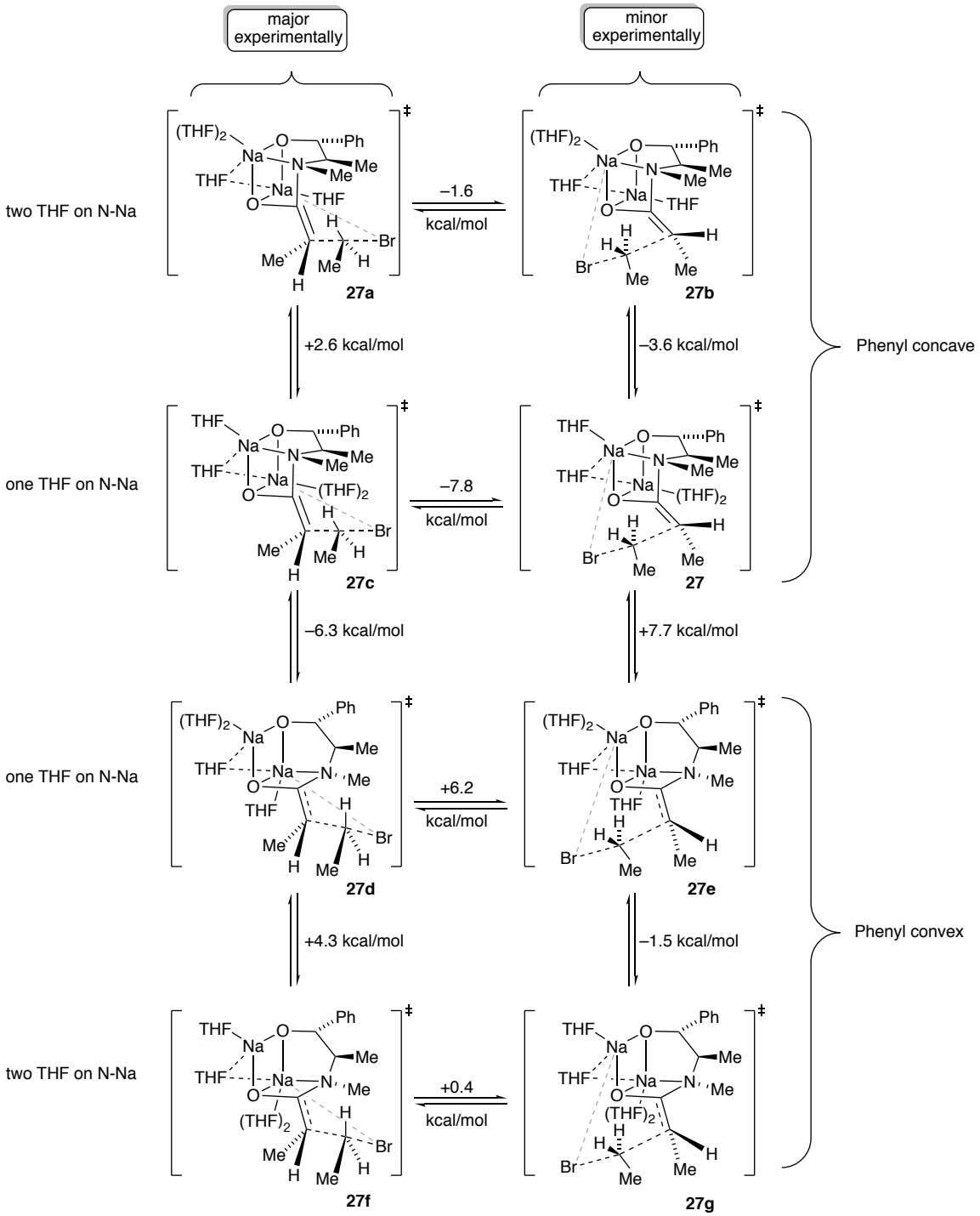
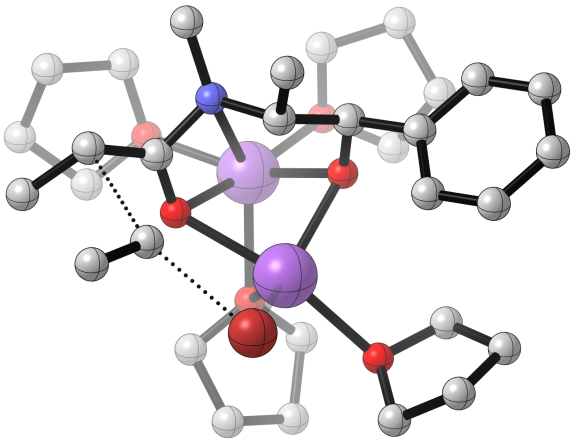


Table 25. Geometric coordinates and thermally corrected M062X energies for transition state **27a**



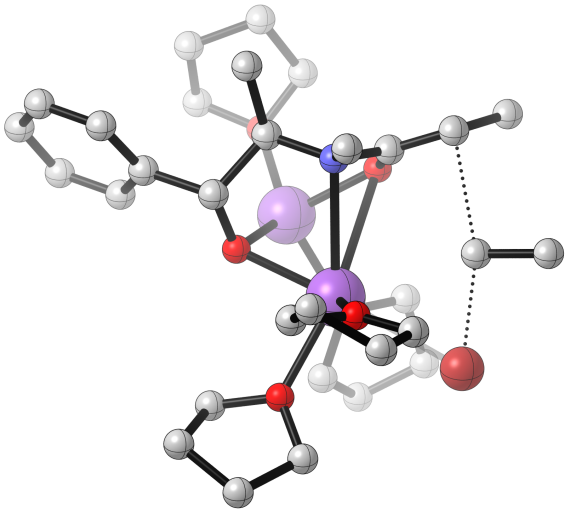
G = –4614.755996

G_{SP} = –4617.669169

Atom	X	Y	Z	Atom	X	Y	Z
Na	0.00000000	0.00000000	0.00000000	C	-4.56353600	-0.57067700	1.24184600
Na	-2.11678600	-1.92398300	-0.17196600	H	-4.02803400	0.05092100	0.51527900
O	-2.04984000	0.24071500	-0.77496200	H	-4.48692400	-0.11567900	2.23998100
C	-2.24426800	0.43945500	-2.11725600	H	-6.36552200	-0.24018900	0.03372800
C	-1.60465600	-0.70776800	-2.94417700	H	-6.68871200	-0.65121600	1.72689900
N	-0.12094600	-0.73726100	-2.79383800	H	-5.80258700	-2.52596900	-0.51292200
C	0.39958500	-1.91110000	-2.17903000	H	-6.98857100	-2.84420800	0.77255500
O	0.05148200	-2.10329200	-0.96549500	H	-5.17196300	-2.97904400	2.44324900
C	1.11821800	-2.85746600	-2.91964500	H	-4.44510700	-3.79869300	1.01997600
C	1.99307900	-3.88403500	-2.25364700	Br	-3.12996000	-4.21198800	-1.49612800
H	1.67377400	-4.03836400	-1.21711300	C	-0.96814400	-4.08943600	-2.69396700
H	3.05323600	-3.58893000	-2.23469500	C	-0.80889000	-5.41751400	-3.35833800
H	1.95288900	-4.85508100	-2.76359900	H	0.07868700	-5.39270400	-4.00255500
H	1.31535700	-2.64187800	-3.96697100	H	-0.67686000	-6.21252000	-2.62223100
C	0.63688700	-0.15465000	-3.88790700	H	-1.67265500	-5.65054000	-3.98454300
H	0.52687500	-0.66952900	-4.85300800	H	-1.40399200	-3.28202300	-3.25643800
H	1.69841100	-0.15673500	-3.62805400	H	-0.58354200	-3.90669200	-1.70735700
H	0.32021800	0.88563800	-4.02512200	O	-0.10327900	2.24124700	0.62725200
H	-1.98002700	-1.62245800	-2.47335700	C	-1.41763600	2.56706600	1.10916500
C	-2.03382400	-0.76713700	-4.41359800	C	-2.13225000	3.29824200	-0.02551000
H	-1.49800900	-1.55955600	-4.94891000	C	-0.96804600	3.88515500	-0.82910800
H	-3.10221800	-0.98285200	-4.47814200	C	0.09726800	2.80419400	-0.67155800
H	-1.85462700	0.18018500	-4.93449000	H	-0.02924100	2.02183600	-1.43653000
C	-3.73156600	0.55835400	-2.45265100	H	1.12165000	3.18670400	-0.71885600
C	-4.27666800	1.75614100	-2.91189600	H	-1.21878900	4.07105300	-1.87703000
C	-5.63828900	1.86947200	-3.19479800	H	-0.62059000	4.82405600	-0.38429800
C	-6.47445800	0.76976500	-3.03695400	H	-2.68111900	2.56187700	-0.61776600
C	-5.94010800	-0.43890500	-2.58659800	H	-2.82407900	4.06094700	0.34065400

C	-4.58671700	-0.53820600	-2.28189100
H	-4.18544400	-1.49476500	-1.94438000
H	-6.58214800	-1.30939500	-2.47293000
H	-7.53271100	0.84753800	-3.26813400
H	-6.04167000	2.81484300	-3.54689400
H	-3.62094300	2.61465100	-3.04969200
H	-1.77352600	1.38432600	-2.49060200
O	-0.73532100	-1.46269100	1.73336900
C	-1.42584200	-1.00340200	2.90118600
C	-1.94163600	-2.26266500	3.62916000
C	-1.39060500	-3.42629900	2.78306200
C	-0.23647200	-2.76894500	2.03272700
H	0.65821200	-2.68358700	2.66811100
H	0.03263000	-3.23646200	1.08279300
H	-1.07092700	-4.27994700	3.38525100
H	-2.14288400	-3.77451800	2.06673800
H	-1.55359800	-2.30202400	4.65060700
H	-3.03208100	-2.27836600	3.67369000
H	-2.22464700	-0.34322700	2.55987500
H	-0.72586700	-0.43243100	3.52460500
O	-3.89404100	-1.84560000	1.26408500
C	-4.88179700	-2.86686800	1.38593900
C	-6.03943900	-2.35420900	0.54227400
C	-6.03428000	-0.85411000	0.87355500
H	-1.29937200	3.19027100	2.00396800
H	-1.93598400	1.63835100	1.36473400
O	2.28217100	-0.05347400	0.07442200
C	2.85326700	-1.31532600	0.45686300
C	4.15739400	-1.43650600	-0.32770700
C	3.82319900	-0.65538500	-1.60143000
C	2.99554100	0.49508100	-1.03661500
H	3.63481200	1.31558500	-0.68407600
H	2.26434400	0.89902700	-1.74504000
H	4.70367100	-0.31334700	-2.15038200
H	3.20317300	-1.27001400	-2.26422500
H	4.97971000	-0.95288600	0.21037700
H	4.43097200	-2.47710200	-0.51793200
H	2.14352700	-2.10526300	0.18433200
H	2.99931000	-1.31008800	1.54127200

Table 26. Geometric coordinates and thermally corrected M062X energies for transition state **27b**

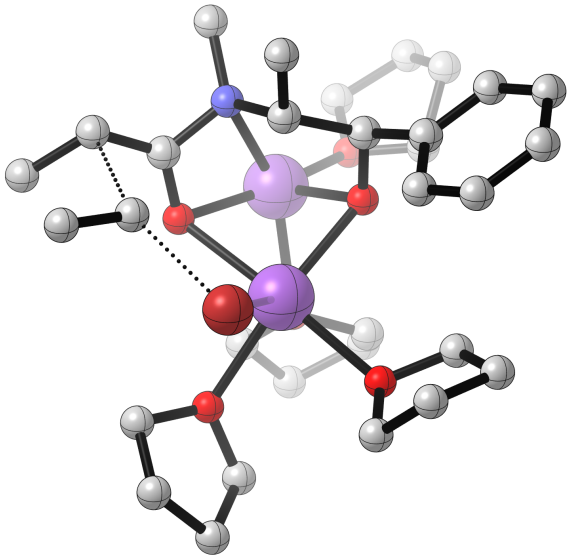


G = –4614.758215
G_{SP} = –4617.671703

Atom	X	Y	Z	Atom	X	Y	Z
Na	0.00000000	0.00000000	0.00000000	O	-4.52110400	-2.26918800	0.92818500
Na	-2.50169200	-1.21538000	0.89068100	C	-4.69008400	-3.18379300	-0.16524100
O	-2.01116300	0.84949200	0.24252700	C	-5.72262100	-2.52361100	-1.10238400
C	-2.79339500	1.20196600	-0.81719000	C	-6.32494900	-1.38305000	-0.24976100
C	-2.96810100	-0.01518900	-1.78821000	C	-5.80920400	-1.70056800	1.15167100
N	-1.64055400	-0.50902200	-2.22086000	H	-6.44723500	-2.43988800	1.65876900
C	-1.38955900	-1.89071400	-2.00299200	H	-5.69195300	-0.82283600	1.78938300
O	-1.69435400	-2.33618800	-0.84431800	H	-7.41571200	-1.34486300	-0.29395900
C	-0.68183900	-2.64071000	-2.94316500	H	-5.93550400	-0.40830300	-0.56305900
C	-0.56229300	-4.12928400	-2.77129200	H	-6.48241500	-3.24526600	-1.41283100
H	-0.58839100	-4.39199500	-1.70850700	H	-5.24675900	-2.13478200	-2.00636100
H	-1.38404500	-4.67564000	-3.25485600	H	-3.70630800	-3.33568400	-0.61373700
H	0.36978700	-4.52246400	-3.19782100	H	-5.07170800	-4.13298100	0.23409100
H	-0.54469100	-2.24266600	-3.94366100	O	1.24709100	1.21584100	-1.56332900
C	-1.11831800	0.10868100	-3.42341200	C	2.44526700	1.06942700	-2.33524500
H	-1.28015700	1.19016100	-3.36395800	C	2.72843100	2.44622100	-2.94185900
H	-0.04043100	-0.06528200	-3.48824700	C	1.33088500	3.07345900	-2.97714200
H	-1.58163600	-0.25965900	-4.35182300	C	0.75893500	2.55301200	-1.66521900
H	-3.40560100	-0.81994000	-1.18598000	H	-0.33248800	2.51419100	-1.60675800
C	-3.90123500	0.17555400	-2.98837700	H	1.13112000	3.14324900	-0.81596000
H	-3.63633900	1.05005100	-3.59322000	H	0.75616100	2.68012400	-3.82340200
H	-3.85475500	-0.70766400	-3.63637400	H	1.34249300	4.16422400	-3.03635800
H	-4.93604900	0.30126900	-2.65995900	H	3.20579000	2.37944600	-3.92189600
H	-2.34912700	2.01832700	-1.43940400	H	3.38152500	3.02765000	-2.28155500
C	-4.16155000	1.73916900	-0.36604000	H	3.23753200	0.69204500	-1.68298700
C	-5.01714700	2.45293800	-1.21432500	H	2.25752000	0.32183700	-3.11891600

C	-6.26725900	2.88491300	-0.78189500
C	-6.68402500	2.63068000	0.52423600
C	-5.82413700	1.96848900	1.39435500
C	-4.57343300	1.53752900	0.95234500
H	-3.87369400	1.06384000	1.63511900
H	-6.12177800	1.79805500	2.42644600
H	-7.65795000	2.96951800	0.86452300
H	-6.91500200	3.43075700	-1.46227300
H	-4.69847300	2.67723700	-2.22975000
O	-0.50100300	-1.49991400	1.94395800
C	0.06806800	-0.84845600	3.09332500
C	0.38705200	-1.97230100	4.06933600
C	0.83567700	-3.07474700	3.10728700
C	-0.12656500	-2.89581800	1.93691500
H	-1.04128900	-3.49054400	2.05606700
H	0.32523000	-3.13202600	0.97356200
H	0.78605300	-4.07788400	3.53684200
H	1.85655000	-2.88029500	2.76437100
H	-0.51239600	-2.27639800	4.61676400
H	1.15599300	-1.68887600	4.79186800
H	0.97548500	-0.31817600	2.78299900
H	-0.66419000	-0.12260400	3.45831600
Br	2.51753900	-1.34518900	0.24703000
O	0.75887400	1.65208900	1.34892400
C	2.08472500	2.14533700	1.47973800
C	1.95332800	3.66465900	1.74716200
C	0.42992000	3.89753300	1.83247800
C	-0.10482700	2.49359000	2.10291100
H	-1.11737600	2.29120000	1.74395500
H	-0.01634800	2.24851800	3.17514100
H	0.03430700	4.26147500	0.87957300
H	0.15382100	4.61373500	2.60997400
H	2.41509300	4.26073800	0.95511200
H	2.44464000	3.93355100	2.68615900
H	2.58776700	1.63377200	2.31257400
H	2.61317900	1.89541200	0.55521800
C	2.36285100	-2.69483100	-2.44233100
H	2.76145800	-3.57812400	-1.93928400
H	3.18693800	-1.99878000	-2.61663100
H	1.95356600	-2.99879800	-3.41031100
C	1.28846200	-2.04608600	-1.61326700
H	0.98483300	-1.03946700	-1.86251700
H	0.62601200	-2.63243600	-0.99472400

Table 27. Geometric coordinates and thermally corrected M062X energies for transition state **27c**



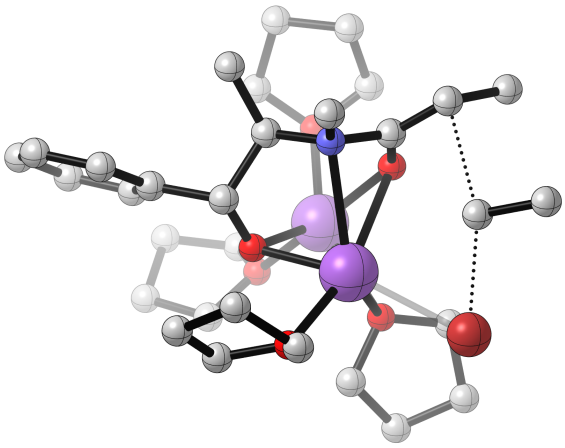
G = –4614.752361

G_{SP} = –4617.665085

Atom	X	Y	Z	Atom	X	Y	Z
Na	0.00000000	0.00000000	0.00000000	H	-6.00060000	-2.75875100	0.62930800
Na	-2.57211100	-0.80544000	1.03398400	H	-7.72267300	-0.58718100	1.08034000
O	-2.09911000	0.97666000	-0.13595800	H	-7.48519700	-1.30138400	-0.52211300
C	-2.40167700	2.06778700	0.64381200	H	-5.96854300	1.09079000	0.64460500
C	-1.60714900	2.01085000	1.97820000	H	-6.77362100	0.99482000	-0.93678700
N	-2.04952800	0.85746200	2.82054300	H	-5.13913400	-0.66255000	-1.72707800
C	-0.99818600	-0.07497600	3.14187500	H	-4.07782000	0.45061200	-0.79000500
O	-0.63186400	-0.82373700	2.17626400	O	0.49180200	0.46488000	-2.21212200
C	-0.35559700	-0.04717800	4.37938100	C	1.80947700	0.88073100	-2.56013300
C	0.45078800	-1.22445800	4.85699100	C	1.68061600	2.37913600	-2.78793800
H	0.90008500	-1.74787200	4.00646100	C	0.33059800	2.46395500	-3.51120700
H	-0.16305800	-1.95433900	5.40269600	C	-0.45897600	1.27806600	-2.92759400
H	1.25644600	-0.92062500	5.53581900	H	-1.22730800	1.56576300	-2.20322500
H	-0.72701100	0.64596300	5.13025300	H	-0.91549000	0.67078600	-3.72080100
C	-2.98405000	1.17854800	3.88918300	H	-0.18191500	3.41329300	-3.34169600
H	-2.58712000	1.84839500	4.66473100	H	0.47450000	2.33743600	-4.58945700
H	-3.29722900	0.24994400	4.37461700	H	1.64088400	2.87670500	-1.81323800
H	-3.86931500	1.65663500	3.45519100	H	2.50952700	2.79792900	-3.36423200
H	-0.58623100	1.78100500	1.65642900	H	2.13616100	0.36265600	-3.47766100
C	-1.55688100	3.31857100	2.77236900	H	2.46995700	0.61164300	-1.73136300
H	-1.05243900	3.17562100	3.73548300	Br	2.27055000	1.67297000	0.91170100
H	-1.00408500	4.07422900	2.21018900	O	1.61999700	-1.67926400	-0.21245900
H	-2.55827900	3.71895500	2.96833300	C	1.99643700	-2.26360000	-1.45271200
C	-2.10954800	3.37235200	-0.09213800	C	3.52500400	-2.06700800	-1.58136600
C	-3.12584000	4.25189700	-0.45743800	C	3.93907600	-1.51867600	-0.19915300

C	-2.84462100	5.42614900	-1.15751100
C	-1.53128400	5.74140200	-1.48877900
C	-0.50310300	4.87098600	-1.12126300
C	-0.79192200	3.69175400	-0.44372600
H	0.02013200	3.02749800	-0.14835900
H	0.52958000	5.11036300	-1.36495900
H	-1.30637700	6.65915900	-2.02418800
H	-3.65274400	6.09620700	-1.43793800
H	-4.15402800	4.01236200	-0.19135300
H	-3.48448800	2.10422600	0.93018200
O	-1.35264400	-1.86036100	-0.62909200
C	-1.20139500	-3.26065700	-0.35697700
C	-1.75312500	-3.99126400	-1.58715900
C	-2.69334100	-2.94302500	-2.19582400
C	-1.89766500	-1.67150400	-1.94113000
H	-1.07406300	-1.56327300	-2.66043200
H	-2.46855000	-0.73952300	-1.91351900
H	-2.90483100	-3.11422400	-3.25389700
H	-3.63782000	-2.90194000	-1.64041900
H	-0.94400100	-4.21683400	-2.29071500
H	-2.24971000	-4.92890400	-1.32725300
H	-1.78068300	-3.49498300	0.54546300
H	-0.14797200	-3.46495000	-0.14993900
O	-4.64232800	-1.25440000	0.20077100
C	-4.95322000	-0.20806900	-0.74219400
C	-6.22085500	0.42398700	-0.18742100
C	-6.97730500	-0.80978600	0.31367200
C	-5.84424400	-1.69694900	0.84629600
H	-5.71117400	-1.57822800	1.92806300
C	2.72457300	-1.83538400	0.66845600
H	2.75005200	-2.86782000	1.05049400
H	2.59049200	-1.13919000	1.49764400
H	4.86017200	-1.96761300	0.17993800
H	4.06317500	-0.43216200	-0.22584800
H	4.01847400	-3.01739400	-1.80142200
H	3.77862200	-1.36894900	-2.38280800
H	1.41053600	-1.76909000	-2.23145900
H	1.74486500	-3.33559300	-1.44344300
C	1.40622600	1.01760900	3.11524800
C	2.58999500	1.09868100	4.02591900
H	2.25277100	1.03208500	5.06671300
H	3.29241700	0.28375100	3.83797800
H	3.10936000	2.05106900	3.90044100
H	0.75539800	1.87260800	3.05075900
H	1.15352300	0.10382500	2.60676700

Table 28. Geometric coordinates and thermally corrected M062X energies for transition state **27**

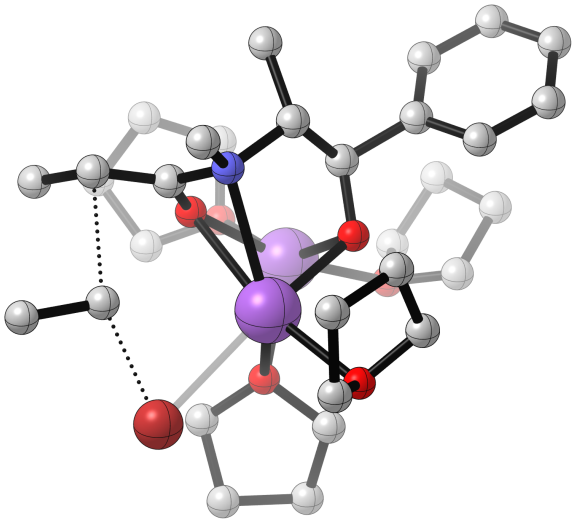


G = –4614.76212
G_{SP} = –4617.677526

Atom	X	Y	Z	Atom	X	Y	Z
Na	0.00000000	0.00000000	0.00000000	O	-1.49848200	0.21982900	1.70657900
Na	2.13995800	1.84261300	-0.71513000	C	-1.74586600	1.54572300	2.19550100
O	-0.04457300	2.13158400	-0.56307100	C	-3.28139400	1.69696600	2.28765200
C	-0.41316300	2.55433200	-1.81083400	C	-3.81662300	0.35568200	1.75406800
C	-0.22786000	1.39499400	-2.84279300	C	-2.63655900	-0.57872800	2.00063300
N	1.22252600	1.18530600	-3.10528100	H	-2.59874200	-1.45304800	1.34696900
C	1.72722700	-0.11083600	-2.79141500	H	-2.60666400	-0.90530600	3.05138500
O	1.40952300	-0.56214300	-1.64337200	H	-4.01715100	0.41478100	0.67852700
C	2.68099100	-0.71978000	-3.60807200	H	-4.73057700	0.03020600	2.25672400
C	3.11025200	-2.12916600	-3.30960400	H	-3.63884100	2.54828400	1.70385400
H	3.17574600	-2.29256600	-2.22758500	H	-3.59144100	1.84668100	3.32567400
H	2.40578400	-2.87765400	-3.70024600	H	-1.27984600	1.65478900	3.18378100
H	4.08946600	-2.35555000	-3.74843000	H	-1.27297200	2.22810600	1.48142400
H	2.82912400	-0.35270200	-4.61859000	O	-1.39942200	-1.62483800	-0.88721300
C	1.72611500	1.85586900	-4.29241900	C	-0.77686500	-2.69757600	-1.59665400
H	1.36114700	2.88733000	-4.29494800	C	-1.03598500	-2.37950900	-3.06251800
H	2.81867800	1.88379800	-4.27399300	C	-2.45515400	-1.78648500	-3.02499500
H	1.42075700	1.37805900	-5.23493700	C	-2.60387100	-1.27603900	-1.57442300
H	-0.57055900	0.49740600	-2.31735500	H	-3.45990700	-1.74371700	-1.06925200
C	-1.03990700	1.48758700	-4.13772700	H	-2.71569400	-0.18879900	-1.51412700
H	-0.85818200	2.41360200	-4.69358300	H	-3.20379300	-2.55530400	-3.23588800
H	-0.80694400	0.64093300	-4.79483900	H	-2.58662200	-0.98457800	-3.75475100
H	-2.10775100	1.45971300	-3.90342700	H	-0.96342100	-3.26120700	-3.70401400
H	0.23302400	3.38629000	-2.19340600	H	-0.30336700	-1.64124100	-3.40354400
C	-1.84318400	3.08778600	-1.84772000	H	0.28221500	-2.69379800	-1.33538500
C	-2.23260200	4.12024800	-2.70255300	H	-1.24373000	-3.64992800	-1.30311200
C	-3.55575600	4.55575100	-2.74543900	C	5.56580500	-0.01560100	-2.76986800
C	-4.51471900	3.95736600	-1.93176100	H	6.07776400	-0.68883700	-2.07937300

C	-4.13596500	2.93118900	-1.06757600
C	-2.80916800	2.51155200	-1.02111400
H	-2.48639700	1.73327500	-0.33397700
H	-4.87755100	2.46498300	-0.42144900
H	-5.54652400	4.29425200	-1.96377500
H	-3.83855700	5.36572100	-3.41192500
H	-1.48686400	4.58764400	-3.34506000
O	1.94670500	0.54353400	1.20623500
C	1.97555900	1.60419900	2.17997500
C	2.65315000	0.99738100	3.40129100
C	3.68491900	0.07708600	2.74280500
C	2.91513700	-0.46756100	1.54295900
H	2.37091000	-1.38920600	1.78254900
H	3.55376500	-0.63871400	0.67304500
H	4.04721000	-0.71568100	3.40121500
H	4.53624800	0.66338600	2.38448400
H	1.93180300	0.41631000	3.98728300
H	3.10156900	1.75424500	4.04886800
H	2.55790400	2.44552500	1.77855400
H	0.94602200	1.93127200	2.34075300
O	2.37742400	4.09309300	-0.35723600
C	3.25203400	4.89381700	-1.14068500
C	2.31091400	5.61665800	-2.10035000
C	1.09454800	5.91548100	-1.20079500
C	1.24368200	4.90744400	-0.03739500
H	0.40097200	4.22267100	0.07914100
H	1.44192300	5.42951000	0.90885900
H	0.14737600	5.78168300	-1.72947900
H	1.12712500	6.94374600	-0.82978700
H	2.02928700	4.93652600	-2.91182400
H	2.75230200	6.51443900	-2.53971800
H	3.78440800	5.60673700	-0.49238200
H	3.98457100	4.22985300	-1.60436200
Br	4.98326800	1.71278700	-0.34448900
H	6.21963900	0.83519400	-2.97115500
H	5.38830700	-0.54956500	-3.70817300
C	4.25854700	0.44503300	-2.18878000
H	3.78482300	1.32028200	-2.60514300
H	3.68161900	-0.19683900	-1.53867800

Table 29. Geometric coordinates and thermally corrected M062X energies for transition state **27d**



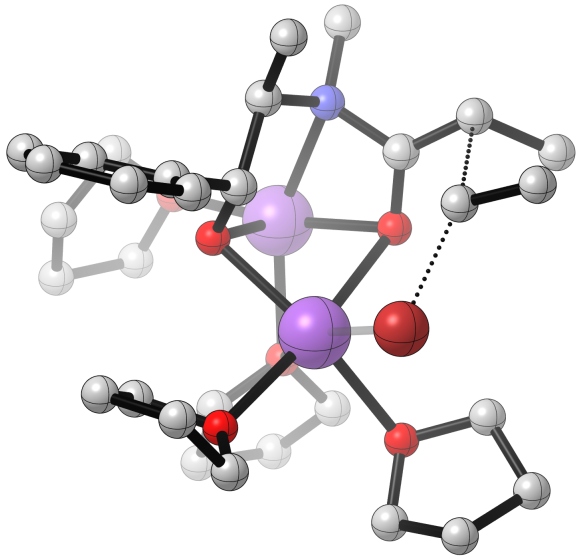
G = – 4614.761279

G_{SP} = –4617.675114

Atom	X	Y	Z	Atom	X	Y	Z
Na	0.00000000	0.00000000	0.00000000	H	0.92936300	-5.71222300	0.70442400
Na	1.97742100	-2.01017200	-0.65556800	H	0.67982800	-4.40067400	-2.01187900
O	-0.20820900	-2.13317400	-0.69403000	H	0.69688400	-6.13677700	-1.64441500
C	-0.95254100	-1.71256000	-1.75317700	H	2.99419200	-4.36053800	-2.30297300
C	-0.27403800	-1.94286800	-3.14372300	H	3.06214000	-6.11409900	-2.08601500
N	1.19715400	-1.69795200	-3.16231200	H	3.37807900	-5.89118900	0.30900900
C	1.58381600	-0.32743300	-2.98517000	H	4.19313300	-4.38104200	-0.21153300
O	1.16551900	0.23428300	-1.92168500	Br	4.81301500	-1.70549100	-0.24606900
C	2.53679700	0.25452900	-3.82197500	O	-1.57996900	-0.20658100	1.64694700
C	2.88504000	1.70752900	-3.66548300	C	-2.18746700	-1.51204700	1.73350100
H	2.83430000	2.00392400	-2.61090600	C	-3.67083200	-1.33213000	1.34660300
H	2.20501500	2.37188700	-4.21834200	C	-3.74922300	0.13809100	0.90860800
H	3.89721800	1.92313600	-4.02920900	C	-2.62124000	0.76242000	1.71909100
H	2.77572200	-0.21262000	-4.77108800	H	-2.22458300	1.69944100	1.32145500
C	1.82116500	-2.41941100	-4.26680400	H	-2.92397400	0.91014200	2.76739700
H	1.53587900	-3.47358900	-4.19681400	H	-3.52346700	0.22501300	-0.16042700
H	2.91047700	-2.35574700	-4.20085900	H	-4.72406500	0.59465400	1.09749500
H	1.52945100	-2.04831300	-5.26047800	H	-3.97281600	-2.01964600	0.55242100
C	-0.97143500	-1.14479100	-4.24900300	H	-4.31784800	-1.50374300	2.21251000
H	-0.47929000	-1.27242100	-5.21784200	H	-2.08312900	-1.88002100	2.76248200
H	-2.01216300	-1.45808900	-4.36118600	H	-1.63171900	-2.15331500	1.04332700
H	-0.95680500	-0.07540700	-4.00249800	O	-0.45023800	2.25291600	-0.27071300
H	-0.37892900	-3.01488700	-3.35759600	C	0.77924000	2.97126900	-0.48214200
C	-2.34177600	-2.36740000	-1.77786600	C	0.54884900	3.84449000	-1.71322000
C	-3.48354300	-1.67601200	-2.18847700	C	-0.44665100	2.99810000	-2.50989700
C	-4.73904500	-2.28120200	-2.17202600	C	-1.31999100	2.43324200	-1.39683300

C	-4.86899900	-3.59886000	-1.74076500
C	-3.73664700	-4.30052400	-1.32762200
C	-2.48781200	-3.68656300	-1.34264500
H	-1.60292600	-4.21289600	-0.99539000
H	-3.83188400	-5.32676600	-0.98338700
H	-5.84525500	-4.07413800	-1.71970200
H	-5.61541800	-1.72117200	-2.48608400
H	-3.38820200	-0.64195400	-2.51878900
H	-1.17150400	-0.61414400	-1.74282200
O	1.84134900	-0.51779100	1.22914400
C	1.63665100	-1.43635500	2.32738700
C	2.36446800	-0.81582600	3.51613800
C	3.51037000	-0.07083000	2.82653100
C	2.81960600	0.47350900	1.58445800
H	2.30073900	1.41928000	1.79128900
H	3.49739900	0.59869400	0.73655600
H	3.95227100	0.71728400	3.44051800
H	4.29381200	-0.77063400	2.51969300
H	1.71025000	-0.11156200	4.04192600
H	2.70639700	-1.57029700	4.22816300
H	2.06788400	-2.40487200	2.04868000
H	0.55835100	-1.54408000	2.47420600
O	2.25609600	-4.15791500	0.40008100
C	3.26007100	-4.94363600	-0.23755300
C	2.69705600	-5.18466100	-1.64244200
C	1.16418900	-5.17665800	-1.41102600
C	1.02754500	-4.81380800	0.07791100
H	0.21833400	-4.10736600	0.27100500
H	-2.12367800	3.12755300	-1.11503500
H	-1.76350800	1.46344900	-1.64978400
H	-1.01899000	3.57193600	-3.24270300
H	0.07878400	2.17843100	-3.00784800
H	0.09902500	4.80209000	-1.42826000
H	1.47491900	4.04337600	-2.25771700
H	1.57332300	2.23941200	-0.66821400
H	0.99960900	3.54345600	0.42393500
C	5.40348400	-0.23185200	-2.82459400
H	5.23904500	0.17856800	-3.82532000
H	5.87584400	0.53605000	-2.20851500
H	6.08720100	-1.07900100	-2.90412400
C	4.09469000	-0.66420400	-2.22364100
H	3.66088400	-1.59794200	-2.54291200
H	3.48047500	0.02727300	-1.66199400

Table 30. Geometric coordinates and thermally corrected M062X energies for transition state **27e**

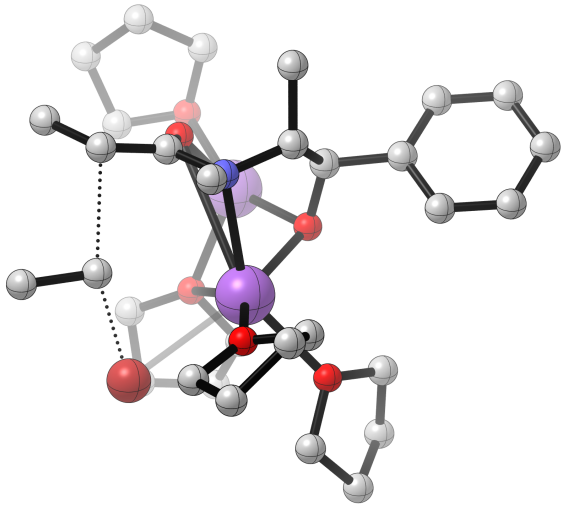


G = –4614.753785
G_{SP} = –4617.665296

Atom	X	Y	Z	Atom	X	Y	Z
Na	0.00000000	0.00000000	0.00000000	H	4.31644000	0.83196100	2.03487900
Na	2.12039800	-0.80288900	2.00577000	H	5.96280600	0.11929200	2.14222300
O	1.98732500	0.88061900	0.66286500	H	4.09441500	0.28384200	-0.26215300
C	1.36863900	1.99303900	1.16983900	H	5.80782800	0.78557700	-0.24196700
C	1.62747700	2.20093200	2.69335700	H	5.19270600	-1.75544000	-1.12231100
N	1.27112100	0.99147800	3.48969300	H	6.60035200	-1.49187700	-0.08917200
C	-0.02754300	0.36248900	3.30190200	H	5.55613900	-2.85668100	1.50521900
O	-0.10242200	-0.49565600	2.36187800	H	3.98028600	-2.75902700	0.68171200
C	-1.11568700	0.69747000	4.10938400	O	0.33159600	0.52594100	-2.30139200
C	-2.22895400	-0.28826700	4.36152400	C	-0.55343600	1.19679300	-3.19555300
H	-2.48855800	-0.84487200	3.45374600	C	-0.08021100	2.64173200	-3.16559600
H	-1.95351000	-1.02926100	5.12464600	C	1.44743200	2.48081800	-3.11707100
H	-3.13746600	0.21115400	4.71552100	C	1.64695300	1.08060800	-2.49999800
H	-0.96183400	1.46026400	4.86857000	H	2.12407800	1.10392700	-1.51533600
C	1.66796200	1.11060400	4.88876600	H	2.20788700	0.42112800	-3.17833000
H	1.52896500	0.14729900	5.38737900	H	1.92142100	3.26012100	-2.51510300
H	2.73259400	1.36992100	4.92554500	H	1.87278100	2.52141600	-4.12474400
H	1.11681800	1.86833700	5.46251800	H	-0.44957600	3.10531600	-2.24606800
H	2.71990700	2.29728200	2.79907800	H	-0.42664200	3.22413800	-4.02313600
C	0.98640600	3.47653100	3.25250600	H	-0.46245900	0.76022400	-4.20320400
H	1.29569100	3.66052000	4.28543500	H	-1.57103600	1.06228000	-2.82314400
H	1.28065600	4.34654800	2.66177400	Br	-2.32128700	1.78443400	-0.25056800
H	-0.10741000	3.41304000	3.24477500	O	-1.34707300	-1.83016700	-0.43130300
H	0.26043800	1.95610800	1.07282100	C	-2.14709400	-1.83200000	-1.61298000
C	1.76467400	3.25569400	0.40585400	C	-3.57537600	-1.45165300	-1.17505300

C	0.80380100	4.15899800	-0.05090200
C	1.18027600	5.30668900	-0.74852400
C	2.52657200	5.56002700	-0.99837100
C	3.49257300	4.65234600	-0.56086700
C	3.11090800	3.50520200	0.12843300
H	3.85095900	2.77559700	0.45097600
H	4.54314800	4.83979300	-0.76620300
H	2.82290400	6.45190700	-1.54278900
H	0.41975400	5.99423300	-1.10823200
H	-0.24935200	3.93237400	0.11357600
O	1.58888200	-2.22136700	0.30000800
C	1.05896000	-3.52945100	0.55232000
C	0.93245200	-4.20048600	-0.81311200
C	2.05951000	-3.52105100	-1.59770800
C	1.94740000	-2.09119500	-1.08395200
H	1.15809100	-1.54866100	-1.61879400
H	2.87080300	-1.50609200	-1.13442800
H	1.93778400	-3.58788900	-2.68125000
H	3.03055100	-3.95462400	-1.32844300
H	-0.03591500	-3.94918800	-1.25707600
H	1.02924400	-5.28711700	-0.75772700
H	1.76682800	-4.06958500	1.19692000
H	0.10786100	-3.42189400	1.07817900
O	4.37956500	-1.21195400	1.95607200
C	4.84995100	-2.18067500	1.01002700
C	5.51147100	-1.39555200	-0.14019700
C	5.08932800	0.05421000	0.13676400
C	4.98053500	0.05253200	1.65279800
C	-3.53105300	-1.56161800	0.36465900
C	-2.19765400	-2.26098500	0.63029000
H	-2.30907800	-3.35699600	0.58021000
H	-1.70952600	-1.97784900	1.56645600
H	-4.37772900	-2.11245100	0.78138100
H	-3.51621800	-0.55605900	0.79389900
H	-4.30965000	-2.13117400	-1.61510100
H	-3.81889500	-0.43020600	-1.47354400
H	-1.69184100	-1.12788600	-2.31217300
H	-2.12427800	-2.83939800	-2.05568900
C	-3.47085200	2.04777200	2.63324200
H	-4.22882200	1.27835300	2.46929300
H	-3.77611300	2.95727200	2.11219600
H	-3.42406000	2.26903200	3.70491500
C	-2.12544500	1.59377600	2.15073700
H	-1.32512600	2.31075300	2.10078400
H	-1.90551100	0.55820900	1.95638400

Table 31. Geometric coordinates and thermally corrected M062X energies for transition state **27f**

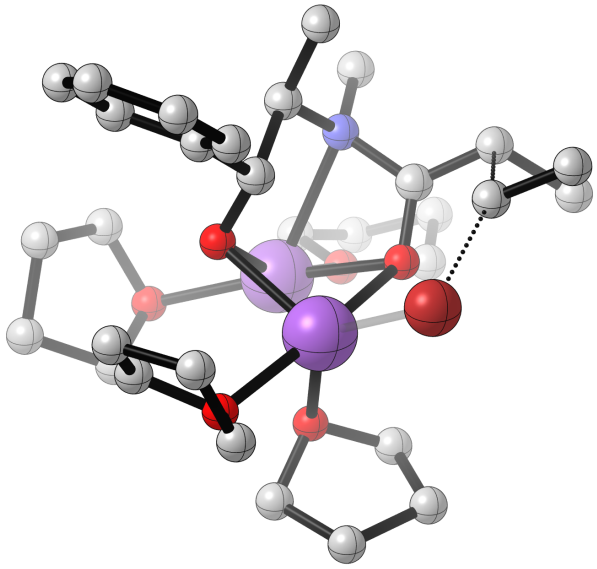


G = –4614.75558
G_{SP} = –4617.668267

Atom	X	Y	Z	Atom	X	Y	Z
Na	0.00000000	0.00000000	0.00000000	H	-5.35808600	0.26488900	-5.22849200
Na	-2.96404800	-0.61852500	-1.31908400	H	-6.94475800	0.73384200	-4.57665400
O	-1.88138500	1.01217200	-0.43379400	H	-6.57513700	-1.87469500	-5.28960400
C	-1.30680400	1.98193100	-1.20792300	H	-7.33363100	-1.52815300	-3.72685600
C	-1.45291600	1.77356300	-2.75918800	H	-5.46507700	-2.76775600	-2.87132500
N	-1.50863300	0.36399400	-3.23324300	H	-4.44549500	-2.34224500	-4.25974100
C	-0.29943000	-0.39323500	-3.14302200	Br	-3.15676000	-3.45941200	-1.16086300
O	0.42951600	-0.19682000	-2.11990200	O	-4.81945000	-0.09738300	-0.08116500
C	-0.03119100	-1.40928200	-4.05948400	C	-4.72786600	0.80340000	1.02840100
C	1.26004500	-2.16568900	-3.91868900	C	-5.27512800	0.01524700	2.21237500
H	1.36069800	-2.61859600	-2.92055500	C	-6.40333300	-0.78426000	1.54937300
H	2.14658900	-1.53011700	-4.05892300	C	-5.83419100	-1.07867100	0.15449700
H	1.32978400	-2.97381700	-4.65527400	H	-6.59338300	-1.00879800	-0.63474800
H	-0.53886100	-1.45204800	-5.01460700	H	-5.36497400	-2.06710000	0.08589400
C	-2.20911600	0.25650000	-4.51061900	H	-7.30251800	-0.16428100	1.47262700
H	-3.08825400	0.90406800	-4.49224500	H	-6.66600000	-1.69614600	2.09044800
H	-2.55525100	-0.76848200	-4.67768800	H	-5.62398300	0.65884800	3.02338900
H	-1.58131600	0.54356800	-5.36689200	H	-4.51129200	-0.65959800	2.61410800
C	-0.39311200	2.57653400	-3.51455300	H	-3.68259000	1.12101400	1.08708300
H	-0.54630100	2.53252700	-4.59792900	H	-5.35502500	1.68678300	0.83422600
H	-0.41767900	3.62785600	-3.21206900	O	2.26199600	-0.13439600	0.29736100
H	0.59829400	2.16925000	-3.28735500	C	2.60814400	-1.44165100	-0.18520100
H	-2.44479300	2.17232900	-3.01192300	C	3.81411700	-1.24202600	-1.09650400
C	-1.88956400	3.36195500	-0.88329300	C	3.52208600	0.13566200	-1.69601800
C	-1.09246600	4.48270900	-0.66032500	C	2.88762800	0.87208400	-0.51958500
C	-1.66166800	5.71968500	-0.35528600	H	3.62946800	1.39454800	0.09623800

C	-3.04377100	5.84802200	-0.27073700
C	-3.85270600	4.73174200	-0.48914100
C	-3.27769300	3.50260400	-0.78822400
H	-3.89543200	2.61900000	-0.93957600
H	-4.93366000	4.82444300	-0.41930300
H	-3.49059900	6.80891100	-0.03266300
H	-1.02326000	6.58115500	-0.17943400
H	-0.00964100	4.38425200	-0.72290800
H	-0.20630000	2.08048000	-1.03871100
O	-1.01243400	-1.81330100	0.85218200
C	-2.14360000	-1.52877200	1.68561900
C	-2.06271500	-2.54487700	2.81783800
C	-1.52714100	-3.77527100	2.07897200
C	-0.55577100	-3.15566400	1.07411500
H	0.46539500	-3.10470600	1.47052100
H	-0.54983100	-3.68706500	0.11769200
H	-1.04055900	-4.49917900	2.73653300
H	-2.33907100	-4.27117600	1.53992900
H	-1.35328500	-2.20960000	3.58234600
H	-3.03102200	-2.71868100	3.29472900
H	-3.06439700	-1.66483400	1.10366200
H	-2.07571600	-0.48252500	1.99809000
O	-4.65132500	-0.87082400	-2.83762300
C	-5.21326600	-1.96629200	-3.56990100
C	-6.42194300	-1.39656300	-4.31976800
C	-6.07520300	0.09200700	-4.41815300
C	-5.40540400	0.31833300	-3.06935700
H	-4.71468200	1.16694500	-3.03825000
H	-6.14468300	0.45129800	-2.26760300
H	2.12164500	1.58413500	-0.84593800
H	4.41463600	0.64177400	-2.07159700
H	2.78094800	0.04346000	-2.49283900
H	4.73826900	-1.22503500	-0.50843300
H	3.89438200	-2.02773200	-1.85196100
H	1.75959400	-1.84663600	-0.75276900
H	2.81330100	-2.07609300	0.68205600
C	-1.34807200	-4.12247000	-3.41839100
H	-0.60231700	-3.99008700	-4.20515500
H	-0.97594300	-4.86684100	-2.71086400
H	-2.26691100	-4.50834900	-3.86597600
C	-1.61121900	-2.81334800	-2.72056800
H	-2.28134500	-2.10008700	-3.17717600
H	-0.89940300	-2.43212900	-1.99615600

Table 32. Geometric coordinates and thermally corrected M062X energies for transition state **26g**



G = –4614.754293
G_{SP} = –4617.667687

Atom	X	Y	Z	Atom	X	Y	Z
Na	0.00000000	0.00000000	0.00000000	H	4.33305800	1.80460500	2.14525000
Na	2.42413200	-1.38459600	0.85784800	H	5.94993700	1.05991800	-0.19947700
O	2.09313700	0.33376700	-0.59676100	H	6.52445300	1.61931100	1.38003800
C	2.56636300	-0.45731200	-1.61033300	H	6.07010200	-1.23530800	0.43746300
C	1.54816900	-0.63557300	-2.76651900	H	7.32062500	-0.64164800	1.55520200
N	0.26547600	-1.19257900	-2.26329400	H	5.63748900	-0.40306400	3.34600700
C	0.27338900	-2.37786100	-1.43316800	H	5.11647000	-1.92005800	2.54089700
O	0.48267300	-2.19627700	-0.19034100	Br	4.06111500	-3.64849600	0.45788300
C	0.06683900	-3.64840200	-1.98409300	O	-0.27016200	2.23902800	0.40079000
C	-0.57512000	-4.75475100	-1.18447200	C	0.76079800	2.52435500	1.35986600
H	-0.50840800	-4.53250500	-0.11393100	C	1.46461200	3.76629400	0.83218700
H	-1.63934700	-4.86846900	-1.43432300	C	1.44176300	3.48112700	-0.67081900
H	-0.10967800	-5.73386200	-1.35391200	C	0.06064700	2.85552700	-0.85560500
H	-0.02602700	-3.71196300	-3.06604100	H	0.06032800	2.08657600	-1.63864500
C	-0.79486400	-1.16861800	-3.25924300	H	-0.71250300	3.60095400	-1.08026000
H	-1.74547800	-1.41780300	-2.77695200	H	2.19318000	2.72059500	-0.90008200
H	-0.86948200	-0.15044800	-3.65992900	H	1.59148100	4.36750100	-1.29225200
H	-0.65654200	-1.85468900	-4.10760500	H	2.47607000	3.87284800	1.23244700
H	1.30309500	0.37887900	-3.11870700	H	0.89171900	4.66814700	1.07562900
C	2.11277200	-1.44196700	-3.94110900	H	0.28161200	2.65187200	2.33452100
H	1.38318900	-1.54102800	-4.75056400	H	1.46068800	1.67877900	1.39558700
H	3.00149500	-0.95594500	-4.35123800	O	-2.23237500	-0.42553500	-0.08555900
H	2.39634200	-2.45332700	-3.62672700	C	-2.87626400	-1.70581300	-0.12089800
H	2.78340000	-1.50023200	-1.28550800	C	-4.18966700	-1.49172000	-0.87428900

C	3.91493800	0.02315400	-2.14371200
C	5.02827900	-0.81826100	-2.10136400
C	6.27116700	-0.38214800	-2.56159900
C	6.41300600	0.90617900	-3.06915400
C	5.30681000	1.75672100	-3.10970400
C	4.07009200	1.31787500	-2.64710300
H	3.20831200	1.98052000	-2.67799500
H	5.41282400	2.76363400	-3.50410000
H	7.37849400	1.25067900	-3.42783500
H	7.12863400	-1.04761400	-2.51064100
H	4.91766100	-1.81293000	-1.66958300
O	0.64991500	-0.67834100	2.32558700
C	1.31793000	-0.24874000	3.51437600
C	1.80184400	-1.54813000	4.17343200
C	0.81952400	-2.61819000	3.63148500
C	-0.12807800	-1.80903800	2.73600500
H	-1.00112600	-1.44843900	3.29903900
H	-0.44854900	-2.32712200	1.83193800
H	0.28182900	-3.13941000	4.42682600
H	1.35184700	-3.36931100	3.03928100
H	1.79252600	-1.47779800	5.26357200
H	2.82705900	-1.76600100	3.85823800
H	2.13105600	0.41808100	3.22493300
H	0.60020000	0.28670200	4.15255000
O	4.08659600	-0.24430400	1.97922400
C	5.30642600	-0.85387200	2.39695000
C	6.27222800	-0.54482800	1.26200200
C	5.87863200	0.89240800	0.87821500
C	4.42387300	1.02097200	1.37855400
H	3.69664600	1.18261300	0.57687100
C	-4.49254300	-0.02096200	-0.57461900
C	-3.09351500	0.58384300	-0.61922600
H	-2.97085200	1.48685100	-0.01628400
H	-2.79415000	0.80533100	-1.65434800
H	-4.91860800	0.08532900	0.42874300
H	-5.17564600	0.43809300	-1.29277100
H	-4.97482300	-2.17607400	-0.54540400
H	-4.04210500	-1.63306000	-1.95078600
H	-2.20478500	-2.42352100	-0.60255400
H	-3.05563300	-2.03052500	0.91166700
C	2.58246600	-5.52297300	-1.62515200
H	2.44242800	-6.25580000	-0.82851300
H	3.61397400	-5.57869300	-1.97923700
H	1.92354200	-5.78586400	-2.46115000
C	2.25864500	-4.14056100	-1.15563700
H	2.61838400	-3.30167300	-1.72453900
H	1.62493000	-3.95166000	-0.30905500

Figure 71. Computation overview for resting state of trisolvated monomers.

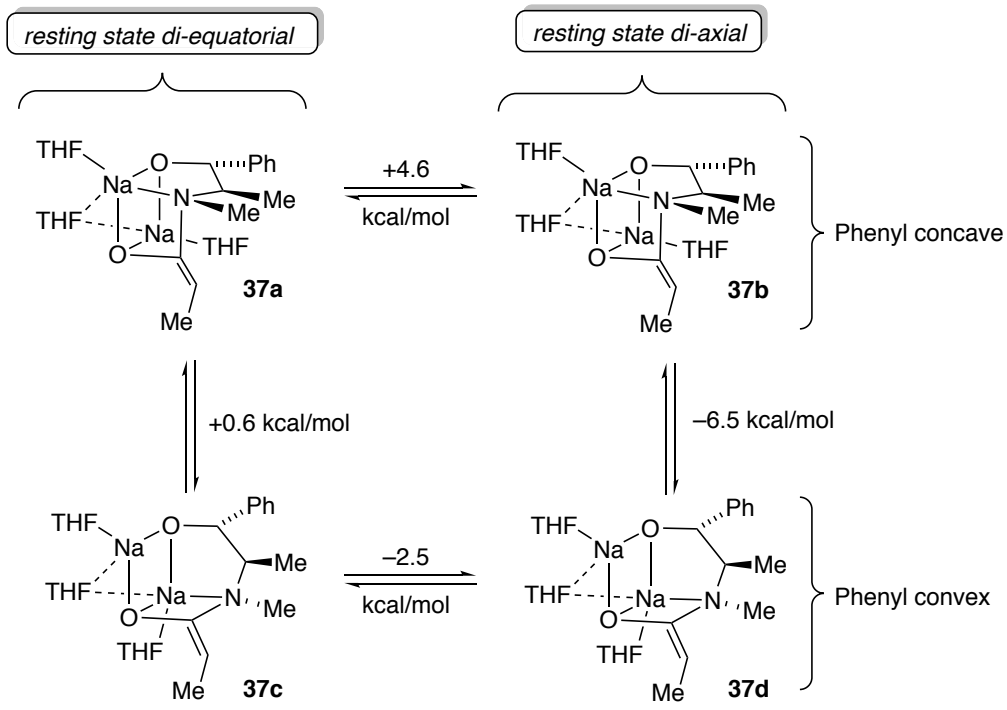
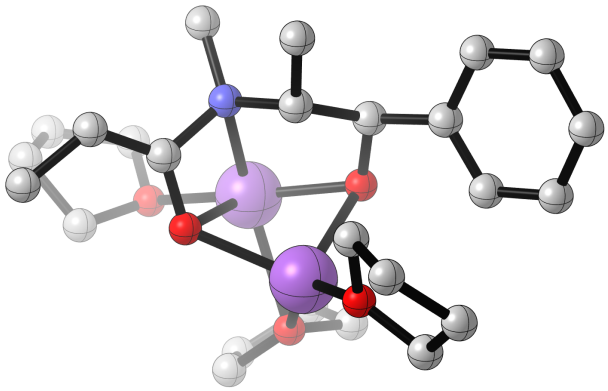


Table 33. Geometric coordinates and thermally corrected M062X energies for resting state **37a**

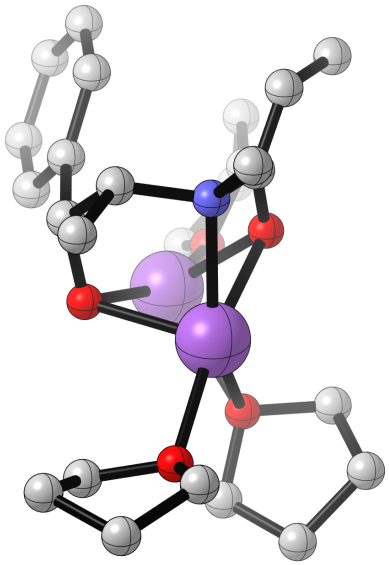


G = –1731.610654
G_{SP} = –1732.054009

Atom	X	Y	Z	Atom	X	Y	Z
Na	0.00000000	0.00000000	0.00000000	H	-4.60332800	-2.57032200	-2.08616300
O	-0.51469200	-0.88236300	2.05863900	H	-2.63627500	-1.57400700	1.10506500
C	-0.33713000	-2.07282700	1.54600600	C	-3.09769000	-3.34518200	0.05210600
N	-0.88795500	-2.20423300	0.20762600	H	-2.98721500	-3.82617600	-0.92619400
C	-2.35756000	-2.00789900	0.13921300	H	-2.69849000	-4.02626400	0.81267000
C	-2.69355800	-0.90152100	-0.92268500	H	-4.16642200	-3.21592500	0.23880900
O	-2.07189100	0.27225500	-0.58222000	C	-0.37296600	-3.27038300	-0.62905800
Na	-2.12194000	0.57228400	1.64718200	H	-0.73735100	-3.13212300	-1.65335800
O	-4.19599600	0.28897800	2.57691500	H	0.72038500	-3.21519500	-0.63302500
C	-4.76568300	-1.02889000	2.58825400	H	-0.65327800	-4.28431000	-0.30335000
C	-6.03269000	-0.88620400	3.41647800	C	0.36415000	-3.09140700	2.11028000
C	-6.54010300	0.47494800	2.93133500	C	1.03821300	-2.94785100	3.44347000
C	-5.23855300	1.26194200	2.73916300	H	0.81568600	-1.96212700	3.86243600
H	-4.99429300	1.87137300	3.61617400	H	0.69385300	-3.69997700	4.16527200
H	-5.26881600	1.90709400	1.85434100	H	2.13337100	-3.05389400	3.38483600
H	-7.22103500	0.96366700	3.63168700	H	0.42168500	-4.05153400	1.60803500
H	-7.04921700	0.35498400	1.96998200	O	2.25168400	-0.04050700	0.16917600
H	-5.78741100	-0.85537100	4.48333200	C	2.69111900	-0.51906200	1.45857100
H	-6.74362600	-1.69636200	3.24102200	C	3.49427200	-1.77245500	1.14908100
H	-4.99908400	-1.33117000	1.55804700	C	4.18313900	-1.38043600	-0.16047800
H	-4.02040400	-1.70858100	3.00958900	C	3.09150700	-0.57262000	-0.86642700
O	-0.49867100	2.14018000	1.07946500	H	2.47744600	-1.21019800	-1.51457100
C	0.71799200	2.54795200	1.71116900	H	3.48552200	0.25733500	-1.46249500
C	1.62457200	3.09758800	0.58699700	H	4.51135900	-2.23580000	-0.75514800
C	0.72850000	3.04720300	-0.66851000	H	5.05443000	-0.74859300	0.04224500
C	-0.67895700	2.95404400	-0.08421000	H	2.79830200	-2.60597600	1.00136100
H	-1.41129500	2.43729500	-0.71054300	H	4.19507300	-2.03174400	1.94588400
H	-1.04901900	3.94555800	0.21552600	H	3.31841300	0.25711000	1.92178600
H	0.94697200	2.14938000	-1.25897500	H	1.79838600	-0.69681300	2.06570100

H	0.85861700	3.91288900	-1.32191400	C	-6.42006400	-1.48391800	-1.73974100
H	2.51945000	2.48508800	0.46083400	C	-6.99983900	-0.32190500	-1.23306000
H	1.93374200	4.12202400	0.80953900	C	-6.18127000	0.65729900	-0.67587300
H	0.49544900	3.31994600	2.45873100	C	-4.80313800	0.46046800	-0.59820800
H	1.11854500	1.66623000	2.21825300	H	-4.14497300	1.23082400	-0.20866400
H	-2.34616200	-1.30614600	-1.90229300	H	-6.61717800	1.58778400	-0.31723500
C	-4.21239700	-0.71680100	-1.06205700	H	-8.07348500	-0.17088200	-1.29864300
C	-5.04265500	-1.66958100	-1.66398600	H	-7.04218900	-2.24241600	-2.20688200

Table 34. Geometric coordinates and thermally corrected M062X energies for resting state **37b**

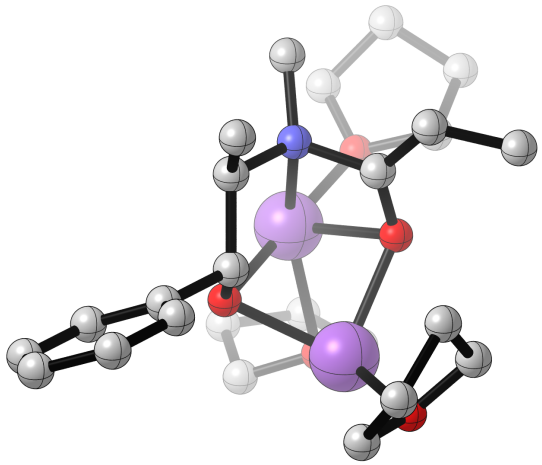


G = –1731.605385
G_{SP} = –1732.046667

Atom	X	Y	Z	Atom	X	Y	Z
Na	0.00000000	0.00000000	0.00000000	H	-3.58429700	-3.30704500	-0.13650800
O	-2.07292400	-0.04460600	0.92238800	H	-6.00017900	-3.15961600	-0.50250200
C	-2.04140800	-1.29374200	1.29137200	H	-6.92497200	-1.68707200	-2.28013600
N	-0.82578700	-2.01741500	0.85856000	H	-5.36204900	-0.36702900	-3.70236000
C	-0.92378700	-2.76927700	-0.41552100	H	-2.91225800	-0.53115600	-3.32420900
C	-1.51434500	-1.98086000	-1.63162000	H	-1.30205800	-2.68301600	-2.47198300
O	-0.91631100	-0.76440800	-1.85209900	H	-1.53363200	-3.67921700	-0.25748900
Na	-2.40835900	0.72105600	-1.12620800	C	0.48437400	-3.22797800	-0.82034200
O	-4.39034700	1.79063500	-0.90301900	H	0.89850200	-3.97536000	-0.13920100
C	-5.00529600	0.96689500	0.11616800	H	0.46499000	-3.66539800	-1.82298500
C	-6.51374900	1.16854800	-0.03396400	H	1.15961000	-2.36281100	-0.84089300
C	-6.60104000	2.53058500	-0.72834500	C	-0.24942100	-2.84120700	1.91879800
C	-5.39688500	2.45606200	-1.65917300	H	0.82161600	-2.99498500	1.75161700
H	-5.63684500	1.86961200	-2.55724300	H	-0.72209300	-3.83578900	1.99684100
H	-5.00503600	3.43036400	-1.96338400	H	-0.38433400	-2.32908600	2.87270500
H	-7.54102600	2.68930900	-1.26208900	C	-2.95111700	-1.94016500	2.05687000
H	-6.46669600	3.34246500	-0.00551200	C	-4.17660200	-1.27197300	2.60260100
H	-6.93271500	0.39008300	-0.67925600	H	-4.42017900	-1.62623100	3.61149000
H	-7.03091400	1.13453700	0.92758400	H	-5.07137900	-1.44464000	1.98123900
H	-4.62594700	1.30849300	1.08263100	H	-4.01615600	-0.19031100	2.65261900
H	-4.69422000	-0.07408400	-0.02534400	H	-2.80455000	-2.99646900	2.26704500
O	-0.74957800	2.24244400	-0.47873000	O	2.11047200	0.34660800	-0.78085600
C	0.25244000	3.00655800	-1.14798700	C	2.13703600	0.03950200	-2.19591600
C	1.26248300	3.42099800	-0.05731900	C	3.29398400	-0.93885300	-2.37442000

C	0.53885300	3.06845700	1.26375500	C	-5.85223700	-1.74125700	-2.11554900
C	-0.90358800	2.83011300	0.81728300	C	-5.33174600	-2.57001400	-1.12410700
H	-1.47265100	2.11896800	1.42031500	C	-3.95463500	-2.65929700	-0.92102200
H	-1.45245100	3.77818400	0.72094000	C	4.25910500	-0.49318800	-1.27216700
H	0.94817900	2.14686900	1.69365900	C	3.29228000	-0.14967500	-0.14286000
H	0.62234100	3.85237600	2.01966200	H	3.03455900	-1.04395700	0.44149100
H	2.19508700	2.86297700	-0.16117200	H	3.66771700	0.61985900	0.53911000
H	1.48901000	4.48809100	-0.12065700	H	4.98110100	-1.26052600	-0.98398100
H	-0.21774600	3.88409900	-1.61165200	H	4.80892000	0.40080300	-1.58554900
H	0.67722100	2.37208600	-1.92805600	H	2.95793900	-1.96554800	-2.19644400
C	-3.06064500	-1.90681600	-1.69169900	H	3.72824400	-0.88766200	-3.37542900
C	-3.60334700	-1.08615500	-2.69144400	H	2.33422500	0.97350500	-2.74013700
C	-4.97766200	-0.99752300	-2.90421000	H	1.14911900	-0.35664600	-2.46249400

Table 35. Geometric coordinates and thermally corrected M062X energies for resting state **37c**

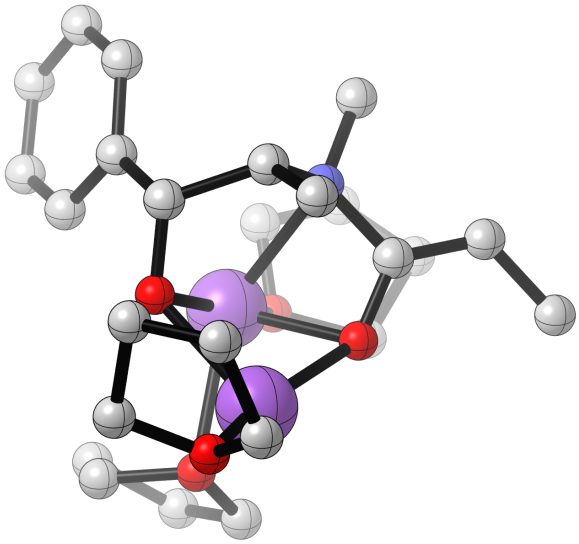


G = –1731.610394
G_{SP} = –1732.052959

Atom	X	Y	Z	Atom	X	Y	Z
Na	0.00000000	0.00000000	0.00000000	C	6.73013100	0.01683400	-0.91942300
O	0.63747300	-1.97754200	0.89956900	C	6.82815000	1.36315600	-1.26236100
C	0.89719200	-2.52980000	-0.25295100	C	5.67329000	2.14123200	-1.32275300
N	0.98463900	-1.57947700	-1.37786800	C	4.43146800	1.57800300	-1.04113500
C	2.33086400	-1.02283400	-1.67172000	H	3.52357400	2.17308300	-1.04652500
C	2.93609200	-0.35383600	-0.39753700	H	5.74388500	3.19430800	-1.58221000
O	2.11076700	0.58696600	0.16475300	H	7.79805300	1.80446100	-1.47296200
Na	1.77943700	-0.50145400	2.04954500	H	7.62463900	-0.59757400	-0.86241300
O	3.29929900	-1.80920400	3.07601200	H	5.40650600	-1.59607500	-0.38309400
C	2.95112000	-3.18668900	2.84510200	C	3.25977100	-2.05966200	-2.31007600
C	3.98826700	-3.68727200	1.85044800	H	4.18868100	-1.60034600	-2.65434300
C	5.24621000	-2.94933000	2.32102000	H	3.50185300	-2.85108500	-1.59151100
C	4.69256900	-1.59816700	2.78672300	H	2.78634700	-2.53528200	-3.17468800
H	4.76929400	-0.83636700	2.00134900	H	2.16225900	-0.20450700	-2.38992000
H	5.18790100	-1.22618200	3.68911200	C	0.27050800	-1.98906100	-2.57668700
H	6.00362600	-2.83303800	1.54217600	H	0.26505000	-1.15269900	-3.28802900
H	5.70337300	-3.48427600	3.16022500	H	0.68751300	-2.86442200	-3.09600800
H	3.69298800	-3.38510700	0.83871100	H	-0.76499300	-2.23010900	-2.31104900
H	4.09728500	-4.77437000	1.86979400	C	0.99853000	-3.86222300	-0.49101100
H	3.00766300	-3.73317900	3.79660400	C	0.76055600	-4.89082800	0.57655900
H	1.93169000	-3.20682900	2.45128900	H	0.17103900	-5.73717100	0.20211000
O	-0.04162000	0.98279000	2.19200900	H	1.68925400	-5.31674200	0.98648000
C	0.24745700	2.34312000	1.84481600	H	0.21269300	-4.43761000	1.40999800
C	-1.03770300	2.81613500	1.16316100	H	1.24626600	-4.20542700	-1.49086500
C	-2.14677600	2.03048500	1.90344600	O	-2.17115600	-0.66130400	-0.14535200
C	-1.37036800	0.97288700	2.71444900	C	-3.02062700	-0.37089500	-1.26385300
H	-1.75775600	-0.04113800	2.59832100	C	-3.81539200	-1.64904200	-1.54589300

H	-1.33853300	1.23015700	3.78124100	C	-3.79571500	-2.34600200	-0.18354600
H	-2.83141200	1.55098600	1.20065600	C	-2.38702300	-2.02082400	0.29089200
H	-2.73130600	2.67727300	2.56177800	H	-1.63806500	-2.67928600	-0.16585500
H	-1.01669500	2.55063200	0.09953900	H	-2.24810700	-2.04803100	1.37294800
H	-1.16802000	3.89870900	1.22489400	H	-3.97879200	-3.42069400	-0.24770700
H	0.44101900	2.91521200	2.76359700	H	-4.54013800	-1.90193500	0.48660200
H	1.13731100	2.32208000	1.21076200	H	-3.29474000	-2.26481400	-2.28652900
H	3.13569000	-1.22314100	0.28368400	H	-4.81981100	-1.43935100	-1.92029100
C	4.31831900	0.22765900	-0.70955100	H	-3.67791700	0.46263800	-0.98691500
C	5.48375900	-0.54088900	-0.64515000	H	-2.40310000	-0.06205100	-2.11509700

Table 36. Geometric coordinates and thermally corrected M062X energies for resting state **37d**



G = –1731.614388

G_{SP} = –1732.056957

Atom	X	Y	Z	Atom	X	Y	Z
Na	0.00000000	0.00000000	0.00000000	H	0.92229000	-3.28253600	2.35464000
Na	2.60213400	-0.94046000	-0.15047800	H	-0.04056500	-2.81277000	0.92783000
O	0.93189400	-1.42962000	-1.43054600	O	4.82676200	-0.64434100	0.12225000
C	0.37415100	-0.91681200	-2.49309100	C	5.01009300	0.64218100	0.72374200
N	0.10385300	0.51713300	-2.38945300	C	5.26763900	1.57042500	-0.45754100
C	1.28864900	1.43030600	-2.30814700	C	6.01907000	0.67161200	-1.46236200
C	1.53548200	2.03828600	-0.88537000	C	5.80475900	-0.75413200	-0.91192700
O	1.94264800	1.13190900	0.04930400	H	5.42289300	-1.46099700	-1.65274900
C	0.27401200	2.81159400	-0.43086600	H	6.73189500	-1.15900200	-0.48591300
C	-0.21754100	2.61620700	0.86276500	H	5.61244000	0.77781500	-2.47076900
C	-1.37940400	3.24752800	1.30970000	H	7.08465500	0.91034200	-1.50587900
C	-2.06818100	4.11317300	0.46767500	H	4.29844300	1.87881500	-0.85702100
C	-1.56358600	4.36167200	-0.80934000	H	5.83447200	2.46083700	-0.17634500
C	-0.40505300	3.72678600	-1.24584200	H	5.86507600	0.59662200	1.41387400
H	-0.02416900	3.95318400	-2.23910800	H	4.09148800	0.89615400	1.25613100
H	-2.07484400	5.05926900	-1.46717200	O	-2.09217400	-0.82493100	0.15366900
H	-2.97347800	4.60881300	0.80543400	C	-2.24476600	-2.04168000	-0.61124200
H	-1.73598600	3.07180000	2.32198800	C	-3.21270300	-1.71367900	-1.74848300
H	0.35968800	1.97631000	1.52446800	C	-3.99316700	-0.51711600	-1.19663500
H	2.30210100	2.83039900	-1.07123100	C	-2.92174500	0.21277800	-0.39574300
C	2.56388900	0.82602200	-2.89204200	H	-2.31232700	0.86570500	-1.03842300
H	3.32339800	1.60899100	-2.99727500	H	-3.31052100	0.80523100	0.43686000
H	2.97818100	0.03504000	-2.26169600	H	-4.42953000	0.11142900	-1.97684500
H	2.36462000	0.39213700	-3.87672000	H	-4.79566200	-0.85407400	-0.53153500
H	1.04703300	2.27573800	-2.96586100	H	-2.63429000	-1.43673100	-2.63500900

C	-0.86518000	1.03186400	-3.34948800
H	-1.16936800	2.03799900	-3.04797200
H	-1.75102400	0.39297900	-3.36377500
H	-0.46663300	1.08310900	-4.37680700
C	-0.03081800	-1.62445800	-3.58007400
C	0.09094600	-3.11957900	-3.63291600
H	0.50362600	-3.48598600	-2.68882600
H	0.75277200	-3.46141100	-4.44033900
H	-0.87905800	-3.61253400	-3.79626200
H	-0.44911600	-1.11989800	-4.44348800
O	1.19472600	-1.36219000	1.63724000
C	0.33483200	-2.47647300	1.89697500
C	-0.75612900	-1.95782800	2.86094500
C	-0.29646300	-0.52366400	3.20368200
C	1.17596100	-0.53266100	2.79806800
H	1.58866100	0.43384900	2.49649000
H	1.80281700	-0.98039900	3.58330100
H	-0.84898300	0.20506000	2.59816500
H	-0.44381500	-0.26731100	4.25536200
H	-1.73923000	-1.94889100	2.38682000
H	-0.80612700	-2.58297800	3.75591600
H	-3.85117300	-2.56251200	-2.00423400
H	-2.64482100	-2.80569900	0.06736600
H	-1.26064200	-2.34754200	-0.98305300

Figure 72. Computational overview for transition state of trisolvated monomers.

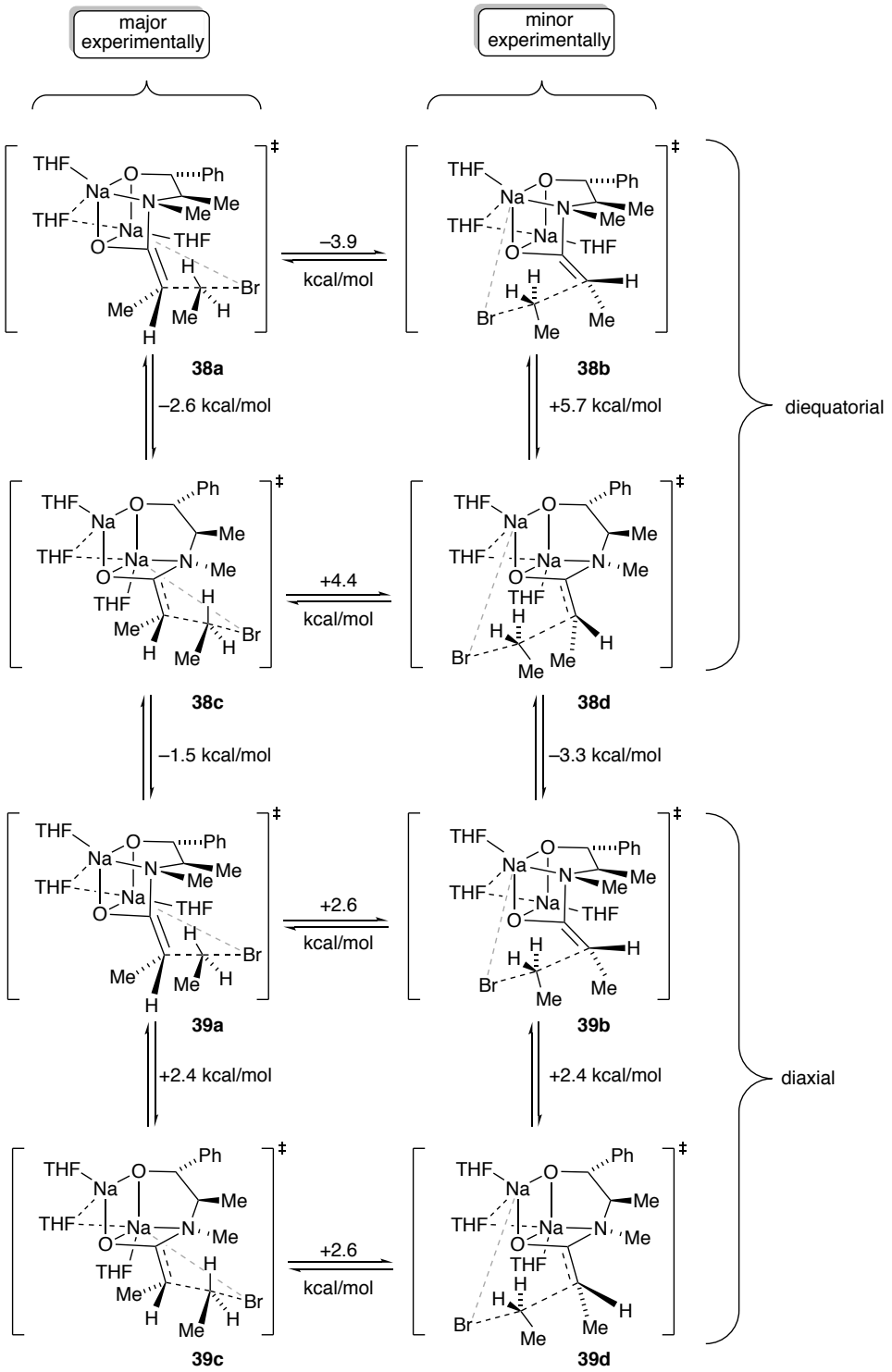
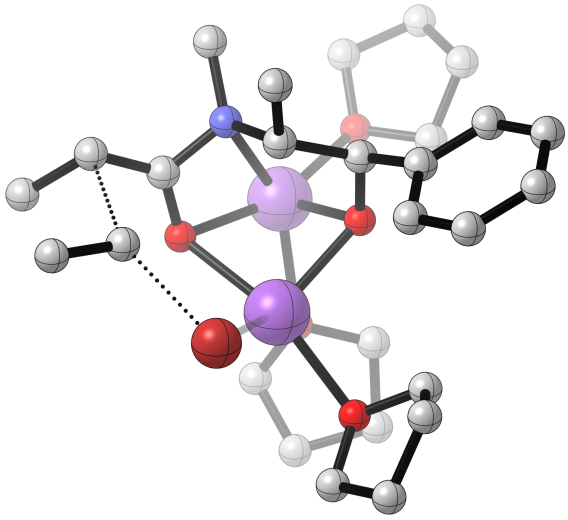


Table 37. Geometric coordinates and thermally corrected M062X energies for transition state **38a**



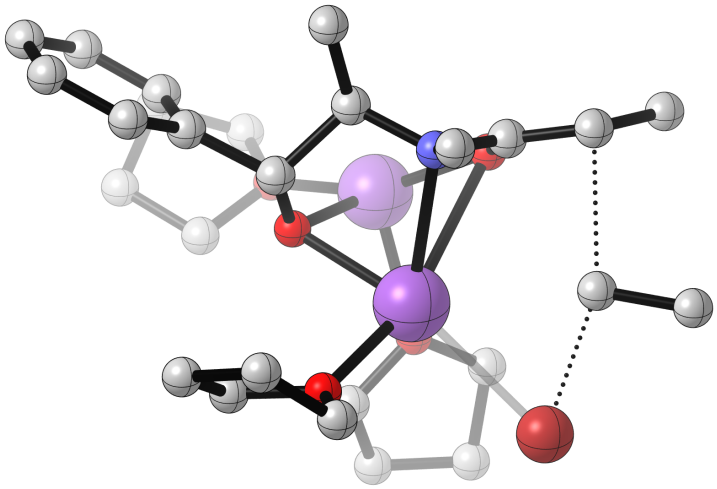
G = –4382.508528

G_{SP} = –4385.350704

Atom	X	Y	Z	Atom	X	Y	Z
Na	0.00000000	0.00000000	0.00000000	H	1.18798600	-2.87436800	0.55826100
Na	2.76549300	-0.70689000	-0.42694800	H	0.04389800	-2.65055100	1.90819300
O	0.87864200	-1.49180900	-1.35024500	O	3.84196300	-2.63920000	0.16438500
C	0.56491400	-1.10606500	-2.63345300	C	5.25687200	-2.71290500	0.40205800
C	1.14859900	0.30177800	-2.93030200	C	5.82961500	-3.68799400	-0.63983500
N	0.47745700	1.34676200	-2.09670500	C	4.70958300	-3.76613600	-1.68242800
C	1.35517400	2.06796000	-1.21512200	C	3.47262600	-3.62826600	-0.80902300
O	1.78401400	1.39600200	-0.21533300	H	2.57747300	-3.26519300	-1.32528900
C	1.78853200	3.35681200	-1.52143100	H	3.24098400	-4.57458700	-0.29406400
C	2.36461600	4.26129200	-0.46642800	H	4.77129900	-2.91049400	-2.36143600
H	2.78754000	3.66854400	0.35022000	H	4.71785000	-4.68888700	-2.26760300
H	1.60454100	4.92571400	-0.03344600	H	6.77360400	-3.32854900	-1.05532000
H	3.15644700	4.90839900	-0.86364300	H	6.00327800	-4.67174000	-0.19159100
H	1.39115400	3.82414600	-2.41912200	H	5.42740100	-3.05628600	1.43028200
C	-0.55722200	2.11922300	-2.76739700	H	5.66303900	-1.70436100	0.28273200
H	-0.20159300	2.74694200	-3.59657700	Br	5.06148200	0.04421600	-1.98729100
H	-1.04126200	2.77087800	-2.03466900	O	-2.12414200	-0.81283500	-0.04708100
H	-1.30911000	1.43094200	-3.16945200	C	-2.10463900	-2.16419600	-0.56154300
H	2.18019800	0.23713300	-2.57048500	C	-3.16678400	-2.19048700	-1.65504200
C	1.20786800	0.69755300	-4.40733600	C	-4.19402600	-1.19228900	-1.11546900
H	1.56549200	1.72773400	-4.52311000	C	-3.28627500	-0.12100500	-0.51688500
H	1.89541300	0.04018500	-4.94330700	H	-2.98196700	0.60908500	-1.27938700
H	0.22907300	0.61889100	-4.89378200	H	-3.73848900	0.41402000	0.32316700
C	1.06586200	-2.14011200	-3.63789800	H	-4.86454500	-0.79337600	-1.87988500
C	0.18399400	-2.99453700	-4.29530400	H	-4.79996400	-1.65769500	-0.33068800
C	0.65077500	-3.99475600	-5.14874500	H	-2.74794700	-1.82798600	-2.59988500

C	2.01679600	-4.14646500	-5.36083500	H	2.35712900	0.24534900	2.70077100
C	2.91094600	-3.29233700	-4.71398400	H	3.01941500	-1.94625500	4.23280600
C	2.43959400	-2.30314300	-3.85809100	H	3.77114200	-1.74241200	2.63669300
H	3.14989200	-1.63627700	-3.36776200	H	1.53862500	-3.63338300	3.39547100
H	3.98071200	-3.39322100	-4.87870800	H	2.76575700	-3.80453600	2.12788500
H	2.38484200	-4.91966000	-6.02881100	H	-3.57446200	-3.19079000	-1.81749500
H	-0.05425100	-4.65332300	-5.64867100	H	-2.37056400	-2.84456300	0.25835100
H	-0.88601300	-2.87869000	-4.13078600	H	-1.08476900	-2.36838700	-0.90707600
H	-0.54009600	-1.01674000	-2.79170200	C	3.84258300	2.18958600	-2.07172100
O	1.35416400	-1.09649900	1.53745800	C	4.87460400	3.22029000	-2.39402500
C	1.08355900	-2.50805500	1.58164600	H	4.37677700	4.17425700	-2.60575000
C	2.07515600	-3.10544400	2.60242600	H	5.56016700	3.36838000	-1.55782000
C	2.82086300	-1.87738000	3.16072200	H	5.44685800	2.93557100	-3.27941100
C	1.87864600	-0.73036900	2.81009900	H	3.28267600	1.75767800	-2.88239400
H	1.05890100	-0.65195300	3.54041000	H	3.60014800	1.94519000	-1.05321700

Table 38. Geometric coordinates and thermally corrected M062X energies for transition state **38b**



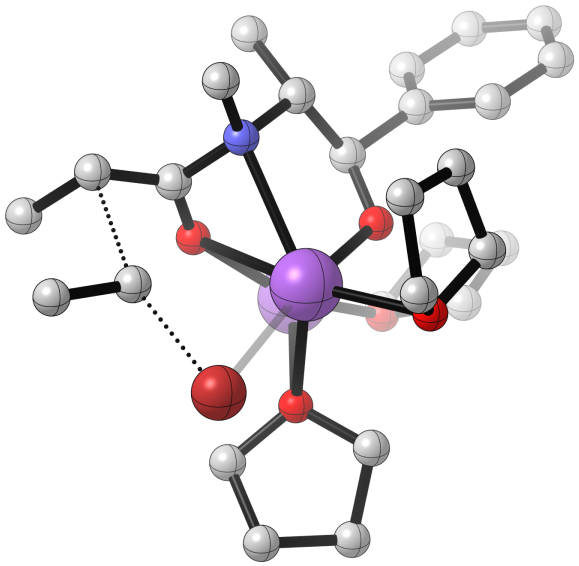
G = –4382.51294

G_{SP} = –4385.356918

Atom	X	Y	Z	Atom	X	Y	Z
Na	0.00000000	0.00000000	0.00000000	C	-5.80419600	3.31711500	1.26048700
Na	-1.73487400	1.72401600	1.54267500	C	-4.47232500	3.88299700	1.74148200
O	-2.20779400	0.15283400	0.10166400	H	-4.31206100	3.81077900	2.81963600
C	-2.60193700	-1.11344100	0.44825700	H	-4.34927300	4.93057200	1.42852500
C	-2.12068200	-1.46588300	1.89001000	H	-6.04691600	2.41913300	1.83750300
N	-0.63481900	-1.58186500	1.92124000	H	-6.62828200	4.02635100	1.36550300
C	0.03410300	-0.68042200	2.80753000	H	-5.98075100	2.02458500	-0.50400000
O	-0.33510200	0.53729700	2.73410300	H	-5.84094800	3.74783200	-0.87945100
C	1.15706000	-1.08818600	3.52460800	H	-3.51999900	3.60170000	-0.90228700
C	1.77932800	-0.13435600	4.50607300	H	-3.59281300	1.84320300	-0.52963300
H	1.83582300	0.87680900	4.08612000	O	-0.25015300	-1.00207500	-2.01292100
H	1.20443300	-0.05364700	5.43869400	C	0.38443100	-2.18937500	-2.46200000
H	2.79336100	-0.44569900	4.78261000	C	-0.76230300	-3.18974800	-2.59207000
H	1.34937700	-2.14761600	3.66083400	C	-1.91794700	-2.30645000	-3.10412400
C	-0.13144100	-2.94223000	1.81197700	C	-1.47527700	-0.87115300	-2.74140600
H	-0.64174500	-3.44176500	0.98282300	H	-2.16494800	-0.34000100	-2.08068900
H	0.93882300	-2.93148200	1.59161100	H	-1.28462200	-0.27860200	-3.64715600
H	-0.27608900	-3.54308700	2.72137200	H	-2.86892800	-2.56281800	-2.63088200
H	-2.36305200	-0.58799800	2.49790100	H	-2.04390800	-2.41291500	-4.18510700
C	-2.80873600	-2.67109100	2.53722600	H	-1.00244800	-3.59948600	-1.60539900
H	-2.75159400	-3.57243300	1.91686800	H	-0.52743700	-4.02094400	-3.26113600
H	-2.36058300	-2.89160700	3.51167800	H	0.87353500	-2.00980000	-3.43101400
H	-3.86765000	-2.45175900	2.69205800	H	1.14876200	-2.46252200	-1.72963900
H	-2.14956400	-1.89664900	-0.21288800	Br	2.73380800	0.41112800	-0.63658300
C	-4.11284600	-1.29922200	0.34137400	C	3.80846500	-0.64268300	1.97982800
C	-4.67648700	-2.46013000	-0.18900600	H	4.33210000	0.31183100	2.06274300
C	-6.05902300	-2.62796200	-0.24934300	H	1.72639100	2.69977100	0.83195200

C	-6.90242400	-1.63058300	0.23080100	H	1.81587400	4.86681900	-0.89551500
C	-6.35159300	-0.46664200	0.76638400	H	2.18912600	3.20826900	-1.42978400
C	-4.97041000	-0.30134900	0.81326200	H	-0.53838500	4.60359900	-1.60580800
H	-4.53476400	0.61174800	1.21590300	H	0.34698400	3.81928000	-2.93380000
H	-7.00730500	0.31456900	1.14530700	H	0.05775200	1.61788400	-1.94186100
H	-7.98006400	-1.75673500	0.18764300	H	-1.51400800	2.34970400	-1.52753000
H	-6.47690600	-3.53750100	-0.67147300	O	-3.50130600	3.06856900	1.09703400
H	-4.01797000	-3.24688700	-0.55503000	C	-3.95907000	2.83654600	-0.24757700
O	-0.13043800	2.36627600	-0.01030100	C	-5.49809800	2.95781000	-0.20602000
C	-0.43225200	2.45081300	-1.41772300	H	4.35397200	-1.27565700	1.27732300
C	0.14691600	3.78682300	-1.86044500	H	3.81045600	-1.12606800	2.96077900
C	1.41613500	3.85648500	-1.00606800	C	2.39462600	-0.43127000	1.51513400
C	0.94566400	3.26699700	0.32058000	H	1.85426300	-1.27140100	1.11014900
H	0.54639100	4.03427000	0.99488500	H	1.83719800	0.44243900	1.82782900

Table 39. Geometric coordinates and thermally corrected M062X energies for transition state **38c**

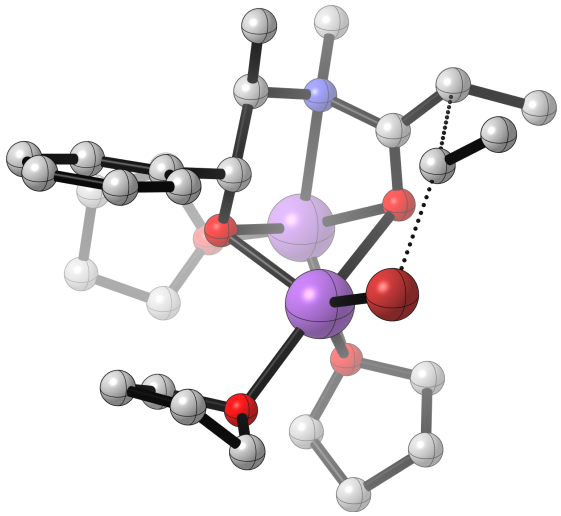


G = –4382.511481
G_{SP} = –4385.354905

Atom	X	Y	Z	Atom	X	Y	Z
Na	0.00000000	0.00000000	0.00000000	H	-0.15637100	-1.12181800	3.94992300
Na	1.79565300	-1.32392000	1.81352100	H	0.41594000	-1.25615500	5.66011200
O	-0.40508800	-1.32019400	1.74446100	H	0.32452200	-3.37894000	3.50145600
C	-1.10647900	-2.16064800	0.92955600	H	0.17939500	-3.60913900	5.25437100
C	-0.43208100	-3.55621700	0.72444500	H	2.63529100	-3.68177900	3.57969100
N	1.05523700	-3.51548700	0.60767200	H	2.54454200	-4.03941100	5.30822200
C	1.55563700	-2.88472200	-0.58521700	H	2.84670100	-1.70990700	5.89944200
O	1.19870100	-1.67522000	-0.76486300	H	3.78956600	-1.71836200	4.37436800
C	2.54513200	-3.49489700	-1.35114000	Br	4.64018300	-0.87607400	1.90309600
C	2.99713500	-2.84003300	-2.62636600	O	-1.86647500	1.24553000	0.26111500
H	3.11202700	-1.75771300	-2.49262800	C	-2.37730800	1.17023900	1.60592400
H	2.27998800	-2.97844600	-3.44678000	C	-3.89599900	0.92545800	1.47722400
H	3.95683800	-3.24504500	-2.96747900	C	-4.16166800	1.01704000	-0.03836100
H	2.74078000	-4.55501300	-1.23409500	C	-2.92228200	1.74316700	-0.55121700
C	1.62537100	-4.81688400	0.94256200	H	-2.67475200	1.53491300	-1.59511600
H	1.25014200	-5.11800200	1.92558900	H	-3.01312200	2.83149500	-0.41505700
H	2.71530100	-4.75587900	0.99692200	H	-4.20880100	0.01462500	-0.47301800
H	1.37815300	-5.60970500	0.22132900	H	-5.08727700	1.54410900	-0.28156400
C	-1.05157300	-4.31114200	-0.45455200	H	-4.18101500	-0.05230900	1.87351300
H	-0.57818600	-5.28515400	-0.60889100	H	-4.45501200	1.69103000	2.02208400
H	-2.11814600	-4.48395600	-0.29117000	H	-2.17290300	2.12691100	2.10644300
H	-0.93071600	-3.72843000	-1.37565300	H	-1.83308000	0.35823400	2.09650100
H	-0.62179800	-4.11877600	1.64850800	C	5.37524100	-2.76193000	-0.35055900
C	-2.53908800	-2.38032600	1.43515400	H	5.24649300	-3.53071800	-1.11788000
C	-3.62636200	-2.49012200	0.56615100	H	5.88830900	-1.90901700	-0.79969900

C	-4.92301200	-2.66055900	1.05036200	H	2.36368800	2.00558800	-0.68859800
C	-5.14944700	-2.72366000	2.42277300	H	3.48608000	0.72240700	-0.14610000
C	-4.07162900	-2.61458200	3.30151400	H	3.98708500	3.35959400	0.50325900
C	-2.78145900	-2.43973800	2.80948100	H	4.31686500	2.03265000	1.64618200
H	-1.93854100	-2.32742400	3.48548800	H	1.75807100	3.72077900	1.49900600
H	-4.24148400	-2.65848900	4.37386900	H	2.76838900	3.44294200	2.93450100
H	-6.15721600	-2.85182800	2.80648100	H	2.13740100	1.09700300	3.03736800
H	-5.75525400	-2.73589200	0.35588600	H	0.60310400	1.80082800	2.45834900
H	-3.45395800	-2.43240700	-0.50788400	O	1.86853800	-1.04253500	4.20631800
H	-1.24743200	-1.77251000	-0.11129900	C	2.81455000	-1.91545900	4.81924200
O	1.78464400	0.96140700	0.99764000	C	2.25618500	-3.31579400	4.54194100
C	1.66919100	1.68732400	2.24098000	C	0.72639300	-3.07518100	4.47322600
C	2.40852400	2.99799200	2.00419800	C	0.59559700	-1.54883900	4.61534500
C	3.53711300	2.54467300	1.07462900	H	6.00520200	-3.16512000	0.44471700
C	2.83016900	1.53013700	0.18388900	C	4.03421400	-2.34980500	0.18941500
H	3.45135800	-1.58251500	-0.30165800	H	3.54894300	-2.98332000	0.91418000

Table 40. Geometric coordinates and thermally corrected M062X energies for transition state **38d**

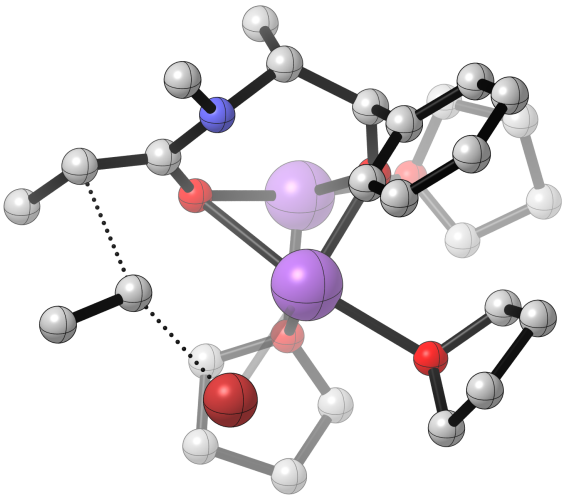


G = –4382.507228
G_{SP} = –4385.347835

Atom	X	Y	Z	Atom	X	Y	Z
Na	0.00000000	0.00000000	0.00000000	H	-3.95126800	-2.44674300	-1.99943300
Na	-2.04012900	-2.04267500	-0.23744200	H	-5.62906000	-2.65750300	-1.42342200
O	-1.83813900	-0.15902700	-1.31167200	H	-4.13457500	-0.08426200	-2.08989600
C	-1.01461200	-0.18575500	-2.40821900	H	-5.81105500	-0.50710200	-2.58936800
C	-1.23555200	-1.43367800	-3.30154100	H	-5.47447800	1.12082200	-0.44180500
N	-1.03462900	-2.68264700	-2.51241400	H	-6.55109500	-0.27874300	-0.21940500
C	0.18267200	-2.83890800	-1.72916900	H	-4.89107400	-0.71497500	1.52107500
O	0.14714500	-2.36925900	-0.54265900	H	-3.58571800	-0.05123300	0.48053400
C	1.31075000	-3.46716500	-2.26148400	O	-0.50543900	2.07075300	0.83655700
C	2.26750900	-4.22957100	-1.37897800	C	0.46816900	3.10729600	0.95628500
H	2.23434300	-3.84523600	-0.35487800	C	0.38602500	3.83879300	-0.37599200
H	2.00701200	-5.29566400	-1.33805800	C	-1.12476600	3.82283500	-0.66899300
H	3.30430900	-4.17200000	-1.73040200	C	-1.64975500	2.63603800	0.16675400
H	1.26086100	-3.77814600	-3.30258100	H	-2.08351800	1.83411400	-0.43916800
C	-1.40270400	-3.88029900	-3.26019700	H	-2.36728800	2.97267500	0.92952800
H	-1.38360200	-4.74527800	-2.59136000	H	-1.33039300	3.68869900	-1.73402700
H	-2.42531200	-3.75421700	-3.63557300	H	-1.59361600	4.75709200	-0.34603200
H	-0.75714800	-4.10752200	-4.11945300	H	0.93335600	3.25815400	-1.12507000
H	-2.30243800	-1.43629100	-3.57706200	H	0.80638600	4.84672900	-0.33468400
C	-0.39484400	-1.40446700	-4.58161900	H	0.20108700	3.76492000	1.79868000
H	-0.61578400	-0.50635500	-5.16314900	H	1.43551900	2.63687700	1.14673800
H	0.67635800	-1.40406700	-4.34899300	Br	2.61336700	0.75230600	-0.72037500
H	-0.59602200	-2.27094300	-5.21810000	C	3.85254300	-1.61491500	-2.39032700
H	0.06399200	-0.25478800	-2.13966300	H	4.52222000	-1.85273100	-1.56197300
C	-1.08167700	1.11028000	-3.21609900	H	4.22976000	-0.73020400	-2.90768300
C	0.07153500	1.87454800	-3.40472900	H	3.86245400	-2.45011600	-3.10022300

C	0.02552400	3.08159600	-4.10261400	H	0.62627300	-2.13304400	1.72704000
C	-1.18131900	3.53963100	-4.62218300	H	1.33967700	-0.65864700	3.94505400
C	-2.34121500	2.78665500	-4.43354500	H	1.25902400	0.15045700	2.37441900
C	-2.29076300	1.58560900	-3.73255100	H	-0.76327500	0.26552800	4.63129800
H	-3.19857600	1.00694400	-3.58327900	H	-0.39729900	1.49553300	3.40726700
H	-3.28750400	3.14154100	-4.83259100	H	-2.16020200	0.66339400	2.07946600
H	-1.22329800	4.47906800	-5.16549000	H	-2.47324700	-0.60763100	3.29729500
H	0.93294900	3.66661000	-4.22518900	O	-4.29231200	-1.93293700	-0.02494700
H	1.00685500	1.53656100	-2.95965500	C	-4.52994300	-0.61167400	0.49410800
O	-1.11926700	-1.07434700	1.80581100	C	-5.52799100	0.02971100	-0.46144800
C	-1.70114500	-0.11048400	2.69629900	C	-5.06780900	-0.56995000	-1.79112900
C	-0.54991000	0.42739600	3.57148900	C	-4.74849500	-2.00466800	-1.38850900
C	0.67152600	-0.39762000	3.12117400	C	2.45305100	-1.38702400	-1.91286800
C	0.02341600	-1.62009300	2.47951900	H	1.75273200	-0.91962900	-2.58400700
H	-0.31182900	-2.34023000	3.23988800	H	2.09941200	-1.74473100	-0.96368600

Table 41. Geometric coordinates and thermally corrected M062X energies for transition state **39a**

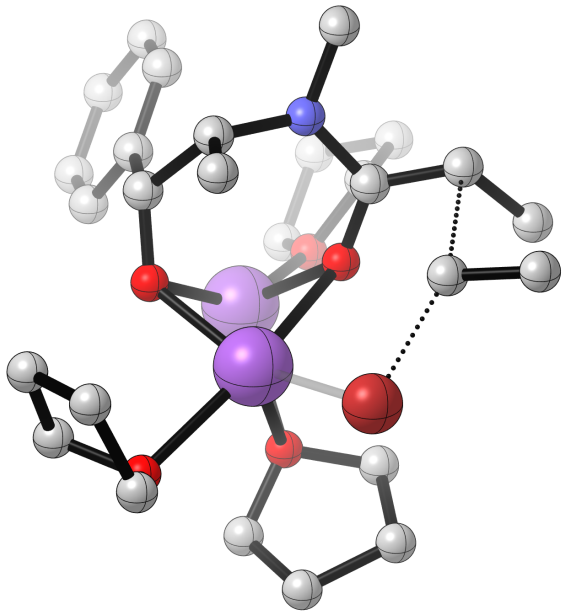


G = –4382.516555
G_{SP} = –4385.357296

Atom	X	Y	Z	Atom	X	Y	Z
Na	0.00000000	0.00000000	0.00000000	C	-4.79127400	-1.05110400	1.38458900
Na	-1.00305400	-1.66628600	2.01819900	C	-4.72189100	-2.06798200	0.24252100
O	-1.84753500	0.15140900	1.19118200	C	-3.29852000	-2.58609100	0.39869800
C	-2.06525500	1.31639200	1.86725400	H	-3.14155400	-3.59441200	0.00498100
C	-1.09518800	1.59333200	3.05767100	H	-2.58871300	-1.88846400	-0.06550900
N	0.33275600	1.75121600	2.68709700	H	-5.44310100	-2.87827000	0.39527100
C	1.21935200	0.65492800	2.81222800	H	-4.89728700	-1.62356500	-0.74020400
O	0.80858200	-0.47812900	2.37134800	H	-5.81203900	-0.81932900	1.69756400
C	2.54507900	0.87152700	3.18689700	H	-4.27233200	-0.13315300	1.09510200
C	3.48687600	-0.28050600	3.38673200	H	-3.42832100	-1.03842200	3.09575900
H	3.17592200	-1.14439900	2.79097000	H	-4.62438500	-2.36607400	3.13005900
H	3.52790000	-0.61524800	4.43243500	O	-1.26256400	-0.21842600	-1.96235500
H	4.51535600	-0.02292800	3.09892600	C	-0.83215900	0.17801000	-3.26212700
H	2.82337100	1.81072100	3.65112800	C	-1.34763100	1.60711900	-3.38684700
C	0.85031100	3.07673100	2.99075200	C	-2.70662400	1.54079700	-2.65923800
H	1.79089300	3.24954200	2.45937200	C	-2.62108100	0.23120000	-1.84786200
H	1.03425700	3.23265200	4.06605200	H	-2.81862700	0.34200300	-0.77867200
H	0.12926900	3.82081400	2.64447700	H	-3.27682900	-0.54075400	-2.27994600
C	-1.30033400	0.63134600	4.23001700	H	-2.85529600	2.40534600	-2.00800100
H	-2.34300800	0.66838200	4.56239100	H	-3.53810700	1.50189900	-3.36858100
H	-1.04736700	-0.40186300	3.98600300	H	-0.66325900	2.27287600	-2.85188600
H	-0.66181900	0.92158800	5.07133400	H	-1.42570200	1.94415100	-4.42326300
H	-1.39631900	2.57707400	3.44146300	H	-1.28738200	-0.48452900	-4.01558600
H	-3.06594100	1.31651800	2.37059800	H	0.25450300	0.09053500	-3.30301300
C	-2.10620100	2.53888400	0.93653100	Br	2.20470100	0.86313800	-1.49298000
C	-3.27600500	3.29345100	0.82106300	C	4.22890600	1.60667300	0.63419200
C	-3.34820000	4.40559500	-0.01789600	H	4.85205400	0.87592000	0.11433500

C	-2.23753300	4.79077900	-0.76329800	H	1.85366900	-2.19081200	1.25243300
C	-1.06288600	4.04557800	-0.66940300	H	3.02463500	-3.59417000	-0.90935700
C	-1.00431300	2.93032700	0.16215000	H	2.78968400	-1.83470100	-0.95714300
H	-0.06656900	2.38612900	0.23011100	H	1.32834300	-3.77940100	-2.59545900
H	-0.18599700	4.32891200	-1.24612500	H	1.16119200	-2.01618000	-2.55092300
H	-2.28555400	5.65917900	-1.41342200	H	-0.96100600	-2.51560000	-1.58139300
H	-4.27319100	4.97149900	-0.08610700	H	-0.38093200	-4.09179900	-0.94371400
H	-4.14778800	3.00222600	1.40392900	O	-3.06329300	-2.62779900	1.81502900
O	0.17077000	-2.41055800	0.12175000	C	-3.99094000	-1.74979600	2.48161100
C	-0.11821200	-3.04122300	-1.13305900	H	4.27282700	2.55122000	0.08809800
C	1.18177800	-2.92065900	-1.93614500	H	4.64032200	1.76279100	1.63636000
C	2.28097400	-2.79605000	-0.85291800	C	2.81295900	1.11893900	0.74486700
C	1.49580900	-2.85249000	0.46211100	H	2.01416600	1.82826700	0.89612000
H	1.43021400	-3.88270200	0.84166900	H	2.61007800	0.07934300	0.95543000

Table 42. Geometric coordinates and thermally corrected M062X energies for transition state **39b**

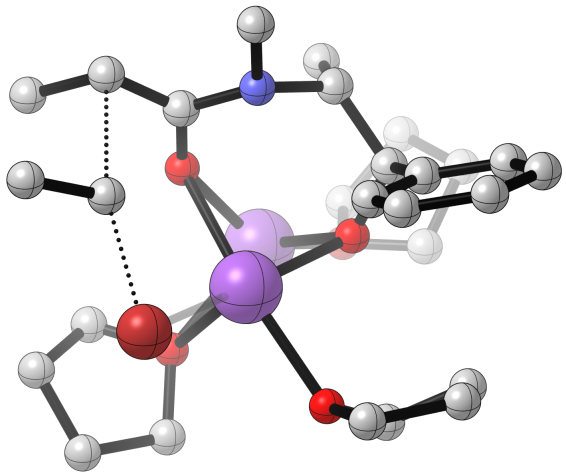


G = –4382.512181
G_{SP} = –4385.353186

Atom	X	Y	Z	Atom	X	Y	Z
Na	0.00000000	0.00000000	0.00000000	C	4.82109800	2.00876600	0.67893600
Na	2.71391700	-0.15637800	0.88420900	C	6.19501800	2.53755800	1.06874600
O	1.62041400	-1.27210200	-0.70810200	C	6.90878100	1.25189200	1.49181800
C	2.41583900	-1.06067700	-1.79425200	C	5.79023200	0.48885800	2.19997100
C	2.11326700	0.19087200	-2.68879000	H	5.75101100	0.73127200	3.26923600
N	2.61189500	1.53395700	-2.30463200	H	5.87779500	-0.59565600	2.08053300
C	2.14952500	2.22447600	-1.17751100	H	7.77234700	1.42131300	2.13934000
O	1.79364400	1.53014900	-0.16028300	H	7.23331800	0.69540300	0.60714900
C	2.01017000	3.62240400	-1.19585900	H	6.11202500	3.22740900	1.91579800
C	2.00107900	4.42235200	0.07914800	H	6.69070800	3.05682200	0.24556400
H	2.94812800	4.95539800	0.24712100	H	4.80943700	1.61733500	-0.34744400
H	1.21054800	5.18647800	0.09673700	H	4.01245600	2.73376100	0.78564300
H	1.84191500	3.76466500	0.94019300	O	-1.37434400	-1.87450800	0.41175900
H	2.24429600	4.17304900	-2.09870100	C	-2.62681300	-1.87892600	-0.27201700
C	3.06598800	2.33154700	-3.43149500	C	-2.25917600	-2.20045700	-1.72290300
H	3.59513100	1.68933700	-4.14079200	C	-0.99193200	-3.07891600	-1.57744500
H	2.24556700	2.82928100	-3.97294600	C	-0.69031600	-3.03710700	-0.07164100
H	3.76037600	3.10049900	-3.08460300	H	0.37335300	-2.90495100	0.12768800
C	0.63550300	0.21795000	-3.08777800	H	-1.09257800	-3.91923800	0.44823100
H	0.45488500	0.98570400	-3.84955400	H	-0.14504400	-2.64674700	-2.11607200
H	0.33402300	-0.74995700	-3.50320200	H	-1.14950400	-4.10095900	-1.93112800
H	-0.02956900	0.43150100	-2.24708400	H	-2.03023600	-1.27162700	-2.25588600
H	2.66635100	-0.02379000	-3.61144700	H	-3.07235700	-2.70211900	-2.25296500
C	3.91566300	-1.18131200	-1.45084800	H	-3.26853300	-2.66146700	0.16035200

C	4.95292900	-0.50708600	-2.10635000	H	0.88050900	2.06176500	1.99185100
C	6.28470300	-0.72372600	-1.75641900	H	-1.17744000	1.99190100	3.95273900
C	6.61442500	-1.62402400	-0.74587000	H	-1.51076200	1.83833400	2.21701300
C	5.59553400	-2.30994600	-0.08815000	H	-1.80927800	-0.30548500	4.18840200
C	4.26613900	-2.08626400	-0.43984900	H	-2.03400100	-0.40197800	2.43324800
H	3.45973400	-2.62862800	0.04894500	H	-0.09777500	-1.78208300	2.53788900
H	5.83661500	-3.03205400	0.68828700	H	0.49389500	-0.97133300	4.02482700
H	7.65418400	-1.79566300	-0.48132900	O	4.56736800	0.92255100	1.59219200
H	7.07099400	-0.18497500	-2.27885500	H	-3.09236000	-0.90213200	-0.13279200
H	4.73029600	0.20278000	-2.89626500	Br	-2.17921100	1.68270800	-0.53751700
H	2.26047200	-1.87442500	-2.54743500	C	-1.05261600	4.43296000	-1.32176400
O	0.78399700	0.04405100	2.24912700	H	-0.30397600	5.16830400	-1.63659100
C	-0.01173400	-0.82765500	3.05922900	H	-1.51281200	4.78298000	-0.39549800
C	-1.34453600	-0.09080700	3.22329900	H	-1.82233900	4.37175100	-2.09382500
C	-0.96505500	1.40261200	3.05767900	C	-0.38559800	3.10555700	-1.12172500
C	0.54073300	1.36345800	2.75906200	H	-0.15969900	2.49703600	-1.98182000
H	1.13674000	1.50072300	3.67249100	H	0.08113600	2.85098900	-0.18735700

Table 43. Geometric coordinates and thermally corrected M062X energies for transition state **39c**



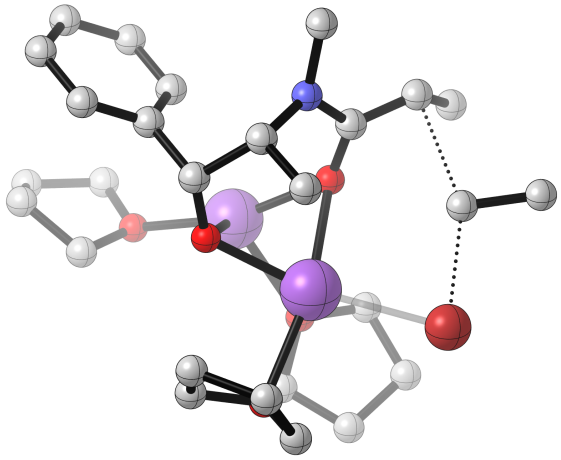
G = –4382.512493

G_{SP} = –4385.353519

Atom	X	Y	Z	Atom	X	Y	Z
Na	0.00000000	0.00000000	0.00000000	O	-4.23733600	-2.11396600	-0.49292100
Na	-2.07857400	-1.79479500	0.07582400	C	-4.88483100	-0.84359000	-0.66989300
O	-2.14019800	0.36993200	0.29574700	C	-5.96818500	-0.77979800	0.42377800
C	-2.52106700	1.08652700	1.39337100	C	-6.09882600	-2.24087000	0.91353100
C	-2.29854300	0.36082500	2.75746200	C	-5.25665600	-3.02293500	-0.09728500
N	-0.87947800	0.07597400	3.07763000	H	-4.77704200	-3.91524300	0.31193000
C	-0.33453000	-1.19908700	2.83110500	H	-5.85207000	-3.30822300	-0.97656000
O	-0.66369700	-1.78069300	1.73737200	H	-5.67266500	-2.34825800	1.91490300
C	0.68355900	-1.70663100	3.63923400	H	-7.13297000	-2.59091800	0.94481100
C	1.19193400	-3.10130400	3.38993500	H	-5.66017200	-0.12054900	1.23817700
H	1.63646400	-3.21780900	2.38910500	H	-6.90898000	-0.39719700	0.02107000
H	0.40163300	-3.86095300	3.46223500	H	-5.33423100	-0.82199800	-1.67221300
H	1.96840900	-3.36557400	4.11545800	H	-4.10724700	-0.07864000	-0.58028300
H	0.86188300	-1.28214000	4.61982300	O	-0.18556700	1.22622900	-1.96178700
C	-0.39375800	0.80094100	4.24157500	C	0.26220900	2.58425000	-1.99527100
H	-0.75108500	1.83161400	4.18897700	C	-1.00523800	3.46427500	-1.97622700
H	0.69977600	0.82696600	4.24515600	C	-2.16306900	2.45687900	-2.13033500
H	-0.72558300	0.35529900	5.19303400	C	-1.45898300	1.19022000	-2.59866900
C	-3.22902400	-0.84724900	2.91291200	H	-1.96507900	0.27561700	-2.27730700
H	-2.91620900	-1.47926400	3.75043700	H	-1.31920700	1.17448400	-3.69154800
H	-4.24670200	-0.49372900	3.11337900	H	-2.61390900	2.24540100	-1.15872900
H	-3.27212200	-1.46943900	2.01630900	H	-2.93136200	2.79427500	-2.83101400
H	-2.61588500	1.07592700	3.52732500	H	-1.09364100	4.02121300	-1.04033400
C	-1.88090800	2.48271500	1.44770400	H	-0.98238500	4.18391400	-2.79935600
C	-2.67922500	3.62793500	1.50011500	H	0.84788900	2.74128200	-2.91117100
C	-2.12158200	4.90572400	1.54181300	H	0.91632200	2.73076800	-1.13247600
C	-0.73889300	5.06556900	1.53567700	Br	2.72347100	0.48817000	0.04343600

C	0.07609200	3.93576900	1.47931900	H	0.38237500	-3.26430900	0.44268000
C	-0.49180700	2.66574800	1.43141400	H	2.64832600	-3.94710400	-0.99735400
H	0.17436600	1.80887200	1.41473600	H	2.53504700	-2.34416700	-0.23722600
H	1.15828600	4.03876400	1.46878900	H	2.30178200	-2.96330400	-3.15902300
H	-0.30014200	6.05833000	1.56952100	H	2.66283600	-1.42860600	-2.34606900
H	-2.76972800	5.77698900	1.57580800	H	0.39603300	-0.83706600	-2.72698400
H	-3.76156500	3.51375100	1.50080000	H	-0.00033800	-2.51966100	-3.19838300
H	-3.62347400	1.28118500	1.39415700	C	3.48524100	-0.81859300	2.65363700
O	-0.05696700	-2.09684900	-1.17573400	H	4.05304300	-1.50365600	2.01967400
C	0.53051100	-1.88935800	-2.47271800	H	4.06100500	0.10212400	2.76765600
C	2.00960700	-2.30335700	-2.33848700	H	3.36040500	-1.27944100	3.63746300
C	2.07822200	-3.01575200	-0.97047000	C	2.13607100	-0.53374900	2.05291900
C	0.61101200	-3.24362900	-0.62460100	H	1.57593500	0.33238300	2.37445200
H	0.22412800	-4.14782300	-1.11939600	H	1.60409700	-1.31663700	1.53248400

Table 44. Geometric coordinates and thermally corrected M062X energies for transition state **39d**

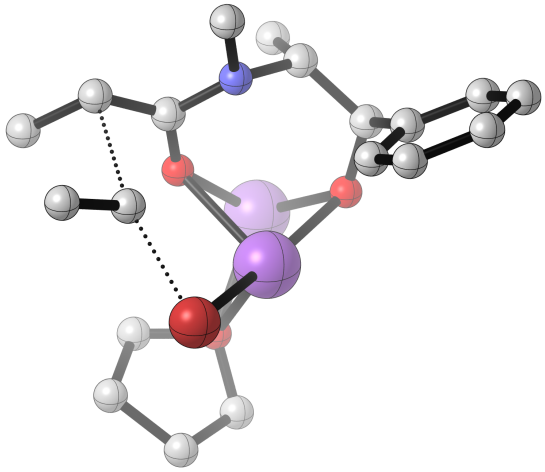


G = –4382.508675
G_{SP} = –4385.349424

Atom	X	Y	Z	Atom	X	Y	Z
Na	0.00000000	0.00000000	0.00000000	H	1.76277200	-3.45002900	-2.60101600
Na	-2.36123400	0.06988300	-1.44342700	H	1.82565200	-2.45994000	-1.12994900
O	-2.09596500	0.03076900	0.72953000	H	-0.51560100	-2.90996200	-1.11160800
C	-2.64254800	1.09072700	1.39467900	H	-0.59994500	-2.97969700	-2.90306400
C	-1.79095600	2.40600900	1.48548700	O	-4.18025200	-1.18507600	-1.84304300
N	-1.68850500	3.29030900	0.30611200	C	-4.54437900	-1.79920300	-0.58876100
C	-0.96696600	2.98067300	-0.85110200	C	-6.02295800	-1.48572300	-0.41273700
O	-0.93879100	1.74946900	-1.22856400	C	-6.52392400	-1.52202000	-1.85812600
C	-0.24141200	3.97129900	-1.52678000	C	-5.35393600	-0.89124900	-2.61203600
C	0.10011700	3.82425100	-2.98456100	H	-5.46668200	0.19810500	-2.67173700
H	-0.08866200	2.79622900	-3.31020100	H	-5.22165100	-1.29361100	-3.62082200
H	-0.50410100	4.48389500	-3.62232300	H	-7.45479100	-0.96978400	-2.00743300
H	1.15185800	4.05627600	-3.20724900	H	-6.67774400	-2.55578600	-2.18584700
H	-0.21368500	4.97605900	-1.11929500	H	-6.14280900	-0.48356500	0.00802500
C	-1.98616900	4.68391500	0.58495400	H	-6.52766300	-2.20375700	0.23809800
H	-1.17160600	5.21093700	1.10816300	H	-4.36864800	-2.88059800	-0.66967100
H	-2.18867300	5.20943400	-0.34968500	H	-3.89930600	-1.37175900	0.18713400
H	-2.88506500	4.73727100	1.20578400	O	0.42094500	-2.08719400	1.00845600
C	-0.43585000	2.15717700	2.15682300	C	1.50344900	-2.12091200	1.93816000
H	0.06604000	3.10895100	2.36754300	C	0.95663900	-1.40877300	3.17936000
H	-0.57772800	1.63125700	3.10803800	C	-0.56487300	-1.69168300	3.10741000
H	0.25740500	1.55984900	1.55923800	C	-0.73186700	-2.44368800	1.77963800
H	-2.36227600	3.00964400	2.20138500	H	-1.61564800	-2.11810200	1.23044000
C	-4.05724200	1.46477000	0.92840400	H	-0.73070800	-3.53411600	1.92638200
C	-5.13754900	1.36688500	1.80915100	H	-1.14001000	-0.76335900	3.05904900
C	-6.42992400	1.72356500	1.42350600	H	-0.92159500	-2.28096700	3.95591400
C	-6.67038100	2.18170500	0.13138900	H	1.15943700	-0.33517500	3.10668800
C	-5.60573300	2.28353600	-0.76365200	H	1.41719400	-1.77599300	4.09967700

C	-4.31659000	1.93151100	-0.36845900	H	0.44601800	0.54928500	-2.86907300
H	-3.48824900	2.08957200	-1.05542200	H	2.14716700	-1.50213700	-3.94314300
H	-5.77530000	2.66594300	-1.76731500	H	2.47680600	-0.65221200	-2.41967600
H	-7.67316000	2.46541200	-0.17401400	H	1.75355600	-3.16959300	2.15751600
H	-7.24826300	1.64002100	2.13335200	H	2.35908500	-1.62660200	1.47638500
H	-4.95796400	1.00946300	2.82101400	Br	2.70554300	0.72930100	0.07317800
H	-2.76565600	0.85169200	2.47907900	C	1.71439600	2.71365600	-0.69392400
O	-0.44122700	-1.09853800	-2.06192200	C	2.88611200	3.57021500	-1.06847900
C	-0.12259300	-2.49394000	-2.04007300	H	2.52236100	4.54465000	-1.41216900
C	1.40190000	-2.52975200	-2.13597100	H	3.46376900	3.11328400	-1.87464300
C	1.74704900	-1.26231900	-2.95514200	H	3.54502200	3.73067500	-0.21262100
C	0.40355000	-0.52297300	-3.07058200	H	1.23407000	2.87479300	0.25680300
H	-0.06344700	-0.68911400	-4.05145300	H	1.18060800	2.14952000	-1.43733300

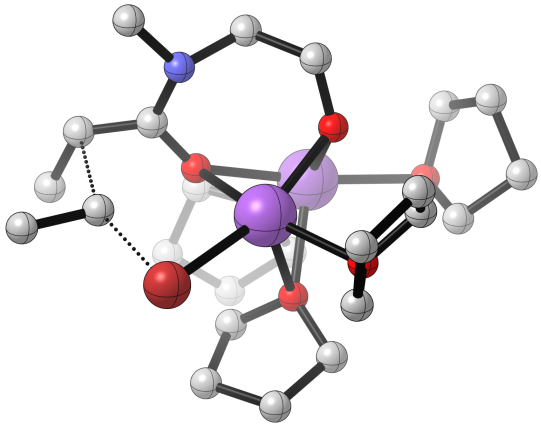
Table 45. Geometric coordinates and single point M062X energy for transition state **26** with one THF



G_{SP} = –3921.14698506

Atom	X	Y	Z	Atom	X	Y	Z
Na	0.00000000	0.00000000	0.00000000	O	-1.54905200	-1.35236600	-0.77549300
Na	0.15636100	-2.71930400	-0.67874500	C	-2.87648300	0.94827700	0.73377900
C	-2.71282700	-1.48916100	-0.08046000	H	-1.86603100	0.89077200	1.12701900
C	-2.58681800	-2.20014500	1.30342400	H	-3.09856400	2.97307500	1.41120000
N	-1.77402300	-1.47500900	2.30876400	H	-5.42691000	3.19224100	0.54943400
C	-0.41877100	-1.81494700	2.49829800	H	-6.47896800	1.26576000	-0.61889300
O	0.29084100	-1.99919300	1.44566900	H	-5.23358000	-0.85230300	-0.88643000
C	0.15295600	-1.73156000	3.77045700	O	1.88290300	-1.12266000	-1.00730100
C	1.57825800	-2.14729900	4.00167400	C	2.50129900	-0.30625600	-2.00698800
H	2.17829600	-1.99820500	3.09608100	C	3.36627000	0.68556500	-1.21759300
H	1.67951800	-3.20721300	4.27812100	C	3.63768400	-0.04368600	0.12151400
H	2.04393800	-1.56833400	4.81058100	C	2.91755100	-1.38592100	-0.05009300
H	-0.48790500	-1.68543900	4.64358400	H	3.59275800	-2.15006000	-0.46701500
C	-2.53977100	-1.05011000	3.46933600	H	2.42620600	-1.77571900	0.84321700
H	-1.99333900	-0.28106600	4.02321800	H	4.70247500	-0.17926400	0.32511800
H	-2.76572600	-1.87456200	4.16502100	H	3.19713900	0.52919900	0.94248600
H	-3.47868800	-0.61037600	3.12487900	H	4.28111900	0.94131700	-1.75721700
C	-2.20285300	-3.67737000	1.18812100	H	2.80824900	1.60758200	-1.03053900
H	-2.91104800	-4.19465400	0.53218500	H	1.70719800	0.16435400	-2.58717000
H	-1.19261800	-3.83154700	0.80480000	H	3.11457200	-0.94955400	-2.65501300
H	-2.24318200	-4.15198500	2.17520500	Br	0.95477200	2.23722100	1.42560900
H	-3.60512800	-2.20021600	1.71450100	C	1.12723000	1.20510900	4.27129600
H	-3.44108900	-2.14699800	-0.62175200	H	2.18731100	1.45271900	4.18408400
C	-3.46018100	-0.15852600	0.10150700	H	0.57364500	2.12184600	4.48441500
C	-4.76313600	-0.01161300	-0.37971100	H	0.99883000	0.51681300	5.11273800
C	-5.46860000	1.18220400	-0.22810000	C	0.62304800	0.55676300	3.01376000
C	-4.88056800	2.26230500	0.42306200	H	-0.43628100	0.54845700	2.80494800
C	-3.57801900	2.13880500	0.90488400	H	1.25375500	-0.11955100	2.45616900

Table 46. Geometric coordinates and single point M062X energy for transition state **26** with no Ph and Me group on the backbone

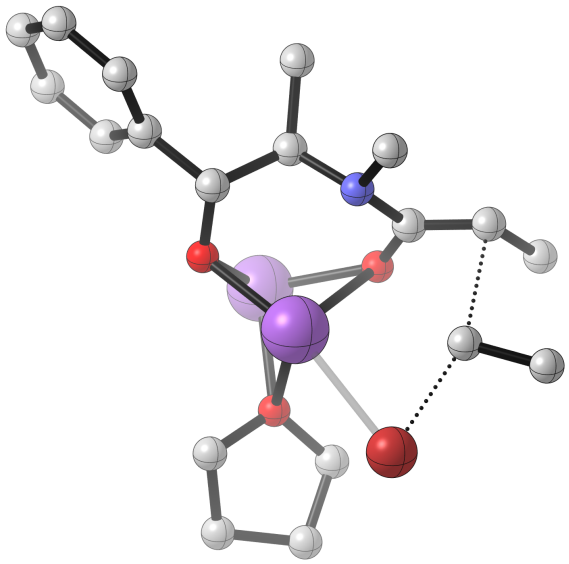


G_{SP} = –4348.12457247

Atom	X	Y	Z	Atom	X	Y	Z
Na	0.00000000	0.00000000	0.00000000	O	-2.01250400	-0.81844100	-0.58784400
Na	2.62363300	-0.94006000	-0.33555100	C	-2.52534000	-2.07540400	-0.15217100
O	1.81791300	0.51146800	1.10449300	C	-2.90003700	-2.78949600	-1.44815100
C	2.02030200	0.30158500	2.43533600	C	-3.38609300	-1.63466500	-2.34891700
C	1.27130900	-0.92662100	3.04116700	C	-2.83843000	-0.36573700	-1.65551900
N	1.69453800	-2.24368900	2.50883600	H	-2.21907800	0.26162500	-2.30287600
C	0.95884200	-2.85533600	1.47306300	H	-3.65360600	0.24904500	-1.25263100
O	0.59530000	-2.10968100	0.49461600	H	-3.01373600	-1.73527500	-3.37131400
C	0.83613500	-4.24643100	1.42819800	H	-4.47738400	-1.60230700	-2.39898500
C	0.00612200	-4.91129500	0.36667900	H	-2.01322100	-3.26859100	-1.87276500
H	-0.01018800	-4.30771600	-0.54863600	H	-3.66032500	-3.55925200	-1.29801700
H	-1.04158800	-5.05947000	0.66741400	H	-3.41033400	-1.91144900	0.48086300
H	0.39892900	-5.90338500	0.10620300	H	-1.73412400	-2.56111100	0.42193000
H	1.05162800	-4.83188600	2.31475600	C	3.33175200	-5.45387700	-0.03400800
C	2.30182000	-3.10175000	3.51321500	H	3.25158900	-5.78410200	-1.07189600
H	2.85774200	-3.91250900	3.03319100	H	4.36703400	-5.57798400	0.29014000
H	1.56684400	-3.55297200	4.19948100	H	2.69381000	-6.09303000	0.58468200
H	3.01136100	-2.50856100	4.09481800	C	2.89511400	-4.02386600	0.10870000
H	1.42640000	-0.92628700	4.09986700	H	3.21033800	-3.45258700	0.96900400
H	0.22464000	-0.80848400	2.85294700	H	2.07418700	-3.64124400	-0.47933000
H	1.70791500	1.17803800	2.96367800	O	-0.37866400	2.25490800	-0.24128700
H	3.06939200	0.16699300	2.59718100	C	-0.35611500	2.75883100	1.10657400
O	1.01183100	-0.52692400	-2.08247900	C	0.93310900	3.56743200	1.24635900
C	1.62857000	0.06678800	-3.22940600	C	1.20084100	3.99355800	-0.19941100
C	2.29560500	-1.10528200	-3.96176100	C	0.76370100	2.74600900	-0.95552800
C	1.48660000	-2.34137200	-3.49670600	H	0.45492700	2.93339100	-1.98845400
C	0.42711500	-1.74465500	-2.56340300	H	1.55825300	1.98793200	-0.93776900
H	-0.49429500	-1.49605300	-3.11371000	H	0.57266600	4.84712200	-0.47806600
H	0.18155600	-2.34298200	-1.68415900	H	2.24572000	4.25373400	-0.38507000
H	1.03266200	-2.89030100	-4.32509700	H	0.82563000	4.40951200	1.93430700

H	2.14547600	-3.02121600	-2.94901300	H	3.45514000	1.78864300	0.38193800
H	2.27767400	-0.96659400	-5.04527200	H	5.71125300	1.56767900	1.18534000
H	3.33787800	-1.20442400	-3.64501500	H	6.19823400	2.72003500	-0.06707500
H	2.32971600	0.82220900	-2.87385700	H	6.28422300	-0.30068800	-0.13416800
H	0.84653100	0.53476600	-3.84526700	H	7.30378600	0.83021400	-1.05056100
O	4.03094700	0.72091300	-1.25125200	H	5.47081100	1.24067200	-2.64557900
C	5.29538600	0.48373300	-1.86437200	H	5.27388900	-0.51067900	-2.31213600
C	6.28423900	0.62815100	-0.71322100	Br	4.43597100	-2.90096100	-1.24076100
C	5.67307300	1.77782600	0.11369500	H	1.73143300	2.90389100	1.59068600
C	4.21917800	1.85959900	-0.39670600	H	-0.38476300	1.91467500	1.80429200
H	4.06824400	2.76865300	-0.99897900	H	-1.25155300	3.37527700	1.24764700

Table 47. Geometric coordinates and single point M062X energy for transition state **27** with one THF

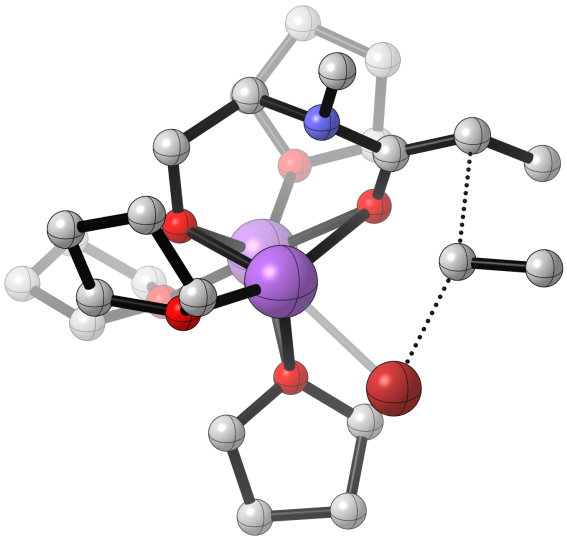


G_{SP} = –3921.15290993

Atom	X	Y	Z	Atom	X	Y	Z
Na	0.00000000	0.00000000	0.00000000	C	-5.45114300	-1.03383100	-3.18621000
Na	1.14224800	-0.78188800	-2.56319600	C	-5.90934800	-0.16707400	-2.19700500
O	-0.89406000	-0.12756400	-2.01173300	C	-4.99991200	0.38934700	-1.29887700
C	-1.69463500	-1.16845900	-2.39527700	C	-3.64593100	0.07894000	-1.39389500
C	-1.41236600	-2.41680400	-1.49789200	H	-2.91570300	0.52400700	-0.72252700
N	-0.09672900	-3.00962900	-1.86415200	H	-5.34868500	1.07518500	-0.52896700
C	0.87241000	-3.05861800	-0.81936100	H	-6.96471100	0.08026800	-2.13243900
O	1.03423000	-1.97630200	-0.16742300	H	-6.15023900	-1.46138000	-3.89944000
C	1.72521900	-4.15572900	-0.69102300	H	-3.74305300	-2.03291800	-4.03775500
C	2.65947100	-4.22526700	0.48458500	O	1.90008700	0.85623600	-1.09390300
H	3.05598900	-3.23139000	0.72277800	C	1.82942800	1.98555100	-1.98478300
H	2.16672800	-4.59556900	1.39518600	C	2.96419900	2.90204300	-1.54739500
H	3.50739400	-4.89263200	0.28880900	C	4.03226900	1.88158200	-1.14368500
H	1.47356200	-5.08679200	-1.18864400	C	3.20112300	0.78684300	-0.48067700
C	-0.17292500	-4.12655900	-2.79109100	H	3.07585900	0.95531400	0.59586500
H	-0.84625200	-3.85791000	-3.61059000	H	3.60924700	-0.21304800	-0.64663700
H	0.81306700	-4.33049200	-3.21658500	H	4.79561100	2.28812900	-0.47640200
H	-0.53790800	-5.05813800	-2.33410700	H	4.51600200	1.47189700	-2.03534700
H	-1.28815100	-2.01130300	-0.48827200	H	2.65611000	3.50421900	-0.68493600
C	-2.51787000	-3.47337700	-1.41812800	H	3.28925300	3.57368700	-2.34521300
H	-2.80538600	-3.86925700	-2.39798300	H	1.97353700	1.63864800	-3.01773200
H	-2.19797700	-4.31268100	-0.78874000	H	0.82979600	2.41558700	-1.89216100
H	-3.41537200	-3.03202600	-0.97579000	Br	3.85972200	-1.04126200	-3.45015800
H	-1.48461700	-1.51230500	-3.44109500	C	4.32622500	-3.81710600	-2.31604800
C	-3.17740300	-0.80587600	-2.36653600	H	5.19402500	-3.38822000	-1.81096000

C	-4.09614200	-1.34991700	-3.26559200	H	4.58434700 -3.98499400 -3.36345100
H	2.31211800	-3.03623100	-2.87927300	H	4.09686100 -4.78182700 -1.85372200
H	3.00025000	-2.27853600	-1.32942500	C	3.14050400 -2.90073500 -2.20159200

Table 48. Geometric coordinates and single point M062X energy for transition state **27** with no Ph and Me group on the backbone

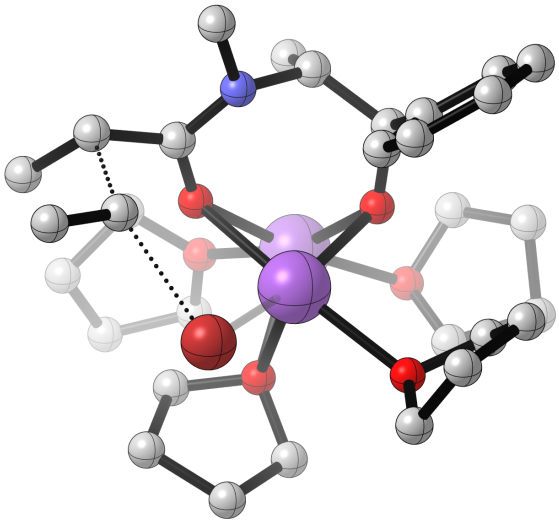


G_{SP} = –4348.1234303

Atom	X	Y	Z	Atom	X	Y	Z
Na	0.00000000	0.00000000	0.00000000	H	-3.14097200	-0.47061000	-0.76938700
Na	2.78529800	-0.32600300	0.78859800	H	-3.19553200	-2.08895800	-1.53299100
O	0.90949700	-0.98532500	1.75060900	H	-3.55939700	-1.43080600	1.43298200
C	0.94476100	-0.40059700	2.98686800	H	-4.60636100	-2.46189600	0.43884900
C	0.80615800	1.15009200	2.84724400	H	-2.51841000	-3.52125200	1.97393800
N	2.06982600	1.71880400	2.30300200	H	-3.01469000	-4.25254800	0.44302100
C	1.95166500	2.41728700	1.06551400	H	-0.98678200	-3.64339100	-0.51455000
O	1.30214500	1.81240200	0.15181000	H	-0.48071300	-2.75982500	0.96530400
C	2.69390500	3.57499000	0.82842900	O	-1.77746800	1.48844500	0.10377300
C	2.46445200	4.34653500	-0.44113300	C	-1.53790600	2.81596100	-0.36735500
H	2.28693100	3.66495200	-1.28118300	C	-1.41189800	3.64817300	0.90095600
H	1.58890400	5.00905300	-0.38115500	C	-2.45715400	3.00006100	1.82535800
H	3.32458400	4.97918100	-0.69135400	C	-2.61364100	1.57051300	1.26079300
H	3.13492400	4.10558700	1.66616700	H	-3.65355200	1.36291900	0.97407200
C	2.98156900	2.23965300	3.30798800	H	-2.28479200	0.79667600	1.96169600
H	3.06967500	1.50720300	4.11599400	H	-3.40904900	3.53587300	1.77223900
H	3.97448500	2.38685300	2.87524900	H	-2.13672400	2.99311700	2.86946400
H	2.66197900	3.19819300	3.74267200	H	-1.60150200	4.71043500	0.72826100
H	-0.00145900	1.37697400	2.18303000	H	-0.39978800	3.53735600	1.30272700
H	0.60796100	1.57774200	3.80783300	H	-0.62319200	2.79410400	-0.96128100
H	1.87456800	-0.63248800	3.46287800	H	-2.38951900	3.14540200	-0.98162500
H	0.13826500	-0.77706400	3.58078600	C	5.44578700	2.96824400	-0.42839600
O	1.78363400	-0.92727900	-1.22429400	H	5.52638500	2.98240700	-1.51717300
C	2.08454400	-2.33534200	-1.19559000	H	6.41032600	2.66771900	-0.01461100
C	2.25755600	-2.72952300	-2.65629500	H	5.21807200	3.98134800	-0.08371700
C	2.91940900	-1.47225800	-3.22754700	C	4.36223200	2.02357500	0.01010300
C	2.19487700	-0.35607100	-2.48054200	H	4.35447200	1.68110500	1.03308200

H	1.29445700	-0.01954200	-3.00875200	H	3.34900300	-3.98544200	2.29895100
H	2.83835100	0.50303300	-2.27616200	H	2.74053300	-2.47926200	4.77319700
H	2.82191600	-1.38076200	-4.31168800	H	3.95094600	-3.74308800	4.53363900
H	3.97984100	-1.45146800	-2.95930600	H	4.28139000	-0.74487400	4.25216000
H	1.28048100	-2.90058300	-3.12259400	H	5.51156500	-1.93304400	4.72749800
H	2.86525600	-3.62925400	-2.77655600	H	5.75232400	-2.68245500	2.39058300
H	3.01238100	-2.49357400	-0.62798700	H	5.55186100	-0.92796900	2.15827400
H	1.26355600	-2.83671500	-0.67850500	Br	5.23663400	-0.04883700	-0.67863600
O	3.85181000	-2.02306700	1.89840100	O	-1.53052700	-1.64981900	-0.37652400
C	5.08683200	-1.82468400	2.57313000	C	-1.29500600	-2.91851600	0.25051400
C	4.68196500	-1.74281900	4.04232800	C	-2.63215500	-3.33715500	0.90319000
C	3.56476700	-2.80199400	4.13208400	C	-3.57208800	-2.15367800	0.60970300
C	3.10865300	-2.97764600	2.66477800	C	-2.92495400	-1.53134000	-0.62333400
H	2.05432500	-2.75404900	2.48856400	H	3.48063600	1.86859400	-0.59508100

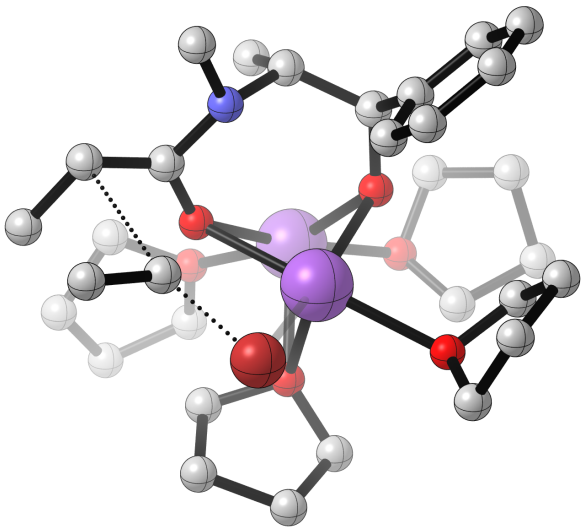
Table 49. Optimized geometries at the M062X level of theory with 6-31G(d) basis set for forward and reverse IRC calculations of transition structures **26**/**27** at 195K with free energies (Hartrees), corrected M062X energies and cartesian coordinates (X, Y, Z). (Note: G_{SP} includes single-point M062X corrections to M062X/6-311+G(2d,p) optimized structures.) The 2D representations below correspond to the transition state, which the IRC has been done.



Forward IRC of 26
G = –4615.59525390
G_{SP} = –4618.50749917

Atom	X	Y	Z
Na	0.00000000	0.00000000	0.00000000
Na	-2.01594400	-1.76096000	0.91303800
O	-2.15673800	0.05346200	-0.33236000
C	-2.79287200	-0.01007600	-1.53228300
C	-2.05010300	-0.83644000	-2.62558200
N	-1.88772700	-2.28556700	-2.34244500
C	-0.75468300	-2.75836100	-1.72529300
O	-0.19858800	-2.09843800	-0.81878900
C	-0.36693100	-4.15691800	-1.93162700
C	1.03355600	-4.57290600	-1.52530400
H	1.28771900	-4.13591000	-0.55478000
H	1.81564600	-4.28742100	-2.24028000
H	1.06551100	-5.66261500	-1.41928400
H	-0.69307200	-4.60091500	-2.87140500
C	-2.62545100	-3.15037000	-3.25810800
H	-2.76243000	-4.14281800	-2.82550200
H	-2.12459800	-3.25087000	-4.23142800
H	-3.61552900	-2.71771300	-3.41123300
C	-0.73165100	-0.20640600	-3.07799200
H	-0.91312300	0.81923300	-3.41360300
H	0.03388800	-0.18415200	-2.30041000
H	-0.31597900	-0.77013700	-3.92127200
H	-2.70455200	-0.80802600	-3.50546200
H	-3.68415800	0.65990000	1.16284500
H	-3.95145700	1.19516000	2.85871000
H	-5.94311800	-0.14241300	1.08433800
H	-6.19312900	0.61151600	2.66534400
H	-5.50037800	-2.26794700	2.02898200
H	-6.35758200	-1.64896600	3.45857000
H	-4.21784500	-0.91323500	4.44384400
H	-3.74635600	-2.45639100	3.63515100
Br	-2.83138800	-4.27982500	1.85104500
O	-0.11571500	2.19535900	0.63721800
C	-0.75708000	2.85313900	-0.46959300
C	-2.16018500	3.23102900	0.00270400
C	-1.96688900	3.34401100	1.51718500
C	-0.99467500	2.19968700	1.77194900
H	-0.37984500	2.32412500	2.66811800
H	-1.53271200	1.24343300	1.82040700
H	-1.50632700	4.30223100	1.78242800
H	-2.89785800	3.23549300	2.07846100
H	-2.52189700	4.15241500	-0.45987400
H	-2.84618400	2.40910900	-0.22113800
H	-0.78403300	2.16918800	-1.32536600
H	-0.15559200	3.73187600	-0.73048000
O	2.21779800	-0.23282900	-0.30953700

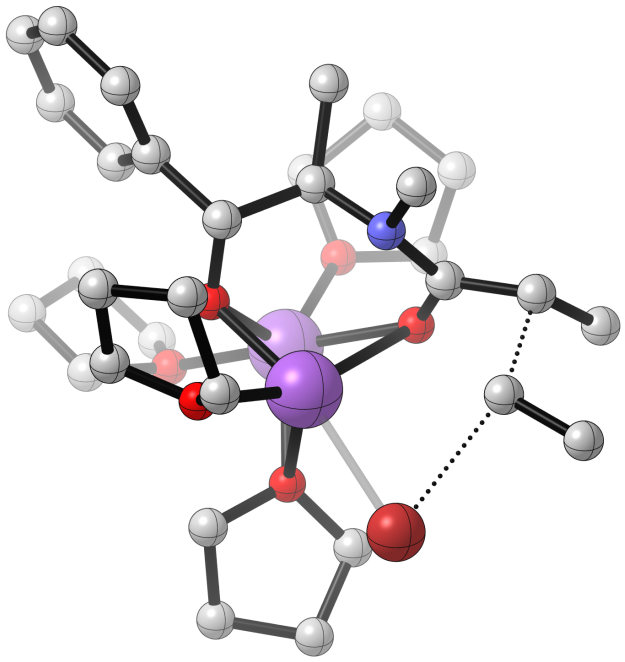
H	-2.86773800	0.99710900	-2.01802000
C	-4.24619300	-0.49838500	-1.42645100
C	-5.29179900	0.30069200	-1.89461900
C	-6.62014400	-0.11630100	-1.81286300
C	-6.92880300	-1.35704200	-1.26280500
C	-5.89931500	-2.16589400	-0.78350800
C	-4.57686900	-1.73489000	-0.85556700
H	-3.80917900	-2.39610900	-0.46109800
H	-6.12007400	-3.13319000	-0.33963400
H	-7.96101400	-1.68855600	-1.20033300
H	-7.41287300	0.52992100	-2.17945700
H	-5.05788700	1.27160000	-2.32763500
O	-0.00442800	-1.11190200	2.08636000
C	-0.28085900	-0.90751500	3.48001200
C	-0.31919100	-2.31796500	4.08221800
C	0.52957000	-3.16420700	3.10277000
C	0.98885000	-2.14503100	2.05568000
H	1.96172000	-1.70182700	2.32373300
H	1.02995000	-2.51812700	1.03084000
H	1.37839500	-3.65494900	3.58527100
H	-0.11134900	-3.92513700	2.64729200
H	0.06960100	-2.32846500	5.10331100
H	-1.34450800	-2.69884100	4.09283000
H	-1.22718200	-0.37051200	3.55088500
H	0.53327800	-0.30451300	3.90897200
O	-3.32527400	-0.75203600	2.58200500
C	-4.17052700	-1.46248800	3.48932400
C	-5.51953300	-1.47190800	2.77988700
C	-5.56096900	-0.08484400	2.10661200
C	-4.08866900	0.37478000	2.13655800
C	2.82077900	-1.19225000	-1.17185000
C	3.80915000	-1.93083700	-0.27369400
C	4.30039000	-0.82079200	0.67888300
C	3.24501100	0.29869200	0.52442500
H	2.77474600	0.59908400	1.46462700
H	3.67502900	1.18885600	0.04845900
H	4.37029300	-1.17573400	1.70979200
H	5.28935900	-0.45740500	0.38875300
H	3.28797600	-2.71632100	0.28088200
H	4.62077800	-2.39526400	-0.83813600
H	3.33919400	-0.67503600	-1.99330800
H	2.01955200	-1.81600200	-1.57033600
C	-1.63419900	-6.17411900	-0.28261900
H	-1.14034700	-6.52728700	0.62467200
H	-2.68257900	-6.47177700	-0.22527100
H	-1.17837200	-6.68080700	-1.14223600
C	-1.48430700	-4.66813700	-0.45313800
H	-2.40389200	-4.13516700	-0.66399000
H	-0.86544400	-4.16872400	0.28110200



Reverse IRC of 26
G = –4615.56379671
G_{SP} = –4618.47663485

Atom	X	Y	Z
Na	0.00000000	0.00000000	0.00000000
Na	0.01557900	0.00156700	2.78339700
O	1.69319000	-0.01175400	1.39653600
C	0.48938900	-2.53933200	5.01058600
C	1.74138800	-2.08315500	5.75184800
C	2.84717000	-2.29140200	4.69655200

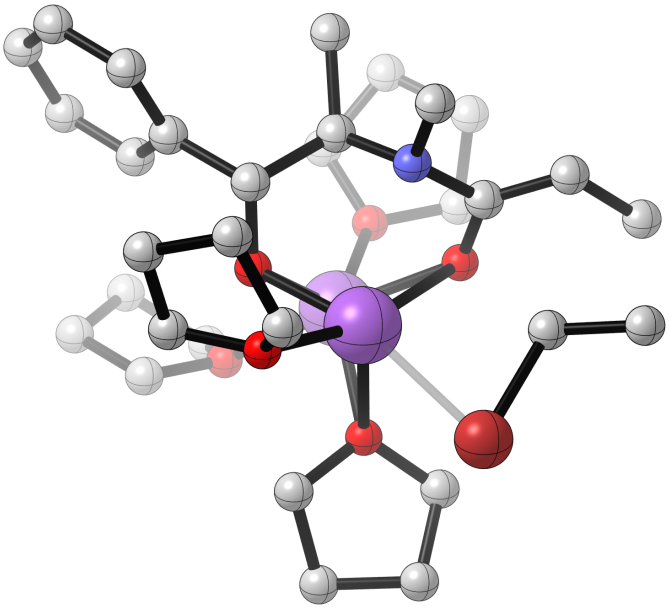
C	2.63113400	0.97420500	1.49432900
C	2.14192800	2.41474900	1.14010500
N	1.10865600	2.95374800	2.05525700
C	-0.26465800	2.90507200	1.66060800
O	-0.68241100	1.74844300	1.23335400
C	-1.09956000	3.96756200	1.89273600
C	-2.57087500	3.88314800	1.59673000
H	-2.88798200	2.83579000	1.51779400
H	-2.85056200	4.36502000	0.64702400
H	-3.18765700	4.36042700	2.37211800
H	-0.70556200	4.92967800	2.19859000
C	1.55041500	4.14054000	2.76569600
H	0.87805300	4.34571500	3.60543800
H	1.58111800	5.04426100	2.13333300
H	2.55045200	3.96056600	3.16910600
C	1.78765000	2.57892300	-0.34066000
H	2.63375200	2.26911000	-0.96377400
H	0.90265200	2.01200800	-0.63706700
H	1.57149200	3.63107700	-0.55667500
H	3.02491000	3.05107300	1.29373100
H	3.46860000	0.81557400	0.76656000
C	3.31795800	1.00000000	2.86980500
C	4.70167300	0.83936100	2.97126600
C	5.35289700	0.86359000	4.20463200
C	4.62476500	1.05800600	5.37452400
C	3.24110100	1.21357000	5.29644400
C	2.59919600	1.17265000	4.06172600
H	1.52397300	1.32147400	4.03044400
H	2.65780200	1.36811100	6.20131200
H	5.12713700	1.08608700	6.33693400
H	6.43065300	0.73305500	4.24967300
H	5.27917400	0.69290300	2.06040100
O	-1.56740200	-1.14248900	1.37486400
C	-1.90131300	-2.43540100	1.88412000
C	-2.93584000	-2.16329200	2.98564900
C	-3.54683400	-0.79685500	2.58782500
C	-2.81365100	-0.43813800	1.28907000
H	-3.36314100	-0.80599100	0.40828000
H	-2.56432800	0.61790500	1.16268300
H	-4.62880300	-0.84096500	2.44337600
H	-3.33672800	-0.05621000	3.36437900
H	-3.68000800	-2.96083700	3.04699600
H	-2.44111000	-2.08761000	3.95871100
H	-0.98149100	-2.89754100	2.24406200
H	-2.33214400	-3.03566600	1.06934000
O	0.70160400	-2.08192200	3.67972900
C	2.06803000	-2.41010300	3.37036500
H	2.37959900	-1.70912900	2.59176500
H	2.09281500	-3.44295300	2.99196400
H	3.54582200	-1.45159100	4.67768600
H	3.41623100	-3.20426200	4.89339800
H	1.64357800	-1.01940300	5.99116600
H	1.91466900	-2.63570500	6.67843400
H	0.39669900	-3.63703900	5.01320400
H	-0.44052000	-2.10320400	5.38139800
Br	-1.27249400	0.55865400	5.25288800
O	1.01374300	-1.76778100	-1.07919400
C	2.32996900	-1.27451900	-1.38902700
C	3.29948400	-2.01886900	-0.47183200
C	2.53805400	-3.31653100	-0.18846800
C	1.10918900	-2.79759200	-0.08829600
H	0.34368400	-3.54727900	-0.31096500
H	0.92816200	-2.36533200	0.90526900
H	2.63093500	-4.01615100	-1.02675500
H	2.86828100	-3.81955400	0.72377600
H	4.27455300	-2.17993000	-0.93785800
H	3.41828700	-1.44949700	0.45428500
H	2.35557000	-0.19282600	-1.21876200
H	2.52083000	-1.47890900	-2.44913200
O	-1.52710500	0.58926200	-1.54235700
C	-2.08139700	1.89966100	-1.64104400
C	-3.59005300	1.66444800	-1.60307500
C	-3.75054600	0.31650700	-2.33775300
C	-2.32454600	-0.28161500	-2.33479100
H	-2.26250600	-1.27734500	-1.88580300
H	-1.91353600	-0.33332600	-3.35132100
H	-4.46818500	-0.33619100	-1.83410900
H	-4.10309000	0.46090400	-3.36221800
H	-3.92238000	1.58513900	-0.56400600
H	-4.15104000	2.47381200	-2.07573300
H	-1.77502400	2.35584900	-2.59449400
H	-1.68854800	2.47515000	-0.79922400
C	-2.17715200	3.35766000	4.98407800
H	-3.21306400	3.04030000	5.12915600
H	-1.73053500	3.56056200	5.96083100
H	-2.16821000	4.27935700	4.39362100
C	-1.38639400	2.32870600	4.21703400
H	-0.33899100	2.57539400	4.08216200
H	-1.82992000	2.01708200	3.27801600



Forward IRC of 27
G = –4615.59493012
G_{SP} = –4618.50990286

Atom	X	Y	Z	Atom	X	Y	Z
Na	0.00000000	0.00000000	0.00000000	C	3.25242000	4.88447600	-1.17466600
Na	2.16154000	1.84550100	-0.72169900	C	2.31260800	5.60216200	-2.14152000
O	-0.04014900	2.11840000	-0.59150200	C	1.09336600	5.90727400	-1.24719300
C	-0.41009200	2.54178500	-1.83508800	C	1.24317900	4.90818300	-0.07569800
C	-0.23465600	1.37560900	-2.85781200	H	0.39617400	4.23080300	0.05067400
N	1.20825900	1.13624400	-3.13938400	H	1.44253500	5.43844000	0.86587900
C	1.72555700	-0.09764200	-2.76384900	H	0.14620800	5.77078200	-1.77609500
O	1.39211500	-0.58578100	-1.66972400	H	1.12464700	6.93840400	-0.88412400
C	2.85430600	-0.66452200	-3.50996000	H	2.03265000	4.91836100	-2.95138100
C	3.11952800	-2.14419600	-3.29380700	H	2.75393700	6.49725900	-2.58653200
H	3.16617700	-2.35254500	-2.22113300	H	3.77829000	5.60176900	-0.52667100
H	2.35965700	-2.80234000	-3.73316400	H	3.98938300	4.21326100	-1.61966600
H	4.08597600	-2.40816900	-3.73374900	Br	4.98937100	1.72718000	-0.33733300
H	2.91258300	-0.35407300	-4.55437000	O	-1.49989500	0.22665400	1.69238100
C	1.73556200	1.82638900	-4.31188300	C	-1.74760900	1.55562400	2.17518000
H	1.36415600	2.85414000	-4.29850500	C	-3.28340100	1.70638900	2.26415500
H	2.82489300	1.86313500	-4.27264100	C	-3.81768000	0.36154100	1.73856600
H	1.43327100	1.36024700	-5.25812900	C	-2.63722800	-0.57034800	1.99250700
H	-0.58272100	0.48306600	-2.32753200	H	-2.59936200	-1.45028500	1.34628800
C	-1.03596900	1.46014600	-4.15846100	H	-2.60715400	-0.88926600	3.04532000
H	-0.85129700	2.38246000	-4.71855600	H	-4.01760700	0.41363900	0.66235400
H	-0.80563000	0.60823200	-4.80964200	H	-4.73202500	0.03880500	2.24216900
H	-2.10338700	1.43754500	-3.92410600	H	-3.64100800	2.55423500	1.67541300
H	0.23566600	3.37116700	-2.22243400	H	-3.59470800	1.86226100	3.30076300
C	-1.84195000	3.07258100	-1.87850200	H	-1.28182000	1.66890000	3.16243500
C	-2.23036500	4.09933600	-2.74039800	H	-1.27343800	2.23517700	1.45967700

C	-3.55384200	4.53345800	-2.78733700
C	-4.51314000	3.93927300	-1.97092900
C	-4.13486100	2.91887200	-1.09989400
C	-2.80768500	2.50015100	-1.04932300
H	-2.48547000	1.72810300	-0.35480800
H	-4.87636100	2.45713700	-0.45070300
H	-5.54489900	4.27577700	-2.00557300
H	-3.83610500	5.33987800	-3.45811900
H	-1.48395000	4.56593200	-3.38261600
O	1.94093000	0.54481900	1.19571200
C	1.97543600	1.61702300	2.16056500
C	2.64996500	1.01770300	3.38714400
C	3.68368400	0.09509800	2.73554400
C	2.91729300	-0.45939800	1.53891200
H	2.37475800	-1.38234400	1.78189800
H	3.56523400	-0.61995800	0.67400200
H	4.04629300	-0.69286700	3.39990700
H	4.52900000	0.68143000	2.36270100
H	1.92758000	0.44199500	3.97809100
H	3.09862900	1.78072300	4.02731700
H	2.56659600	2.44672500	1.75023300
H	0.94629000	1.94798800	2.31856800
O	2.37003800	4.09020500	-0.39164300
O	-1.39320100	-1.63250900	-0.89003600
C	-0.77363700	-2.71170100	-1.59018300
C	-1.03140000	-2.40350000	-3.05880500
C	-2.45009700	-1.80972100	-3.02585300
C	-2.60009700	-1.29042900	-1.57829700
H	-3.45362900	-1.75759900	-1.06974800
H	-2.71450100	-0.20330200	-1.52319900
H	-3.19734900	-2.58041500	-3.23315300
H	-2.58167600	-1.01315100	-3.76138200
H	-0.95603900	-3.28772900	-3.69612000
H	-0.30383500	-1.66355500	-3.40665200
H	0.28412600	-2.71597000	-1.32291100
H	-1.24267400	-3.66127300	-1.29334700
C	5.54838400	-0.05603700	-2.80660700
H	6.02783900	-0.67034300	-2.04214200
H	6.13976200	0.85413500	-2.91493800
H	5.57561000	-0.60372400	-3.75664700
C	4.09884100	0.25248100	-2.44397700
H	3.82694600	1.29496600	-2.56939800
H	3.76299400	-0.15322200	-1.49778300



Forward IRC of 27
G = – -4615.56693022
G_{SP} = – -4618.48221221

Atom	X	Y	Z
Na	0.00000000	0.00000000	0.00000000
Na	2.10393100	1.83039400	-0.71501800
O	-0.05465100	2.15084700	-0.52111500
C	-0.41801400	2.57515600	-1.77294200
C	3.25538300	4.90502900	-1.09553400
C	2.30873800	5.63501000	-2.04286100
C	1.09814900	5.92433600	-1.13357700
C	1.24901200	4.90182200	0.01662100

C	-0.22297600	1.42543500	-2.81515300
N	1.23211900	1.23515300	-3.06518000
C	1.71288200	-0.10447800	-2.80037000
O	1.44388200	-0.52394300	-1.60492100
C	2.51028600	-0.76295400	-3.69246400
C	3.08045600	-2.10865100	-3.33762100
H	3.20339500	-2.19897300	-2.25090200
H	2.43024200	-2.94183400	-3.64380400
H	4.05581600	-2.29009000	-3.80708400
H	2.66815400	-0.37725900	-4.69336800
C	1.72007400	1.89710500	-4.26161700
H	1.36947900	2.93470200	-4.26531100
H	2.81473400	1.90409000	-4.25957200
H	1.39656000	1.42201200	-5.20047500
H	-0.55941100	0.52040200	-2.29761100
C	-1.04204500	1.52491600	-4.10577400
H	-0.86687400	2.45655900	-4.65489300
H	-0.80422000	0.68490400	-4.76958600
H	-2.10967700	1.48773500	-3.87020800
H	0.22891600	3.41041100	-2.14817200
C	-1.84596700	3.10948900	-1.80417800
C	-2.23563600	4.14972600	-2.64895100
C	-3.55813400	4.58763700	-2.68488300
C	-4.51611800	3.98365400	-1.87432400
C	-4.13694800	2.94932100	-1.01994200
C	-2.81089300	2.52775600	-0.98001900
H	-2.48711400	1.74248000	-0.30156400
H	-4.87811600	2.47787600	-0.37701600
H	-5.54766000	4.32191400	-1.90153900
H	-3.84156400	5.40327700	-3.34426200
H	-1.49068300	4.61972200	-3.29050900
O	1.95747600	0.54495800	1.21982500
C	1.97755900	1.58748800	2.20999700
C	2.66008100	0.96739600	3.42245600
C	3.68837600	0.05095800	2.75259800
C	2.91138500	-0.47965000	1.55044400
H	2.35807800	-1.39522100	1.79053700
H	3.53664000	-0.66614000	0.67393300
H	4.05064800	-0.74887000	3.40218300
H	4.54452500	0.63740300	2.40524100
H	1.94046400	0.37913000	4.00276600
H	3.10955500	1.71549800	4.07937100
H	2.54897600	2.44301700	1.82122000
H	0.94641900	1.90549300	2.37707600
O	2.39197300	4.09557600	-0.30960600
H	0.41161400	4.20800700	0.11962600
H	1.44283600	5.41147200	0.97034600
H	0.14890600	5.79769800	-1.65983500
H	1.13447300	6.94784900	-0.74993900
H	2.02320400	4.96110100	-2.85762300
H	2.74801900	6.53689400	-2.47577600
H	3.79600200	5.61274900	-0.44777500
H	3.98211200	4.24831100	-1.57984800
Br	4.97864200	1.69420300	-0.35075500
O	-1.49421500	0.21090800	1.72829800
C	-1.74135500	1.53311700	2.22580400
C	-3.27653500	1.68440900	2.32253000
C	-3.81312300	0.34831400	1.77769700
C	-2.63352500	-0.58952000	2.01380700
H	-2.59634300	-1.45621400	1.35009100
H	-2.60388600	-0.92740000	3.06116100
H	-4.01507900	0.41731800	0.70312200
H	-4.72648600	0.01878000	2.27886500
H	-3.63440600	2.54093500	1.74666200
H	-3.58460000	1.82492900	3.36251300
H	-1.27422200	1.63636800	3.21462600
H	-1.27035100	2.21983200	1.51443700
O	-1.40862900	-1.61447200	-0.87999800
C	-0.77987700	-2.67629500	-1.60262400
C	-1.04215100	-2.34521900	-3.06479500
C	-2.46186700	-1.75368000	-3.02102200
C	-2.60974200	-1.25502600	-1.56669900
H	-3.46930600	-1.72216300	-1.06631100
H	-2.71675900	-0.16761600	-1.49869700
H	-3.21138100	-2.52048000	-3.23721500
H	-2.59386500	-0.94536600	-3.74362700
H	-0.97191000	-3.22286600	-3.71236000
H	-0.30561100	-1.60814400	-3.40061700
H	0.28056400	-2.66326100	-1.34644800
H	-1.23981500	-3.63413300	-1.31497700
C	5.59573300	0.05421500	-2.70149700
H	6.12639500	-0.69064900	-2.10373200
H	6.29702600	0.84071500	-2.99072200
H	5.21269700	-0.42702000	-3.60527500
C	4.41245900	0.61876400	-1.95421600
H	3.84811600	1.33346800	-2.54918700
H	3.73857200	-0.13359900	-1.54614600