

SUPPORTING INFORMATION

Lithium Amino Alkoxide–Evans Enolate Mixed Aggregates: Aldol Addition with Matched and Mismatched Stereocontrol

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Chart 1. Substrates and aggregates S-14

Part 1. Substrates And Products

Figure 1.	¹ H NMR spectrum of 11	S-15
Figure 2.	¹³ C NMR spectrum of 11	S-16
Figure 3.	¹ H NMR spectrum of 8	S-17
Figure 4.	¹³ C NMR spectrum of 8	S-18
Figure 5.	¹ H NMR spectrum of 1a	S-19
Figure 6.	¹³ C NMR spectrum of 1a	S-20
Figure 7.	¹ H NMR spectrum of (<i>R,S</i>)- 2a	S-21
Figure 8.	¹³ C NMR spectrum of (<i>R,S</i>)- 2a	S-22
Figure 9.	¹ H NMR spectrum of (<i>S,R</i>)- 2a	S-23
Figure 10.	¹³ C NMR spectrum of (<i>S,R</i>)- 2a	S-24
Figure 11.	¹ H NMR spectrum of (<i>R,R</i>)- 2a	S-25
Figure 12.	¹³ C NMR spectrum of (<i>R,R</i>)- 2a	S-26
Figure 13.	¹ H NMR spectrum of (<i>S,S</i>)- 2a	S-27
Figure 14.	¹³ C NMR spectrum of (<i>S,S</i>)- 2a	S-28
Figure 15.	¹ H NMR spectrum of 2a aldol products	S-29

Figure 16.	^1H NMR spectrum of 1b	S-30
Figure 17.	^{13}C NMR spectrum of 1b	S-31
Figure 18.	^1H NMR spectrum of (<i>R,S</i>)- 2b	S-32
Figure 19.	^{13}C NMR spectrum of (<i>R,S</i>)- 2b	S-33
Figure 20.	^1H NMR spectrum of (<i>S,R</i>)- 2b	S-34
Figure 21.	^{13}C NMR spectrum of (<i>S,R</i>)- 2b	S-35
Figure 22.	^1H NMR spectrum of (<i>R,R</i>)- 2b	S-36
Figure 23.	^{13}C NMR spectrum of (<i>R,R</i>)- 2b	S-37
Figure 24.	^1H NMR spectrum of (<i>S,S</i>)- 2b	S-38
Figure 25.	^{13}C NMR spectrum of (<i>S,S</i>)- 2b	S-39
Figure 26.	^1H NMR spectrum of 2b aldol products	S-40
	Pivaldehyde- <i>d</i> Synthesis	S-41
Figure 27.	^1H NMR spectrum of neopentyl alcohol- d_2	S-42
Figure 28.	^{13}C NMR spectrum of neopentyl alcohol- d_2	S-43
Figure 29.	^1H NMR spectrum of pivaldehyde- <i>d</i>	S-44
Figure 30.	^{13}C NMR spectrum of pivaldehyde- <i>d</i>	S-45
	Synthesis of 51	S-46
Figure 31.	^1H NMR spectrum of ethyl 2-morpholinoacetate	S-47
Figure 32.	^1H NMR spectrum of 51	S-48

Part 2. Aggregate Characterization

Figure 33.	^6Li NMR spectra of the method of continuous variation of 11 and CyOLi in THF	S-49
Figure 34.	Job plot of 11 and CyOLi in THF	S-50
Figure 35.	^6Li NMR spectra of the method of continuous variation of 11 and (<i>S</i>)- 1a in toluene	S-51

Figure 36.	^6Li NMR spectra of the method of continuous variation of 11 and (R)- 1a in toluene	S-52
Figure 37.	^6Li NMR spectra of the method of continuous variation of 11 and (S)- 1b in toluene	S-53
Figure 38.	^6Li NMR spectra of the method of continuous variation of 11 and (R)- 1b in toluene	S-54
Figure 39.	^6Li NMR spectra of the method of continuous variation of (S)- 15a and (S)- 15b in toluene	S-55
Figure 40.	Job plot of (S)- 15a and (S)- 15b in toluene	S-56
Figure 41.	^6Li NMR spectra of the method of continuous variation of (S)- 15a and (R)- 15b in toluene	S-57
Figure 42.	Job plot of (S)- 15a and (R)- 15b in toluene	S-58
Figure 43.	^6Li NMR spectra of the method of continuous variation of (R)- 15a and (S)- 15b in toluene	S-59
Figure 44.	Job plot of (R)- 15a and (S)- 15b in toluene	S-60
Figure 45.	^6Li NMR spectra of the method of continuous variation of (R)- 15a and (R)- 15b in toluene	S-61
Figure 46.	Job plot of (R)- 15a and (R)- 15b in toluene	S-62
Figure 47.	^6Li NMR spectra of the method of continuous variation of 8 and (S)- 1a in toluene	S-63
Figure 48.	^6Li NMR spectra of the method of continuous variation of 8 and (R)- 1a in toluene	S-64
Figure 49.	^6Li NMR spectra of the method of continuous variation of 8 and (S)- 1b in toluene	S-65
Figure 50.	^6Li NMR spectra of the method of continuous variation of (S)- 36a and (S)- 36b in toluene	S-66
Figure 51.	Job plot of (S)- 36a and (S)- 36b in toluene	S-67
Figure 52.	^6Li NMR spectra of the method of continuous variation of (S)- 1b and 8 in toluene	S-68
Figure 53.	Job plot of (S)- 1b and 8 in toluene	S-69

Figure 54.	^6Li NMR spectra of (<i>S</i>)- 15a with changing pyridine concentration	S-70
Figure 55.	^6Li NMR spectra of an unaged mixture of (<i>S</i>)- 15b and (<i>S</i>)- 15a	S-71
Figure 56.	^6Li NMR spectra of (<i>S</i>)- 16a with changing THF concentration	S-72
Figure 57.	^6Li NMR spectra of the method of continuous variation of 11 and (<i>S</i>)- 1a in THF	S-73
Figure 58.	^6Li NMR spectra of the method of continuous variation of 11 and (<i>R</i>)- 1a in THF	S-74
Figure 59.	^6Li NMR spectra of the method of continuous variation of 11 and (<i>S</i>)- 1b in THF	S-75
Figure 60.	^6Li NMR spectra of the method of continuous variation of (<i>S</i>)- 16a and (<i>R</i>)- 16a in THF	S-76
Figure 61.	^6Li NMR and $^6\text{Li}\{^{15}\text{N}\}$ NMR spectra of [$^6\text{Li},^{15}\text{N}$]- (<i>S</i>)- 16a in THF	S-77
Figure 62.	^{15}N NMR and $^{15}\text{N}\{^6\text{Li}\}$ NMR spectra of [$^6\text{Li},^{15}\text{N}$]- (<i>S</i>)- 16a in THF	S-78
Figure 63.	^6Li NMR spectra of (<i>S</i>)- 16a with changing pyridine concentration in THF	S-79
Figure 64.	^6Li NMR spectra of (<i>S</i>)- 16a with changing HMPA concentration in THF	S-80
Figure 65.	^6Li NMR spectra of (<i>R</i>)- 16a with varying temperature	S-81
Figure 66.	^6Li NMR spectra of the method of continuous variation of 51 and (<i>S</i>)- 1b in toluene	S-82
	2D NMR analysis of 2:2 mixed aggregate (<i>S</i>)- 15a	S-83
Table 1.	^1H and ^{13}C chemical shift assignments for (<i>S</i>)- 15a	S-84
Figure 67.	^1H NMR spectrum of (<i>S</i>)- 15a	S-85
Figure 68.	Full display HSQC spectrum of (<i>S</i>)- 15a	S-86
Figure 69.	Expansion HSQC spectrum of (<i>S</i>)- 15a	S-87

Figure 70.	Full display HMBC spectrum of (<i>S</i>)- 15a	S-88
Figure 71.	Expansion HMBC spectrum of (<i>S</i>)- 15a	S-89
Figure 72.	Full display HSQC-TOCSY spectrum of (<i>S</i>)- 15a	S-90
Figure 73.	Expansion HSQC-TOCSY spectrum of (<i>S</i>)- 15a	S-91
Figure 74.	Full display ROESY spectrum of (<i>S</i>)- 15a	S-92
Figure 75.	Expansion ROESY spectrum of (<i>S</i>)- 15a	S-93
Figure 76.	Full display HSQC-NOESY spectrum of (<i>S</i>)- 15a	S-94
Figure 77.	Expansion HSQC-NOESY spectrum of (<i>S</i>)- 15a	S-95
Figure 78.	Expansion HSQC-NOESY spectrum of (<i>S</i>)- 15a	S-96
	2D NMR analysis of 2:2 mixed aggregate (<i>R</i>)- 15a	S-97
Table 2.	¹ H and ¹³ C chemical shift assignments for (<i>R</i>)- 15a	S-98
Figure 79.	¹ H NMR spectrum of (<i>R</i>)- 15a	S-99
Figure 80.	Full display HSQC spectrum of (<i>R</i>)- 15a	S-100
Figure 81.	Expansion HSQC spectrum of (<i>R</i>)- 15a	S-101
Figure 82.	Full display HMBC spectrum of (<i>R</i>)- 15a	S-102
Figure 83.	Expansion HMBC spectrum of (<i>R</i>)- 15a	S-103
Figure 84.	Full display HSQC-TOCSY spectrum of (<i>R</i>)- 15a	S-104
Figure 85.	Expansion HSQC-TOCSY spectrum of (<i>R</i>)- 15a	S-105
Figure 86.	Full display ROESY spectrum of (<i>R</i>)- 15a	S-106
Figure 87.	Expansion ROESY spectrum of (<i>R</i>)- 15a	S-107
Figure 88.	Full display HSQC-NOESY spectrum of (<i>R</i>)- 15a	S-108
Figure 89.	Expansion HSQC-NOESY spectrum of (<i>R</i>)- 15a	S-109
Figure 90.	Expansion HSQC-NOESY spectrum of (<i>R</i>)- 15a	S-110
	2D NMR analysis of 1:3 mixed aggregate (<i>S</i>)- 16a	S-111
Table 3.	¹ H and ¹³ C chemical shift assignments for (<i>S</i>)- 16a	S-113

Figure 91.	^1H NMR spectrum of (<i>S</i>)- 16a	S-116
Figure 92.	Full display HSQC spectrum of (<i>S</i>)- 16a	S-117
Figure 93.	Expansion HSQC spectrum of (<i>S</i>)- 16a	S-118
Figure 94.	Expansion HSQC spectrum of (<i>S</i>)- 16a	S-119
Figure 95.	Full display HMBC spectrum of (<i>S</i>)- 16a	S-120
Figure 96.	Expansion HMBC spectrum of (<i>S</i>)- 16a	S-121
Figure 97.	Full display HSQC-TOCSY spectrum of (<i>S</i>)- 16a	S-122
Figure 98.	Expansion HSQC-TOCSY spectrum of (<i>S</i>)- 16a	S-123
Figure 99.	Full display ROESY spectrum of (<i>S</i>)- 16a	S-124
Figure 100.	Expansion ROESY spectrum of (<i>S</i>)- 16a	S-125
Figure 101.	Expansion ROESY spectrum of (<i>S</i>)- 16a	S-126
Figure 102.	Full display HSQC-NOESY spectrum of (<i>S</i>)- 16a	S-127
Figure 103.	Expansion HSQC-NOESY spectrum of (<i>S</i>)- 16a	S-128
Figure 104.	Expansion HSQC-NOESY spectrum of (<i>S</i>)- 16a	S-129
Figure 105.	^1H - ^{15}N HMBC spectrum of (<i>S</i>)- 16a	S-130
Figure 106.	Selectively decoupled ^6Li NMR spectrum of (<i>S</i>)- 16a	S-131
	2D NMR analysis of 1:3 mixed aggregate (<i>R</i>)- 16a	S-132
Table 4.	^1H and ^{13}C chemical shift assignments for (<i>R</i>)- 16a	S-134
Figure 107.	^1H NMR spectrum of (<i>R</i>)- 16a	S-136
Figure 108.	Full display HSQC spectrum of (<i>R</i>)- 16a	S-137
Figure 109.	Expansion HSQC spectrum of (<i>R</i>)- 16a	S-138
Figure 110.	Expansion HSQC spectrum of (<i>R</i>)- 16a	S-139
Figure 111.	Full display HMBC spectrum of (<i>R</i>)- 16a	S-140
Figure 112.	Expansion HMBC spectrum of (<i>R</i>)- 16a	S-141
Figure 113.	Full display HSQC-TOCSY spectrum of (<i>R</i>)- 16a	S-142

Figure 114.	Expansion HSQC-TOCSY spectrum of (<i>R</i>)- 16a	S-143
Figure 115.	Full display ROESY spectrum of (<i>R</i>)- 16a	S-144
Figure 116.	Expansion ROESY spectrum of (<i>R</i>)- 16a	S-145
Figure 117.	Expansion ROESY spectrum of (<i>R</i>)- 16a	S-146
Figure 118.	Full display HSQC-NOESY spectrum of (<i>R</i>)- 16a	S-147
Figure 119.	Expansion HSQC-NOESY spectrum of (<i>R</i>)- 16a	S-148
Figure 120.	Expansion HSQC-NOESY spectrum of (<i>R</i>)- 16a	S-149
Table 5.	¹ H and ¹³ C chemical shift assignments for (<i>S</i>)- 15b	S-150
Figure 121.	¹ H NMR spectrum of (<i>S</i>)- 15b	S-152
Figure 122.	Full display HSQC spectrum of (<i>S</i>)- 15b	S-153
Figure 123.	Full display HMBC spectrum of (<i>S</i>)- 15b	S-154
Figure 124.	Full display HSQC-TOCSY spectrum of (<i>S</i>)- 15b	S-155
Figure 125.	Full display HSQC-NOESY spectrum of (<i>S</i>)- 15b	S-156
Table 6.	¹ H and ¹³ C chemical shift assignments for (<i>R</i>)- 15b	S-157
Figure 126.	¹ H NMR spectrum of (<i>R</i>)- 15b	S-159
Figure 127.	Full display HSQC spectrum of (<i>R</i>)- 15b	S-160
Figure 128.	Full display HMBC spectrum of (<i>R</i>)- 15b	S-161
Figure 129.	Full display HSQC-TOCSY spectrum of (<i>R</i>)- 15b	S-162
Figure 130.	Full display HSQC-NOESY spectrum of (<i>R</i>)- 15b	S-163
Table 7.	¹ H and ¹³ C chemical shift assignments for (<i>S</i>)- 36a	S-164
Figure 131.	¹ H NMR spectrum of (<i>S</i>)- 36a	S-166
Figure 132.	Full display HSQC spectrum of (<i>S</i>)- 36a	S-167
Figure 133.	Full display HMBC spectrum of (<i>S</i>)- 36a	S-168
Figure 134.	Full display HSQC-TOCSY spectrum of (<i>S</i>)- 36a	S-169
Figure 135.	Full display ROESY spectrum of (<i>S</i>)- 36a	S-170

Table 8.	^1H and ^{13}C chemical shift assignments for (<i>R</i>)- 36a	S-171
Figure 136.	^1H NMR spectrum of (<i>R</i>)- 36a	S-173
Figure 137.	Full display HSQC spectrum of (<i>R</i>)- 36a	S-174
Figure 138.	Full display HMBC spectrum of (<i>R</i>)- 36a	S-175
Figure 139.	Full display HSQC-TOCSY spectrum of (<i>R</i>)- 36a	S-176
Figure 140.	Full display HSQC-NOESY spectrum of (<i>R</i>)- 36a	S-177
Table 9.	^1H and ^{13}C chemical shift assignments for (<i>S</i>)- 52b	S-178
Figure 141.	^1H NMR spectrum of (<i>S</i>)- 52b	S-180
Figure 142.	Full display HSQC spectrum of (<i>S</i>)- 52b	S-181
Figure 143.	Full display HMBC spectrum of (<i>S</i>)- 52b	S-182
Figure 144.	Full display HSQC-TOCSY spectrum of (<i>S</i>)- 52b	S-183
Figure 145.	Full display HSQC-NOESY spectrum of (<i>S</i>)- 52b	S-184

Part 3. Selectivity Studies

Figure 146.	^1H NMR spectrum of aldol products from (<i>S</i>)- 1a	S-185
Figure 147.	^1H NMR spectrum of aldol products from (<i>S</i>)- 15a	S-186
Figure 148.	^1H NMR spectrum of aldol products from (<i>R</i>)- 15a	S-187
Figure 149.	^1H NMR spectrum of aldol product from (<i>S</i>)- 1a dependence on THF concentration	S-188
Figure 150.	^1H NMR spectra showing temperature dependency of aldolate the equilibration in (<i>S</i>)- 16a	S-189
Figure 151.	^1H NMR spectrum of aldol products from (<i>S</i>)- 16a	S-190
Figure 152.	^1H NMR spectrum of aldol products from (<i>R</i>)- 16a	S-191
Figure 153.	^1H NMR spectrum of aldol products from (<i>S</i>)- 1b	S-192
Figure 154.	^1H NMR spectrum of aldol products from (<i>S</i>)- 15b	S-193
Figure 155.	^1H NMR spectrum of aldol products from (<i>S</i>)- 16b	S-194

Figure 156.	^1H NMR spectrum of aldol products from (<i>R</i>)- 16b	S-195
Figure 157.	^1H NMR spectrum of aldol products from (<i>S</i>)- 36a	S-196
Figure 158.	^1H NMR spectrum of aldol products from (<i>R</i>)- 36a	S-197
Figure 159.	^1H NMR spectrum of aldol products from (<i>S</i>)- 37a	S-198
Figure 160.	^1H NMR spectrum of aldol products from (<i>R</i>)- 37a	S-199
Figure 161.	^1H NMR spectrum of aldol products from (<i>S</i>)- 1b and (<i>S</i>)- 16b with benzaldehyde	S-200
Figure 162.	^1H NMR spectrum of aldol products from (<i>S</i>)- 1b and (<i>S</i>)- 16b with pivaldehyde	S-201
Figure 163.	^1H NMR spectrum of aldol products from (<i>S</i>)- 1b and (<i>S</i>)- 16b with ethynyl methyl ketone	S-202
Figure 164.	^1H NMR spectrum of aldol products from (<i>S</i>)- 52b	S-203

Part 4. Rate Studies

Figure 165.	Plot of aldolate concentration versus time under stoichiometric conditions for the formation of (<i>S</i>)- 44a	S-204
Figure 166.	Plot of aldolate concentration versus time under pseudo-first-order conditions for the formation of (<i>S</i>)- 44a	S-205
Figure 167.	Plot of k_{obsd} versus concentration of <i>t</i> -BuCHO for the formation of (<i>S</i>)- 44a	S-206
Figure 168.	Plot of k_{obsd} versus concentration of (<i>S</i>)- 16a for the formation of (<i>S</i>)- 44a	S-207
Figure 169.	Plot of k_{obsd} versus concentration of 11 for the formation of (<i>S</i>)- 44a	S-208
Figure 170.	Plot of k_{obsd} versus concentration of HMPA for the formation of (<i>S</i>)- 44a	S-209
Figure 171.	Kinetic isotope effect for the formation of (<i>S</i>)- 44a	S-210

Part 5. Computations

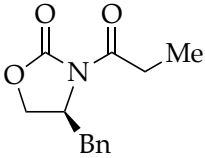
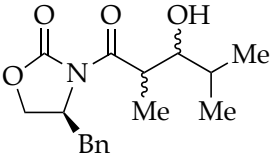
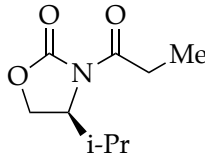
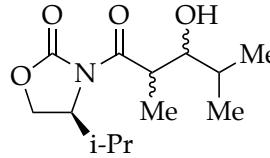
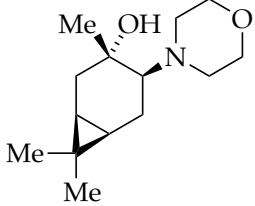
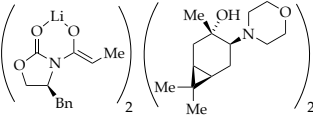
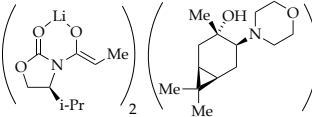
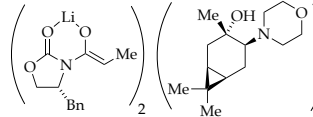
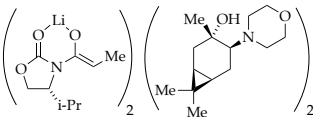
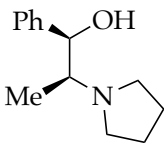
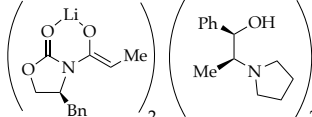
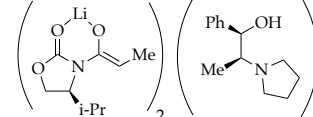
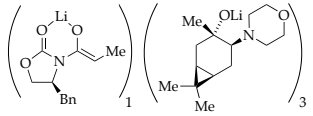
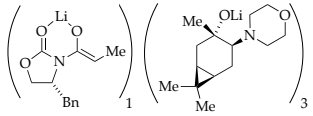
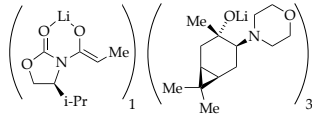
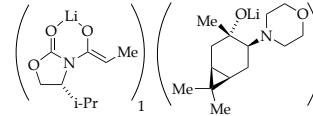
Table 10.	Geometric coordinates and thermally corrected MP2 energies for THF	S-211
Table 11.	Geometric coordinates and thermally corrected MP2 energies for isobutyraldehyde	S-211
Table 12.	Geometric coordinates and thermally corrected MP2 energies for 18a	S-212
Table 13.	Geometric coordinates and thermally corrected MP2 energies for 18b	S-214
Table 14.	Geometric coordinates and thermally corrected MP2 energies for 18c	S-216
Figure 172.	Computational overview of ground states for (S)-15a	S-218
Figure 173.	Computational overview of ground states for (R)-15a	S-219
Figure 174.	Computational overview of ground states for (S)-16a	S-220
Figure 175.	Computational overview of ground states for (R)-16a	S-221
Figure 176.	Computational overview of transition states	S-222
Figure 177.	Computational overview of alternative transition states	S-223
Table 15.	Geometric coordinates and thermally corrected MP2 energies for (S)-22a	S-224
Table 16.	Geometric coordinates and thermally corrected MP2 energies for (S)-21a	S-227
Table 17.	Geometric coordinates and thermally corrected MP2 energies for (S)-15a	S-230
Table 18.	Geometric coordinates and thermally corrected MP2 energies for (S)-23a	S-233
Table 19.	Geometric coordinates and thermally corrected MP2 energies for (S)-24a	S-236
Table 20.	Geometric coordinates and thermally corrected MP2 energies for (R)-22a	S-239

Table 21.	Geometric coordinates and thermally corrected MP2 energies for (<i>R</i>)- 15a	S-242
Table 22.	Geometric coordinates and thermally corrected MP2 energies for (<i>R</i>)- 23a	S-245
Table 23.	Geometric coordinates and thermally corrected MP2 energies for (<i>R</i>)- 24a	S-248
Table 24.	Geometric coordinates and thermally corrected MP2 energies for (<i>R</i>)- 21a	S-251
Table 25.	Geometric coordinates and thermally corrected MP2 energies for (<i>S</i>)- 32a	S-254
Table 26.	Geometric coordinates and thermally corrected MP2 energies for (<i>S</i>)- 33a	S-257
Table 27.	Geometric coordinates and thermally corrected MP2 energies for (<i>S</i>)- 34a	S-260
Table 28.	Geometric coordinates and thermally corrected MP2 energies for (<i>S</i>)- 35a	S-263
Table 29.	Geometric coordinates and thermally corrected MP2 energies for (<i>S</i>)- 29a	S-266
Table 30.	Geometric coordinates and thermally corrected MP2 energies for (<i>S</i>)- 30a	S-269
Table 31.	Geometric coordinates and thermally corrected MP2 energies for (<i>S</i>)- 31a	S-272
Table 32.	Geometric coordinates and thermally corrected MP2 energies for (<i>S</i>)- 16a *	S-275
Table 33.	Geometric coordinates and thermally corrected MP2 energies for (<i>S</i>)- 26a	S-278
Table 34.	Geometric coordinates and thermally corrected MP2 energies for (<i>S</i>)- 27a	S-281
Table 35.	Geometric coordinates and thermally corrected MP2 energies for (<i>S</i>)- 28a	S-284
Table 36.	Geometric coordinates and thermally corrected MP2 energies for (<i>S</i>)- 16a	S-287

Table 37.	Geometric coordinates and thermally corrected MP2 energies for (R)-32a	S-290
Table 38.	Geometric coordinates and thermally corrected MP2 energies for (R)-33a	S-293
Table 39.	Geometric coordinates and thermally corrected MP2 energies for (R)-34a	S-296
Table 40.	Geometric coordinates and thermally corrected MP2 energies for (R)-35a	S-299
Table 41.	Geometric coordinates and thermally corrected MP2 energies for (R)-29a	S-302
Table 42.	Geometric coordinates and thermally corrected MP2 energies for (R)-30a	S-305
Table 43.	Geometric coordinates and thermally corrected MP2 energies for (R)-31a	S-308
Table 44.	Geometric coordinates and thermally corrected MP2 energies for (R)-16a	S-311
Table 45.	Geometric coordinates and thermally corrected MP2 energies for (R)-26a	S-314
Table 46.	Geometric coordinates and thermally corrected MP2 energies for (R)-27a	S-317
Table 47.	Geometric coordinates and thermally corrected MP2 energies for (R)-28a	S-320
Table 48.	Geometric coordinates and thermally corrected MP2 energies for precomplex pre-(S)-48a	S-323
Table 49.	Geometric coordinates and thermally corrected MP2 energies for precomplex pre-(S)-47a	S-326
Table 50.	Geometric coordinates and thermally corrected MP2 energies for precomplex pre-(R)-49a	S-329
Table 51.	Geometric coordinates and thermally corrected MP2 energies for precomplex pre-(R)-50a	S-332
Table 52.	Geometric coordinates and thermally corrected MP2 energies for transition state (S)-48a	S-335

Table 53.	Geometric coordinates and thermally corrected MP2 energies for transition state (S)-47a	S-338
Table 54.	Geometric coordinates and thermally corrected MP2 energies for transition state (R)-49a	S-341
Table 55.	Geometric coordinates and thermally corrected MP2 energies for transition state (R)-50a	S-344
Table 56.	Geometric coordinates and thermally corrected MP2 energies for transition state (S)-46a	S-347
Table 57.	Geometric coordinates and thermally corrected MP2 energies for transition state (S)-45a	S-350
Table 58.	Geometric coordinates and thermally corrected MP2 energies for transition state (R)-45a	S-353
Table 59.	Geometric coordinates and thermally corrected MP2 energies for transition state (R)-46a	S-356
Table 60.	Geometric coordinates and thermally corrected MP2 energies for transition state (S)-37a (isomer A)	S-359
Table 61.	Geometric coordinates and thermally corrected MP2 energies for transition state (S)-37a (isomer B)	S-361
Table 62.	Geometric coordinates and thermally corrected MP2 energies for transition state (S)-37a (isomer C)	S-363
Part 6. Full reference (Gaussian)		S-365

Chart 1. Substrates And Aggregates

 <p>(S)-1a</p>	 <p>(S)-2a</p>	 <p>(S)-1b</p>	 <p>(S)-2b</p>
 <p>11</p>	 <p>(S)-15a</p>	 <p>(S)-15b</p>	 <p>(R)-15a</p>
 <p>(R)-15b</p>	 <p>8</p>	 <p>(S)-36a</p>	 <p>(S)-36b</p>
 <p>(S)-16a</p>	 <p>(R)-16a</p>	 <p>(S)-16b</p>	 <p>(R)-16b</p>

Part 1: Substrates And Products

Standard ^1H , ^6Li , and ^{13}C NMR spectra were recorded on a 500 MHz spectrometer at 500, 73.57, and 125.79 MHz, respectively. The ^6Li resonances were referenced to 0.30 M [^6Li]LiCl/methanol at $-80\text{ }^\circ\text{C}$ (0.0 ppm).

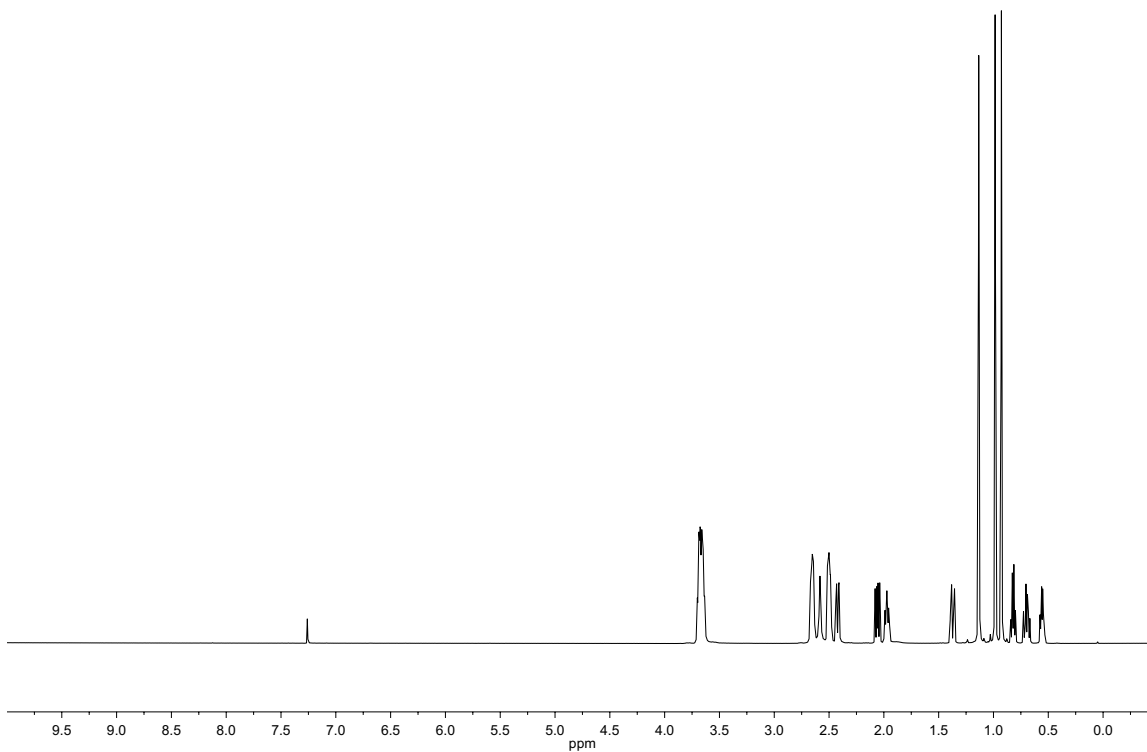
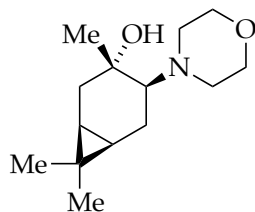


Figure 1. ^1H NMR spectrum of **11** in CDCl_3 at $25\text{ }^\circ\text{C}$.

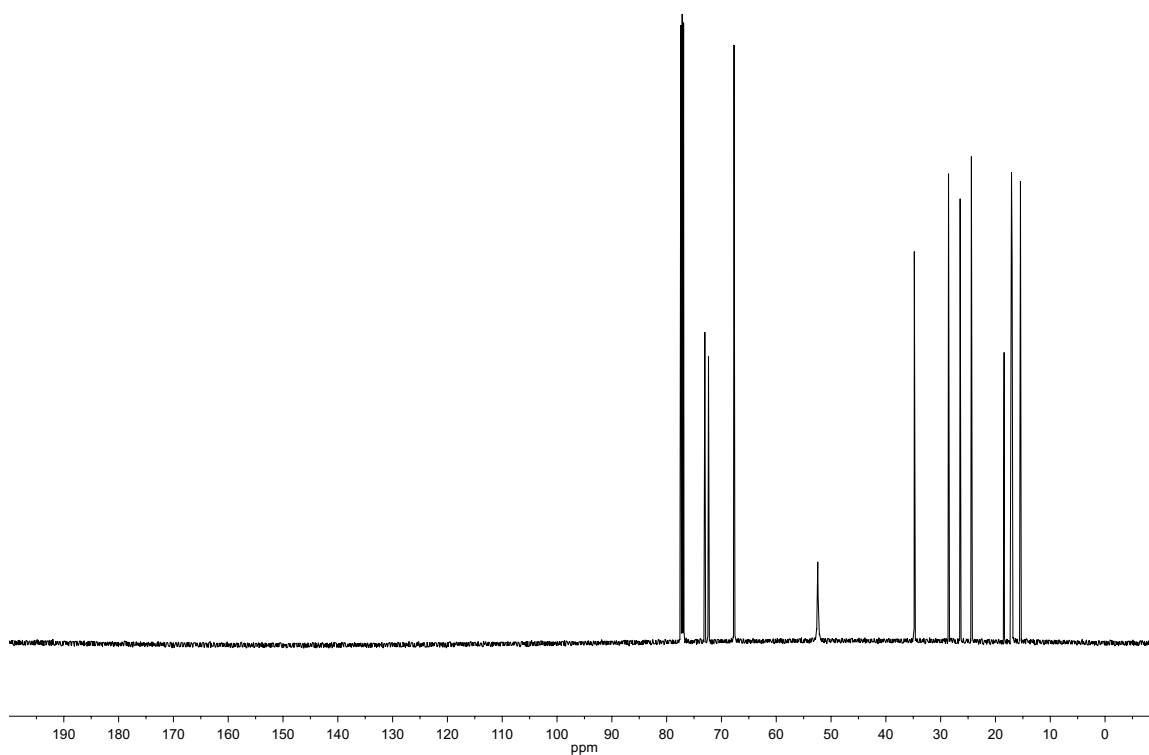
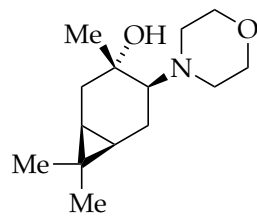


Figure 2. ¹³C NMR spectrum of **11** in CDCl₃ at 25 °C.

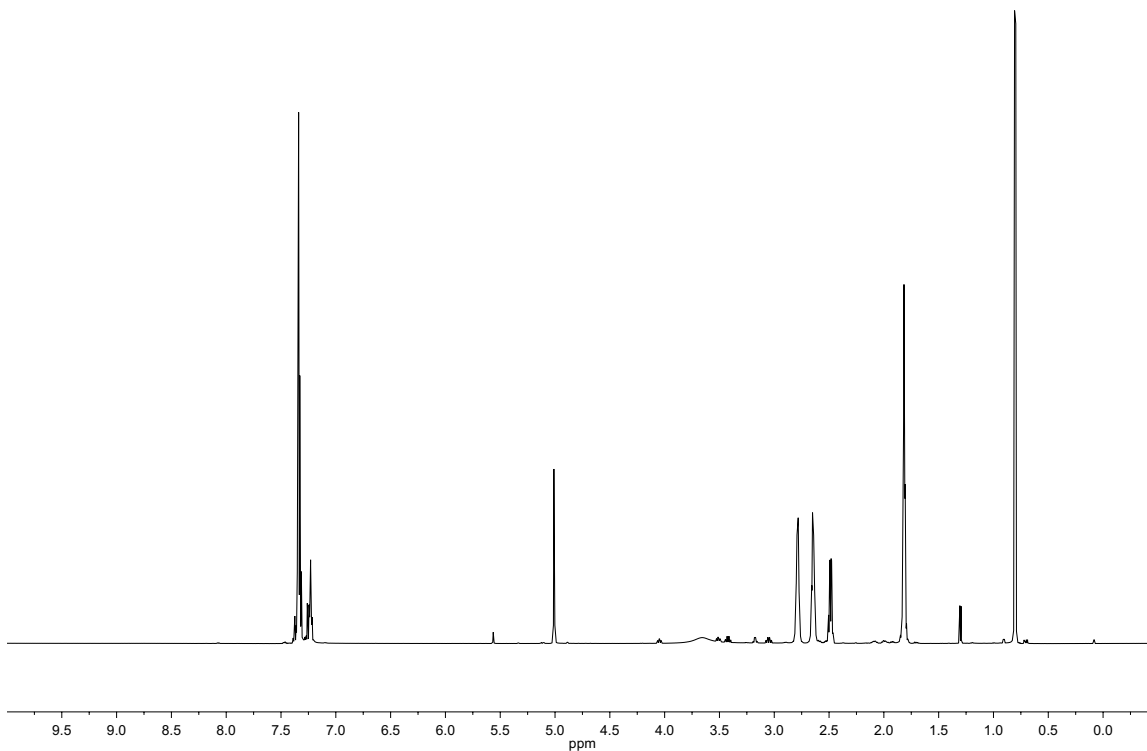
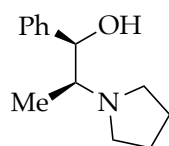


Figure 3. ¹H NMR spectrum of **8** in CDCl₃ at 25 °C.

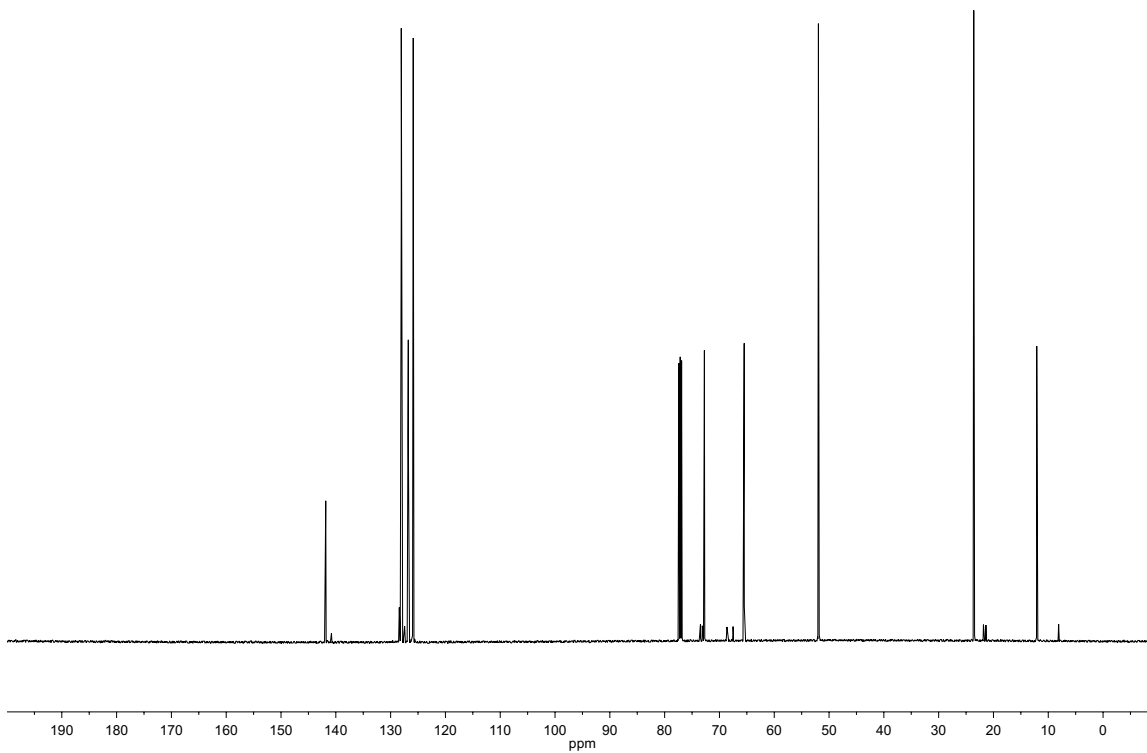
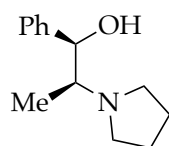


Figure 4. ^{13}C NMR spectrum of **8** in CDCl_3 at 25°C .

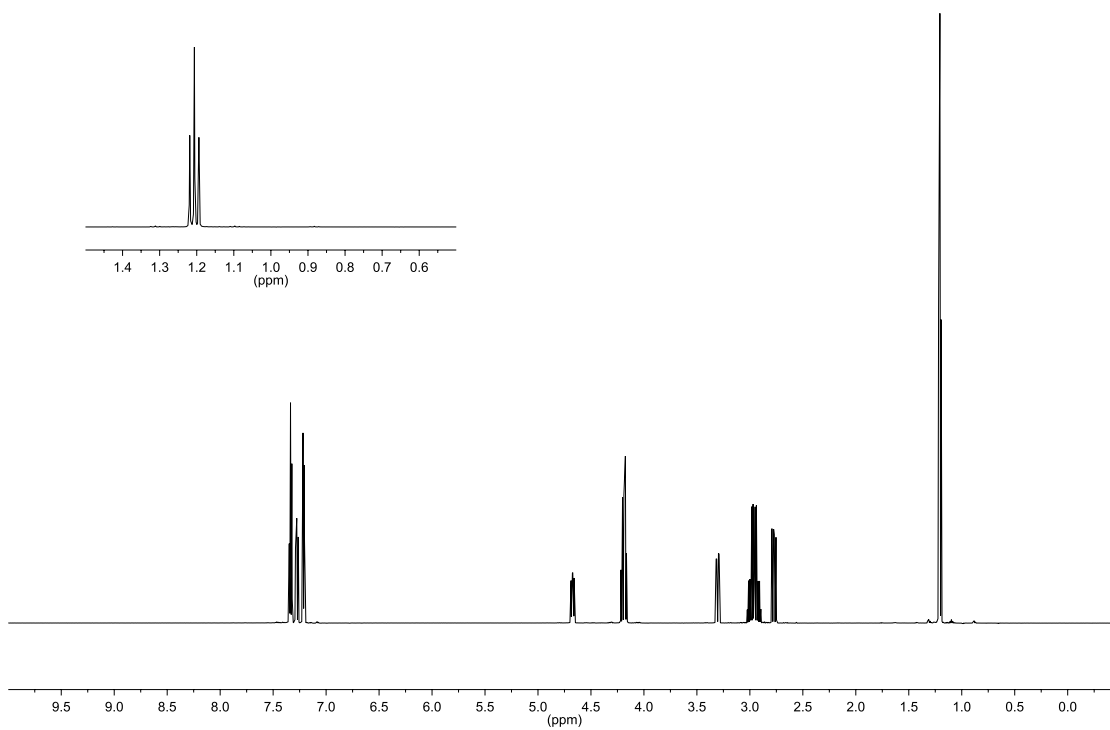
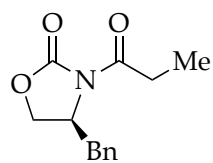


Figure 5. ¹H NMR spectrum of **1a** in CDCl₃ at 21 °C.

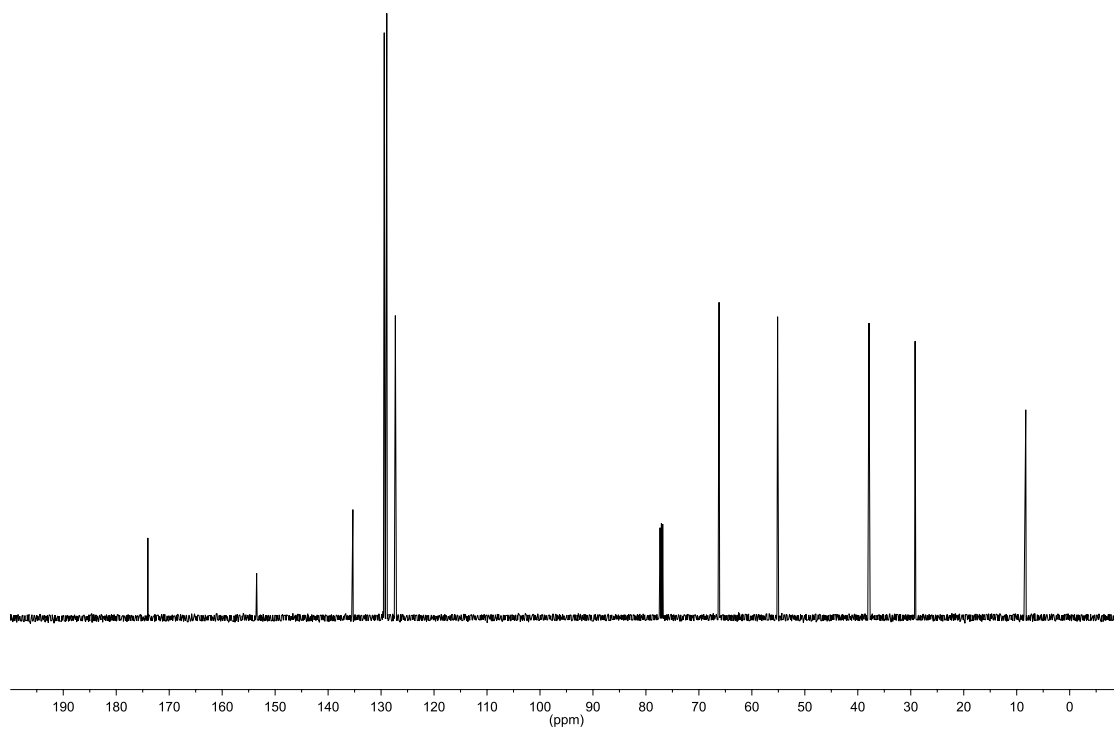
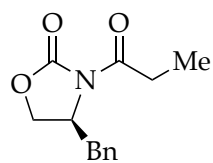


Figure 6. ^{13}C NMR spectrum of **1a** in CDCl_3 at 21°C .

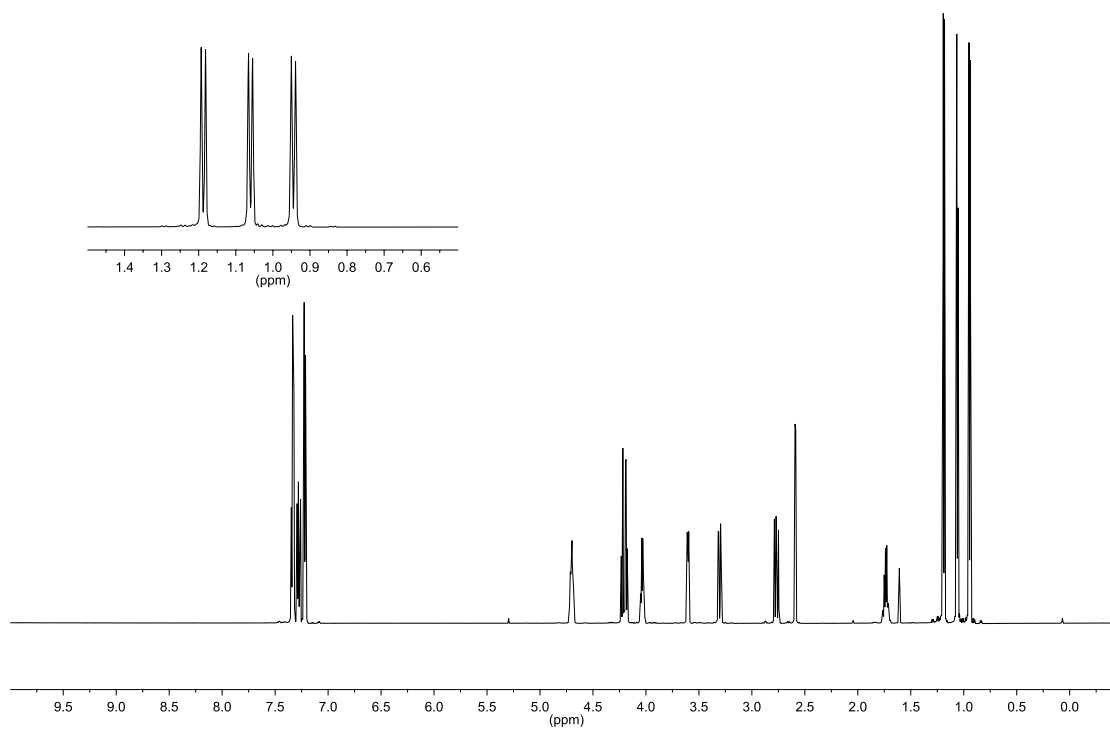
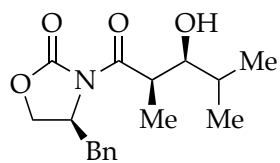


Figure 7. ¹H NMR spectrum of (R,S)-2a aldol product in CDCl₃ at 25 °C.

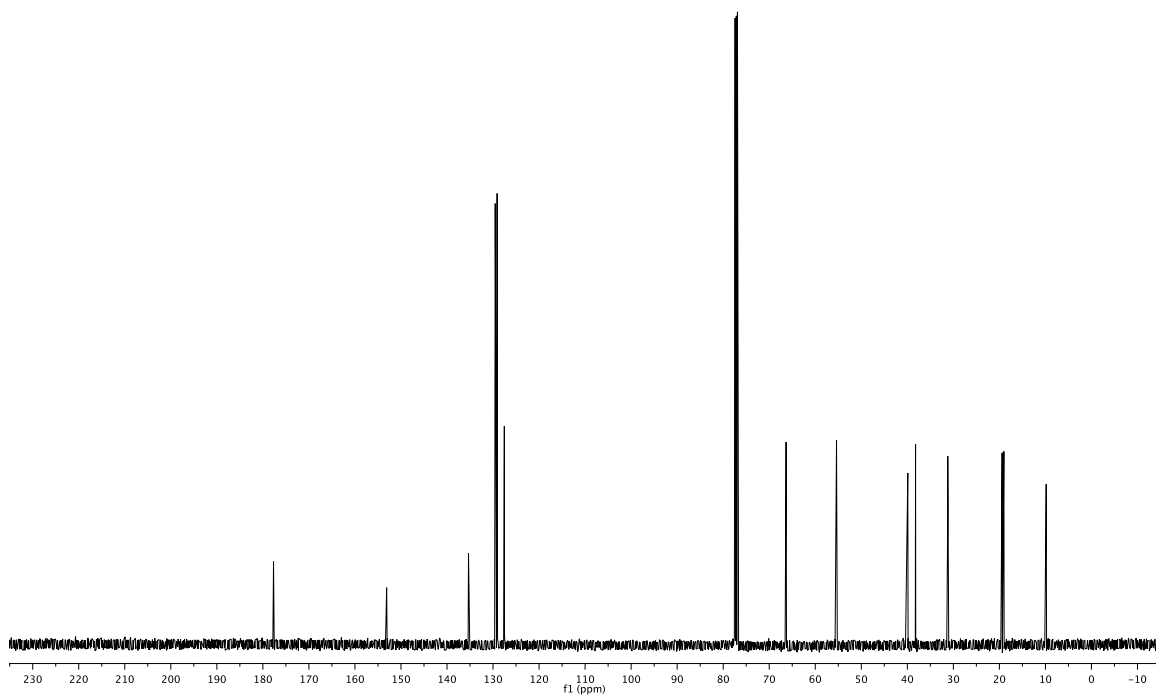
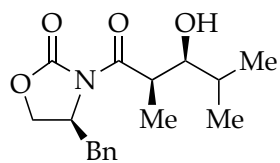


Figure 8. ^{13}C NMR spectrum of (R,S)-2a aldol product in CDCl_3 at 25 °C.

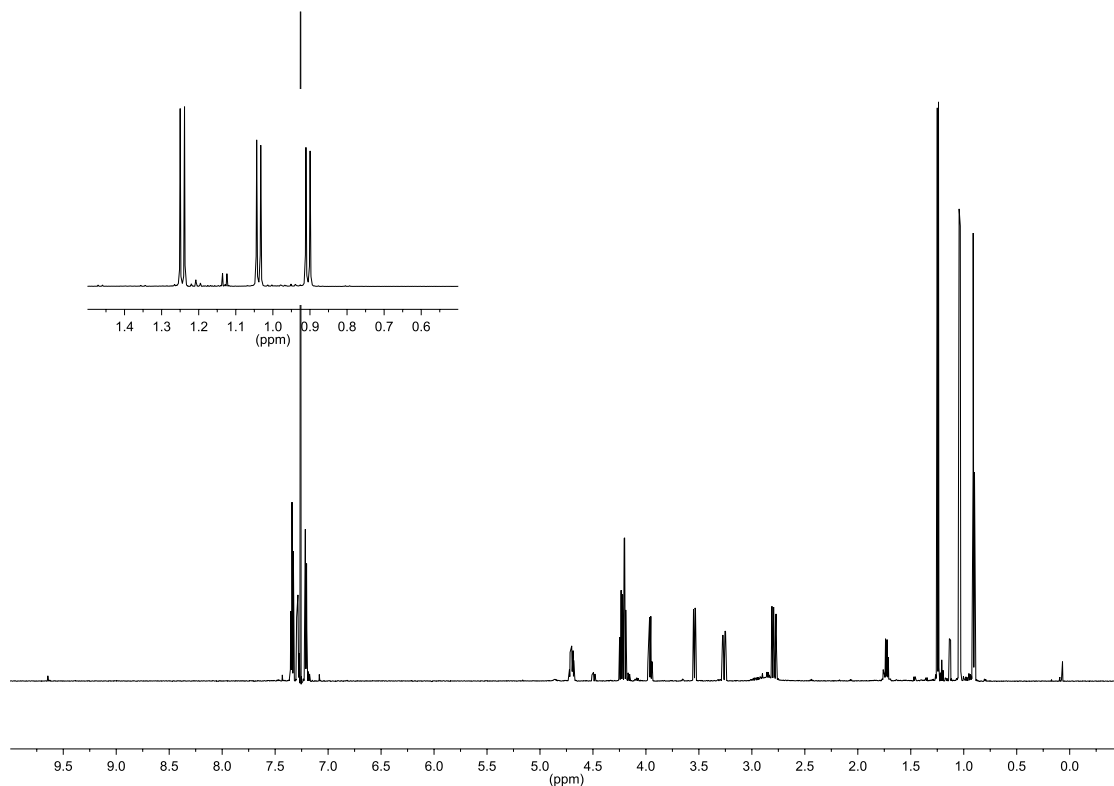
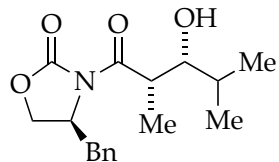


Figure 9. ¹H NMR spectrum of (S,R)-2a aldol product in CDCl₃ at 21 °C.

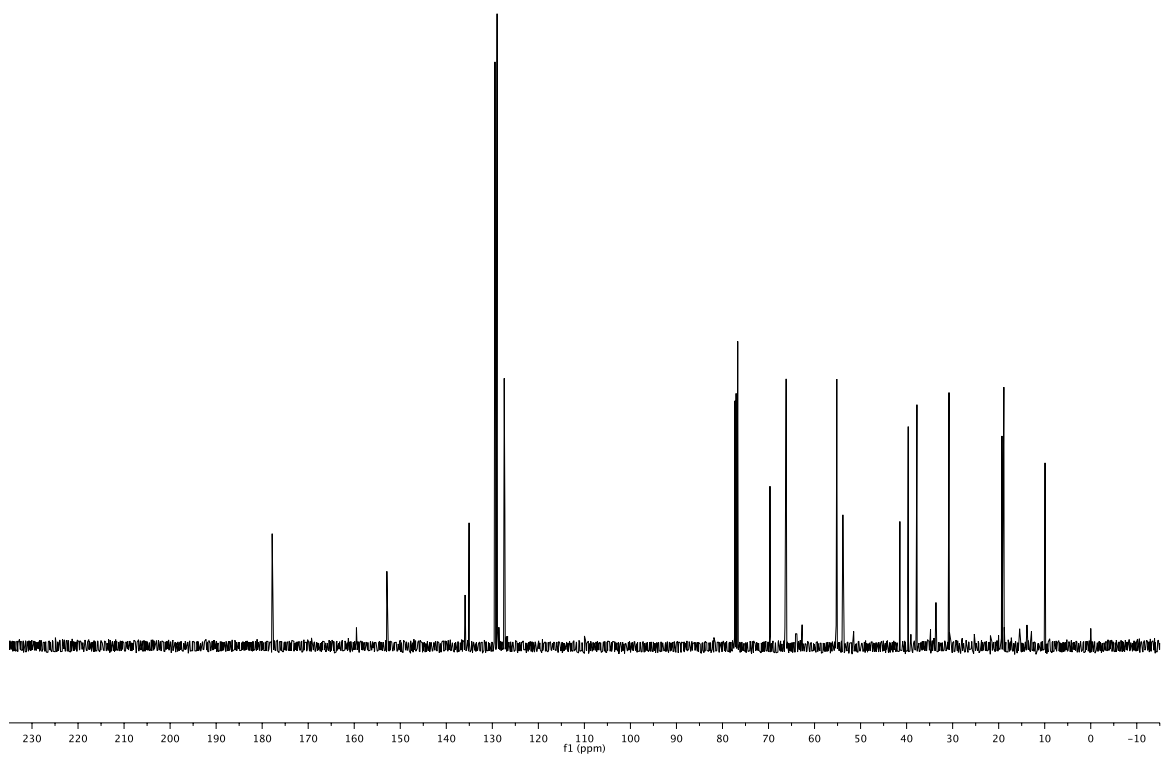
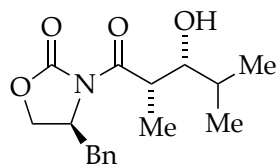


Figure 10. ^{13}C NMR spectrum of (S,R)-2a aldol product in CDCl_3 at 21 °C.

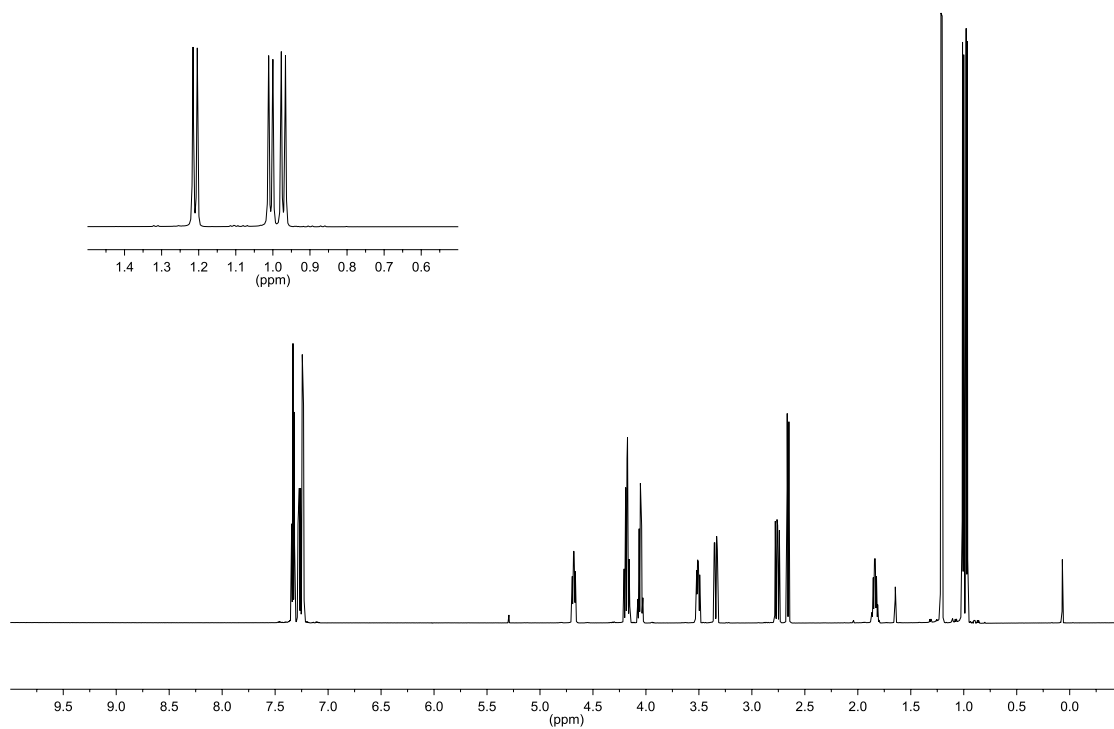
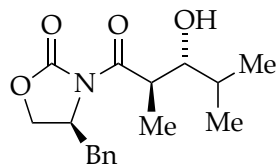


Figure 11. ^1H NMR spectrum of (R,R)-2a aldol product in CDCl_3 at 25°C .

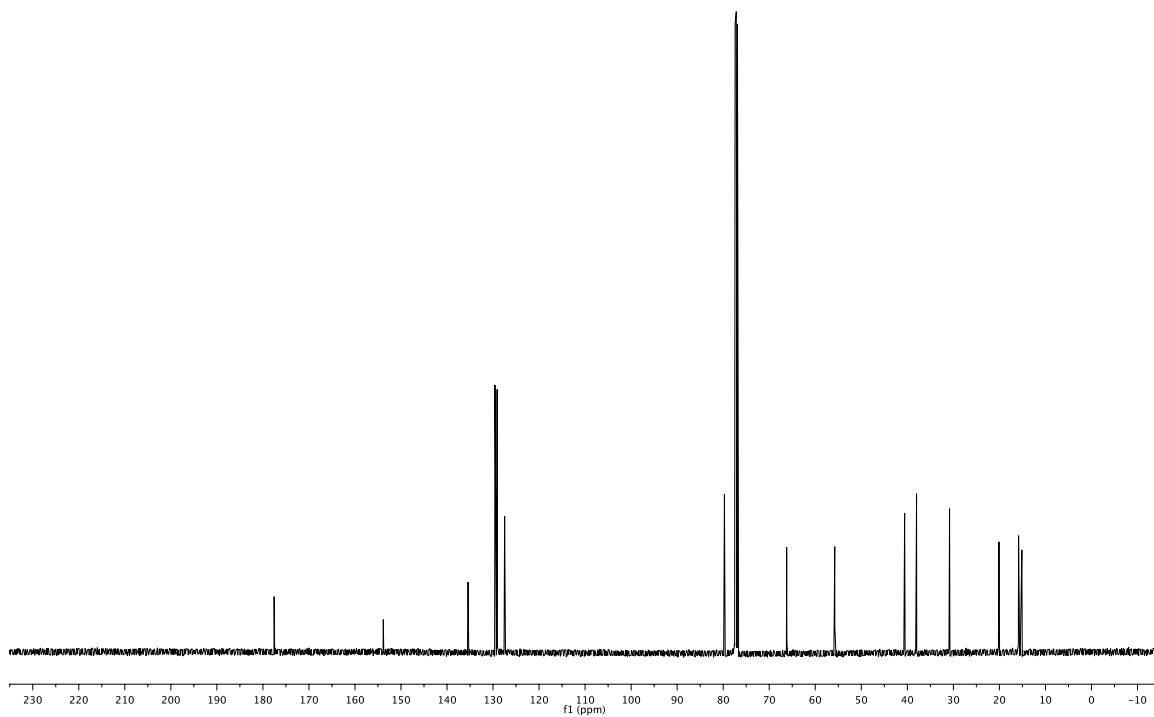
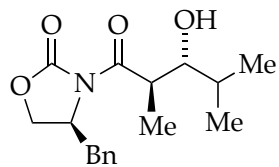


Figure 12. ¹³C NMR spectrum of (R,R)-2a aldol product in CDCl₃ at 25 °C.

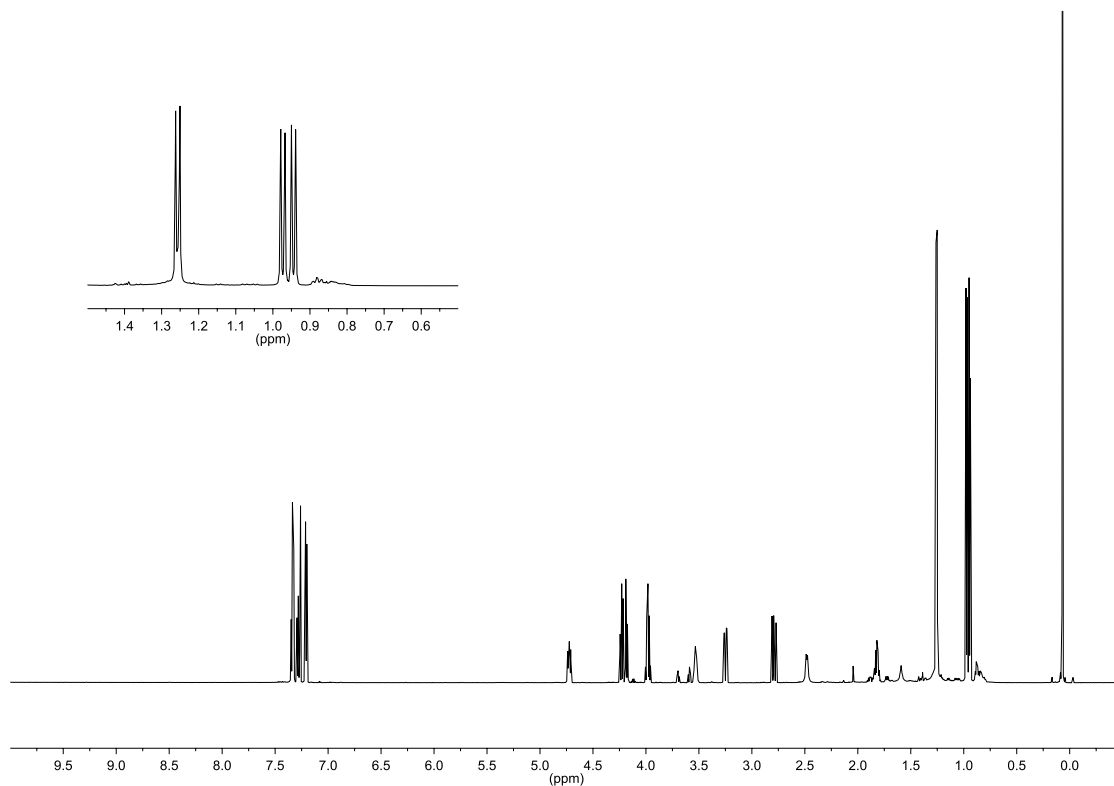
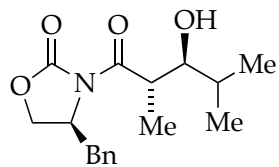


Figure 13. ¹H NMR spectrum of (S,S)-2a aldol product in CDCl₃ at 23 °C.

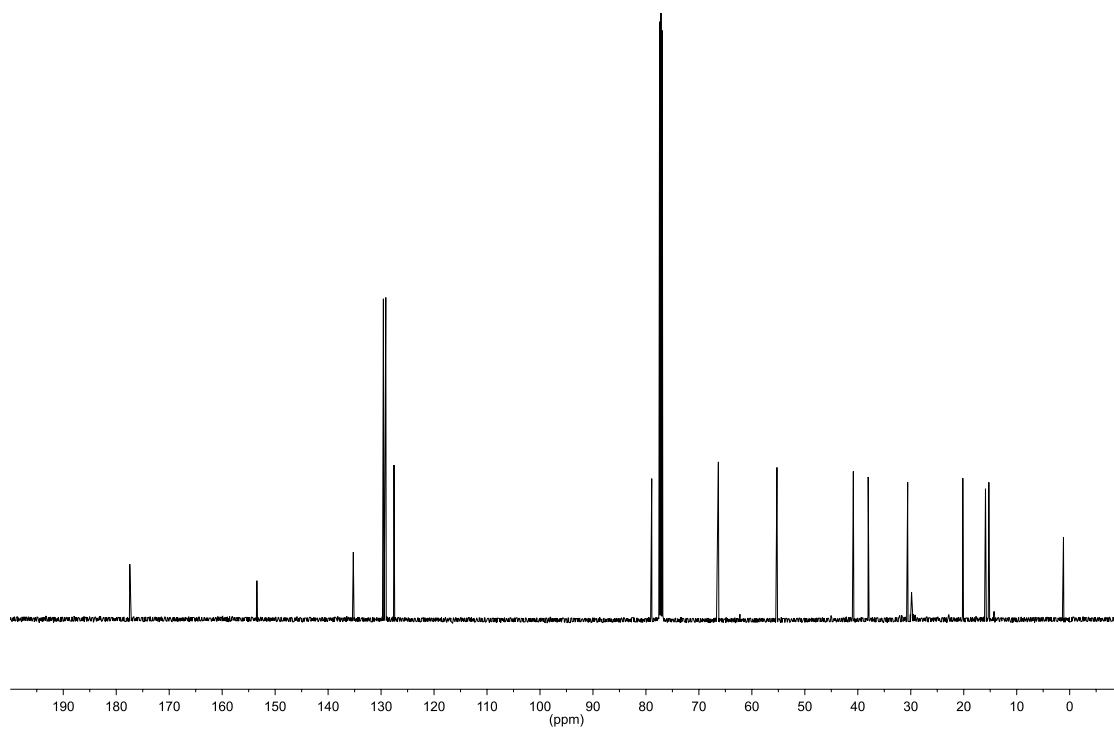
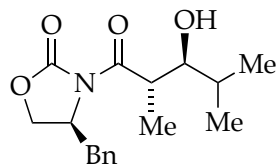


Figure 14. ^{13}C NMR spectrum of (*S,S*)-**2a** aldol product in CDCl_3 at 23 °C.

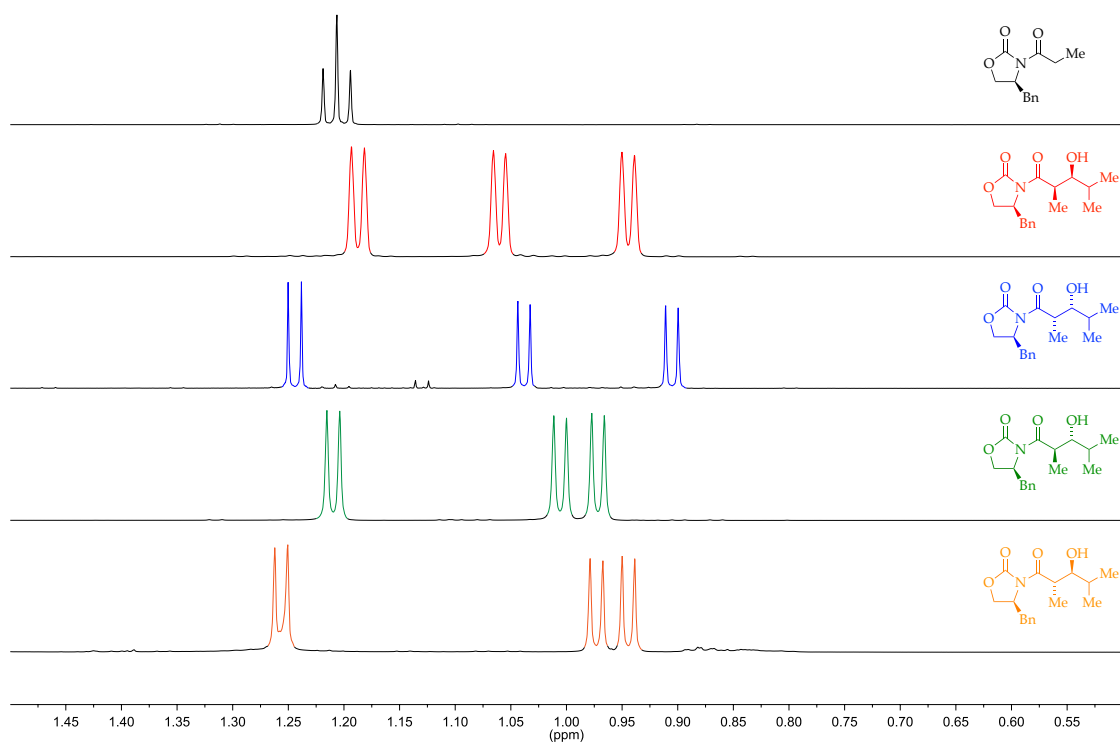


Figure 15. ¹H NMR spectrum of **1a**, (*R,S*)-**2a**, (*S,R*)-**2a**, (*R,R*)-**2a**, (*S,S*)-**2a** aldol products in CDCl₃.

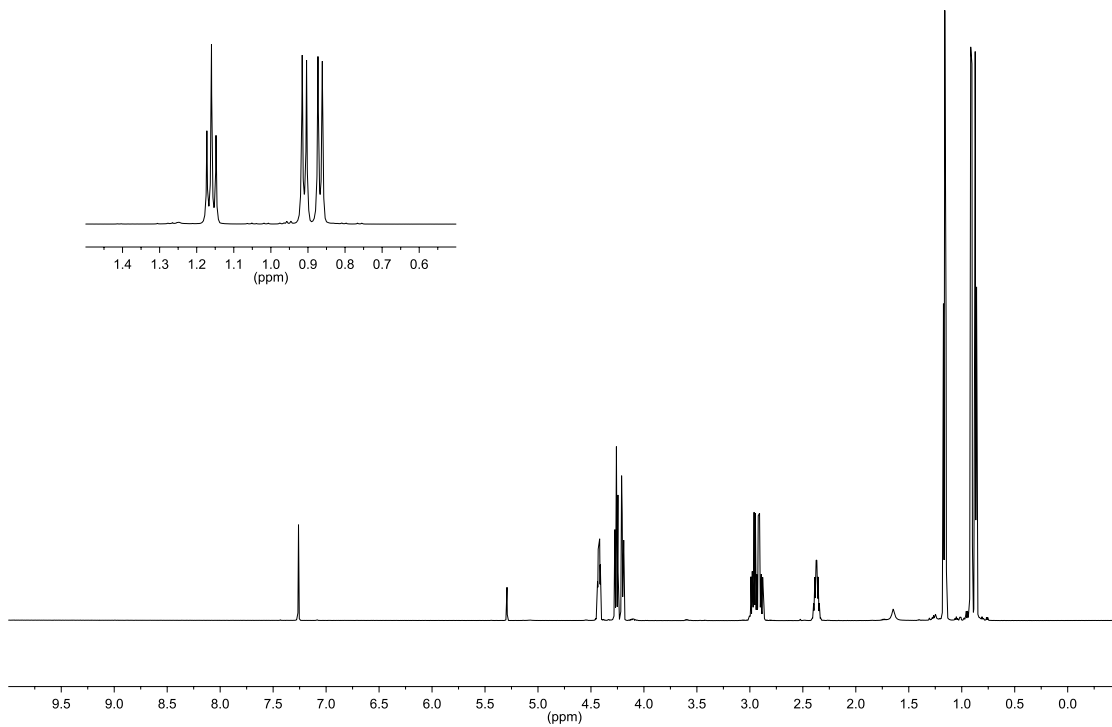
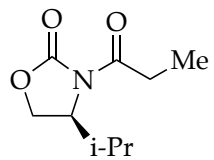


Figure 16. ¹H NMR spectrum of **1b** in CDCl₃ at 25 °C.

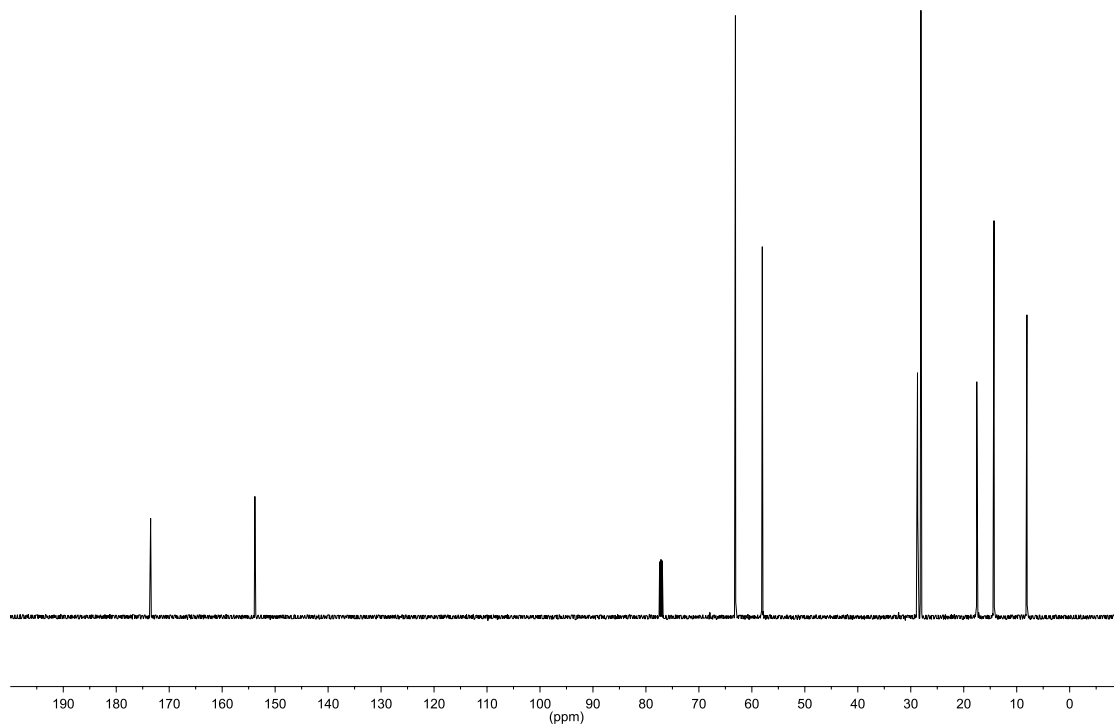
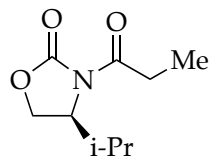


Figure 17. ^{13}C NMR spectrum of **1b** in CDCl_3 at $25\text{ }^\circ\text{C}$.

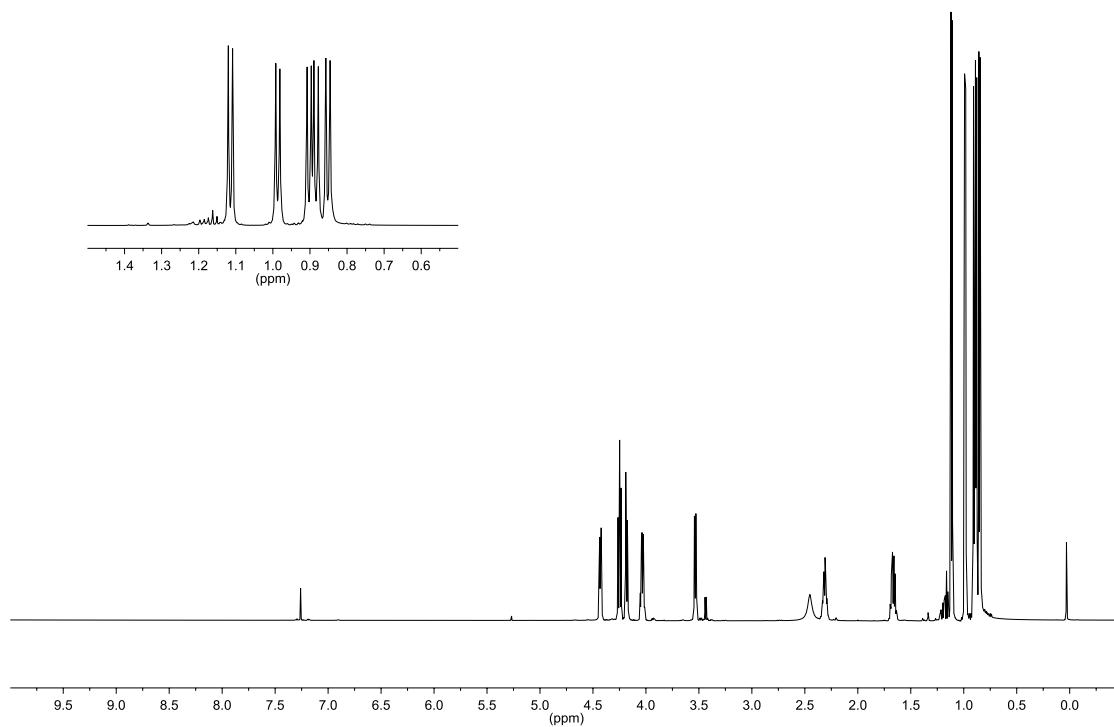
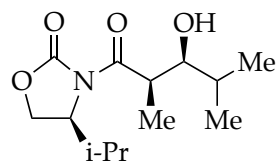


Figure 18. ^1H NMR spectrum of (R,S)-**2b** aldol product in CDCl_3 at 25°C .

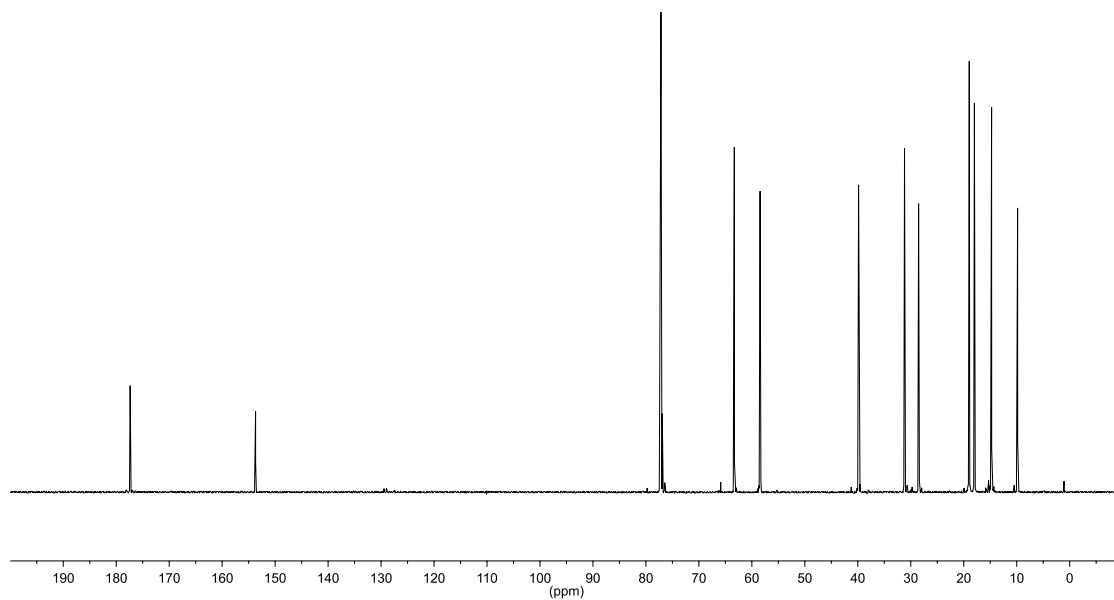
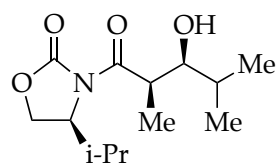


Figure 19. ¹³C NMR spectrum of (R,S)-2b aldol product in CDCl₃ at 25 °C.

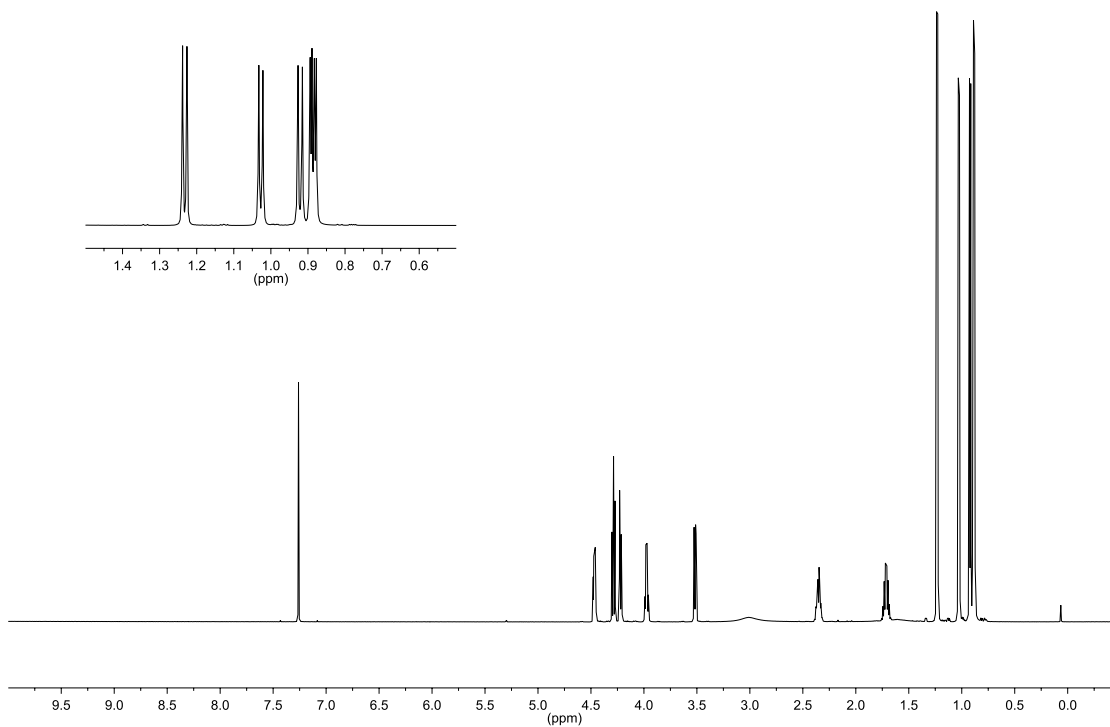
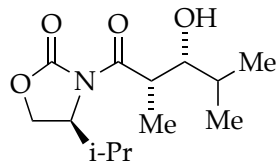


Figure 20. ¹H NMR spectrum of (S,R)-**2b** aldol product in CDCl₃ at 25 °C.

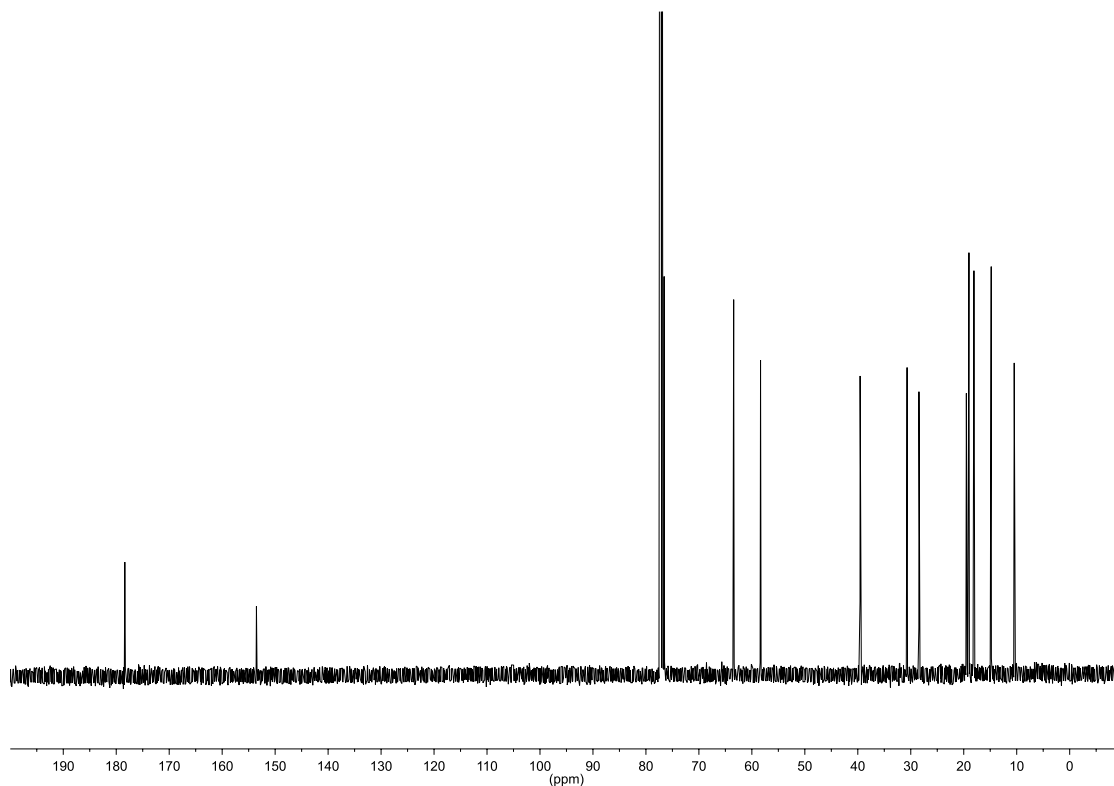
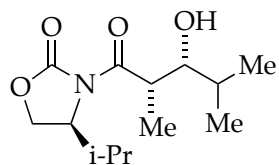


Figure 21. ¹³C NMR spectrum of (S,R)-2b aldol product in CDCl₃ at 25 °C.

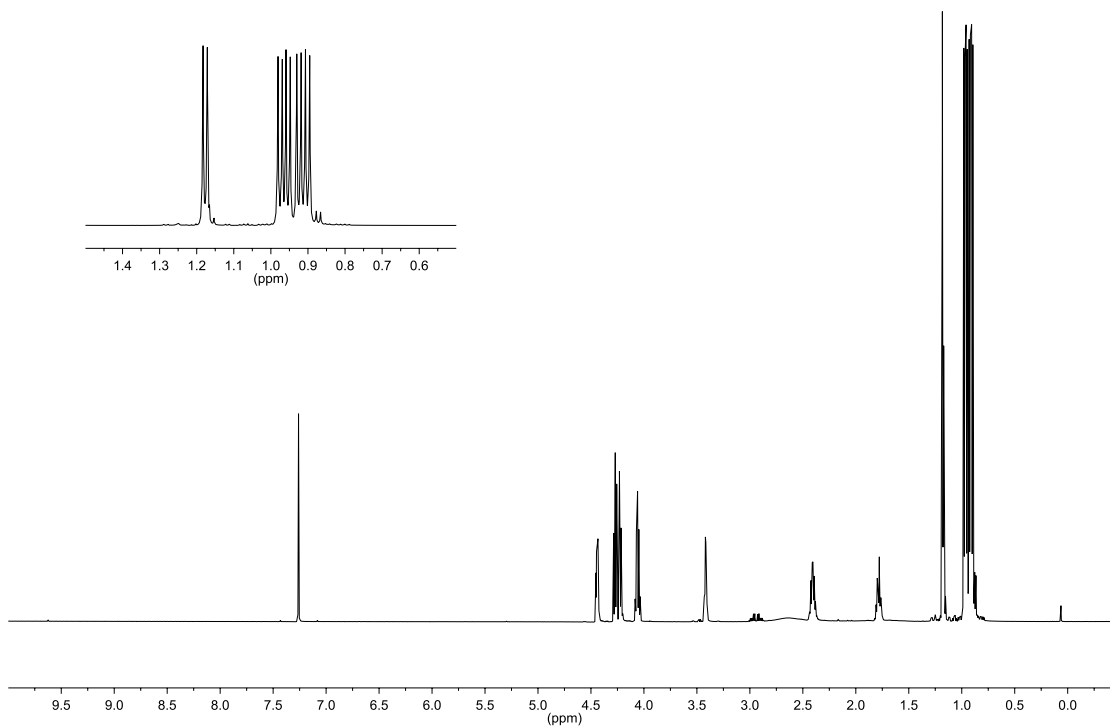
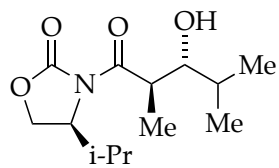


Figure 22. ^1H NMR spectrum of (R,R)-2b aldol product in CDCl_3 at 25°C .

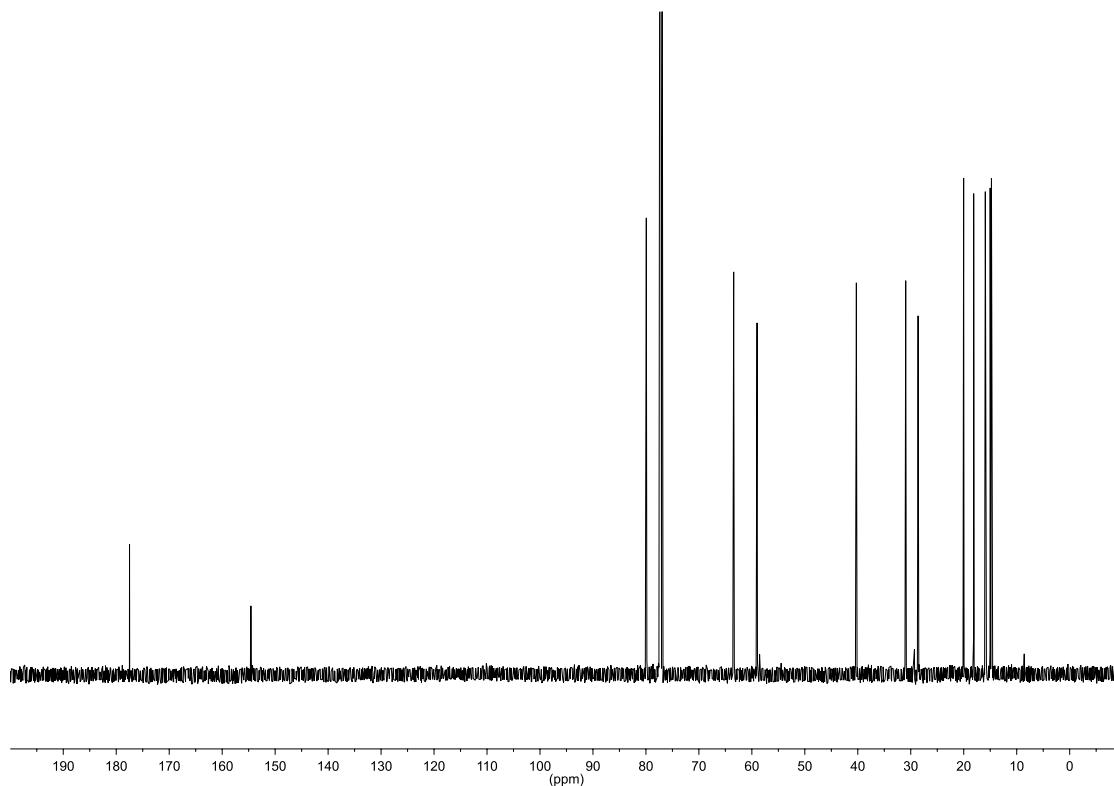
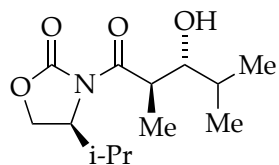


Figure 23. ¹³C NMR spectrum of (R,R)-2b aldol product in CDCl₃ at 25 °C.

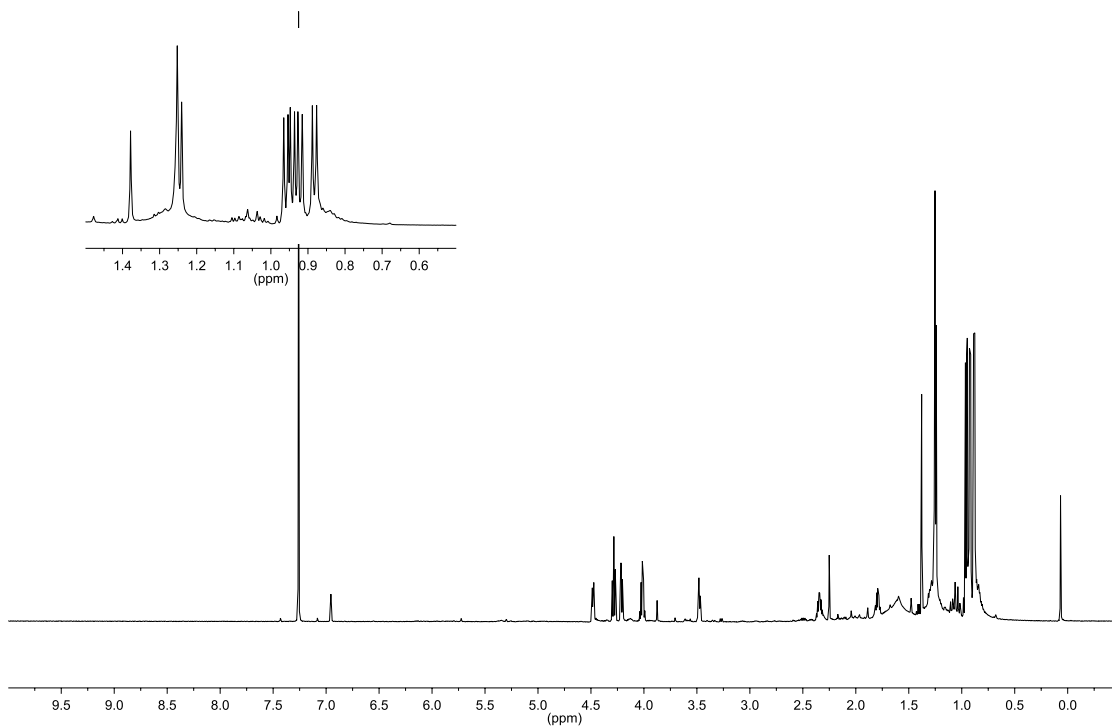
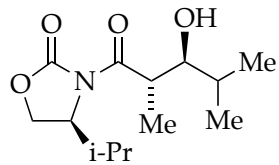


Figure 24. ¹H NMR spectrum of (S,S)-2b aldol product in CDCl₃ at 25 °C.

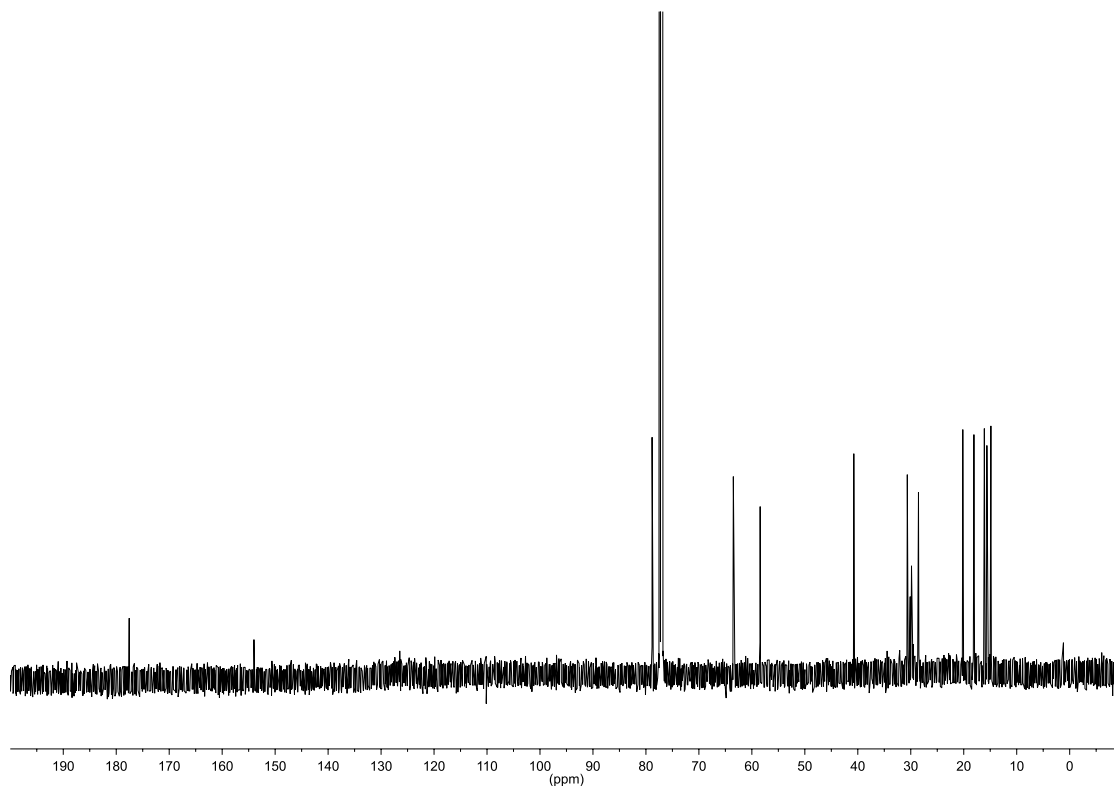
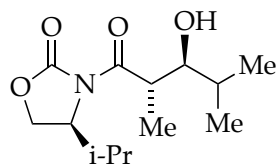


Figure 25. ¹³C NMR spectrum of (S,S)-2b aldol product in CDCl₃ at 25 °C.

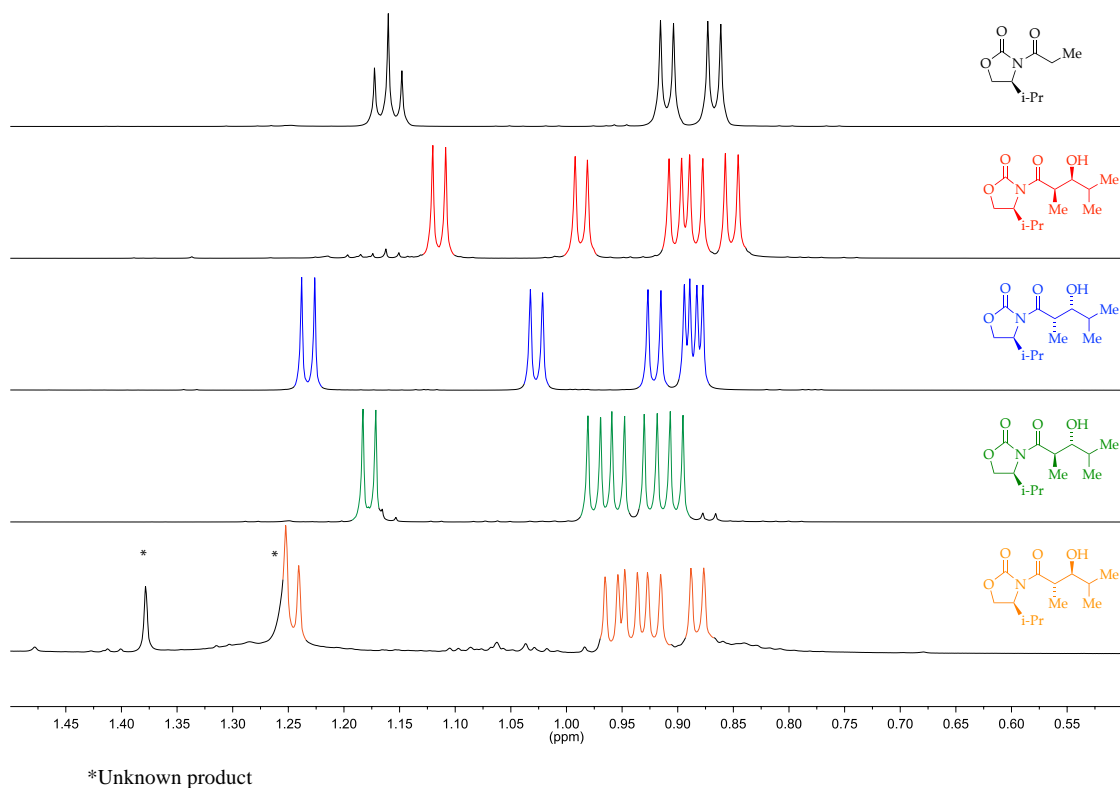


Figure 26. ^1H NMR spectrum of **1b**, (*R,S*)-**2b**, (*S,R*)-**2b**, (*R,R*)-**2b**, (*S,S*)-**2b** aldol products in CDCl_3 .

Pivaldehyde-*d* Synthesis

Neopentyl alcohol-*d*₂ was synthesized using a modified prep from *J. Org. Chem.* **2014**, *79*, 6743 and *J. Org. Chem.* **2017**, *82*, 1285 to avoid using LiAlD₄ as a reducing reagent. Pivaldehyde-*d* was synthesized using a slightly modified procedure from *J. Am. Chem. Soc.* **1992**, *114*, 1800.

Neopentyl alcohol-*d*₂. To a solution of methyl pivalate (11.6 g, 0.10 mol) in anhydrous hexane (250 mL) was added MeOD (18.36 mL, 0.45 mol) followed by sodium dispersion in mineral oil (40 wt %, 0.45 mol) at 0 °C while purging the reaction vessel with a stream of Ar. Na dispersion can be easily added with a graduated pipette (the approximate amount 8 × 4 mL). The reaction mixture was stirred vigorously and after 5 min the temperature was raised to rt. After 20 min, the mixture was quenched with 200 mL of 3 M aqueous HCl solution, and diluted with 200 mL Et₂O. The mixture was sequentially washed with water, brine, NaHCO₃, and brine. The solution was dried over MgSO₄, filtered, and distilled to afford the desired product in 30% yield. ¹H NMR (500 MHz, CDCl₃) δ 0.91 (s, 9H); ¹³C NMR (126 MHz, CDCl₃) δ 72.87, 34.81, 26.10.

Pivaldehyde-*d*. To a stirred solution of PCC (32.0 g, 150 mmol) in 200 mL of anhydrous DCM at rt was added neopentyl alcohol-*d*₂ (8.7 g, 96 mmol) in 16 mL of DCM. The solution was stirred overnight, and afterwards diluted with pentane. The crude mixture was filtered through a thin layer of Florisil[®], and the filtrate was fractionally distilled at ambient pressure to afford 3.1 g (37%) of desired aldehyde. ¹H NMR (500 MHz, CDCl₃) δ 1.08 (s, 9H); ¹³C NMR (126 MHz, CDCl₃) δ 206.00 (t, *J* = 25.7 Hz), 42.57 (t, *J* = 3.1 Hz), 23.57.

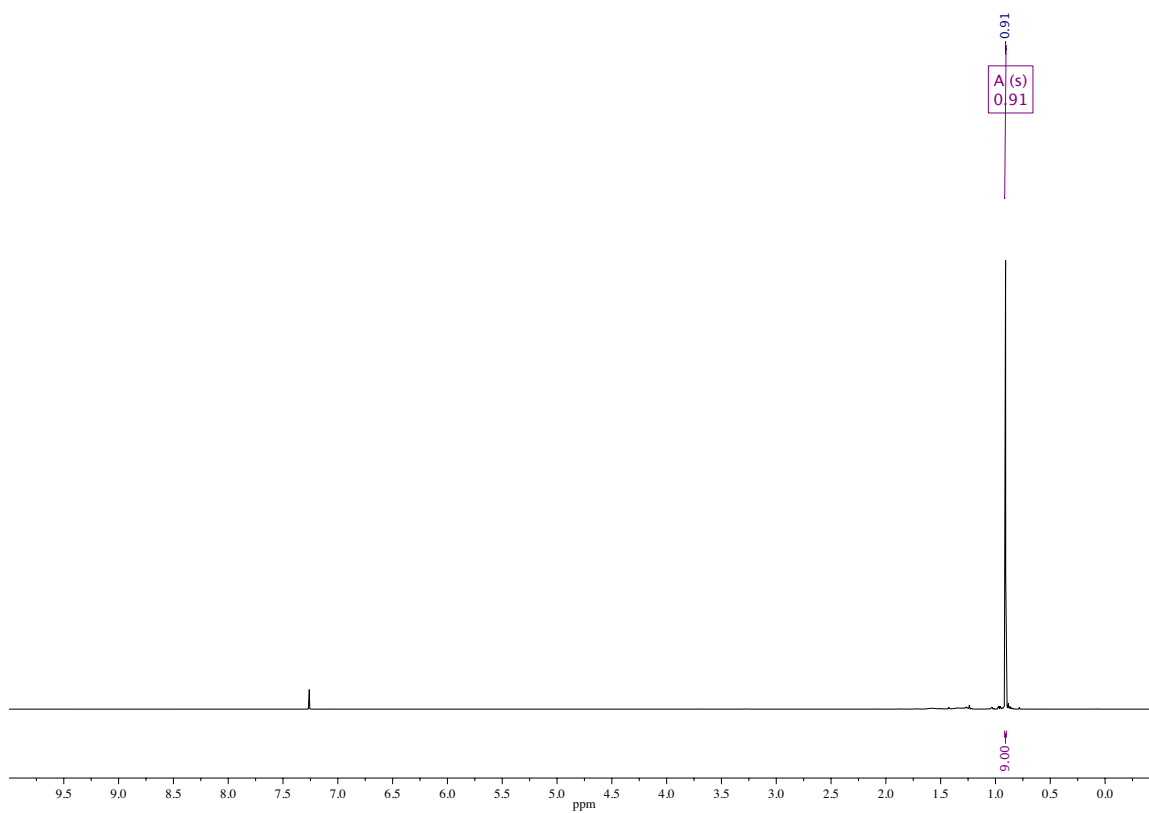
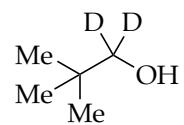


Figure 27. ^1H NMR spectrum of neopentyl alcohol- d_2 in CDCl_3 .

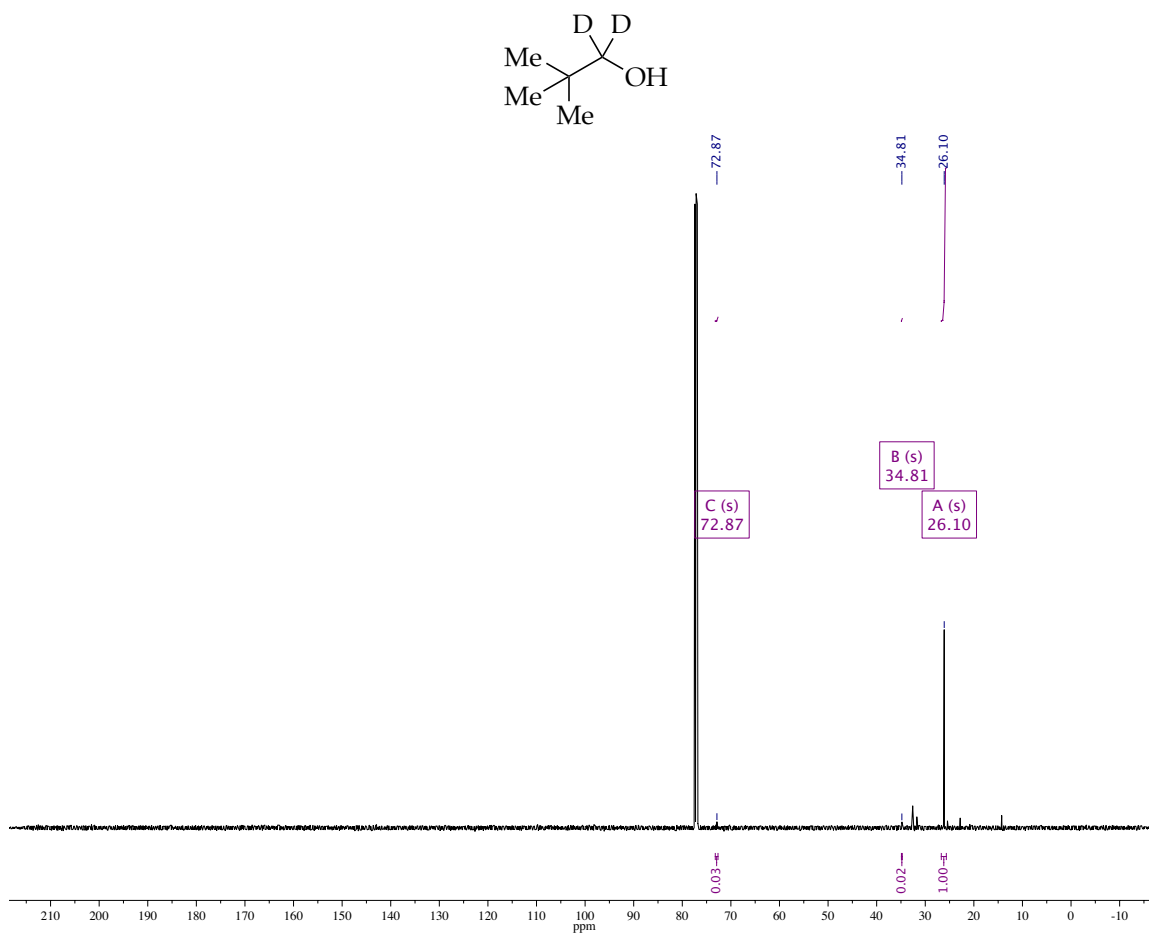


Figure 28. ^{13}C NMR spectrum of neopentyl alcohol- d_2 in CDCl_3 .

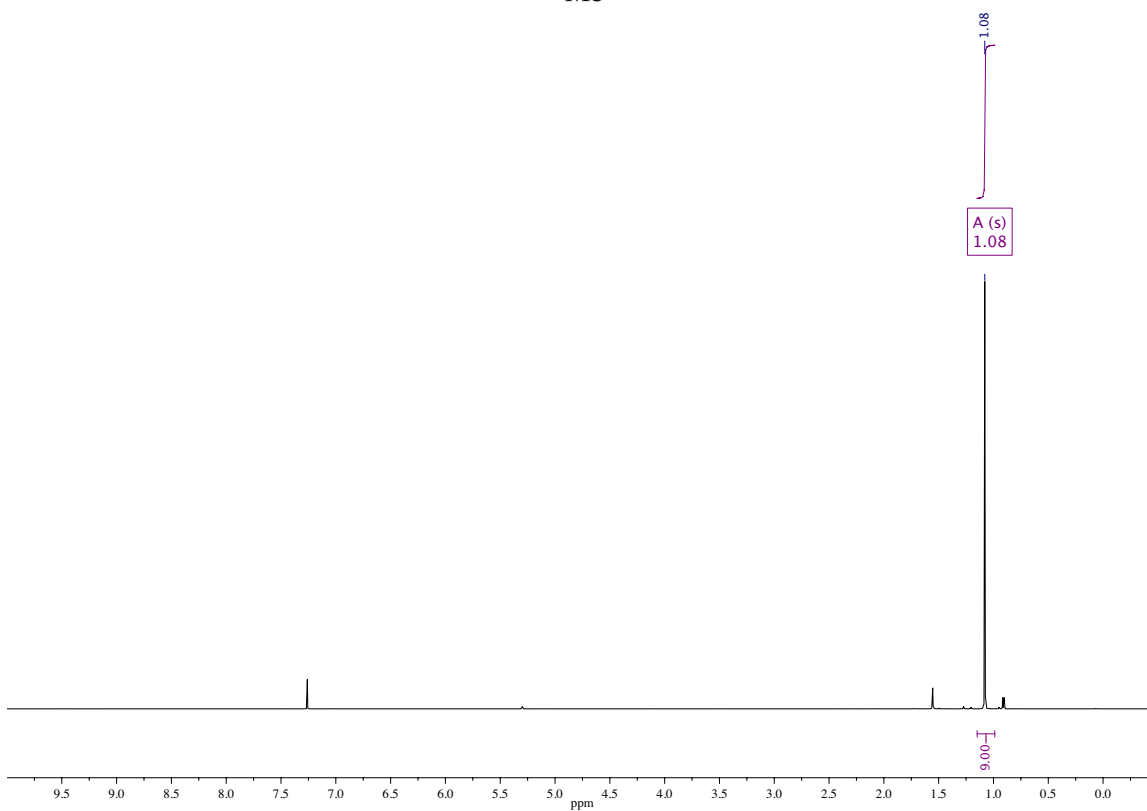
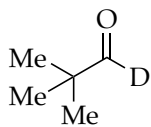


Figure 29. ^1H NMR spectrum of pivalaldehyde-*d* in CDCl_3 .

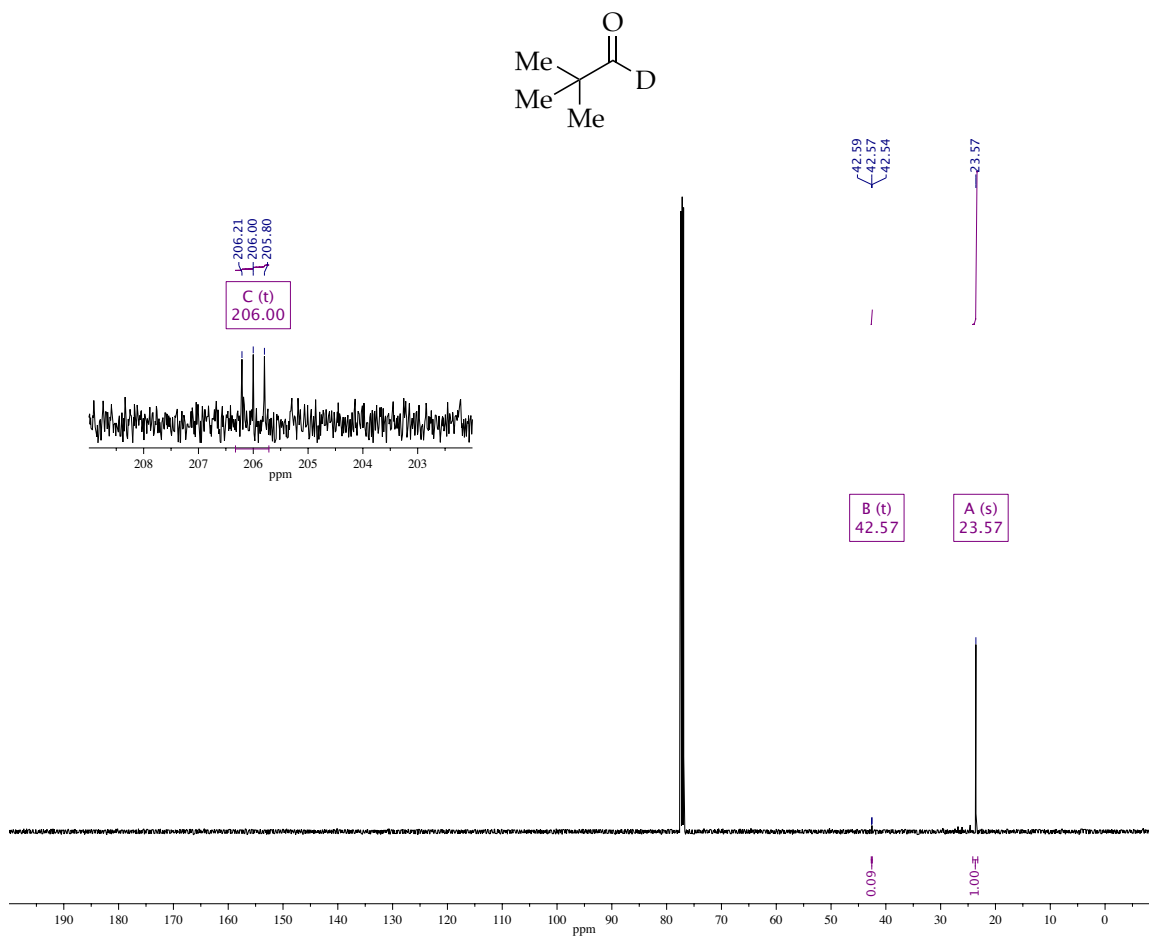


Figure 30. ^{13}C NMR spectrum of pivaldehyde-*d* in CDCl_3 .

Synthesis of 51.

Ethyl 2-morpholinoacetate. Add K_2CO_3 (27.6 g, 0.20 mol) to a solution of morpholine (8.71 g, 0.10 mol) in 500 mL of THF. The resulting mixture was stirred at rt for 15 min and chloroethyl acetate (12.3 g, 10.7 mL, 0.10 mol) was then added. The reaction was stirred for 48 h at rt. Quenched by adding 200 mL of water, extracted with EtOAc (3x), and dried over Na_2SO_4 . Concentrated in vacuo and purified by flash chromatography (hexanes/ethyl acetate). The desired product was obtained in 90% yield. 1H NMR (400 MHz, $CDCl_3$) δ 4.14 (q, $J = 7.1$ Hz, 1H), 3.70 (dd, $J = 4.7$ Hz, 2H), 3.15 (s, 1H), 2.53 (dd, $J = 5.7, 3.7$ Hz, 2H), 1.22 (t, $J = 7.1$ Hz, 2H).

2-Methyl-1-morpholinopropan-2-ol (51). 3.0 M MeMgBr in Et_2O (46.2 mL) was added dropwise to a solution of ethyl 2-morpholinoacetate (8.0 g, 46.2 mmol) in 200 mL of anhydrous THF under Ar at -78 °C, and the reaction mixture was stirred overnight allowing the temperature to rise to rt. Water (200 mL) was added and the resulting mixture was extracted with Et_2O (3x). The combined organic extracts were washed with brine and dried over $MgSO_4$. 6.9 g (94%) of the desired amino alcohol was obtained. 1H NMR (400 MHz, $CDCl_3$) δ 3.75 – 3.67 (m, 4H), 3.00 (s, 1H), 2.68 – 2.59 (m, 4H), 2.32 (s, 2H), 1.17 (s, 6H).

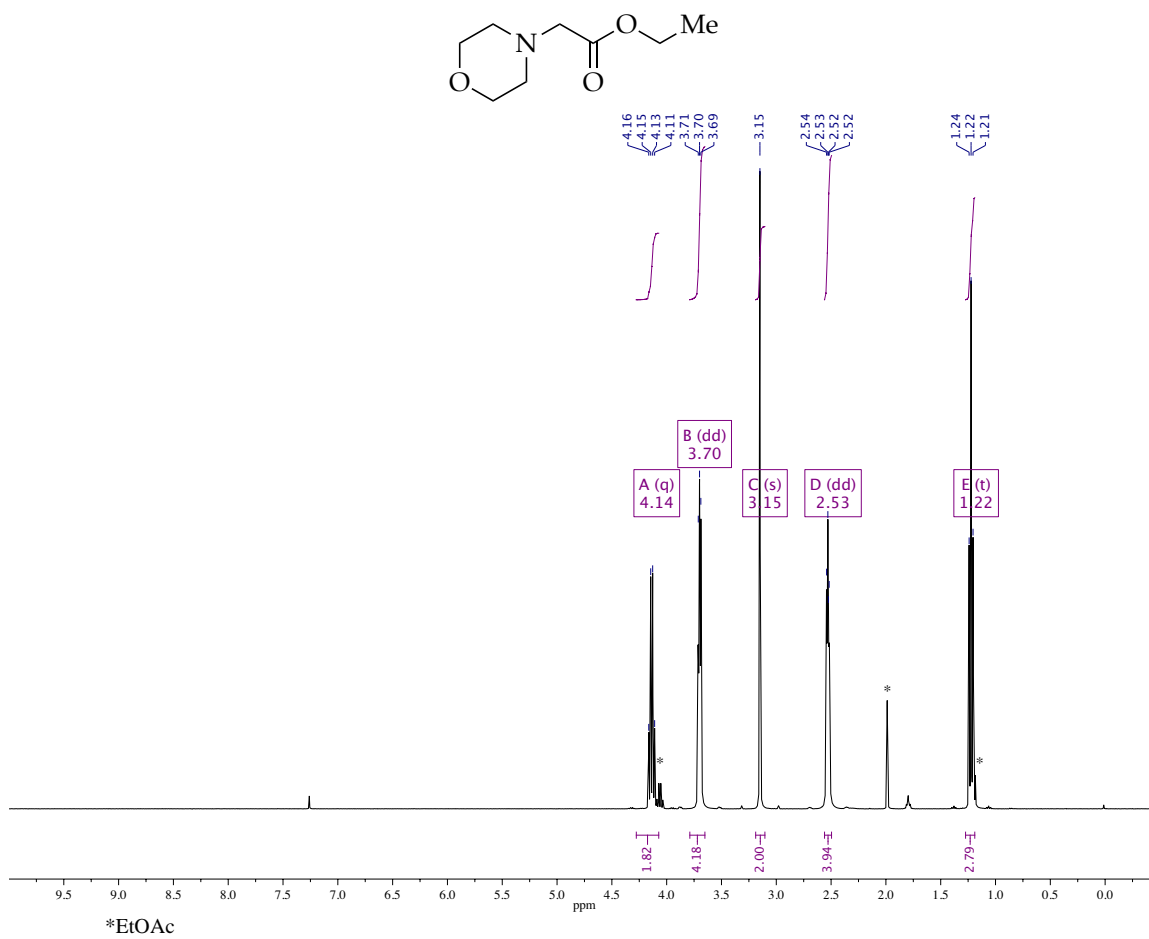


Figure 31. ¹H NMR spectrum of ethyl 2-morpholinoacetate in CDCl₃.

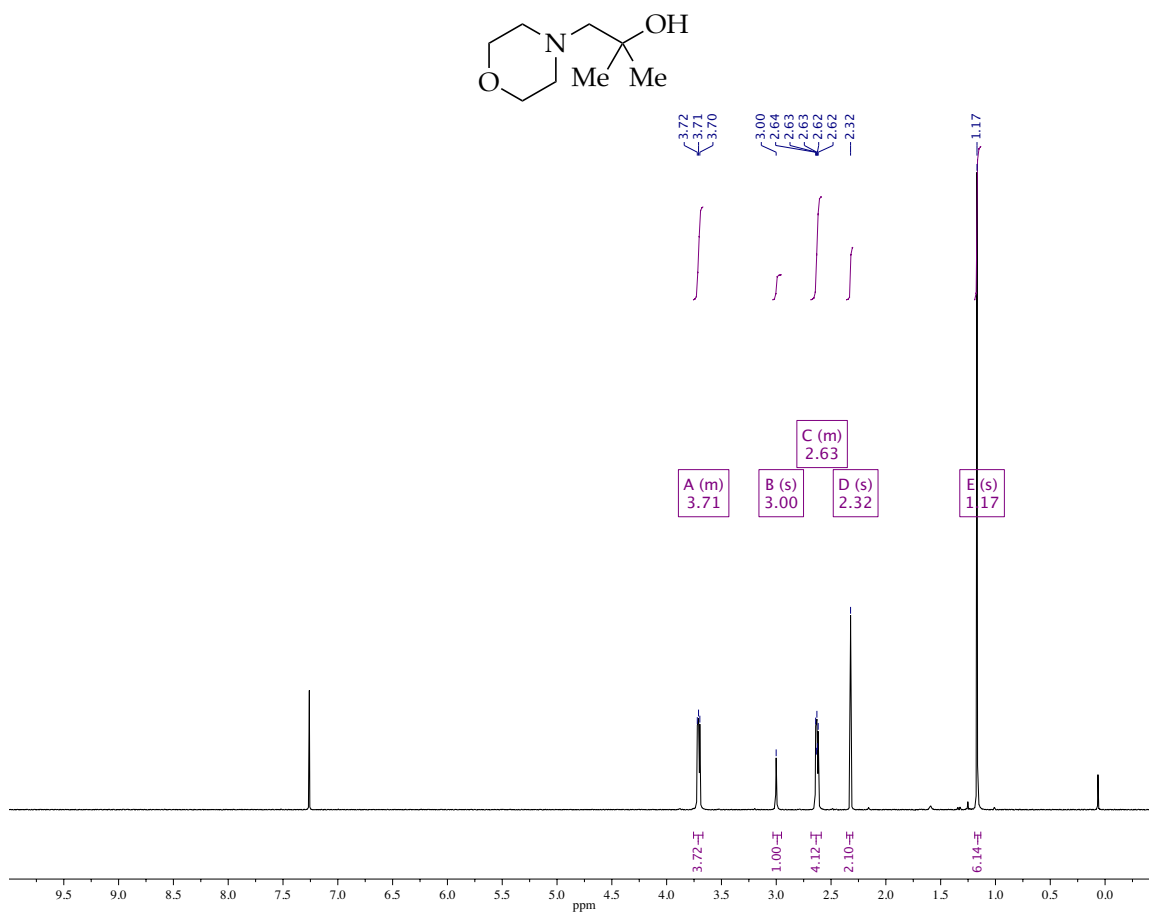


Figure 32. ¹H NMR spectrum of **51** in CDCl₃.

Part 2. Aggregate Characterization

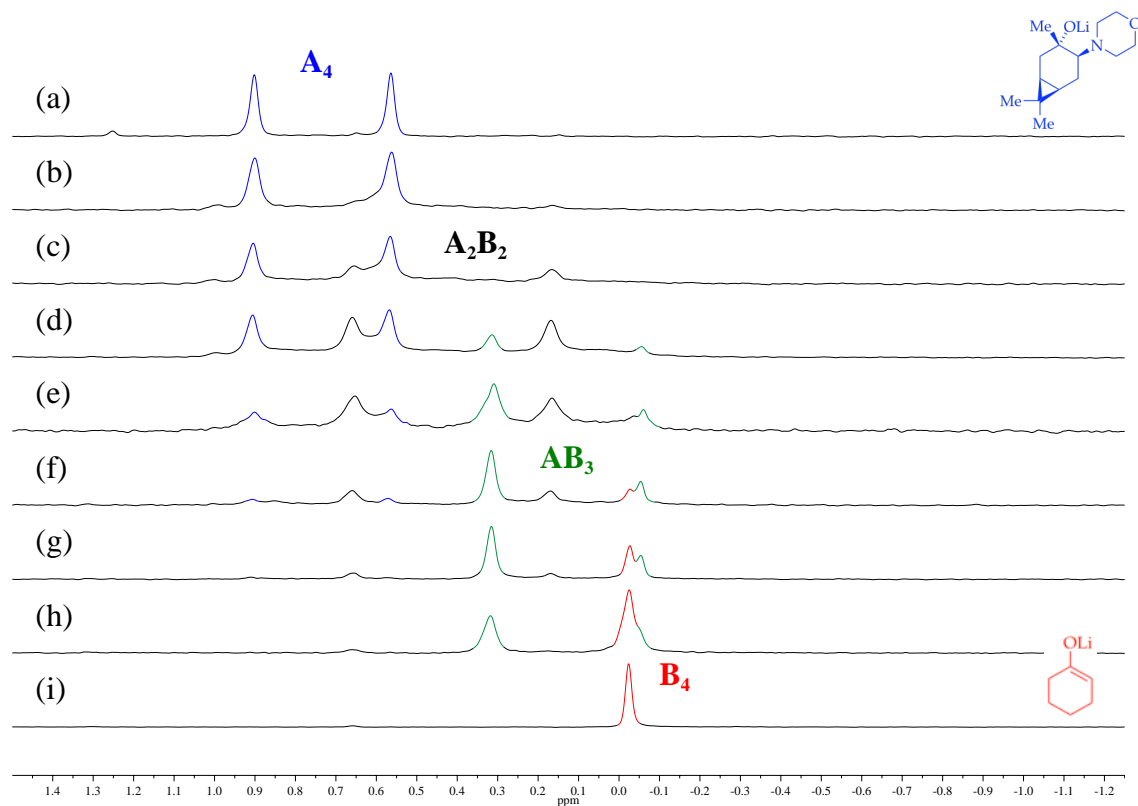


Figure 33. ^6Li NMR spectra for 0.10 M solutions of $[\text{}^6\text{Li}]\text{-11}$ (A) and $[\text{}^6\text{Li}]\text{-CyOLi}$ (B) in THF at $-80\text{ }^\circ\text{C}$ (substrates were deprotonated with 0.11 M $[\text{}^6\text{Li}]\text{LDA}$ and aged for 10 min at $25\text{ }^\circ\text{C}$). The intended mole fractions, X_B , in (a)–(i) are 0.00, 0.02, 0.13, 0.32, 0.45, 0.55, 0.78, 0.89 and 1.00, respectively.

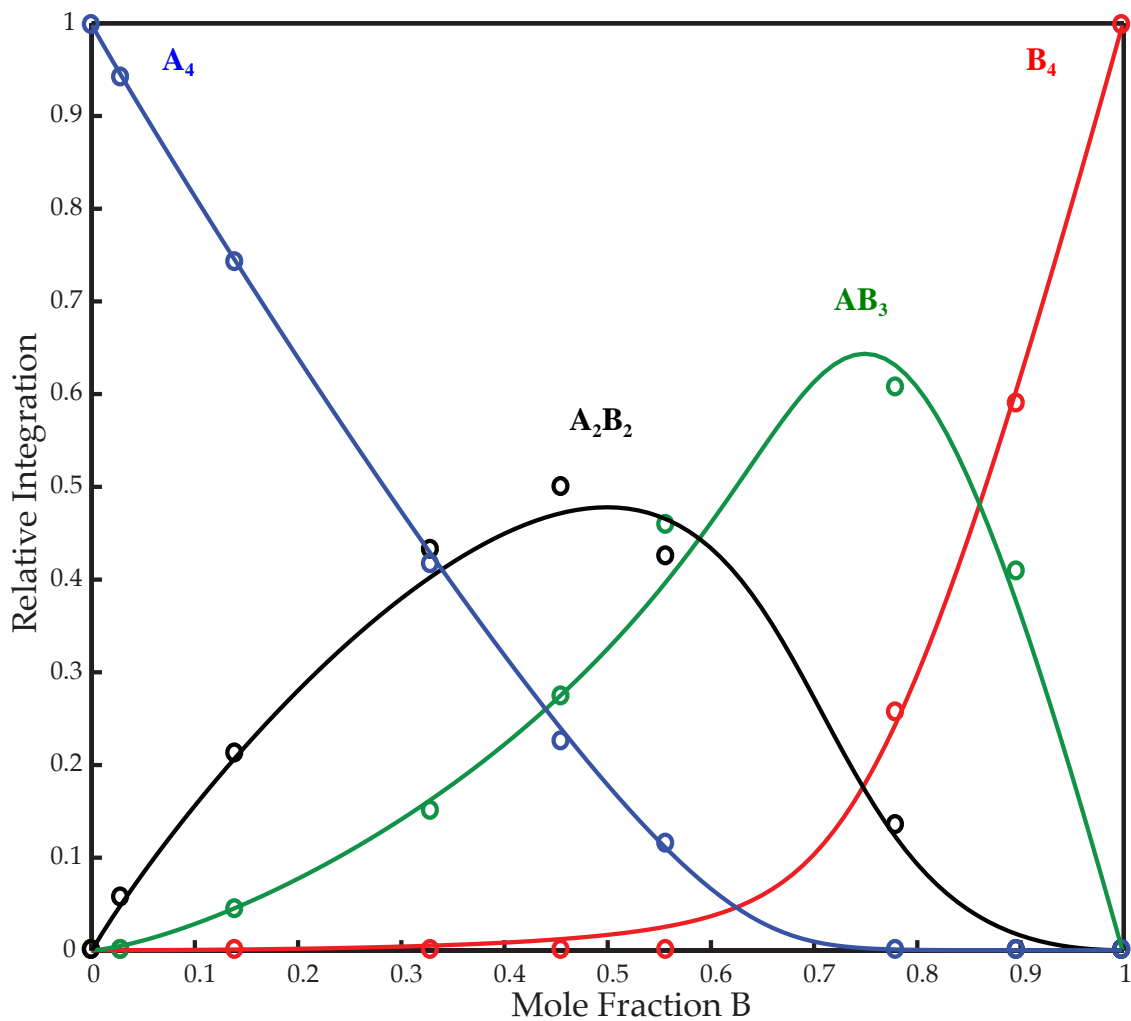


Figure 34. Job plot showing the relative integrations versus the measured mole fraction of CyOLi for 0.10 M mixtures of [⁶Li]-**11** (**A**) and [⁶Li]- **CyOLi** (**B**) in THF at $-80\text{ }^{\circ}\text{C}$.

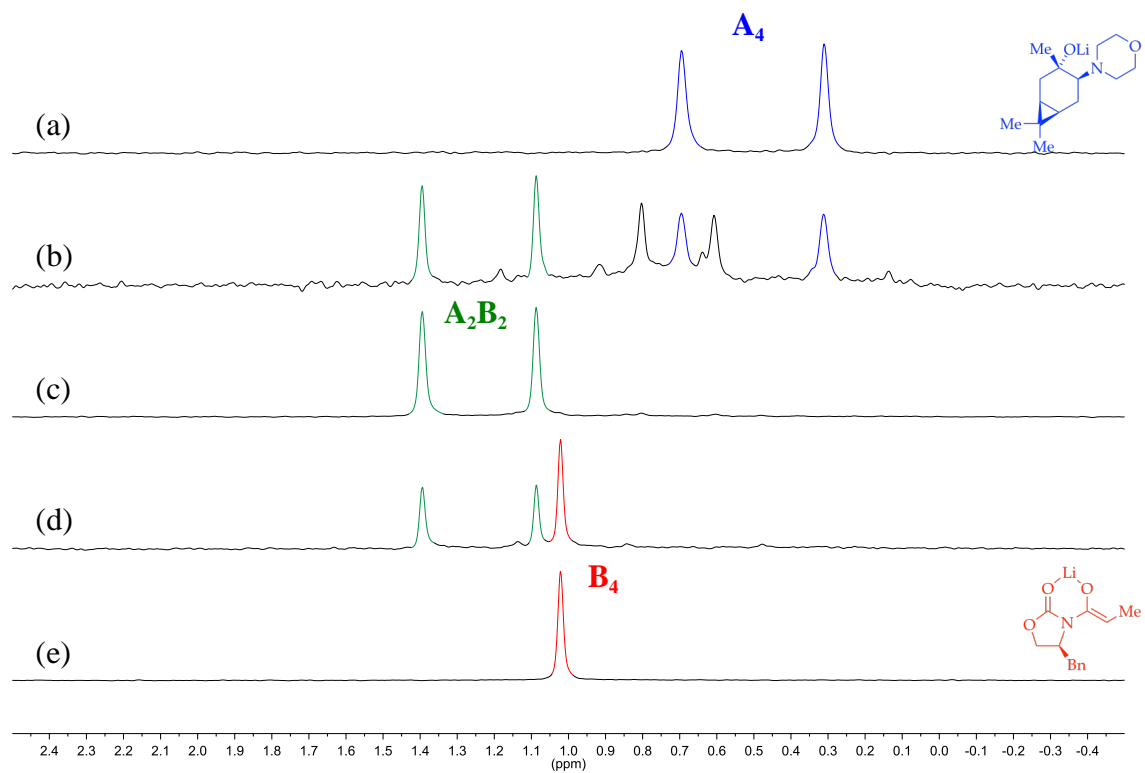


Figure 35. ^6Li NMR spectra for 0.10 M solutions of $[\text{}^6\text{Li}]\text{-11}$ (A) and $[\text{}^6\text{Li}]\text{-(S)-1a}$ (B) in toluene (1.0 equiv of THF per Li) at $-80\text{ }^\circ\text{C}$ (substrates were deprotonated with 0.11 M $[\text{}^6\text{Li}]\text{LDA}$ and aged for 10 min at $25\text{ }^\circ\text{C}$). The intended mole fractions, X_B , in (a)–(e) are 0.00, 0.25, 0.50, 0.75, and 1.00, respectively.

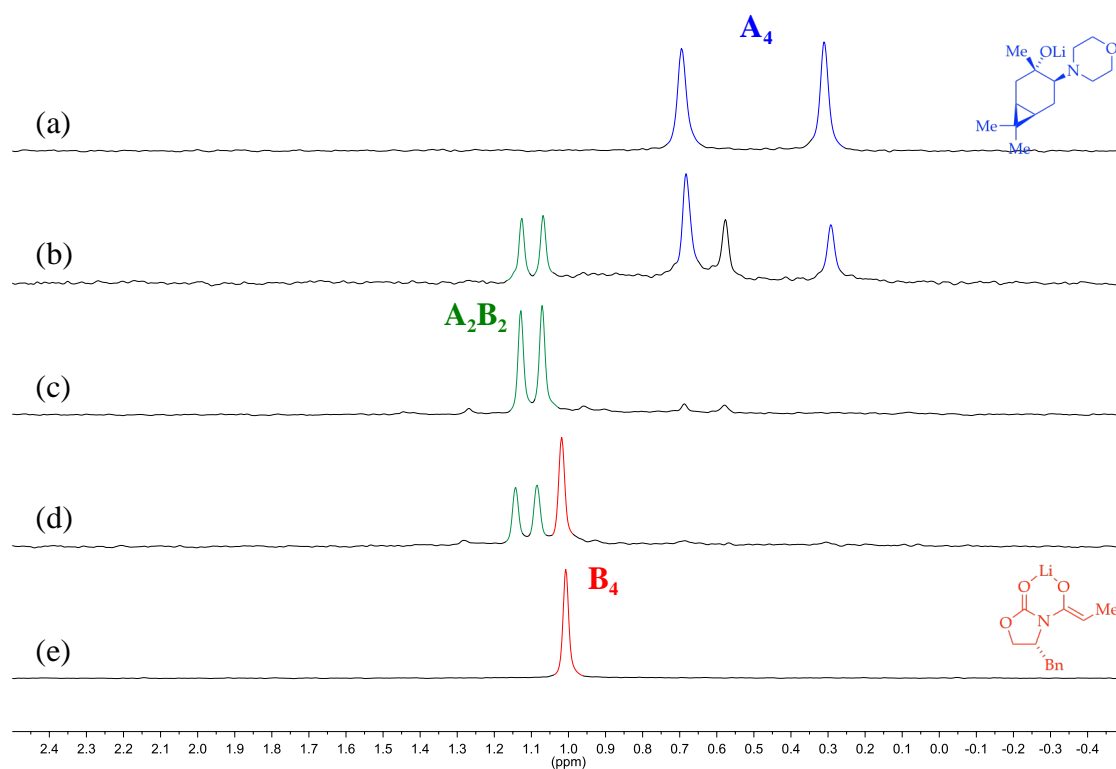


Figure 36. ^6Li NMR spectra for 0.10 M solutions of $[\text{}^6\text{Li}]\text{-5}$ (A) and $[\text{}^6\text{Li}]\text{-(R)-1}$ (B) in toluene (1.0 equiv of THF per Li) at $-80\text{ }^\circ\text{C}$ (substrates were deprotonated with 0.11 M $[\text{}^6\text{Li}]\text{LDA}$ and aged for 10 min at $25\text{ }^\circ\text{C}$). The intended mole fractions, X_B , in (a)–(e) are 0.00, 0.25, 0.50, 0.75, and 1.00, respectively.

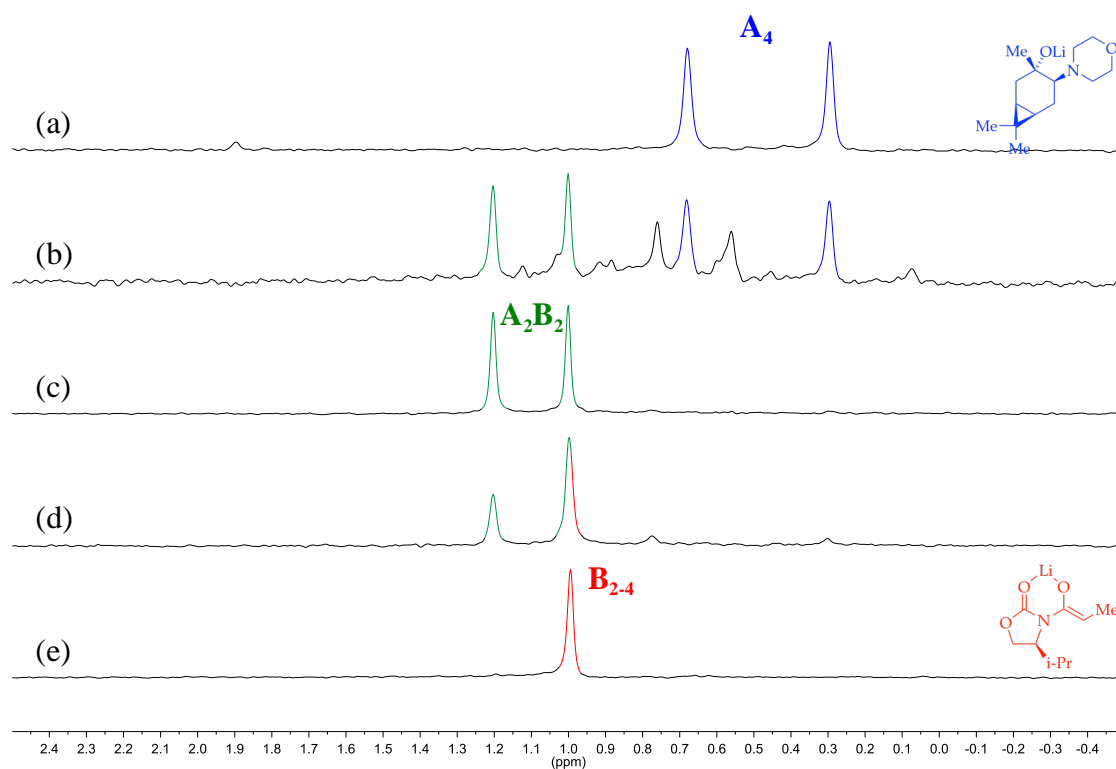


Figure 37. ^6Li NMR spectra for 0.10 M solutions of $[\text{}^6\text{Li}]\text{-11}$ (A) and $[\text{}^6\text{Li}]\text{-(S)-1b}$ (B) in toluene (1.0 equiv of THF per Li) at $-80\text{ }^\circ\text{C}$ (substrates were deprotonated with 0.11 M $[\text{}^6\text{Li}]\text{LDA}$ and aged for 10 min at $25\text{ }^\circ\text{C}$). The intended mole fractions, X_B , in (a)-(e) are 0.00, 0.25, 0.50, 0.75, and 1.00, respectively.

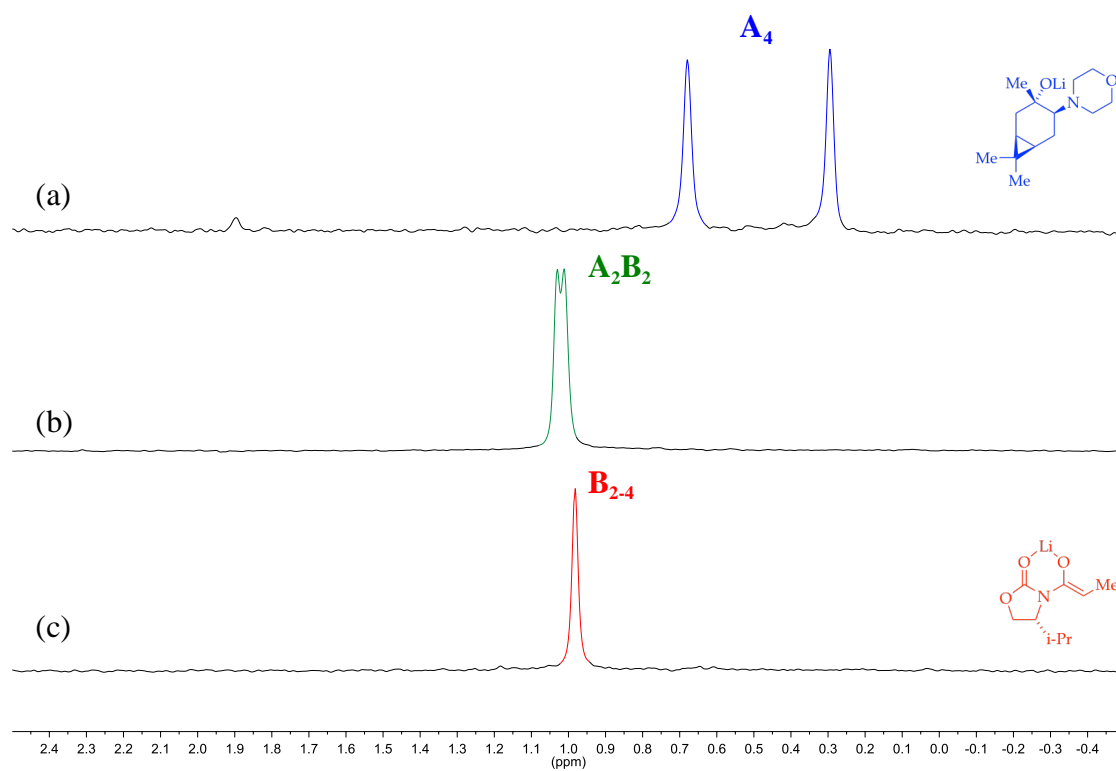


Figure 38. ^6Li NMR spectra for 0.10 M solutions of $[\text{}^6\text{Li}]\text{-11}$ (A) and $[\text{}^6\text{Li}]\text{-(R)-1b}$ (B) in toluene (1.0 equiv of THF per Li) at $-80\text{ }^\circ\text{C}$ (substrates were deprotonated with 0.11 M $[\text{}^6\text{Li}]\text{LDA}$ and aged for 10 min at $25\text{ }^\circ\text{C}$). The intended mole fractions, X_B , in (a)-(c) are 0.00, 0.50, and 1.00, respectively.

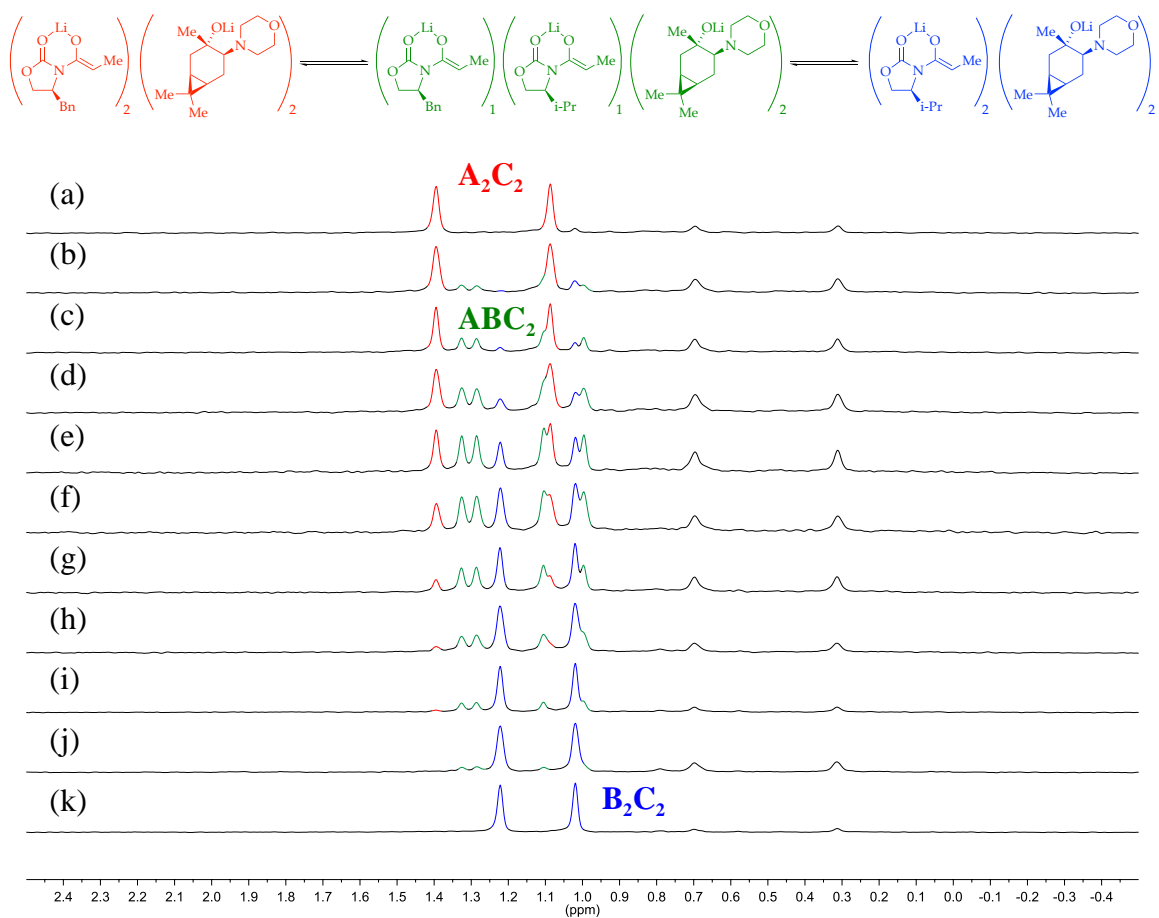


Figure 39. ^6Li NMR spectra for 0.10 M solutions of $[\text{}^6\text{Li}]$ -(*S*)-**15a** (**A**) and $[\text{}^6\text{Li}]$ -(*S*)-**15b** (**B**) in toluene (1.0 equiv of THF per Li) at $-80\text{ }^\circ\text{C}$ (substrates were deprotonated with 0.11 M $[\text{}^6\text{Li}]$ LDA and aged for 10 min at $25\text{ }^\circ\text{C}$). The measured mole fractions, X_B , in (a)-(k) are 0.00, 0.11, 0.24, 0.38, 0.45, 0.55, 0.65, 0.74, 0.81, 0.93, and 1.00, respectively.

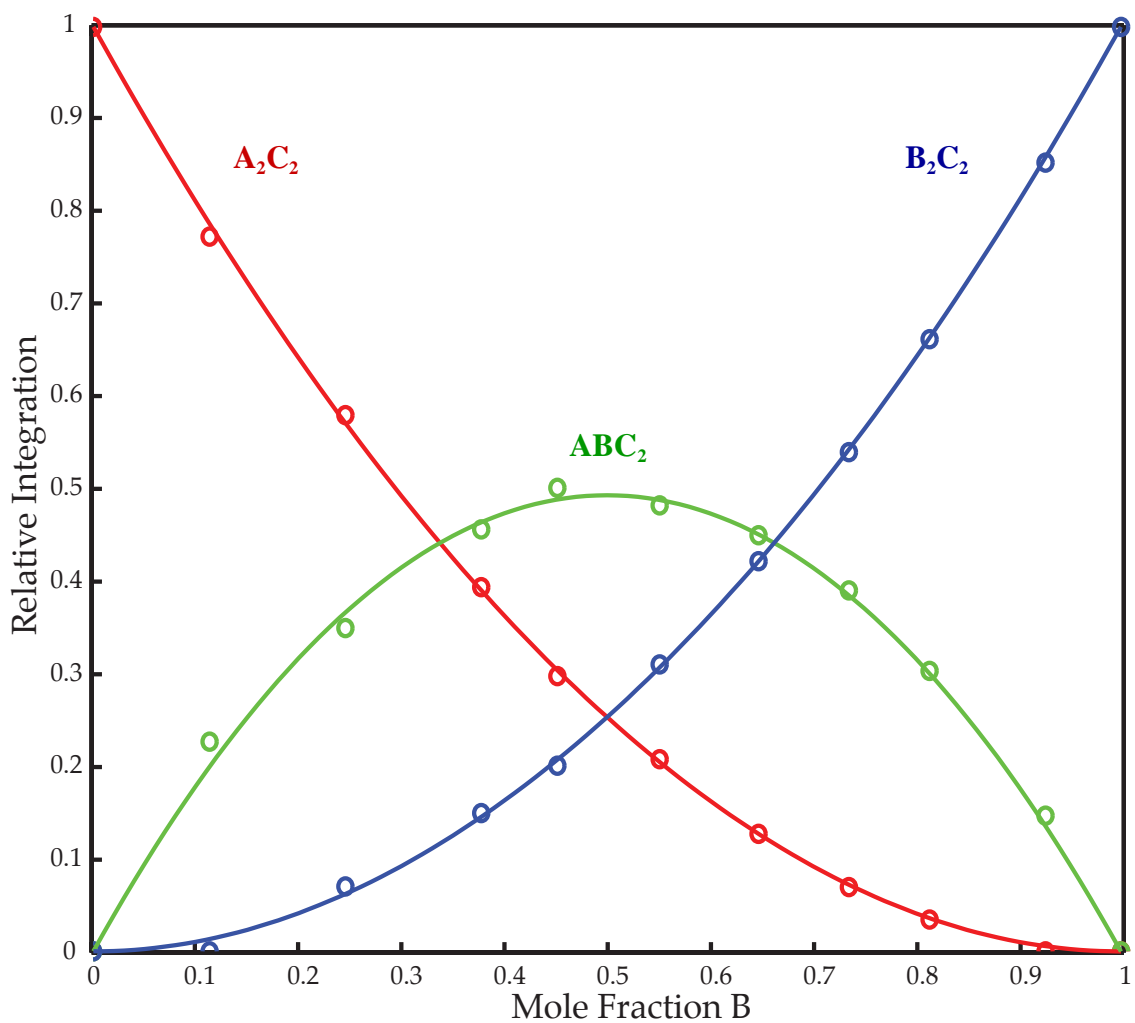
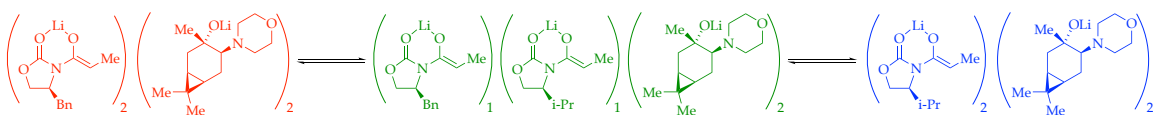


Figure 40. Job plot showing the relative integrations versus the measured mole fraction of (*S*)-**1b** for 0.10 M mixtures of [⁶Li]-(*S*)-**15a** (**A**) and [⁶Li]-(*S*)-**15b** (**B**) in toluene (1.0 equiv of THF per Li) at $-80\text{ }^{\circ}\text{C}$.

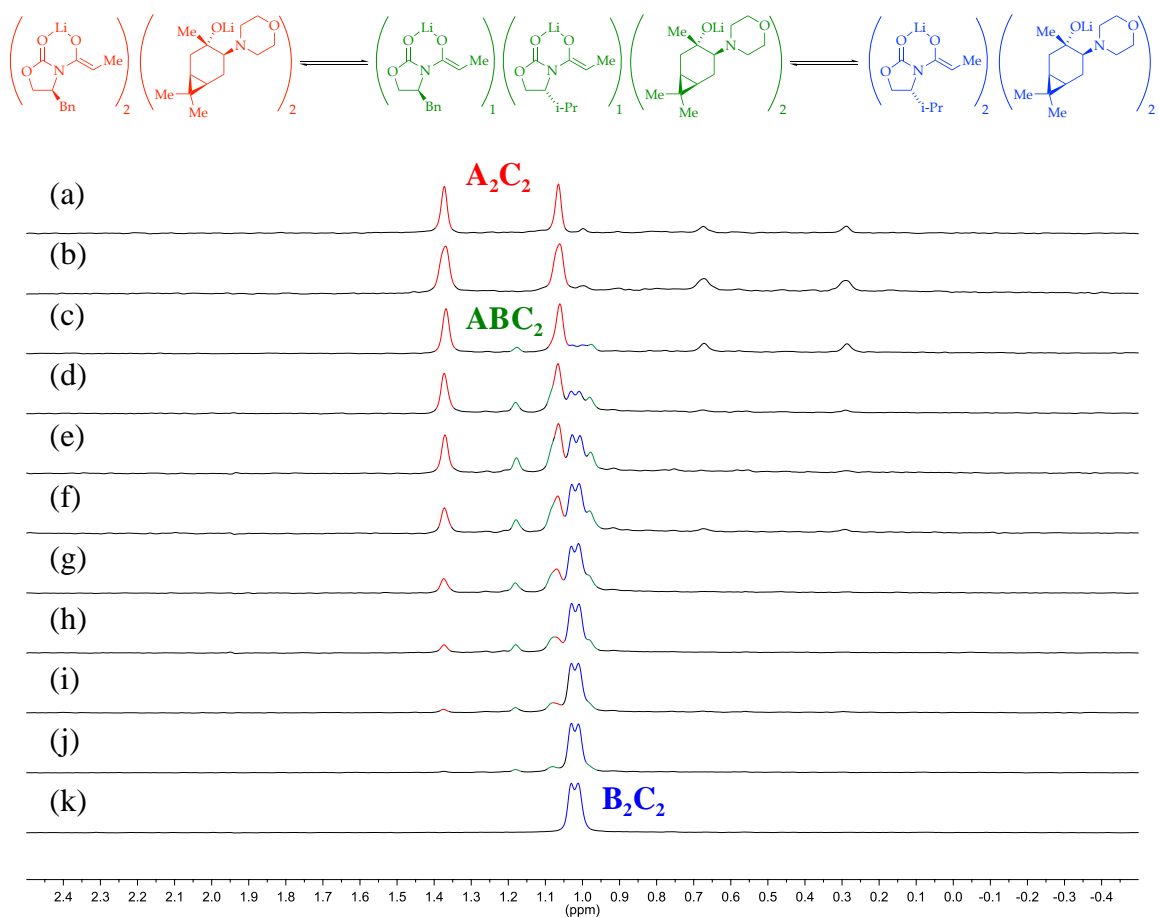


Figure 41. ^6Li NMR spectra for 0.10 M solutions of [^6Li]-(*S*)-15a (**A**) and [^6Li]-(*R*)-15b (**B**) in toluene (1.0 equiv of THF per Li) at $-80\text{ }^\circ\text{C}$ (substrates were deprotonated with 0.11 M [^6Li]LDA and aged for 10 min at $25\text{ }^\circ\text{C}$). The measured mole fractions, X_B , in (a)-(k) are 0.00, 0.06, 0.22, 0.30, 0.45, 0.56, 0.62, 0.77, 0.82, 0.91, and 1.00, respectively.

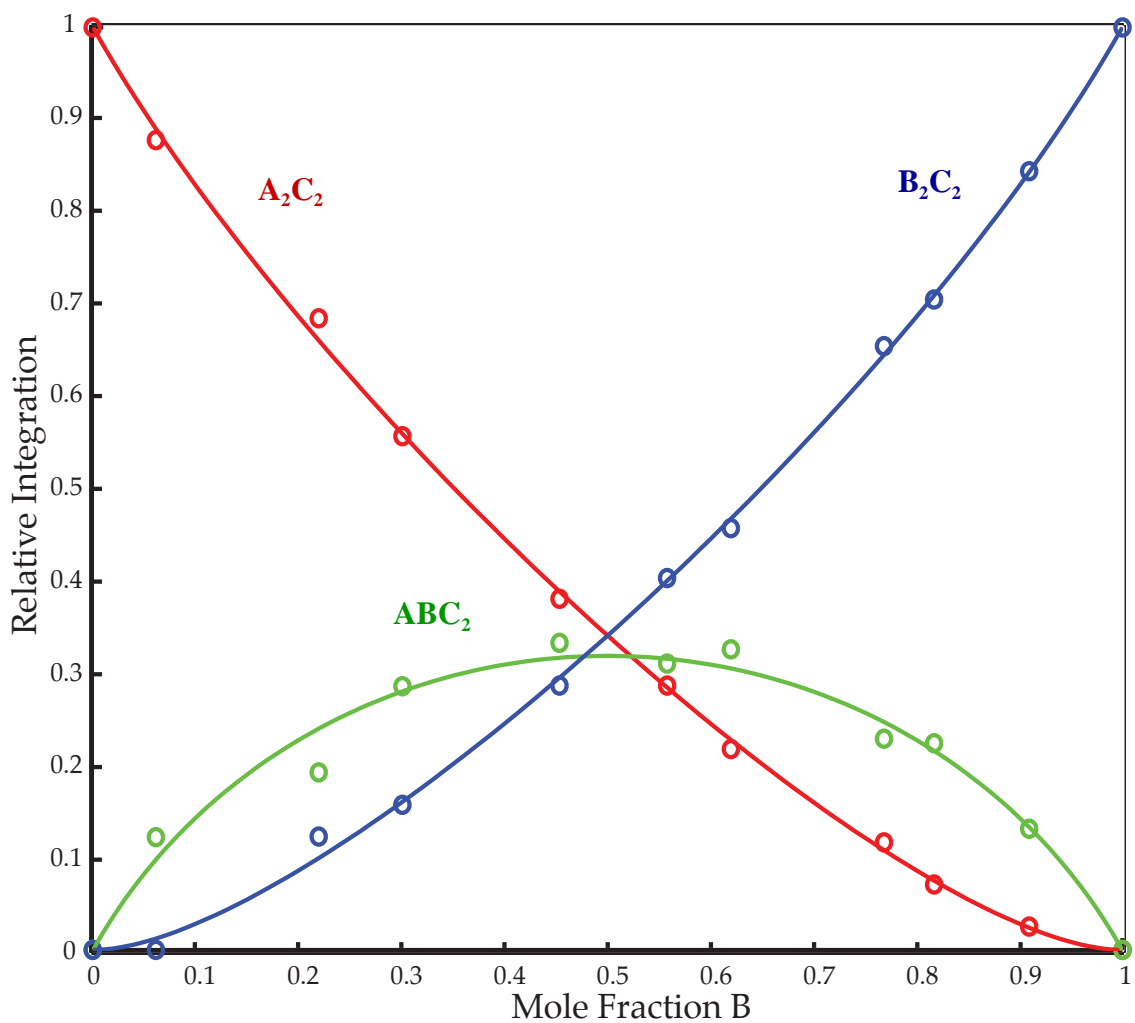
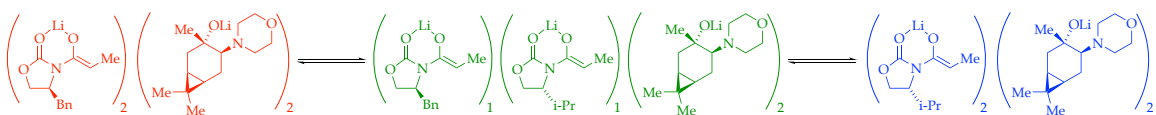


Figure 42. Job plot showing the relative integrations versus the measured mole fraction of (*R*)-**1b** for 0.10 M mixtures of [⁶Li]-(*S*)-**15a** (**A**) and [⁶Li]-(*R*)-**15b** (**B**) in toluene (1.0 equiv of THF per Li) at $-80\text{ }^{\circ}\text{C}$.

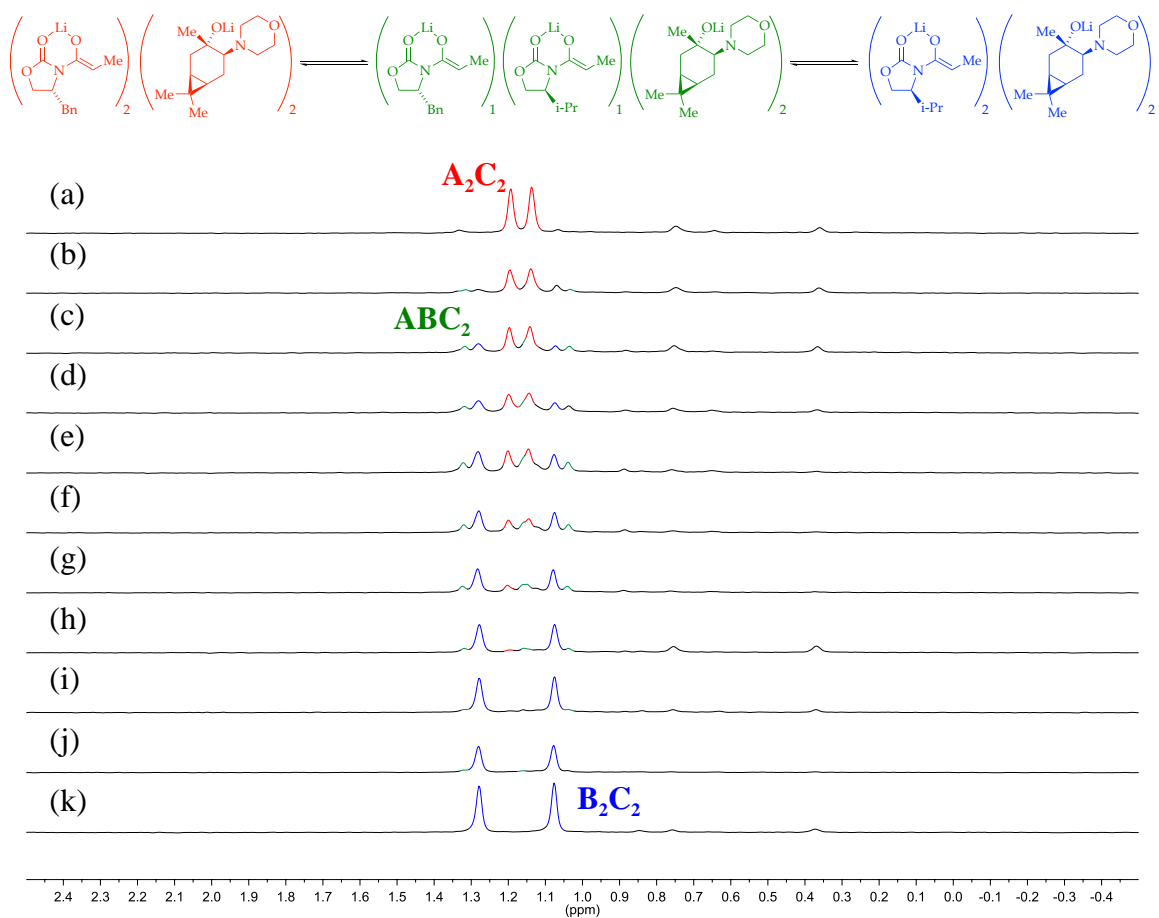


Figure 43. ^6Li NMR spectra for 0.10 M solutions of [^6Li]-(*R*)-15a (**A**) and [^6Li]-(*S*)-15b (**B**) in toluene (1.0 equiv of THF per Li) at $-80\text{ }^\circ\text{C}$ (substrates were deprotonated with 0.11 M [^6Li]LDA and aged for 10 min at $25\text{ }^\circ\text{C}$). The measured mole fractions, X_B , in (a)-(k) are 0.00, 0.14, 0.34, 0.44, 0.49, 0.60, 0.72, 0.82, 0.90, 0.93, and 1.00, respectively.

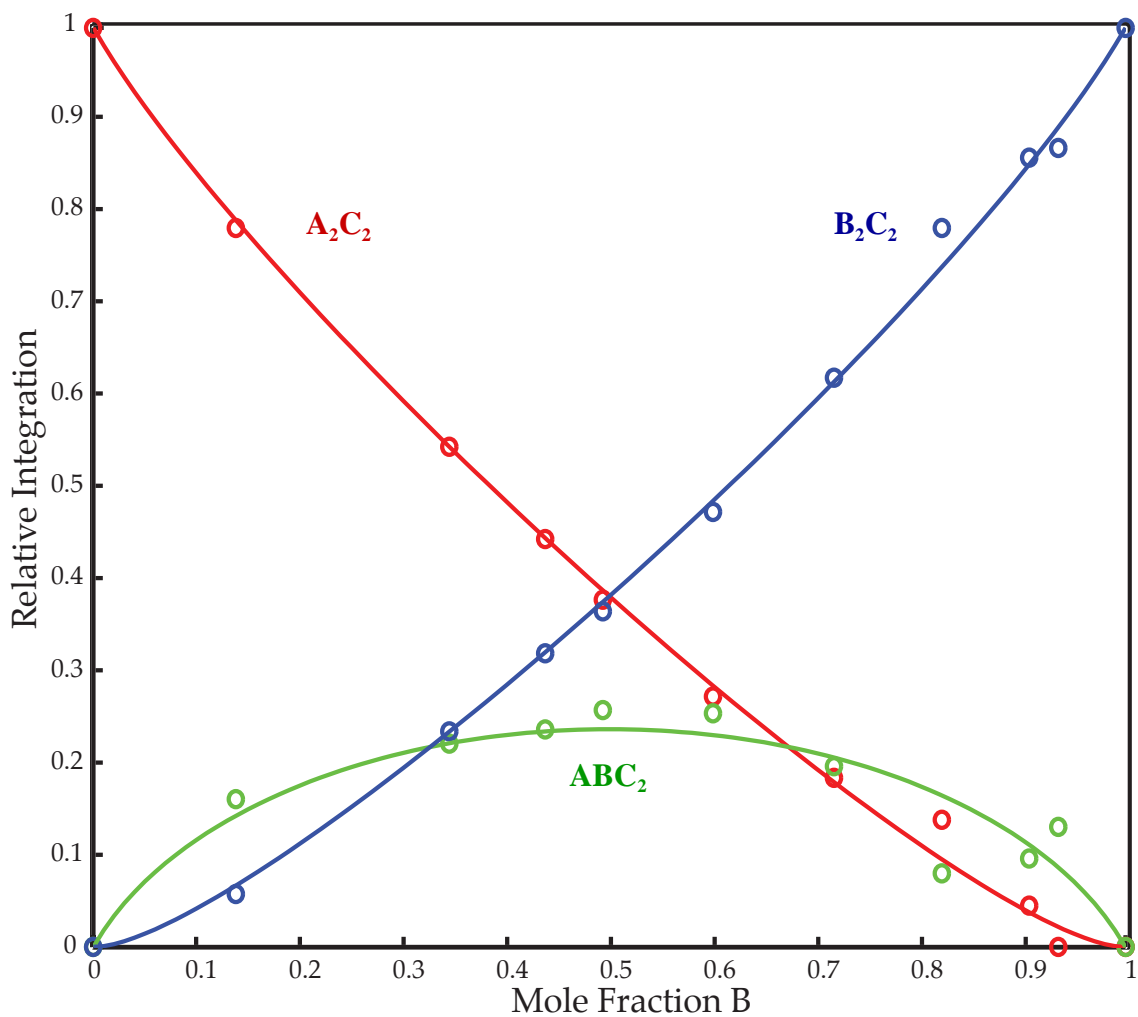
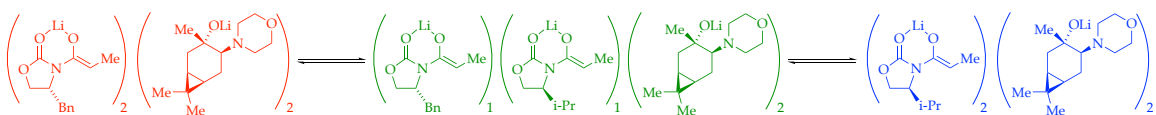


Figure 44. Job plot showing the relative integrations versus the measured mole fraction of (*S*)-**1b** for 0.10 M mixtures of [⁶Li]-(*R*)-**15a** (**A**) and [⁶Li]-(*S*)-**15b** (**B**) in toluene (1.0 equiv of THF per Li) at $-80\text{ }^{\circ}\text{C}$.

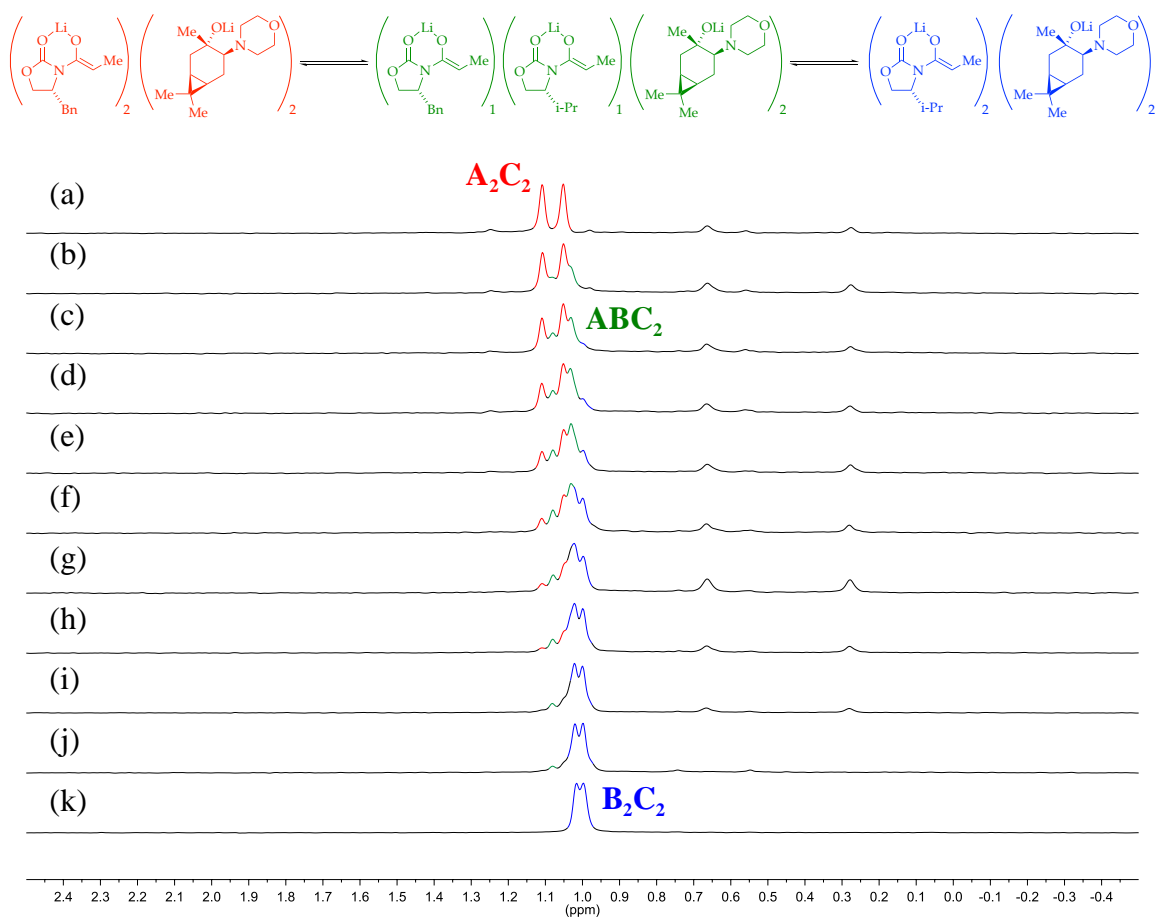


Figure 45. ^6Li NMR spectra for 0.10 M solutions of [6Li]-(R)-15a (A) and [6Li]-(R)-15b (B) in toluene (1.0 equiv of THF per Li) at -80°C (substrates were deprotonated with 0.11 M [6Li]LDA and aged for 10 min at 25°C). The measured mole fractions, X_B , in (a)-(k) are 0.00, 0.13, 0.28, 0.37, 0.53, 0.68, 0.70, 0.80, 0.88, 0.93, and 1.00, respectively.

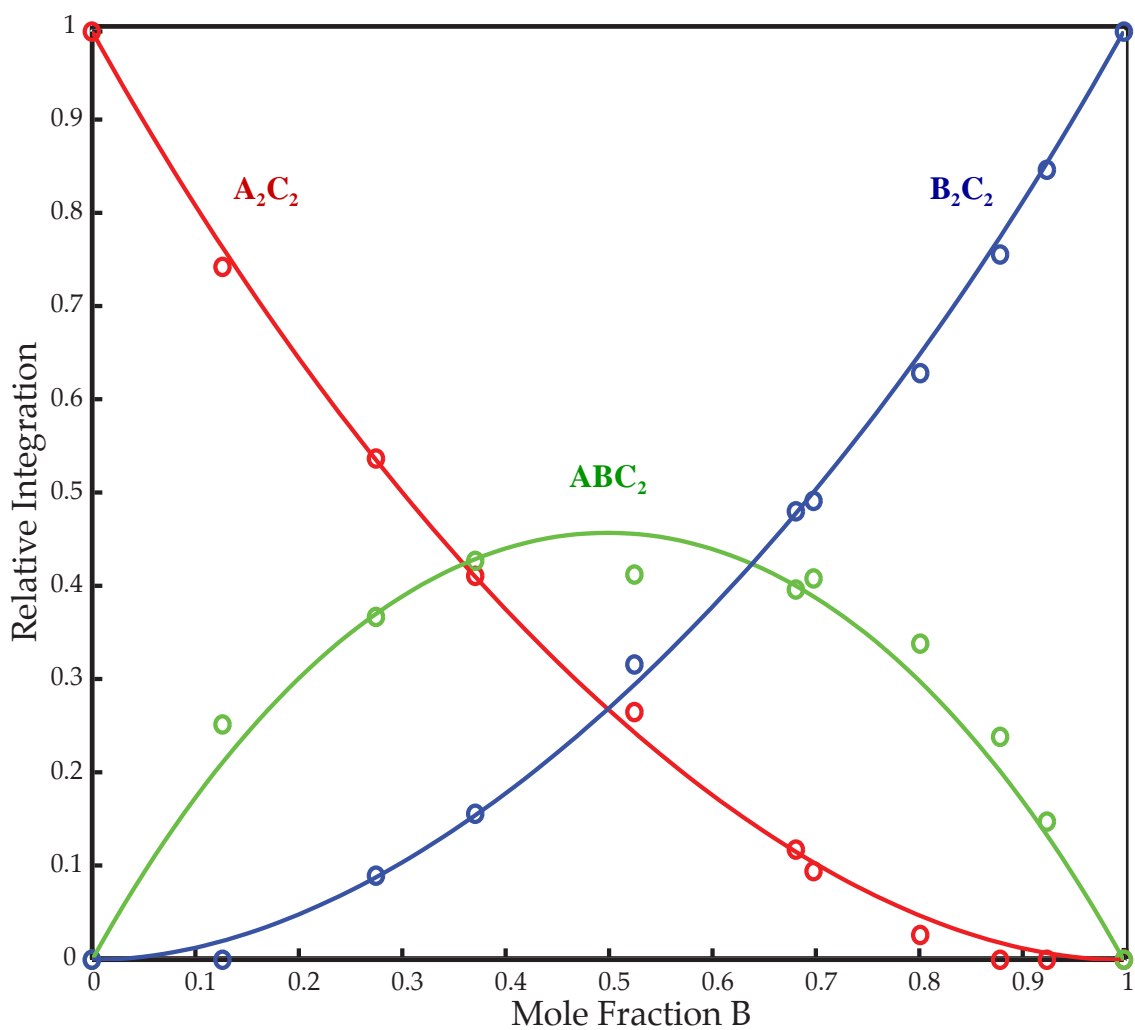
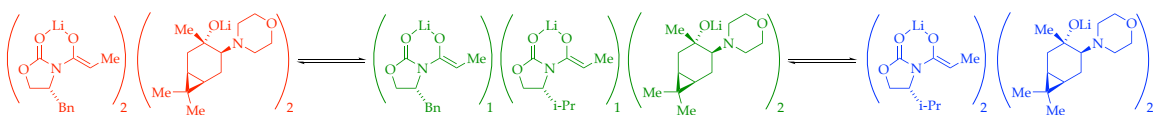


Figure 46. Job plot showing the relative integrations versus the measured mole fraction of (*R*)-**1b** for 0.10 M mixtures of [⁶Li]-(*R*)-**15a** (A) and [⁶Li]-(*R*)-**15b** (B) in toluene (1.0 equiv of THF per Li) at $-80\text{ }^{\circ}\text{C}$.

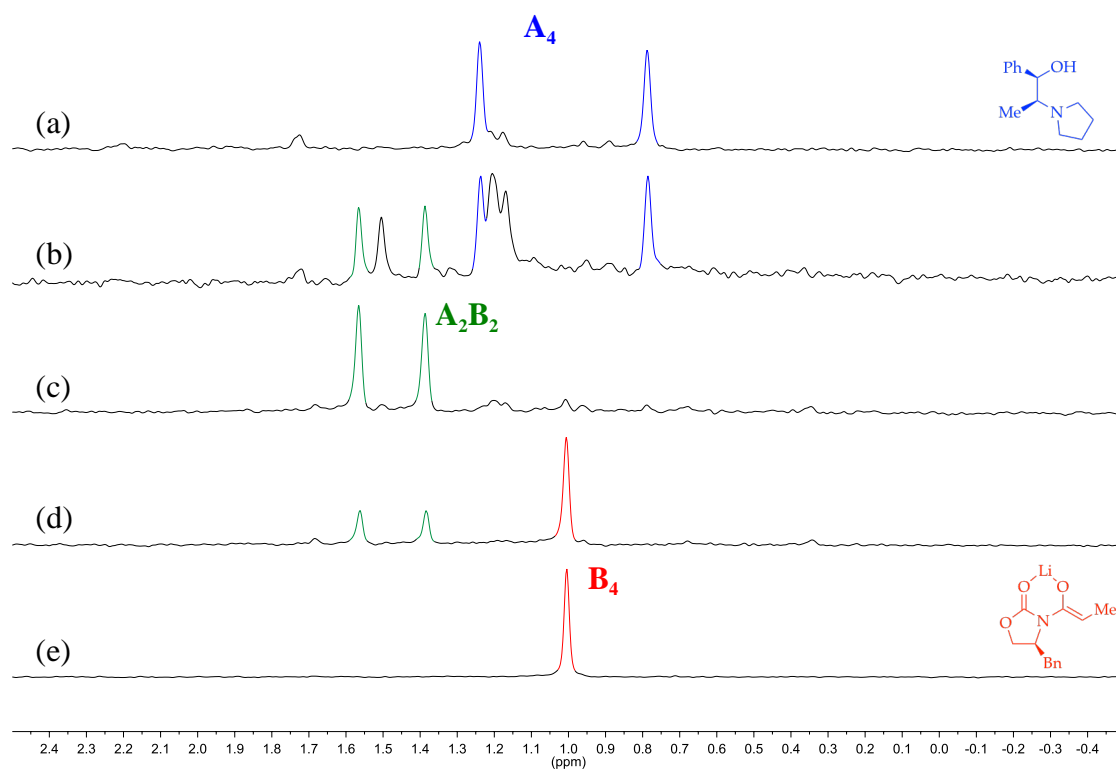


Figure 47. ^6Li NMR spectra for 0.10 M solutions of $[\text{}^6\text{Li}]\text{-8}$ (A) and $[\text{}^6\text{Li}]\text{-(S)-1a}$ (B) in toluene (1.0 equiv of THF per Li) at $-80\text{ }^\circ\text{C}$ (substrates were deprotonated with 0.11 M $[\text{}^6\text{Li}]\text{LDA}$ and aged for 10 min at $25\text{ }^\circ\text{C}$). The intended mole fractions, X_B , in (a)-(e) are 0.00, 0.25, 0.50, 0.75, and 1.00, respectively.

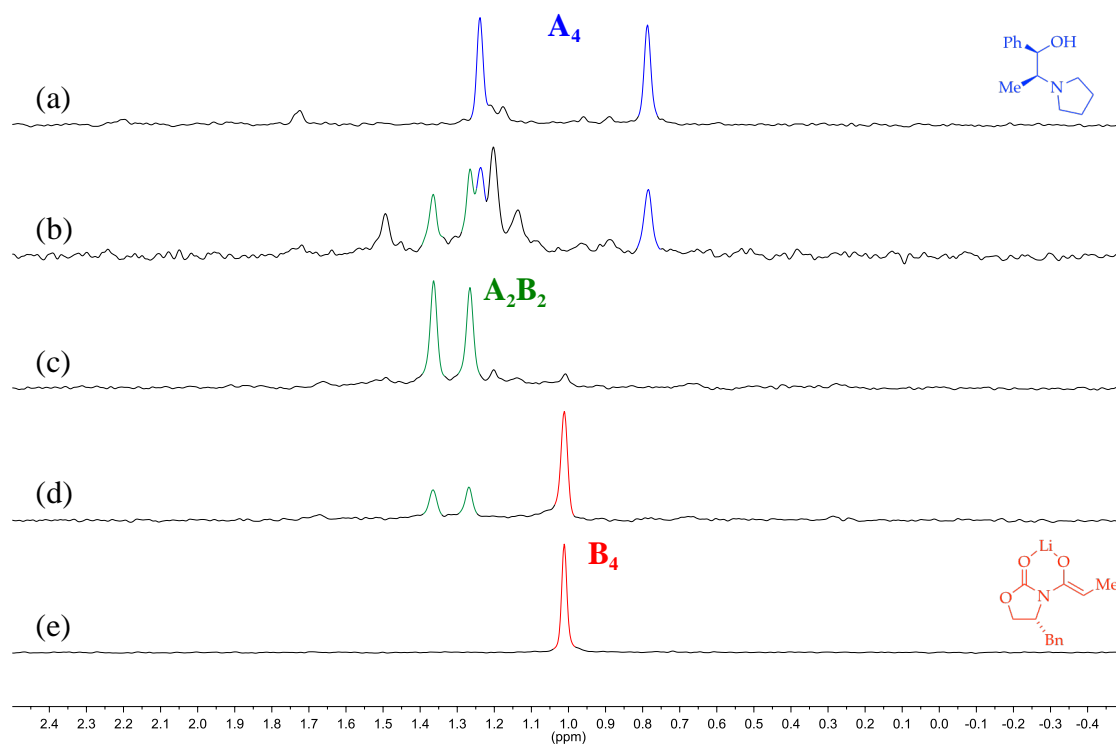


Figure 48. ^6Li NMR spectra for 0.10 M solutions of $[\text{}^6\text{Li}]\text{-8}$ (A) and $[\text{}^6\text{Li}]\text{-(R)-1a}$ (B) in toluene (1.0 equiv of THF per Li) at $-80\text{ }^\circ\text{C}$ (substrates were deprotonated with 0.11 M $[\text{}^6\text{Li}]\text{LDA}$ and aged for 10 min at $25\text{ }^\circ\text{C}$). The intended mole fractions, X_B , in (a)-(e) are 0.00, 0.25, 0.50, 0.75, and 1.00, respectively.

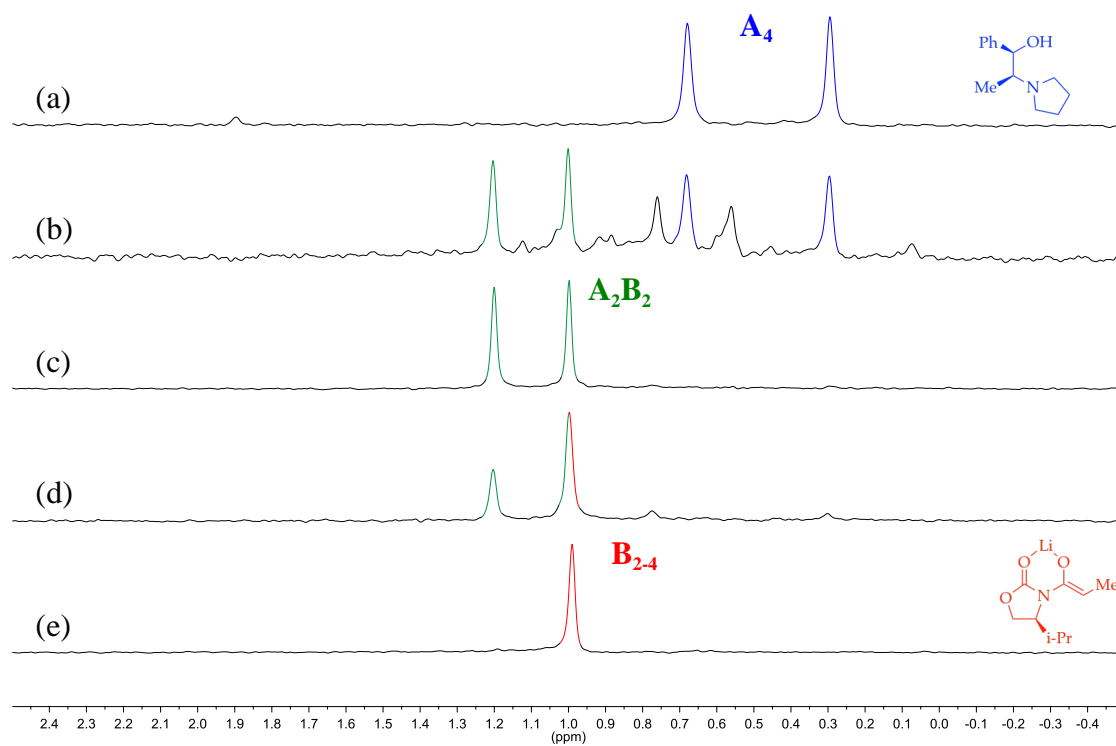


Figure 49. ^6Li NMR spectra for 0.10 M solutions of $[\text{}^6\text{Li}]\text{-8}$ (A) and $[\text{}^6\text{Li}]\text{-(S)-1b}$ (B) in toluene (1.0 equiv of THF per Li) at $-80\text{ }^\circ\text{C}$ (substrates were deprotonated with 0.11 M $[\text{}^6\text{Li}]\text{LDA}$ and aged for 10 min at $25\text{ }^\circ\text{C}$). The intended mole fractions, X_B , in (a)-(e) are 0.00, 0.25, 0.50, 0.75, and 1.00, respectively.

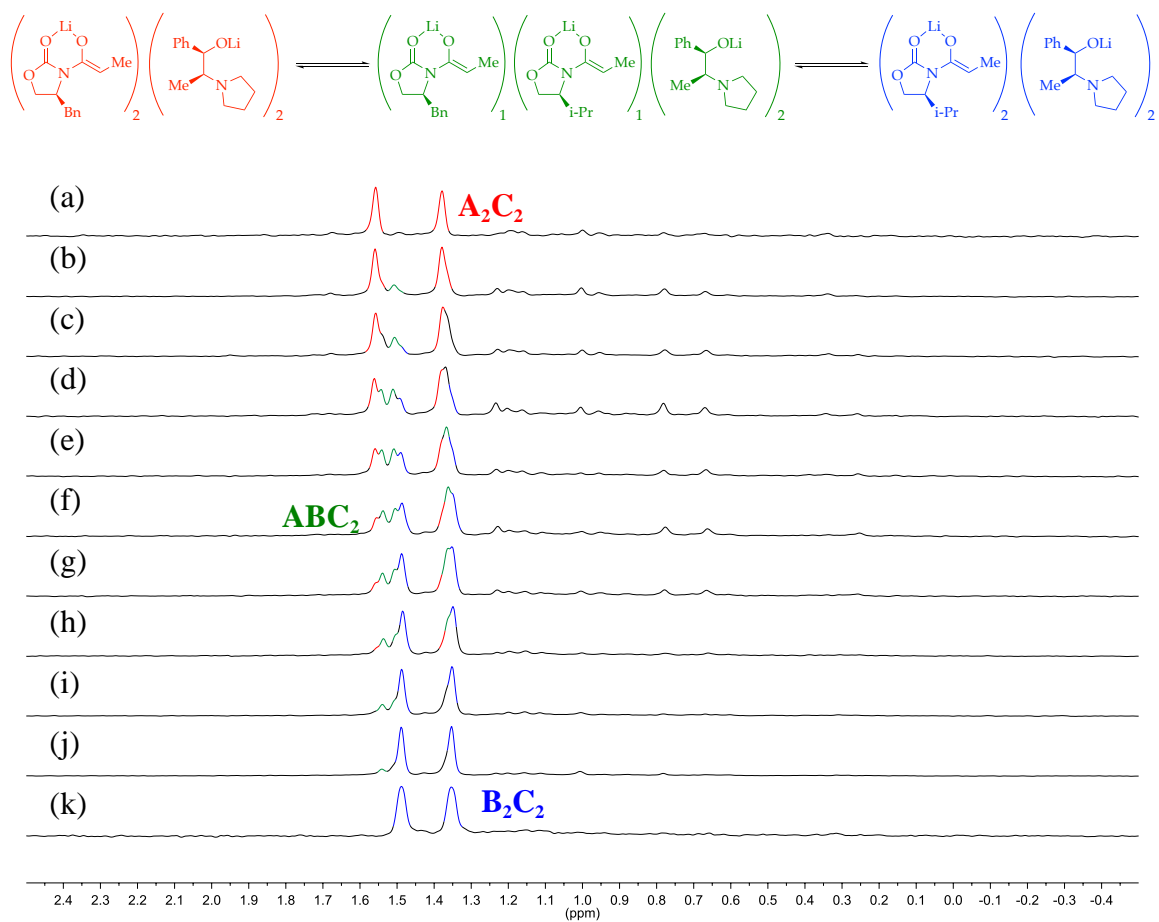


Figure 50. ^6Li NMR spectra for 0.10 M solutions of $[\text{}^6\text{Li}]$ -(*S*)-**36a** (**A**) and $[\text{}^6\text{Li}]$ -(*S*)-**36b** (**B**) in toluene (1.0 equiv of THF per Li) at $-80\text{ }^\circ\text{C}$ (substrates were deprotonated with 0.11 M $[\text{}^6\text{Li}]$ LDA and aged for 10 min at $25\text{ }^\circ\text{C}$). The measured mole fractions, X_B , in (a)-(k) are 0.00, 0.19, 0.26, 0.36, 0.48, 0.63, 0.70, 0.78, 0.86, 0.92, and 1.00, respectively.

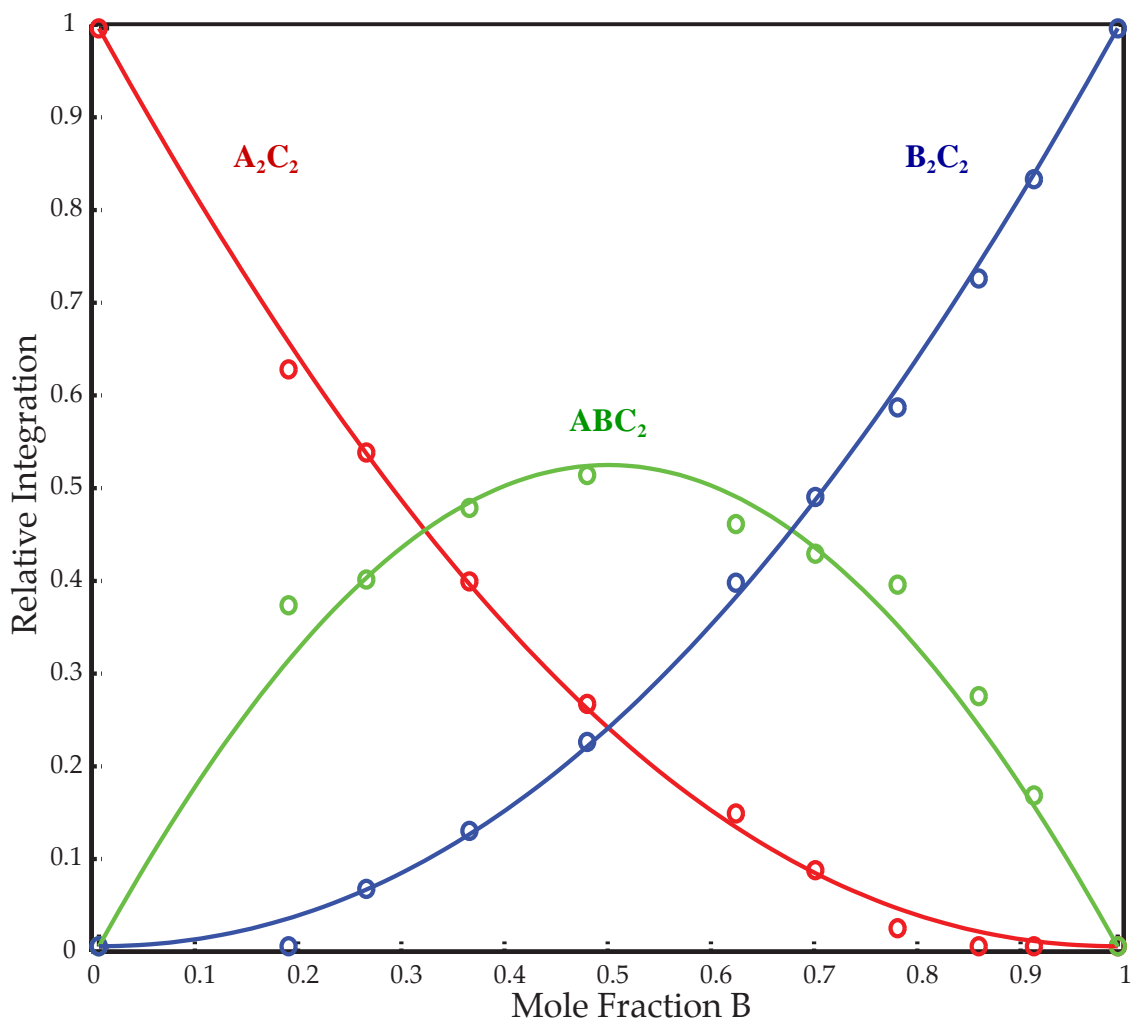
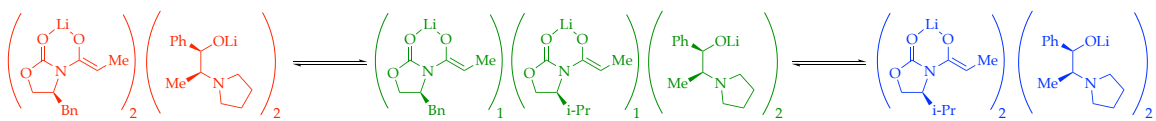


Figure 51. Job plot showing the relative integrations versus the measured mole fraction of (*S*)-**1b** for 0.10 M mixtures of [⁶Li]-(*S*)-**36a** (A) and [⁶Li]-(*S*)-**36b** (B) in toluene (1.0 equiv of THF per Li) at $-80\text{ }^{\circ}\text{C}$.

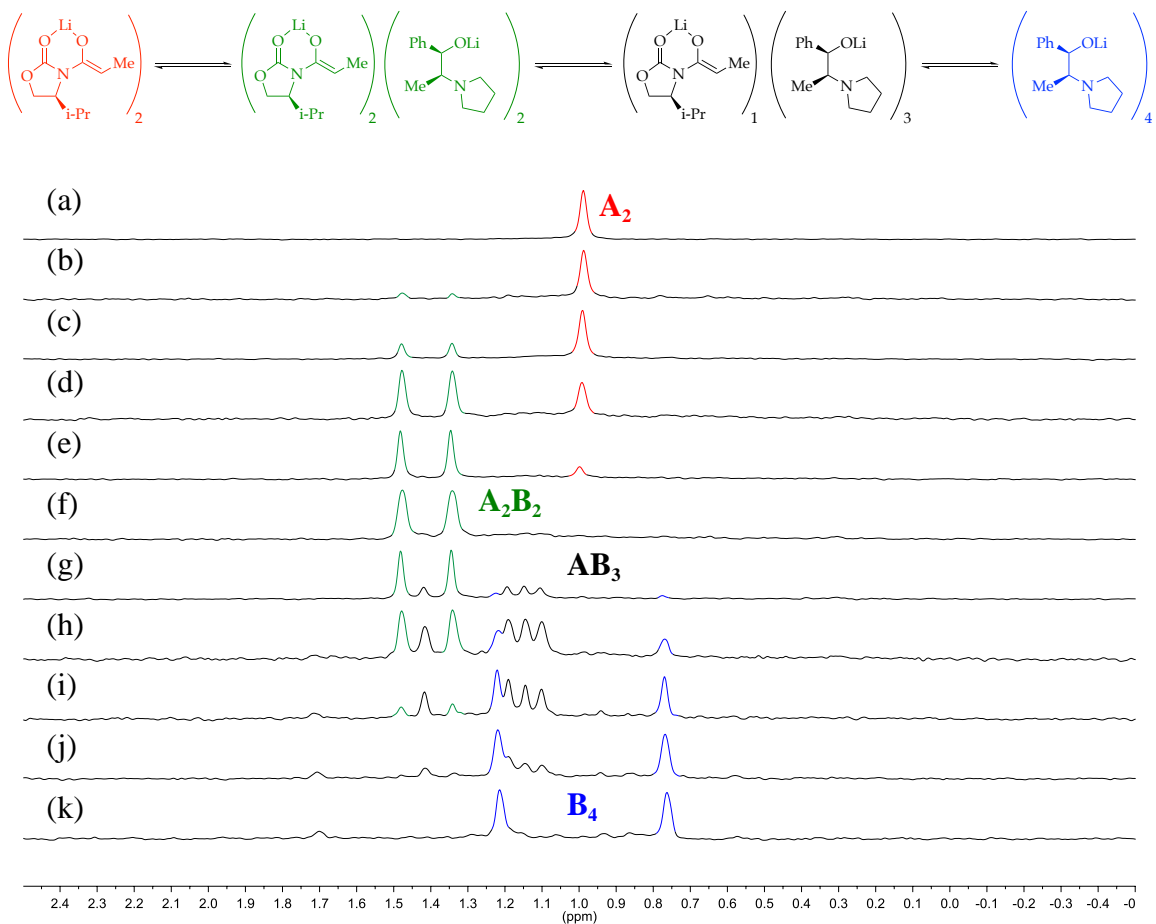


Figure 52. ^6Li NMR spectra for 0.10 M solutions of $[\text{}^6\text{Li}]$ -**(S)**-**1b** (**A**) and $[\text{}^6\text{Li}]$ -**8** (**B**) in toluene (1.0 equiv of THF per Li) at $-80\text{ }^\circ\text{C}$ (substrates were deprotonated with 0.11 M $[\text{}^6\text{Li}]$ LDA and aged for 10 min at $25\text{ }^\circ\text{C}$). The measured mole fractions, X_B , in (a)-(k) are 0.00, 0.10, 0.17, 0.36, 0.44, 0.50, 0.61, 0.70, 0.80, 0.91, and 1.00, respectively.

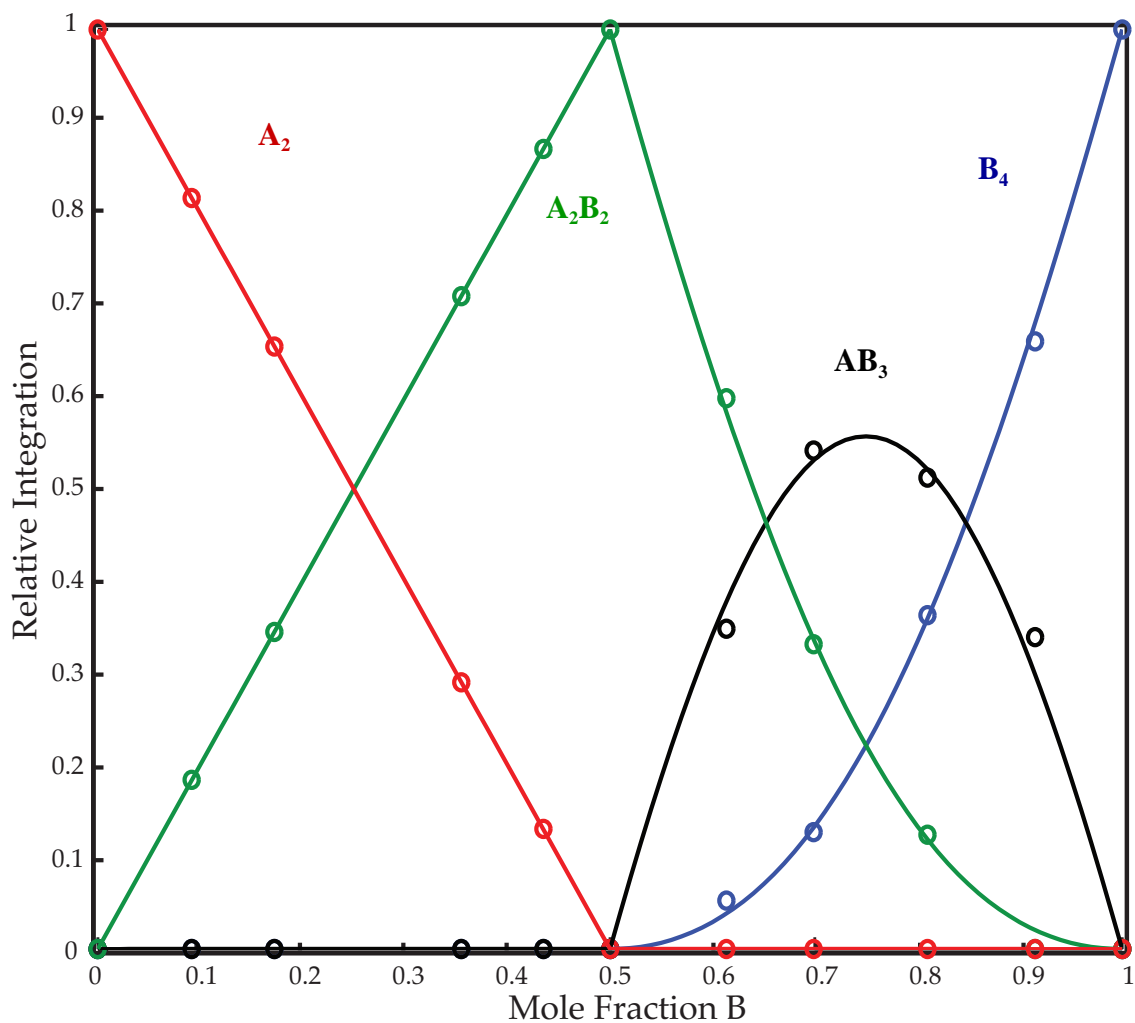
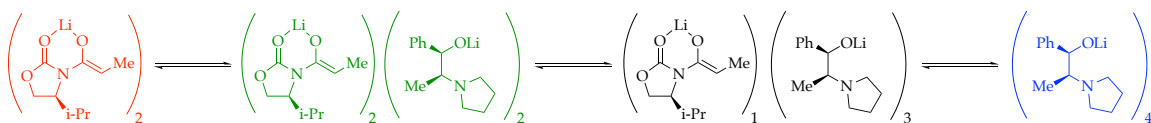


Figure 53. Job plot showing the relative integrations versus the measured mole fraction of 10 for 0.10 M mixtures of [⁶Li]-(S)-1b (A) and [⁶Li]-8 (B) in toluene (1.0 equiv of THF per Li) at -80 °C.

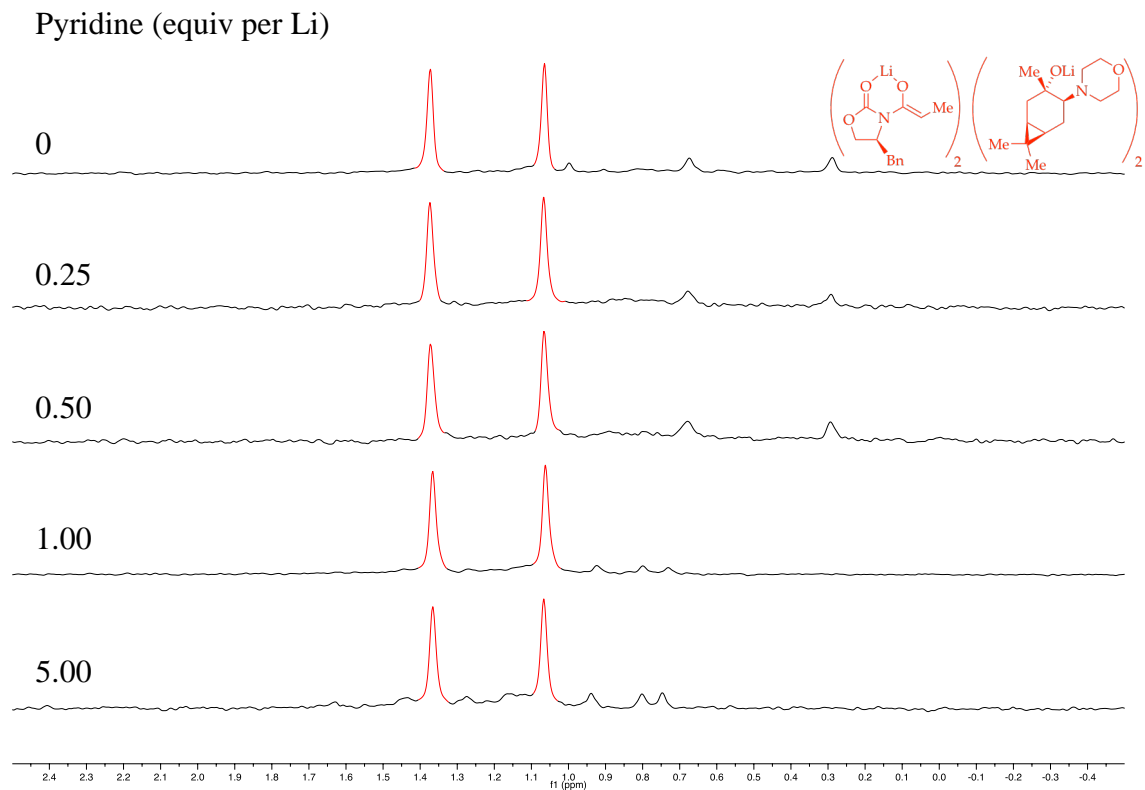


Figure 54. ^6Li NMR spectra for 0.10 M solutions of $[\text{}^6\text{Li}]$ -**(S)-15a** with varying concentrations of pyridine in toluene (1.0 equiv of THF per Li) at $-80\text{ }^\circ\text{C}$ (substrates were deprotonated with 0.11 M $[\text{}^6\text{Li}]$ LDA and aged for 10 min at $25\text{ }^\circ\text{C}$).

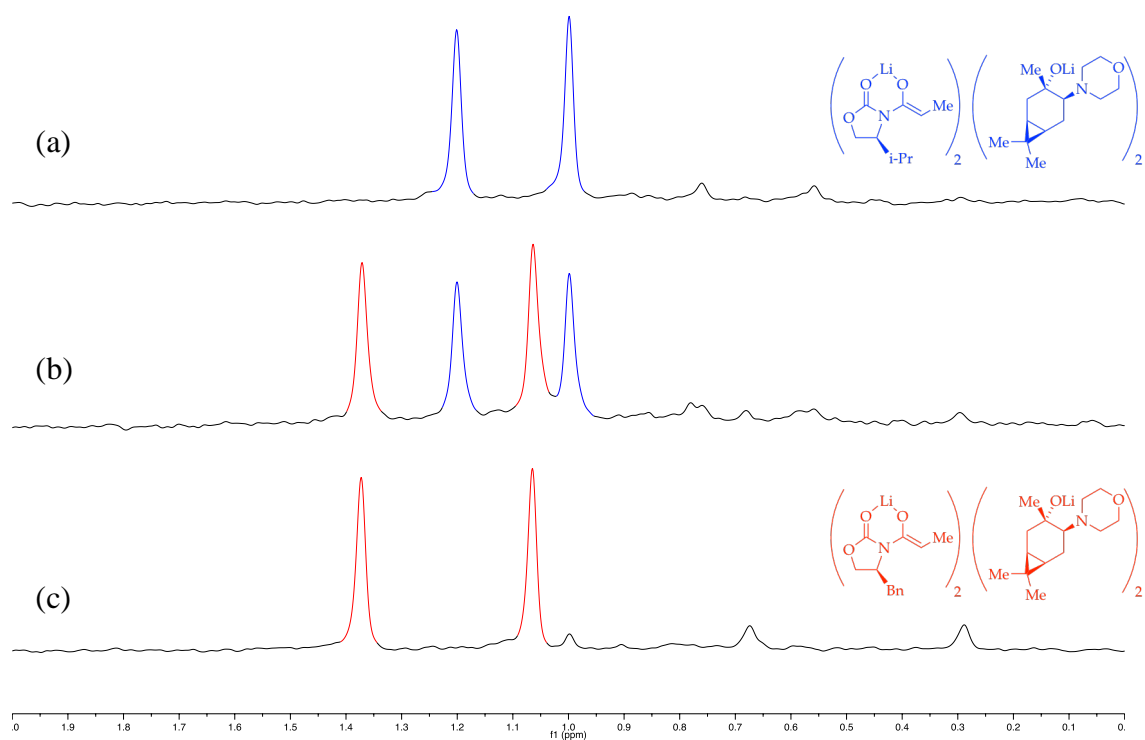


Figure 55. ^6Li NMR spectra for **unaged** 0.10 M solutions of $[\text{}^6\text{Li}]$ -(S)-15b (A) and $[\text{}^6\text{Li}]$ -(S)-15a (B) in toluene (1.0 equiv of THF per Li) at $-80\text{ }^\circ\text{C}$ (substrates were deprotonated with 0.11 M $[\text{}^6\text{Li}]$ LDA). The intended mole fractions, X_B , in (a)-(c) are 0.00, 0.50, and 1.00, respectively.

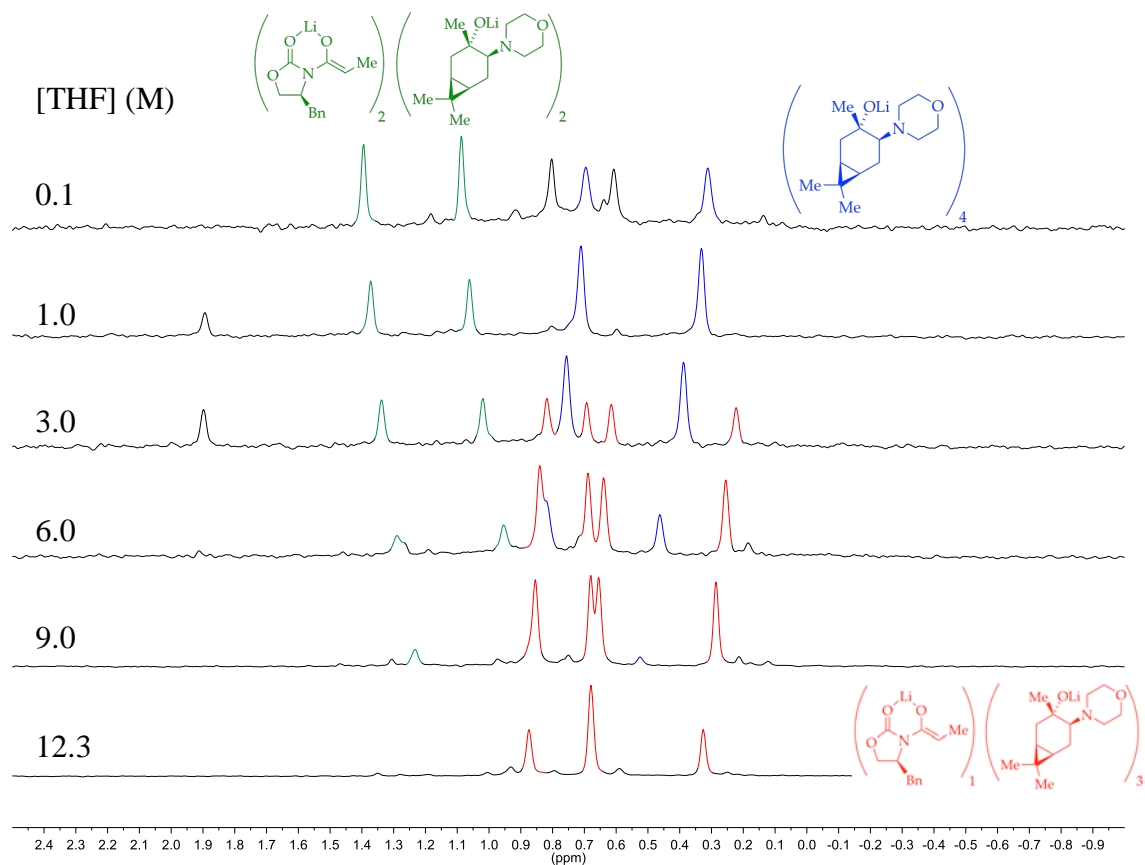


Figure 56. ^6Li NMR spectra for 0.10 M solutions of $[\text{}^6\text{Li}]$ -(S)-16a with varying concentrations of THF at $-80\text{ }^\circ\text{C}$ in toluene cosolvent (substrates were deprotonated with 0.11 M $[\text{}^6\text{Li}]$ LDA and aged for 10 min at $25\text{ }^\circ\text{C}$).

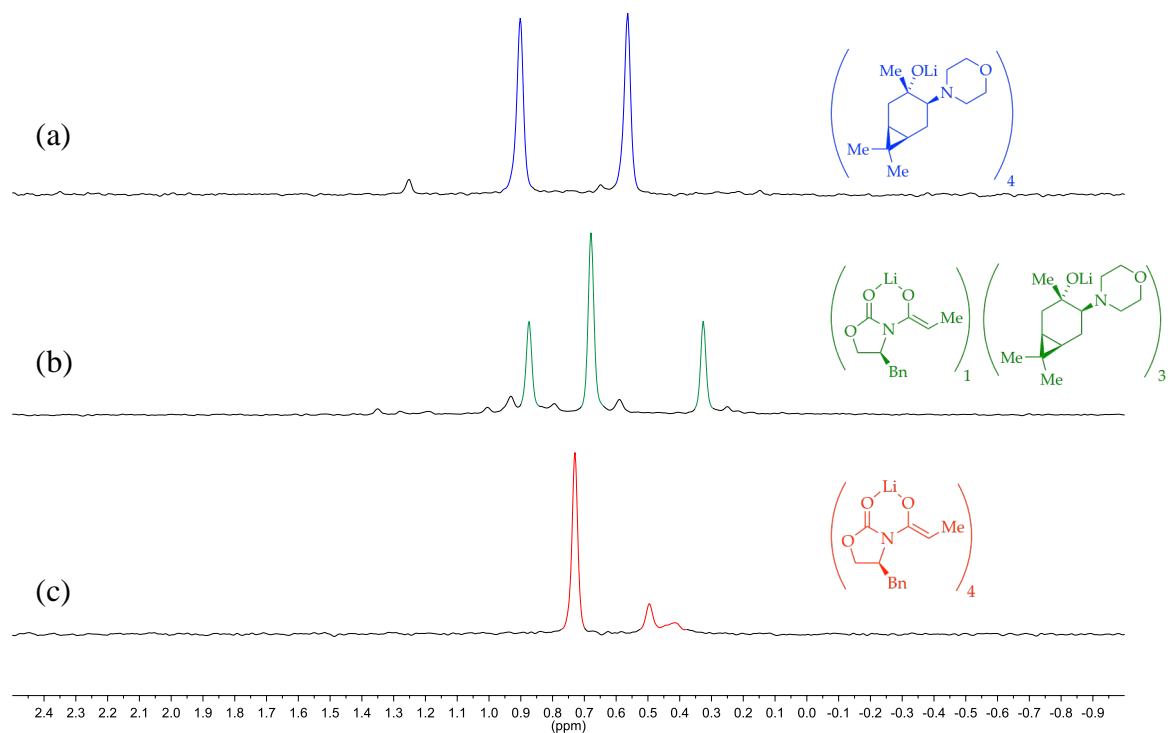


Figure 57. ^6Li NMR spectra for 0.10 M solutions of $[\text{}^6\text{Li}]\text{-11}$ (**A**) and $[\text{}^6\text{Li}]\text{-(S)-1a}$ (**B**) in 12.3 M THF at $-80\text{ }^\circ\text{C}$ (substrates were deprotonated with 0.11 M $[\text{}^6\text{Li}]\text{LDA}$ and aged for 10 min at $25\text{ }^\circ\text{C}$). The intended mole fractions, X_B , in (a)-(c) are 0.00, 0.25, and 1.00, respectively.

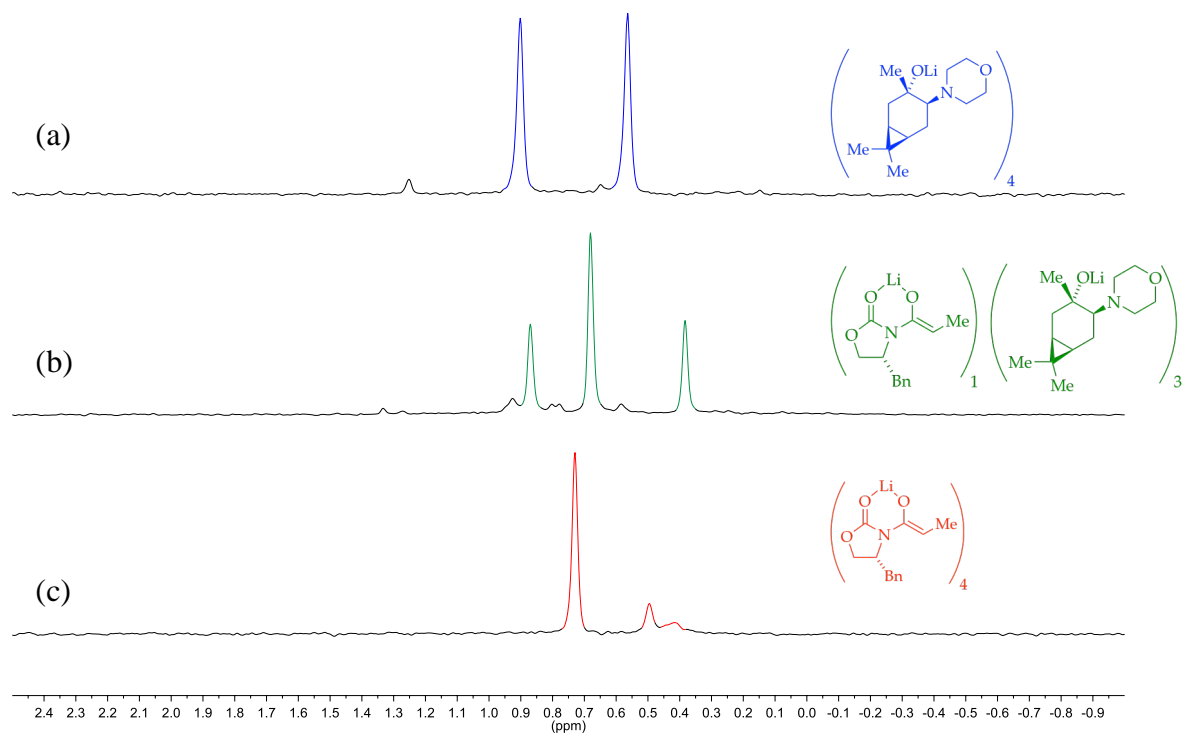


Figure 58. ^6Li NMR spectra for 0.10 M solutions of $[\text{}^6\text{Li}]\text{-11}$ (A) and $[\text{}^6\text{Li}]\text{-(R)-1a}$ (B) in 12.3 M THF at $-80\text{ }^\circ\text{C}$ (substrates were deprotonated with 0.11 M $[\text{}^6\text{Li}]\text{LDA}$ and aged for 10 min at $25\text{ }^\circ\text{C}$). The intended mole fractions, X_B , in (a)-(c) are 0.00, 0.25, and 1.00, respectively.

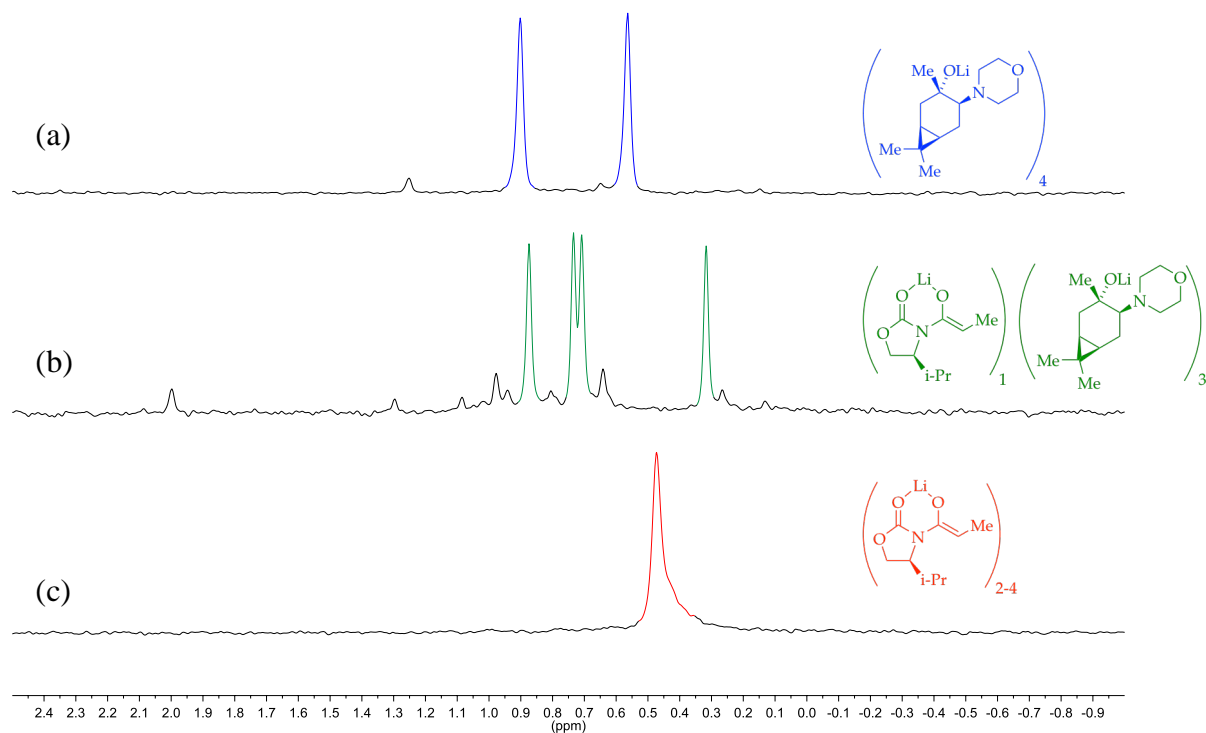


Figure 59. ^6Li NMR spectra for 0.10 M solutions of $[\text{}^6\text{Li}]\text{-11}$ (**A**) and $[\text{}^6\text{Li}]\text{-(S)-1b}$ (**B**) in 12.3 M THF at $-80\text{ }^\circ\text{C}$ (substrates were deprotonated with 0.11 M $[\text{}^6\text{Li}]\text{LDA}$ and aged for 10 min at $25\text{ }^\circ\text{C}$). The intended mole fractions, X_B , in (a)-(c) are 0.00, 0.25, and 1.00, respectively.

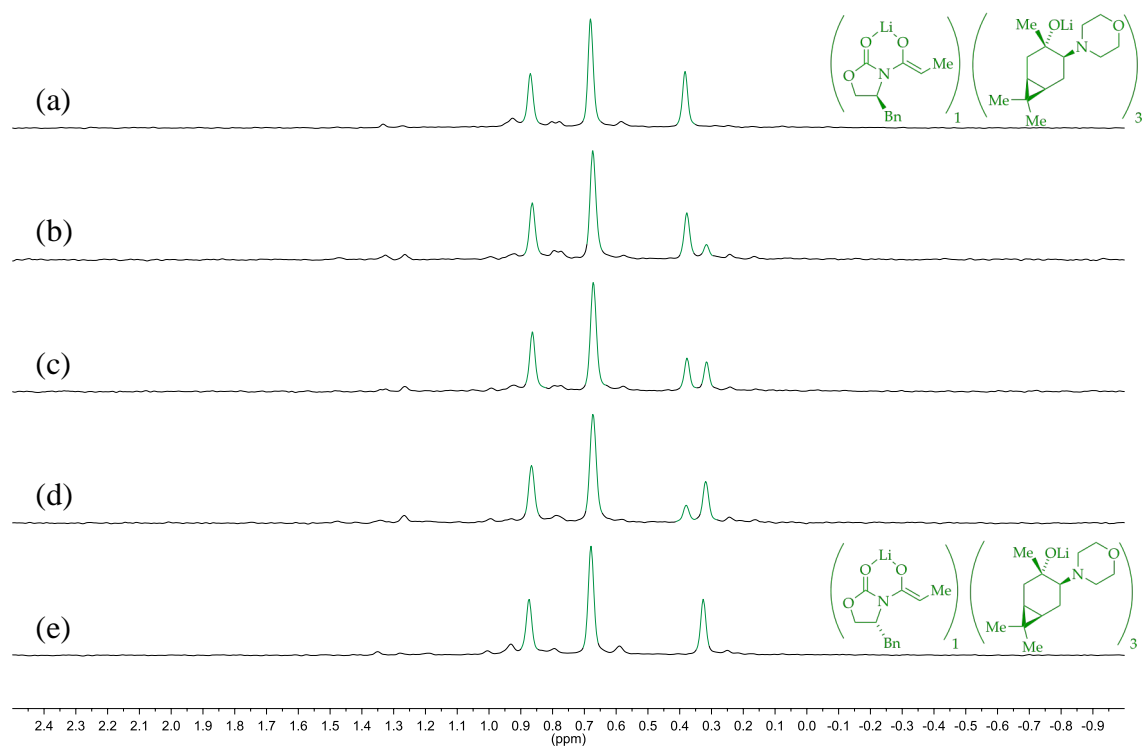


Figure 60. ^6Li NMR spectra for 0.10 M solutions of $[\text{}^6\text{Li}]$ -(S)-**16a** (A) and $[\text{}^6\text{Li}]$ -(R)-**16a** (B) in 12.3 M THF at $-80\text{ }^\circ\text{C}$ (substrates were deprotonated with 0.11 M $[\text{}^6\text{Li}]$ LDA and aged for 10 min at $25\text{ }^\circ\text{C}$). The intended mole fractions, X_B , in (a)-(e) are 0.00, 0.25, 0.50, 0.75, and 1.00, respectively.

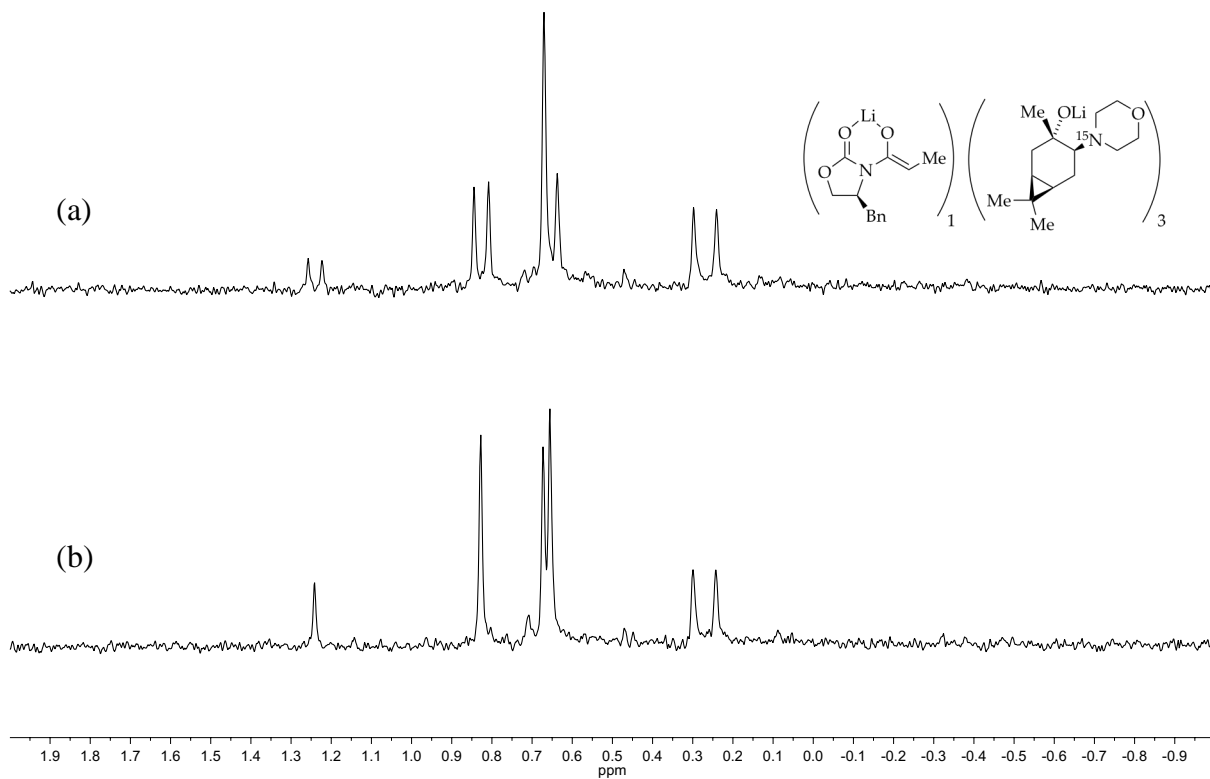


Figure 61. ${}^6\text{Li}$ NMR (a) and ${}^6\text{Li}\{^{15}\text{N}\}$ NMR (b) spectra for 0.10 M solution of $[{}^6\text{Li}, {}^{15}\text{N}]$ -(*S*)-**16a** in 12.3 M THF at $-80\text{ }^\circ\text{C}$ with 0.11 M $[{}^6\text{Li}]$ LDA and 0.055 M HMPA.

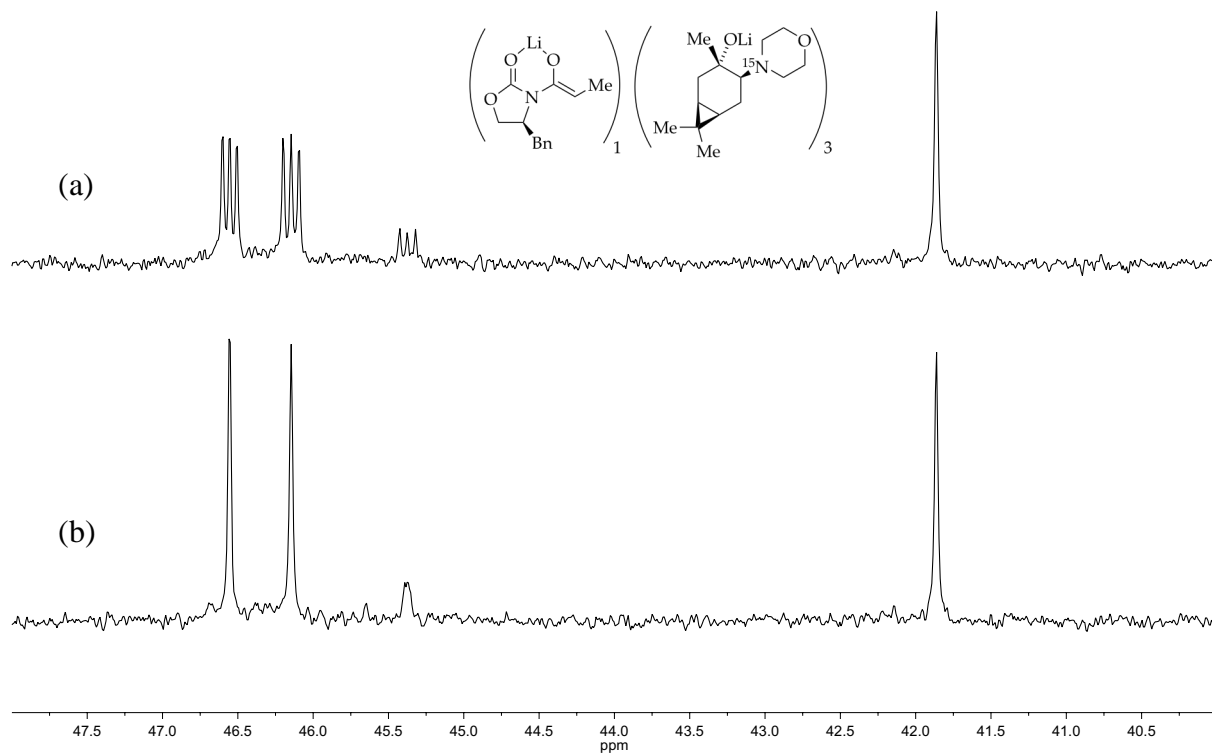


Figure 62. ^{15}N NMR (a) and $^{15}\text{N}\{\text{}^6\text{Li}\}$ NMR (b) spectra for 0.10 M solution of $[\text{}^6\text{Li}, \text{}^{15}\text{N}]$ -(S)-16a in 12.3 M THF at $-80\text{ }^\circ\text{C}$ with 0.11 M $[\text{}^6\text{Li}]$ LDA and 0.055 M HMPA.

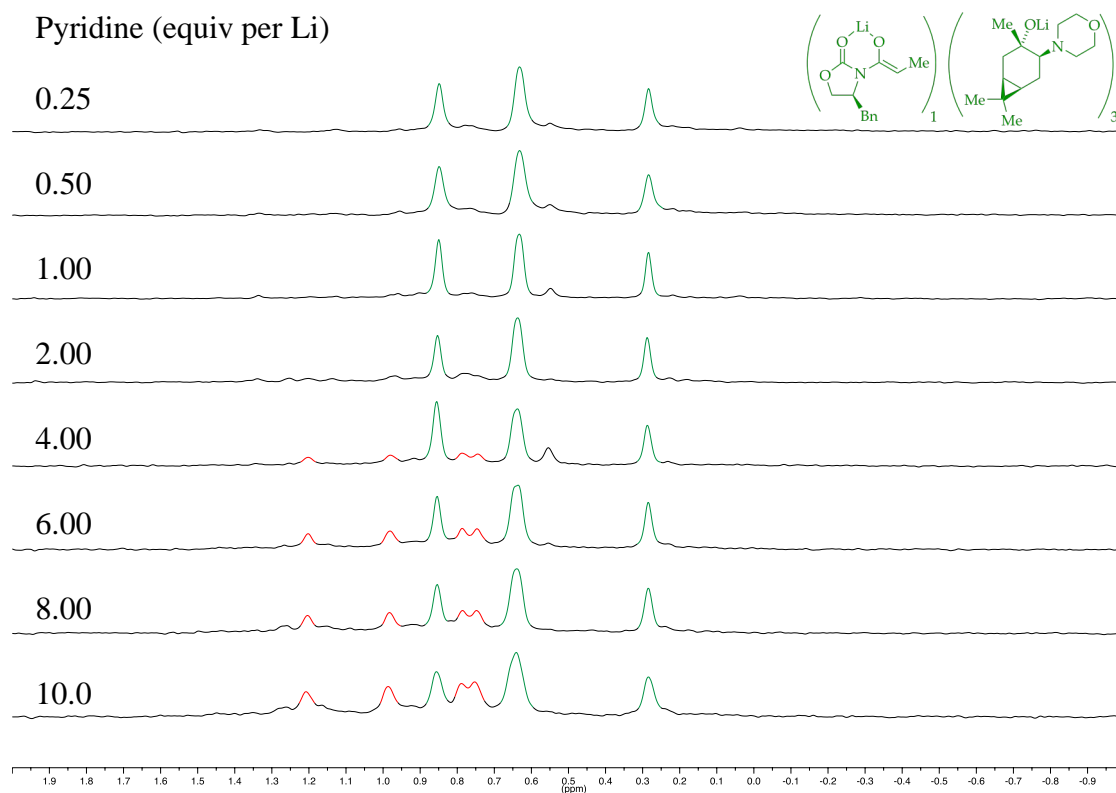


Figure 63. ^6Li NMR spectra for 0.10 M solutions of $[\text{}^6\text{Li}]$ -(*S*)-**16a** with varying concentrations of pyridine in 12.3 M THF at $-105\text{ }^\circ\text{C}$ with 0.11 M $[\text{}^6\text{Li}]$ LDA.

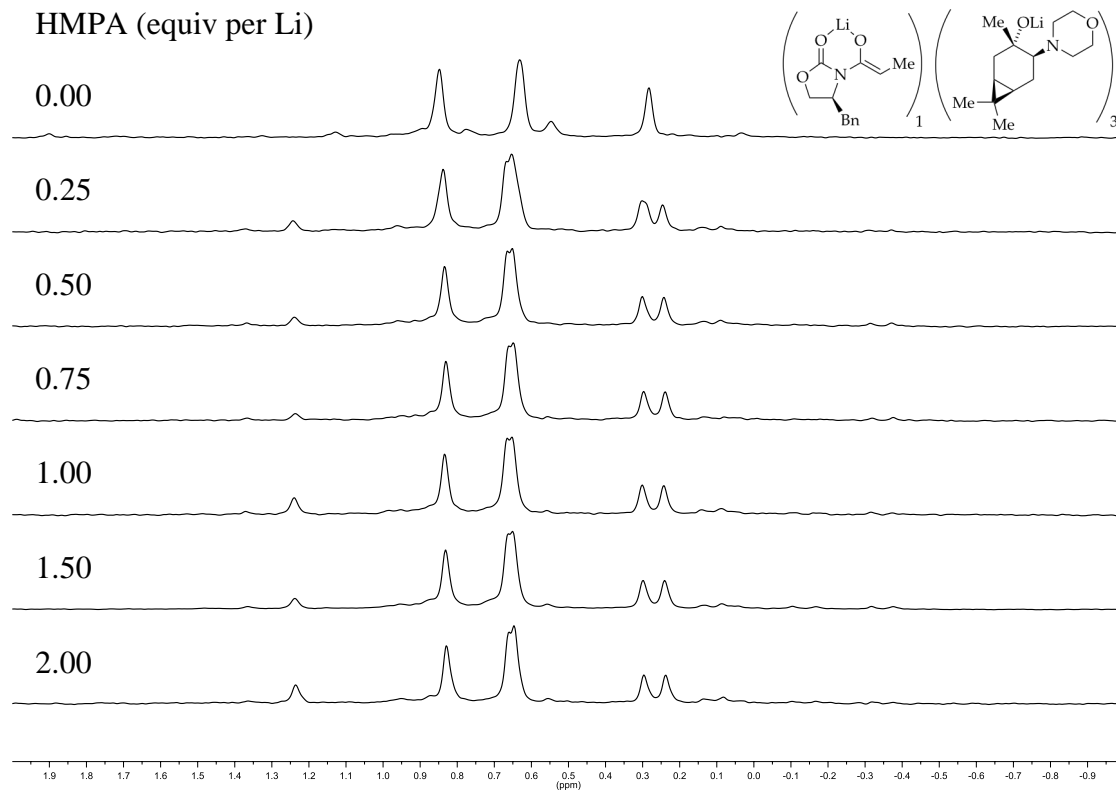


Figure 64. ^6Li NMR spectra for 0.10 M solutions of $[\text{}^6\text{Li}]$ -(*S*)-**16a** with varying concentrations of HMPA in 12.3 M THF at $-105\text{ }^\circ\text{C}$ with 0.11 M $[\text{}^6\text{Li}]$ LDA.

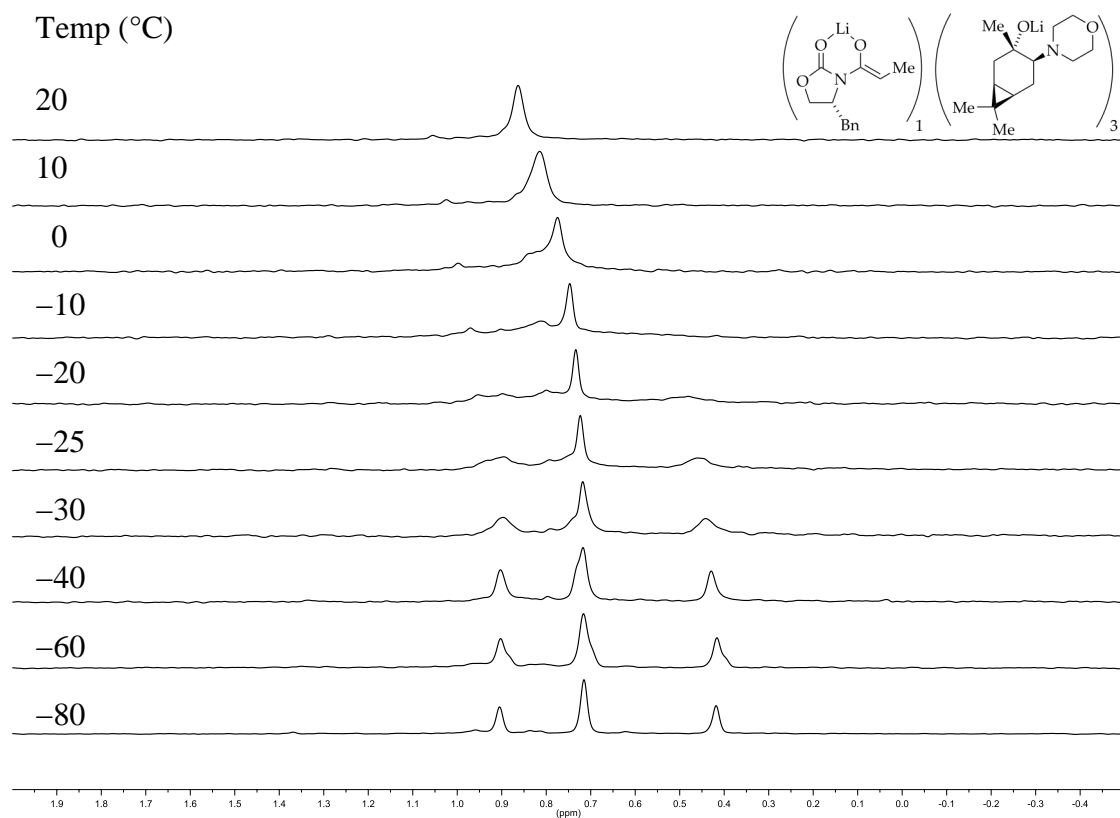


Figure 65. ^6Li NMR spectra of a 0.10 M solution of $[\text{}^6\text{Li}]\text{-(R)-16a}$ in 12.3 M THF with 0.11 M $[\text{}^6\text{Li}]\text{LDA}$, and varying temperature.

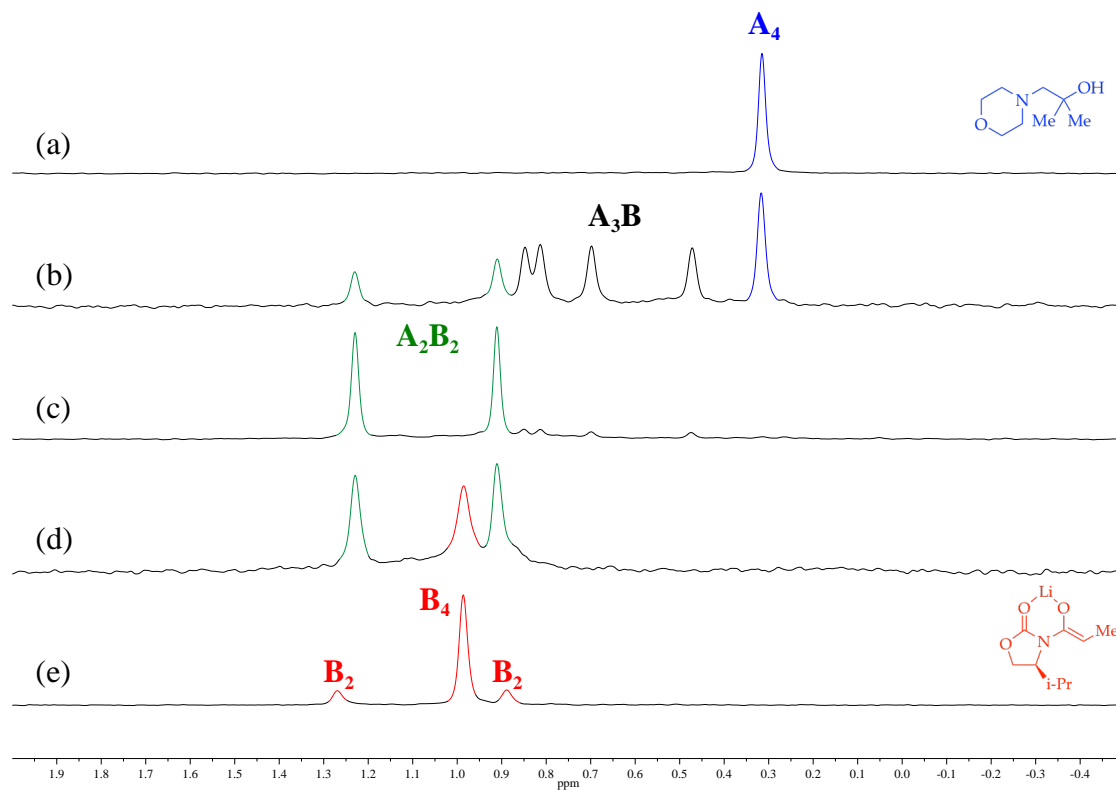


Figure 66. ${}^6\text{Li}$ NMR spectra for 0.10 M solutions of ${}^6\text{Li}$ -51 (A) and ${}^6\text{Li}$ -(S)-1b (B) in toluene at $-80\text{ }^\circ\text{C}$ (substrates were deprotonated with 0.11 M ${}^6\text{Li}$ LiHMDS and aged for 10 min at $25\text{ }^\circ\text{C}$). The intended mole fractions, X_B , in (a)-(e) are 0.00, 0.25, 0.50, 0.75, and 1.00, respectively.

2D NMR analysis of 2:2 mixed aggregate (S)-15a: A sample prepared from 0.40 M [⁶Li]LiHMDS, 0.20 M (S)-1a and 0.20 M 11 in neat toluene-*d*₈, after aging at 25 °C for 10 min, was studied by standard 2D NMR techniques. All chemical shifts with the exception of quaternary C-7's in the carene amino alkoxide (CAA) residues were assigned using high field indirect-resolution 2D HSQC, HSQC-TOCSY, and HMBC experiments.

Experimental: 2D NMR spectra were acquired on a 500 MHz Varian INOVA spectrometer operating at 499.92 MHz for ¹H observation using a 5 mm Varian inverse-detect probehead with Z-axis pulsed field-gradient. Sample temperature was maintained at -40 °C as calibrated with a neat methanol sample. ¹H and ¹³C chemical shifts were referenced to the residual downfield toluene-*d*₇ resonance at 2.09 ppm and 20.40 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 NOESY, 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-4 and C-7. Reciprocal H-7 to C-4 correlation is also observed. The starting point for solving the structure is H-8 methyl of the enolate, which gives nOe correlations to C-13' and C-12', as well as C-2'. Reciprocal correlations from H-12' and H-13' to C-8 are also observed. This indicates that the methyl groups project over the O-1/Li-2/O-3/Li-4 and O-4/Li-1/O-2/Li-3 faces of the cube and are sandwiched between the morpholine ring of CAA' and the other enolate. The correlations with both H-12' and H-13' allow the assignment of CAA' specifically to O-3 and O-4 with N' coordinating to Li-3 and Li-4 resulting in a barrel-shaped arrangement on chelates. Alternative isomers would result in a close contact with the C-11'/C-12' edge of the morpholine based on computational data. Correlations from C-4 to H-13' and H-12' to H-5b further support this assignment. Consequently, CAA' units are adjacent and oriented anti-parallel to each other.

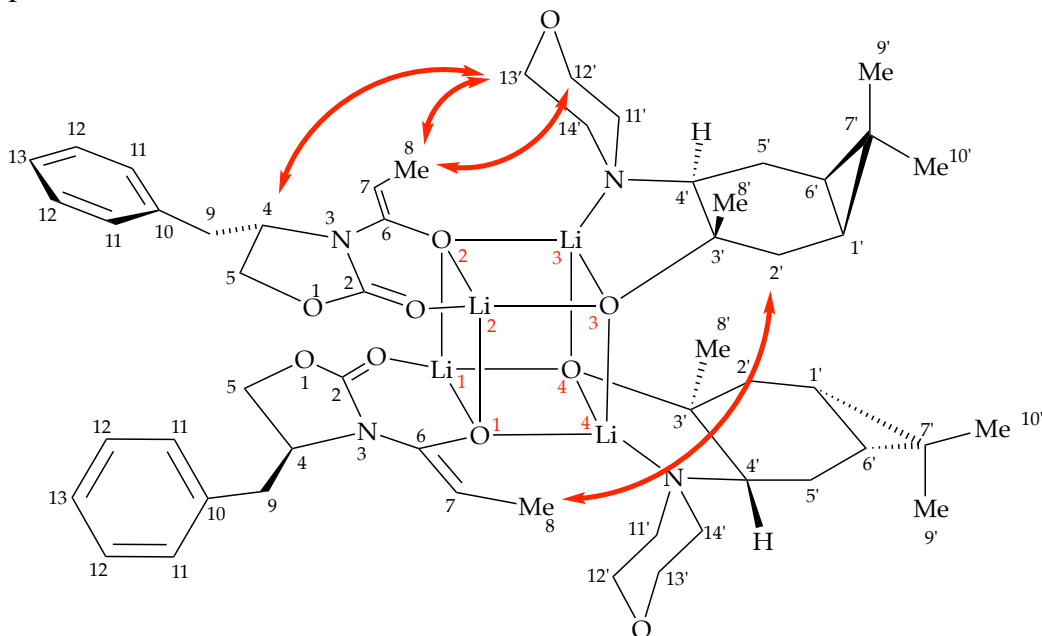


Table 1. ¹H and ¹³C chemical shift assignments for mixed aggregate (*S*)-**15a** at –40 °C.

Atom	δC, ppm	δH, ppm	HMBC	HSQC-TOCSY ¹	ROESY ²	HSQC-NOESY ^{1,2}
1' C	19.39	0.91	9',10'	2',6'	2',6'	2',6',10'
2 C	156.79	–	5b			
2' C	44.43	2.01(a)	8'	1',6'	8',9'	8,5',8',9',1',6'
		2.65(b)				
3' C	70.47	–	8',2',4'			
4 C	57.05	3.61	9,5	9,5	11,7, 13'a ,5	11,7,9,5,8
4' C	76.48	2.63	8'	5'	11',5'a	11',2',5'
5 C	63.84	2.64(a)	4	4,9	11,4	12,11,7,4,9
		3.26(b)				
5' C	17.08	0.81(a)		1',6',4'	5'b,8',9',10'	11',14',4',2',8',9'
		1.99(b)				
6 C	150.26	–	8			
6' C	25.21	0.81	9',10'	2',5',1'	1',10',9'	2',9',10',1',5'
7 C	72.67	3.69	8	8	11,4,9b,8	11,4,9,8
7' C ³	–	–				
8 C	10.97	2.33	7	7	12'a ,4,7, 2'b	12' ,13',7,4,2'
8' C	31.26	1.26	2',3',4'		14'b,2',9',5'	13',14',2',9',5'
9 C	37.33	2.12(a)	11,5	4,5	11,7,5	11,7,4,9,5
		3.37(b)				
9' C	15.71	1.1	10'	10',1',6'	2',5',8',10'	2',8',10',5'
10 C	136.34	–	12,13,9			
10' C	28.68	1	9'	9',1',6'	5',1',6',9'	2',9',6'
11 C	128.94	6.6	12,13	12,13	7,4,5,9	7,4,5,9
11' C	54.46	2.76(a)		12'	4',11'b	12',4',5'
		2.89(b)			11'a	
12 C	128.55	6.98	9,10,11	11,13	11,13	11,13
12' C	68.01	3.89(a)		11'	12'b, 5b ,8	13',11', 8
		4.03(b)			12'a	
13 C	126.62	6.98	10,11	11,12	11,12	11,12
13' C	67.19	3.78(a)		14'	5b ,4	12',14', 8 ,8'
		3.81(b)				
14' C	49.62	2.31(a)		13'	14'b	13',11'
		2.57(b)			8',14'a	

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

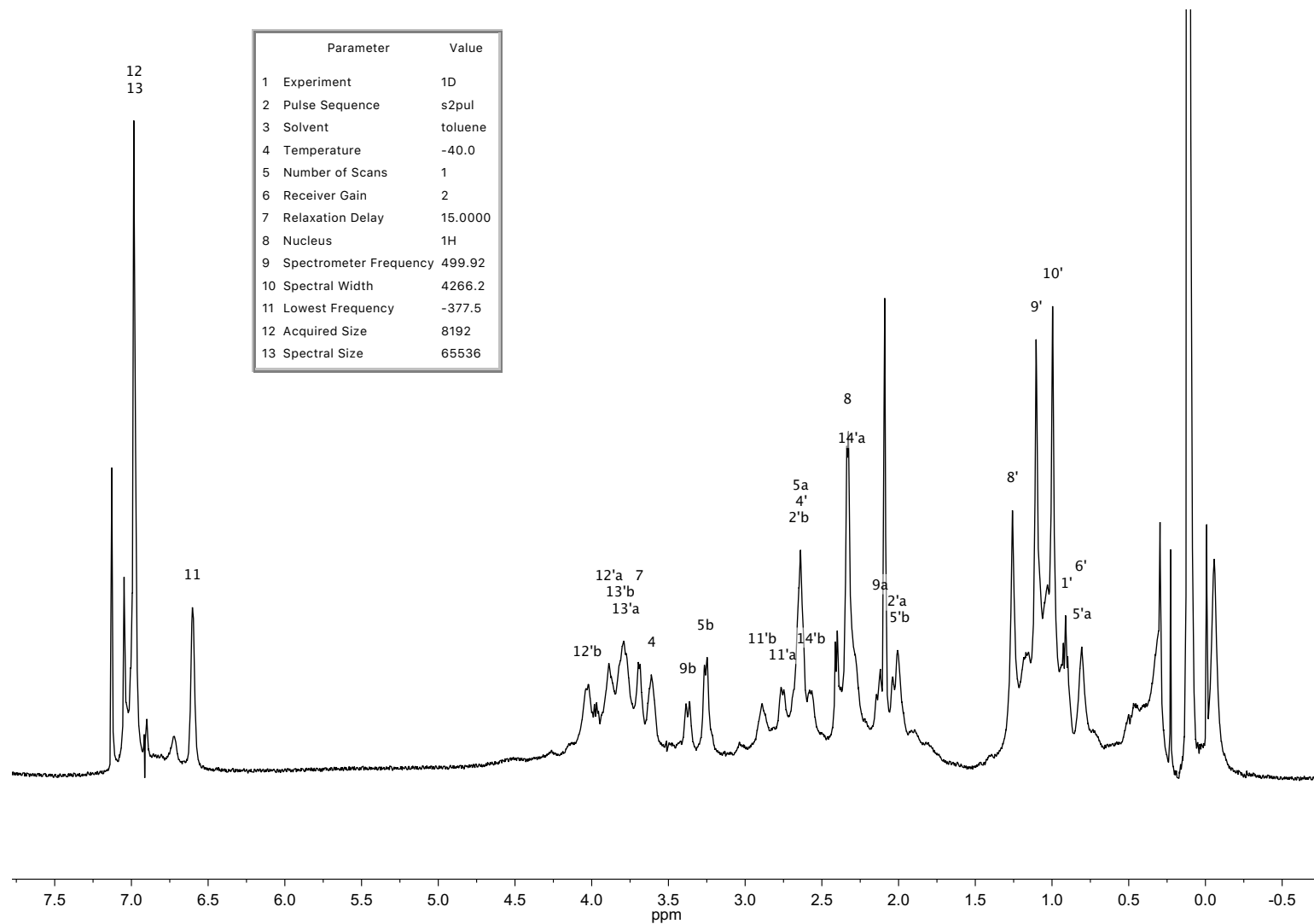


Figure 67. ^1H NMR spectrum of 0.10 M mixed aggregate (*S*)-**15a** in neat toluene- d_8 at -40 °C. Labels indicate assignments by 2D NMR.

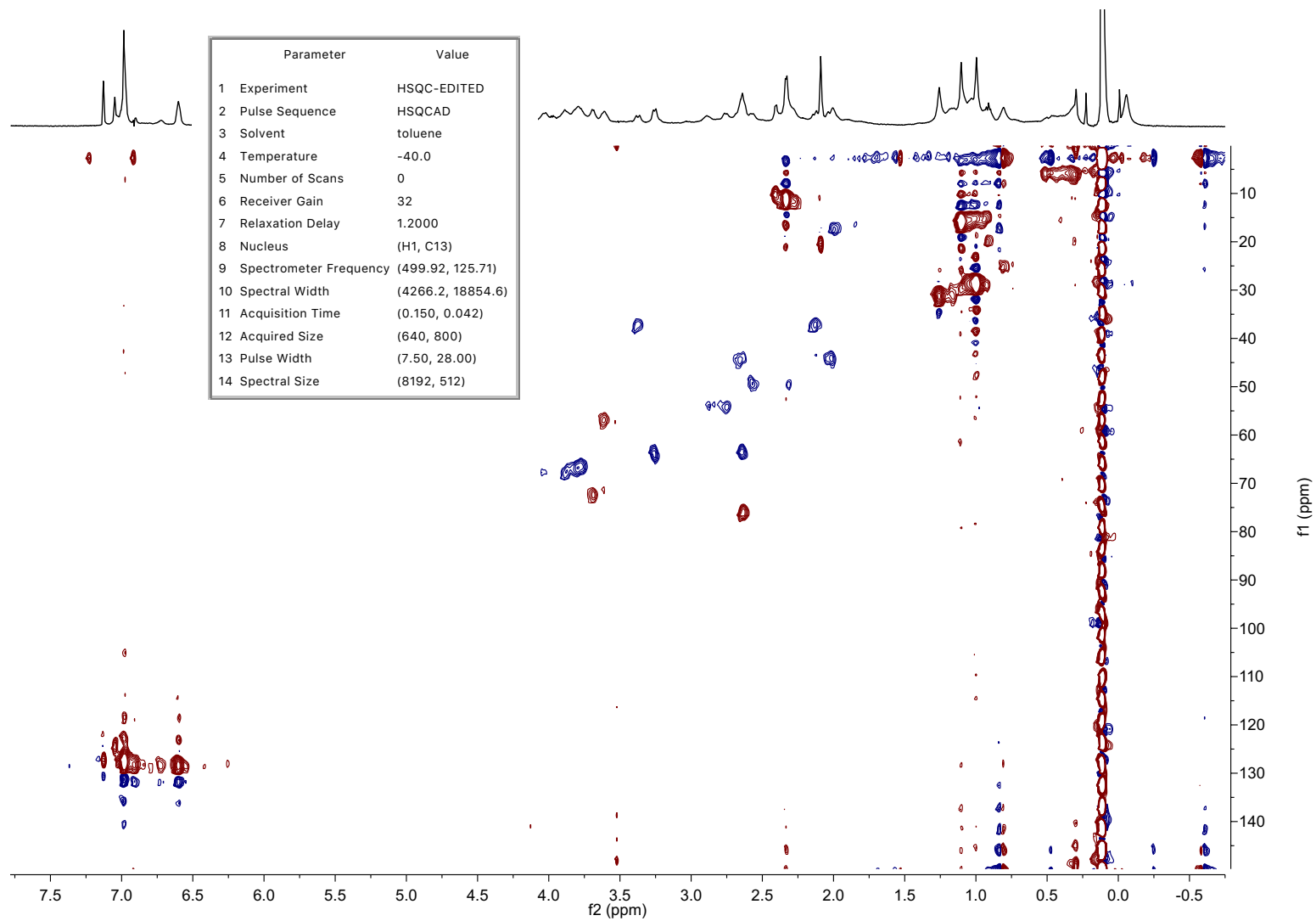


Figure 68. Full display HSQC spectrum of 0.10 M (*S*)-**15a** in neat toluene-*d*₈ at -40 °C.

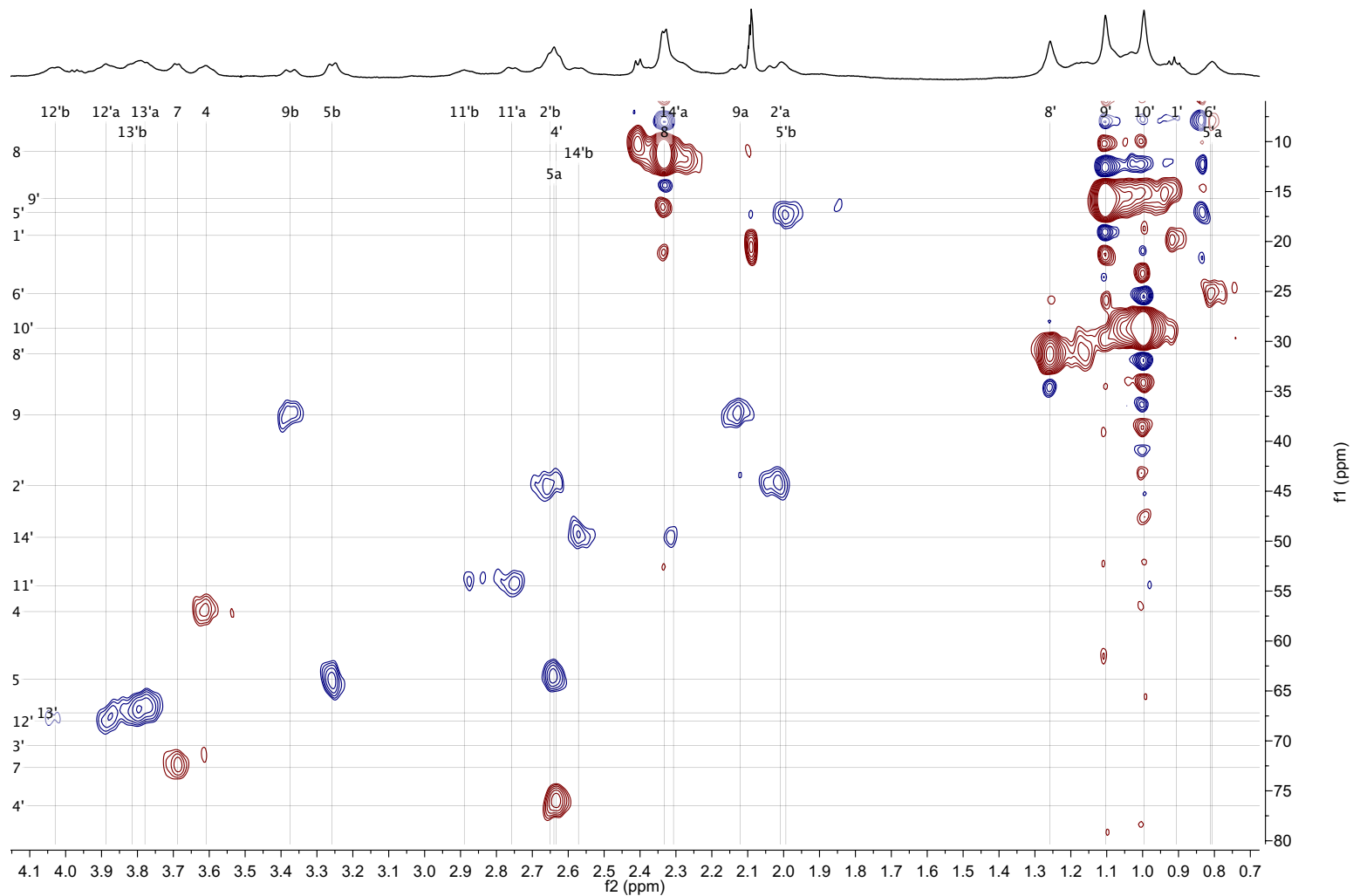


Figure 69. Expansion of the HSQC spectrum of 0.10 M (*S*)-**15a** in neat toluene-*d*₈ at -40 °C. Labels indicate assignments.

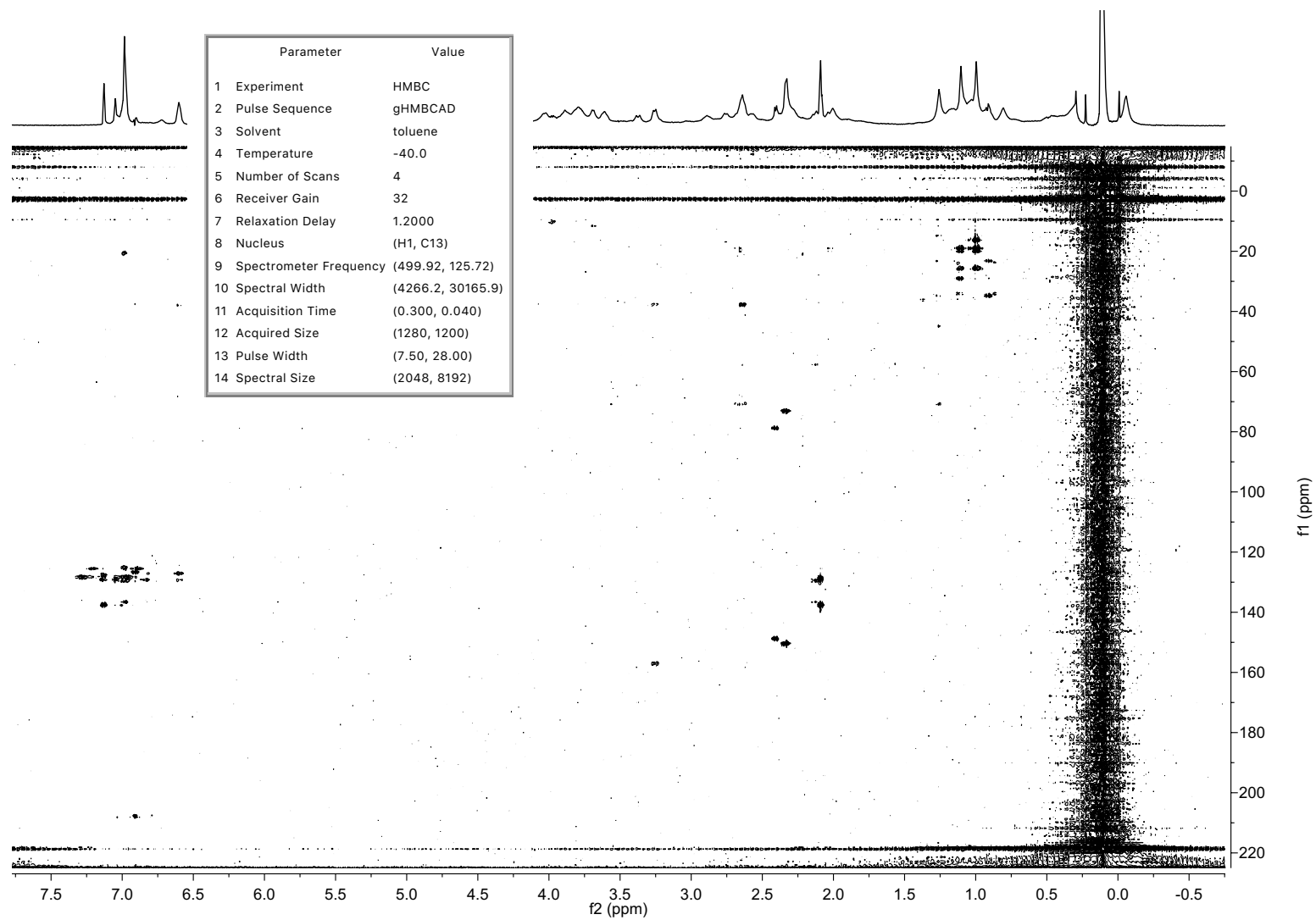


Figure 70. Full display HMBC spectrum of 0.10 M (S)-15a in neat toluene- d_8 at $-40\text{ }^\circ\text{C}$.

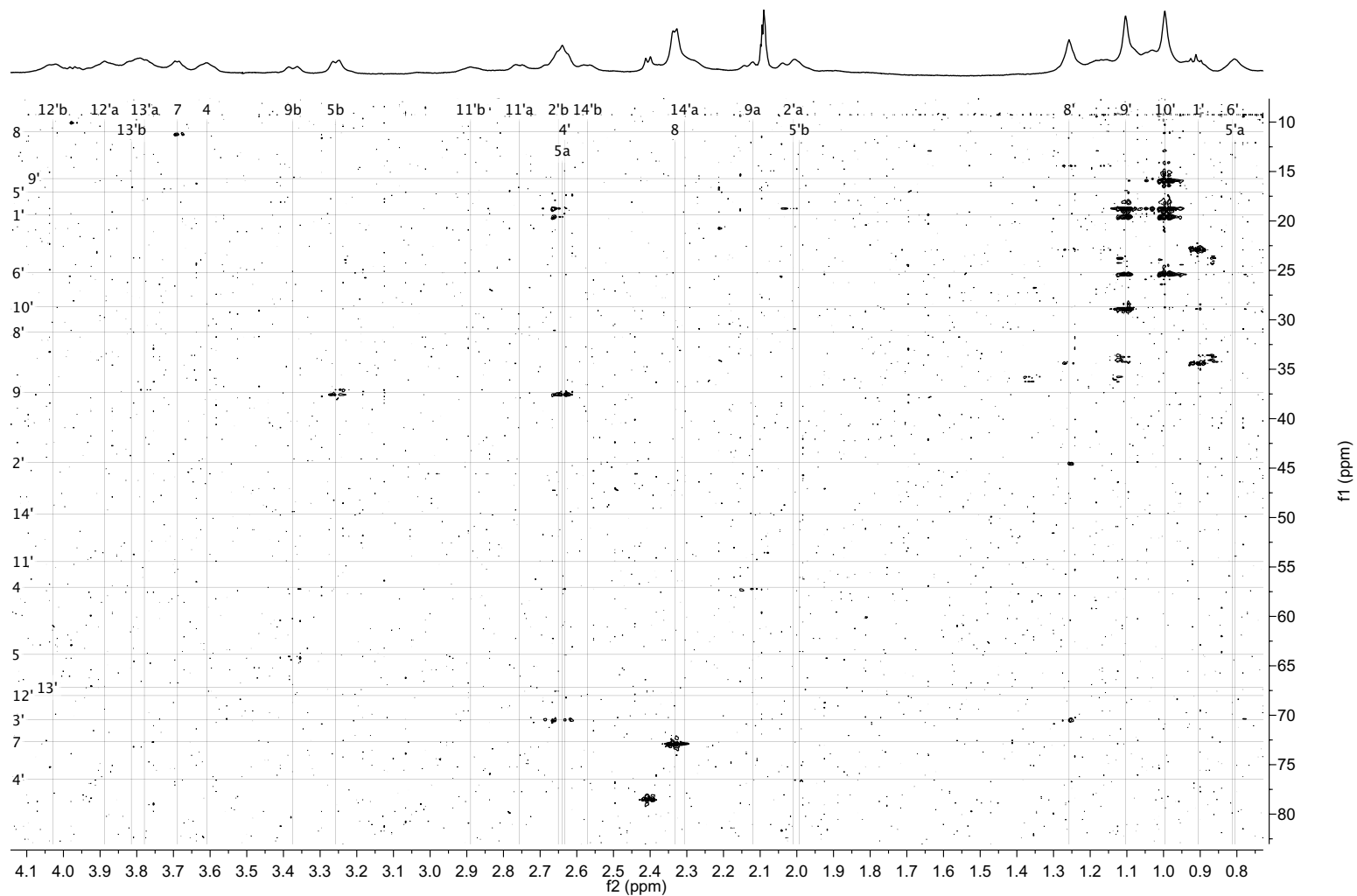


Figure 71. Expansion of the HMBC spectrum of 0.10 M (S)-15a in neat toluene-*d*₈ at -40 °C. Labels indicate assignments.

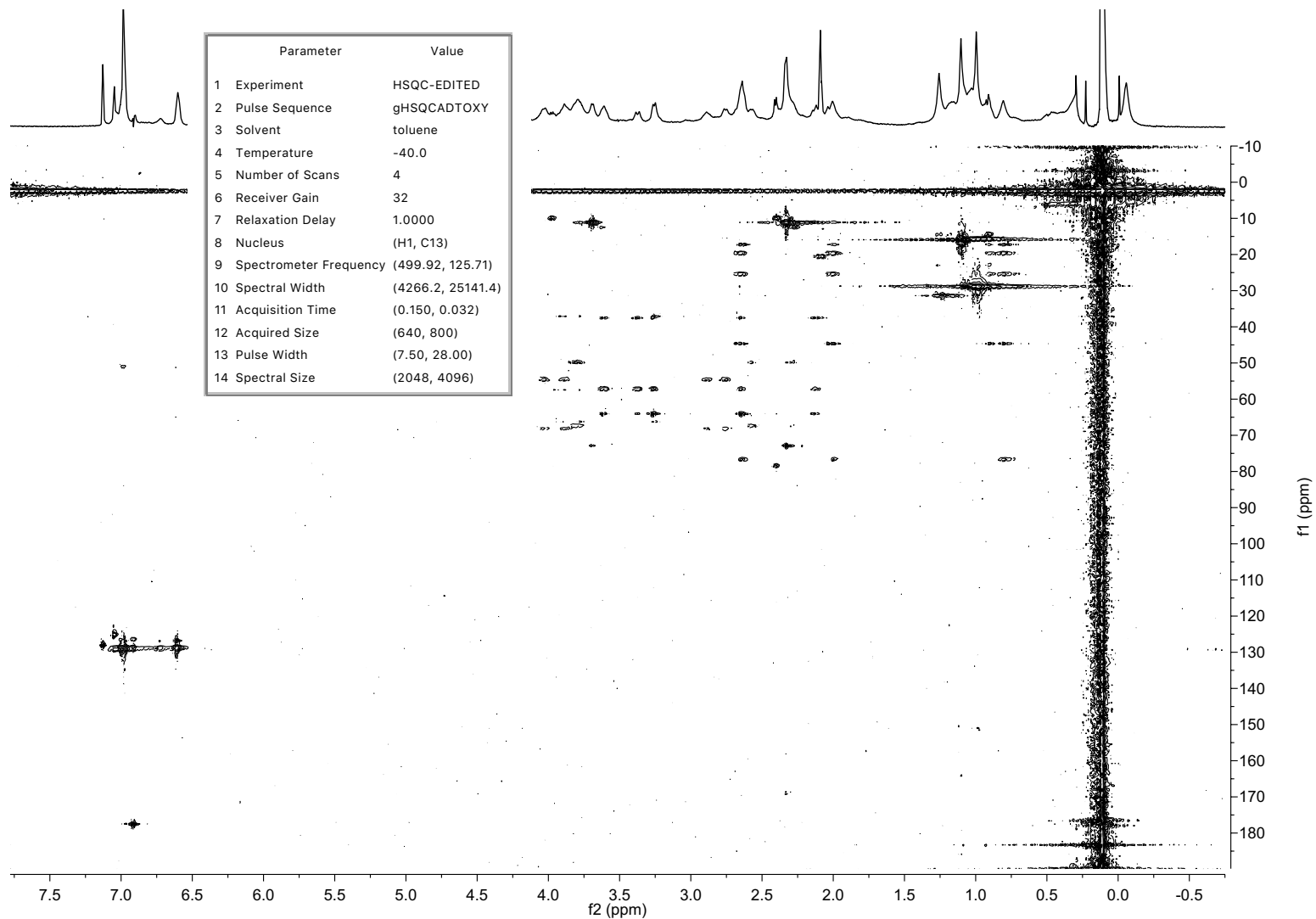


Figure 72. Full display HSQC-TOCSY spectrum of 0.10 M (*S*)-**15a** in neat toluene-*d*₈ at -40 °C.

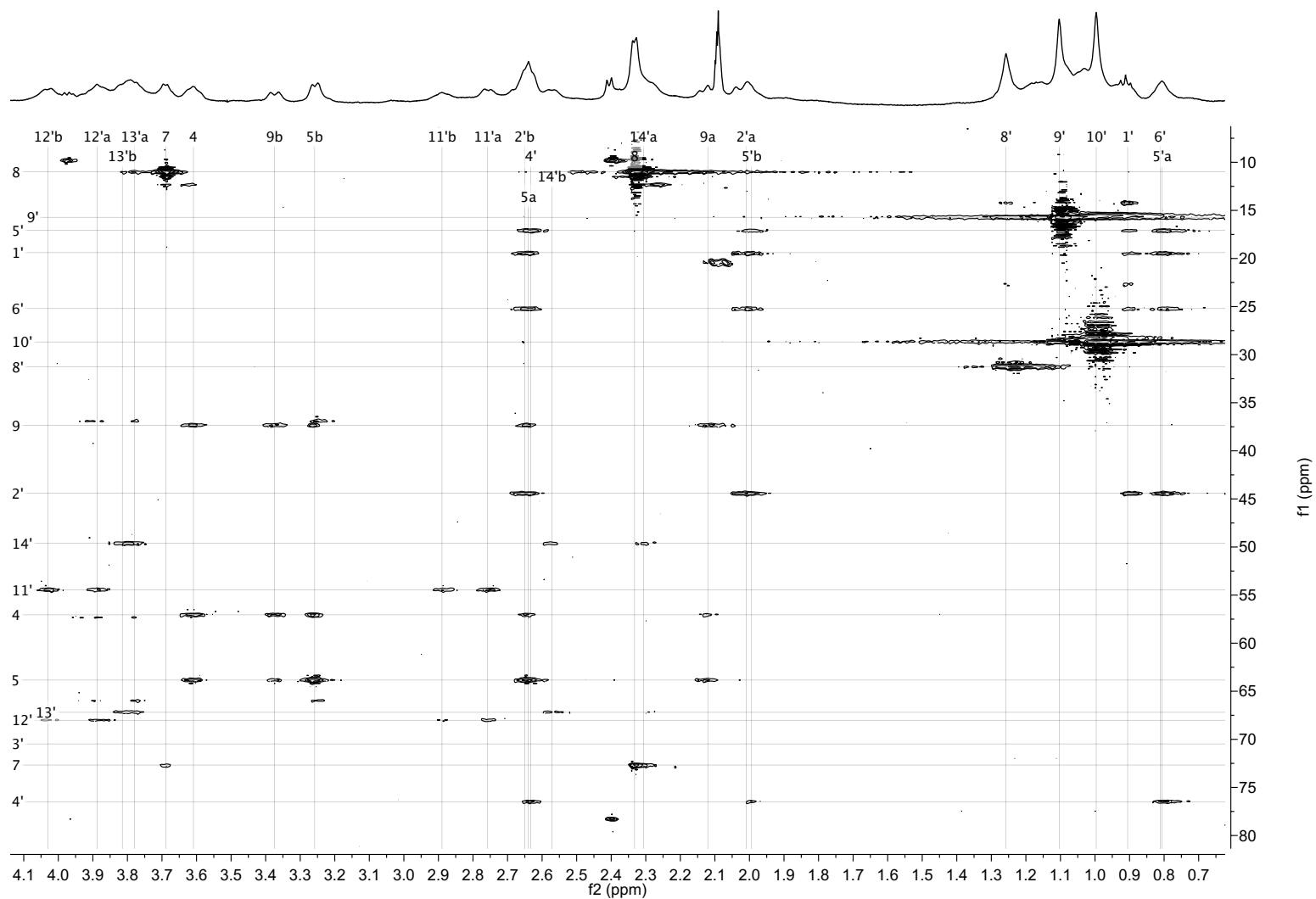


Figure 73. Expansion of the HSQC-TOCSY spectrum of 0.10 M (*S*)-**15a** in neat toluene-*d*₈ -40 °C. Labels indicate assignments.

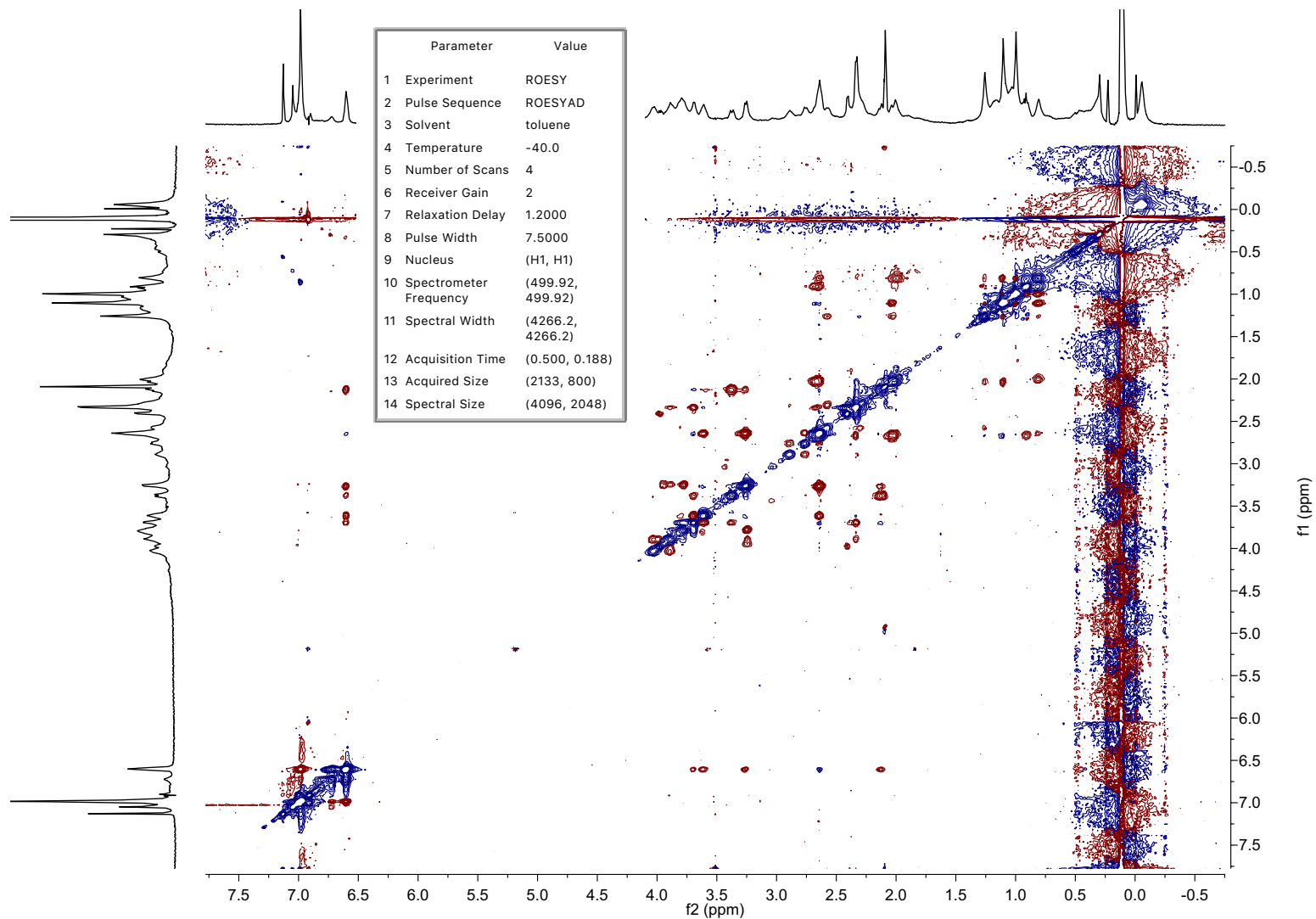


Figure 74. Full display ROESY spectrum of 0.10 M (*S*)-**15a** in neat toluene-*d*₈ at -40 °C.

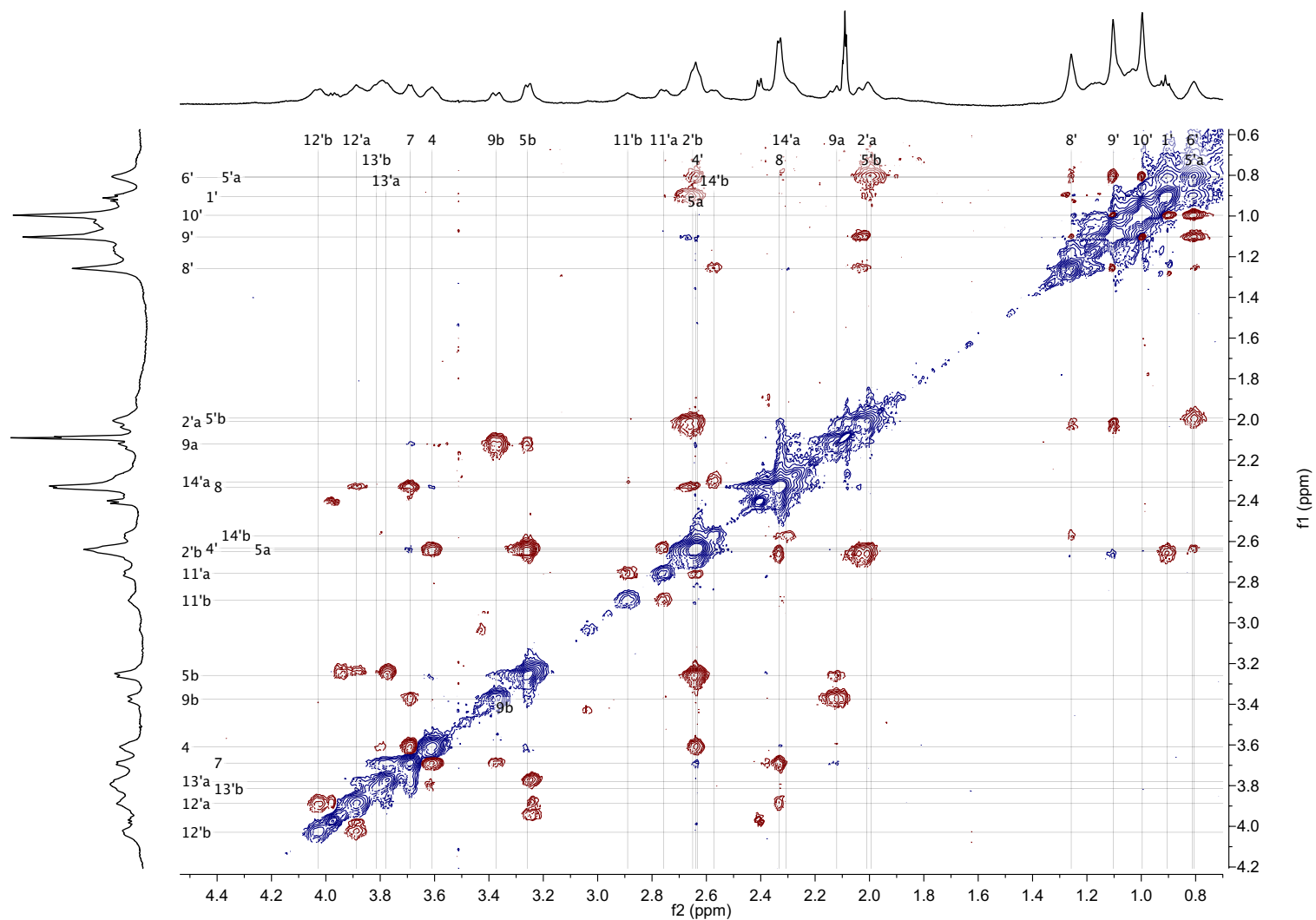


Figure 75. Expansion of the ROESY spectrum of 0.10 M (S)-15a in neat toluene-*d*₈ at -40 °C. Labels indicate assignments.

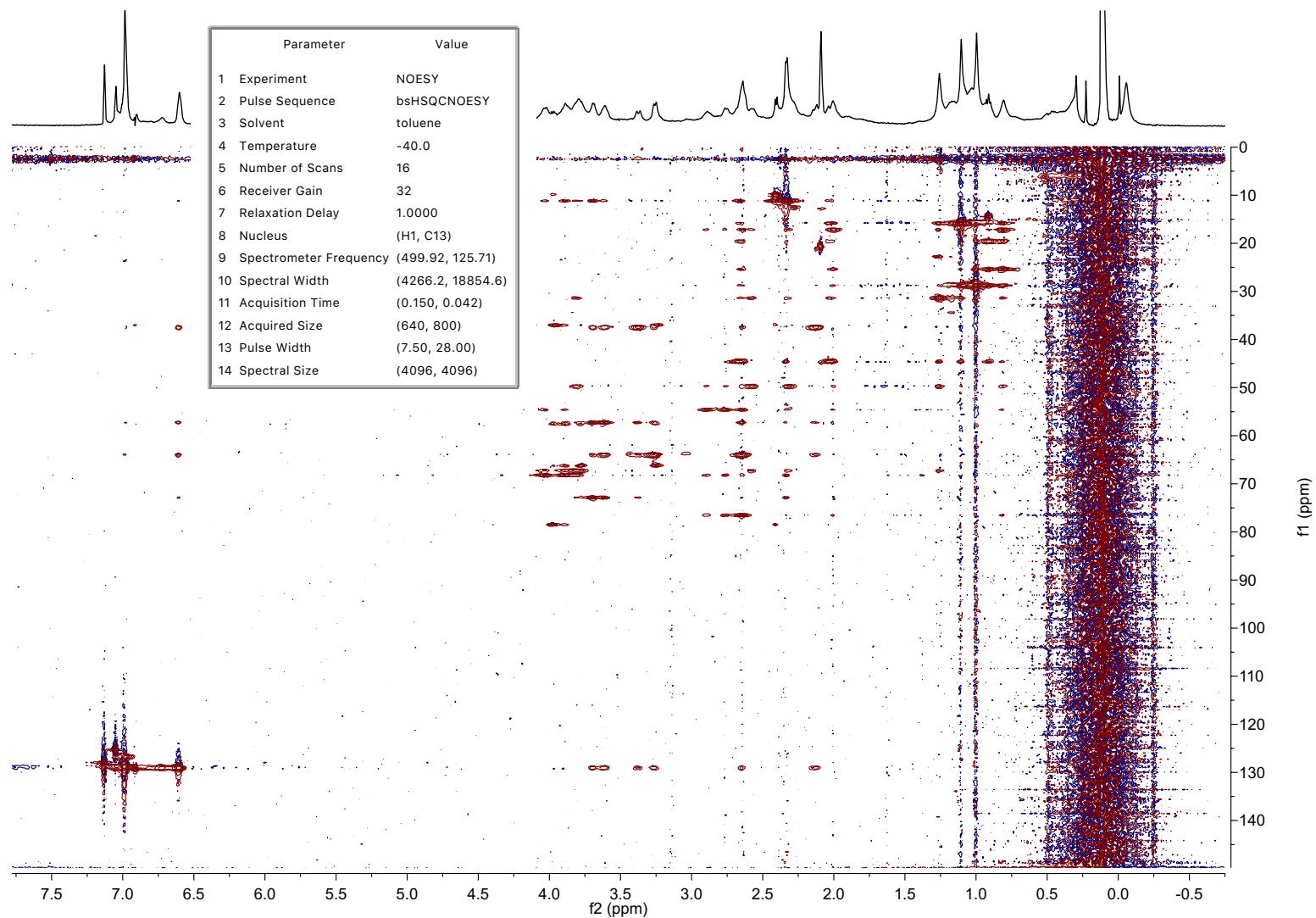


Figure 76. Full display HSQC-NOESY spectrum of 0.10 M (*S*)-**15a** in neat toluene-*d*₈ at -40 °C.

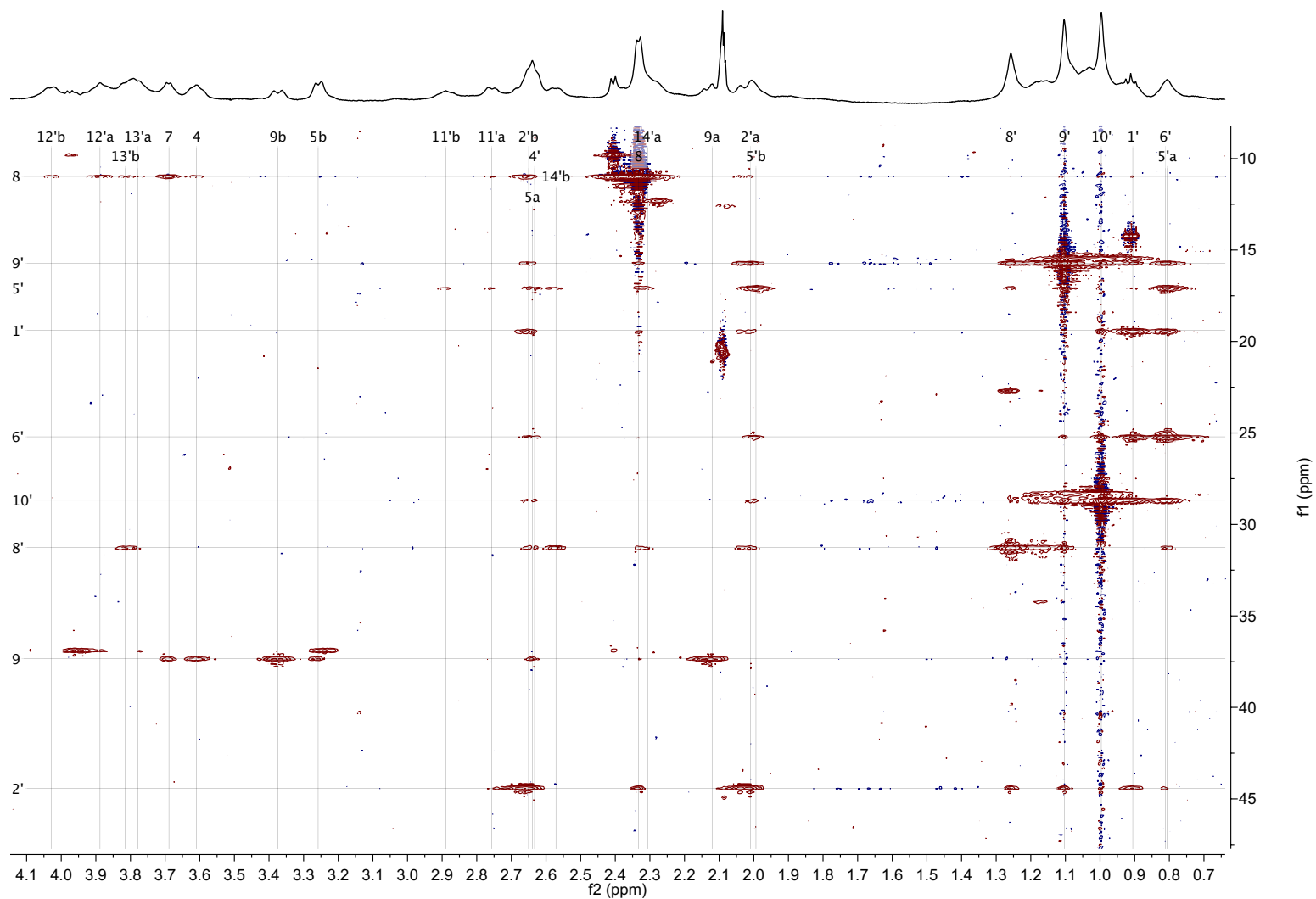


Figure 77. Expansion of the HSQC-NOESY spectrum of 0.10 M (*S*)-**15a** in neat toluene-*d*₈ -40 °C. Labels indicate assignments.

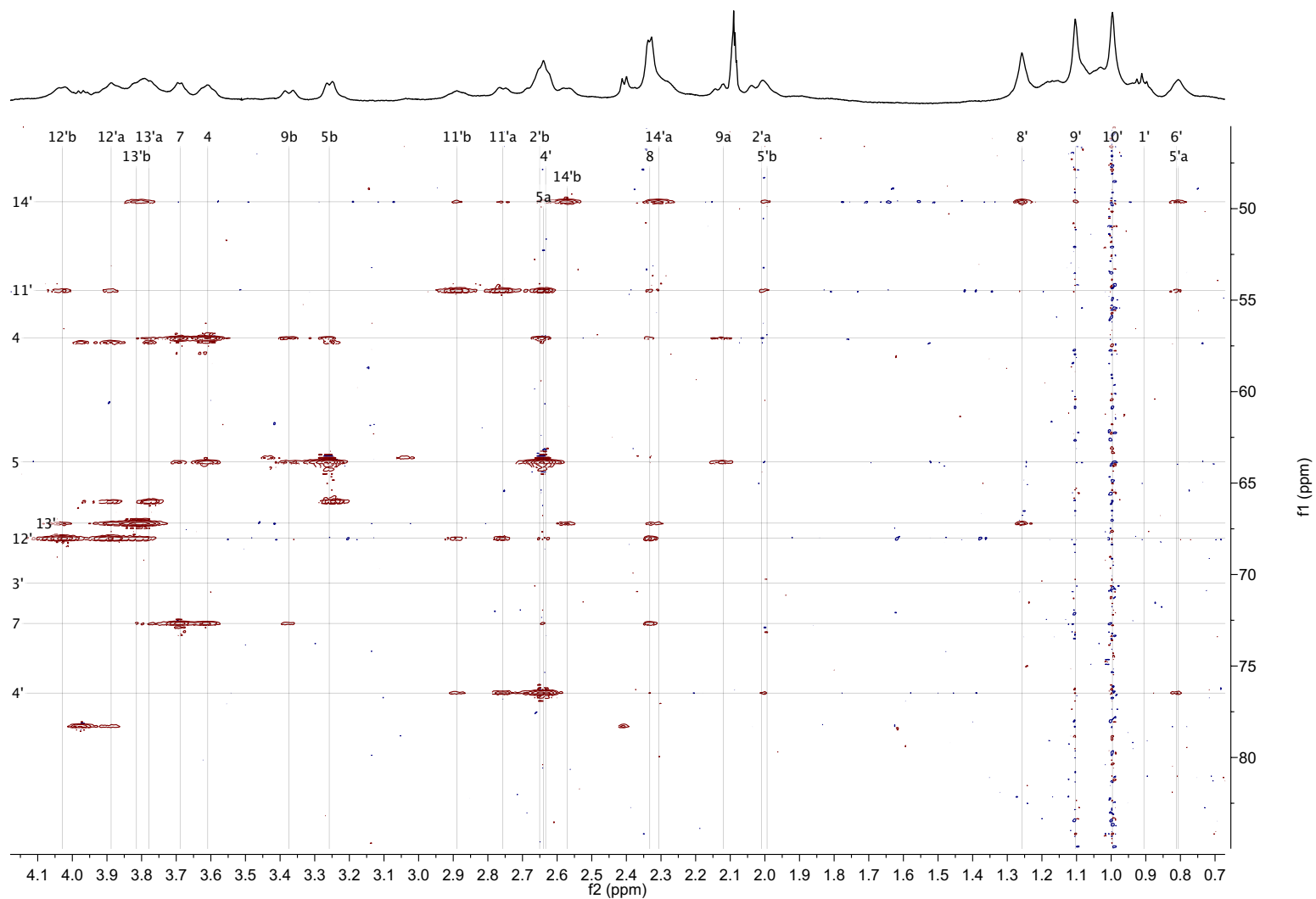


Figure 78. Expansion of the HSQC-NOESY spectrum of 0.10 M (*S*)-**15a** in neat toluene- d_8 -40 °C. Labels indicate assignments.

2D NMR analysis of 2:2 mixed aggregate (R)-15a: A sample prepared from 0.40 M [⁶Li]LiHMDS, 0.20 M (R)-1a and 0.20 M 11 in neat toluene-*d*₈, after aging at 25 °C for 10 min, was studied by standard 2D NMR techniques. All chemical shifts with the exception of quaternary C-7's in the carene amino alkoxide (CAA) residues were assigned using high field indirect-resolution 2D HSQC, HSQC-TOCSY, and HMBC experiments.

Experimental: 2D NMR spectra were acquired on a 500 MHz Varian INOVA spectrometer operating at 499.92 MHz for ¹H observation using a 5 mm Varian inverse-detect probehead with Z-axis pulsed field-gradient. Sample temperature was maintained at -40 °C as calibrated with a neat methanol sample. ¹H and ¹³C chemical shifts were referenced to the residual downfield toluene-*d*₇ resonance at 2.09 ppm and 20.40 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 NOESY, 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-4 and C-7. Reciprocal H-7 to C-4 correlation is also observed. The starting point for solving the structure is H-8 methyl of the enolate, which gives nOe correlations to C-13' and C-12', as well as C-2' and C-8'. Reciprocal correlations from H-12' and H-13' to C-8 are also observed. This indicates that the methyl groups project over the O-1/Li-2/O-3/Li-4 and O-4/Li-1/O-2/Li-3 faces of the cube and are sandwiched between the morpholine ring of CAA' and the other enolate. The correlations with both H-12' and H-13' allow the assignment of CAA' specifically to O-3 and O-4 with N' coordinating to Li-3 and Li-4 resulting in a barrel-shaped arrangement on chelates. Alternative isomers would result in a close contact with the C-11'''/C-12''' edge of the morpholine based on computational data. Correlations from C-13' to H-9b and H-14' to H-9 further support this assignment. Consequently, CAA' units are adjacent and oriented anti-parallel to each other.

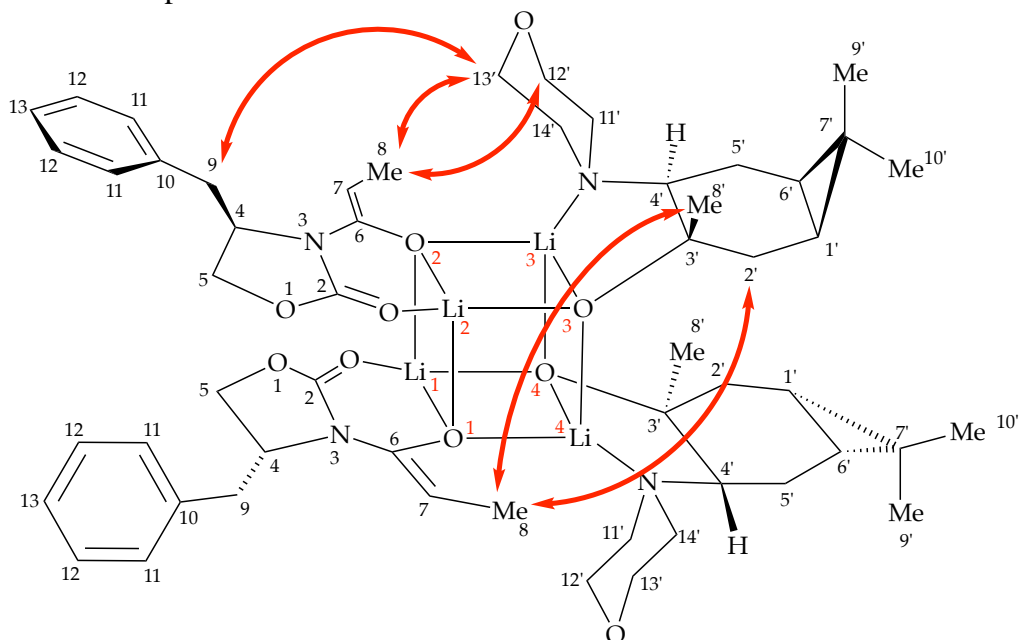


Table 2. ¹H and ¹³C chemical shift assignments for mixed aggregate (**R**)-**15a** at –40 °C.

Atom	δC, ppm	δH, ppm	HMBC	HSQC-TOCSY	ROESY	HSQC-NOESY
1' C	18.72	0.36	2',9',10'	2',5',6'	10',6',2',12'a	12',11',2',10',9',6',5'
2 C	156.55	–	5b			
2' C	43.44	1.87(a)	8'	1',6'	12'b,2'b	12',11',8,5',10',9',6',1'
		2.29(b)			2'a,1'	
3' C	70.54	–	2'b			
4 C	57.16	3.67	5,9	5,9	5,9,8	12,11,7,5,9,8
4' C	77.72	2.35		5',6'	11',6',1'	11',5'b,10',9',6'
5 C	63.94	2.85(a)	4,2,9	4,9	4,7	12,11,7,4,9
		3.38(b)				
5' C	16.67	0.65(a)		4',1',6'	5'b	11',14',4',8',10',9',6',1'
		1.83(b)			5'a,6'	
6 C	150.11	–	8			
6' C	25.69	0.73	10',9'	2',5',1'	5',1',10'	8,2',5',8',10',9',5',1'
7 C	72.96	3.76	8	8	4,8,9	11,4,9,5,8
7' C	–	–				
8 C	10.97	2.36	7	7	7,12'b,11'b,6'	12',13',2',8',10'
8' C	30.14	1.29			14'b,2'a	14',8,2',9',5'
9 C	37.07	2.40(a)	11,4	4,5	11,4,7,5b,9b	12,11,4,7,5,8
		3.12(b)			9a	
9' C	15.62	1.02	10'	10'	2',8',6',5'a	14'b,2',8',5',1',6',10'
10 C	148.46	–	9a			
10' C	28.53	1.07	6',9'	9'	1',5',6'	2',8',9',6',1',5'
11 C	129.24	6.75	9,13	12,13	7,4,5,9,12	7,4,12,5,9,8,8',9'
11' C	54.18	2.80(a)		12'	11'b	12',4',14',5',6',1',8',10',9'
		2.89(b)			11'a,4'	
12 C	128.71	7.02	13,	11,13	11,13	11,13,9,4,5
12' C	67.73	4.04(a)		11'	12'b	13',11',2'b,8
		4.22(b)			12'a,13'b	
13 C	126.83	7.01	12,11	12,13	11,12	11,12
13' C	66.79	3.63(a)		14'	12',13'b	12',14',8,9b,8'
		3.74(b)			13'a	
14' C	50.02	2.12(a)		13'	14'b	13',11',8,5',8',9'
		2.66(b)			14'a	

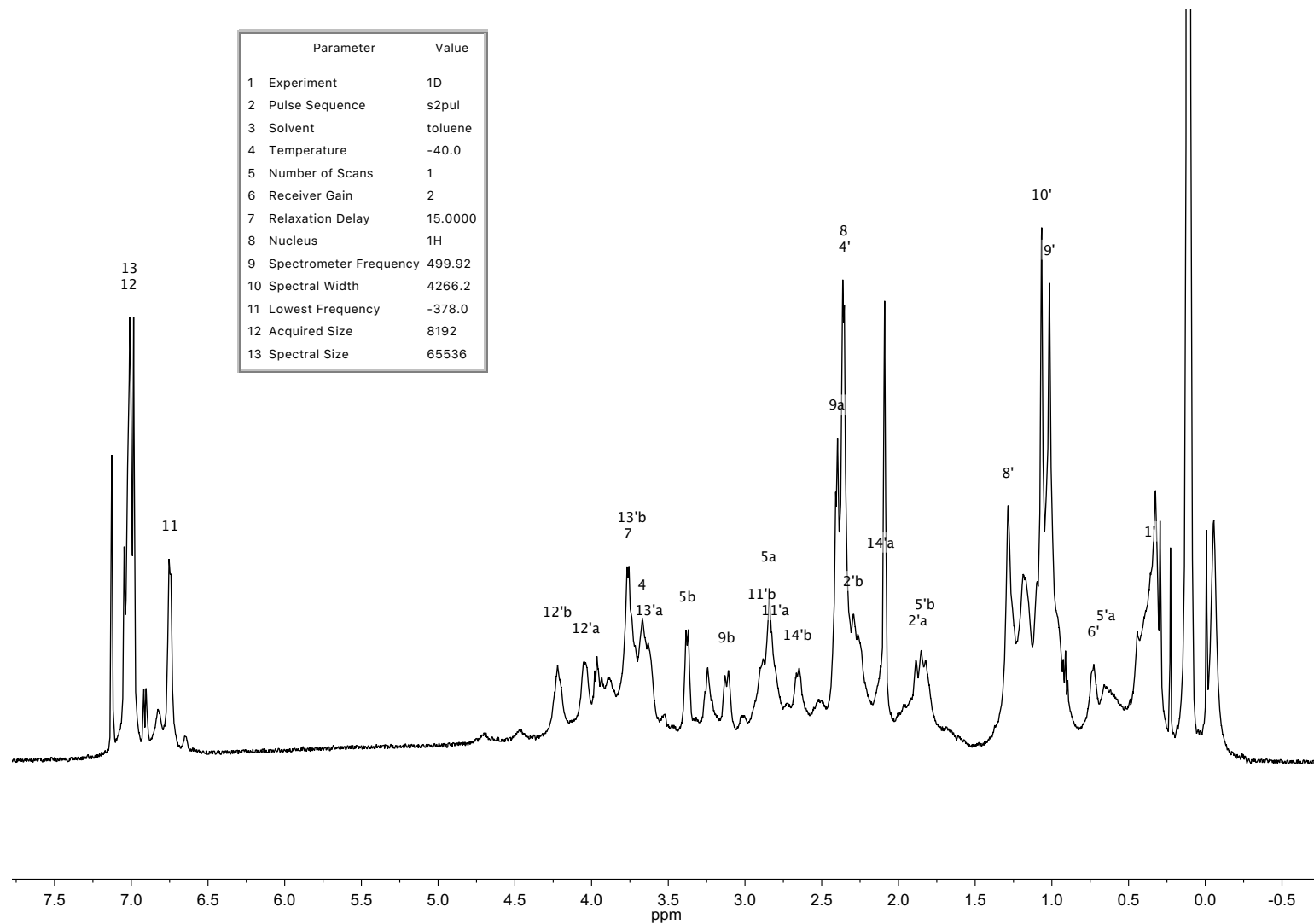


Figure 79. ¹H NMR spectrum of 0.10 M mixed aggregate (*R*)-**15a** in neat toluene-*d*₈ -40 °C. Labels indicate assignments by 2D NMR.

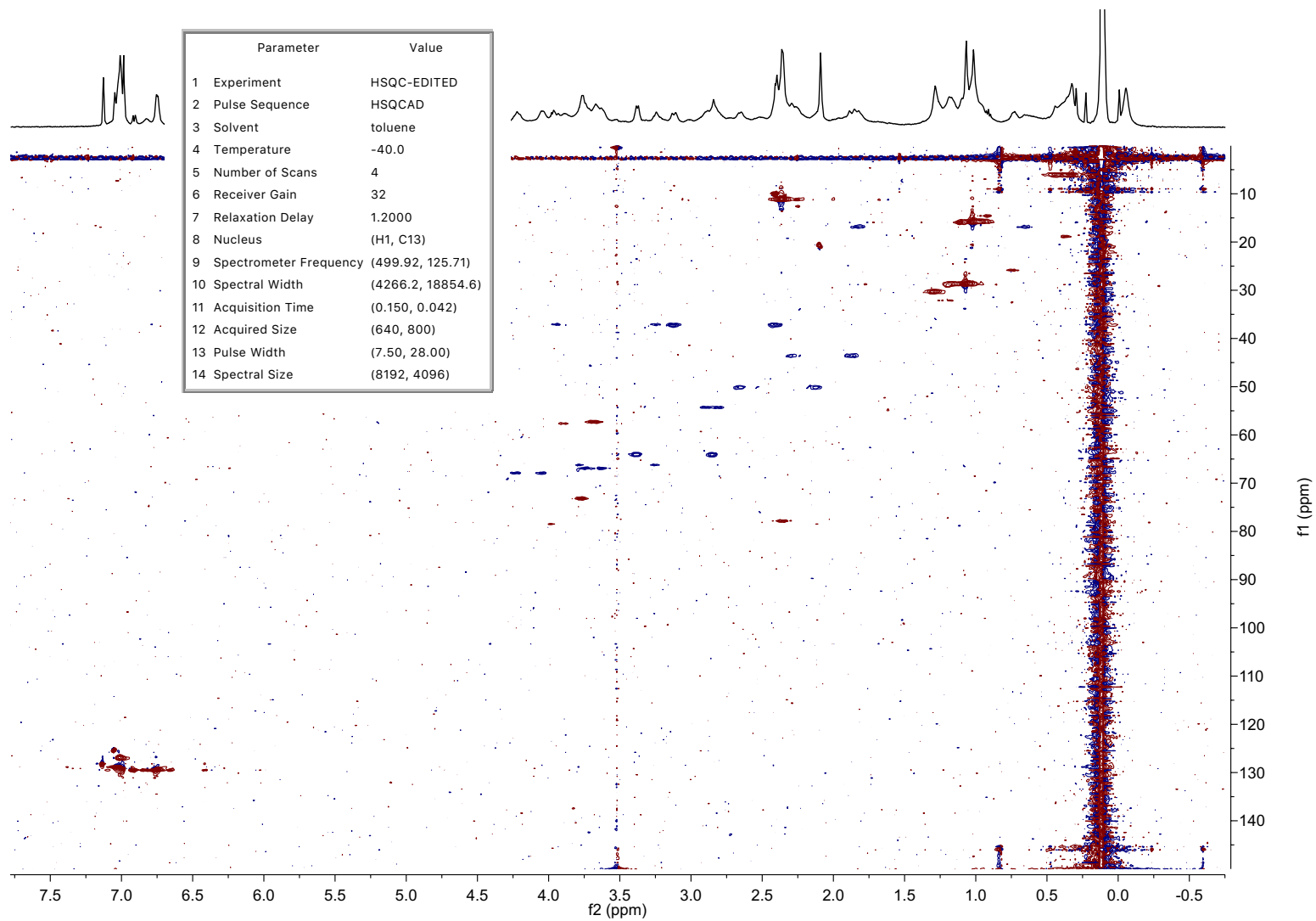


Figure 80. Full display HSQC spectrum of 0.10 M (*R*)-**15a** in neat toluene-*d*₈ at -40 °C.

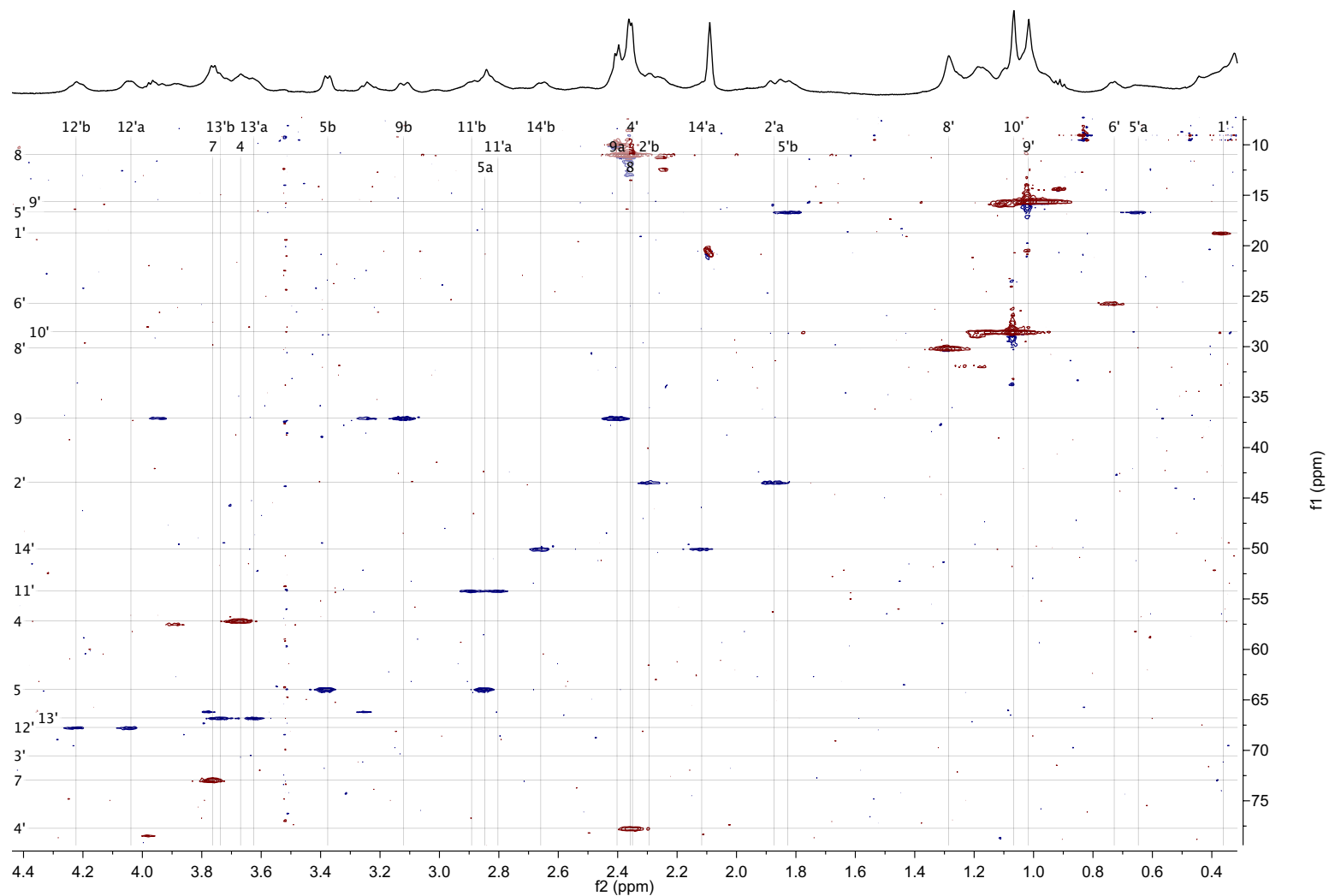


Figure 81. Expansion of the HSQC spectrum of 0.10 M (*R*)-**15a** in neat toluene-*d*₈ at -40 °C. Labels indicate assignments.

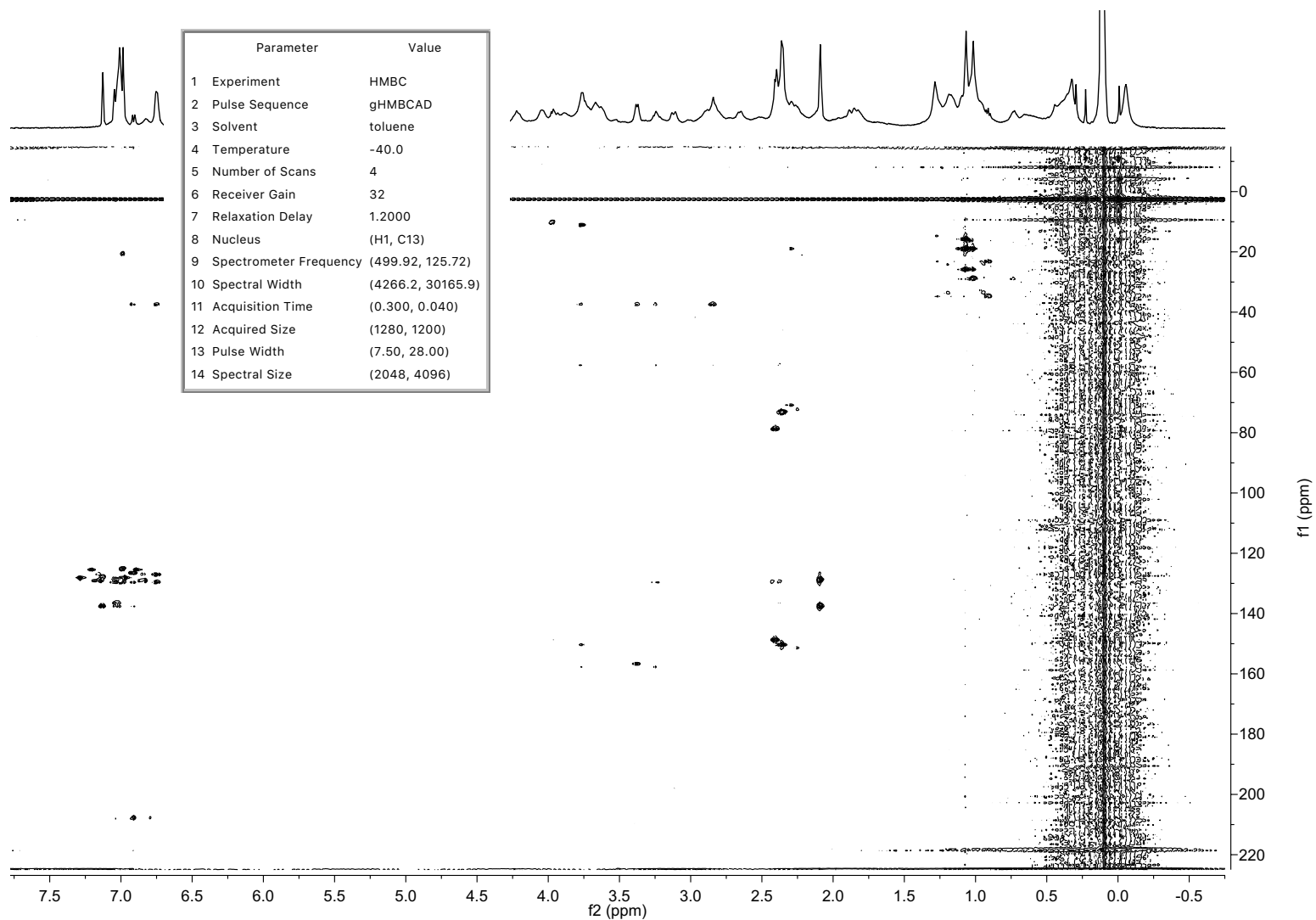


Figure 82. Full display HMBC spectrum of 0.10 M (*R*)-**15a** in neat toluene-*d*₈ at -40 °C.

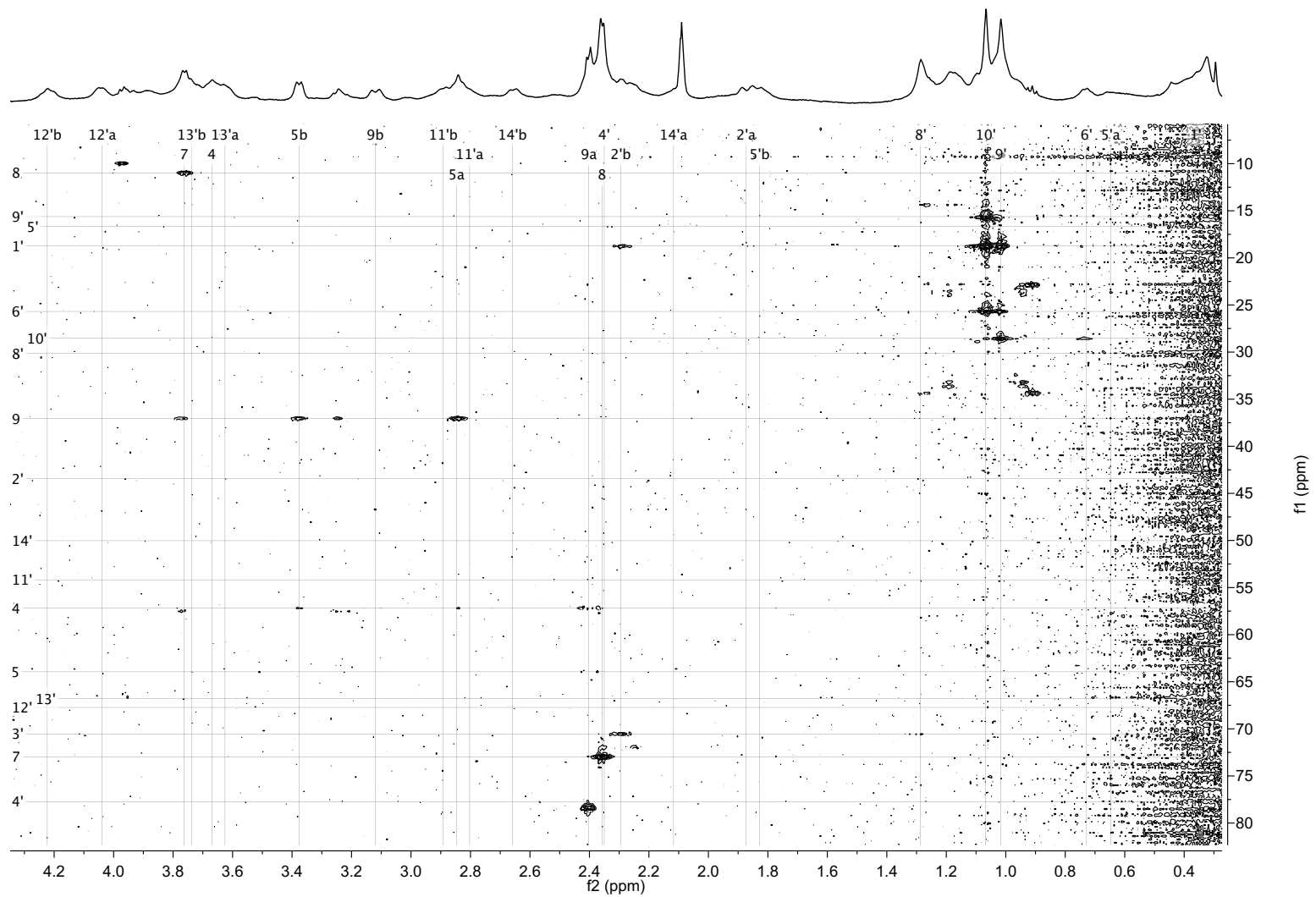


Figure 83. Expansion of the HMBC spectrum of 0.10 M (*R*)-**15a** in neat toluene-*d*₈ at -40 °C. Labels indicate assignments.

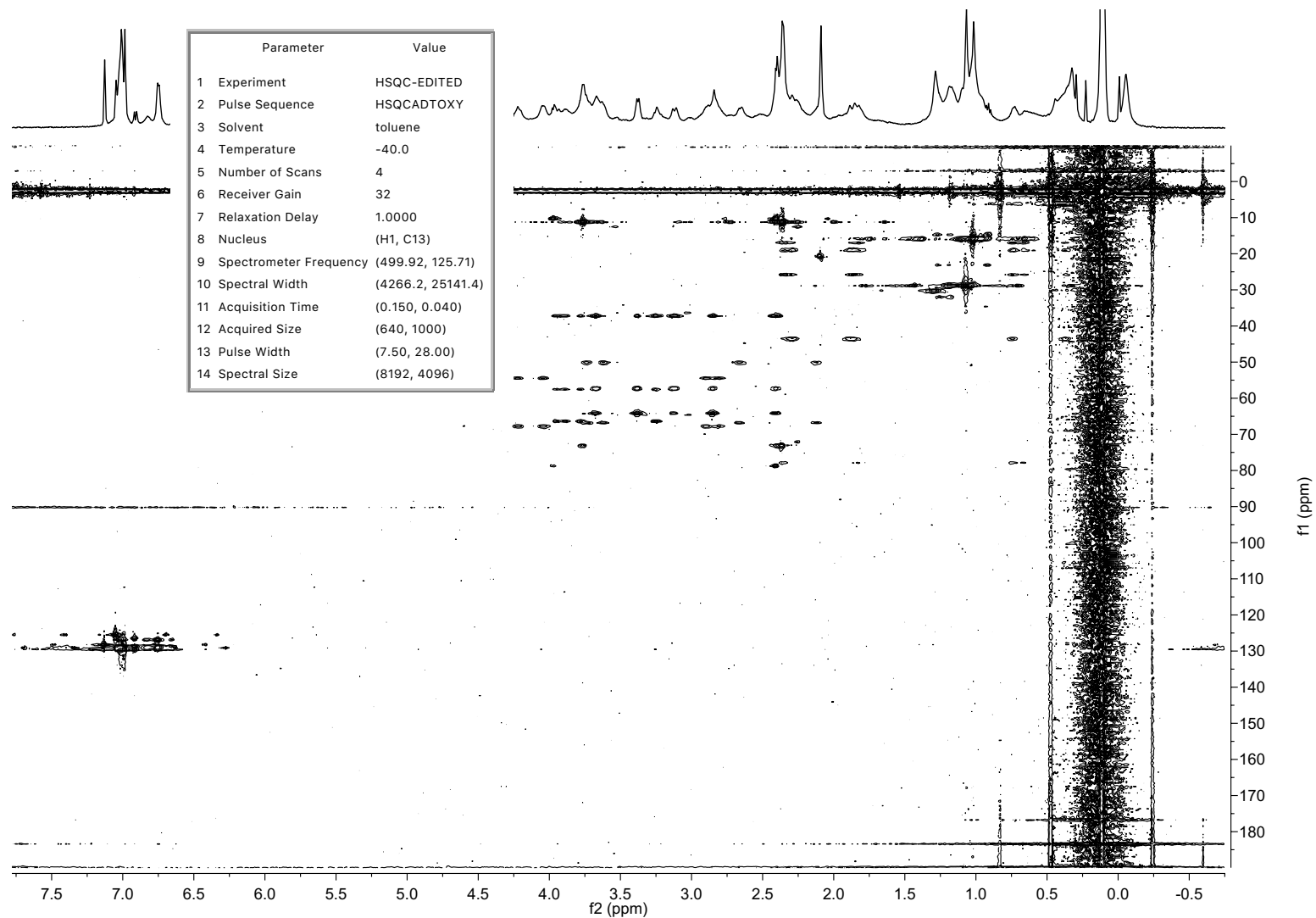


Figure 84. Full display HSQC-TOCSY spectrum of 0.10 M (*R*)-15a in neat toluene-*d*₈ at -40 °C.

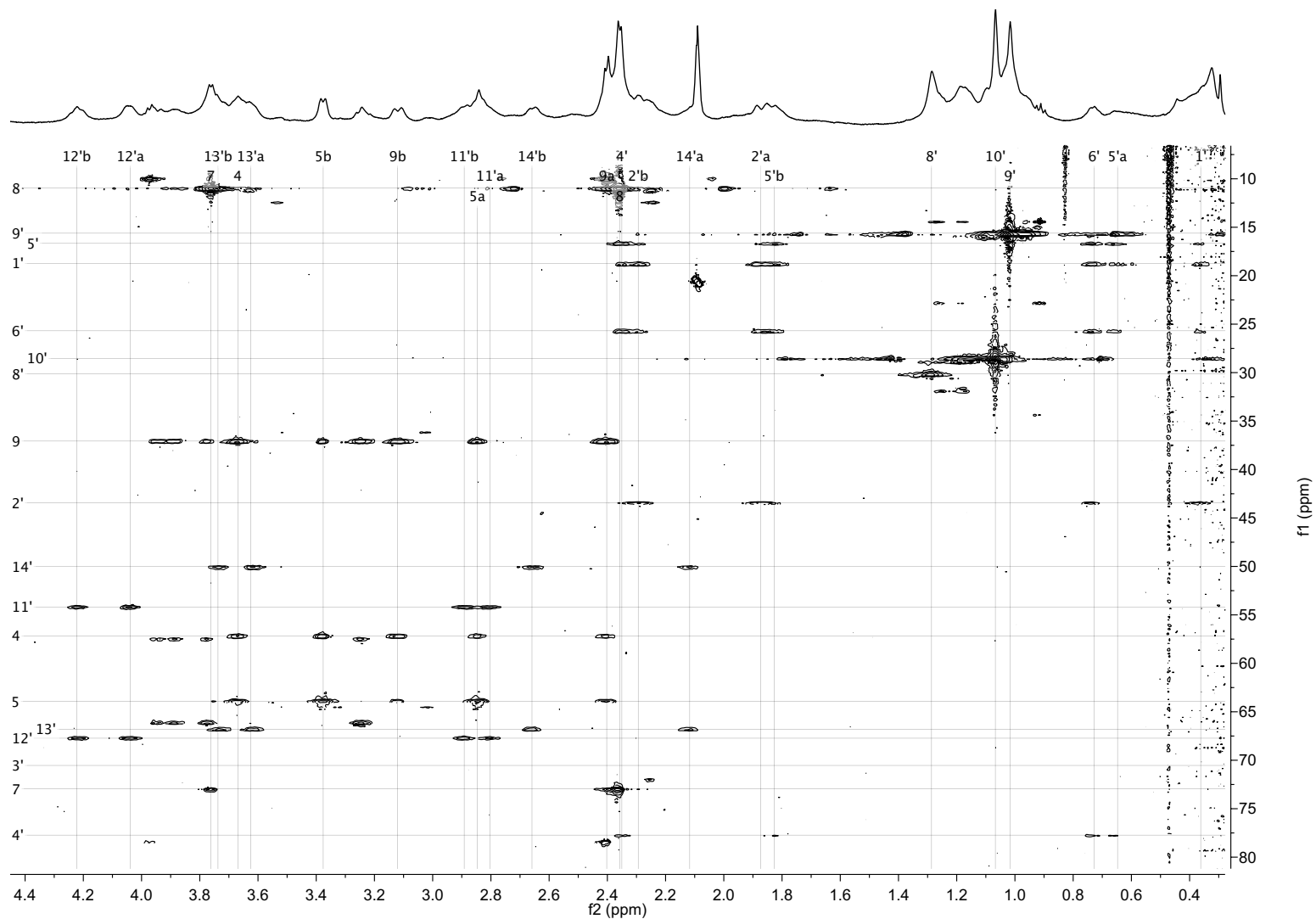


Figure 85. Expansion of the HSQC-TOCSY spectrum of 0.10 M (*R*)-**15a** in neat toluene- d_8 at -40 °C. Labels indicate assignments.

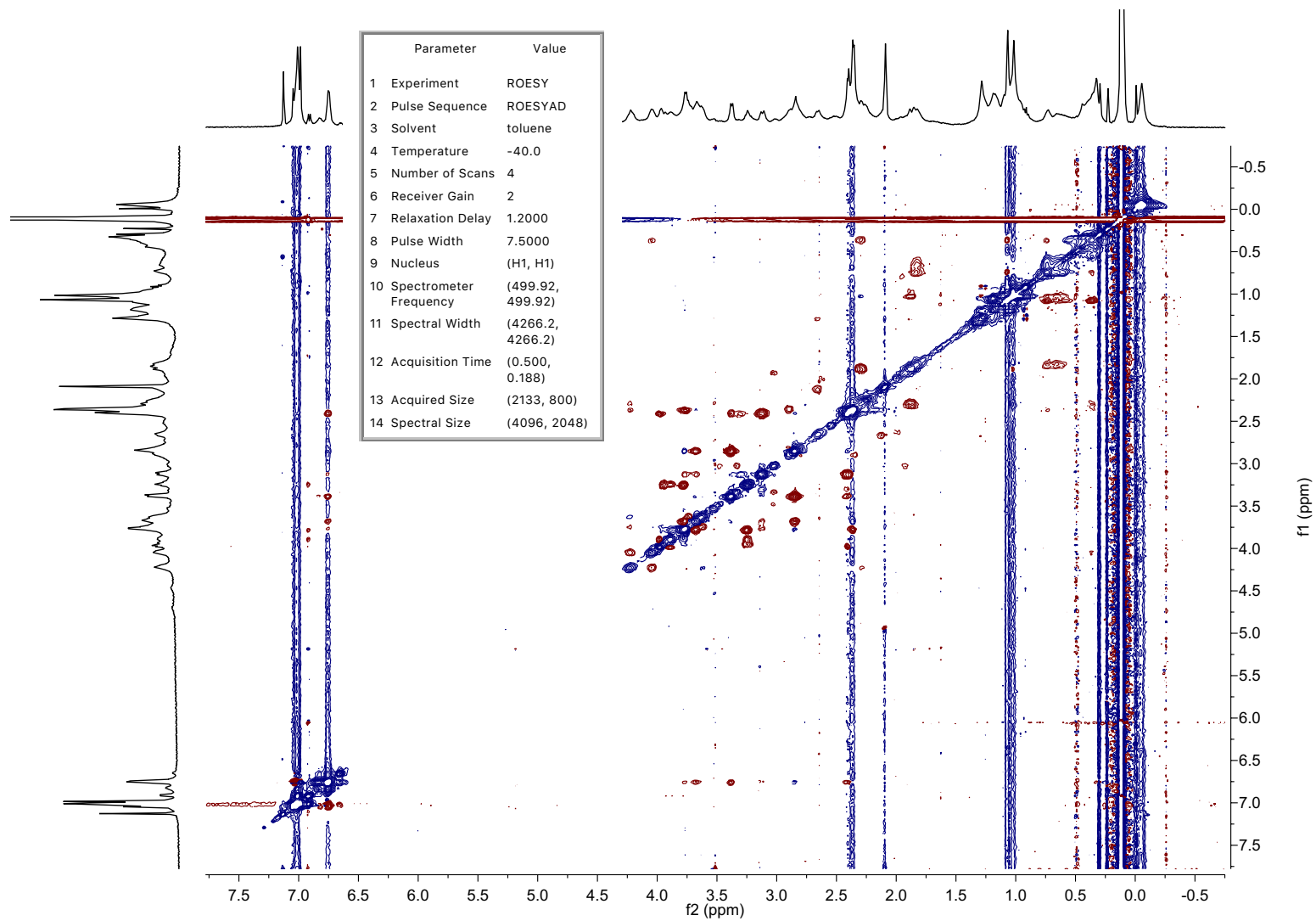


Figure 86. Full display ROESY spectrum of 0.10 M (*R*)-**15a** in neat toluene-*d*₈ at -40 °C.

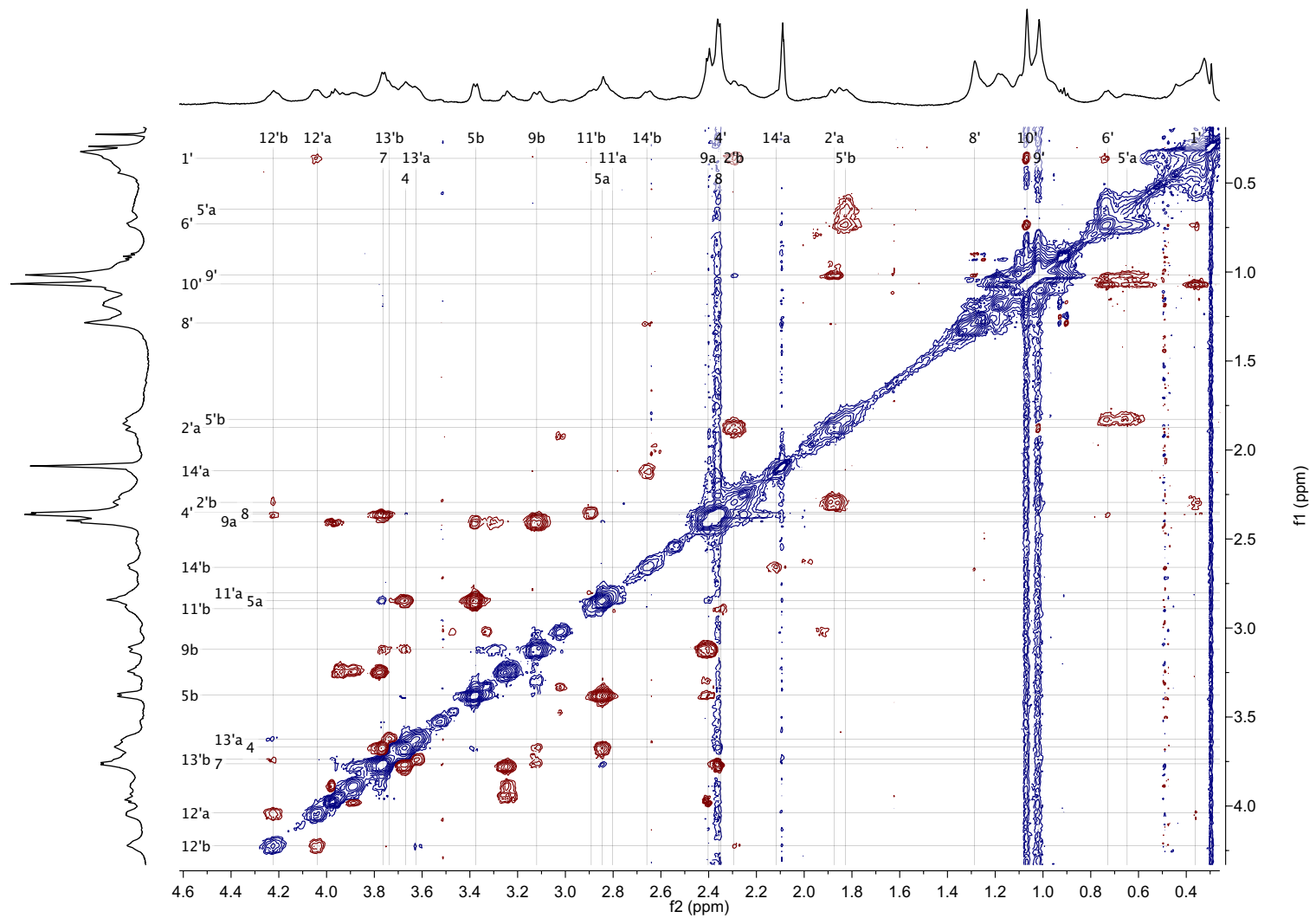


Figure 87. Expansion of the ROESY spectrum of 0.10 M (*R*)-15a in neat toluene-*d*₈ at -40 °C. Labels indicate assignments.

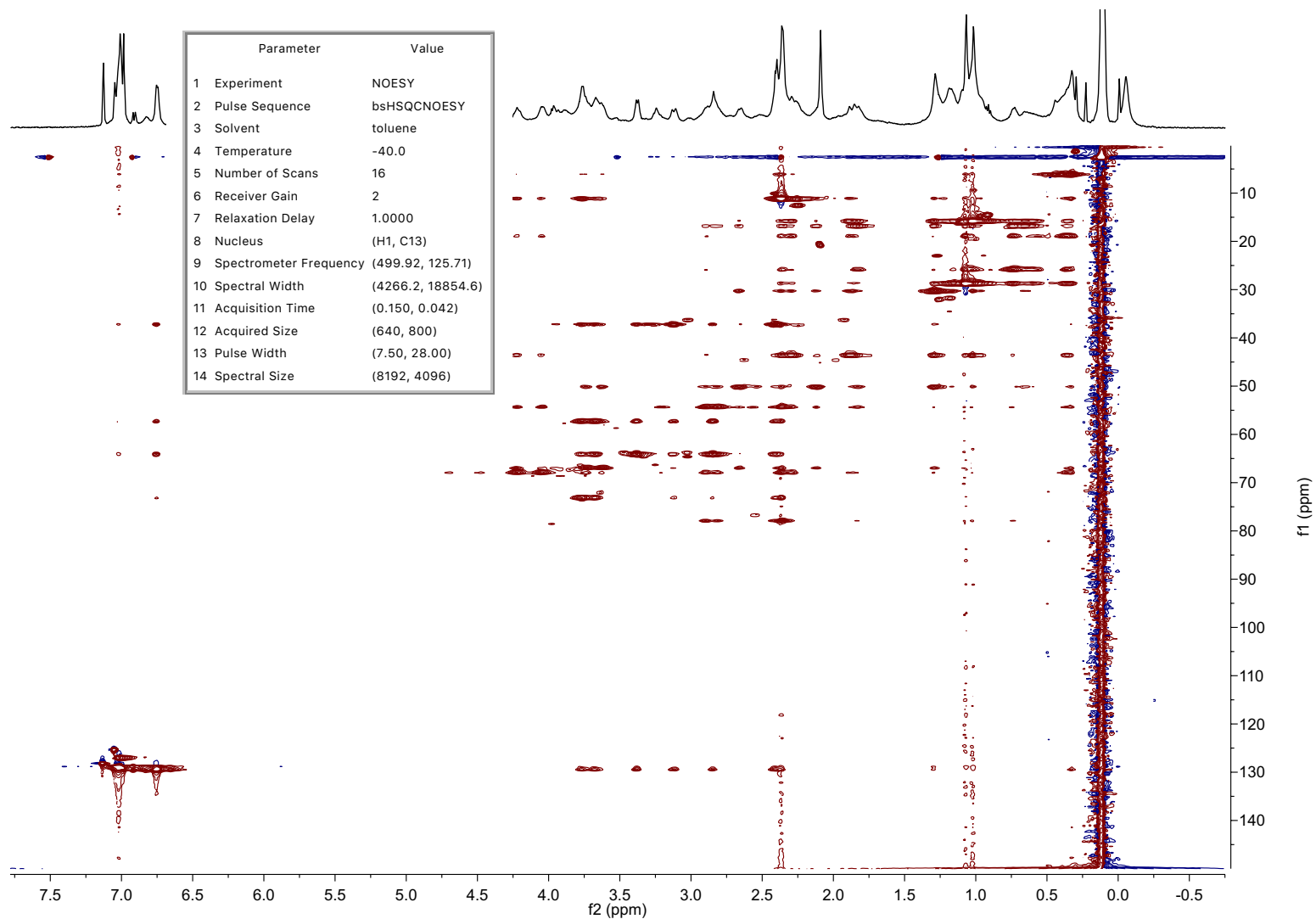


Figure 88. Full display HSQC-NOESY spectrum of 0.10 M (*R*)-**15a** in neat toluene- d_8 at -40 °C.

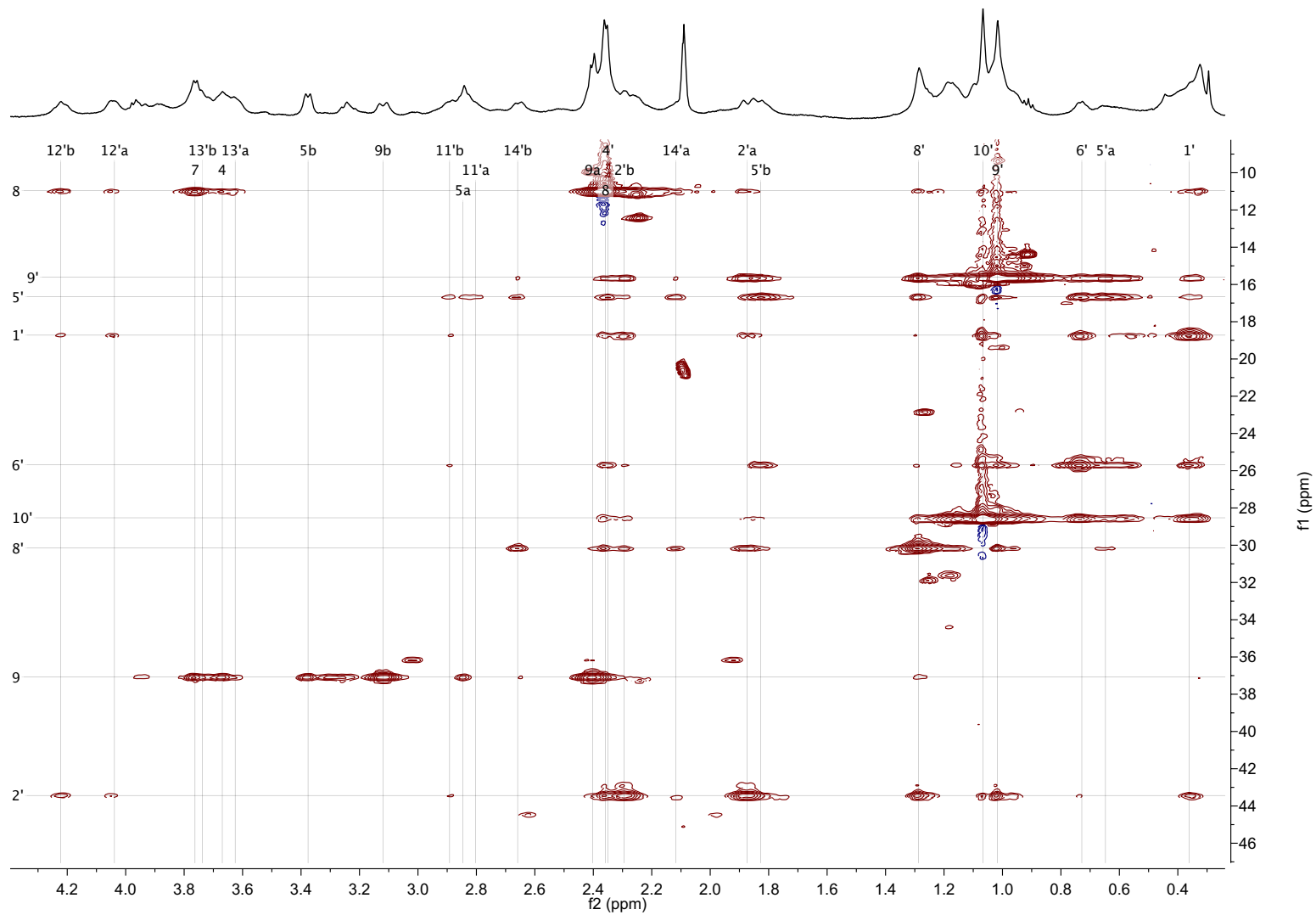


Figure 89. Expansion of the HSQC-NOESY spectrum of 0.10 M (*R*)-**15a** in neat toluene-*d*₈ at -40 °C. Labels indicate assignments.

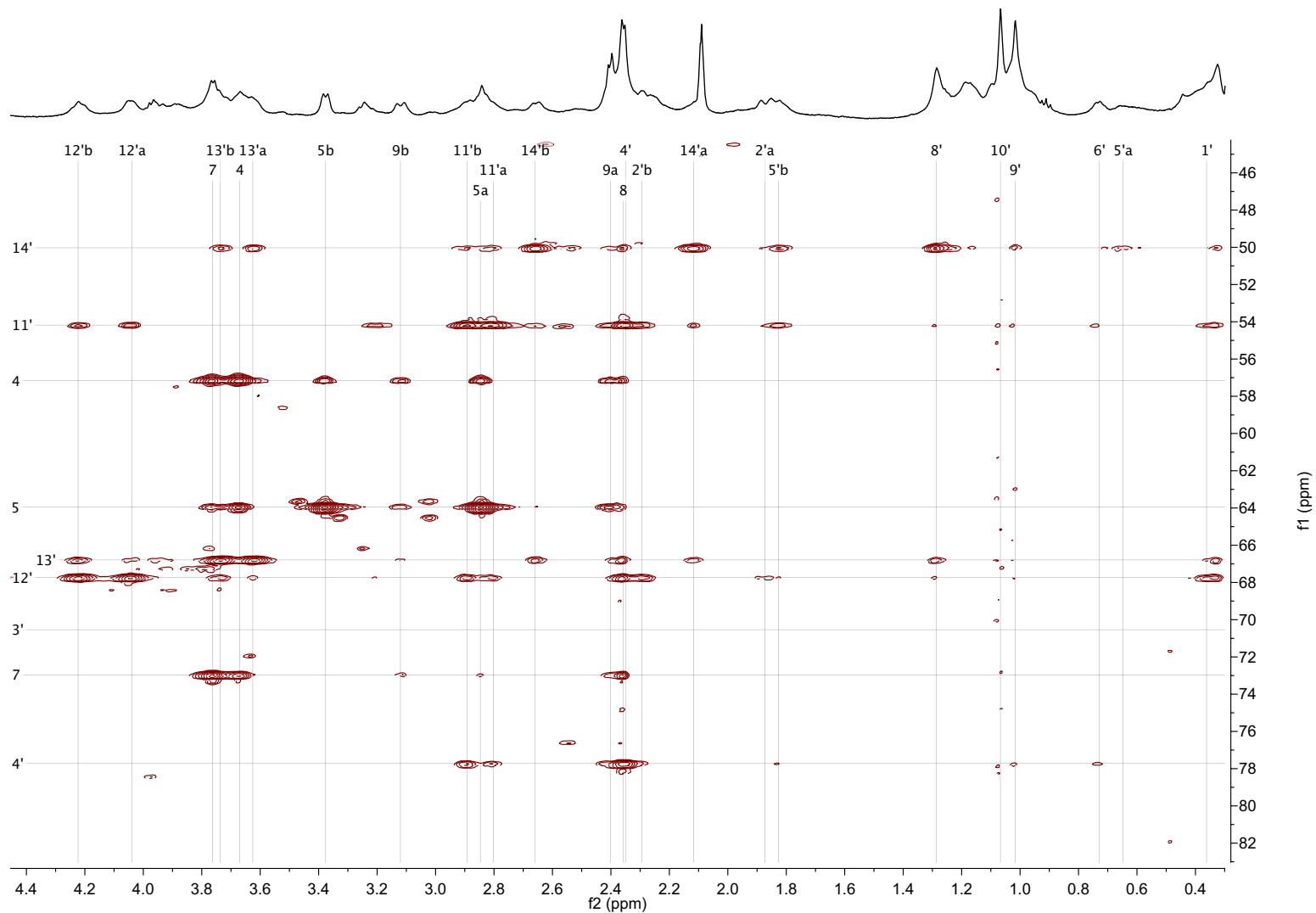


Figure 90. Expansion of the HSQC-NOESY spectrum of 0.10 M (*R*)-**15a** in neat toluene-*d*₈ at -40 °C. Labels indicate assignments.

2D NMR analysis of 1:3 mixed aggregate (S)-16a: A sample prepared from 0.40 M [⁶Li]LiHMDS, 0.10 M (S)-**1a** and 0.30 M amino alkoxide **11** with 0.05 M HMPA in neat THF-*d*₈, after aging at 20 °C for 10 min, was studied by standard 2D NMR techniques. All chemical shifts with the exception of quaternary C-7's in the carene amino alkoxide (CAA) residues were assigned using high field indirect-resolution 2D HSQC, HSQC-TOCSY, and HMBC experiments.

Experimental: 2D NMR spectra were acquired on a 500 MHz Varian INOVA spectrometer operating at 499.92 MHz for ¹H observation using a 5 mm Varian inverse-detect probehead with Z-axis pulsed field-gradient. Sample temperature was maintained at -60 °C as calibrated with a neat methanol sample. ¹H and ¹³C 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: All morpholine rings display four non-equivalent methylenes, however the ROESY spectrum shows exchange crosspeaks between H-12'ax and H-13'eq as well as H-12'eq and H-13'ax indicating that the morpholine fragment of CAA' undergoes rotation around C-4'-N' bond followed by a chair flip and that this process is slow on the ¹H timescale ($\Delta\nu = 300$ and 250 Hz, respectively).

The 3D structure of the aggregate was derived from 2D NOESY, 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-4 and C-7. Reciprocal H-7 to C-4 correlations are observed but cannot be unambiguously assigned due to the coincidental chemical shifts of H-4 and H-9. The starting point for solving the structure is H-8 methyl of the enolate, which gives nOe correlations to bound HMPA, C-13''' and C-12''', as well as C-2''. Reciprocal correlations to H-12''' and H-13''' to C-8 are also observed. This indicates that the methyl group projects over the O-1/Li-2/O-3/Li-4 face of the cube and is sandwiched between the morpholine ring of CAA''' and HMPA. Contacts with both H-12''' and H-13''' show that the N-O axis of the morpholine is perpendicular to the O-1/Li-2/O-3/Li-4 face and therefore O-3 cannot be part of CAA'''. The same correlations also allow the assignment of CAA''' specifically to O-4 with N''' coordinating to Li-4 as opposed to O-2/Li-2 which would result in a close contact with the C-11'''/C-12''' edge of the morpholine based on computational data. Correlations from C-4''' to H-11'' and H-4'' further support this assignment.

CAA'' and CAA''' are adjacent and oriented anti-parallel to each other as evidenced by correlations between the morpholine of CAA''' and the carene fragment of CAA'' (H-11'''ax/eq to C-4'', C-12''' to H-1'') as well as the carene of CAA''' and the morpholine of CAA'' (C-4''' to H-11'' and H-4'') leading us to assign O-3 to CAA'' with N'' coordinating to Li-3.

CAA' contributes O-2 and is oriented so the morpholine is proximal to Li-1 and the carene is adjacent to HMPA as determined by correlations between HMPA and H-2'ax, HMPA and H-8', H-2'eq and H-8'' as well as H-4' and C-13''

HMPA is bound to Li-2 and is sitting in a "cavity" defined by the Re face of the enolate, C-8', C-2' and C-8''.

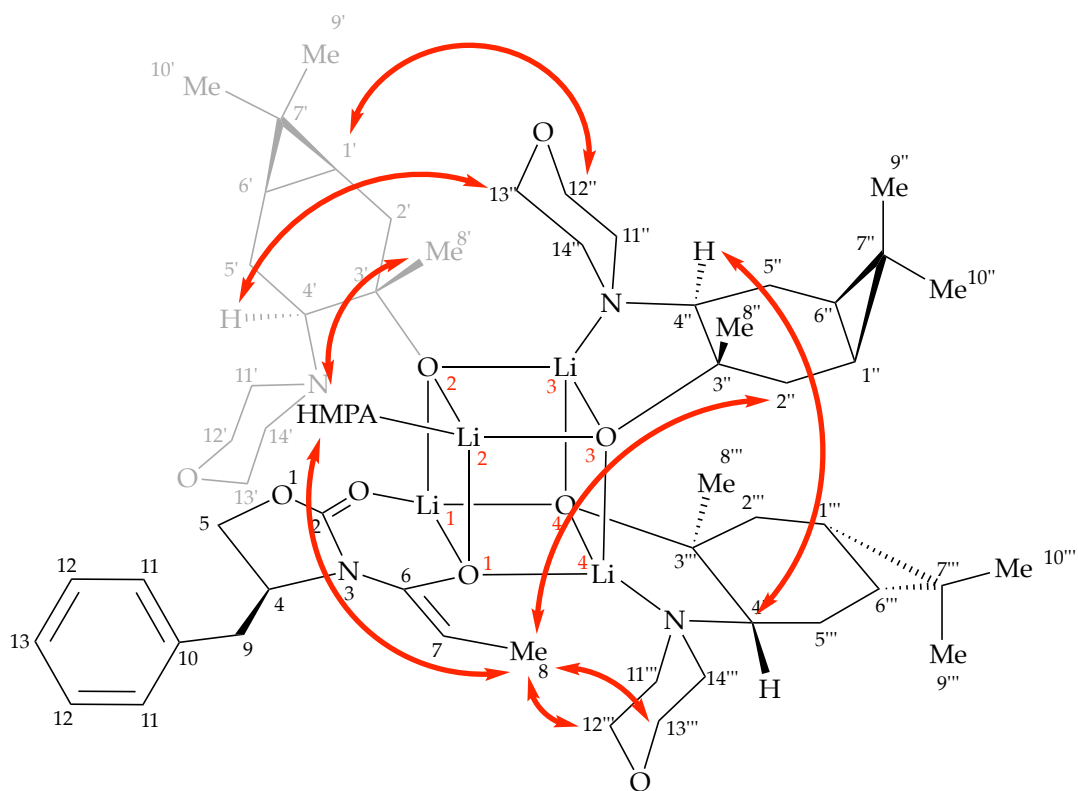


Table 3. ^1H , ^6Li , ^{13}C , and ^{15}N chemical shift assignments for mixed aggregate (*S*)-**16a** at $-60\text{ }^\circ\text{C}$.

Atom	δC , ppm	δH , ppm	HMBC	HSQC-TOCSY	ROESY	HSQC-NOESY
N''' N	46.15	–	$12'''\text{Heq}$, $13\text{H}'''\text{eq}$			
Li4 Li	0.83	–				
N'' N	46.55	–	$12''\text{Heq}$, $13\text{H}''\text{eq}$			
Li3 Li	0.66	–				
Li1 Li	0.67	–				
N' N	41.86	–	$12'\text{Heq}$, $3\text{H}'\text{eq}$			
Li2 Li	0.27	–				
1' C	19.51	0.29	9',10'	4',2',6'	13'',2',9',10',6'	2',6',8'',9',13'',14''
1'' C	19.52	0.25	9'',10'',2''	4'',2'',6''	12''',2'',9'',10'',6'''	2'',6'',9'',11''',12'''
1''' C	19.75	0.24	9''',10'''	4''',2''',6'''	12''',2''',9''',10''',6'''	2''',6''',9''',11''',12'''
2 C	155.95	–	5a			
2' C	40.92	1.24(ax)		5',6',1'	2'eq,10'	8',10',1'
		2.12(eq)	3',6'		2'ax	
2'' C	44.19	1.59(ax)		5'',6'',1''	2''eq,10''	1'',10'',8'',12'''
		2.08(eq)	1'',3'',6''		2''ax	
2''' C	44.3	1.49(ax)		5''',6''',1'''	2'''eq,10'''	12''',12'',11'',8''',10''',1'''
		1.85(eq)	3''',6'''		2'''ax	
3' C	71.99	–	4',6'			
3'' C	71.76	–	4'',6''			
3''' C	71.48	–	4''',6'''			
4 C	59.25	4.1	–	9,5	5,7,9	5,9,8,11,7
4' C	79.92	2.35	3',5'	5',6'	12'',13'',11',5',6'	13'',12'',11',5',6'
4'' C	78.67	2.31	3'',5''	5'',6''	11'',5'',6''	11'',11''',5'',6''
4''' C	77.95	2.27	3''',5'''	5''',6'''	11''',11''',5''',6'''	12''',11'',11''',5''',6'''
5 C	64.95	3.91(a)	9	4,9	4,5b	11,4,9
		3.86(b)			5a,13'''ax	
5' C	17.88	0.54(ax)	4'	4',6',1'	5'eq	4',6',8',10',11',14'
		1.94(eq)			5'ax	
5'' C	17.61	0.70(ax)	4''	4'',6'',1''	5''eq	4'',6'',8'',10'',11'',14''
		2.01(eq)			5''ax	
5''' C	17.48	0.68(ax)	4'''	4''',6''',1'''	5'''eq	4''',6''',8''',10''',11''',14'''
		1.99(eq)			5'''ax	
6 C	152.98	–	8			

6' C	28.31	0.78	2',9',10'	4',2',5',1'	13'ax,4',5',9',1'	13',4',5',9',10',1'
6" C	26.57	0.82	2",9",10"	4",2",5",1"	4",5",9",1"	4",5",9",10",1"
6''' C	26.1	0.79	2''',9''',10'''	4''',2''',5''',1'''	4''',5''',9''',1'''	11'',4''',5''',9''',10''',1'''
7 C	70.3	3.4	8	8	4,8,11	11,4,8,9
7' C	–	–				
7" C	–	–				
7''' C	–	–				
8 C	13.18	1.94	7,6	7	7,9,13'ax,12'ax,2'aq	4,12''',13''',7,HMPA,2''
8' C	29.29	1.03				14',2',5',10'
8" C	30.04	1.29			10"	14'',2'',2'',5'',10''
8''' C	31.62	1.03			10'''	14''',2''',5''',10'''
9 C	37.59	3.39	5,11	4,5	4,11	11,4,5,7,8,8'
		3.39				
9' C	29.42	0.95	10',6'	10',6'	13'eq,10',6',1'	10',6',1'
9" C	28.91	0.97	10",6"	10",6"	10",6",1"	10",6",1"
9''' C	28.93	0.94	10''',6'''	10''',6'''	10''',6''',1'''	10''',6''',1'''
10 C	138.59	–	11,12,13			
10' C	16.18	0.93	9',6'	9',6'	5',9',2',HMPA	2',5',8',9'
10" C	16.33	0.9	9",6"	9",6"	5",9",2"	14'',2'',5'',8'',9''
10''' C	16.18	0.87	9''',6'''	9''',6'''	5''',9''',2'''	14''',2''',5''',8''',9'''
11 C	130.54	7.32	10,12,13	12,13	HMPA,9,5,4,12	12,4,5,7,9
11' C	56.88	2.79(a)		12'	12',11'b,14',4'	12',13',14',4',5',2'''eq,8'
		2.88(b)			11'a	
11" C	54.81	2.75(a)		12"	12",11"b,14",4"	12'',14'',4'',5'',1'''
		2.99(b)			11"a	
11''' C	55	2.73		12'''	12''',11'''b,14''',4'''	12''',14''',4''',5''',1'''
		2.9			11'''a	
12 C	129.66	7.32	10,11,13	11,13	11,13	11,13
12' C	68.67	4.03(ax)	13'	11'	13'eq,12'eq,13'	13',11',14',14',2''',8'
		3.62(eq)			13'ax,12'ax,11'a	
12" C	69.06	3.92(ax)	13"	11"	12'eq,1'''	13'',11'',11'',14'',4',2''',1'''
		3.80(eq)			12'ax,11'ax	
12''' C	67.81	4.01(ax)	13'''	11'''	12'''eq,8,1"	13''',2'',11''',2'',8,1"
		3.82(eq)			12'''ax,11'''ax	
13 C	127.66	7.22	10,11,12	11,12	12	12
13' C	66.91	4.13(ax)	12'	14'	12'eq,13'eq	12',11',14',8'
		3.42(eq)			12'ax,13'ax	

13" C	68.85	3.83(ax)	12"	14"	13"eq,4',1'	12",14",11",8",6',1'
		3.56(eq)			13'ax,6',9'	
13''' C	67.07	3.76(ax)	12'''	14'''	13'''eq,8	12''',11'''14''',8,8'''
		3.47(eq)			13'''ax	
14' C	50.72	2.31(a)	–	13'	13'eq,11'a	13',12',11',5',8'
		2.64(b)				
14" C	51.26	2.34(a)	–	13"	11"a,14"b	13",12",11",5",8",1'
		2.93(b)			14"a	
14''' C	51.35	2.22(a)	–	13'''	13'''eq,14'''b,11'''a	13''',11''',5''',8'''
		2.75(b)			14'''a	

Parameter	Value
1 Experiment	1D
2 Pulse Sequence	s2pul
3 Solvent	thf
4 Temperature	-60.0
5 Number of Scans	1
6 Receiver Gain	2
7 Relaxation Delay	6.0000
8 Nucleus	¹ H
9 Spectrometer Frequency	499.92
10 Spectral Width	7998.4
11 Lowest Frequency	-1002.7
12 Acquired Size	15997
13 Spectral Size	65536

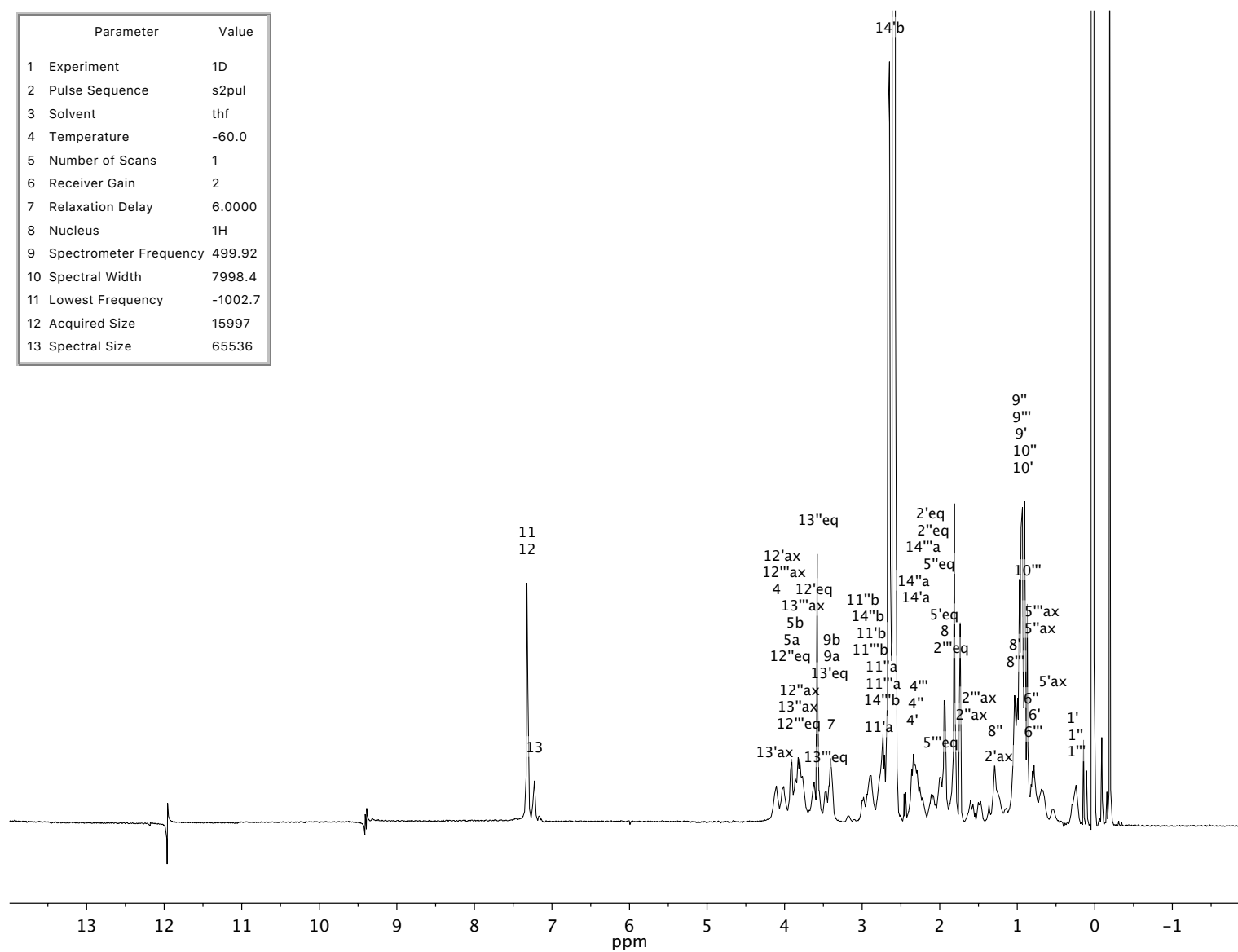


Figure 91. ¹H NMR spectrum of 0.10 M mixed aggregate (*S*)-**16a** with 0.05 M HMPA in neat THF-*d*₈ -60 °C. Labels indicate assignments by 2D NMR.

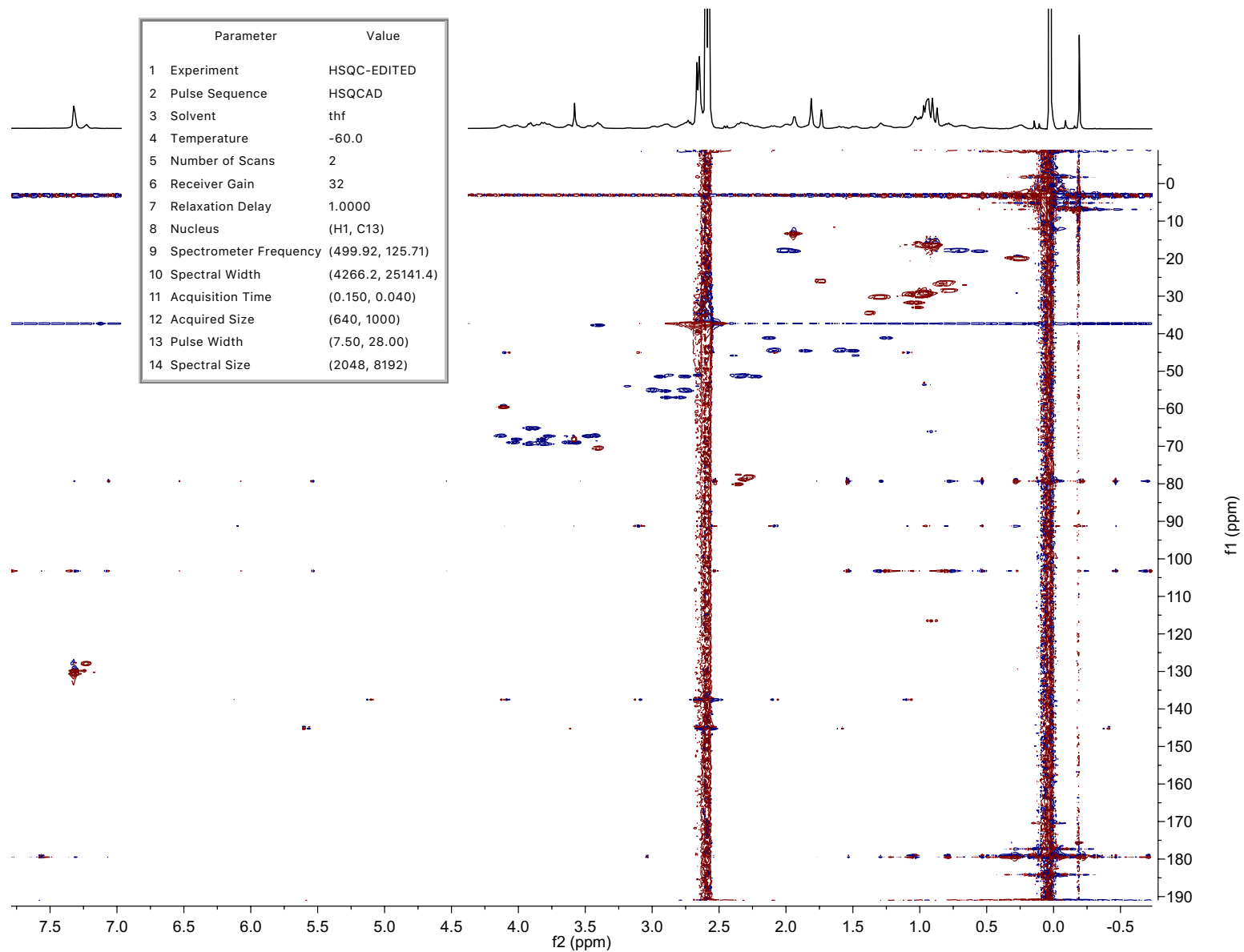


Figure 92. Full display HSQC spectrum of 0.10 M (*S*)-**16a** with 0.05 M HMPA in neat THF-*d*₈ -60 °C.

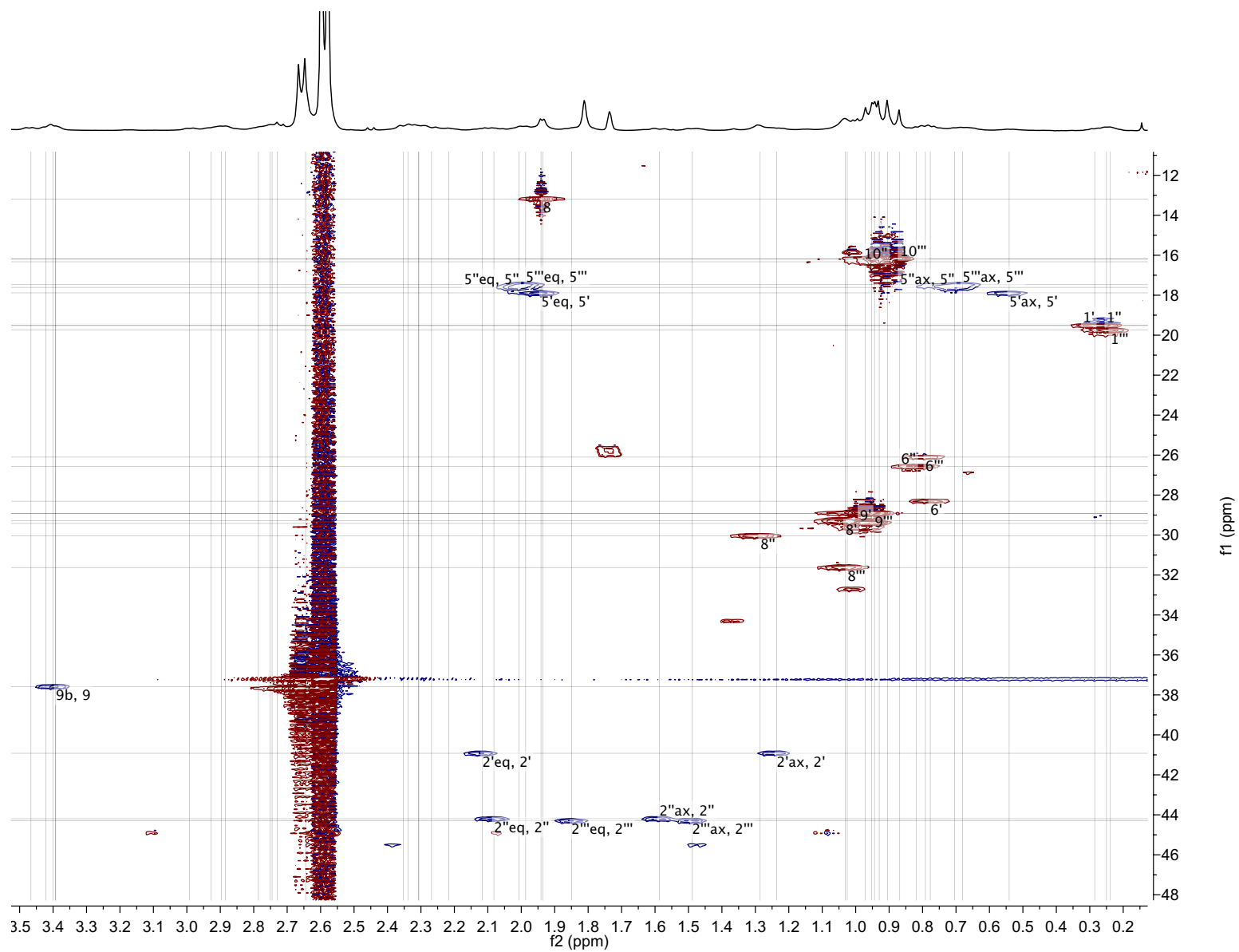


Figure 93. Expansion of HSQC spectrum of 0.10 M (*S*)-**16a** with 0.05 M HMPA in neat THF-*d*₈ -60 °C. Labels indicate assignments.

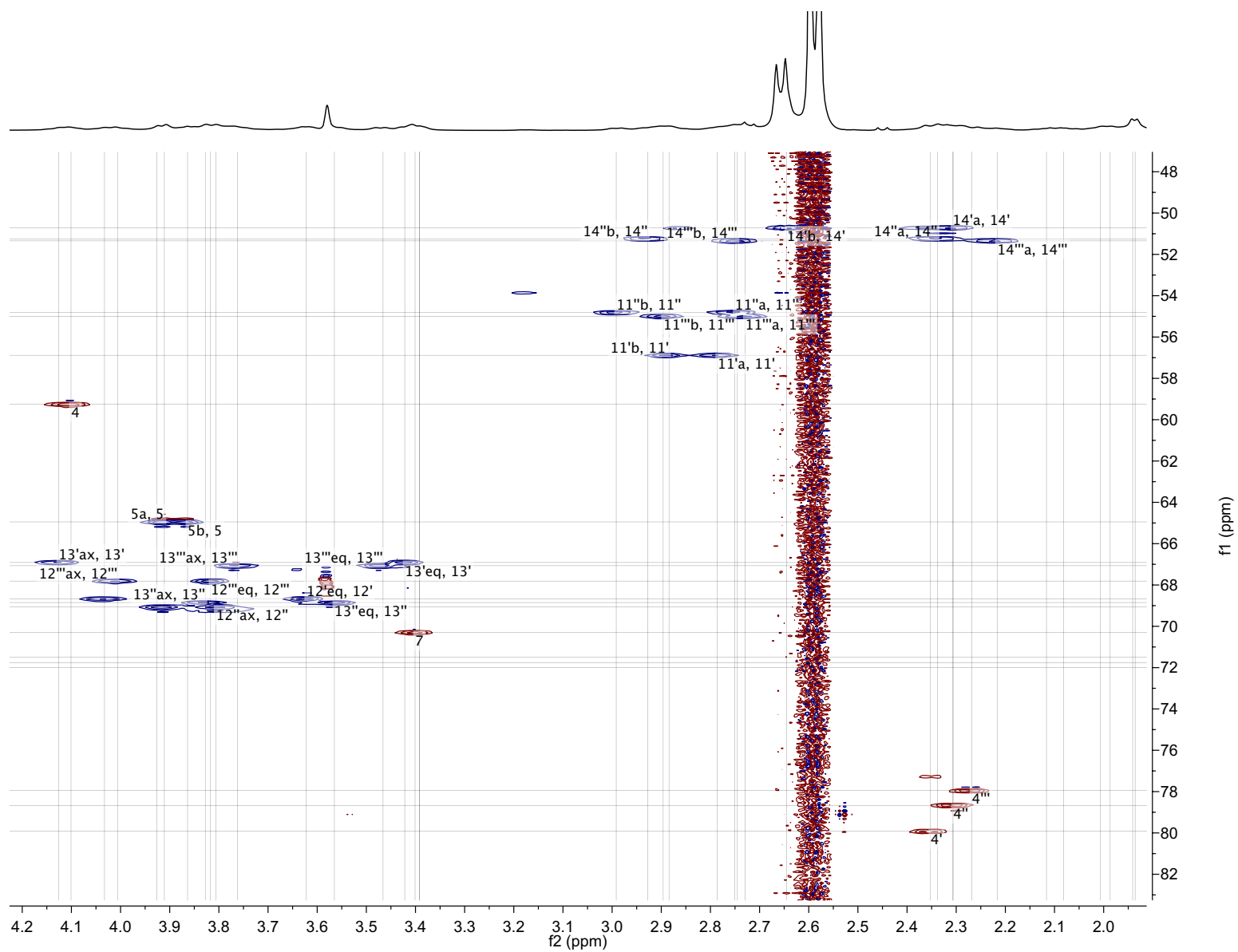


Figure 94. Expansion of HSQC spectrum of 0.10 M (*S*)-**16a** with 0.05 M HMPA in neat THF-*d*₈ -60 °C. Labels indicate assignments.

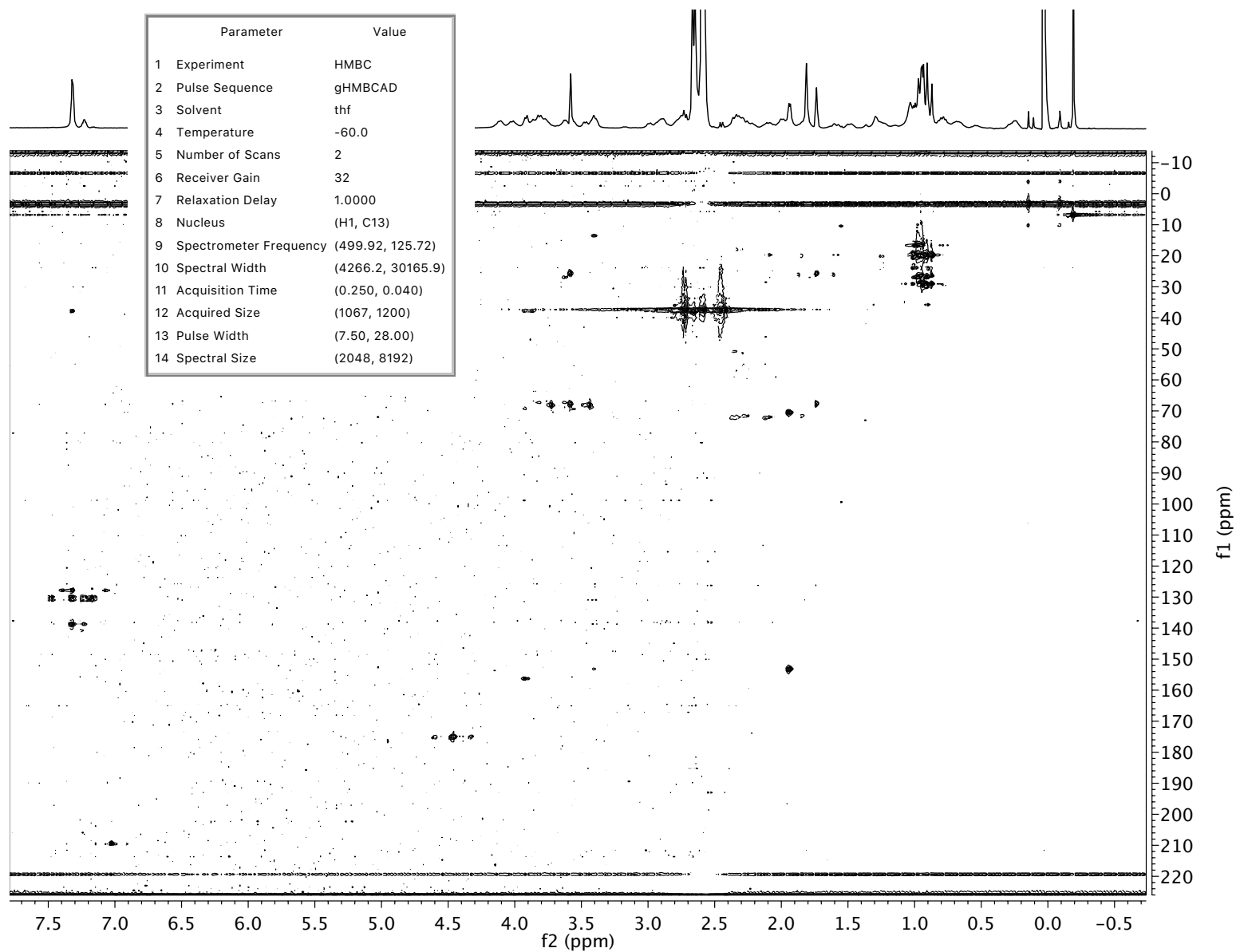


Figure 95. Full display HMBC spectrum of 0.10 M (*S*)-**16a** with 0.05 M HMPA in neat THF-*d*₈ -60 °C.

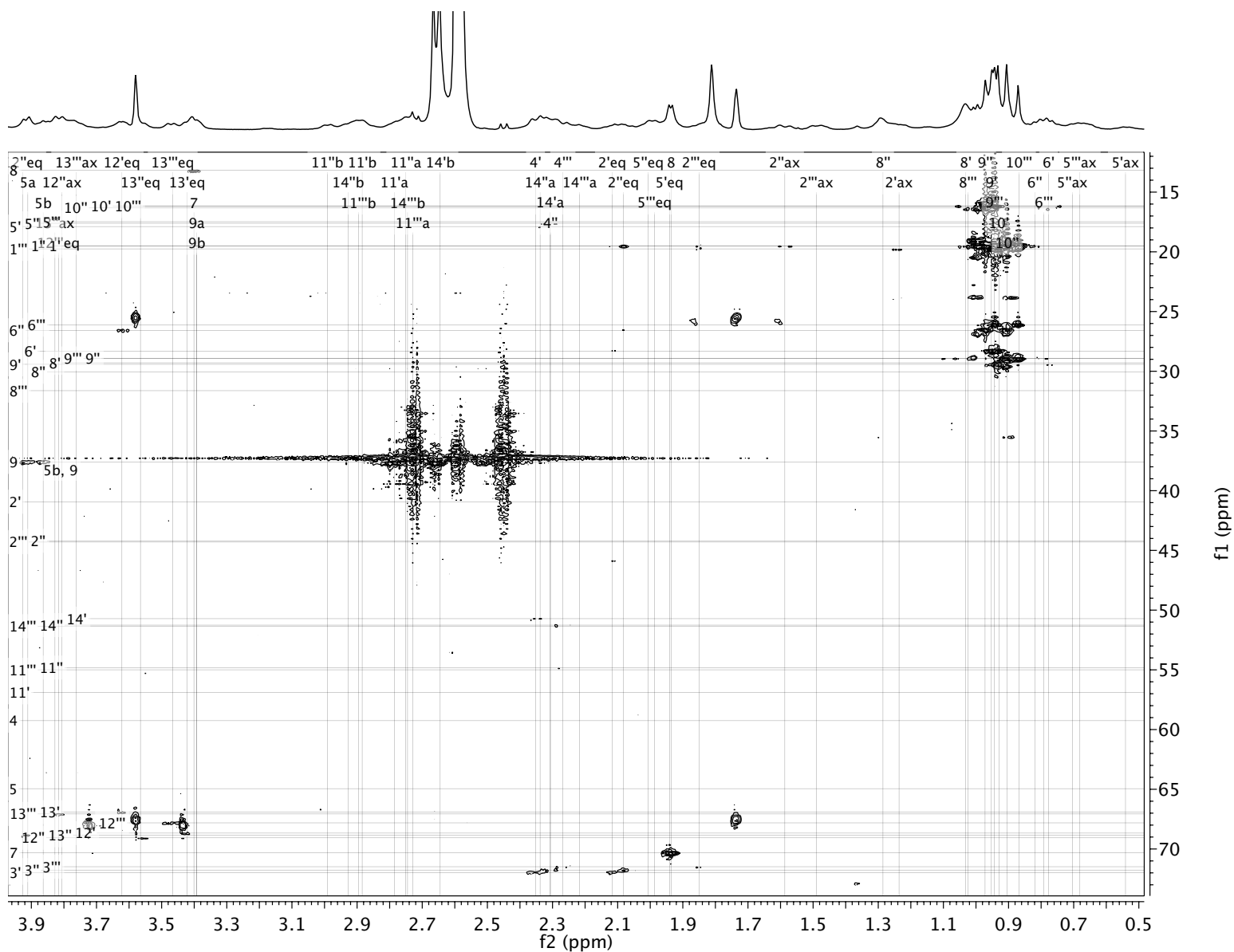


Figure 96. Expansion of HMBC spectrum of 0.10 M (S)-16a with 0.05 M HMPA in neat THF-*d*₈ -60 °C. Labels indicate assignments.

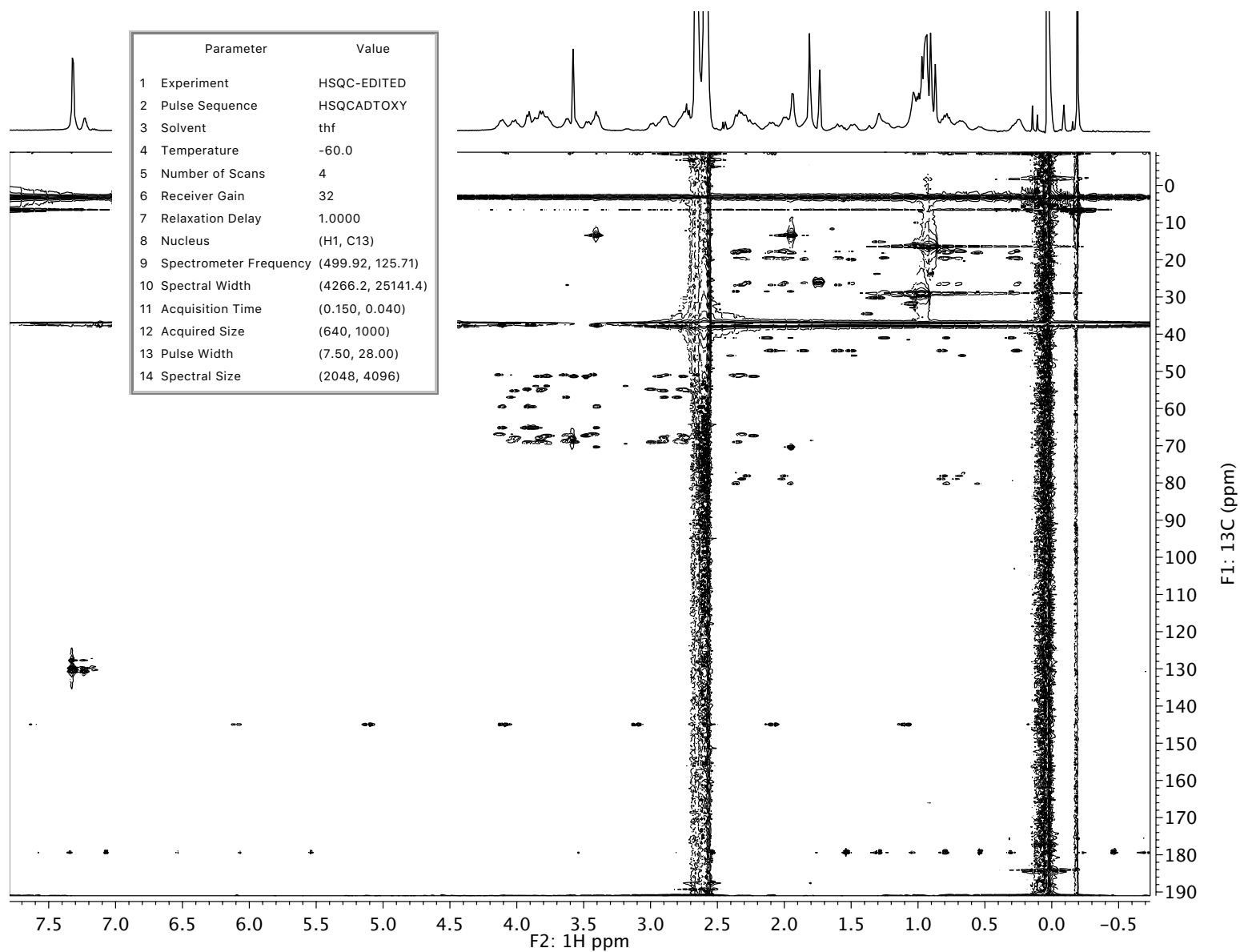


Figure 97. Full display HSQC-TOCSY spectrum of 0.10 M (*S*)-**16a** with 0.05 M HMPA in neat THF-*d*₈ -60 °C.

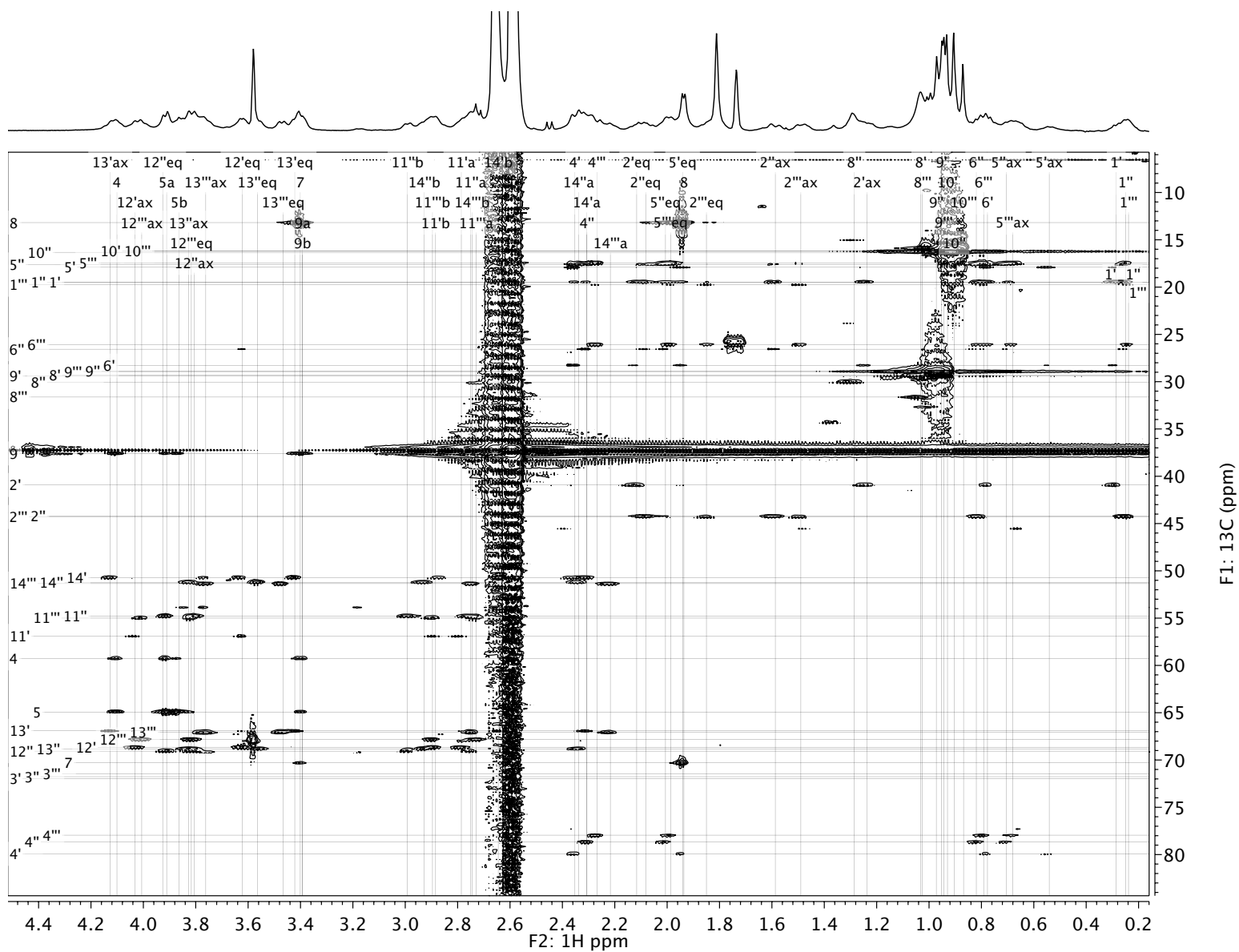


Figure 98. Expansion of HSQC-TOCSY spectrum of 0.10 M (*S*)-**16a** with 0.05 M HMPA in neat THF-*d*₈ –60 °C. Labels indicate assignments.

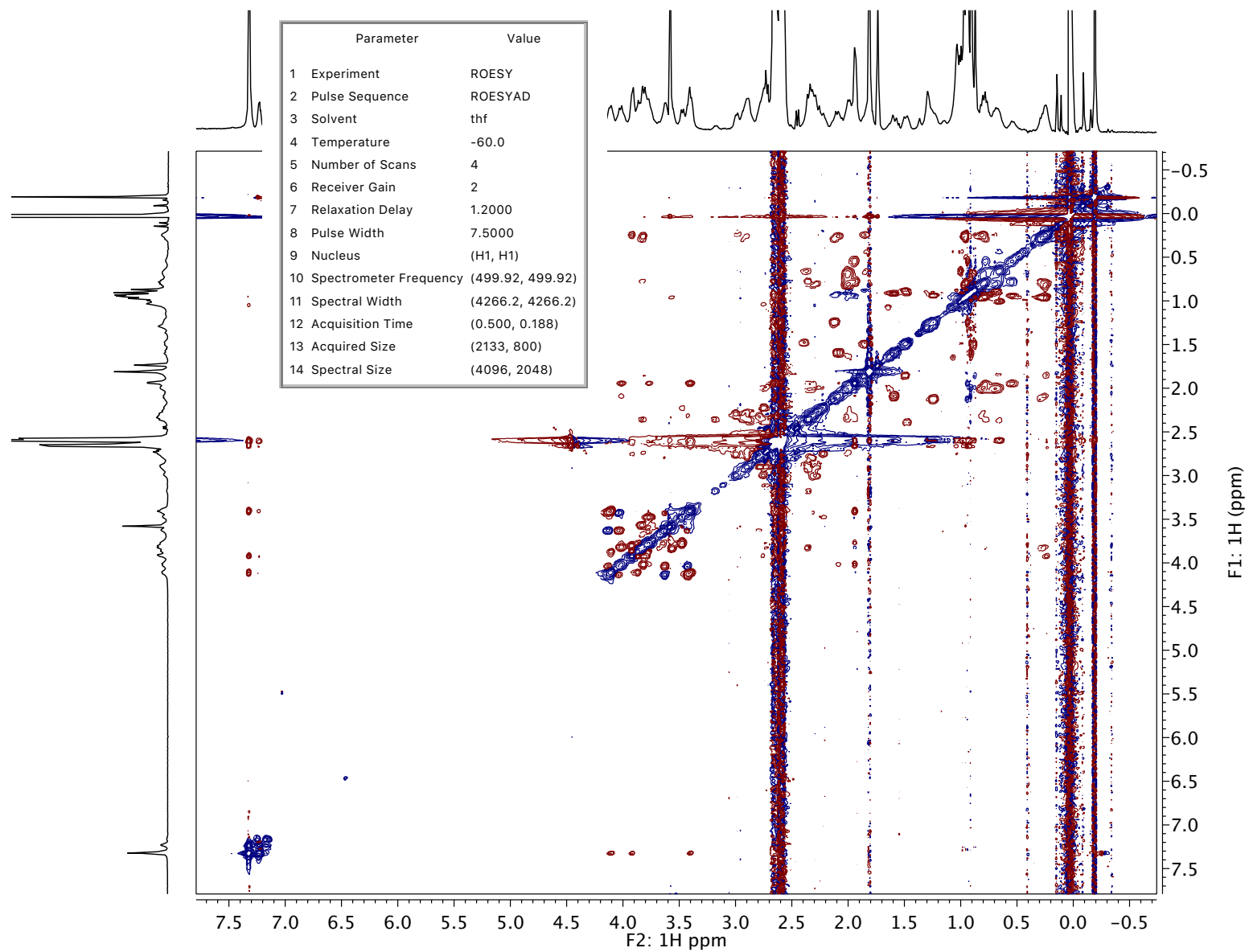


Figure 99. Full display ROESY spectrum of 0.10 M (*S*)-**16a** with 0.05 M HMPA in neat THF-*d*₈ -60 °C.

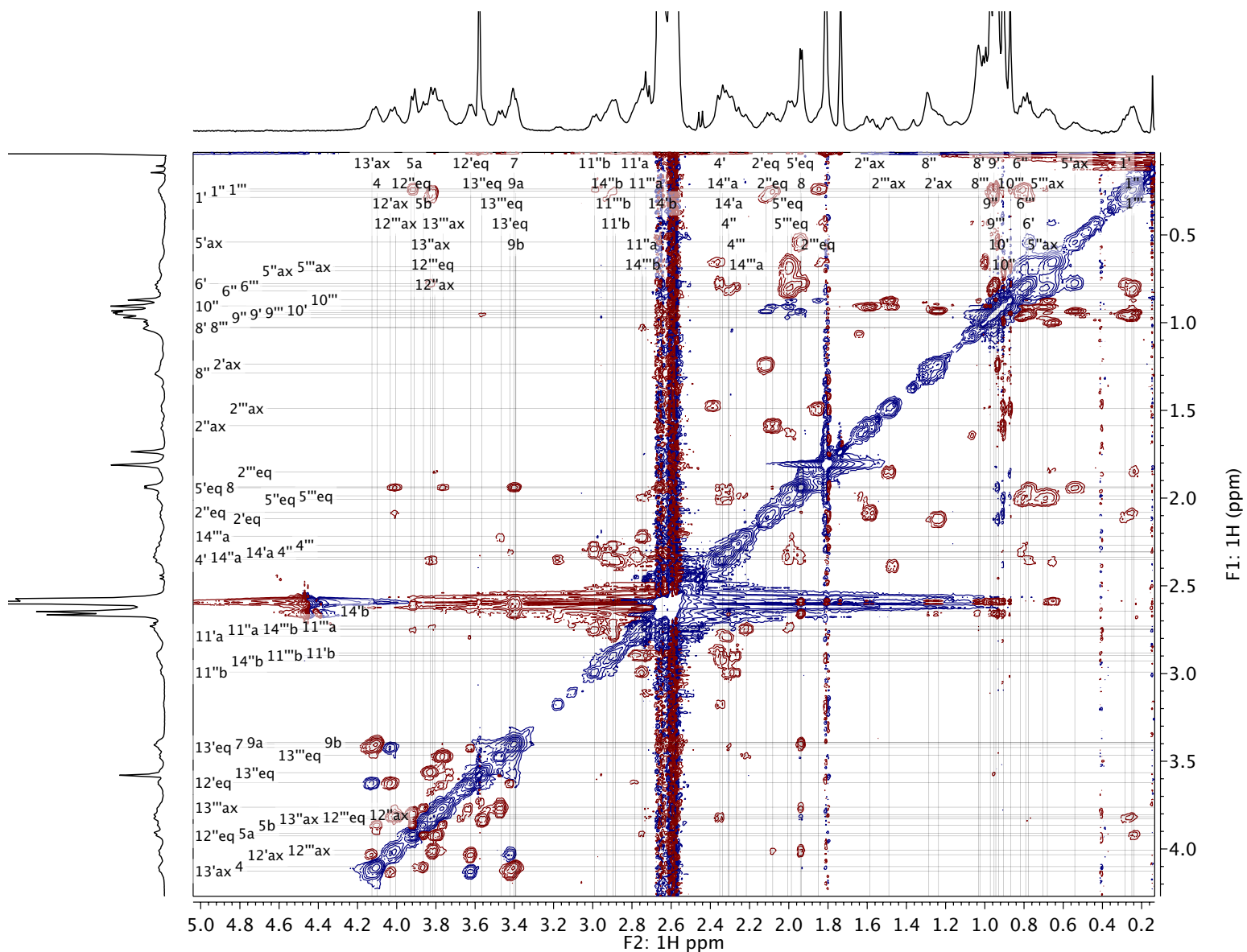


Figure 100. Expansion of ROESY spectrum of 0.10 M (*S*)-**16a** with 0.05 M HMPA in neat THF-*d*₈ -60 °C. Labels indicate assignments.

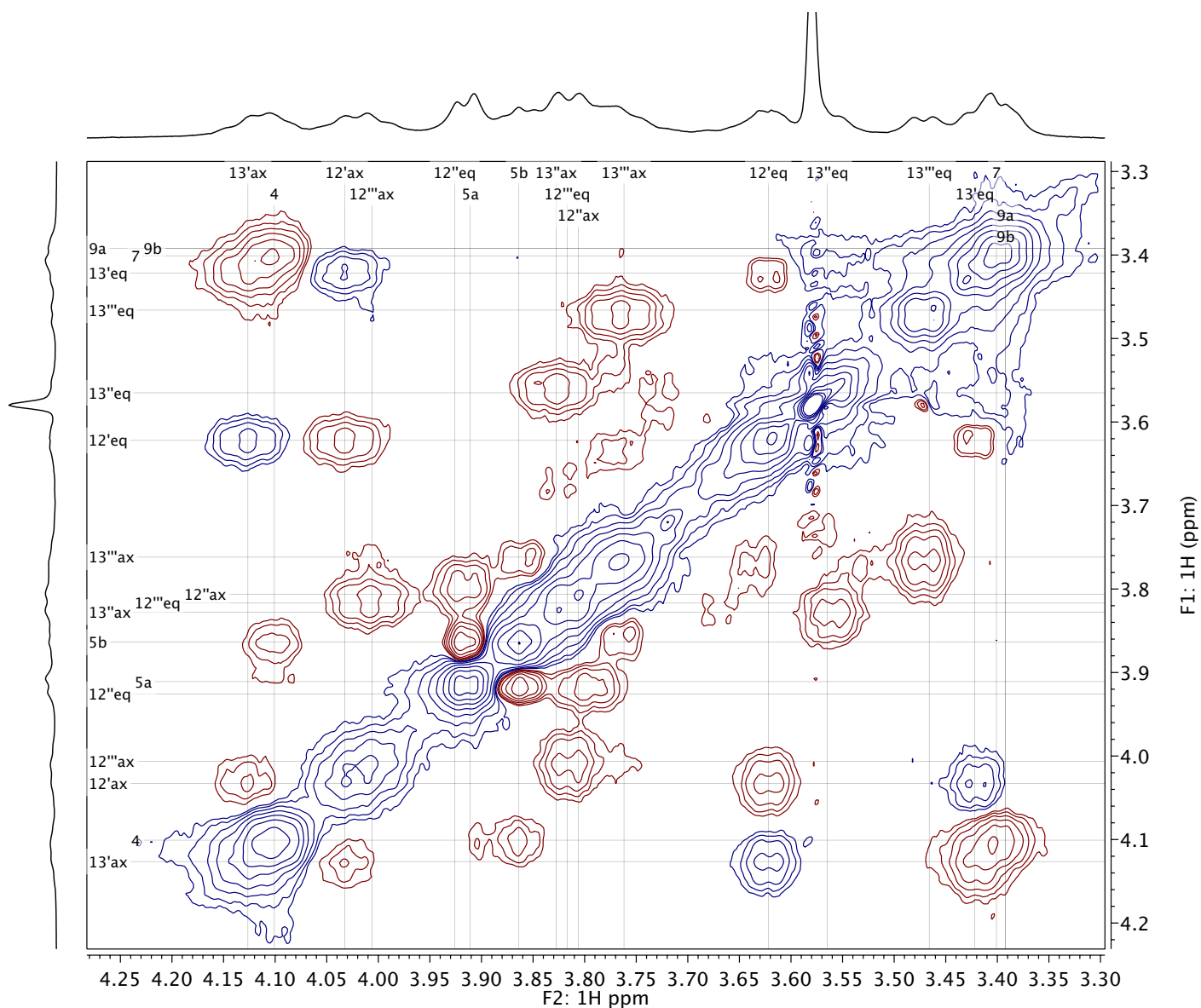


Figure 101. Expansion of the morpholine ring region in the ROESY spectrum of 0.10 M (S)-16a with 0.05 M HMPA in neat THF-*d*₈ -60 °C. Labels indicate assignments.

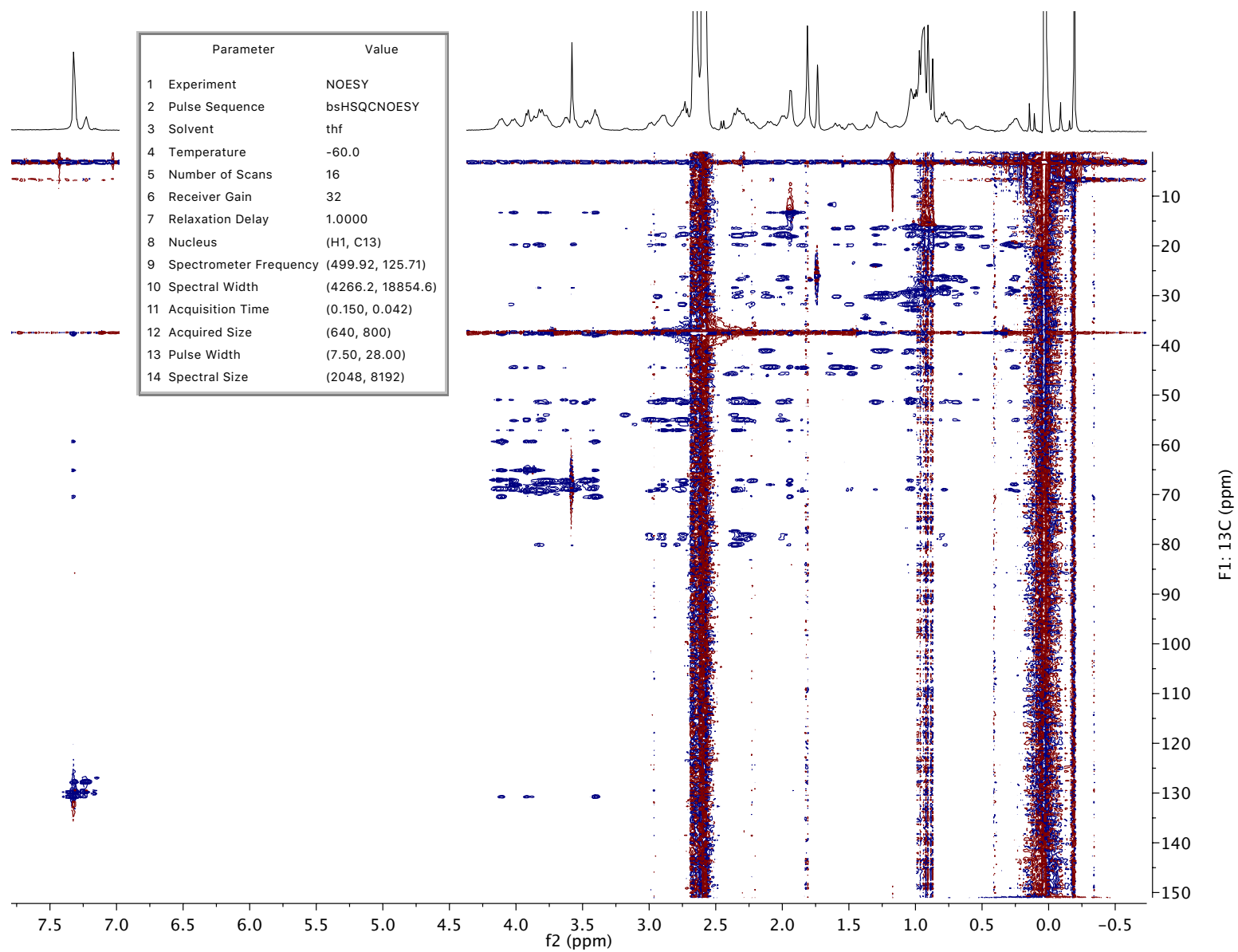


Figure 102. Full display HSQC-NOESY spectrum of 0.10 M (*S*)-**16a** with 0.05 M HMPA in neat THF-*d*₈ -60 °C.

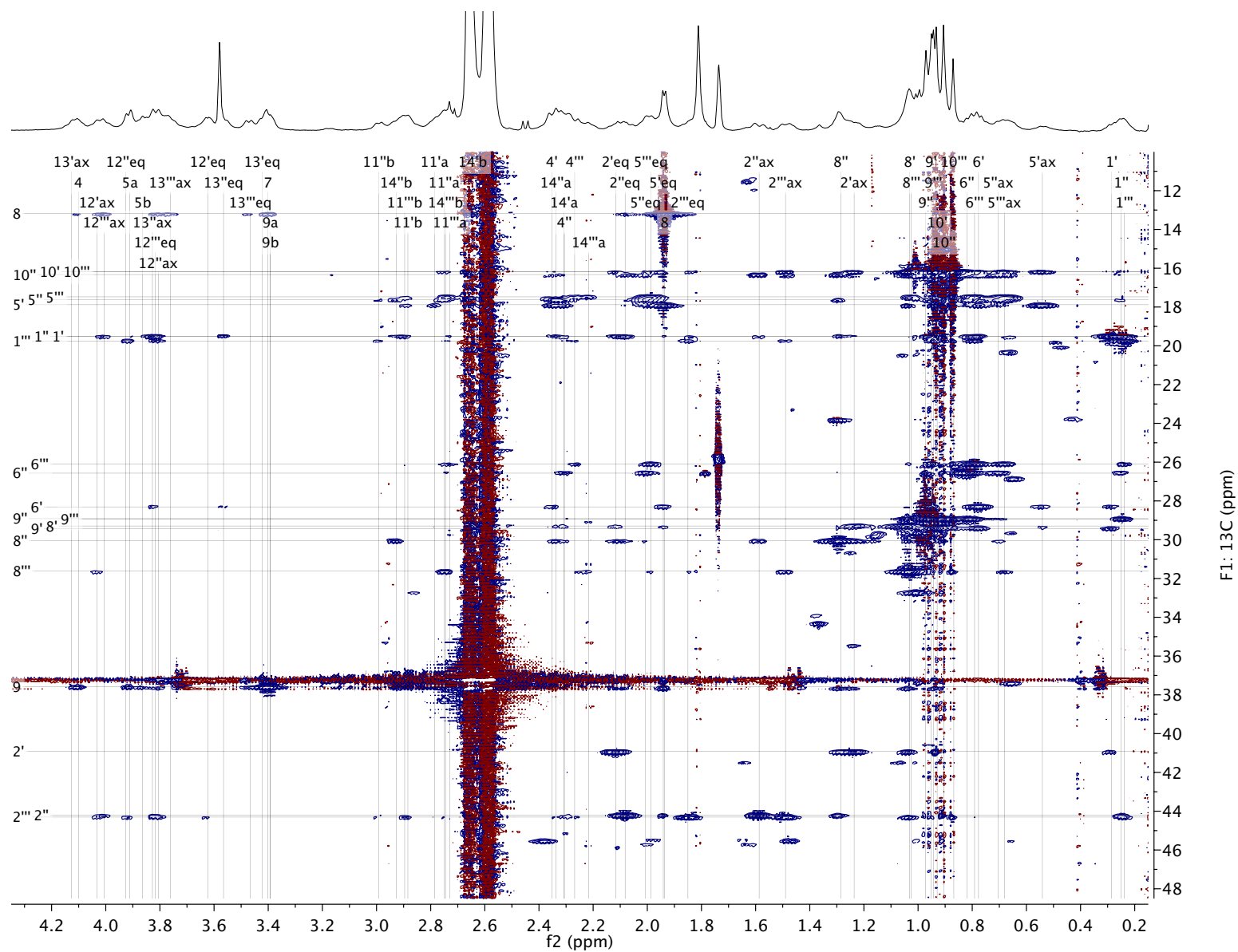


Figure 103. Expansion of HSQC-NOESY spectrum of 0.10 M (S)-16a with 0.05 M HMPA in neat THF-*d*₈ -60 °C. Labels indicate assignments.

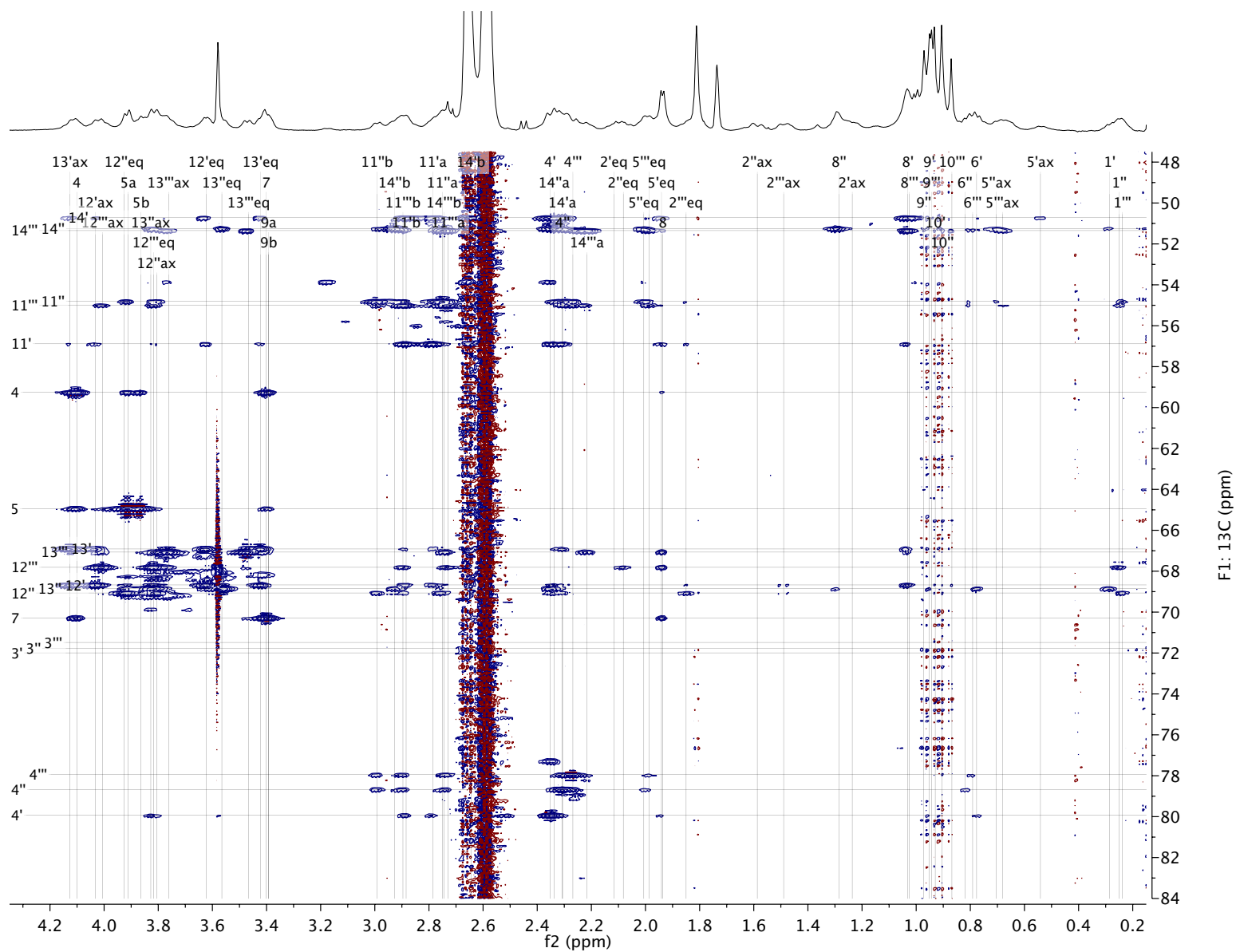


Figure 104. Expansion of HSQC-NOESY spectrum of 0.10 M (*S*)-**16a** with 0.05 M HMPA in neat THF-*d*₈ -60 °C. Labels indicate assignments.

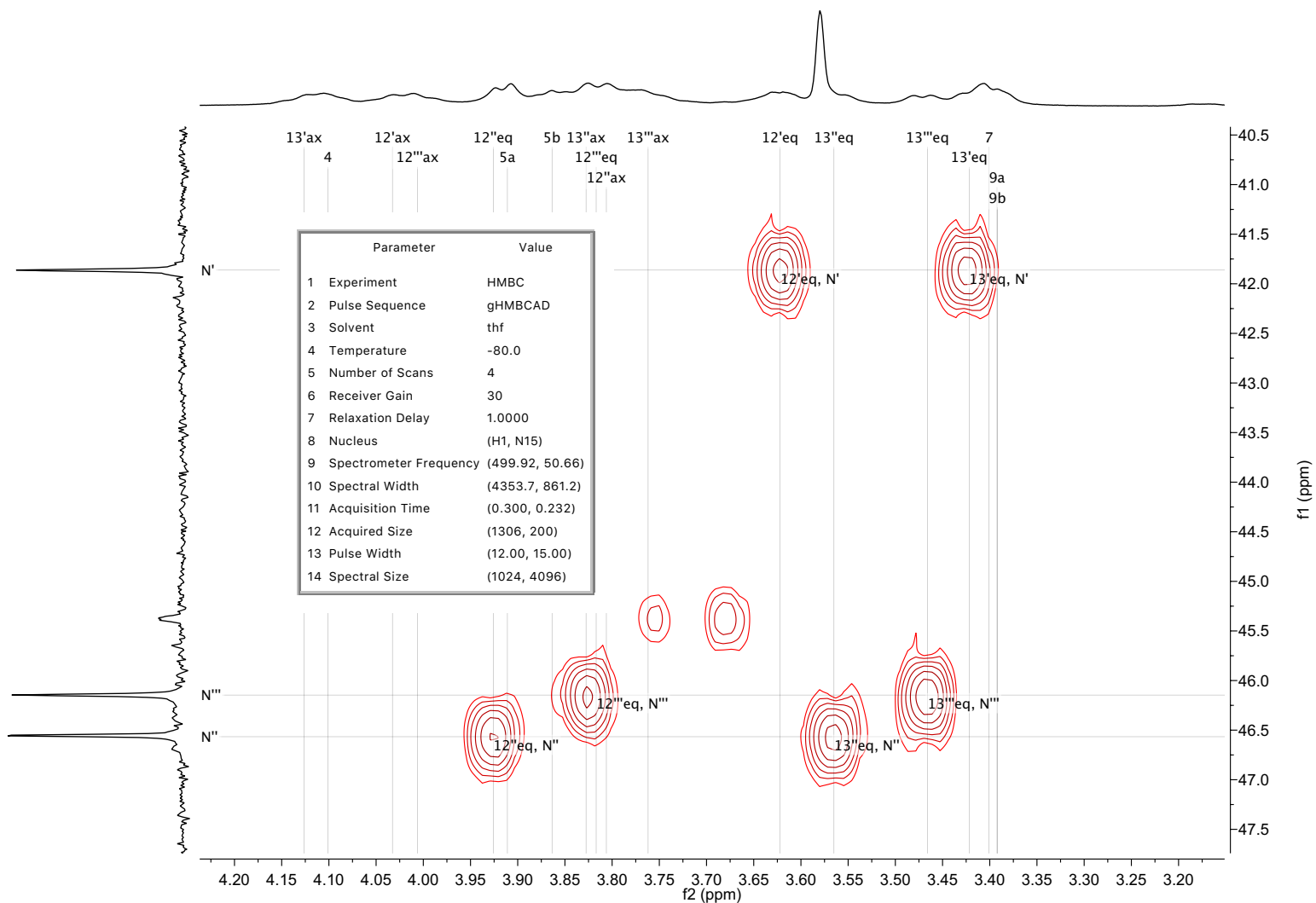


Figure 105. ^1H - ^{15}N HMBC spectrum of 0.10 M (S)-**16a** with 0.05 M HMPA in neat $\text{THF-}d_8$ -80°C . Labels indicate assignments.

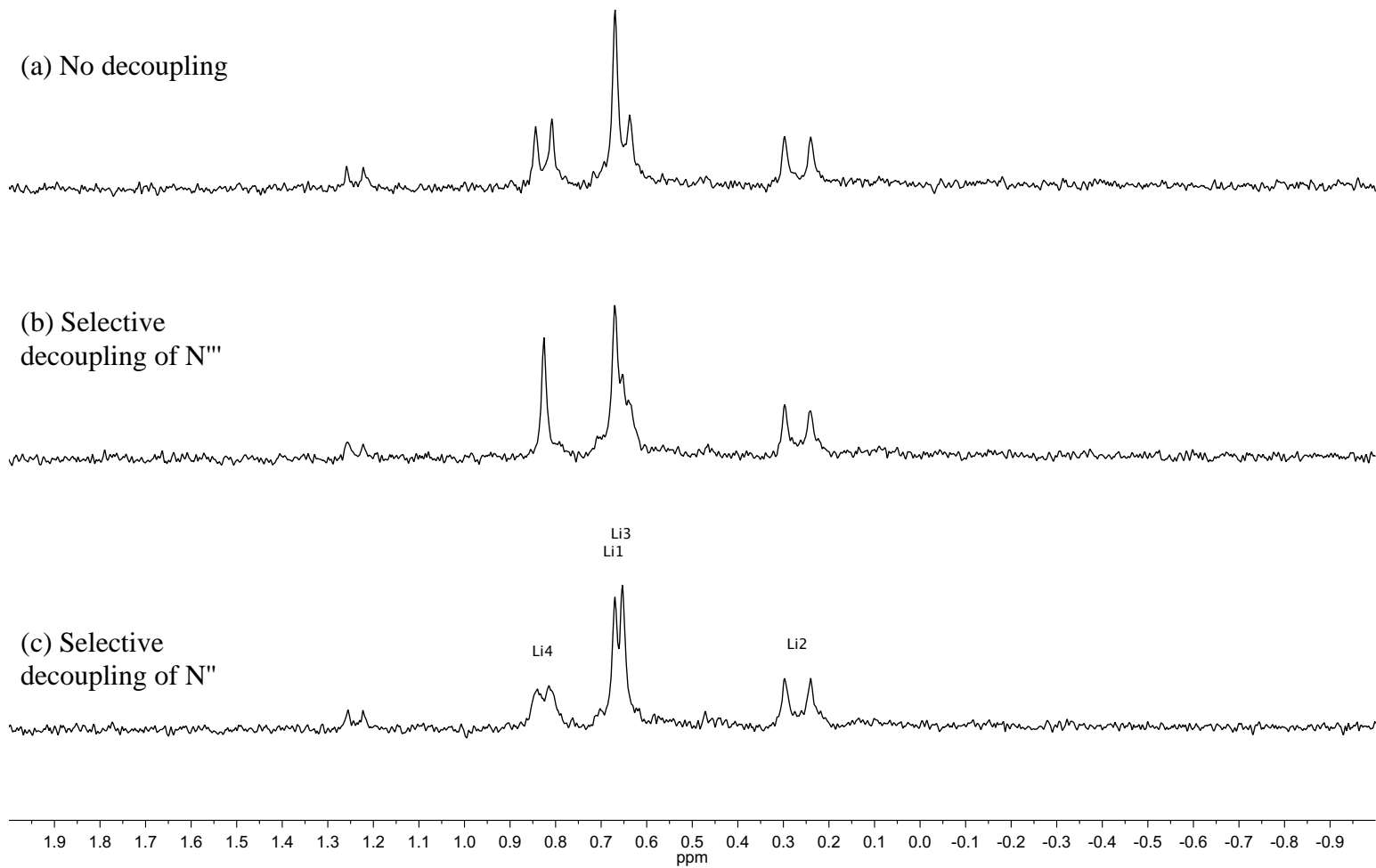


Figure 106. ^6Li NMR spectrum of 0.10 M (S)-16a with 0.05 M HMPA in neat THF- d_8 -80°C with selective decoupling on ^{15}N . Labels indicate assignments.

2D NMR analysis of 1:3 mixed aggregate (R)-16a: A sample prepared from 0.40 M [⁶Li]LiHMDS, 0.10 M (R)-1a and 0.30 M amino 11 with 0.05 M HMPA in neat THF-*d*₈, after aging at 20 °C for 10 min, was studied by standard 2D NMR techniques. All chemical shifts with the exception of quaternary C-7's in the carene amino alkoxide (CAA) residues were assigned using high field indirect-resolution 2D HSQC, HSQC-TOCSY, and HMBC experiments.

Experimental: 2D NMR spectra were acquired on a 500 MHz Varian INOVA spectrometer operating at 499.92 MHz for ¹H observation using a 5 mm Varian inverse-detect probehead with Z-axis pulsed field-gradient. Sample temperature was maintained at -60 °C as calibrated with a neat methanol sample. ¹H and ¹³C 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: All morpholine rings display four non-equivalent methylenes, however the ROESY spectrum shows exchange crosspeaks between H-12'a and H-13'b as well as H-12'b and H-13'a indicating that the morpholine fragment of CAA' undergoes rotation around C-4'-N' bond followed by a chair flip and that this process is slow on the ¹H timescale ($\Delta\nu = 270$ and 295 Hz, respectively). The 3D structure of the aggregate was derived from 2D NOESY, 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-4 and C-7. Reciprocal H-7 to C-4 correlation is also observed. The starting point for solving the structure is H-8 methyl of the enolate, which gives nOe correlations to bound HMPA, C-13'' and C-12'', as well as C-2'''. Reciprocal correlations to H-12'' and H-13'' to C-8 are also observed. This indicates that the methyl group projects over the O-1/Li-2/O-3/Li-4 face of the cube and is sandwiched between the morpholine ring of CAA'' and HMPA. Contacts with both H-12'' and H-13'' show that the N-O axis of the morpholine is perpendicular to the O-1/Li-2/O-3/Li-4 face and therefore O-3 cannot be part of CAA''. The same correlations also allow the assignment of CAA'' specifically to O-4 with N'' coordinating to Li-4 as opposed to O-2/Li-2 which would result in a close contact with the C-11''/C-12'' edge of the morpholine based on computational data. Correlations from C-4'' to H-11''' and H-4''' further support this assignment. CAA'' and CAA''' are adjacent and oriented anti-parallel to each other as evidenced by correlations between the morpholine of CAA''' and the carene fragment of CAA'' (H-11''' to C-1'') as well as the carene of CAA''' and the morpholine of CAA'' (C-1''' to H-11'') leading us to assign O-3 to CAA''' with N''' coordinating to Li-3. CAA' contributes O-2 and is oriented so the morpholine is proximal to Li-1 and the carene is adjacent to HMPA as determined by correlation between HMPA and H-8'. HMPA is bound to Li-2 and is sitting in a "cavity" defined by the *Si* face of the enolate, C-8', C-2' and C-8''.

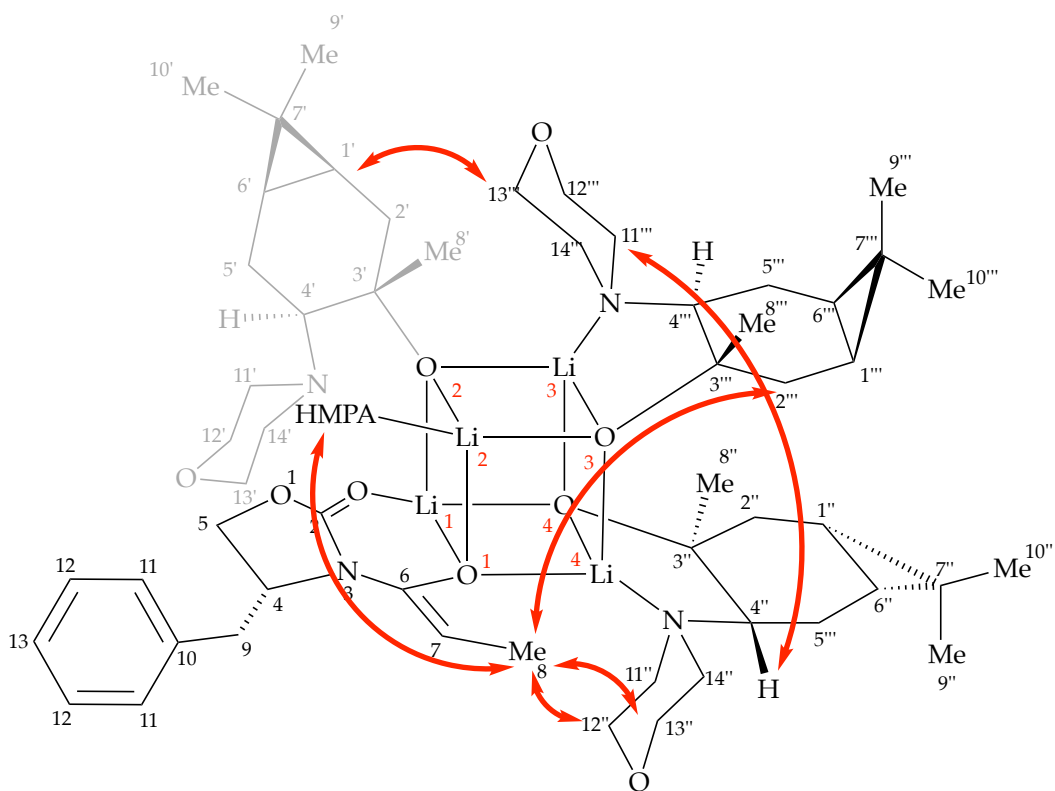


Table 4. ¹H and ¹³C chemical shift assignments for mixed aggregate (**R**)-**16a** at –60 °C

Atom	δC, ppm	δH, ppm	HMBC	HSQC-TOCSY	ROESY	HSQC-NOESY
1' C	19.35	0.27	10',6',2',5',9'	6',2'	6',10',2'	12'''b,13''',10',6'
1'' C	19.3	0.26	10'',6'',2'',5'',9''	6'',2''	6'',10'',2''	10'',6''
1''' C	19.14	0.26	10''',6''',2''',5''',9'''	6''',2'''	6''',10''',2'''	12'',11''b,2''a,10''',6'''
2 C	155.66	–	5a			
2' C	40.82	1.23(a)	1',6',3'	6',1'	2'b,9'	8',9'
		2.12(b)			2'a	
2'' C	44.2	1.52(a)	1'',6'',3''	6'',1''	2''b,9''	12''',12'',8'',9'',2''
		1.88(b)			2''a	
2''' C	43.98	1.58(a)	1''',6''',3'''	6''',1'''	8,2'''a,9'''	8,8''',9''',2'''
		2.09(b)				
3' C	71.68	–	2',4'			
3'' C	71.21	–	2'',4'',5''			
3''' C	71.41	–	2''',4'''			
4 C	58.45	4.18	9	9,5	5,7,9	5,7,9
4' C	79.57	2.34	5',3',11',14'	5'	13'''b,11',6',5'	11',5'
4'' C	78.46	2.29	5'',3'',11'',14''	5''	11'',11''',6'',5''	11'',11''',5'',4'''
4''' C	77.82	2.28	5''',3''',11''',14'''	5'''	11''',11'',6''',5'''	11''',5''',4''
5 C	64.43	3.94(a)	2,4,9	4,9	4,9	4
		3.94(b)				
5' C	17.62	0.53(a)	4',1',6',3'	4',6'	5'b,9'	4',6'
		1.94(b)			5'a,6',11'a	
5'' C	17.28	0.72(a)	4'',1'',6'',3''	4'',6''	5''b,9''	4'',14'',8'',6''
		2.00(b)			5''a,6'',11''a	
5''' C	17.4	0.70(a)	4''',1''',6''',3'''	4''',6'''	5'''b,9'''	14''',11''',4''',8''',6'''
		2.01(b)			5'''a,6''',11'''a	
6 C	152.2	–	7,8			
6' C	27.93	0.77	9',1',10',2'	4',2'	13''',4',5',10',1'	10'
6'' C	25.87	0.8	9'',1'',10'',2''	4'',2''	4'',5'',10'',1''	4''',5'',10'',6''
6''' C	26.24	0.81	9''',1''',10''',2'''	4''',2'''	4''',5''',10''',1'''	4''',5''',10''',6'''
7 C	70.63	3.44	8,6	8	4,5a,8	4,8
7' C	–	–				
7'' C	–	–				
7''' C	–	–				
8 C	12.83	1.93	7,6	7	4,12'',7,2'''b	12'',13'',7,HMPA,2'''b
8' C	29.16	1.01	3',4'			14',11',2',9'

8" C	31	1.12	3",4"		14"	14",2",9"
8" C	29.69	1.29	3",4"		14"	14",2",2"b,9"
9 C	38.17	2.41(a)	4,5,10,11	4,5	11,12,5,7,9b	11,4,5,13",7
		3.38(b)			9a	
9' C	15.89	0.92	10',6'	10'	2',5',8',10',1'	2',5',8'
9" C	15.93	0.9	10",6"	10"	2",5",8",10",1"	2",5",8"
9" C	16.05	0.91	10",6"	10"	2",5",8",10",1"	2",5",8"
10 C	137.95	–	9,11,12			
10' C	29.09	0.95	9',1',6'	9'	1',6',5'b	9',6',1'
10" C	28.61	0.95	9",1",6"	9"	1",6",5'b	9",6",1"
10" C	28.62	0.97	9",1",6"	9"	1",6",5"b,13" a	9",6",1"
11 C	130.1	7.29	9,10,12,13	12,13	12,13,4,5,7,9a	12,4,5,9
11' C	56.58	2.79(a)	4'	12'	12',11'b,4'	12',4',5'
		2.89(b)			11'a	
11" C	54.72	2.75(a)	4"	12"	12",13",11"b,4"	12",13",4",5",1"
		2.88(b)			11"a	
11" C	54.65	2.75(a)	4"	12"	12",13",11"b,4"	12",13",4",5",1"
		3.00(b)			11"a	
12 C	129.4	7.32	10,11,13	11,13	11,13	11,13
12' C	68.45	3.64(a)	13'	11'	13'b,12'b,13'a,11'a	12'b,13',11',8"
		4.02(b)			13'a,12'a,13'b,11'b	12'a
12" C	67.67	3.83(a)	13"	11"	12"b,11"a	12"b,13",11",8,2"
		4.01(b)			12"a,2"b,11"b,8	12"a
12" C	68.78	3.80(a)	13"	11"	12"b	12"b,13",11",4",2"
		3.92(b)			12"a	12"a
13 C	127.41	7.23	10,11,12	11,12	11,12	12
13' C	66.63	3.42(a)	12'	14'	12'b,13'b,12'a,14'a	13'b,12',14',8"
		4.18(b)			12'a,13'a,12'b	13'a
13" C	67.06	3.45(a)	12"	14"	12"b,13"b,14"a	13"b,12",14",8
		3.82(b)			13"a	13"a
13" C	68.6	3.56(a)	12"	14"	13"b,12"a,14"a	13"b,12",14",10',6',1'
		3.83(b)			13"a,14"b,6'	13"a
14' C	50.47	2.30(a)	4'	13'	8',13'a,11'b,14'b	13',11',5',8'
		2.65(b)			14'a,13'a,5'b	
14" C	50.77	2.24(a)	4"	13"	8",13"a	13",11",5",8"
		2.80(b)			11"b,5"b	
14" C	50.95	2.34(a)	4"	13"	8",13"b,12"a	13",11",5",8"
		2.92(b)			11"a,5"b	

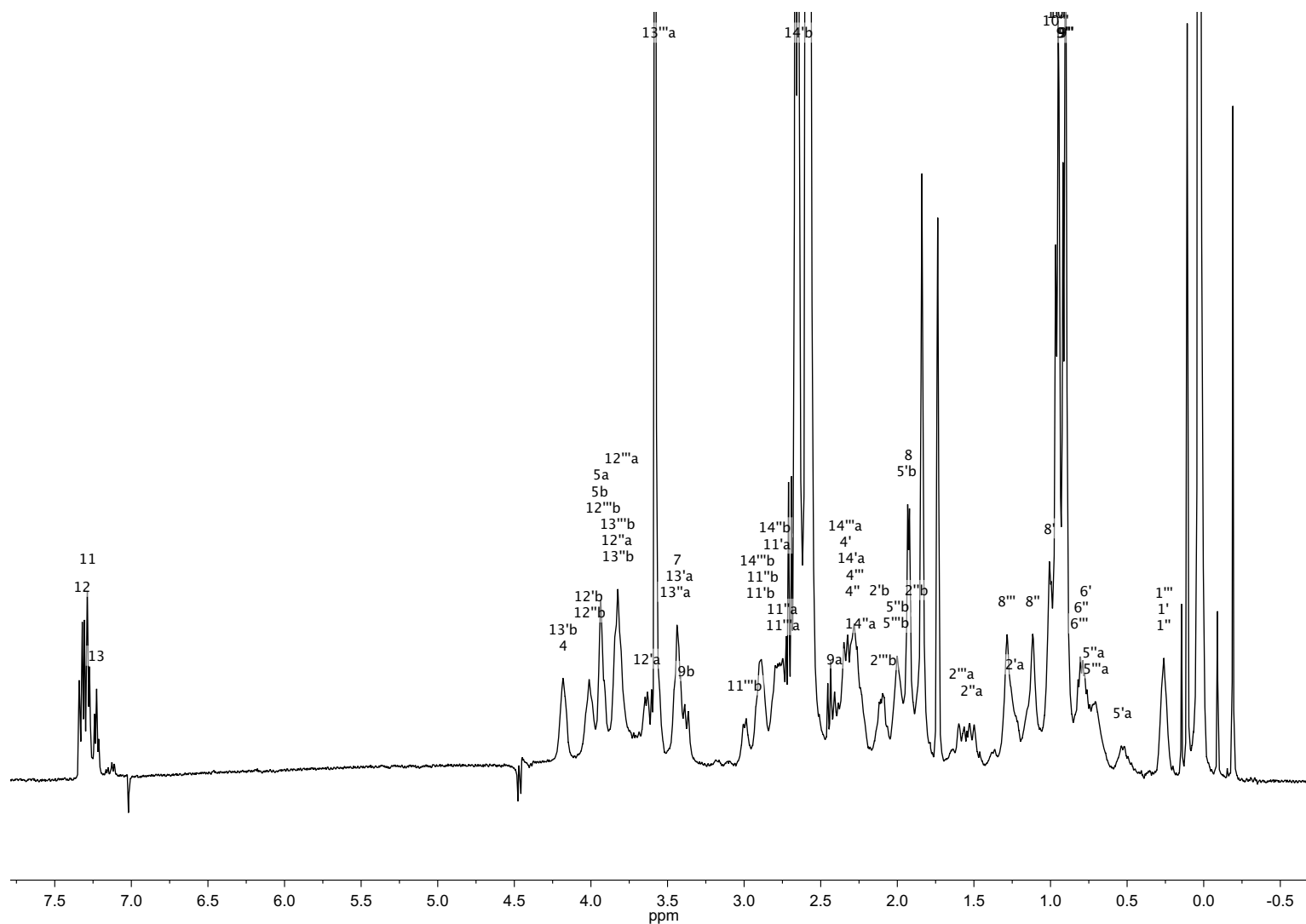


Figure 107. ^1H NMR spectrum of 0.10 M mixed aggregate (*R*)-**16a** with 0.05 M HMPA in neat $\text{THF-}d_8$ $-60\text{ }^\circ\text{C}$. Labels indicate assignments by 2D NMR.

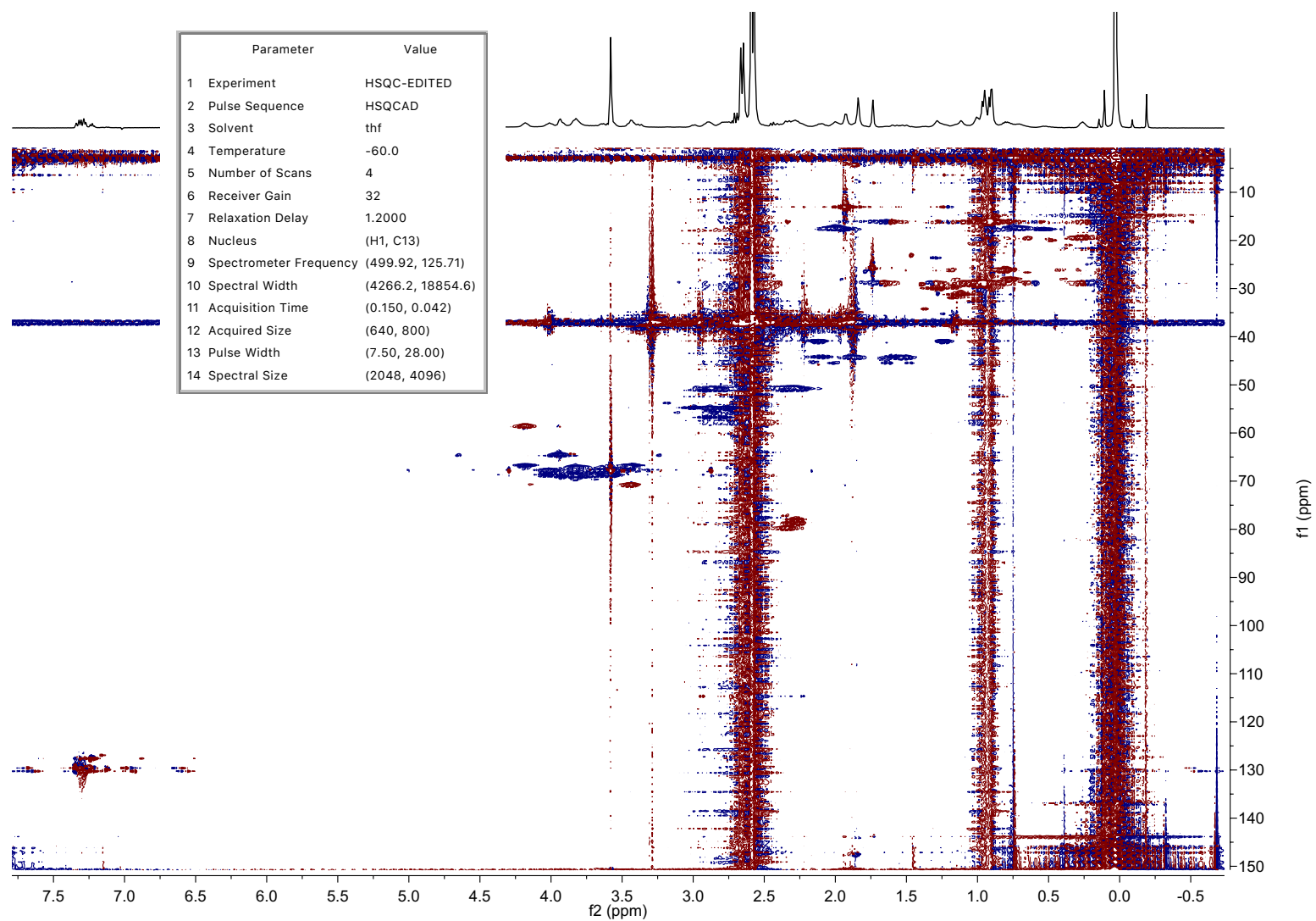


Figure 108. Full display HSQC spectrum of 0.10 M (*R*)-**16a** with 0.05 M HMPA in neat THF-*d*₈ -60 °C.

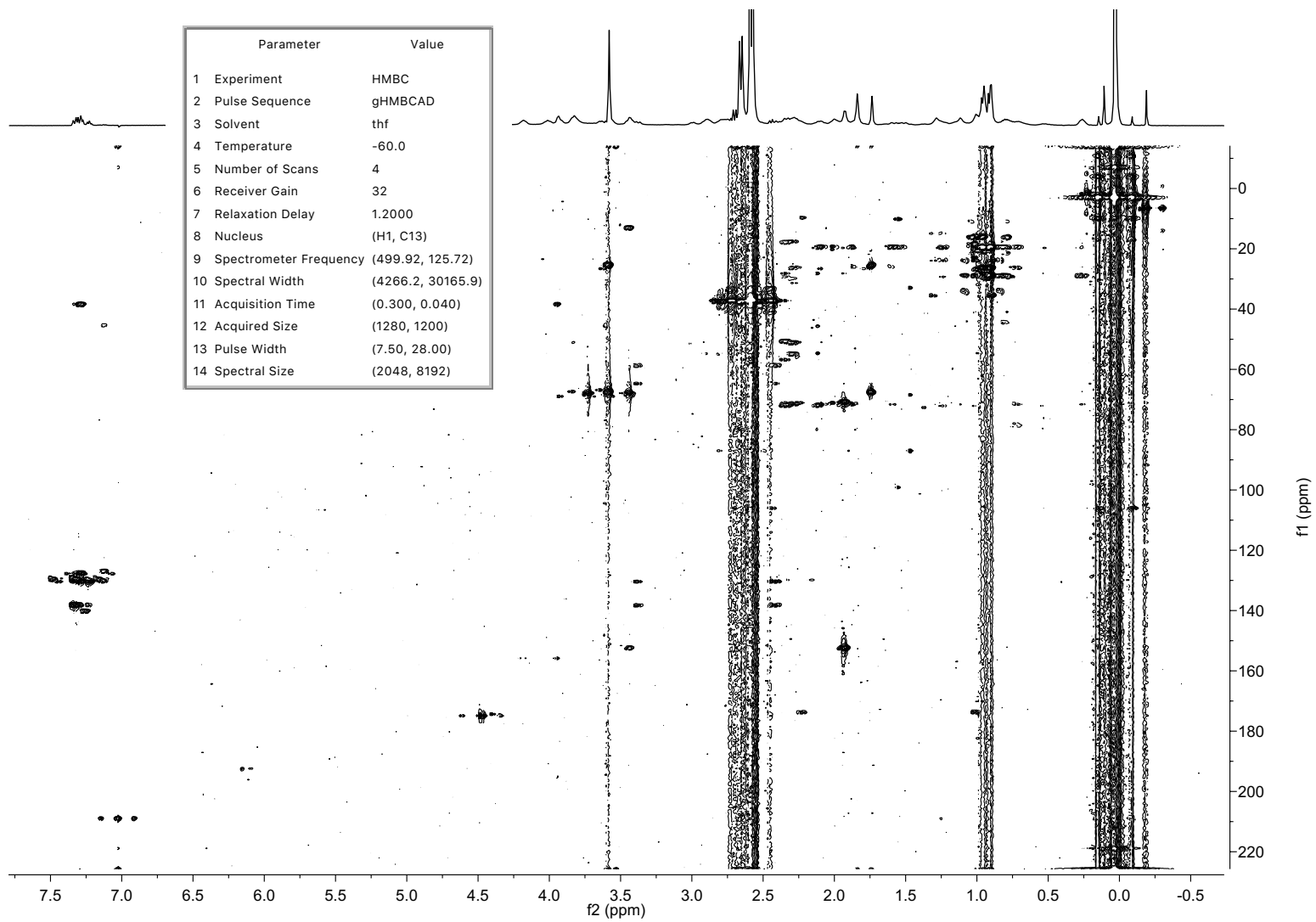


Figure 111. Full display HMBC spectrum of 0.10 M (*R*)-**16a** with 0.05 M HMPA in neat THF-*d*₈ -60 °C.

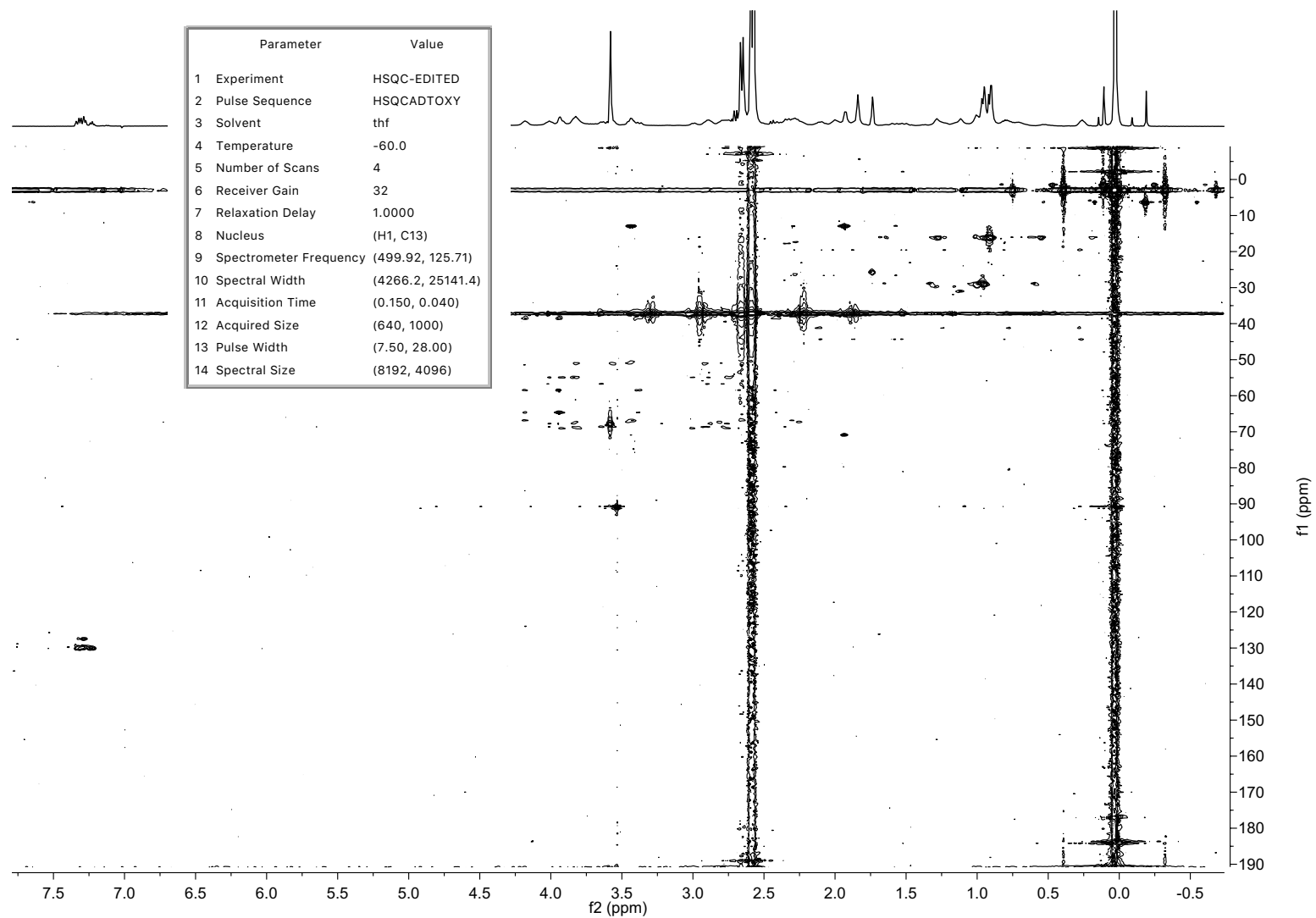


Figure 113. Full display HSQC-TOCSY spectrum of 0.10 M (*R*)-**16a** with 0.05 M HMPA in neat THF-*d*₈ -60 °C.

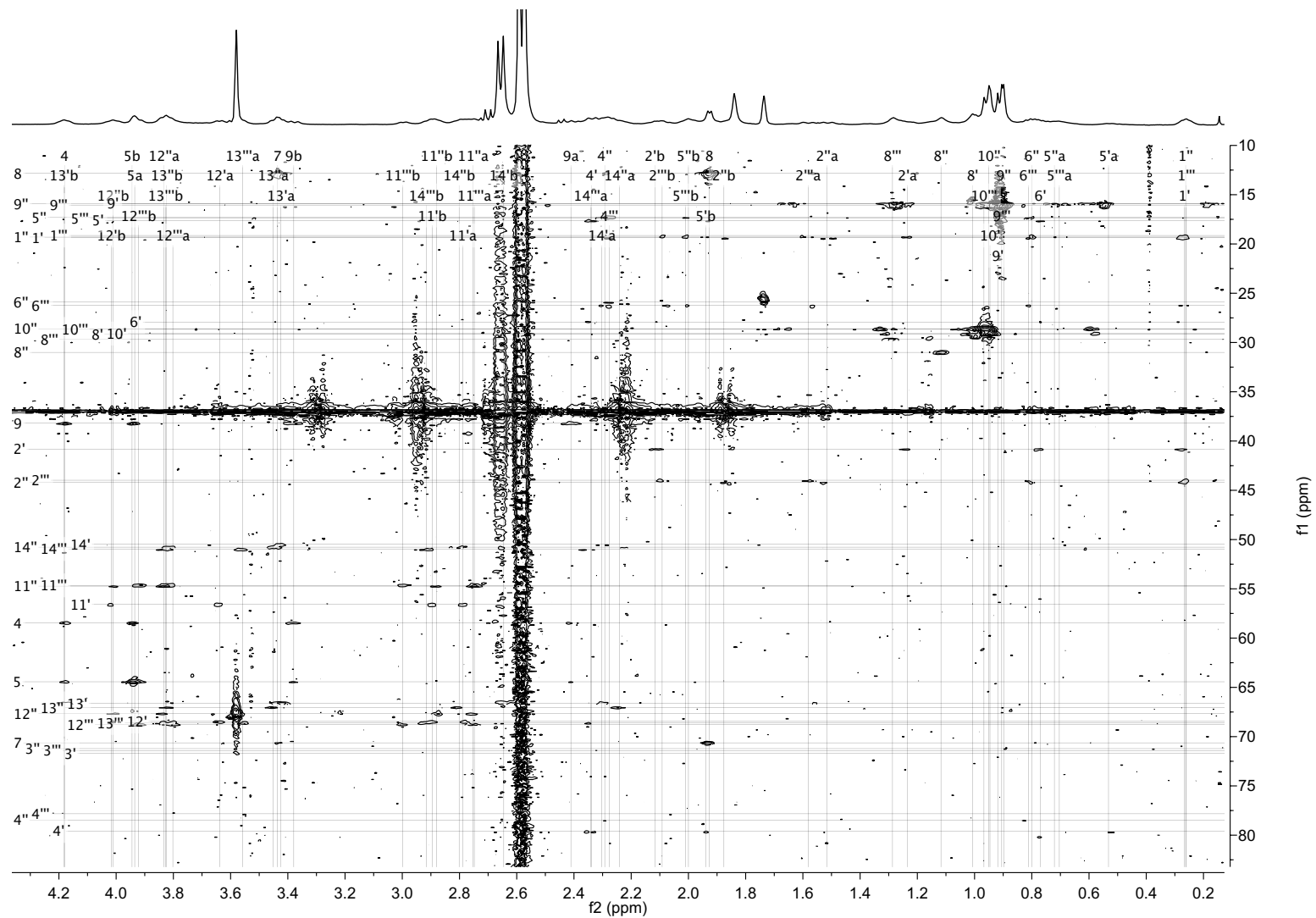


Figure 114. Expansion of HSQC-TOCSY spectrum of 0.10 M (*R*)-**16a** with 0.05 M HMPA in neat THF-*d*₈ -60 °C. Labels indicate assignments.

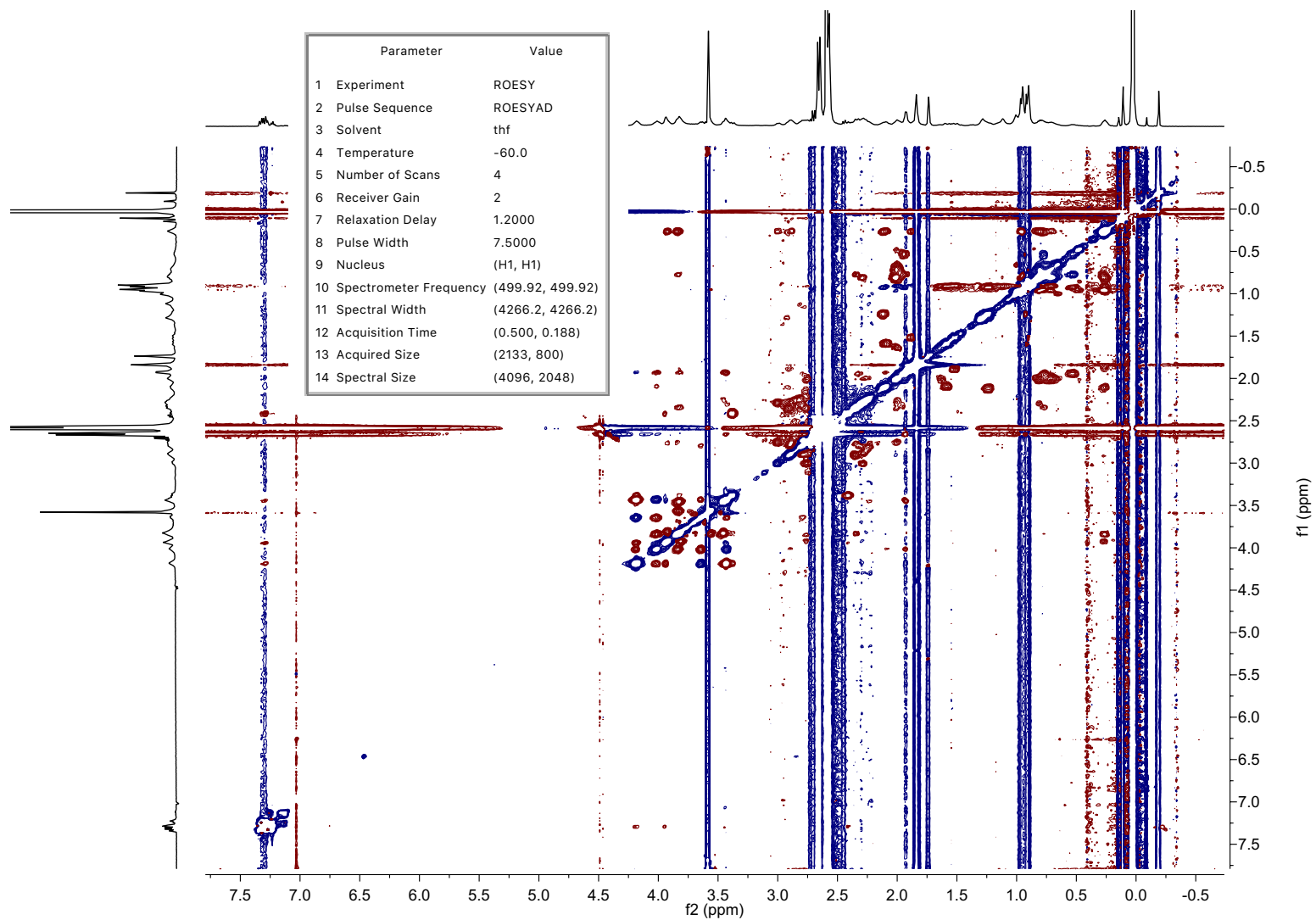


Figure 115. Full display ROESY spectrum of 0.10 M (*R*)-**16a** with 0.05 M HMPA in neat THF-*d*₈ -60 °C.

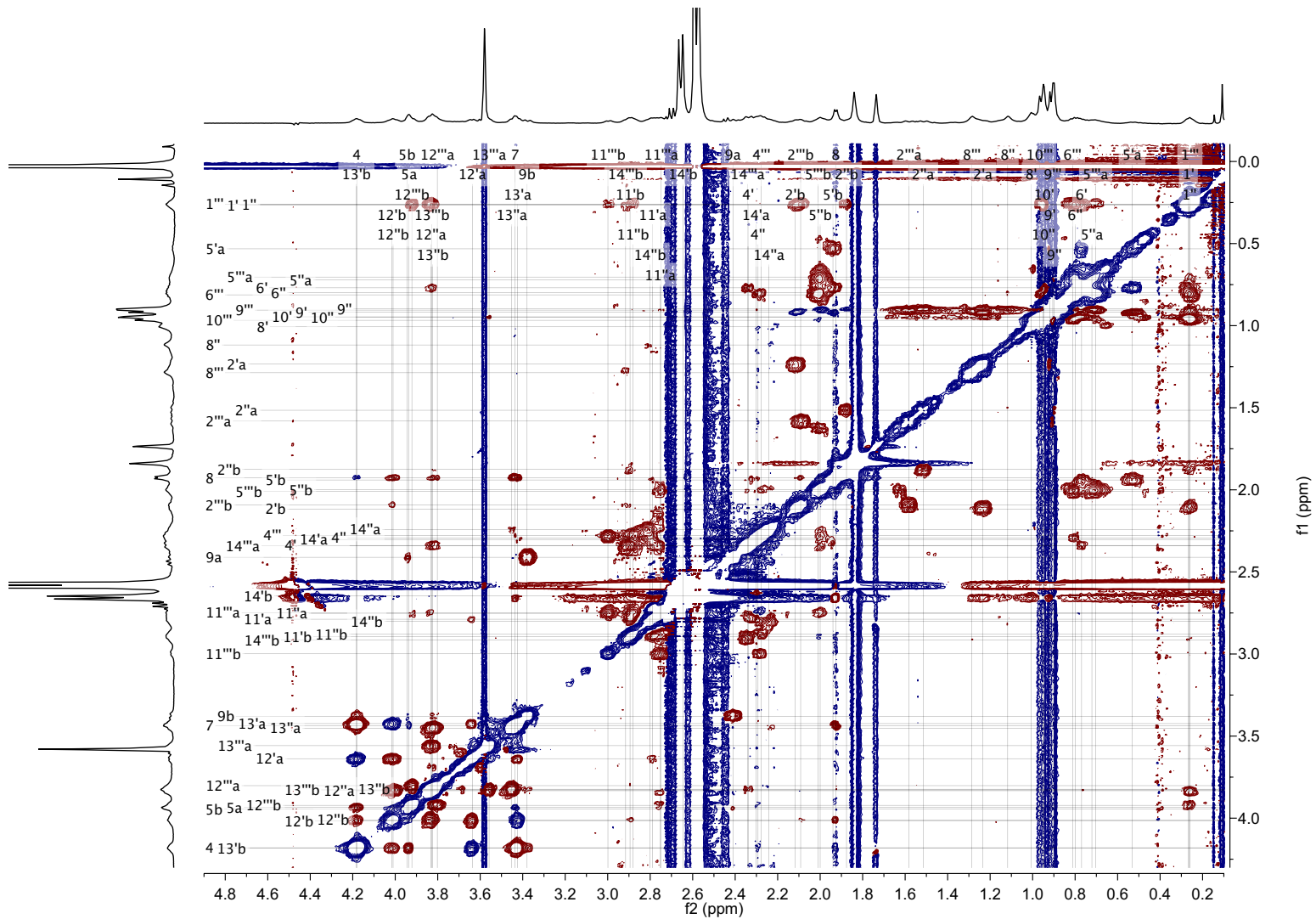


Figure 116. Expansion of ROESY spectrum of 0.10 M (*R*)-**16a** with 0.05 M HMPA in neat THF-*d*₈ -60 °C. Labels indicate assignments.

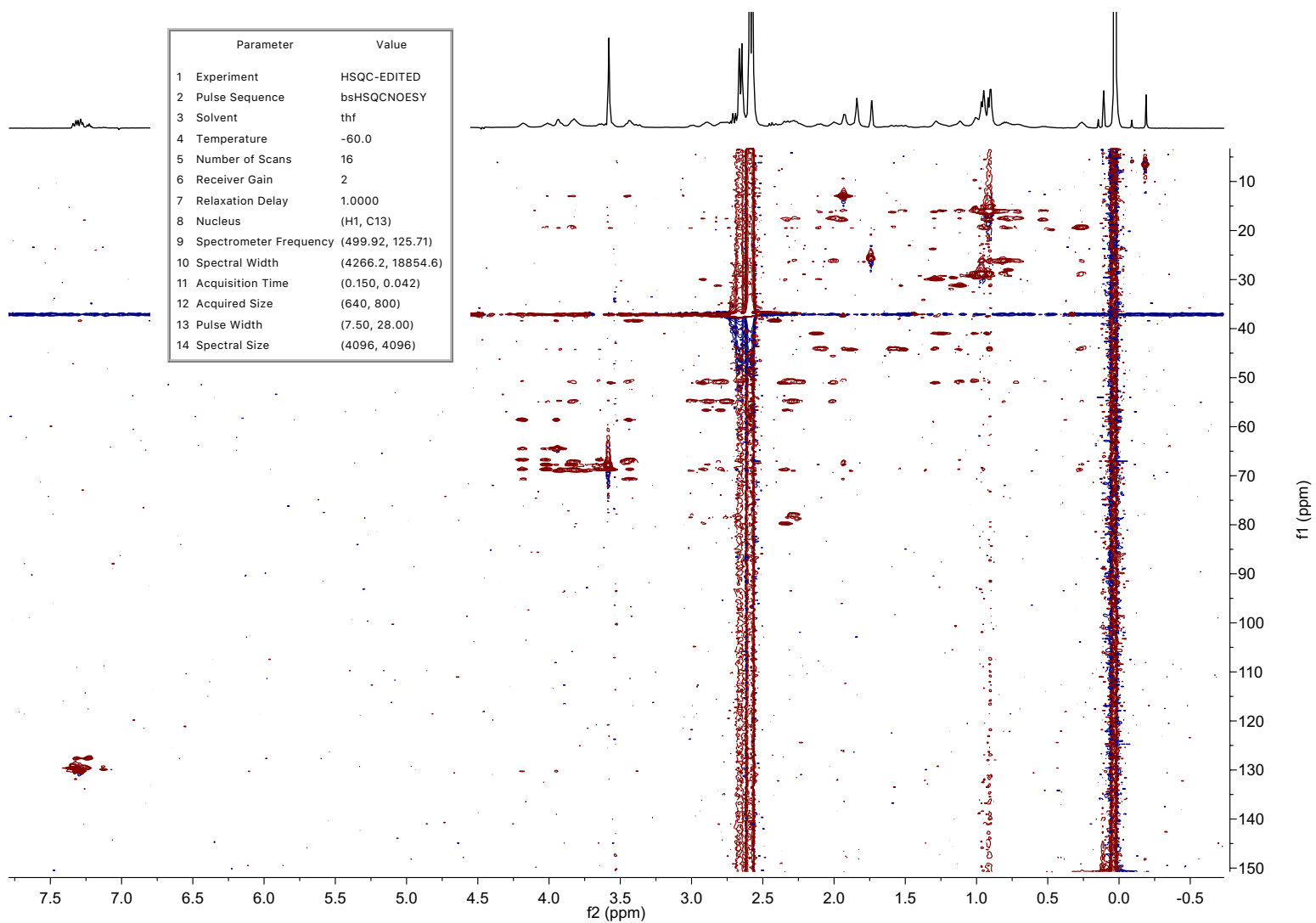


Figure 118. Full display HSQC-NOESY spectrum of 0.10 M (**R**)-**16a** with 0.05 M HMPA in neat THF- d_8 -60 °C.

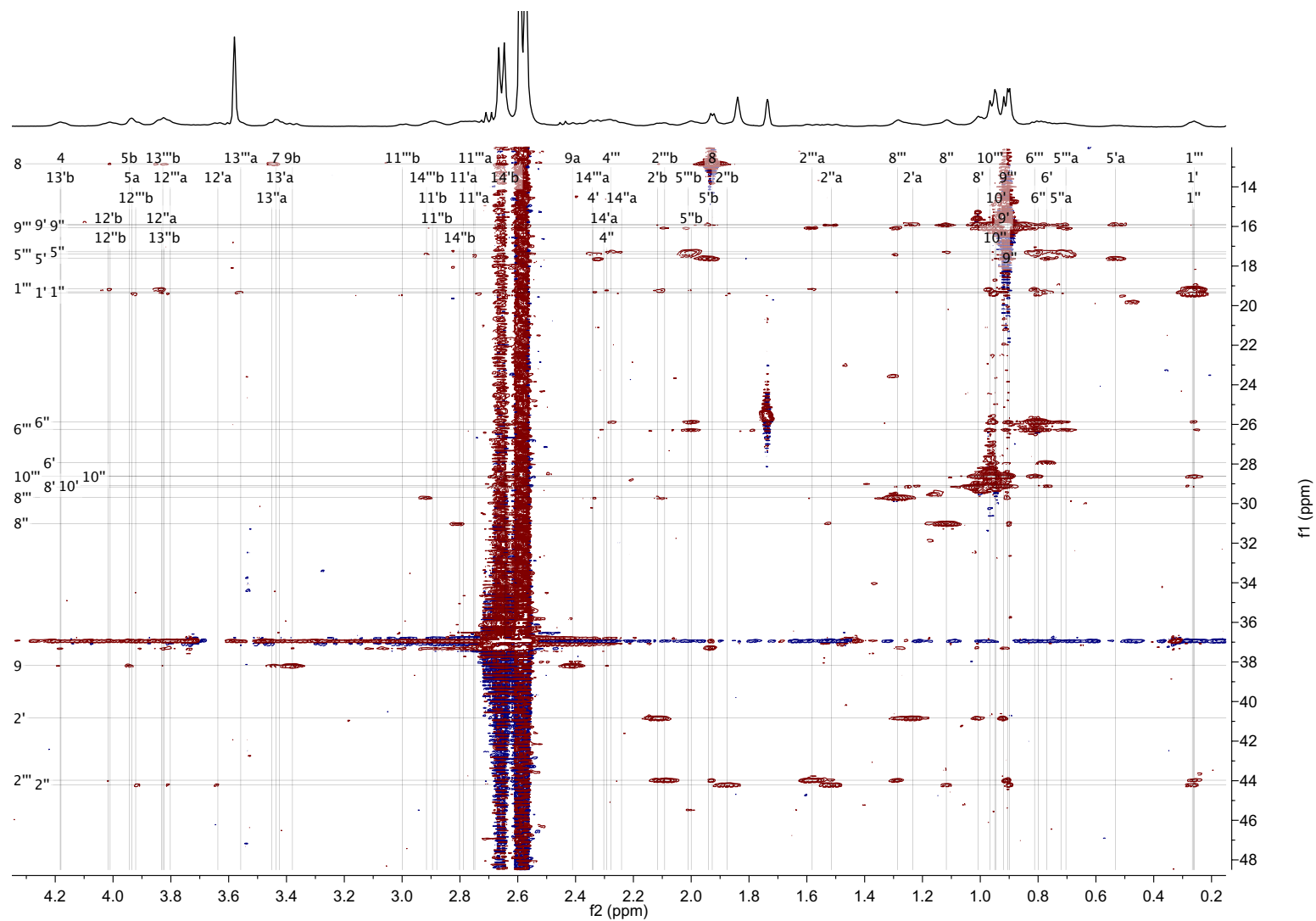


Figure 119. Expansion of HSQC-NOESY spectrum of 0.10 M (*R*)-**16a** with 0.05 M HMPA in neat THF-*d*₈ -60 °C. Labels indicate assignments.

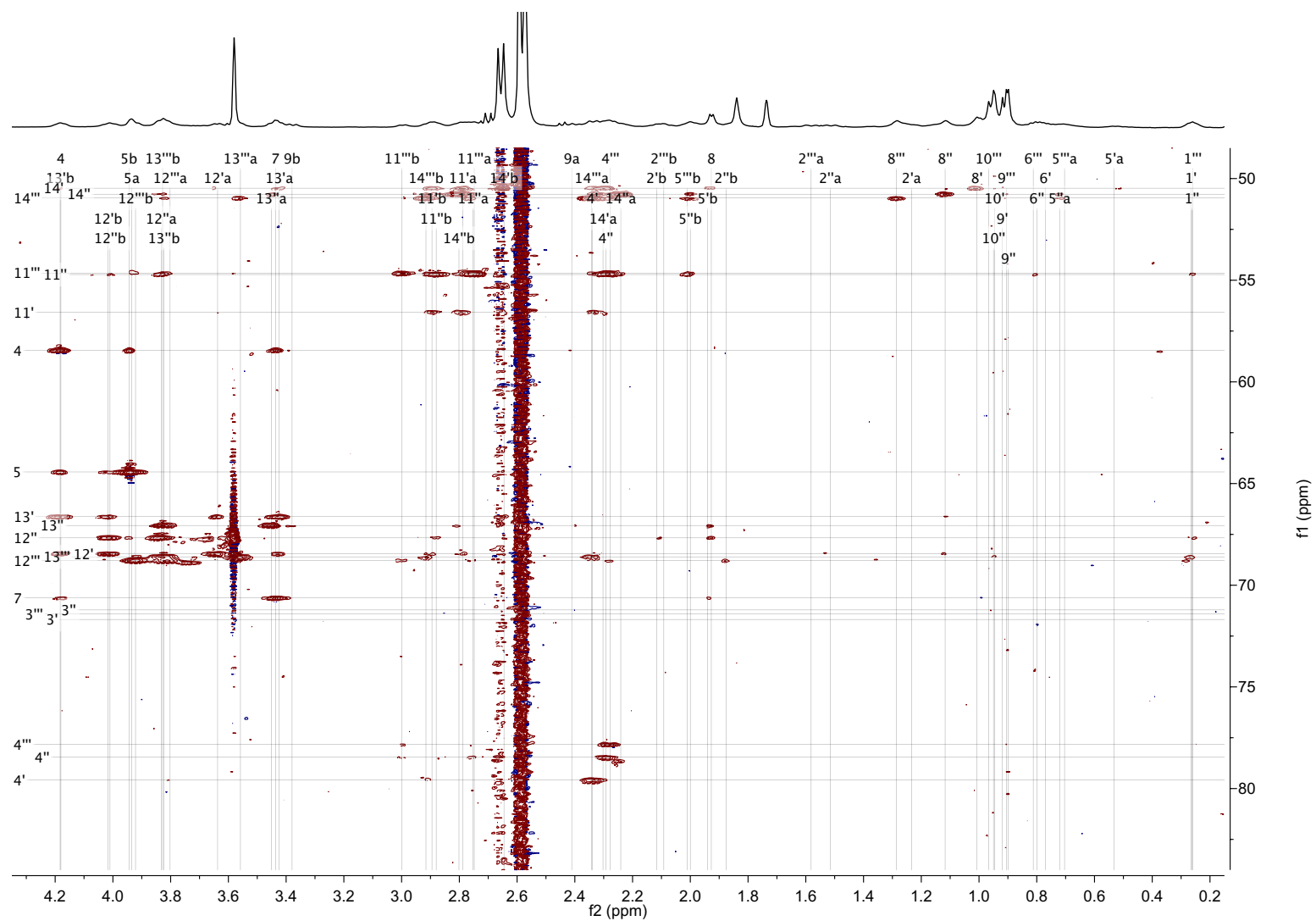


Figure 120. Expansion of HSQC-NOESY spectrum of 0.10 M (*R*)-**16a** with 0.05 M HMPA in neat THF-*d*₈ –60 °C. Labels indicate assignments.

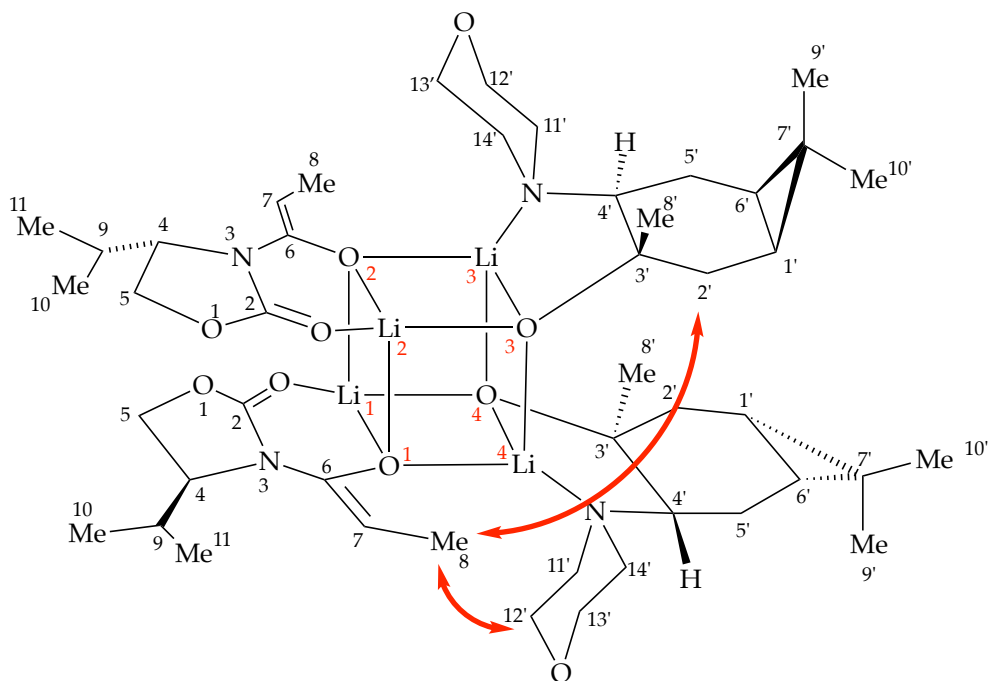


Table 5. ^1H and ^{13}C chemical shift assignments for mixed aggregate (*S*)-**15b** at $-40\text{ }^\circ\text{C}$.

Atom	δC , ppm	δH , ppm	HMBC	HSQC-TOCSY	HSQC-NOESY
1' C	18.22	0.81	6',9',10'	2',4',5',6'	2',6',10',8'
2 C	156.28	–	5b	–	–
2' C	43.11	1.84(a) 2.48(b)		1',6'	8,10',8',9',1'
3' C	69.83	–	8',2'	–	–
4 C	59.10	3.32	10,5	5	11,7,9,5,8
4' C	75.85	2.55	2',8'	5'	11',2',5',6'
5 C	59.68	2.76(a) 3.14(b)	4	4	11,4,9,10
5' C	16.25	0.70(a) 1.88(b)	1',3'	1',6',4'	11',14',4',2',8',9'
6 C	149.52	–	7,8	–	–
6' C	25.12	0.74	1',9',10'	2',4',5',1'	4',1',5'
7 C	71.69	3.37	6,8	8	4,9,8
7' C	–	–			
8 C	10.29	2.12	6,7	7	12',7',2'
8' C	31.04	1.18	2',3',4'		13',14',2',9',5'
9 C	25.73	2.11	10,11,5	10,11	7,4,10,11
9' C	15.25	1.03	1',10'	10'	2',8',10'
10 C	13.14	0.65	4,11,9	9,11	11

10' C	27.78	0.93	1',9',6'	9'	9',1'
11 C	17.10	0.26	10,9	9,10	10
11' C	53.65	2.63(a)	4'	12'	12',4',5',14'
		2.74(b)			
12' C	67.45	3.81(a)	11'	11'	13',11',8
		3.94(b)			
13' C	66.52	3.73(a)	–	14'	12',14'
		3.75(b)			
14' C	49.06	2.23(a)	4'	13'	13',11',8',5'
		2.55(b)			

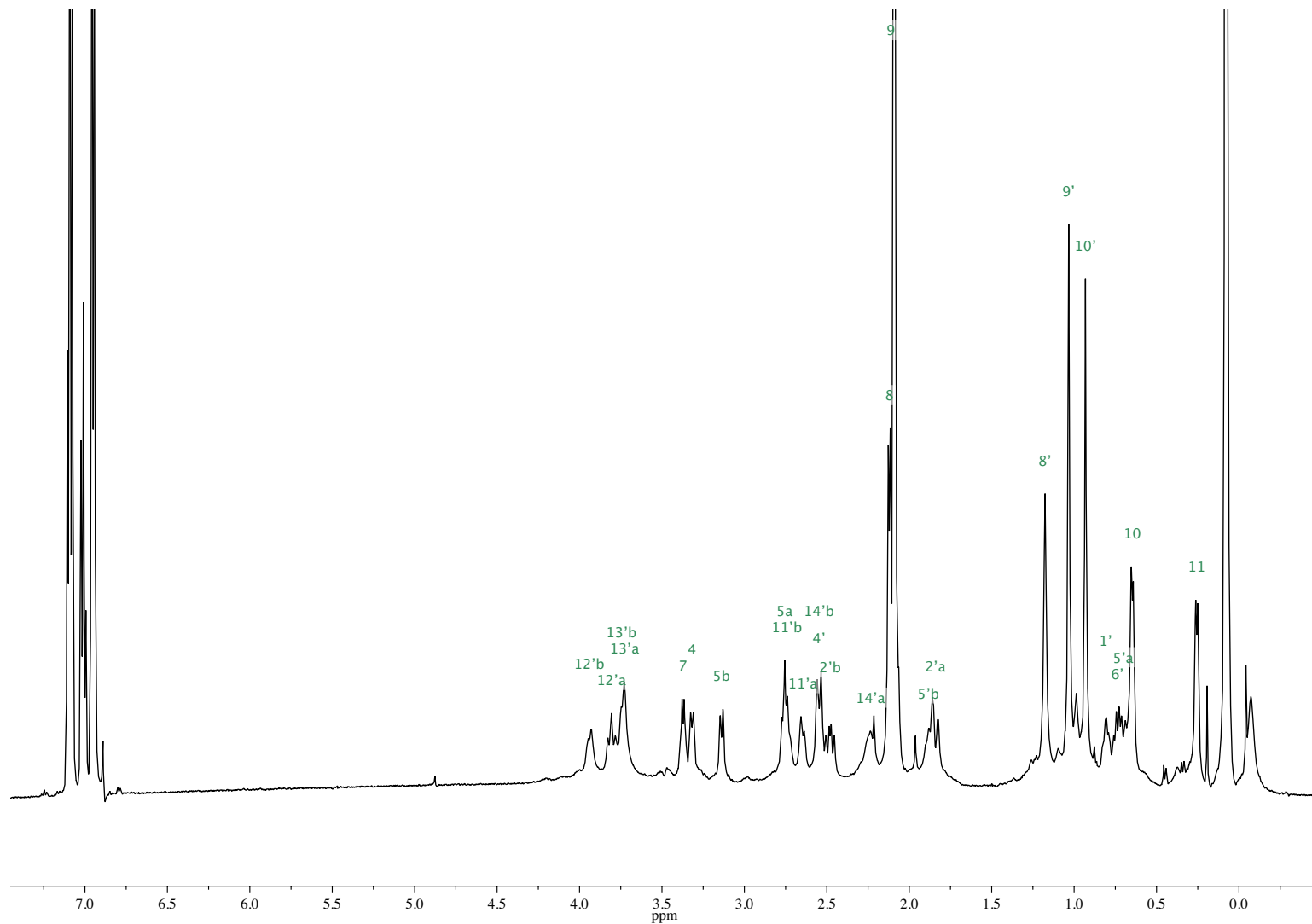


Figure 121. ¹H NMR spectrum of 0.10 M mixed aggregate (*S*)-**15b** in neat toluene-*d*₈ at -40 °C. Labels indicate assignments by 2D NMR.

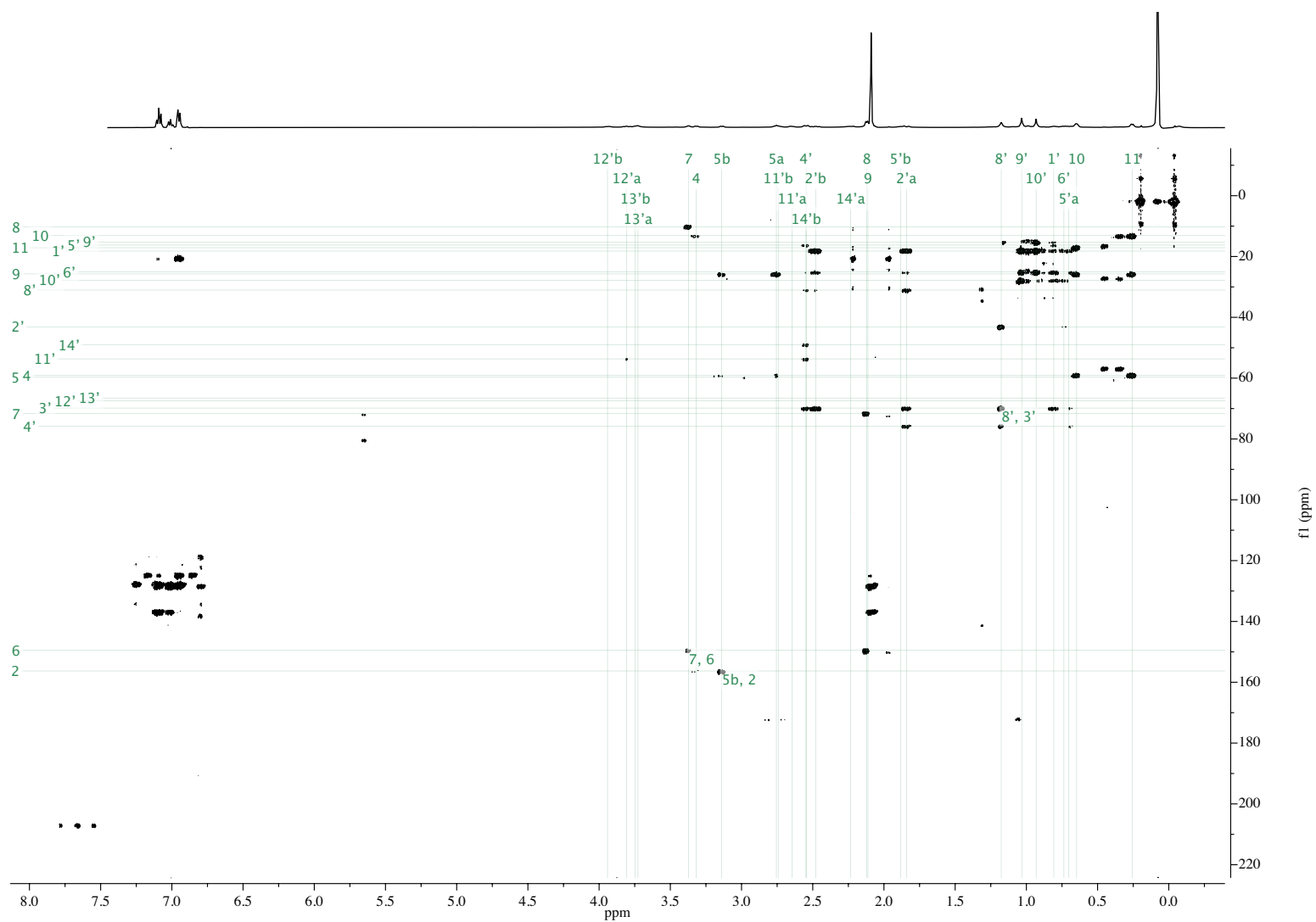


Figure 123. Full display HMBC spectrum of 0.10 M (S)-15b in neat toluene- d_8 at $-40\text{ }^\circ\text{C}$. Labels indicate assignments.

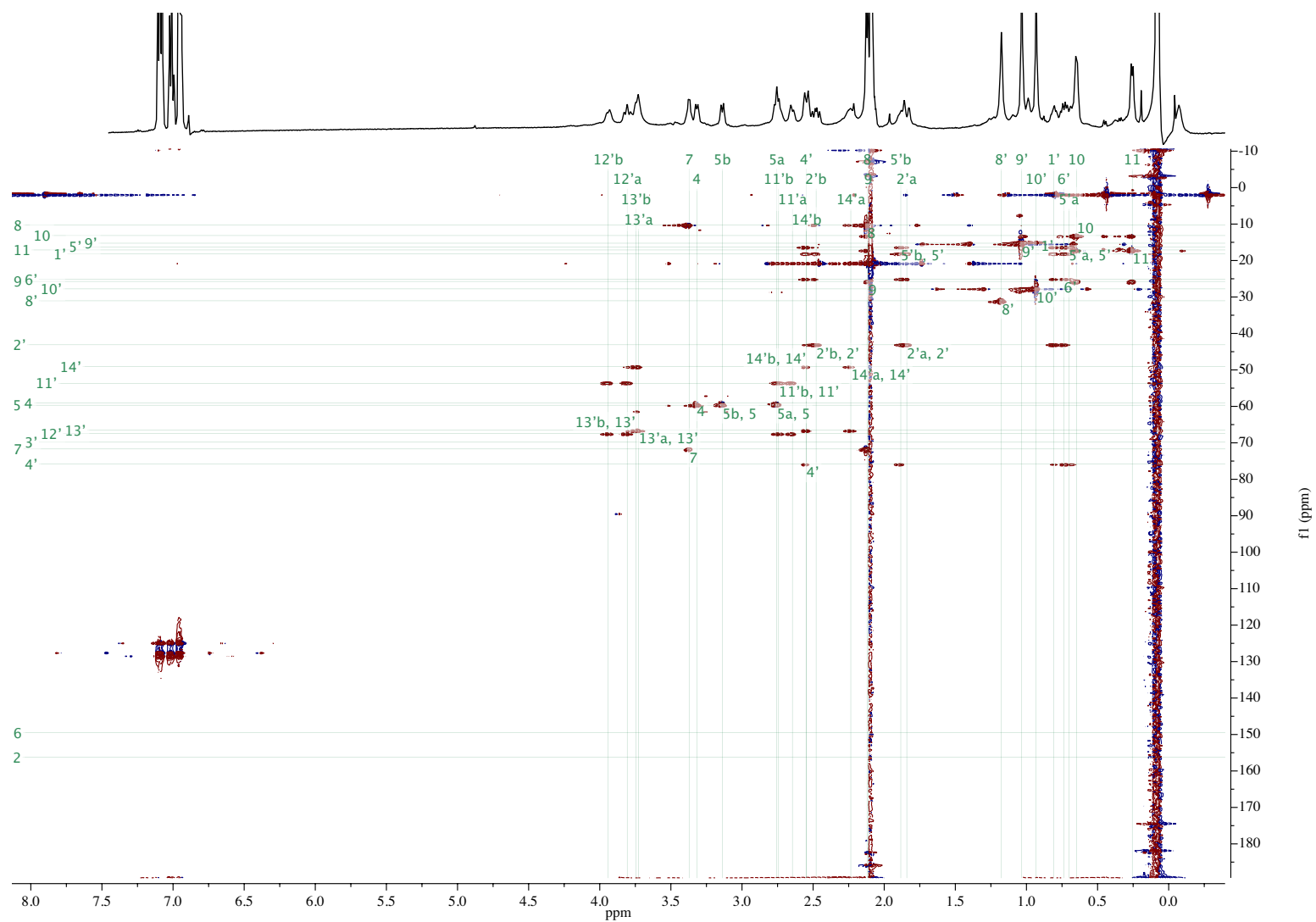


Figure 124. Full display HSQC-TOCSY spectrum of 0.10 M (*S*)-**15b** in neat toluene-*d*₈ at -40 °C. Labels indicate assignments.

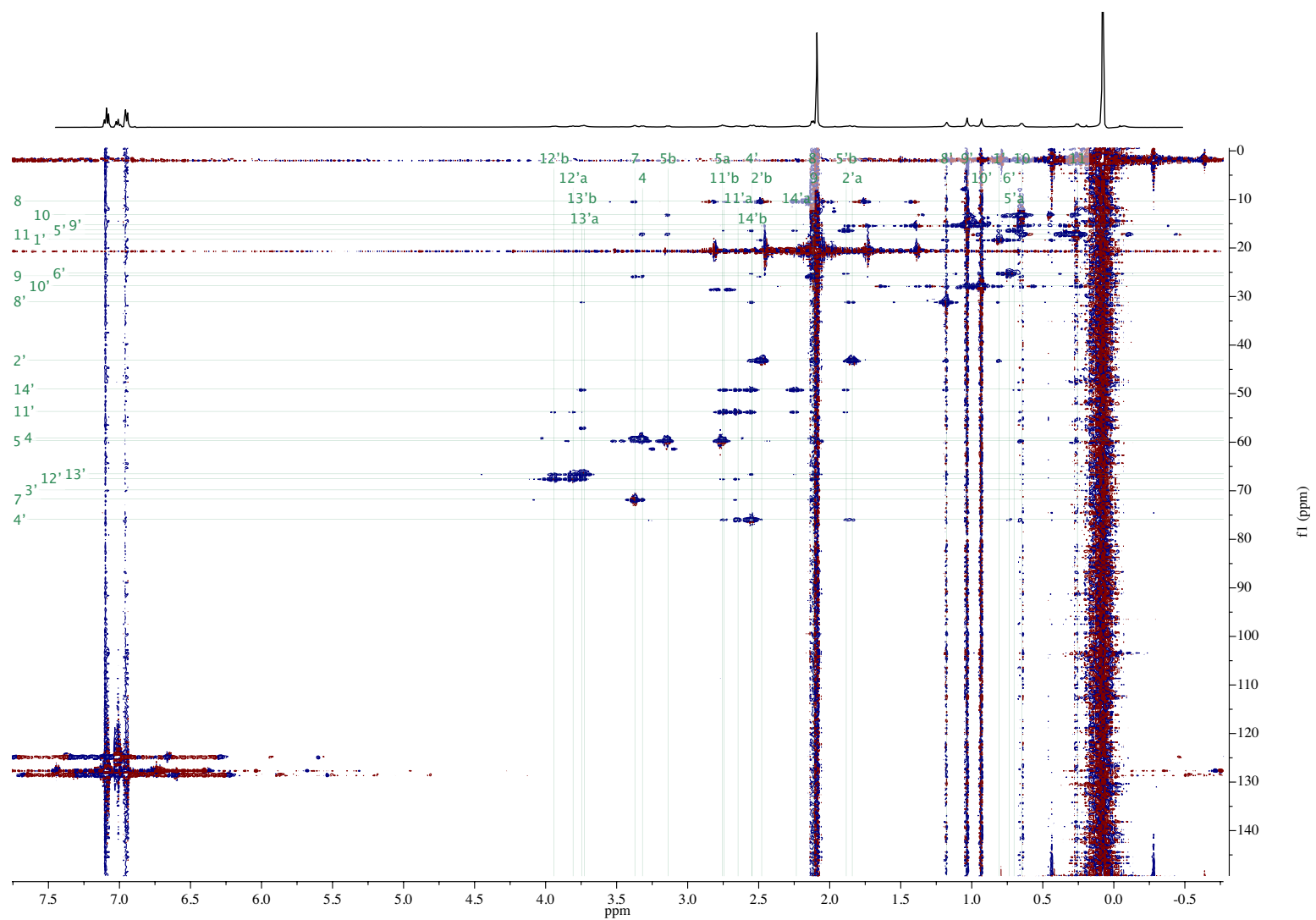


Figure 125. Full display HSQC-NOESY spectrum of 0.10 M (S)-15b in neat toluene- d_8 at -40 °C. Labels indicate assignments.

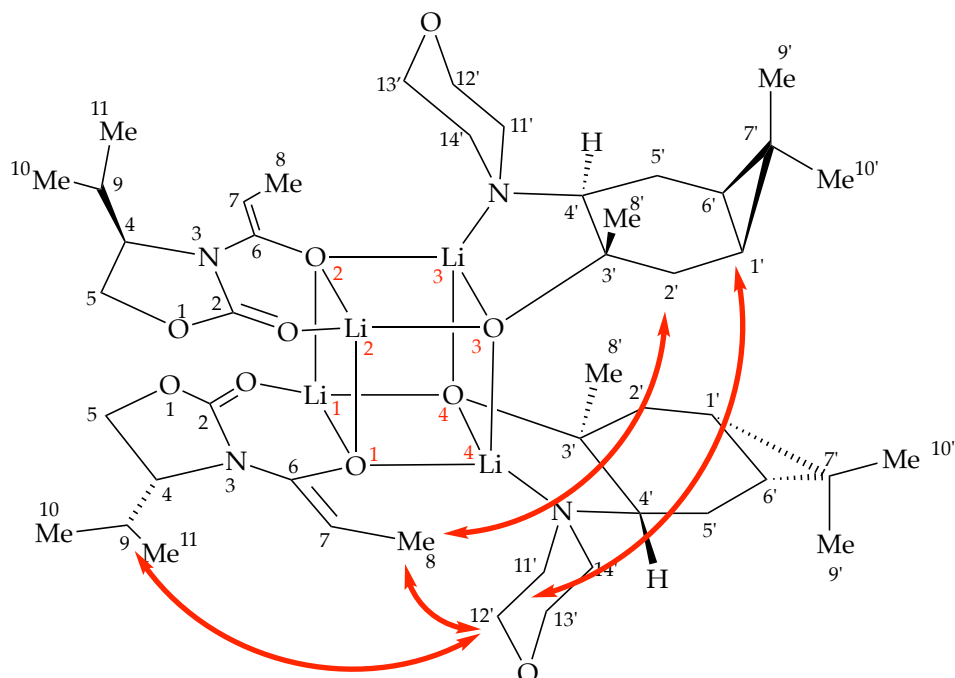


Table 6. ^1H and ^{13}C chemical shift assignments for mixed aggregate (**R**)-**15b** at $-40\text{ }^\circ\text{C}$.

Atom	δC , ppm	δH , ppm	HMBC	HSQC-TOCSY	HSQC-NOESY
1' C	18.18	0.30	2',5',6',9',10'	2',4',5',6'	2',6',11',12'
2 C	156.01	–	4,5b	–	–
2' C	42.66	1.76(a) 2.18(b)	6',8'	1',6'	8,11',12',8',9',1'
3' C	69.70	–	8',2',5',4'	–	–
4 C	58.84	3.43	10,11,9,5	5	7,9,5
4' C	76.95	2.29	2',8',5'	5',6'	11',2',5',6'
5 C	59.67	3.00(a) 3.26(b)	4,9	4	11,4,9,10
5' C	15.95	0.58(a) 1.78(b)	1',4'	1',2',6',4'	11',14',4',2'
6 C	149.10	–	7,8	–	–
6' C	25.03	0.69	1',2',4',5',9',10'	2',4',5',1'	4',1',5'
7 C	72.26	3.47	6,8	8	4,9,8
7' C	–	–			
8 C	10.05	2.22	6,7	7	12',7,2'
8' C	29.76	1.16	2',4'		14',2',9',5'
9 C	25.31	2.35	10,11,5	10,11	7,4,10,11
9' C	14.94	0.91	1',2',6',10'	10'	2',8',10'
10 C	12.71	0.54	4,11,9	9,11	9,5,11

10' C	27.90	1.01	1',9',6'	9'	9',1'
11 C	16.74	0.27	10,9,4	9,10	4,9,5,10
11' C	53.48	2.78(a)	4',14'	12'	12',4',5',14'
		2.84(b)			
12' C	67.14	3.98(a)	13'	11'	13',11',1',2',8
		4.12(b)			
13' C	66.18	3.56(a)	12'	14'	12',14',9
		3.65(b)			
14' C	49.47	2.15(a)	13',4'	13'	13',11',8',5'
		2.65(b)			

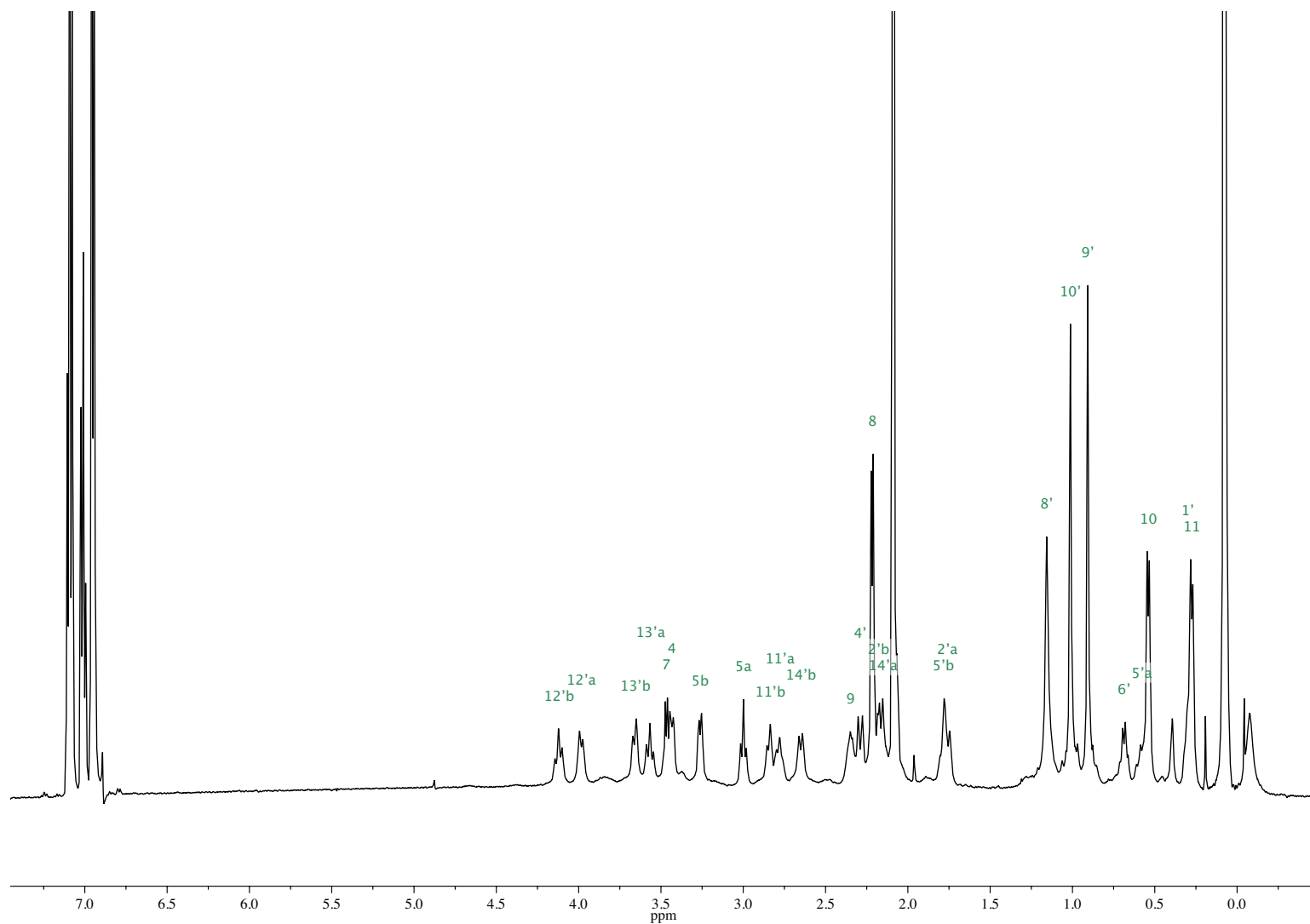


Figure 126. ^1H NMR spectrum of 0.10 M mixed aggregate (*R*)-**15b** in neat toluene- d_8 at $-40\text{ }^\circ\text{C}$. Labels indicate assignments by 2D NMR.

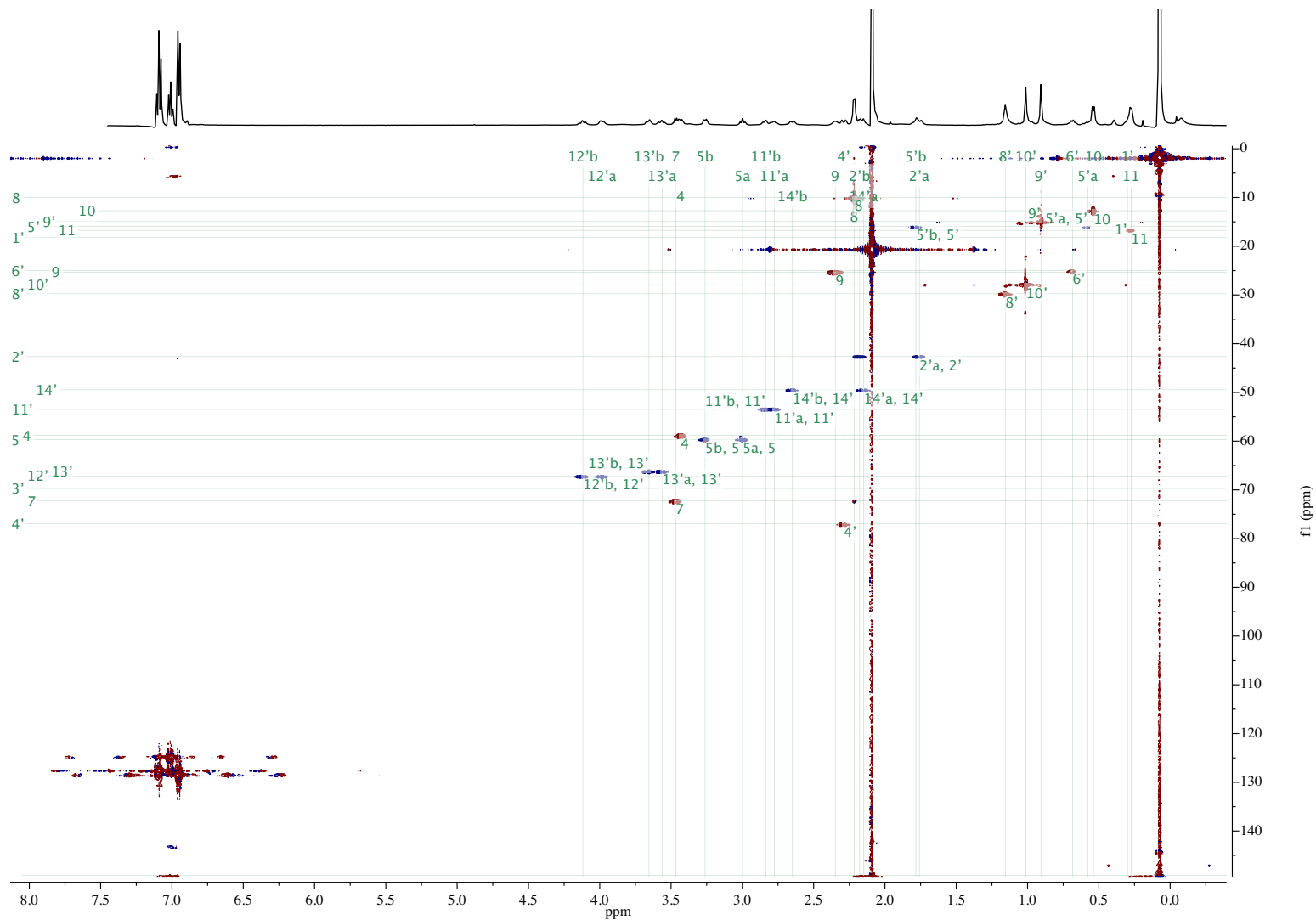


Figure 127. Full display HSQC spectrum of 0.10 M (*R*)-**15b** in neat toluene-*d*₈ at -40 °C. Labels indicate assignments.

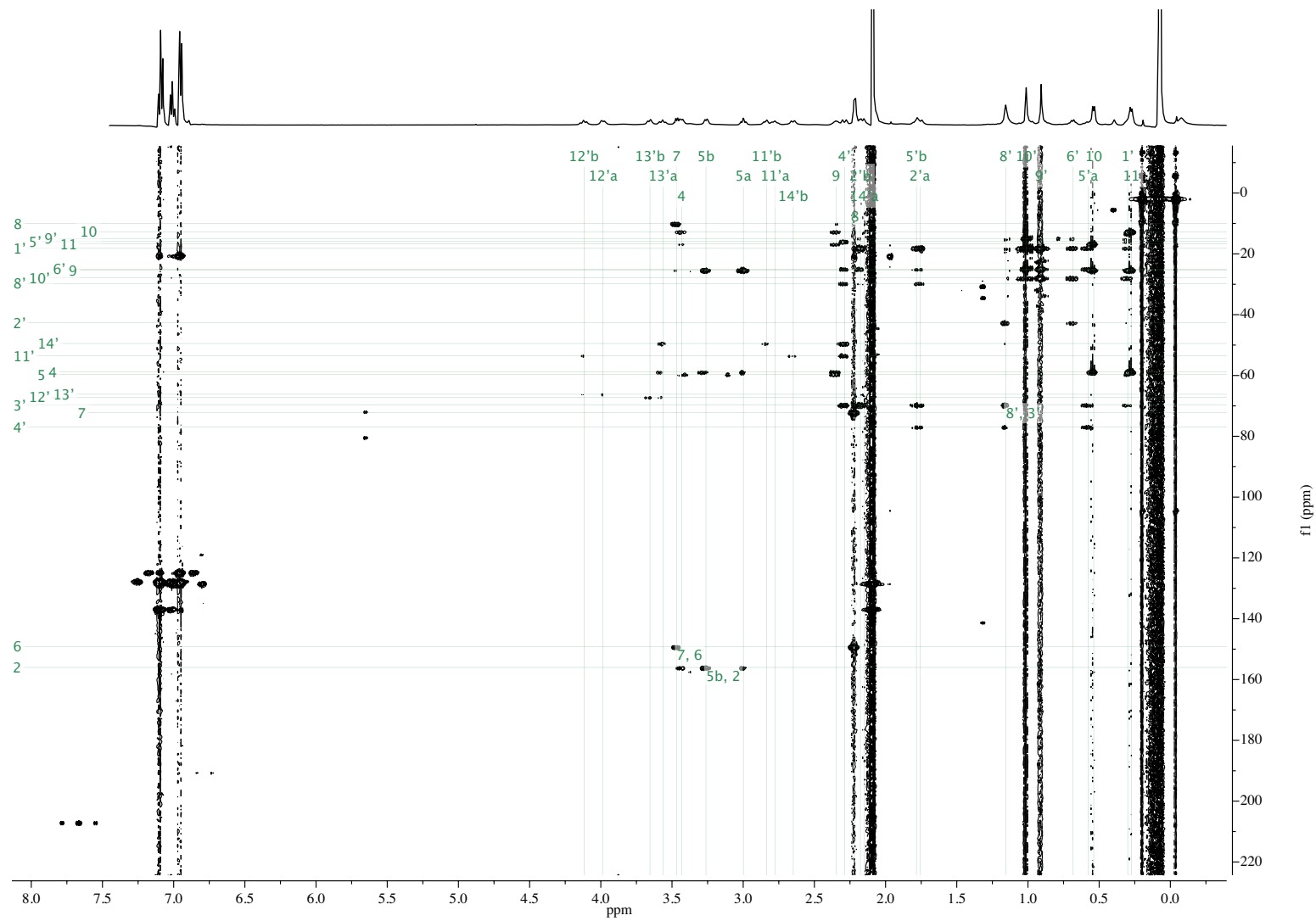


Figure 128. Full display HMBC spectrum of 0.10 M (*R*)-**15b** in neat toluene-*d*₈ at -40 °C. Labels indicate assignments.

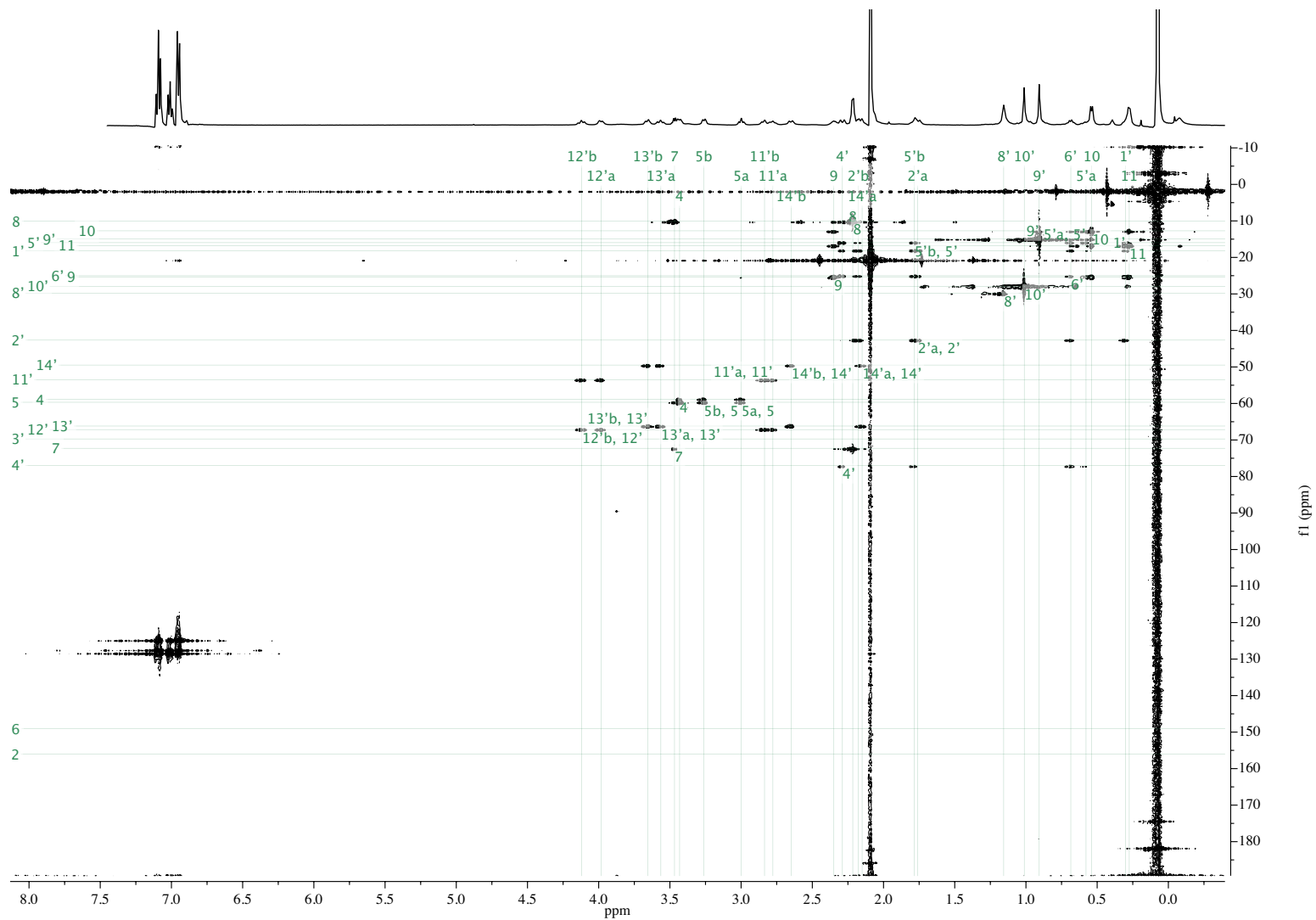


Figure 129. Full display HSQC-TOCSY spectrum of 0.10 M (*R*)-**15b** in neat toluene-*d*₈ at -40 °C. Labels indicate assignments.

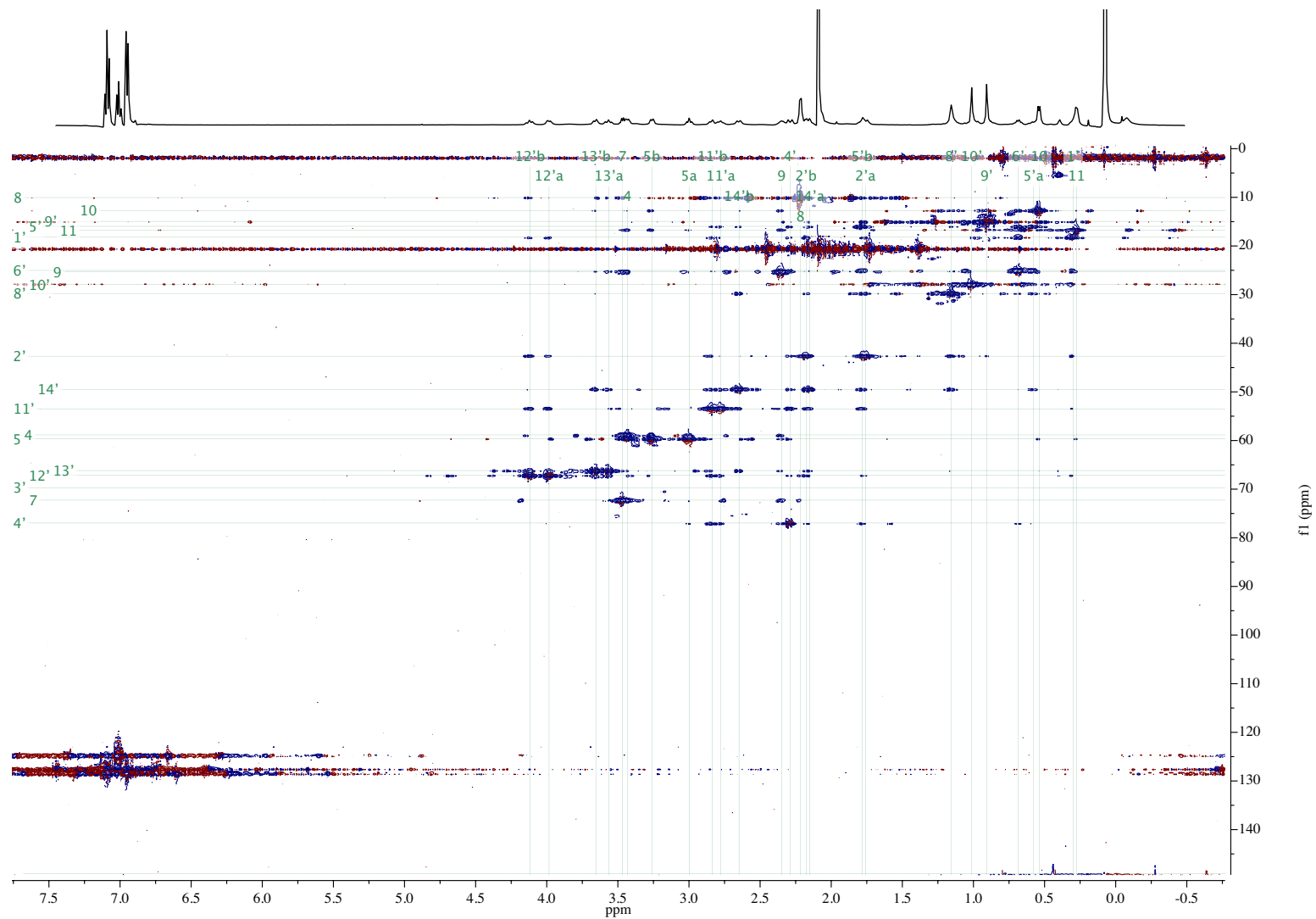


Figure 130. Full display HSQC-NOESY spectrum of 0.10 M (*R*)-**15b** in neat toluene-*d*₈ at -40 °C. Labels indicate assignments.

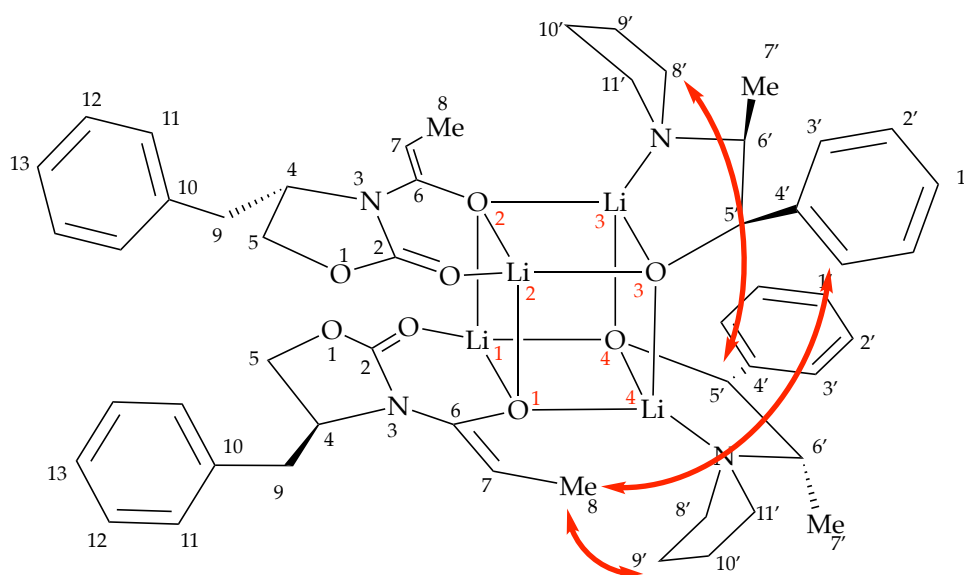


Table 7. ^1H and ^{13}C chemical shift assignments for mixed aggregate (*S*)-**36a** at $-40\text{ }^\circ\text{C}$.

Atom	δC , ppm	δH , ppm	HMBC	HSQC-TOCSY	ROESY
1' C	125.73	7.11	2',3',4'	2',3'	2'
2 C	156.41	–	5b	–	–
2' C	127.58	7.37	1',3',4'	1',3'	1',3',5'
3' C	126.44	7.71	1',5'	1',2'	2',7',8
4 C	57.83	3.73	9,5	9,5	11,7,5
4' C	149.24	–	2',5'	–	–
5 C	63.81	2.77 (a)	4,9	4,9	4,9
		3.34 (b)			
5' C	76.71	5.57	3',7'	7'	2',8',6',10'
6 C	150.45	–	8,7	–	–
6' C	70.27	2.29	5',11',8',7'	5',7'	2',5',8',7',11'
7 C	72.29	3.82	8	8	11,4,9,8
7' C	11.50	1.04	5',8',6'	5',6'	2',5',11',6'
8 C	11.13	2.22	7	7	7,2',9',10'
8' C	52.82	1.93 (a)	11',6'	11',9',10'	6',9',10',5'
		3.77 (b)			
9 C	36.73	2.30 (a)	11,5	4,5	11,7,5,4
		3.40 (b)			
9' C	22.63	1.26 (a)	8',11'	8',11',10'	11',8',10'
		1.51 (b)			
10 C	136.27	–	12,13,9	–	–

10' C	23.09	1.50 (a)	8',6'	8',9',11'	11',8',9'
		1.67 (b)			
11 C	129.10	6.67	12,13,9	12,13	7,4,5,9
11' C	51.53	1.69 (a)	8'	8',9',10'	6',9',7'
		2.99 (b)			
12 C	128.50	6.95	9,10,11	11,13	11,13
13 C	126.53	6.95	10,11	11,12	11,12

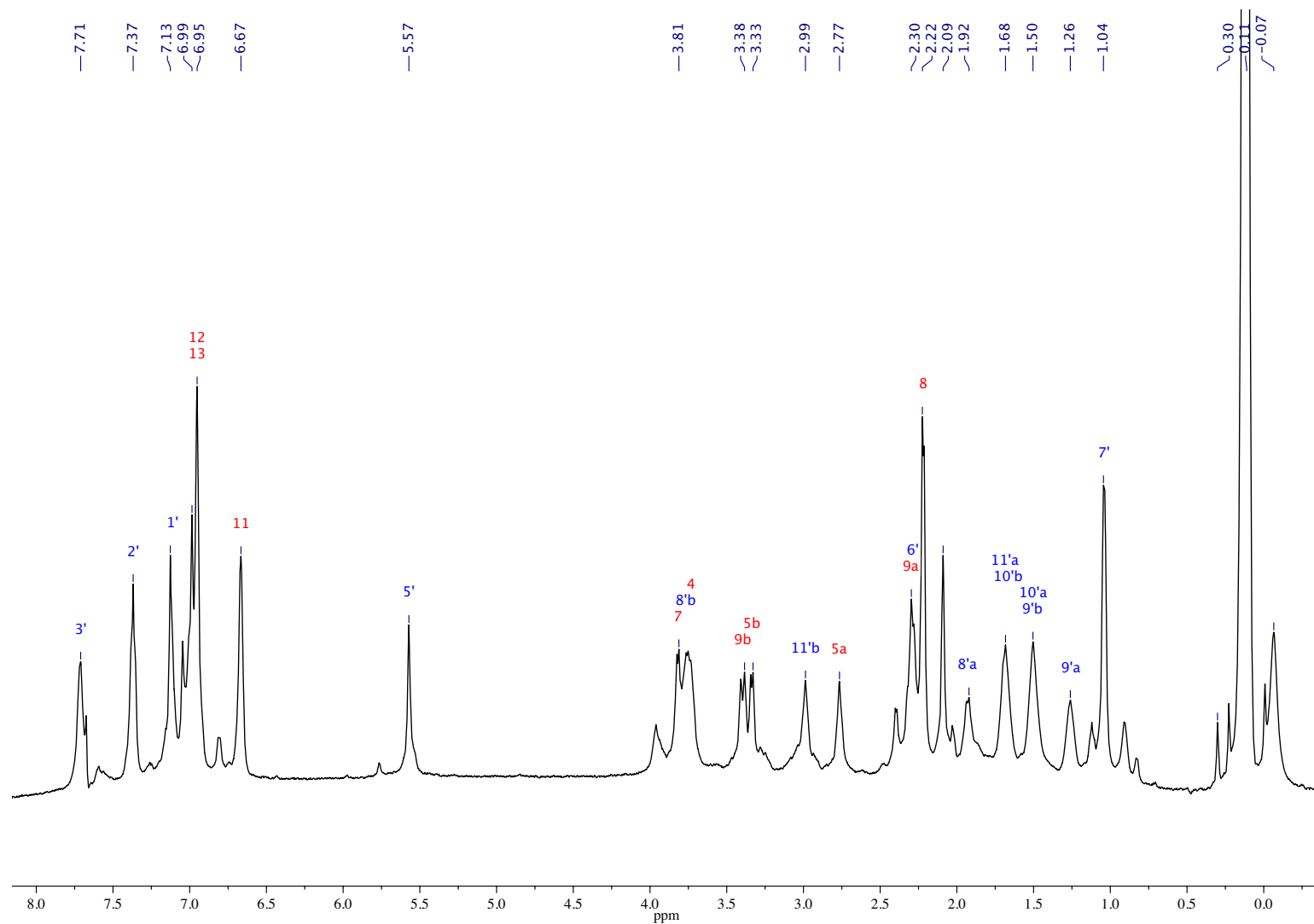


Figure 131. ¹H NMR spectrum of 0.10 M mixed aggregate (*S*)-**36a** in neat toluene-*d*₈ at -40 °C. Labels indicate assignments by 2D NMR.

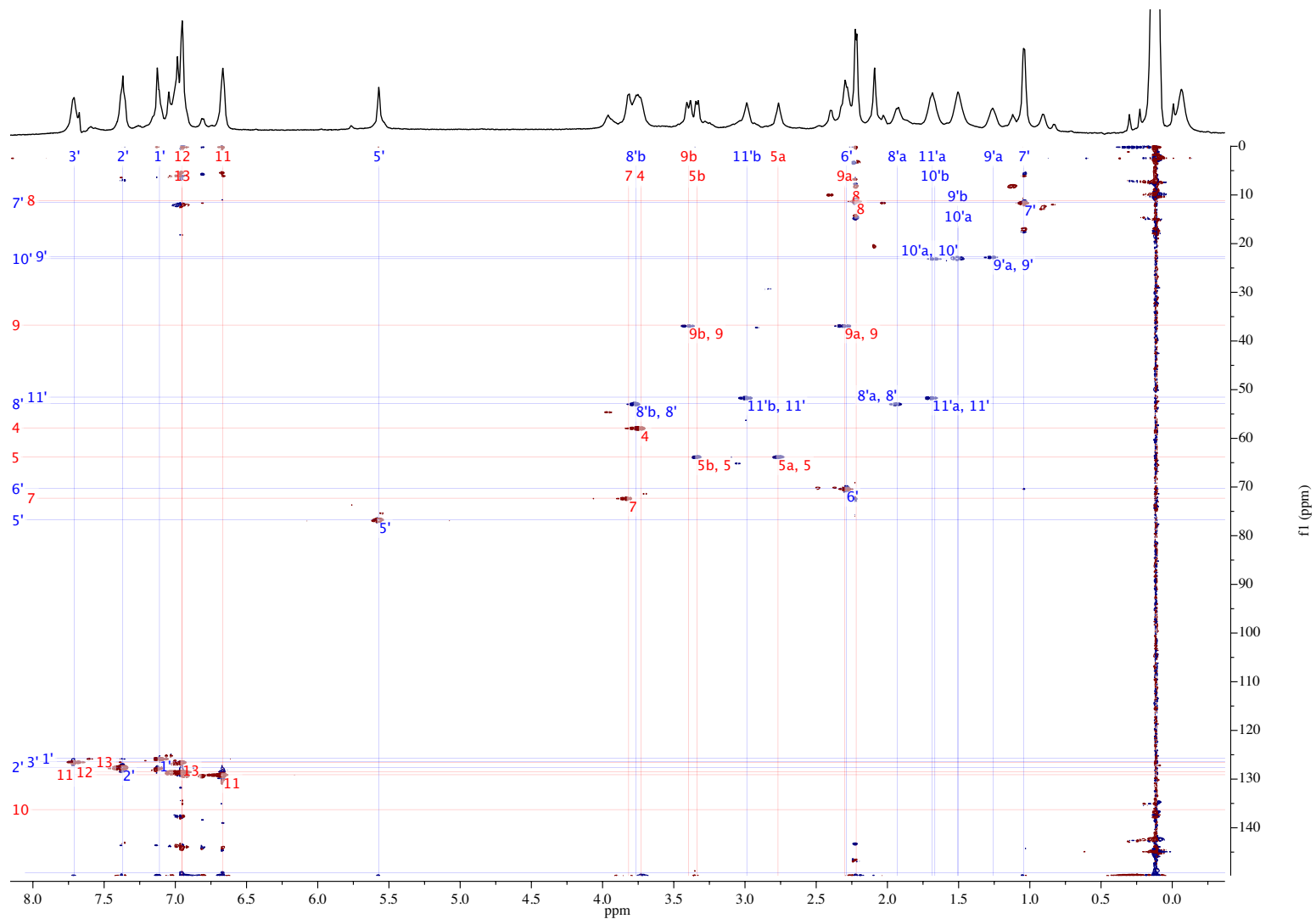


Figure 132. Full display HSQC spectrum of 0.10 M (*S*)-**36a** in neat toluene-*d*₈ at -40 °C. Labels indicate assignments.

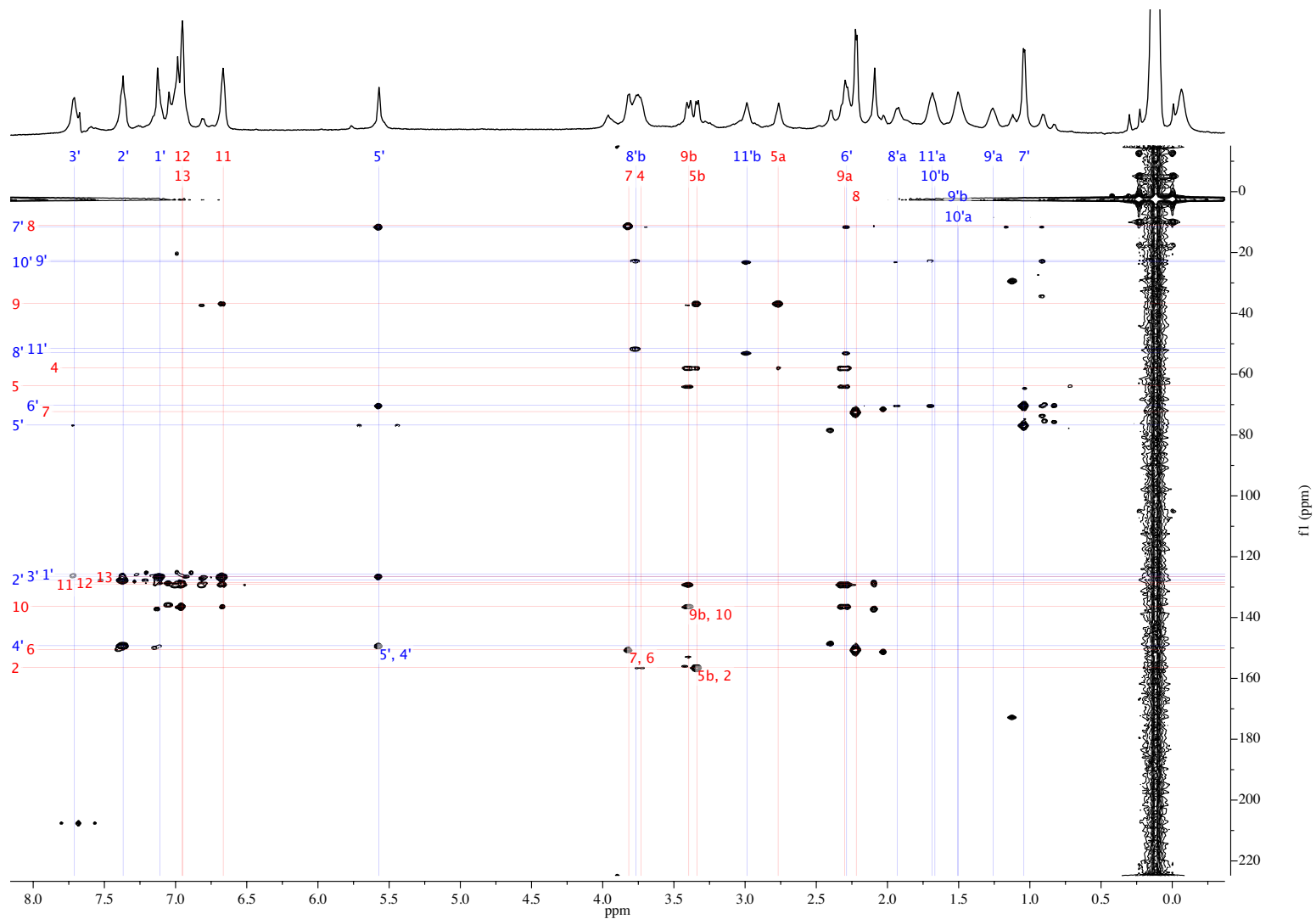


Figure 133. Full display HMBC spectrum of 0.10 M (*S*)-**36a** in neat toluene-*d*₈ at -40 °C. Labels indicate assignments.

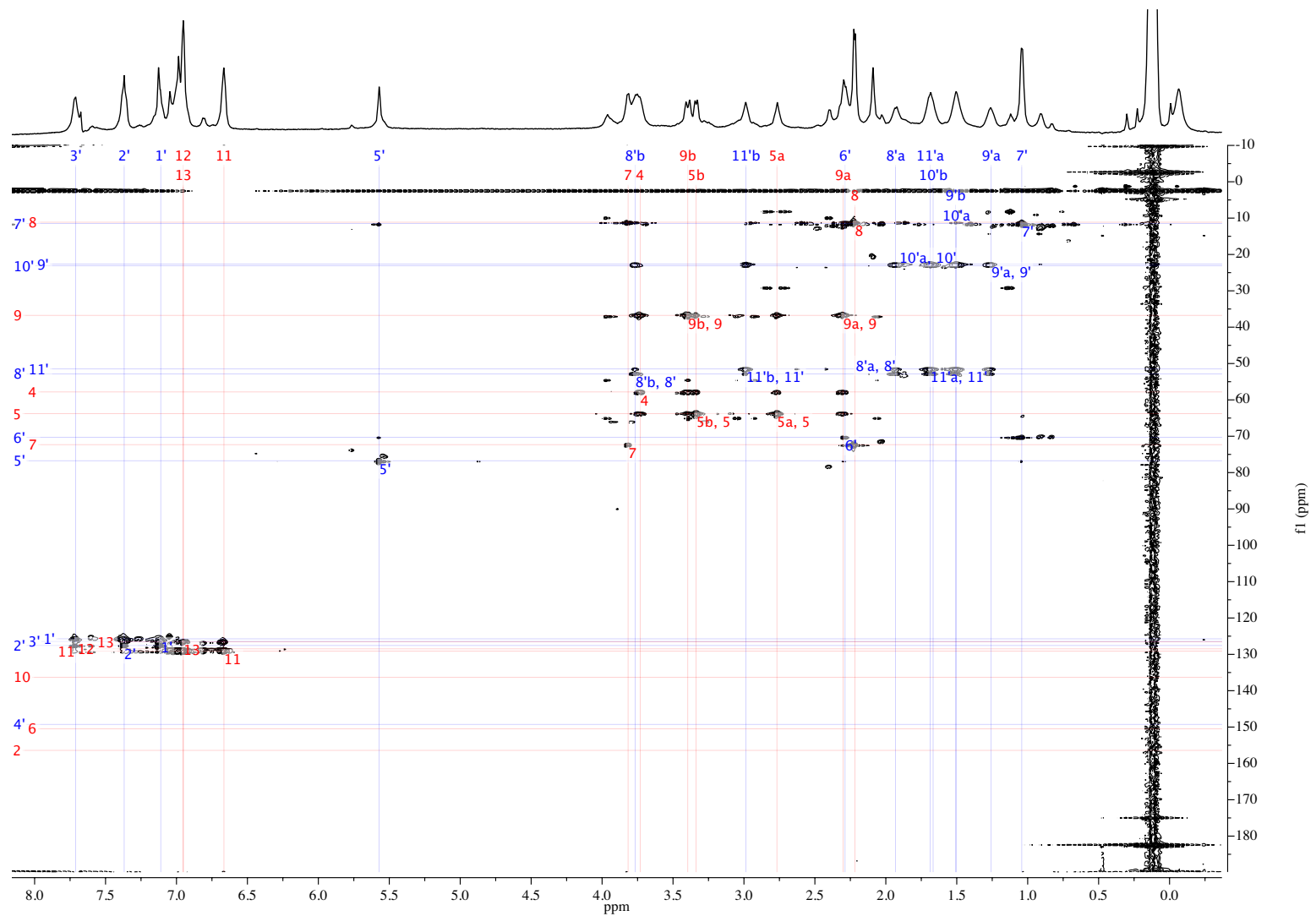


Figure 134. Full display HSQC-TOCSY spectrum of 0.10 M (*S*)-**36a** in neat toluene-*d*₈ at -40 °C. Labels indicate assignments.

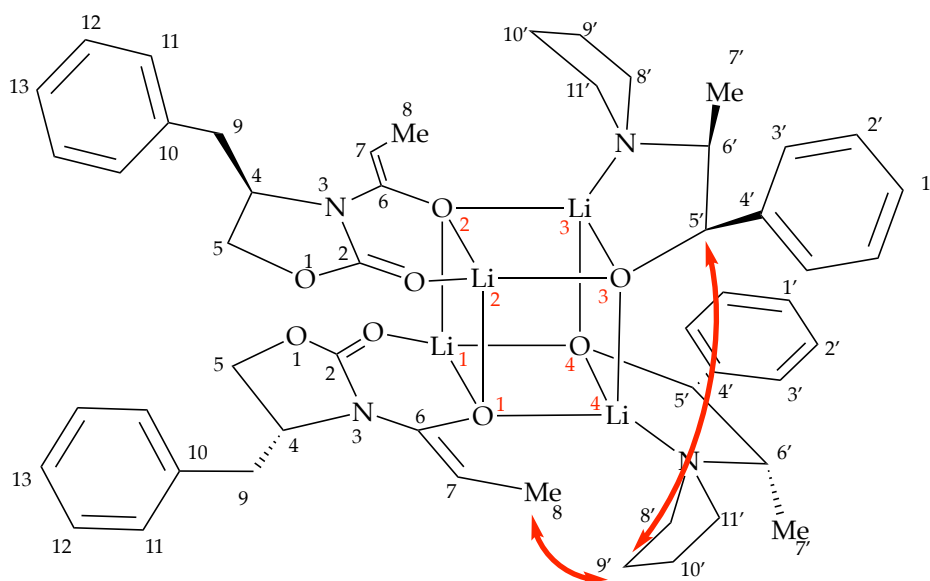


Table 8. ^1H and ^{13}C chemical shift assignments for mixed aggregate (**R**)-**36a** at $-40\text{ }^\circ\text{C}$.

Atom	δC , ppm	δH , ppm	HMBC	HSQC-TOCSY	HSQC-NOESY
1' C	125.62	7.08	2',3',4'	2',3'	2'
2 C	156.89	–	5	–	–
2' C	122.71	7.33	1',3',4'	1',3'	1',3'
3' C	125.95	7.67	1',5'	1',2'	2',7'
4 C	57.74	3.78	9,5	9,5	11,7,5
4' C	149.32	–	2',5'	–	–
5 C	64.89	3.10 (a)	4,9	4,9	4,9
		3.55 (b)			
5' C	76.23	5.57	3',7',6',4'	7'	2',8',6',10',9'
6 C	149.50	–	8,7,4	–	–
6' C	70.58	2.27	5',11',7'	5',7'	2',5',8',7',11'
7 C	74.45	3.80	8	8	11,4,9,8
7' C	11.79	1.01	5',8',6'	5',6'	2',5',11',6'
8 C	10.80	2.05	7,6	7	7,11'
8' C	52.85	1.95 (a)	11',6'	11',9',10'	6',9',10'
		3.79 (b)			
9 C	37.42	2.53 (a)	11,5	4,5	11,7,5,4
		3.76 (b)			
9' C	22.37	1.30 (a)	8',11'	8',11',10'	11',8',10'
		1.53 (b)			
10 C	136.85	–	11,12,13,9	–	–

10' C	23.46	1.54 (a)	11'	8',9',11'	11',8',9'
		1.65 (b)			
11 C	128.93	6.88	12,13,9	12,13	7,4,5,9
11' C	51.82	1.69 (a)	8'	8',9',10'	6',9',7'
		3.06 (b)			
12 C	128.53	7.05	9,10,11	11,13	11,13
13 C	126.45	7.01	10,11	11,12	11,12

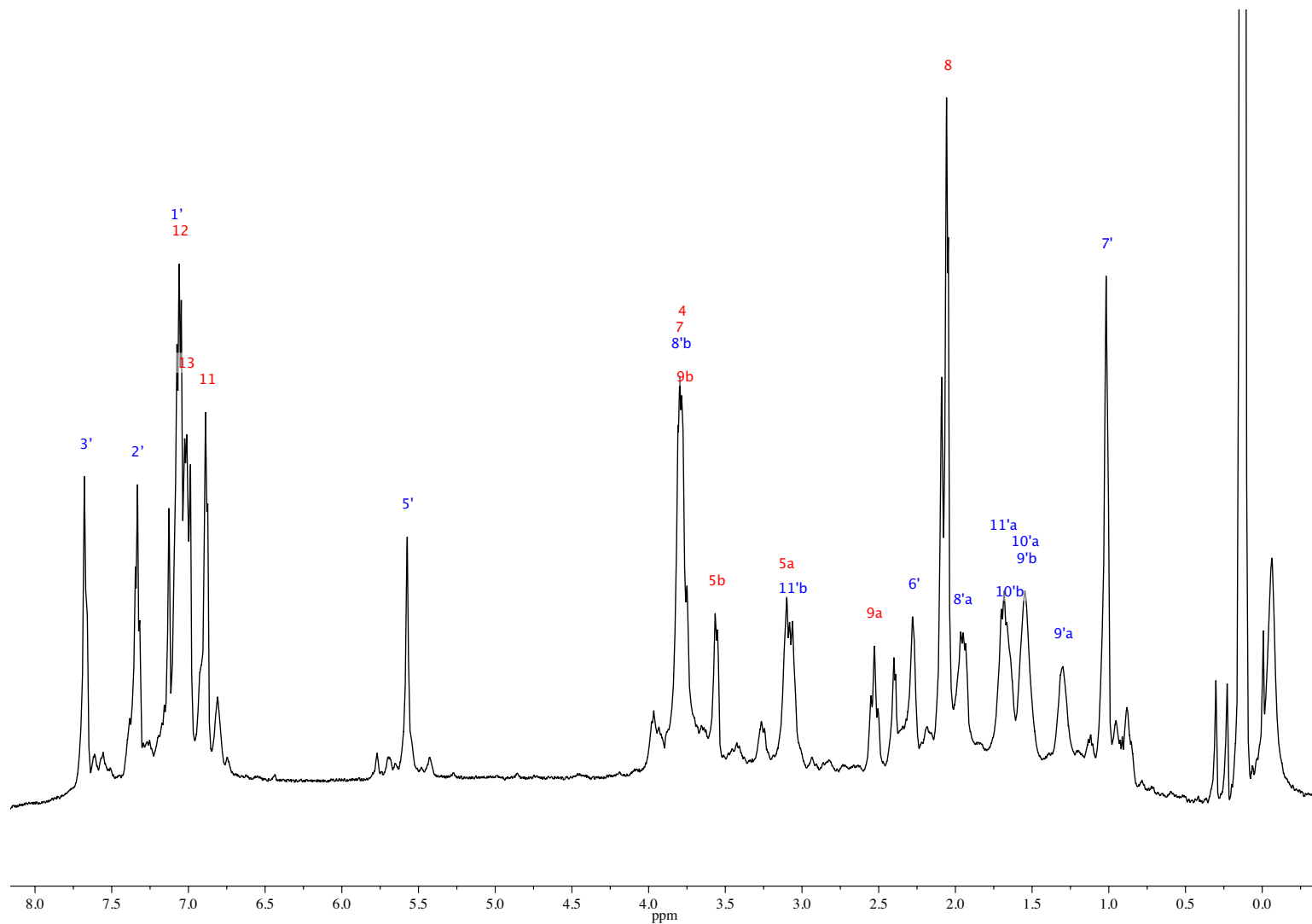


Figure 136. ^1H NMR spectrum of 0.10 M mixed aggregate (*R*)-**36a** in neat toluene- d_8 at $-40\text{ }^\circ\text{C}$. Labels indicate assignments by 2D NMR.

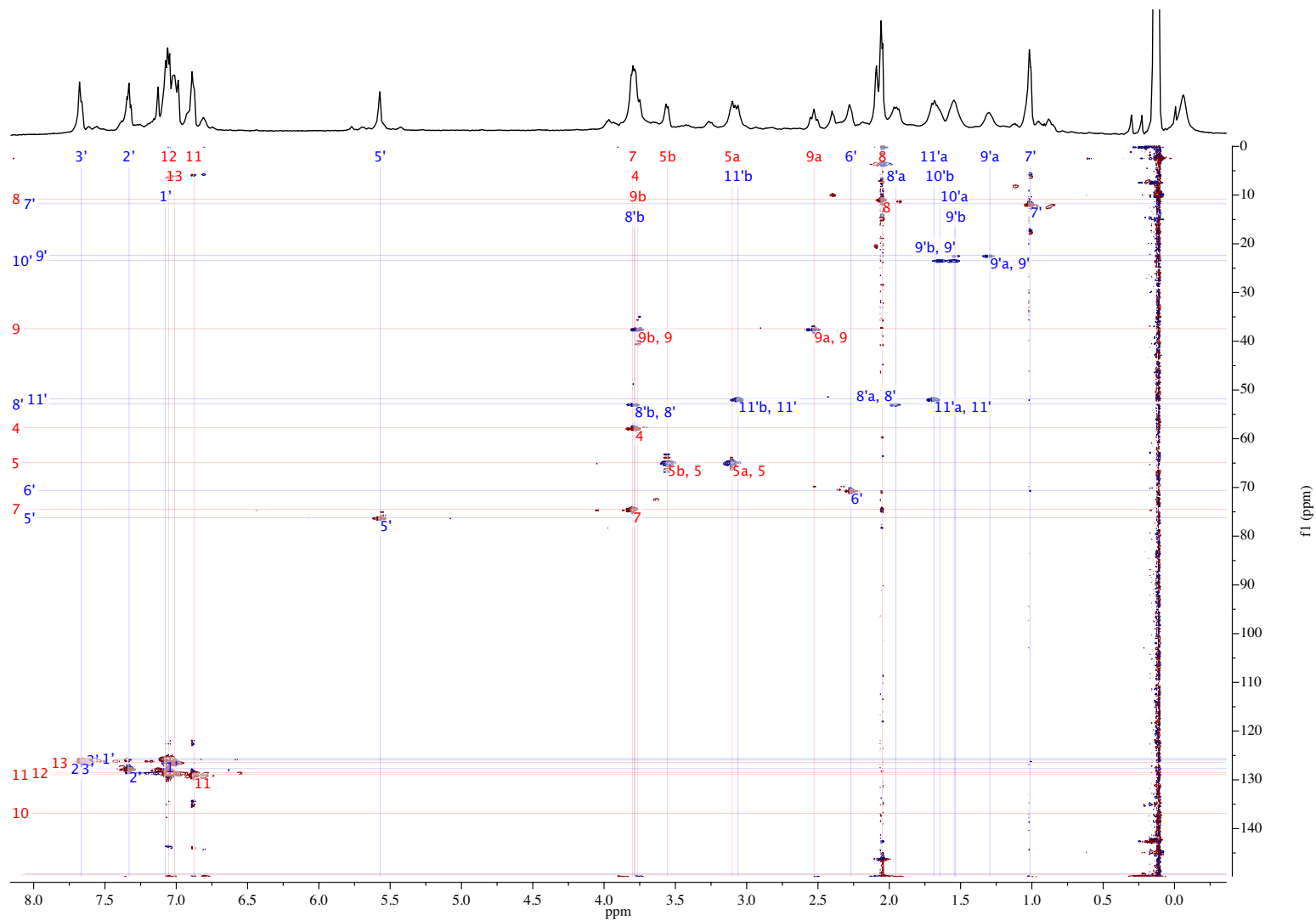


Figure 137. Full display HSQC spectrum of 0.10 M (*R*)-**36a** in neat toluene-*d*₈ at -40 °C. Labels indicate assignments.

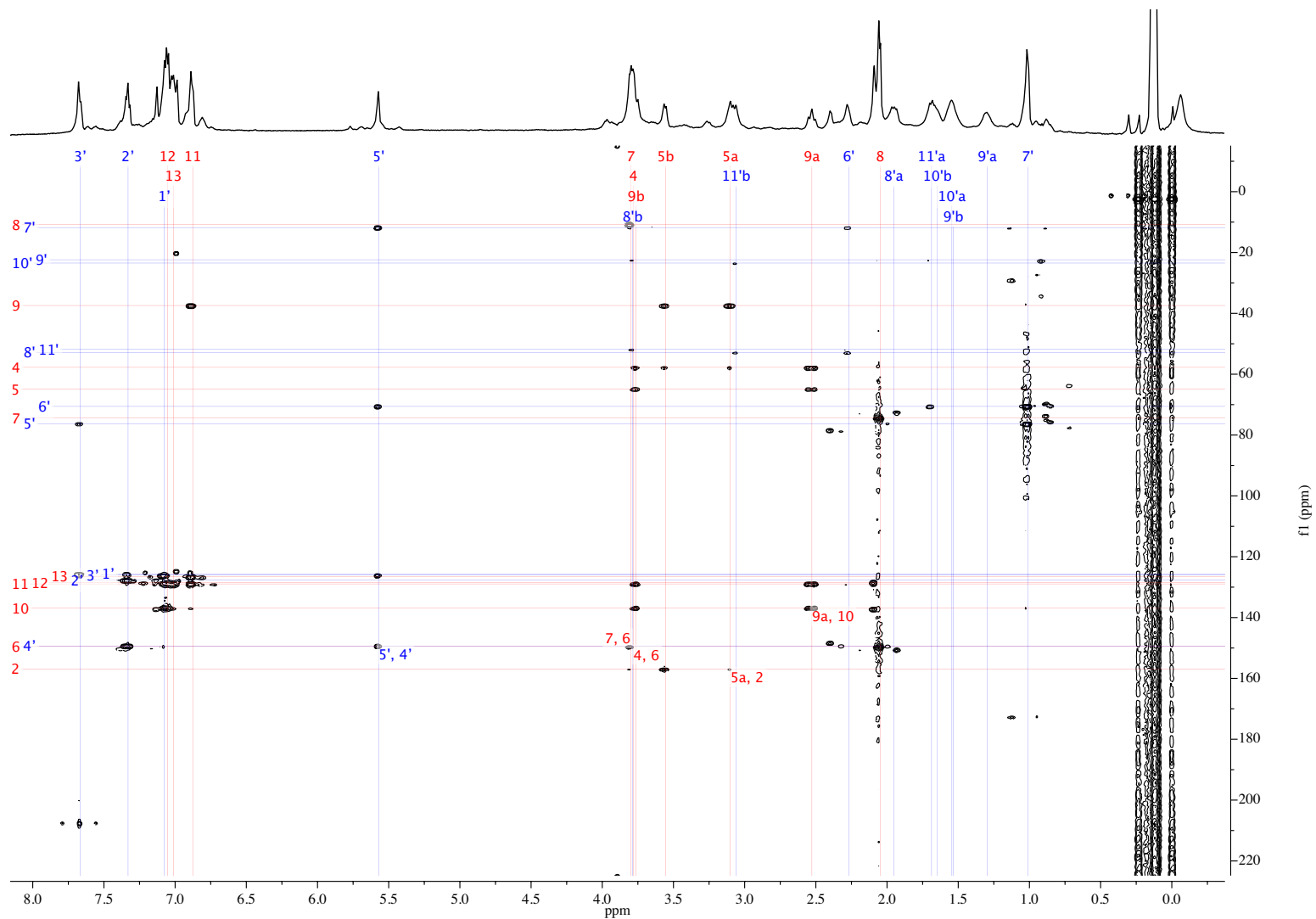


Figure 138. Full display HMBC spectrum of 0.10 M (*R*)-**36a** in neat toluene- d_8 at $-40\text{ }^\circ\text{C}$. Labels indicate assignments.

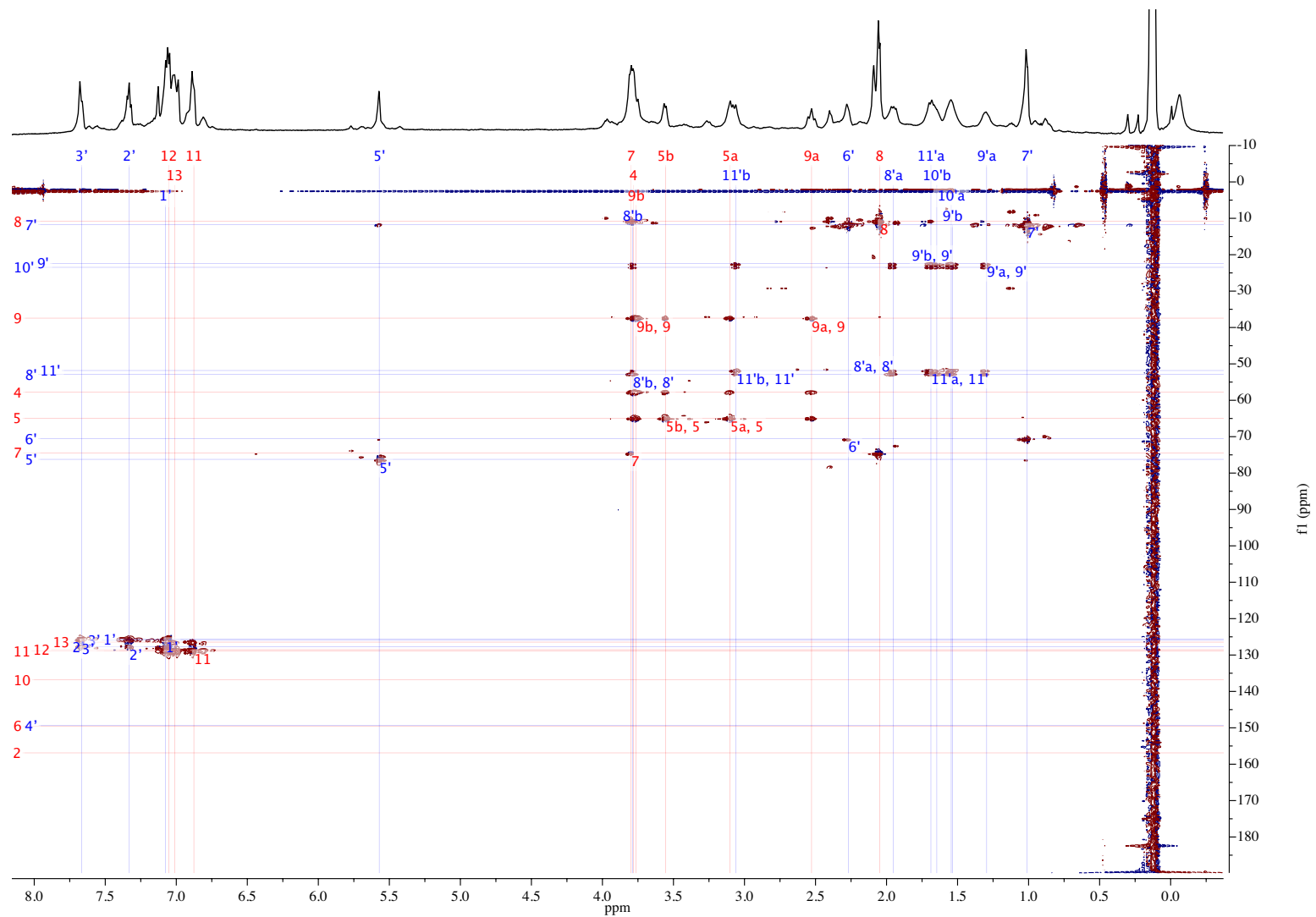


Figure 139. Full display HSQC-TOCSY spectrum of 0.10 M (*R*)-**36a** in neat toluene-*d*₈ at -40 °C. Labels indicate assignments.

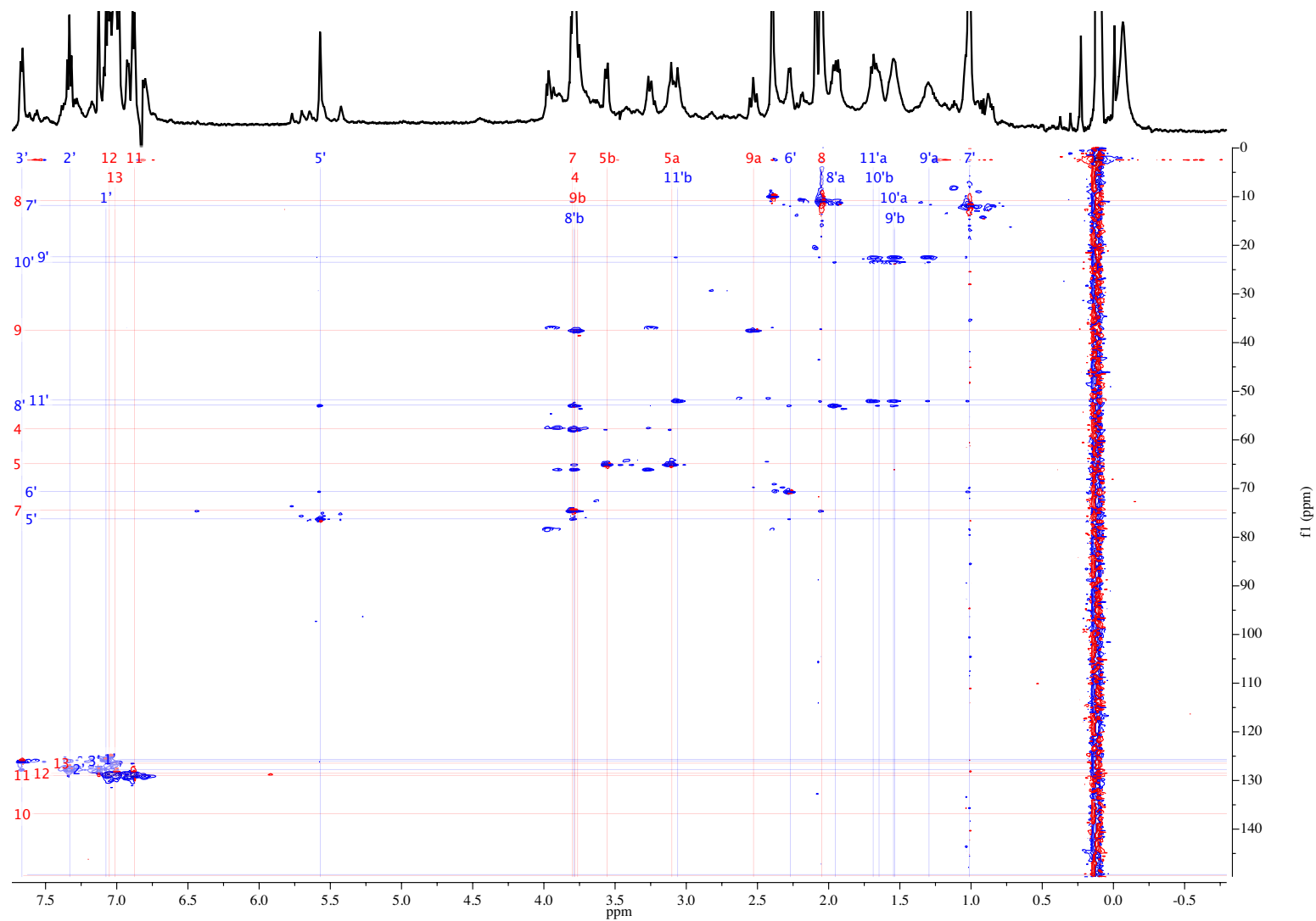


Figure 140. Full display HSQC-NOESY spectrum of 0.10 M (*R*)-**36a** in neat toluene-*d*₈ at -40 °C. Labels indicate assignments.

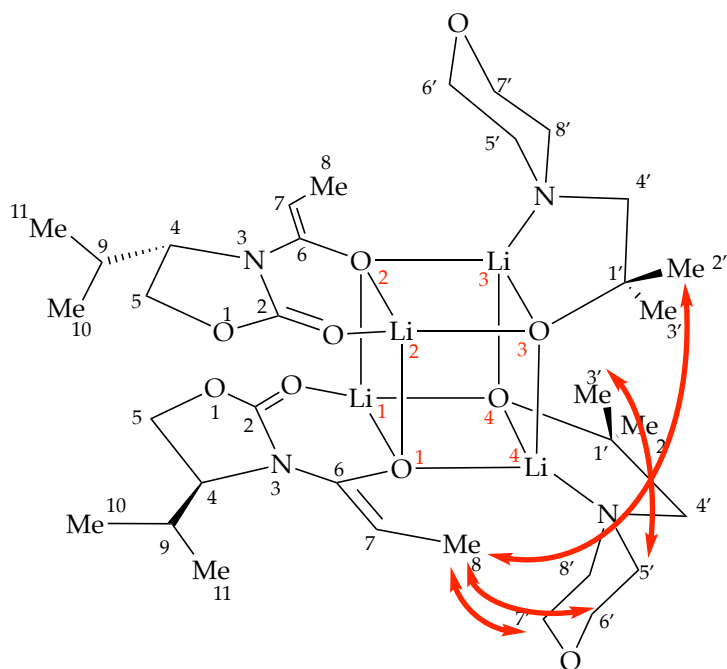


Table 9. ^1H and ^{13}C chemical shift assignments for mixed aggregate (*S*)-**52b** at $-40\text{ }^\circ\text{C}$.

Atom	δC , ppm	δH , ppm	HMBC	HSQC-TOCSY	ROESY
1' C	68.51	–	2',3',4'	–	–
2 C	156.29	–	4,5	–	–
2' C	33.57	1.36	1',3',4'	–	4',8',8
3' C	34.58	1.17	1',2',5'	–	4',5'
4 C	59.12	3.33	9,5,10,11	5	8,9,10
4' C	73.90	2.19 (a) 2.28 (b)	2',3'	–	2',3',5',8'
5 C	59.69	2.71 (a) 3.14 (b)	9	4	4,9,10,11
5' C	55.79	2.11 (a) 2.71 (b)	6'	6'	6',3',8'
6 C	149.65	–	7	–	–
6' C	66.38	3.69 3.70	5'	5'	5',8',3'
7 C	71.24	3.36	8,6	8	8
7' C	66.41	3.78 (a) 3.78 (b)	8'	8'	–
8 C	10.03	2.10	7	7	7,5',6',2'
8' C	55.70	2.20 (a)	7'	7'	5',4',2'

		2.94 (b)			
9 C	25.63	2.13	11,5,10	10,11	4,5,10,11
10 C	16.92	0.19	11,9	9,11	5,4,9,11
11 C	13.02	0.50	4,9,10	9,10	5,9,10

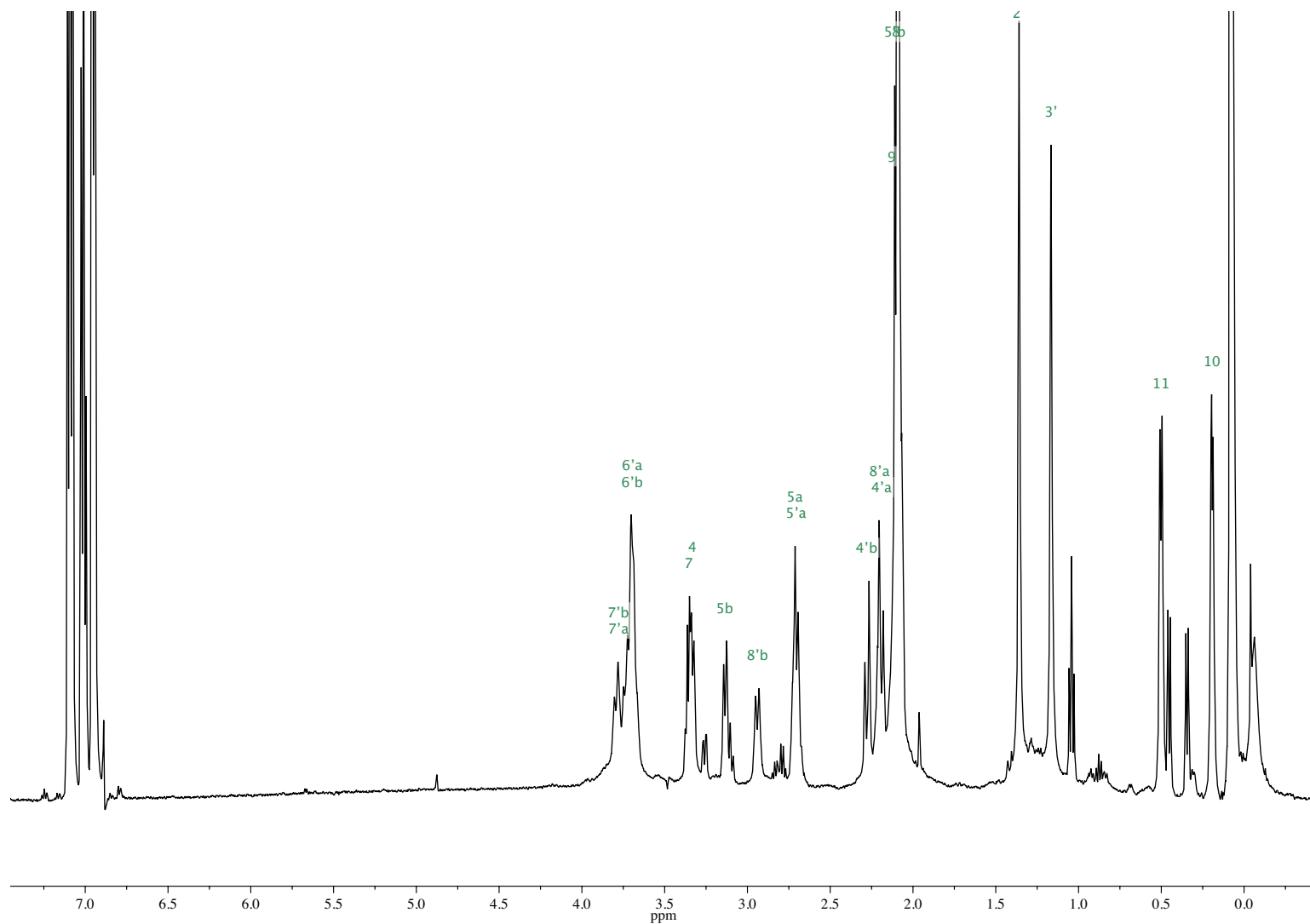


Figure 141. ^1H NMR spectrum of 0.10 M mixed aggregate (*S*)-**52b** in neat toluene- d_8 at $-40\text{ }^\circ\text{C}$. Labels indicate assignments by 2D NMR.

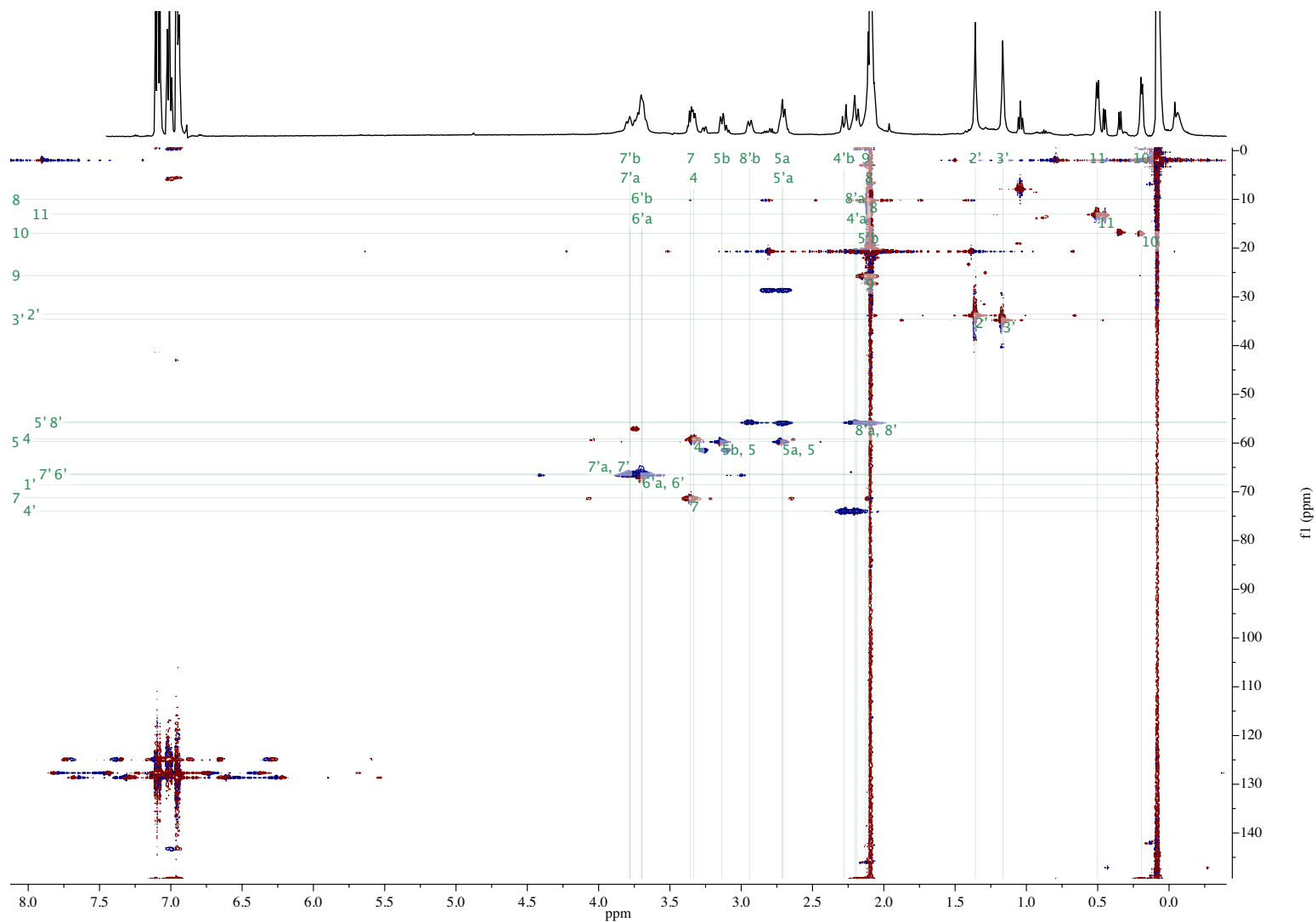


Figure 142. Full display HSQC spectrum of 0.10 M (*S*)-**52b** in neat toluene-*d*₈ at -40 °C. Labels indicate assignments.

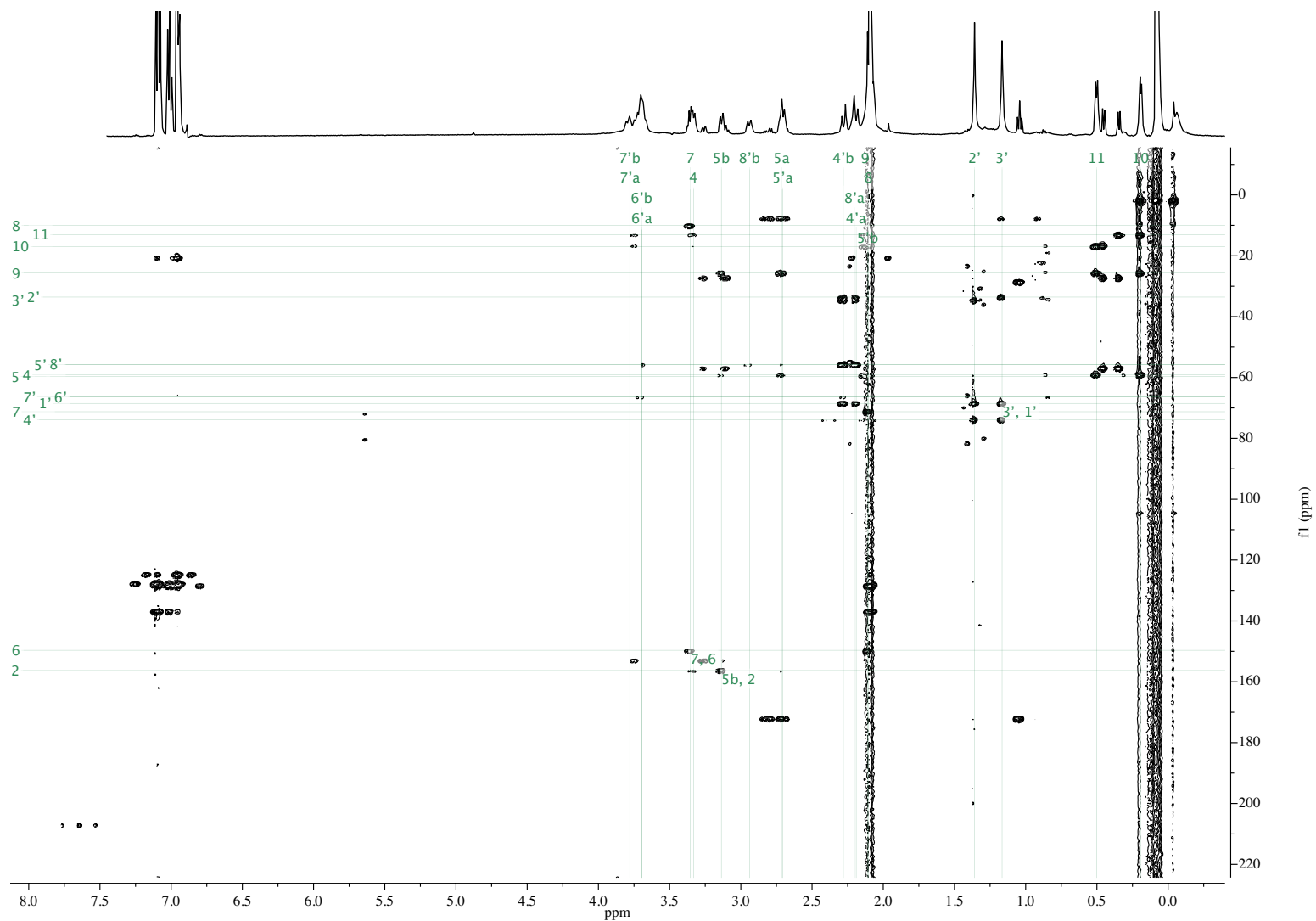


Figure 143. Full display HMBC spectrum of 0.10 M (*S*)-**52b** in neat toluene- d_8 at $-40\text{ }^\circ\text{C}$. Labels indicate assignments.

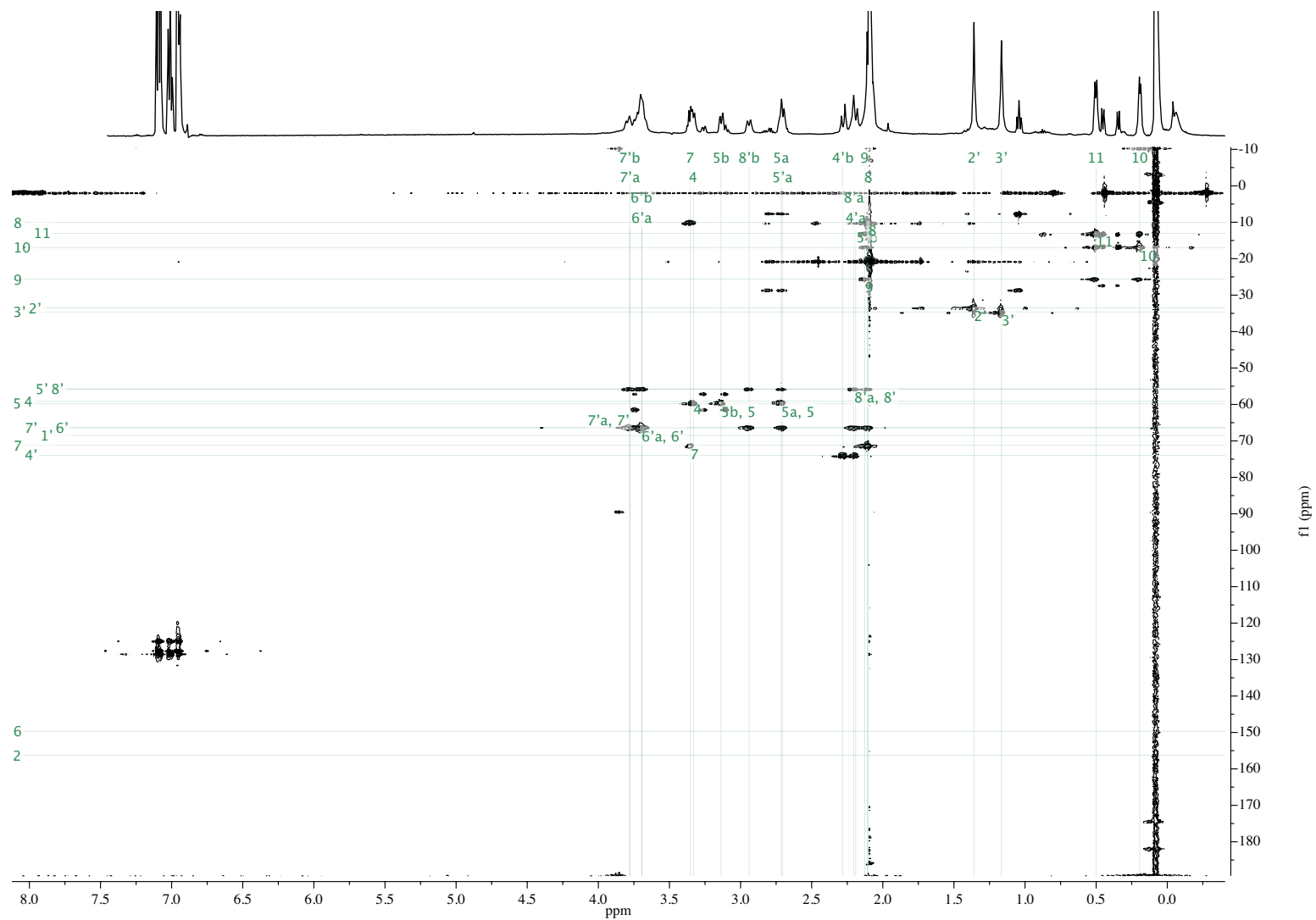


Figure 144. Full display HSQC-TOCSY spectrum of 0.10 M (*S*)-**52b** in neat toluene-*d*₈ at -40 °C. Labels indicate assignments.

Part 3. Selectivity Studies

Product ratio:

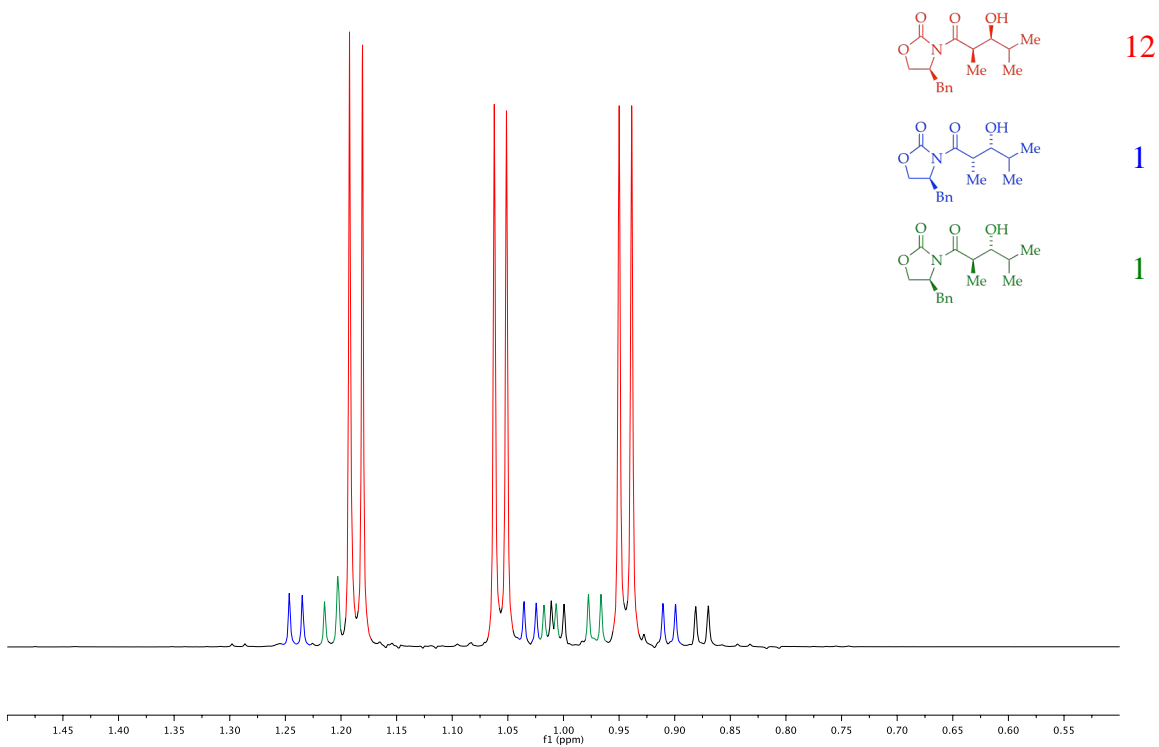


Figure 146. Crude ^1H NMR spectrum of the aldol reaction products between enolate (*S*)-**1a** and isobutyraldehyde.

Product ratio:

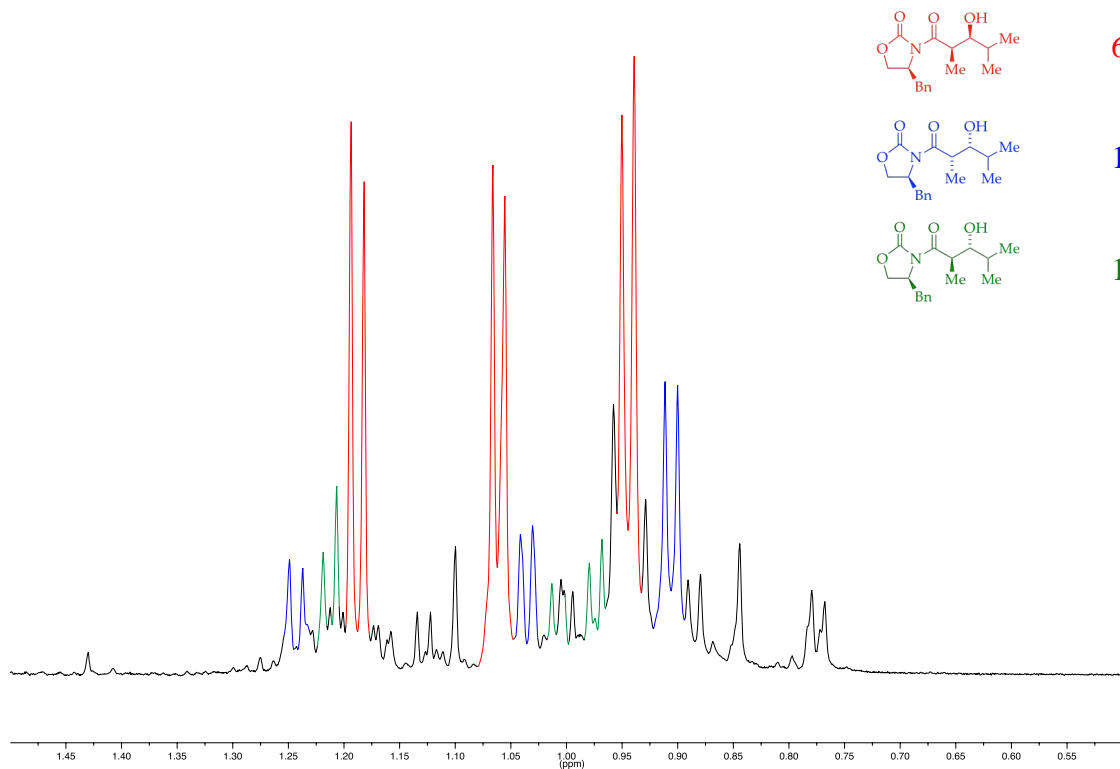


Figure 147. Crude ¹H NMR spectrum of the aldol reaction products between mixed aggregate (S)-15a and isobutyraldehyde.

Product ratio:

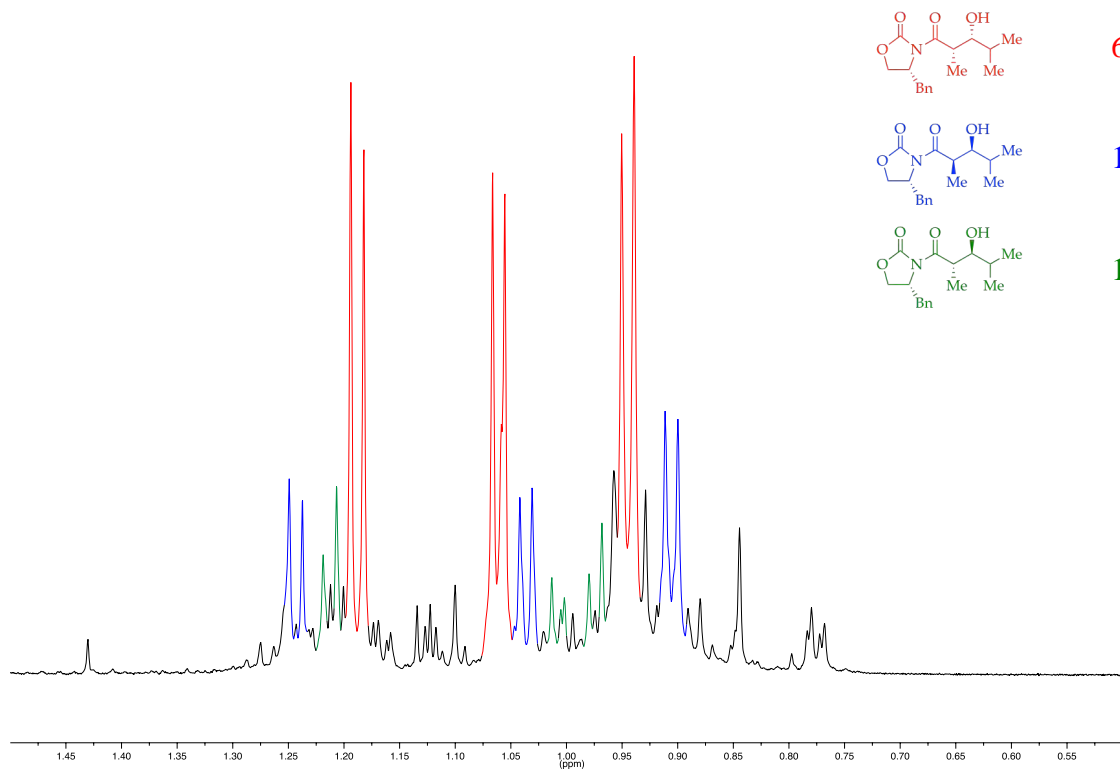


Figure 148. Crude ¹H NMR spectrum of the aldol reaction products between mixed aggregate **(R)-15a** and isobutyraldehyde.

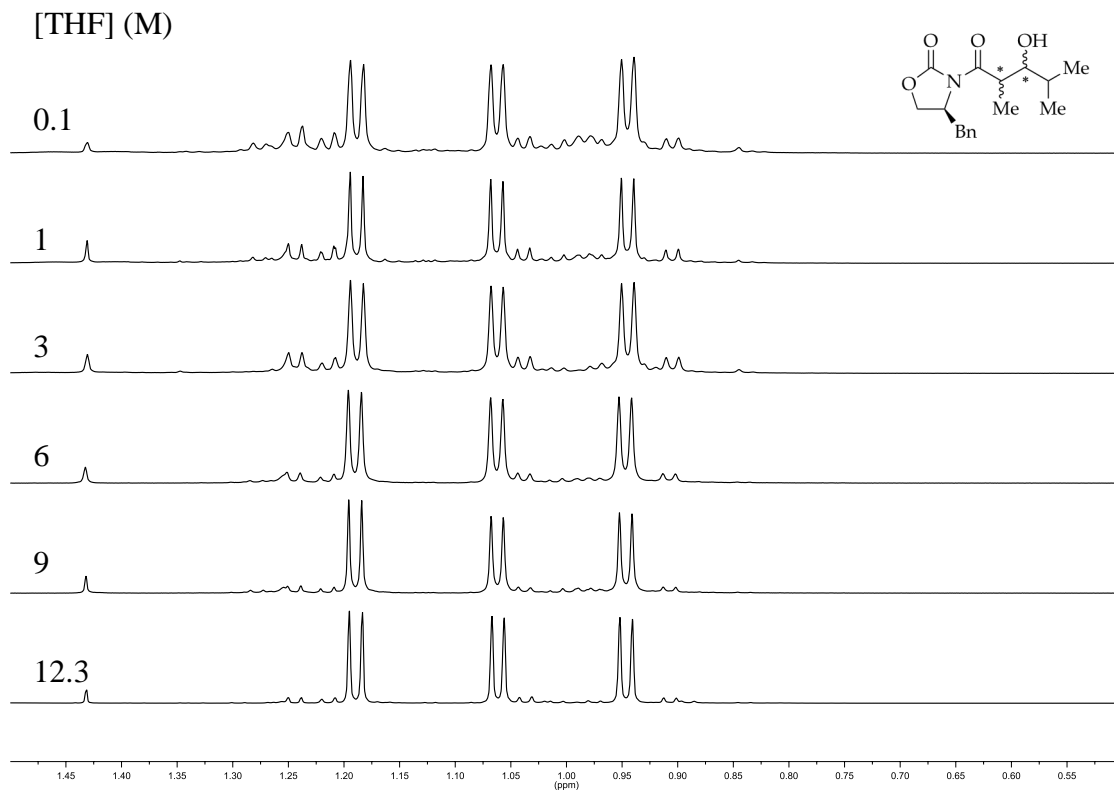


Figure 149. ^1H NMR spectra of the aldol reaction products between mixed aggregate (*S*)-**16a** and isobutyraldehyde with dependence on THF concentration of the reaction.

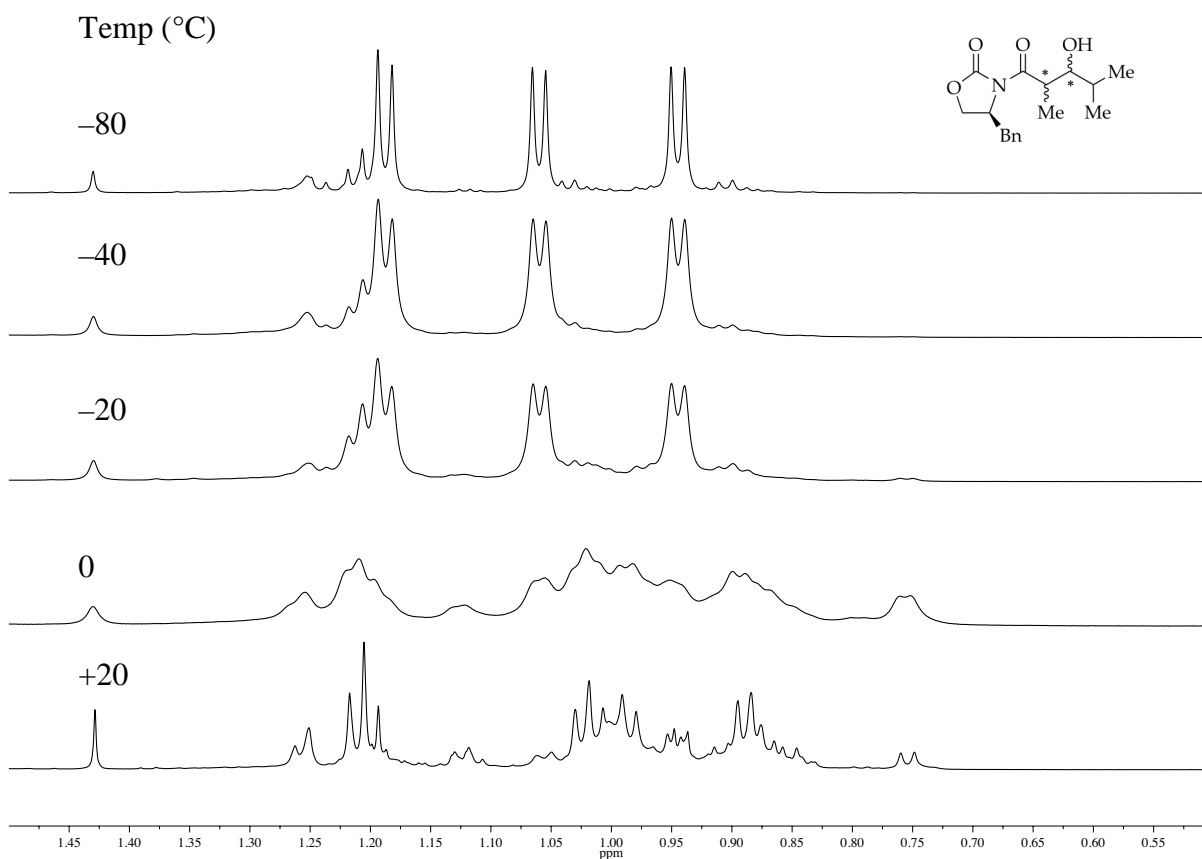


Figure 150. Crude ^1H NMR spectra of the aldol reaction products between mixed aggregate (*S*)-**16a** and isobutyraldehyde. The reactions were quenched at the mentioned temperature to show the extent of product equilibration in the mixed aggregate.

Product ratio:

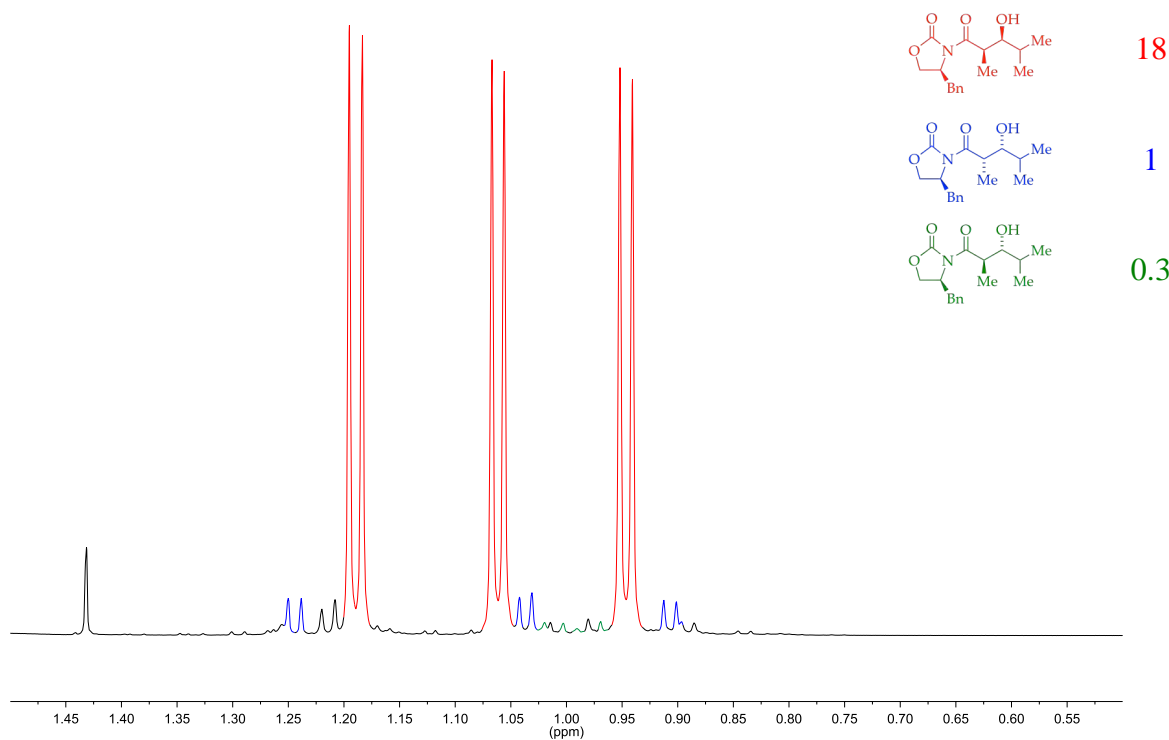


Figure 151. Crude ¹H NMR spectrum of the aldol reaction products between mixed aggregate (*S*)-**16a** and isobutyraldehyde.

Product ratio:

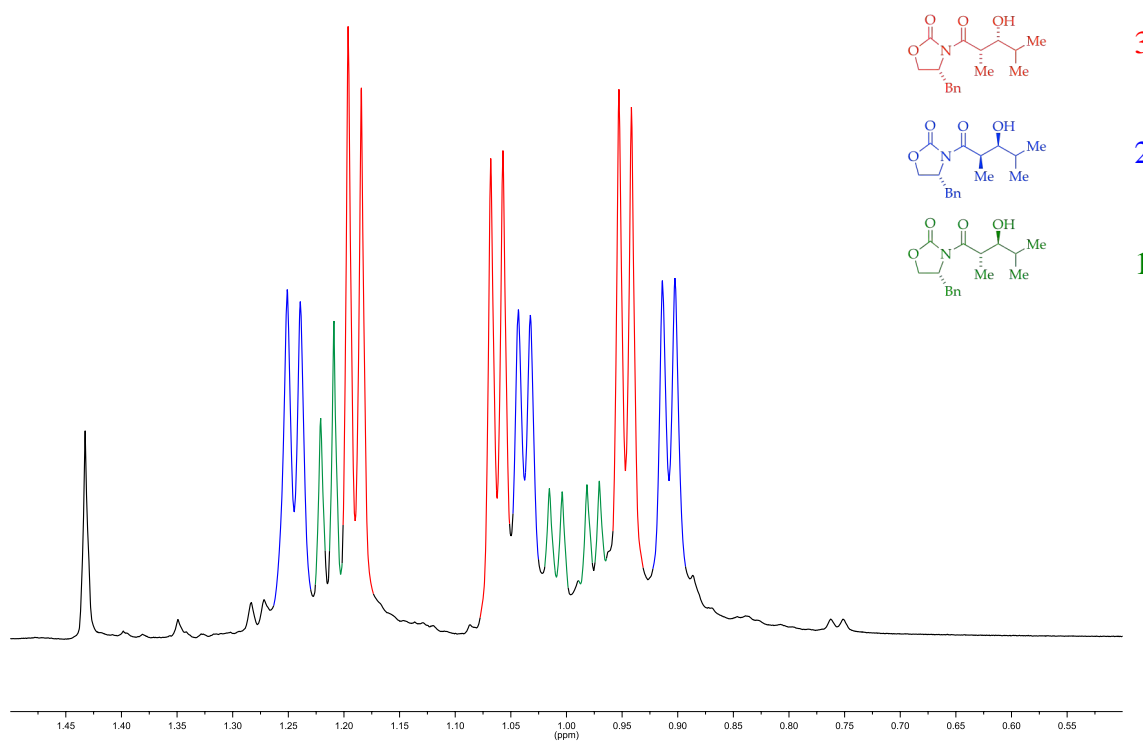


Figure 152. Crude ¹H NMR spectrum of the aldol reaction products between mixed aggregate **(R)-16a** and isobutyraldehyde.

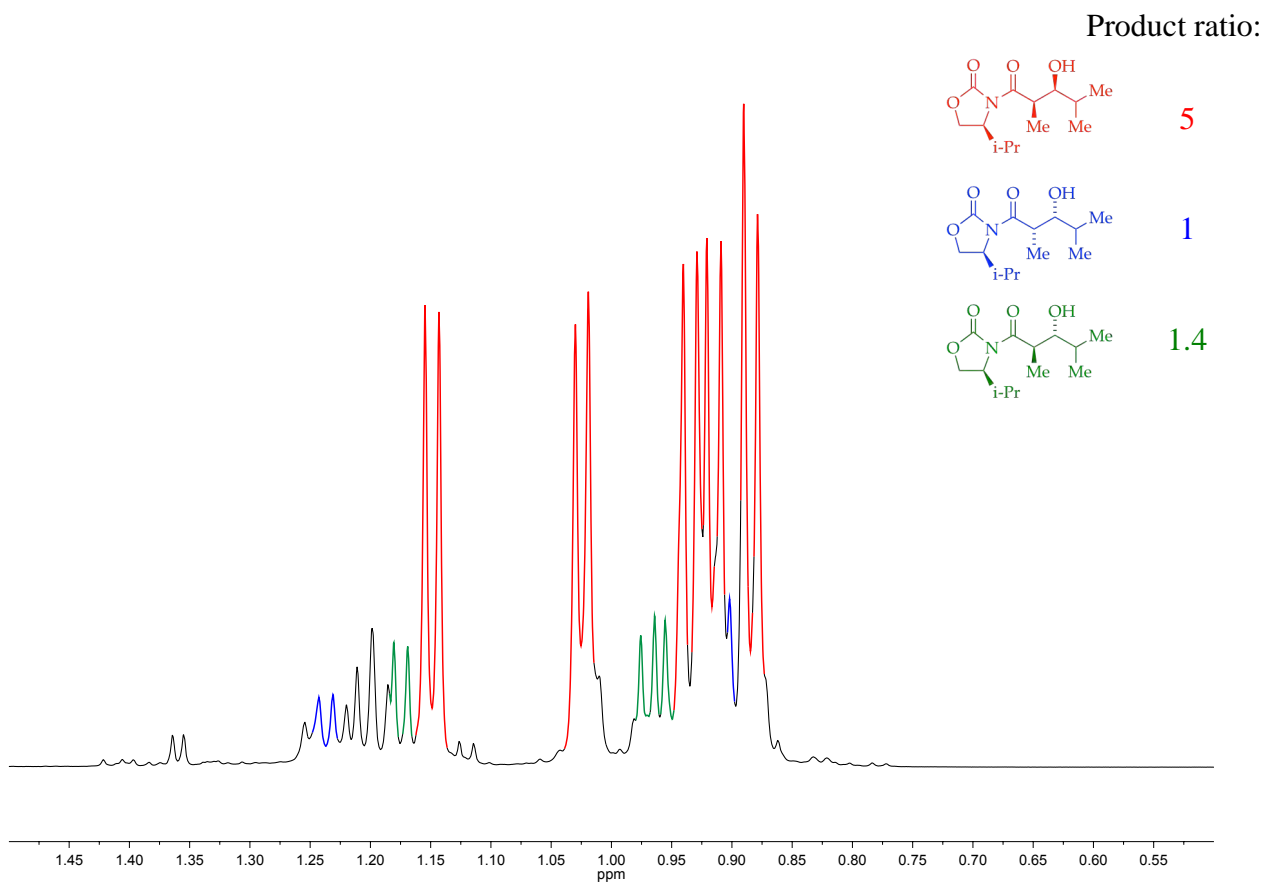


Figure 153. Crude ^1H NMR spectrum of the aldol reaction products between enolate (*S*)-**1b** and isobutyraldehyde.

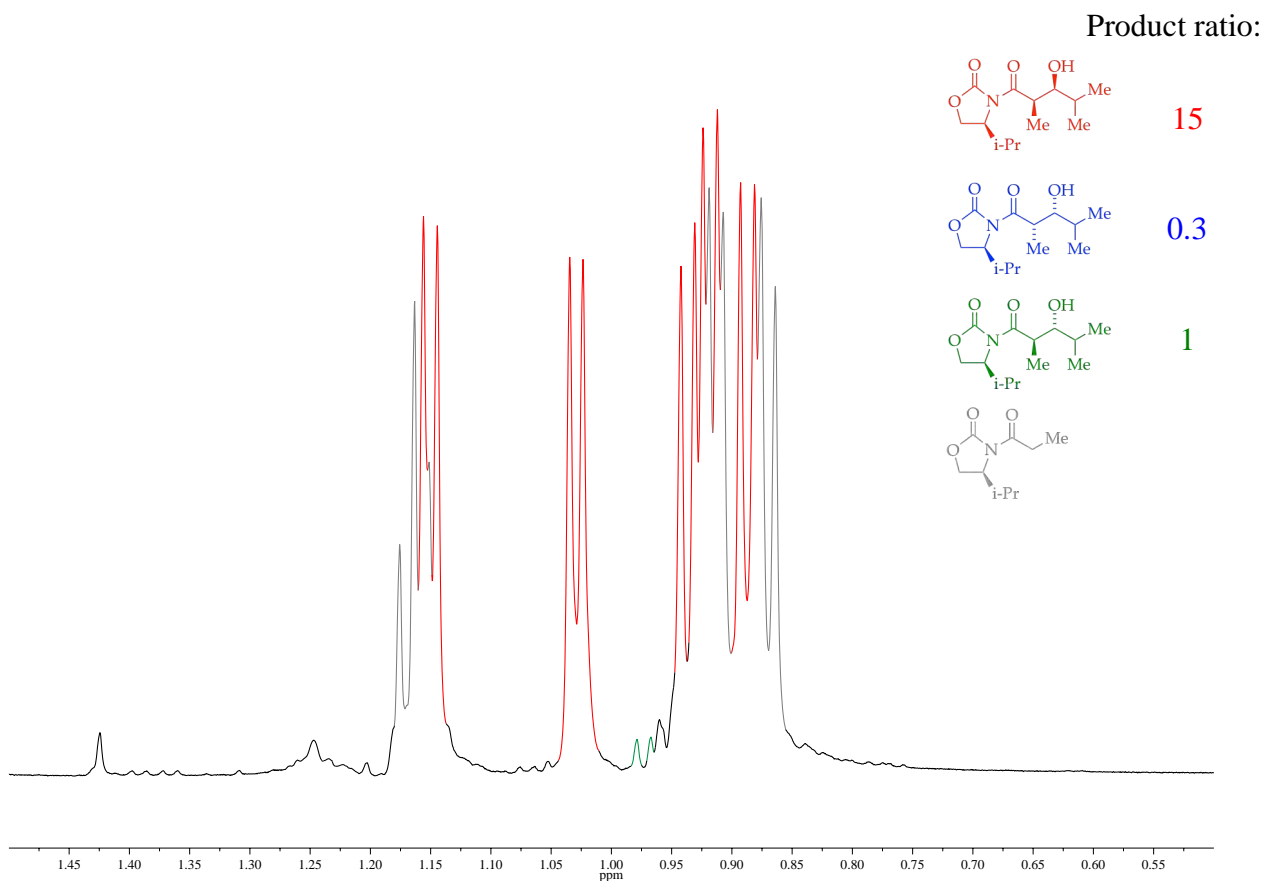


Figure 154. Crude ^1H NMR spectrum of the aldol reaction products between mixed aggregate (*S*)-**15b** and isobutyraldehyde.

* (*R*)-**15b** displays an analogous result

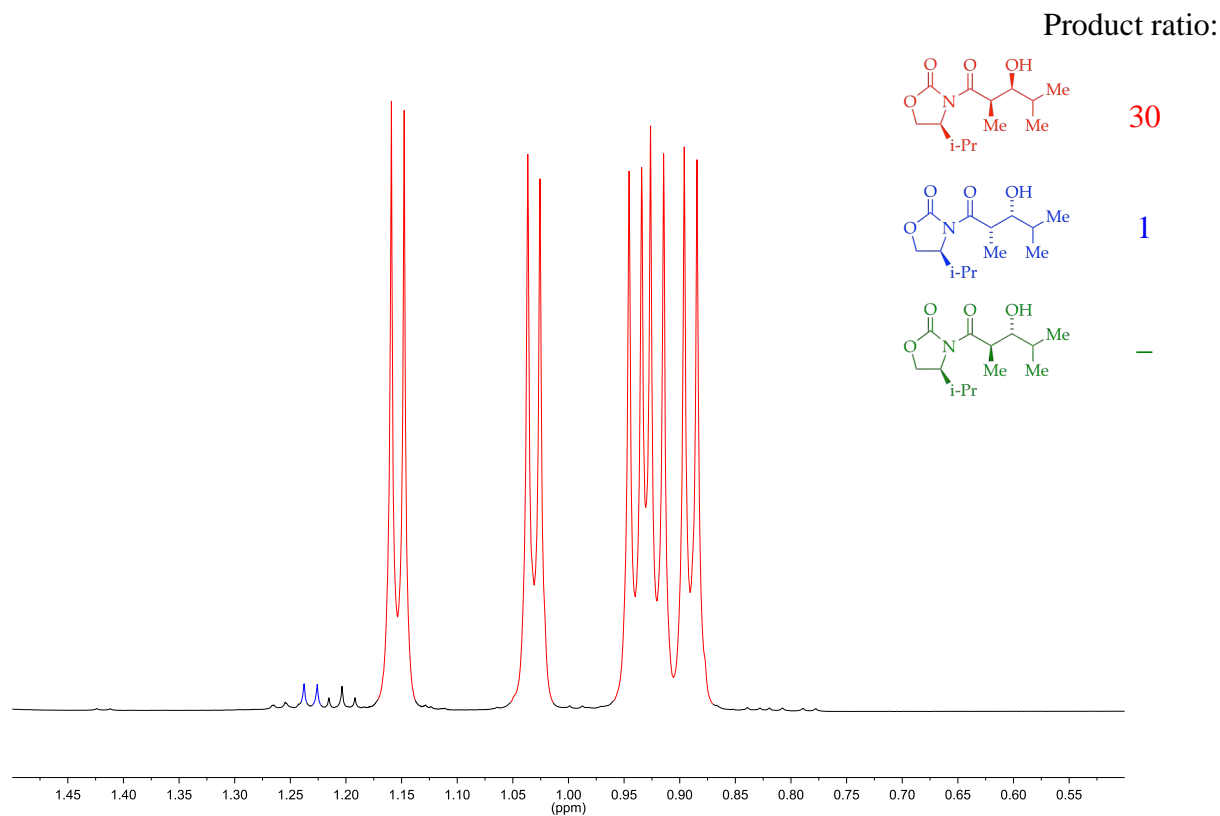


Figure 155. Crude ^1H NMR spectrum of the aldol reaction products between mixed aggregate (*S*)-**16b** and isobutyraldehyde.

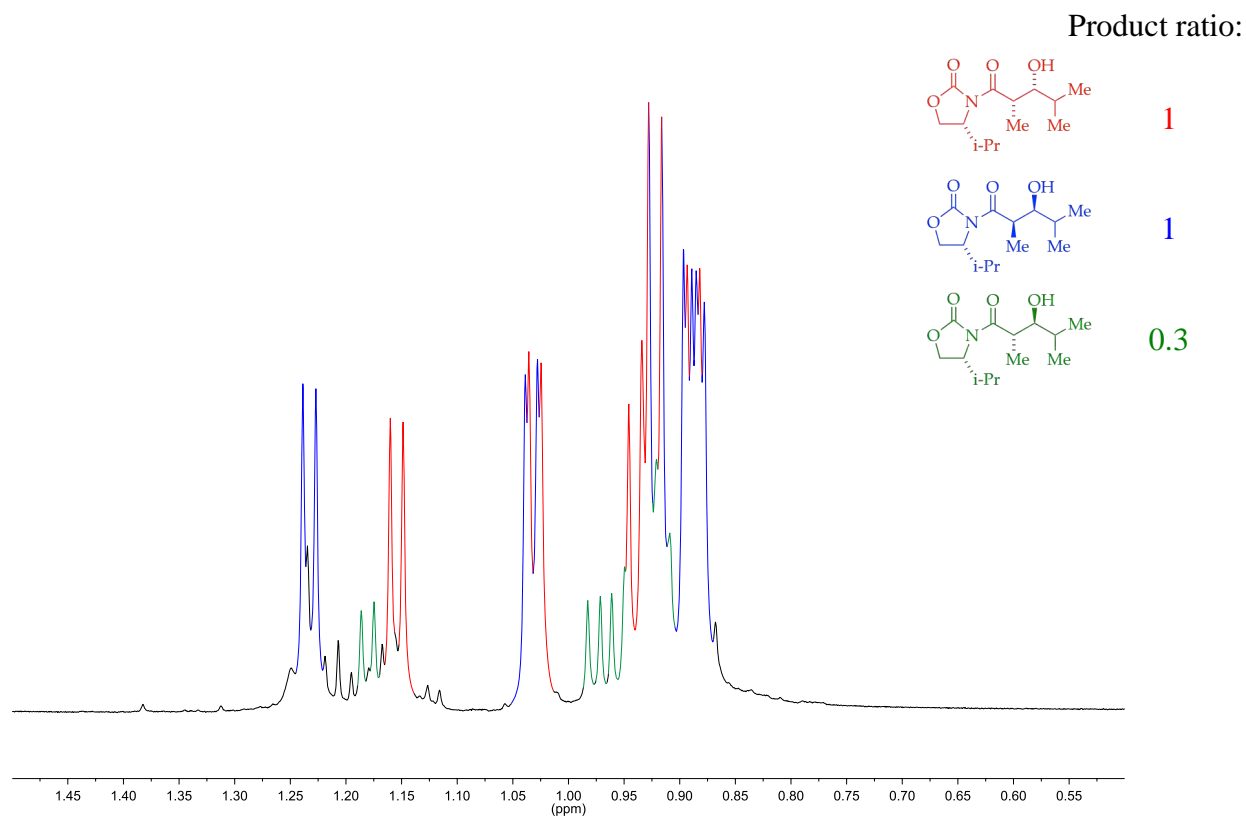


Figure 156. Crude ^1H NMR spectrum of the aldol reaction products between mixed aggregate **(R)-16b** and isobutyraldehyde.

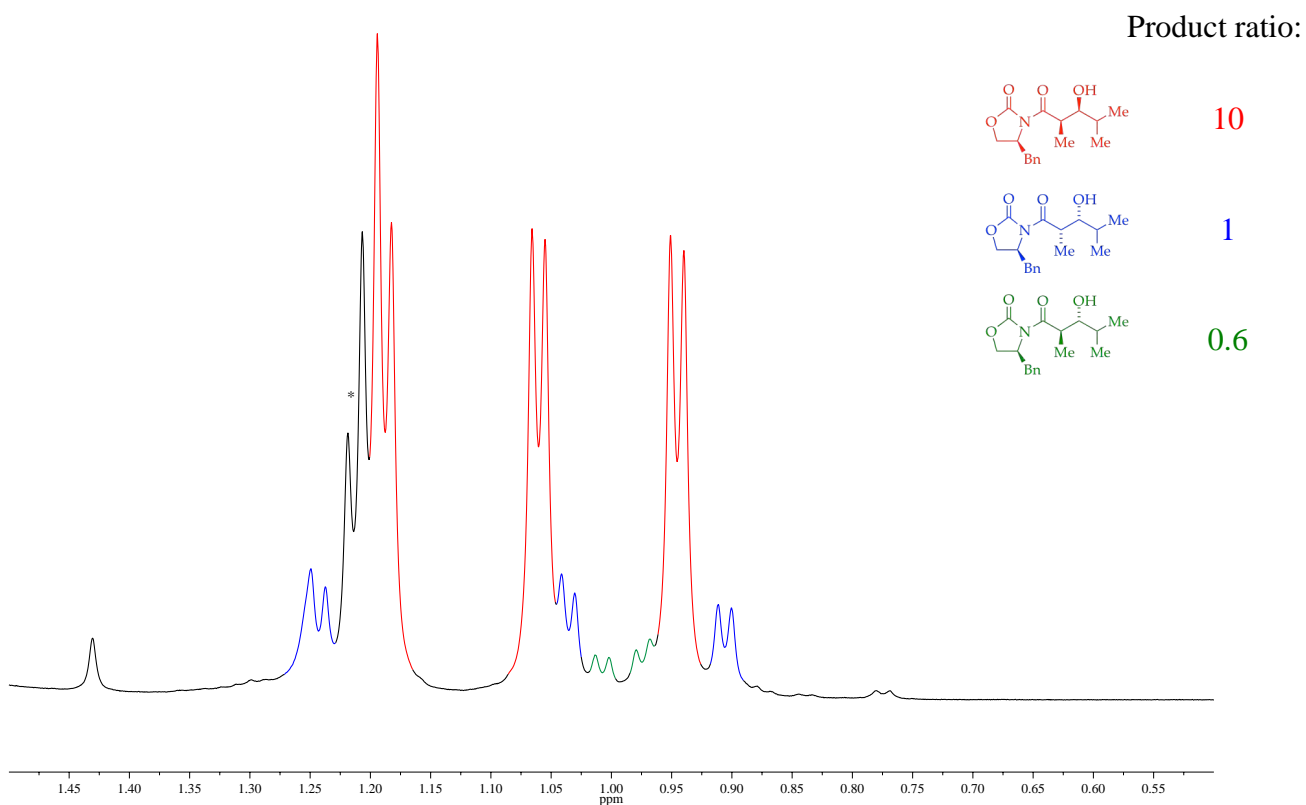


Figure 157. Crude ^1H NMR spectrum of the aldol reaction products between mixed aggregate (*S*)-**36a** and isobutyraldehyde.

* Overlapping peak of the starting material and anti aldol product.

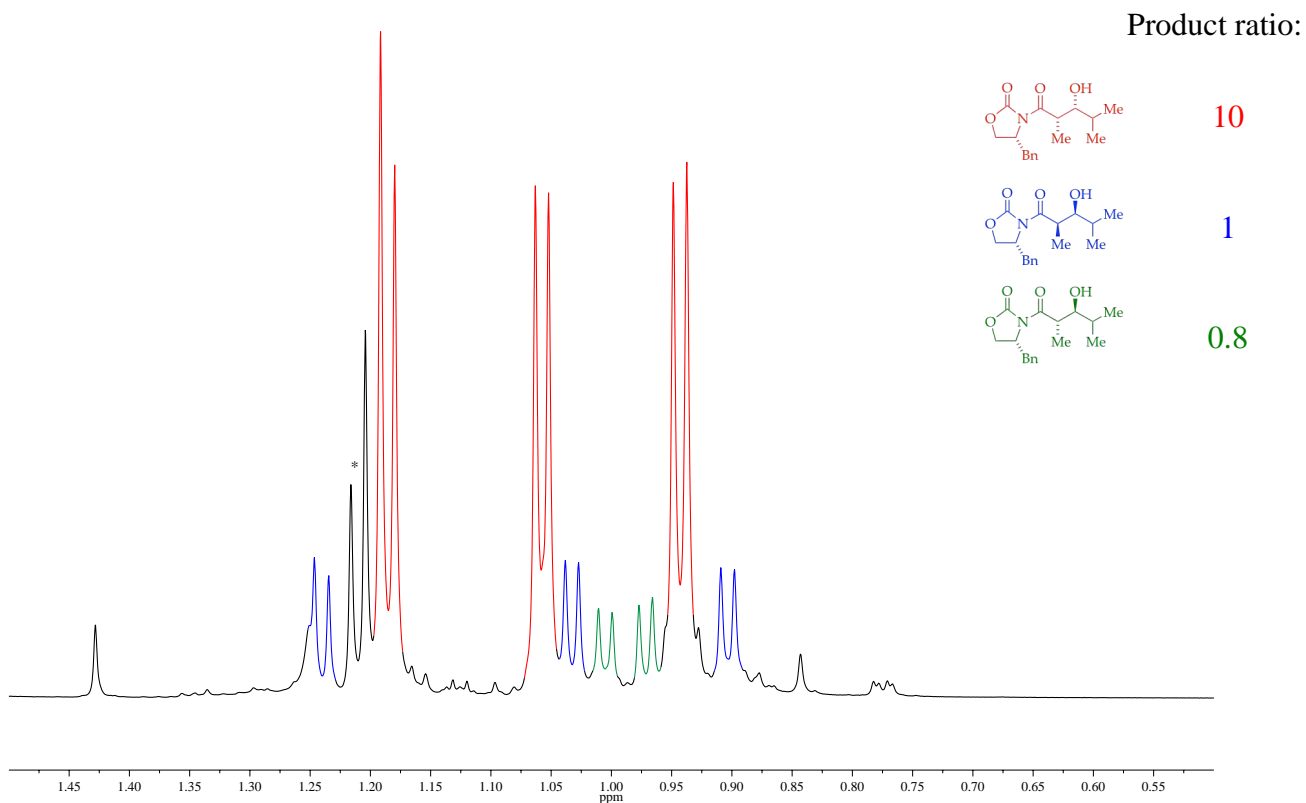


Figure 158. Crude ^1H NMR spectrum of the aldol reaction products between mixed aggregate **(R)-36a** and isobutyraldehyde.

* Overlapping peak of the starting material and anti aldol product.

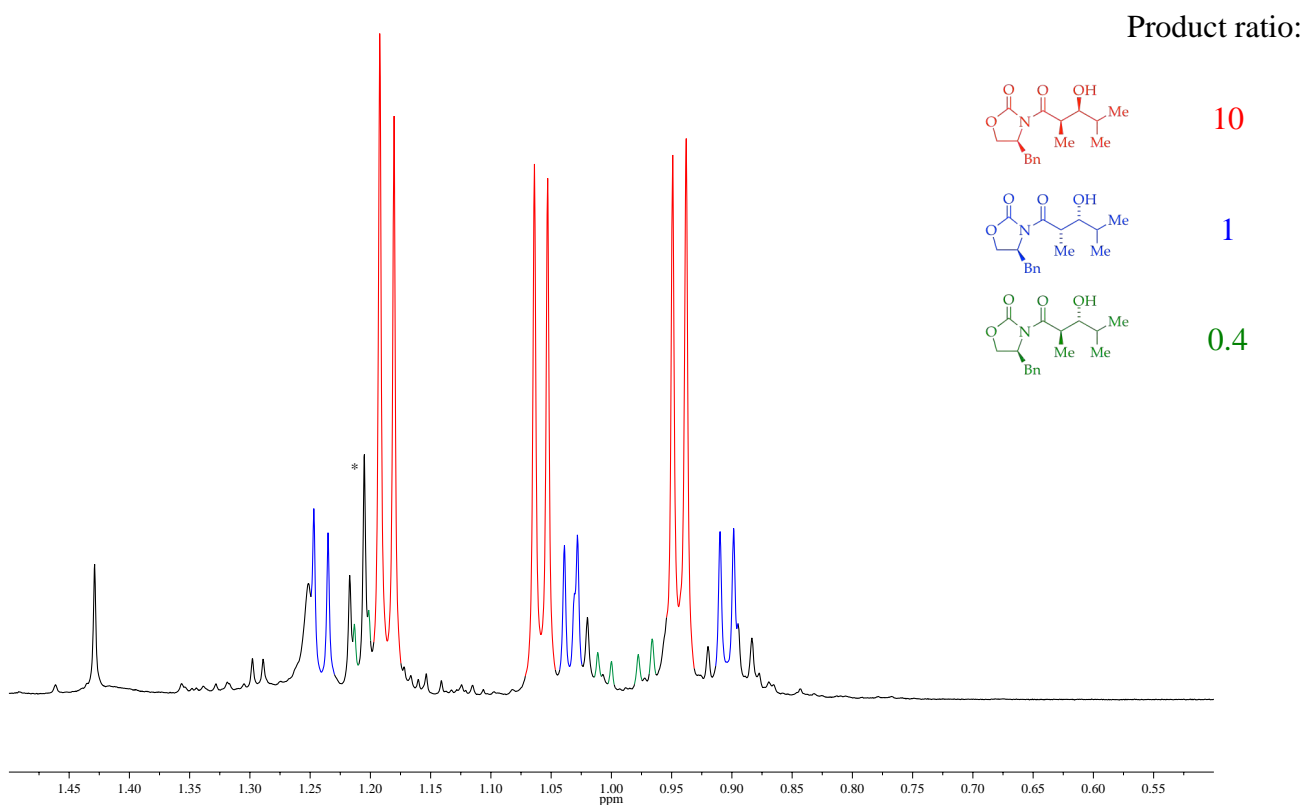


Figure 159. Crude ^1H NMR spectrum of the aldol reaction products between mixed aggregate (*S*)-**37a** and isobutyraldehyde.

* Starting material.

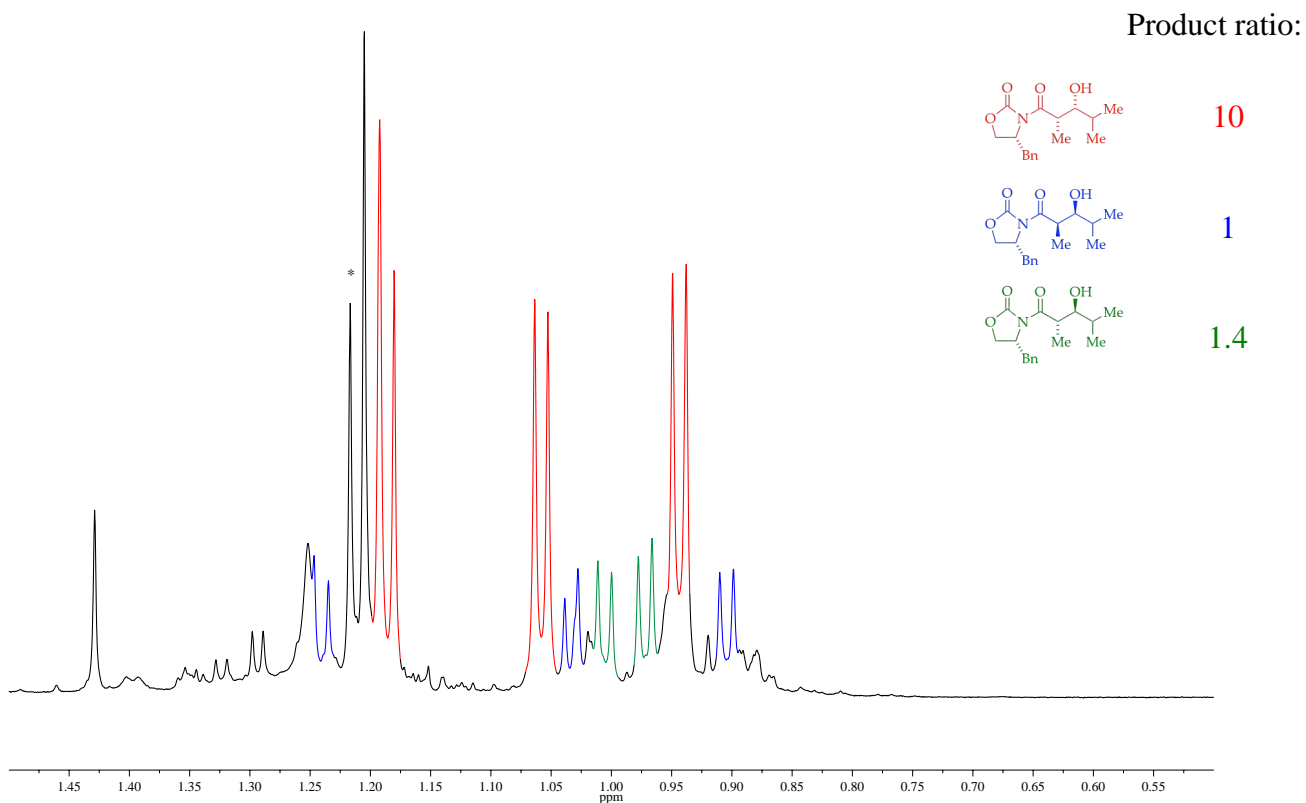


Figure 160. Crude ^1H NMR spectrum of the aldol reaction products between mixed aggregate **(R)-37a** and isobutyraldehyde.

* Overlapping peak of the starting material and anti aldol product.

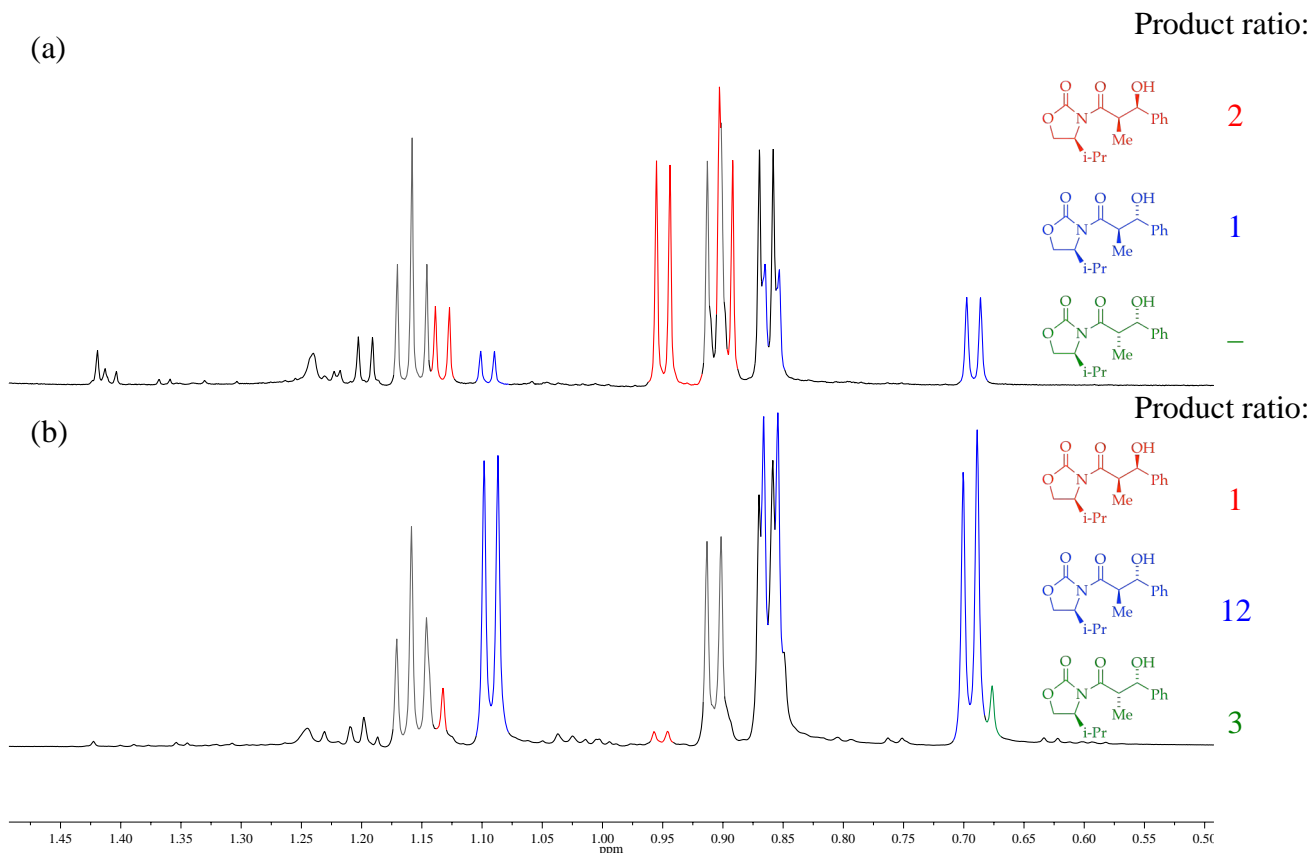


Figure 161. Crude ^1H NMR spectrum of the aldol reaction products between (a) mixed aggregate (*S*)-**16b** and (b) enolate (*S*)-**1b** with benzaldehyde. Gray peaks indicate excess starting material.

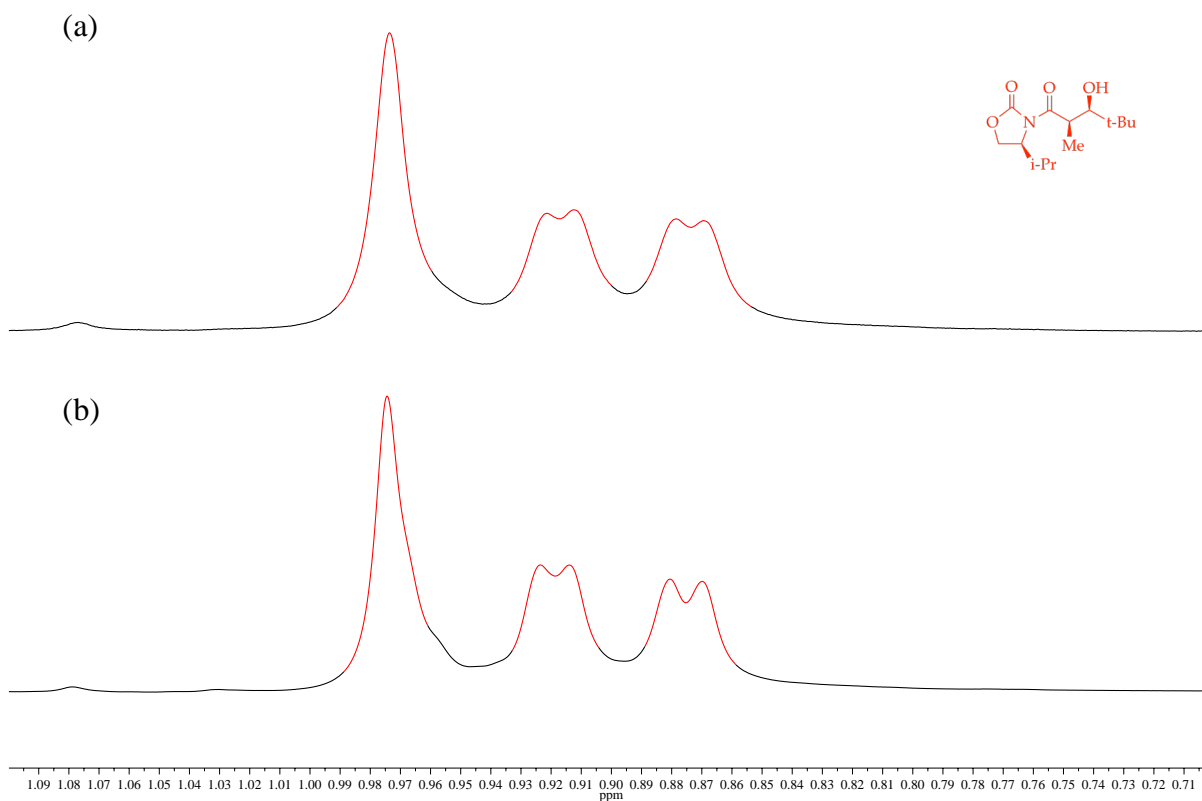


Figure 162. Crude ^1H NMR spectrum of the aldol reaction products between (a) mixed aggregate (**S**)-**16b** and (b) enolate (**S**)-**1b** with pivaldehyde.

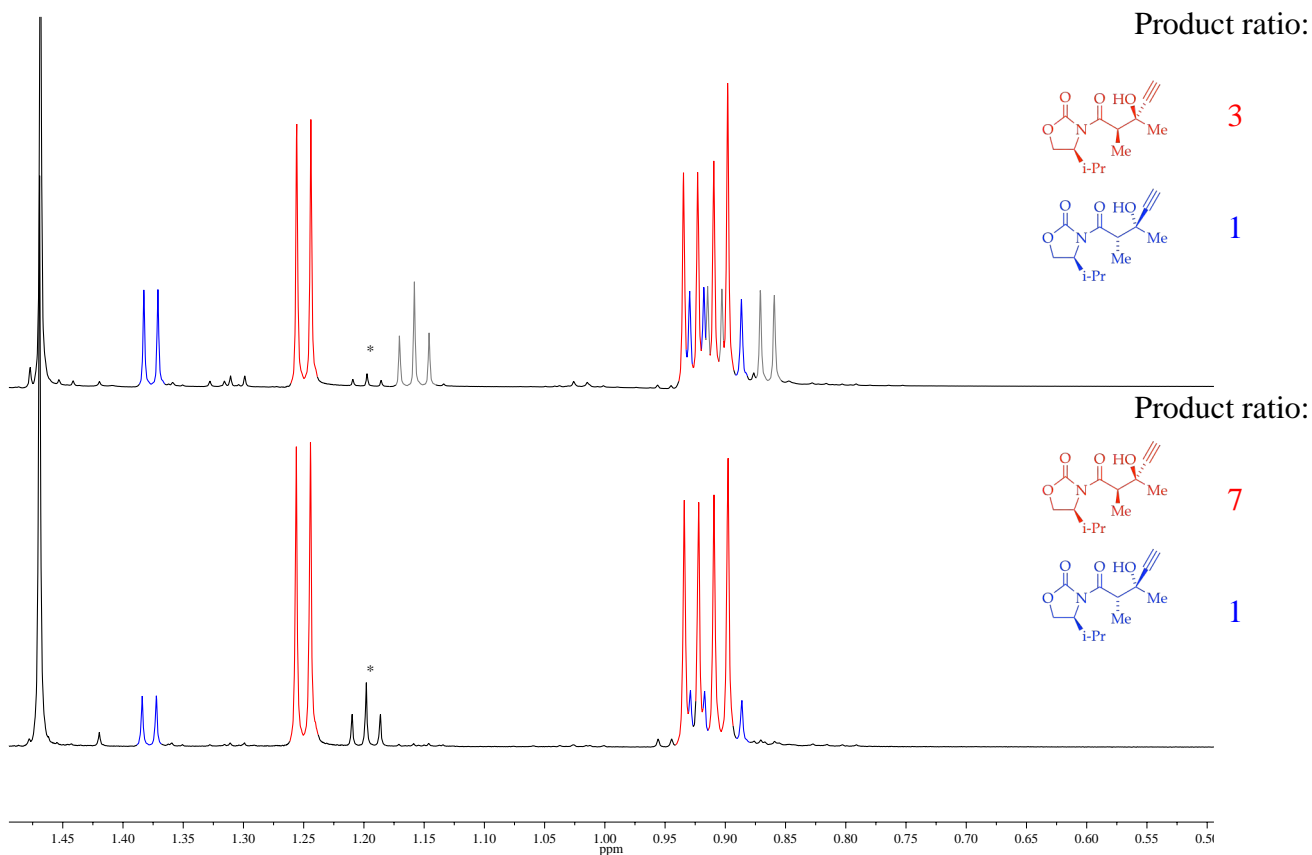


Figure 163. Crude ^1H NMR spectrum of the aldol reaction products between (a) enolate (*S*)-**1b** and (b) mixed aggregate (*S*)-**16b** with ethynyl methyl ketone. Gray peaks indicate excess starting material.

* Unknown product

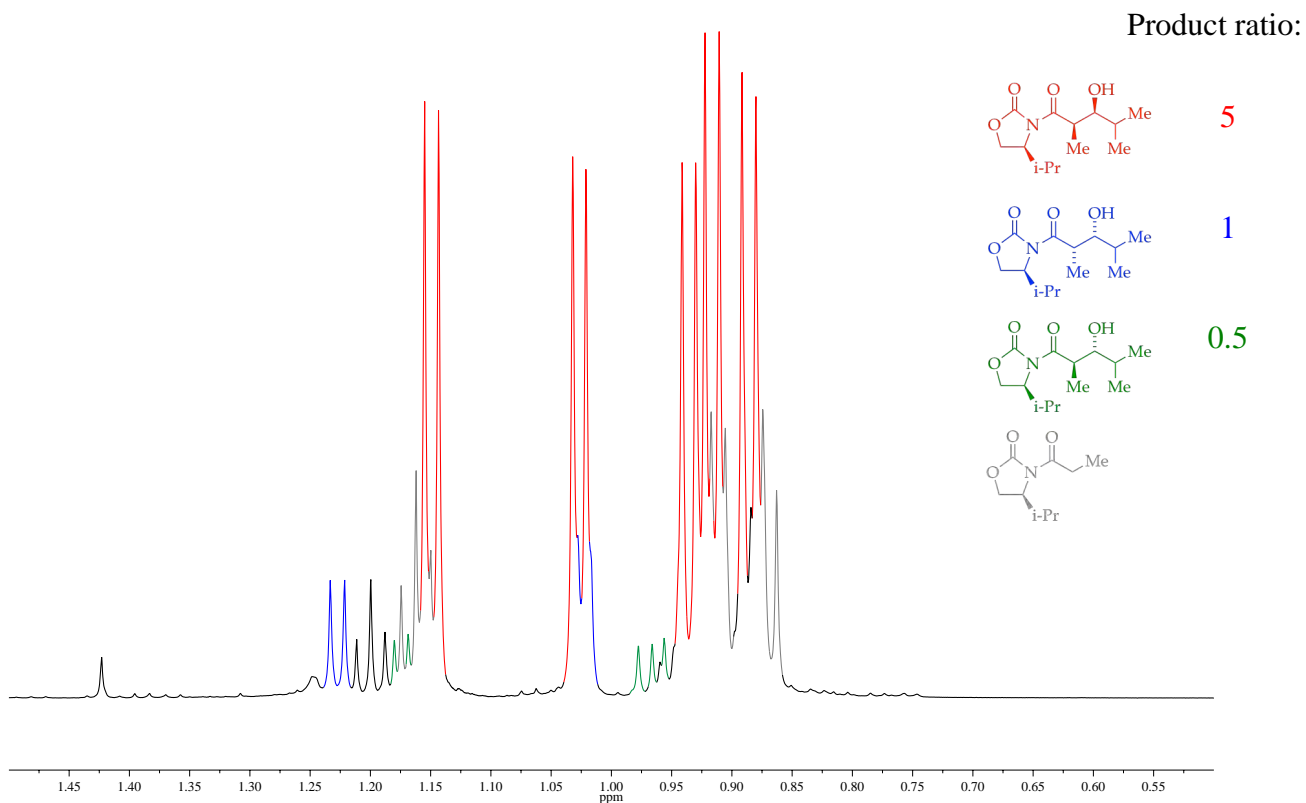


Figure 164. Crude ^1H NMR spectrum of the aldol reaction products between mixed aggregate (*S*)-**52b** and isobutyraldehyde. Gray peaks indicate excess starting material.

Part 4. Rate Studies

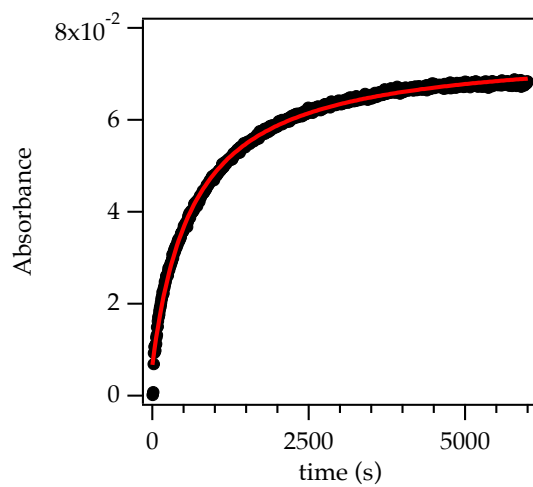


Figure 165. Plot of aldolate concentration versus time (IR spectroscopy) for the formation of **(S)-44a** (1788 cm^{-1}) carried out using mixed tetramer **(S)-16a** (0.10 M) at $-78\text{ }^{\circ}\text{C}$ under second-order conditions with pivaldehyde (0.10 M). Red curve represents a fit to $f(x) = a - a/(1 + bx) + c$.

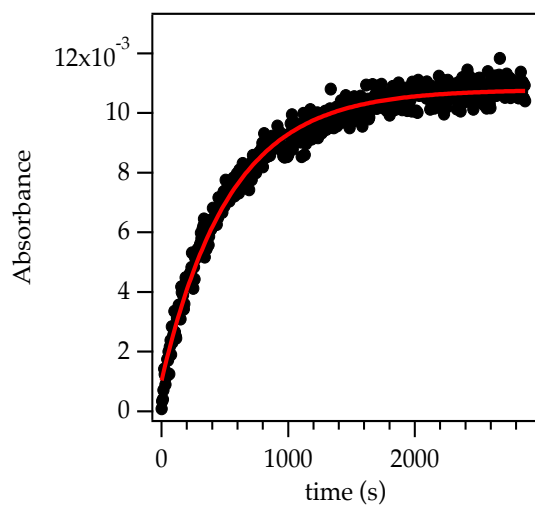


Figure 166. Plot of aldolate concentration versus time (IR spectroscopy) for the formation of **(S)-44a** (1788 cm^{-1}) carried out using mixed tetramer **(S)-16a** (0.10 M) at $-78\text{ }^{\circ}\text{C}$ under pseudo-first-order conditions with pivaldehyde (0.010 M). Red curve represents a fit to $f(x) = (a-1)e^{-bx} + c$.

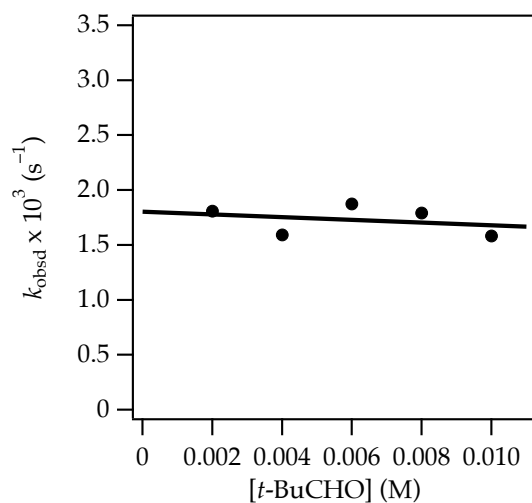


Figure 167. Plot of pseudo-first-order rate constants (k_{obsd}) vs t -BuCHO concentration in neat tetrahydrofuran (THF) at $-78\text{ }^{\circ}\text{C}$ (0.10 M (S)-**16a**, neat THF, $-78\text{ }^{\circ}\text{C}$). The curve depicts an unweighted least-squares fit to the function $f(x) = ax + b$: $a = (-1.3 \pm 2.3) \times 10^{-2}$; $b = (2 \pm 2) \times 10^{-3}$.

[t -BuCHO] M	$k_{\text{obsd}} \times 10^3 \text{ (s}^{-1}\text{)}$
0.002	1.81
0.004	1.59
0.006	1.87
0.008	1.79
0.010	1.58

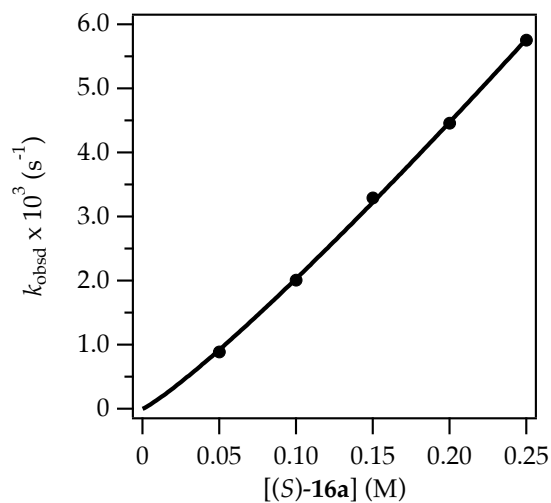


Figure 168. Plot of pseudo-first-order rate constants (k_{obsd}) vs (*S*)-**16a** concentration at 0.0050 M pivaldehyde in neat tetrahydrofuran (THF) at -78 °C. The data were fit to $y = ax^n$, such that $n = 1.14 \pm 0.02$.

[(<i>S</i>)- 16a] M	$k_{\text{obsd}} \times 10^3$ (s^{-1})
0.050	0.886
0.100	2.01
0.150	3.29
0.200	4.46
0.250	5.76

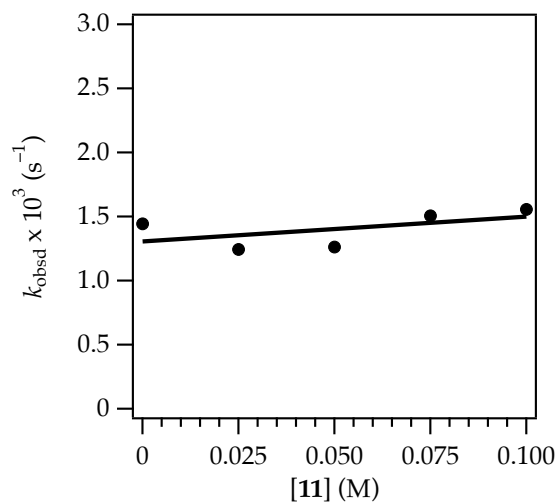


Figure 169. Plot of pseudo-first-order rate constants (k_{obsd}) vs **11** concentration in neat tetrahydrofuran (THF) at $-78\text{ }^{\circ}\text{C}$ (0.10 M **(S)-16a**, neat THF, $-78\text{ }^{\circ}\text{C}$). The curve depicts an unweighted least-squares fit to the function $f(x) = ax + b$: $a = (1.94 \pm 1.8) \times 10^{-3}$; $b = (1.31 \pm 0.11) \times 10^{-3}$.

[11] M	$k_{\text{obsd}} \times 10^3 \text{ (s}^{-1}\text{)}$
0	1.44
0.025	1.24
0.050	1.26
0.075	1.50
0.10	1.57

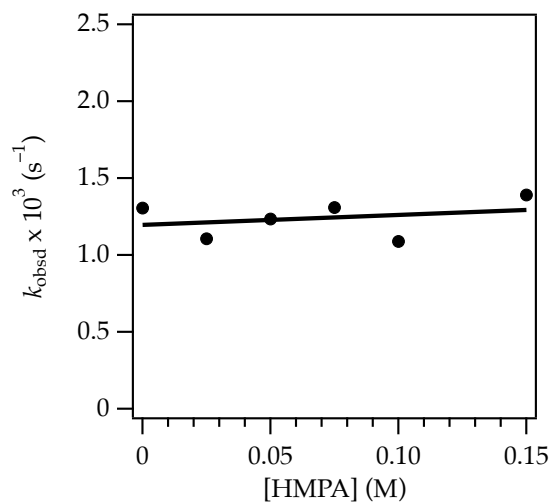


Figure 170. Plot of pseudo-first-order rate constants (k_{obsd}) vs HMPA concentration in neat tetrahydrofuran (THF) at $-78\text{ }^{\circ}\text{C}$ (0.10 M (S)-**16a**, neat THF, $-78\text{ }^{\circ}\text{C}$). The curve depicts an unweighted least-squares fit to the function $f(x) = ax + b$: $a = (6.4 \pm 10.6) \times 10^{-4}$; $b = (1.20 \pm 0.09) \times 10^{-3}$.

[HMPA] M	$k_{\text{obsd}} \times 10^3 \text{ (s}^{-1}\text{)}$
0	1.31
0.025	1.11
0.050	1.23
0.075	1.09
0.10	1.39

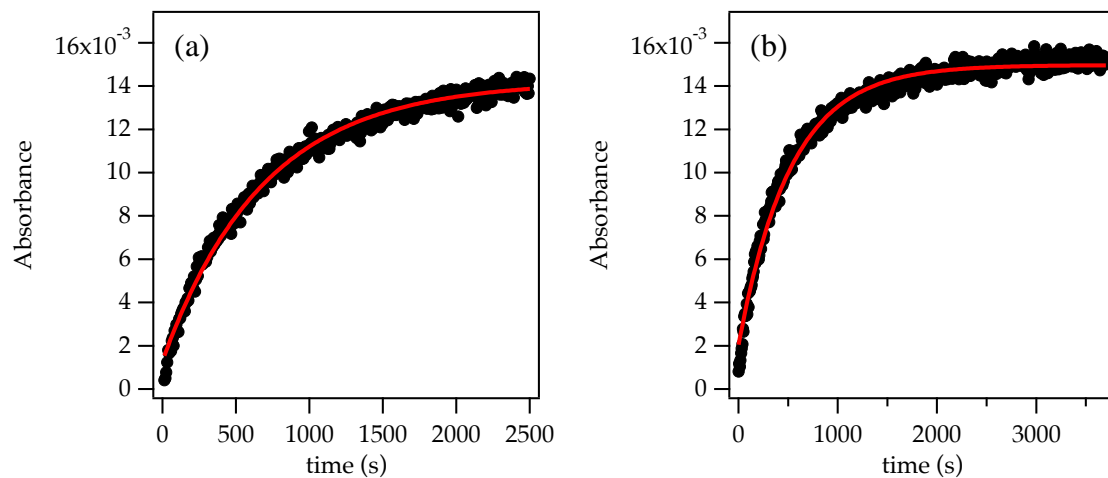
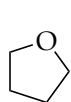


Figure 171. Plot of aldolate concentration versus time (IR spectroscopy, 1788 cm^{-1}) carried out using mixed tetramer (**S**)-**16a** (0.10 M) at $-78 \text{ }^\circ\text{C}$ under pseudo-first-order conditions with: (a) pivaldehyde (0.010 M); (b) pivaldehyde-*d* (0.010 M). Red curves represent fits to $f(x) = (a-1)e^{-bx} + c$. $k_H/k_D = 0.77 \pm 0.016$.

Part 5. Computations

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

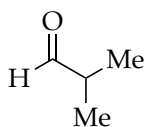
Table 10. Geometric coordinates and thermally corrected MP2 energies for **THF**



$$G = -232.349384$$
$$G_{\text{MP2}} = -231.569879$$

Atom	X	Y	Z	Atom	X	Y	Z
C	0.00000000	0.00000000	0.00000000	O	-0.73331100	-2.24858800	-0.22715800
H	0.06320400	0.15873800	1.08328900	C	0.43208200	-1.42748600	-0.35845700
H	0.61015700	0.76456500	-0.49095800	H	1.21529000	-1.82013100	0.30070600
C	-1.46729300	-0.00033900	-0.45381300	H	0.80244900	-1.48014300	-1.39416900
H	-1.53059400	0.15785900	-1.53717400	H	-2.68246900	-1.82083900	-0.75299500
H	-2.07768600	0.76422300	0.03685600	H	-2.26811000	-1.48024900	0.94140300
C	-1.89874200	-1.42780200	-0.09469900				

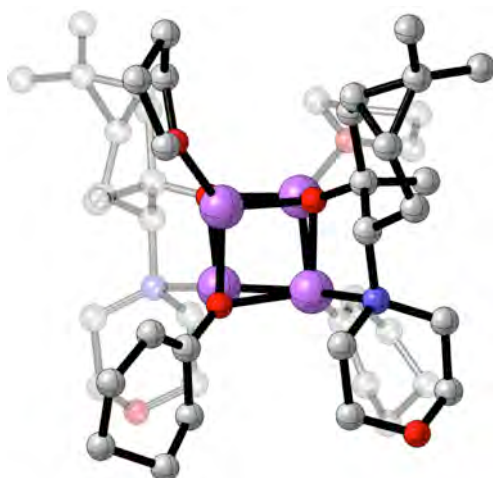
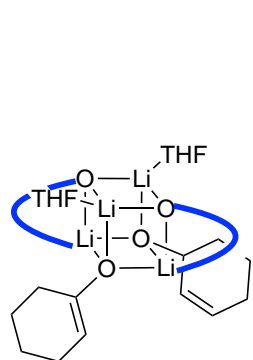
Table 11. Geometric coordinates and thermally corrected MP2 energies for **isobutyraldehyde**



$$G = -232.363544$$
$$G_{\text{MP2}} = -231.5853565$$

Atom	X	Y	Z	Atom	X	Y	Z
C	0.00000000	0.00000000	0.00000000	H	-0.97876300	-0.84739100	-1.76264900
C	1.35825200	-0.64247100	-0.21642300	H	-1.03772400	-1.90679400	-0.34086300
O	2.32728500	-0.08817100	-0.68588300	C	-0.02488200	1.45908100	-0.45726000
H	1.41543300	-1.71265200	0.09428100	H	-0.99317700	1.91827800	-0.23079400
H	-0.17199100	-0.04888300	1.08902500	H	0.76022900	2.04023200	0.03518600
C	-1.08708400	-0.86257100	-0.67179900	H	0.14434900	1.52988600	-1.53710400
H	-2.08343300	-0.48022400	-0.42704300				

Table 12. Geometric coordinates and thermally corrected MP2 energies for **18a**

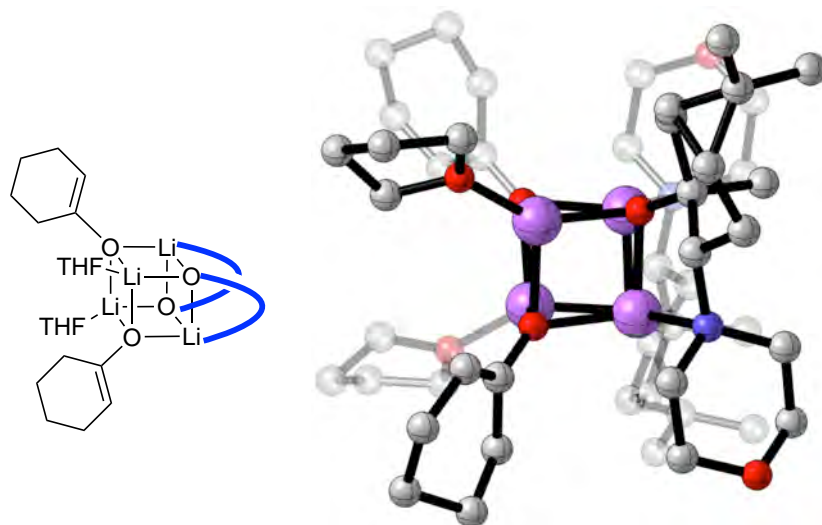


$G = -2618.987508$
 $G_{\text{MP2}} = -2611.435743$

Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	H	5.36896700	2.22933400	-2.58101400
O	-0.08023400	2.02256100	-0.26406100	H	5.64596400	2.47079400	-0.07718200
Li	-0.87456600	1.43685900	-1.97089400	H	4.21686800	2.26646700	0.95035500
Li	0.85467900	-0.48874700	-2.41846300	C	5.98957400	-2.63068100	-0.20646600
O	0.79292100	1.47635000	-2.99965400	C	6.06414600	-2.42402800	1.29509600
Li	1.61073700	1.69097300	-1.22602700	H	7.07598300	-2.12478900	1.59895100
O	1.78601600	-0.16260200	-0.75878800	H	5.36890500	-1.66578300	1.66072300
C	3.05490000	-0.41436900	-0.22434300	H	5.82777900	-3.35920200	1.81952600
C	3.37017900	-1.96939500	-0.31700800	C	6.88860700	-3.76130300	-0.68623400
H	3.25481200	-2.41584900	0.68009900	H	7.93951400	-3.56526100	-0.43467100
H	2.55037000	-2.36813100	-0.91753100	H	6.60841200	-4.71494200	-0.21908500
C	4.67880400	-2.44593500	-0.95539900	H	6.82757200	-3.89249200	-1.77281700
C	5.82021800	-1.46465100	-1.16249100	H	4.53223100	-3.16518500	-1.76064000
H	6.36608800	-1.55407700	-2.10134200	C	3.03951500	-0.00249600	1.26647700
C	5.57404900	-0.02779100	-0.72490000	H	2.38485800	-0.69199900	1.80851500
H	6.27947000	0.62798200	-1.24789900	H	4.02289300	-0.03084100	1.75214100
H	5.77612400	0.10428300	0.34342300	H	2.62171000	1.00210800	1.38502600
C	4.12001300	0.37341500	-1.06094300	C	1.08437000	2.04697200	-4.17603400
H	3.93678200	0.04667400	-2.09222500	C	0.71842800	3.52101800	-4.29715500
N	3.86661500	1.85540700	-1.09721900	H	0.99319300	4.03058300	-3.36343200
C	4.55509800	2.61420100	-0.02706000	H	-0.37672300	3.60809600	-4.36122900
C	4.28215500	4.10976100	-0.15534900	C	1.35989500	4.22263900	-5.50277100
H	4.83838600	4.65842500	0.61123400	H	0.89607200	5.20536900	-5.65783100
H	3.20792900	4.31518600	-0.01981000	H	2.42412100	4.40844800	-5.29674300
O	4.71770400	4.60890400	-1.41035600	C	1.23943300	3.35575500	-6.76023400
C	4.05019900	3.92070500	-2.45892900	C	1.96311700	2.01620100	-6.56032700
H	4.43398000	4.32895000	-3.39856300	H	1.68250200	1.32508100	-7.36919800
H	2.96908300	4.12659400	-2.40921400	H	3.04953200	2.17442400	-6.68061300
C	4.29518900	2.41564100	-2.40238600	C	1.65617000	1.39441200	-5.21658200
H	3.72360000	1.93225900	-3.20152000	H	1.90375900	0.34276400	-5.08343800

H	1.64355600	3.88187300	-7.63481400	C	2.03757500	-4.50028100	-3.39438200
H	0.17545000	3.16823400	-6.96496100	H	2.77369000	-4.55282800	-2.58441800
O	-0.93816000	-0.46941000	-1.65043900	H	1.64489300	-5.50723200	-3.56497700
C	-2.11364500	-0.94905600	-2.24687200	C	0.93753800	-3.49656900	-3.05197800
C	-2.40674200	-2.43209400	-1.75511500	H	0.69708700	-3.44422400	-1.98741600
H	-2.28558400	-3.11799900	-2.60366200	H	0.01559700	-3.70806400	-3.60835100
H	-1.58649100	-2.66012000	-1.06889000	H	2.05455000	-4.10012300	-5.53267200
C	-3.72381700	-2.74096800	-1.03805100	H	3.68368300	-4.20386200	-4.84257900
C	-4.91680300	-1.82210100	-1.24290500	H	2.44735600	-1.74682400	-5.21200800
H	-5.52447800	-1.61981600	-0.36129300	H	3.48245500	-2.02908100	-3.79112200
C	-4.69160300	-0.60735300	-2.13096100	C	-0.50043600	2.97135200	0.57842200
H	-5.47454600	0.13274600	-1.92824700	C	0.15270000	4.33474400	0.39380900
H	-4.78369100	-0.86140100	-3.19262900	H	0.21508700	4.54644800	-0.68316400
C	-3.29873300	-0.00985100	-1.83162900	H	1.19437200	4.26813000	0.74554500
H	-3.21264600	0.04923500	-0.73965200	C	-0.56710600	5.47612000	1.12589900
N	-3.10412600	1.40631600	-2.29279500	H	0.06219600	6.37544200	1.13475200
C	-3.72695000	1.72107600	-3.59938700	H	-1.48388700	5.74099800	0.57953500
C	-3.45699000	3.17324700	-3.98264600	C	-0.93918100	5.05257200	2.55019900
H	-3.95868500	3.41337600	-4.92526700	C	-1.89093700	3.84844200	2.51773800
H	-2.37429500	3.32611700	-4.11561000	H	-1.98281600	3.42789100	3.53084600
O	-3.96345700	4.07607100	-3.01195400	H	-2.90565100	4.20226400	2.26226300
C	-3.39634900	3.79893400	-1.73804100	C	-1.43008900	2.78106100	1.54901100
H	-3.85676400	4.49570800	-1.03149900	H	-1.88386300	1.79437600	1.63493000
H	-2.31105400	3.99400600	-1.75563400	H	-1.39660300	5.88700900	3.09742800
C	-3.65350700	2.36039100	-1.30111600	H	-0.02292800	4.77891000	3.09339400
H	-3.16474100	2.19681300	-0.33724000	O	-0.55807000	-0.73389700	1.82856000
H	-4.74140000	2.21717600	-1.17275400	C	-0.16321000	-0.18614300	3.11408900
H	-4.81855400	1.57791200	-3.56104400	C	-1.20666100	-0.67368900	4.13447700
H	-3.32860100	1.06297400	-4.37267500	C	-2.40364500	-1.06387300	3.25210300
C	-4.97033700	-3.25006600	-1.74946600	H	-3.00886600	-0.18319300	3.00878500
C	-4.94200100	-3.56354400	-3.23407200	H	-3.05523700	-1.81129500	3.71521200
H	-4.60438900	-4.59501300	-3.40079100	C	-1.70659700	-1.58520500	1.99795900
H	-5.94554500	-3.47273200	-3.67007400	H	-2.30625600	-1.51387500	1.08923300
H	-4.27480600	-2.90969300	-3.80055900	H	-1.37862600	-2.62769600	2.12625900
C	-5.85412600	-4.20748600	-0.96318900	H	-0.83546400	-1.55048800	4.67748900
H	-6.89246800	-4.17108900	-1.31896600	H	-1.45136500	0.09660800	4.87144700
H	-5.50454900	-5.24349700	-1.06591700	H	0.84607300	-0.53432900	3.35269300
H	-5.86120700	-3.96390100	0.10558300	H	-0.15147800	0.90240400	3.00892400
H	-3.59921700	-3.13687400	-0.03086100				
C	-1.90530900	-0.98436100	-3.78170400				
H	-1.12529100	-1.71383500	-4.02192700				
H	-2.80632200	-1.26923100	-4.34060900				
H	-1.55286300	-0.01737600	-4.15231200				
O	1.44364500	-2.20461500	-3.45886500				
C	2.58931100	-2.37245300	-4.32709400				
C	2.66045100	-3.86863600	-4.64881300				

Table 13. Geometric coordinates and thermally corrected MP2 energies for **18b**

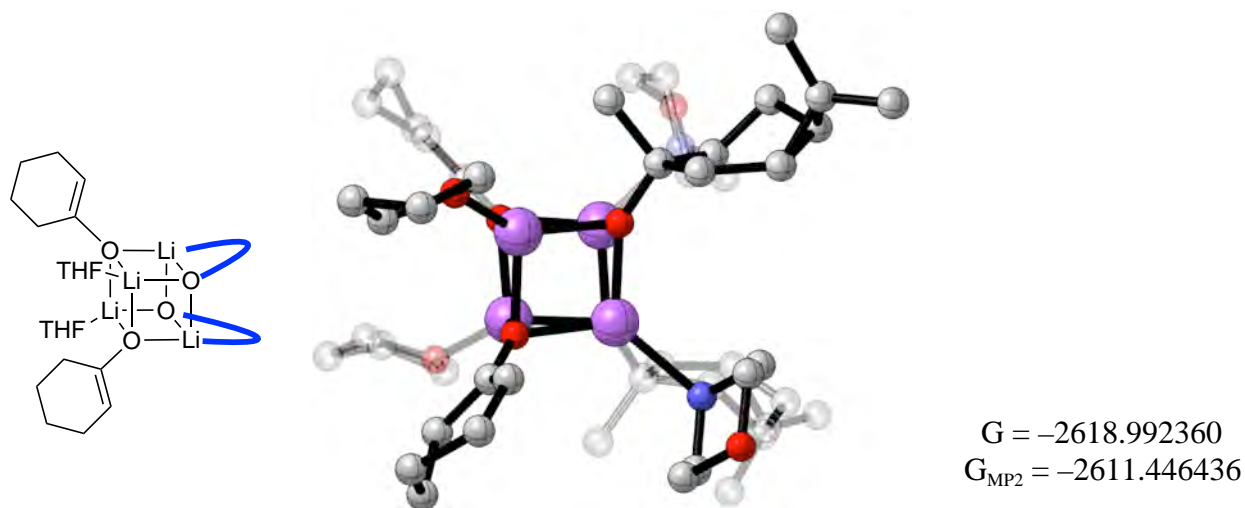


G = -2618.993062
G_{MP2} = -2611.441668

Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	H	2.54624700	6.64088300	-2.01858200
Li	-1.70021100	1.86646900	-0.72672100	C	1.48324500	4.72395000	-1.95794100
O	-0.95375700	1.97090600	-2.55767700	H	0.55437500	4.77917300	-2.53163700
Li	-0.92534800	0.00071200	-2.34668500	H	1.26399800	4.89744100	-0.89805800
O	0.90648900	-0.06026000	-1.72798600	H	4.10154600	5.00947500	-1.04859600
Li	0.77493600	1.86665900	-1.61905900	H	4.73262200	5.14982800	-2.70060300
O	0.02845100	1.97021400	0.21204100	H	3.92244800	2.69226700	-1.71228900
C	0.32337000	2.70001500	1.29217900	H	3.59431100	3.12549700	-3.40778200
C	-0.74335900	2.70866900	2.38315800	C	1.99270400	-0.94189800	-1.71005900
H	-1.11367300	1.68200900	2.51040200	C	3.03465000	-0.51398300	-2.83205400
H	-1.61003800	3.28239600	2.02343000	H	2.93123500	-1.19155500	-3.69070600
C	-0.25451200	3.27332000	3.72514900	H	2.66964600	0.45610200	-3.18213200
H	-1.10849800	3.46413700	4.38831900	C	4.51432400	-0.34324300	-2.47312400
H	0.37239200	2.52565300	4.23255000	C	5.04584200	-0.90584100	-1.16473000
C	0.56991200	4.54712300	3.51210400	H	5.75821400	-0.27963200	-0.62817500
C	1.80963900	4.24329300	2.65902000	C	4.04055500	-1.60747900	-0.26054200
H	2.27815200	5.18843500	2.34465300	H	4.43309300	-1.62194000	0.76273500
H	2.56549700	3.74644300	3.29264100	H	3.90668000	-2.65668700	-0.54580400
C	1.47745900	3.39717000	1.45031400	C	2.69436900	-0.84973700	-0.31032300
H	2.22302900	3.33404800	0.65849400	H	2.93381400	0.21656800	-0.21028900
H	0.86495800	4.98521800	4.47448100	N	1.76871200	-1.11532600	0.84278500
H	-0.05181300	5.29589800	2.99913400	C	1.67917400	-2.53536400	1.24975900
O	2.00981900	3.37880900	-2.09259900	C	0.72218400	-2.69694300	2.42858100
C	3.42671500	3.41853500	-2.36276100	H	0.69674000	-3.74240800	2.75167500
C	3.85845800	4.86470600	-2.10758300	H	-0.29713900	-2.39908400	2.13112500
C	2.58774100	5.64730100	-2.47484100	O	1.14188200	-1.93506500	3.54953400
H	2.51370100	5.76831500	-3.56222200	C	1.22893200	-0.56137300	3.19596900

H	1.58237500	-0.02974700	4.08445700	H	-3.58920200	-2.92153000	-3.90646800
H	0.22712700	-0.17786900	2.93980600	H	-2.25381200	-3.14093900	-2.76236100
C	2.18735500	-0.33284200	2.03080000	C	-6.47122200	-1.46153200	0.13792700
H	2.19053200	0.73133200	1.77539100	C	-6.10633100	-2.85846300	0.60449600
H	3.20409800	-0.61614800	2.35545100	H	-5.07228400	-3.13130000	0.38512000
H	2.66348500	-2.92313400	1.55833400	H	-6.23894500	-2.94365100	1.69098600
H	1.32818000	-3.14187000	0.41400300	H	-6.75651200	-3.60876500	0.13525100
C	5.54578200	-1.46121300	-2.48518000	C	-7.88742200	-1.06614100	0.53214100
C	5.18078500	-2.85788900	-2.95242900	H	-8.62530300	-1.75623200	0.10146100
H	4.14658000	-3.13056200	-2.73359500	H	-8.01372500	-1.08366200	1.62284400
H	5.31383700	-2.94270300	-4.03889400	H	-8.13550000	-0.05663300	0.18459000
H	5.83059800	-3.60851500	-2.48319200	H	-5.84421000	0.62498100	0.41791600
C	6.96203100	-1.06575000	-2.87913500	C	-2.39276200	-2.35922500	-0.31110900
H	7.69982900	-1.75616000	-2.44882300	H	-2.04612600	-2.37357300	0.72845200
H	7.08836500	-1.08267200	-3.96984300	H	-3.13850900	-3.15560800	-0.41972600
H	7.21021000	-0.05646400	-2.53100500	H	-1.53449000	-2.60311100	-0.94246200
H	4.91895900	0.62549600	-2.76409400	C	-1.24828000	2.70127300	-3.63754700
C	1.46721600	-2.35882100	-2.03682800	C	-0.18145400	2.70995900	-4.72843500
H	1.12058800	-2.37255400	-3.07640300	H	0.18852600	1.68322300	-4.85602500
H	2.21288700	-3.15533300	-1.92863900	H	0.68538500	3.28327200	-4.36842400
H	0.60891100	-2.60297600	-1.40562200	C	-0.67001300	3.27527700	-6.07024800
O	-1.83186000	-0.06052800	-0.61874400	H	0.18408000	3.46598600	-6.73331300
C	-2.91813900	-0.94207700	-0.63708400	H	-1.29719100	2.52803800	-6.57794000
C	-3.96000200	-0.51469900	0.48519600	C	-1.49392400	4.54934100	-5.85678500
H	-3.85661300	-1.19276800	1.34345900	C	-2.73381400	4.24573400	-5.00385500
H	-3.59490400	0.45515400	0.83581800	H	-3.20191100	5.19096400	-4.68913400
C	-5.43967700	-0.34364100	0.12641400	H	-3.48987800	3.74946900	-5.63768800
C	-5.97129400	-0.90551200	-1.18225600	C	-2.40206000	3.39898000	-3.79547400
H	-6.68364700	-0.27897200	-1.71845100	H	-3.14769600	3.33584000	-3.00371800
C	-4.96609100	-1.60673600	-2.08686000	H	-1.78875300	4.98789800	-6.81901700
H	-5.35868200	-1.62064000	-3.11012500	H	-0.87190500	5.29768000	-5.34353200
H	-4.83227000	-2.65609700	-1.80214700	O	-2.93528000	3.37835300	-0.25224100
C	-3.61985500	-0.84911300	-2.03673600	C	-2.40895700	4.72364500	-0.38620400
H	-3.85922600	0.21726500	-2.13618400	C	-3.51383200	5.64654500	0.13066400
N	-2.69426600	-1.11414900	-3.19003300	C	-4.78422700	4.86394100	-0.23768200
C	-2.60484700	-2.53397700	-3.59776700	H	-5.02679700	5.00928600	-1.29670900
C	-1.64796300	-2.69498700	-4.77675100	H	-5.65874200	5.14858200	0.35505100
H	-1.62259500	-3.74028500	-5.10039000	C	-4.35239700	3.41767800	0.01688700
H	-0.62859900	-2.39732700	-4.47923000	H	-4.84755800	2.69175800	-0.63441000
O	-2.06773400	-1.93251100	-5.89727500	H	-4.52068800	3.12392200	1.06158400
C	-2.15466300	-0.55900100	-5.54299600	H	-3.44034800	5.76695900	1.21815000
H	-2.50817300	-0.02689300	-6.43117000	H	-3.47226900	6.64038700	-0.32502300
H	-1.15280900	-0.17569000	-5.28674900	H	-1.48030300	4.77884200	0.18783500
C	-3.11294200	-0.33099800	-4.37760200	H	-2.18938100	4.89764300	-1.44594000
H	-3.11597100	0.73304300	-4.12162900				
H	-4.12975000	-0.61401600	-4.70229500				

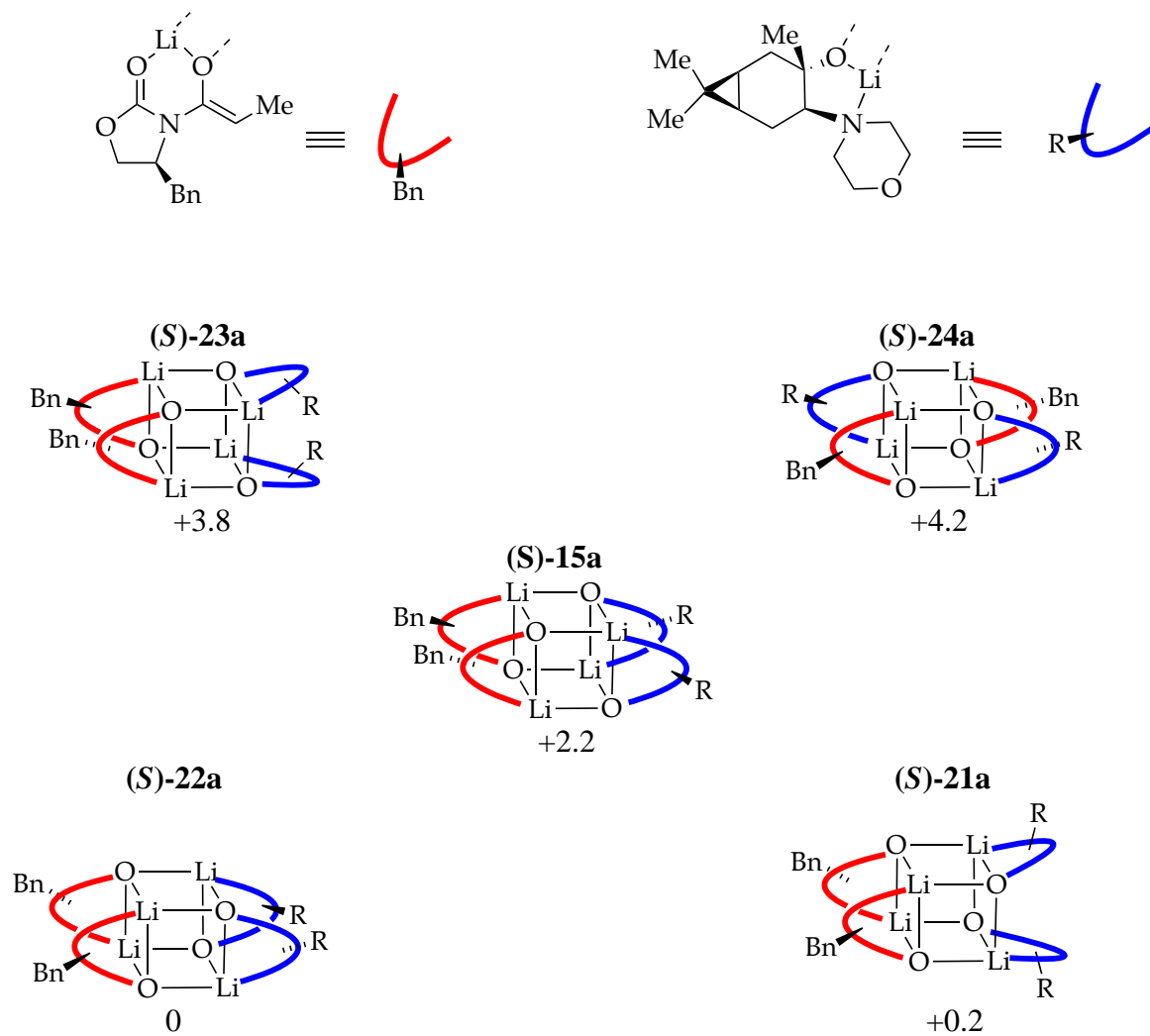
Table 14. Geometric coordinates and thermally corrected MP2 energies for **18c**



Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	H	4.76575300	3.13915900	0.20795300
Li	-0.00097700	0.59999700	2.44129700	C	3.11610900	2.72575300	-1.18905000
Li	-1.84113300	-1.00213800	1.49679700	H	3.86727300	2.12639900	-1.71646600
O	-1.96105500	0.59848000	2.64276400	H	2.65203200	3.36382700	-1.94885000
Li	-1.84510500	1.59683700	0.94488500	C	2.06032200	1.81068700	-0.52828900
O	-1.96008100	-0.00435900	-0.20099300	H	2.54369300	1.36605100	0.35055800
C	-2.56006100	-0.38607700	-1.33178800	N	1.64061100	0.62440900	-1.34583400
C	-3.53208900	0.62652200	-1.92289000	C	1.41650300	0.90700000	-2.78301300
H	-3.07748900	1.62377300	-1.85420200	C	0.96471500	-0.35494600	-3.51201900
H	-4.42623600	0.66457100	-1.27914700	O	1.93979700	-1.38696100	-3.40663400
C	-3.94182600	0.31889200	-3.37019900	C	2.17947800	-1.68897800	-2.04186500
H	-4.79381500	0.94593900	-3.66430100	H	1.26622600	-2.10100300	-1.58138800
H	-3.11428900	0.57869400	-4.04612600	H	2.95439500	-2.46181200	-2.02193100
C	-4.27240000	-1.16745300	-3.53870500	C	2.64323800	-0.46137000	-1.25905900
C	-3.04564800	-2.03010800	-3.20890800	H	2.77889900	-0.73549800	-0.20806000
H	-3.35091900	-3.08462300	-3.12832700	H	3.62146200	-0.13795600	-1.65659300
H	-2.34723500	-2.00068400	-4.06335600	H	0.84825800	-0.14812900	-4.58047000
C	-2.35792500	-1.58498700	-1.93631100	H	-0.00157800	-0.69923900	-3.11062800
H	-1.64082200	-2.27147300	-1.48490400	H	2.34103700	1.26911900	-3.26149100
H	-4.62182900	-1.37466100	-4.55849900	H	0.65625000	1.67932300	-2.89636300
H	-5.09838300	-1.42964800	-2.86096900	C	3.64259600	5.03953500	0.07664500
O	0.10052600	1.74617700	0.89054700	C	2.87721600	5.87936500	-0.92917200
C	0.85005900	2.60765700	0.07824300	H	1.99060700	5.37784800	-1.32405800
C	1.40303100	3.82406200	0.94058400	H	2.54105200	6.81709700	-0.46752700
H	0.89033100	4.74274100	0.62630900	H	3.51707200	6.14405900	-1.78122400
H	1.05075200	3.62269200	1.95519000	C	4.83633200	5.77454500	0.66876900
C	2.91151500	4.07754700	1.00418700	H	5.54862400	6.06861500	-0.11376100
C	3.80314200	3.54341100	-0.10442100	H	4.51900500	6.68787500	1.18920200

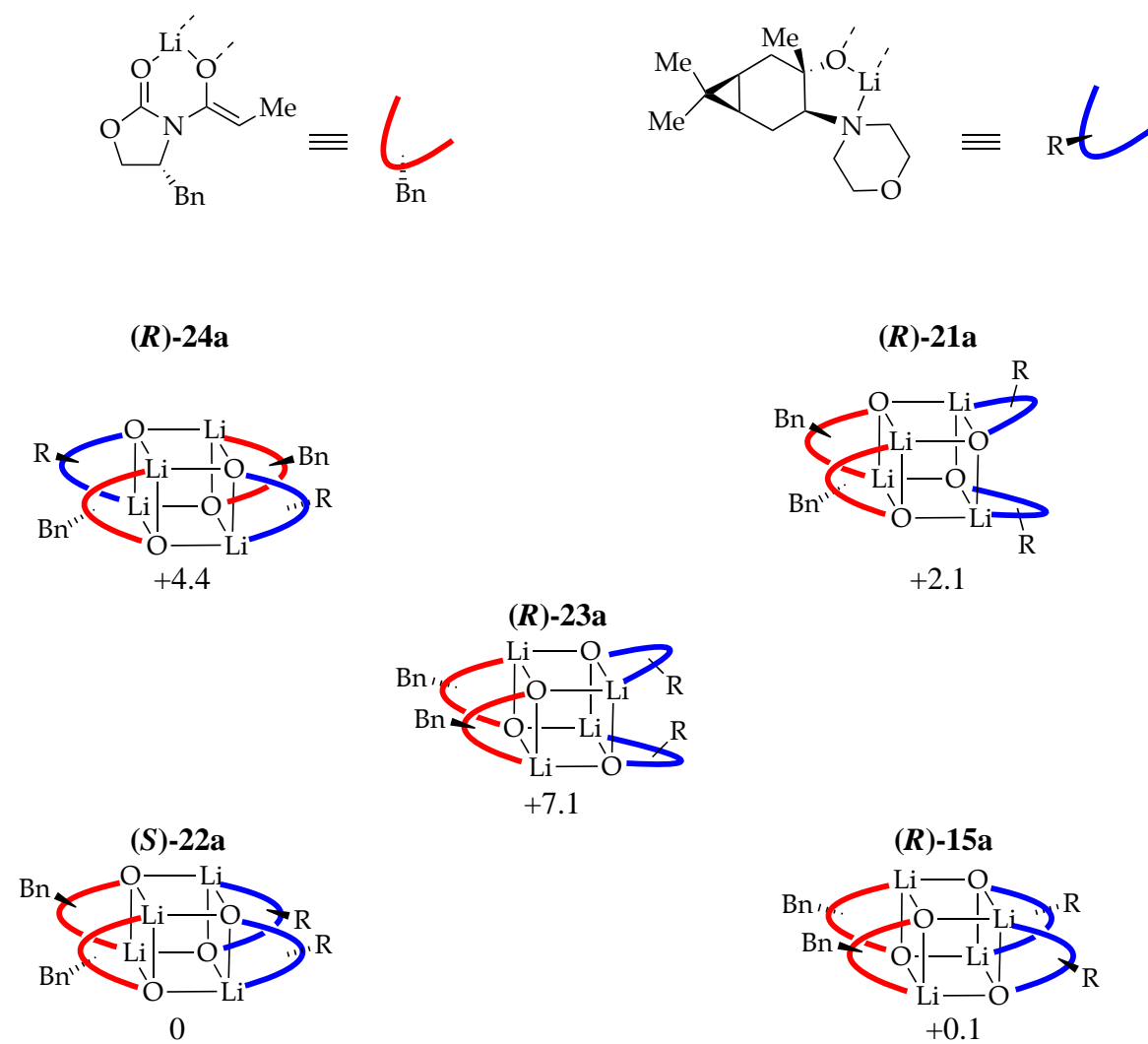
H	5.37596100	5.15110600	1.39093200	H	2.54632000	-0.75811800	2.09225500
H	3.32792400	4.02837700	2.00962800	N	1.64029000	-0.01951000	3.78829600
C	-0.08670100	3.18892200	-1.00984200	C	2.63988000	1.06913900	3.70247100
H	-0.82424000	3.84132800	-0.53127700	C	2.17210000	2.29526900	4.48520100
H	0.43378400	3.78753500	-1.76824300	O	1.93233900	1.99225100	5.84973600
H	-0.64303200	2.39247000	-1.51146600	C	0.96003200	0.95751300	5.95416300
O	-3.18435600	3.10542800	0.88263100	H	0.84333900	0.75014800	7.02248200
C	-4.55422900	2.78886900	1.23197300	H	-0.00689400	1.29923600	5.55210100
C	-5.21767500	4.12949300	1.54692500	C	1.41584000	-0.30303600	5.22522200
C	-4.04913200	4.92122800	2.15325000	H	2.34098400	-0.66276800	5.70432600
H	-3.89508800	4.62740100	3.19674000	H	0.65758100	-1.07743600	5.33778400
H	-4.19047800	6.00559600	2.11391200	H	1.25798700	2.70479500	4.02420600
C	-2.86978600	4.45703900	1.29618400	H	2.94483600	3.07030500	4.46595800
H	-1.91900700	4.43882100	1.83555500	H	2.77553200	1.34384900	2.65161100
H	-2.75590800	5.07514100	0.39617700	H	3.61872600	0.74843700	4.10064300
H	-5.57419400	4.60990000	0.62777500	C	3.65806100	-4.42731000	2.36459700
H	-6.06695200	4.02278100	2.22846800	C	2.89591500	-5.27094000	3.36969100
H	-5.00195300	2.26174100	0.38545000	H	2.00760700	-4.77308800	3.76543200
H	-4.54441500	2.13132000	2.10858300	H	2.56300400	-6.20938300	2.90713100
C	-2.56207400	0.97957900	3.77322100	H	3.53697800	-5.53421900	4.22127000
C	-3.53023600	-0.03568000	4.36607100	C	4.85469300	-5.15720100	1.77197700
H	-3.07209200	-1.03139400	4.29854100	H	5.56813100	-5.44903600	2.55430000
H	-4.42455000	-0.07784200	3.72281900	H	4.54099300	-6.07140200	1.25087400
C	-3.94049600	0.27245400	5.81313900	H	5.39184000	-4.53110100	1.05027500
H	-4.79007700	-0.35728500	6.10844700	H	3.33959600	-3.41585900	0.43234000
H	-3.11175700	0.01663000	6.48910900	C	-0.07900100	-2.58975500	3.45090900
C	-4.27642100	1.75782600	5.97969600	H	-0.81397400	-3.24448600	2.97155900
C	-3.05293100	2.62447200	5.64821600	H	0.44301500	-3.18691600	4.20940700
H	-3.36208100	3.67775100	5.56623200	H	-0.63845500	-1.79546200	3.95248000
H	-2.35412100	2.59881700	6.50245600	O	-3.17565100	-2.51479000	1.55840500
C	-2.36401900	2.18003100	4.37603500	C	-2.85757500	-3.86467400	1.14186600
H	-1.64937500	2.86838500	3.92357800	C	-4.03661100	-4.33067200	0.28534600
H	-4.62621600	1.96518800	6.99933200	C	-5.20671900	-3.54357500	0.89468100
H	-5.10361500	2.01604600	5.30191400	H	-5.56051500	-4.02673400	1.81343600
O	0.10489300	-1.14582600	1.55094200	H	-6.05724000	-3.43814800	0.21449200
C	0.85658100	-2.00508700	2.36361400	C	-4.54681200	-2.20158200	1.21121400
C	1.41391400	-3.21986500	1.50167600	H	-4.99503000	-1.67720400	2.05918000
H	0.90504100	-4.14036200	1.81680000	H	-4.54000600	-1.54243500	0.33576300
H	1.06029600	-3.02062000	0.48710800	H	-3.88472500	-4.03430200	-0.75773700
C	2.92334100	-3.46743800	1.43771900	H	-4.17469700	-5.41553100	0.32271900
C	3.81282700	-2.93074500	2.54683600	H	-1.90752500	-3.84257200	0.60137400
H	4.77391000	-2.52259300	2.23481100	H	-2.74079400	-4.48414900	2.04055300
C	3.12250100	-2.11626200	3.63174900				
H	3.87135800	-1.51472500	4.15996500				
H	2.66014800	-2.75636700	4.39090100				
C	2.06402800	-1.20440500	2.97085600				

Figure 172. Computational overview of ground states for **(S)-15a**



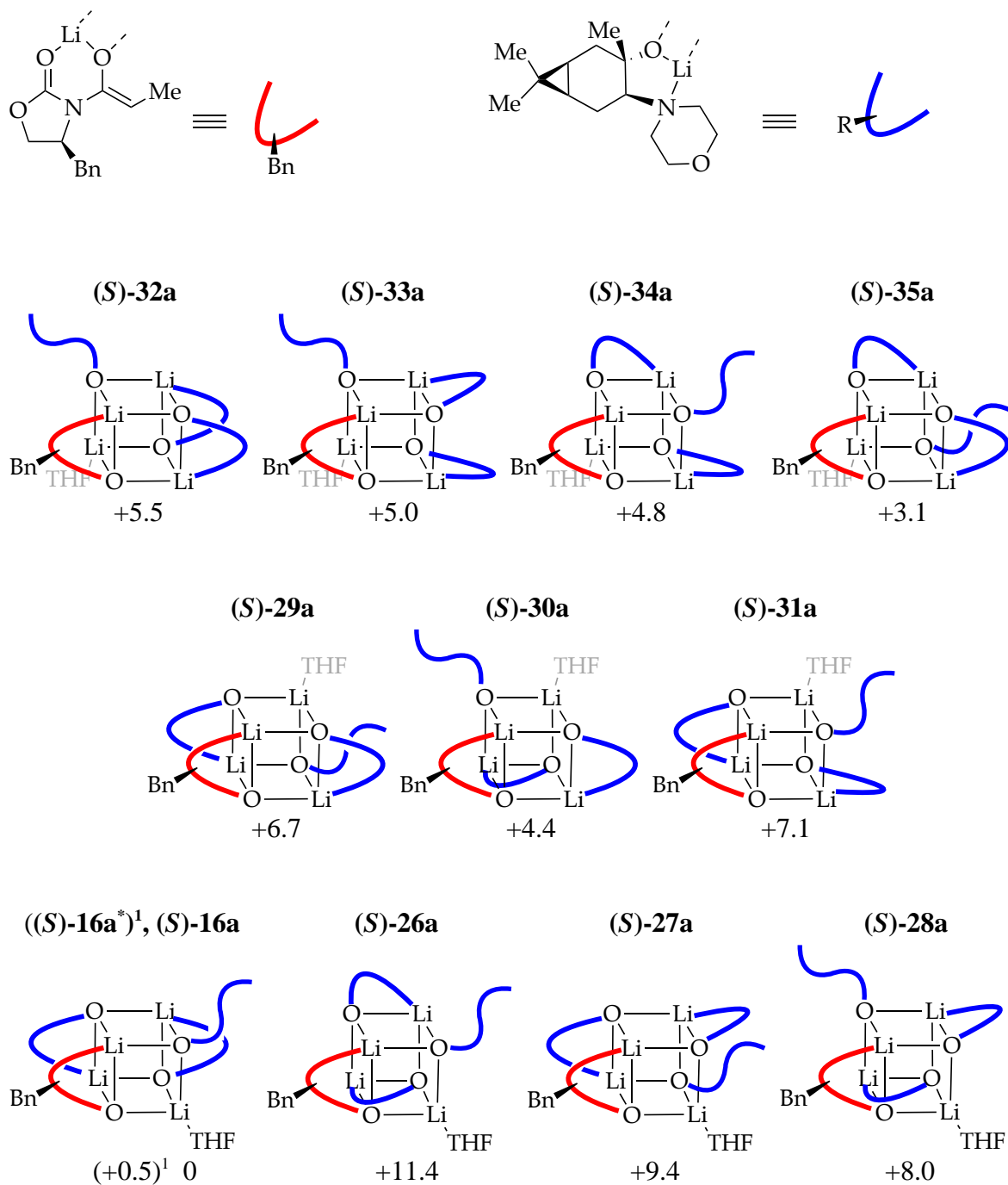
* Relative energies are given in kcal/mol

Figure 173. Computational overview of ground states for (*R*)-15a



* Relative energies are given in kcal/mol

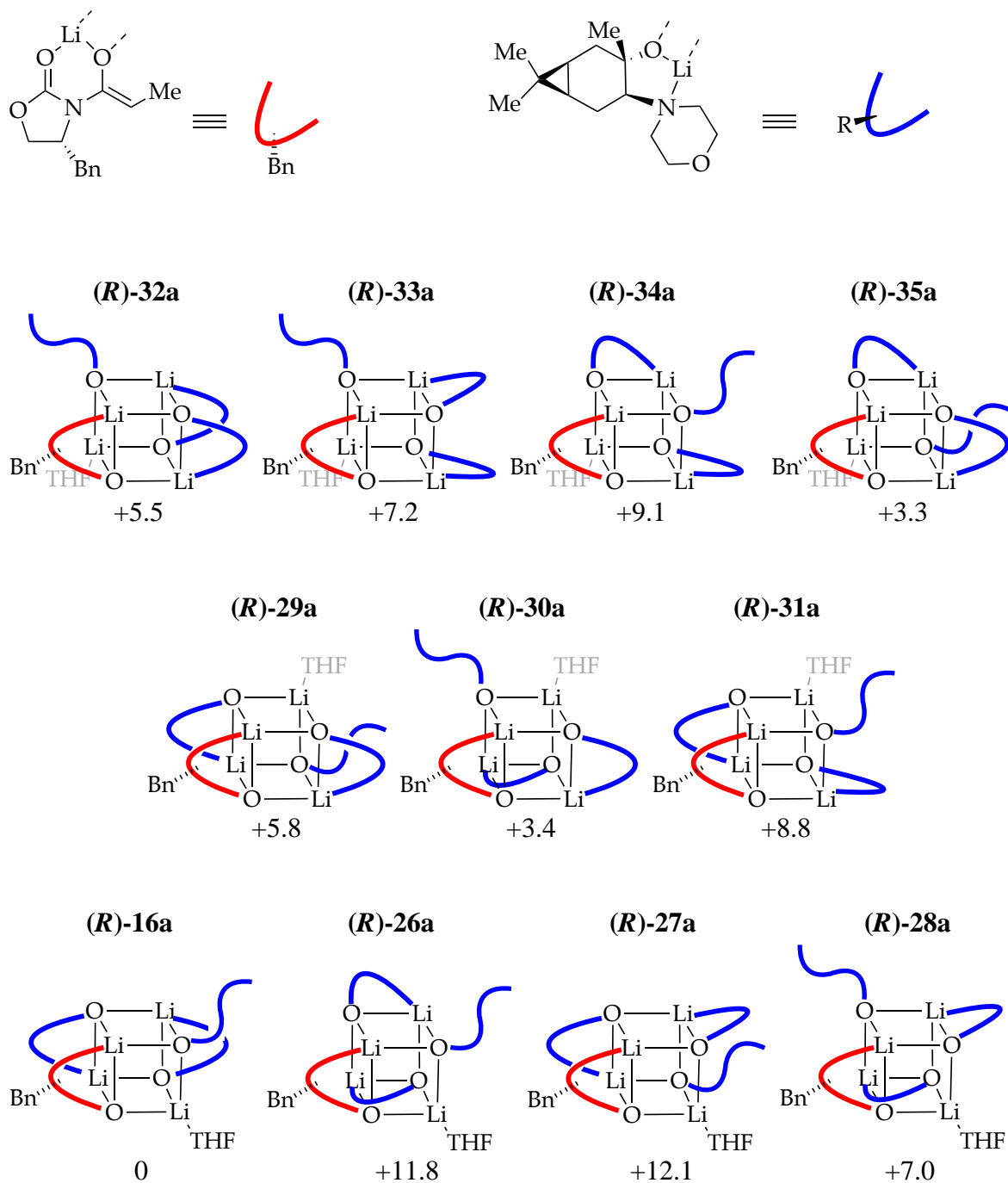
Figure 174. Computational overview of ground states for **(S)-16a**



* Relative energies are given in kcal/mol

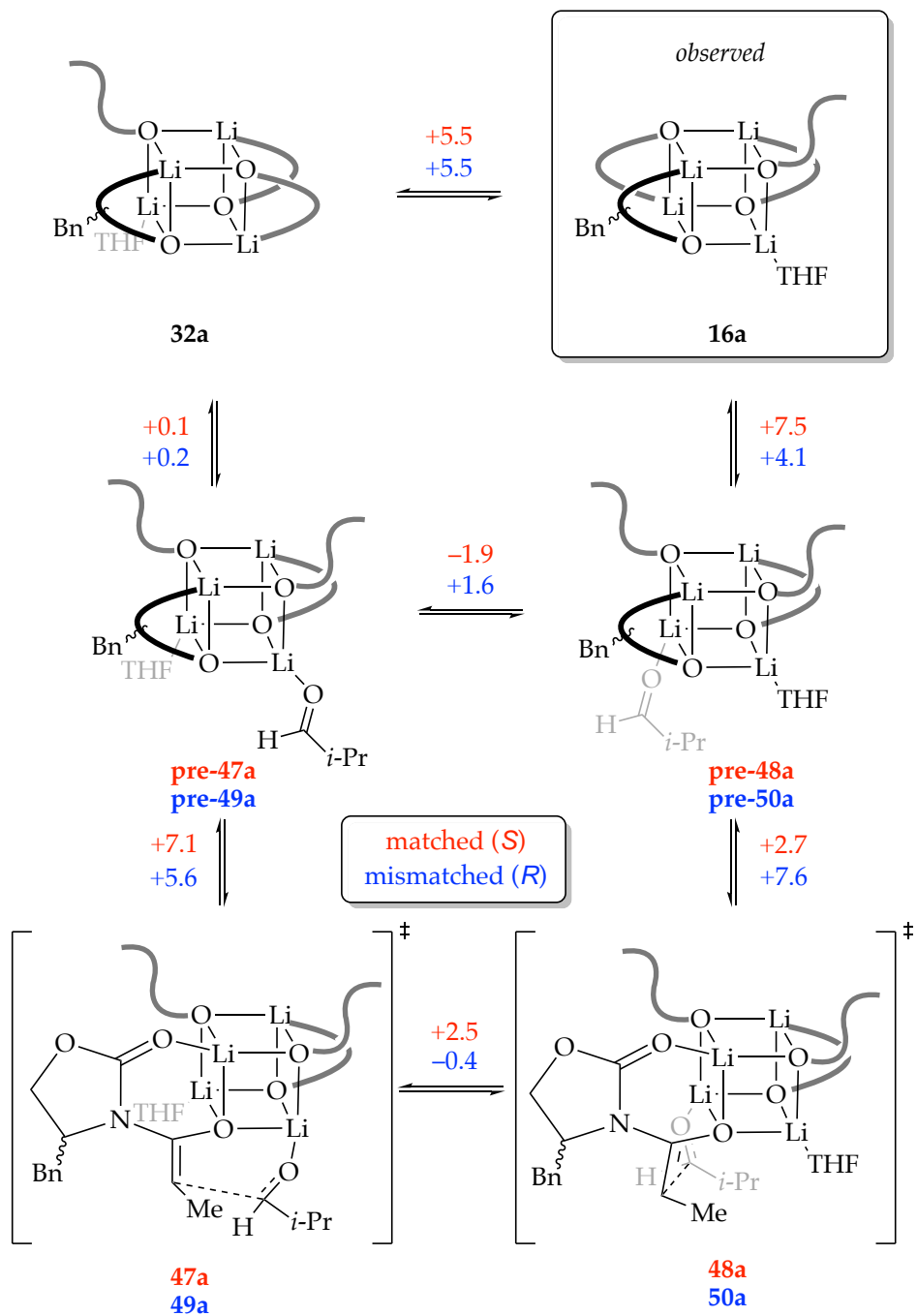
¹Rotational isomer

Figure 175. Computational overview of ground states for **(R)-16a**



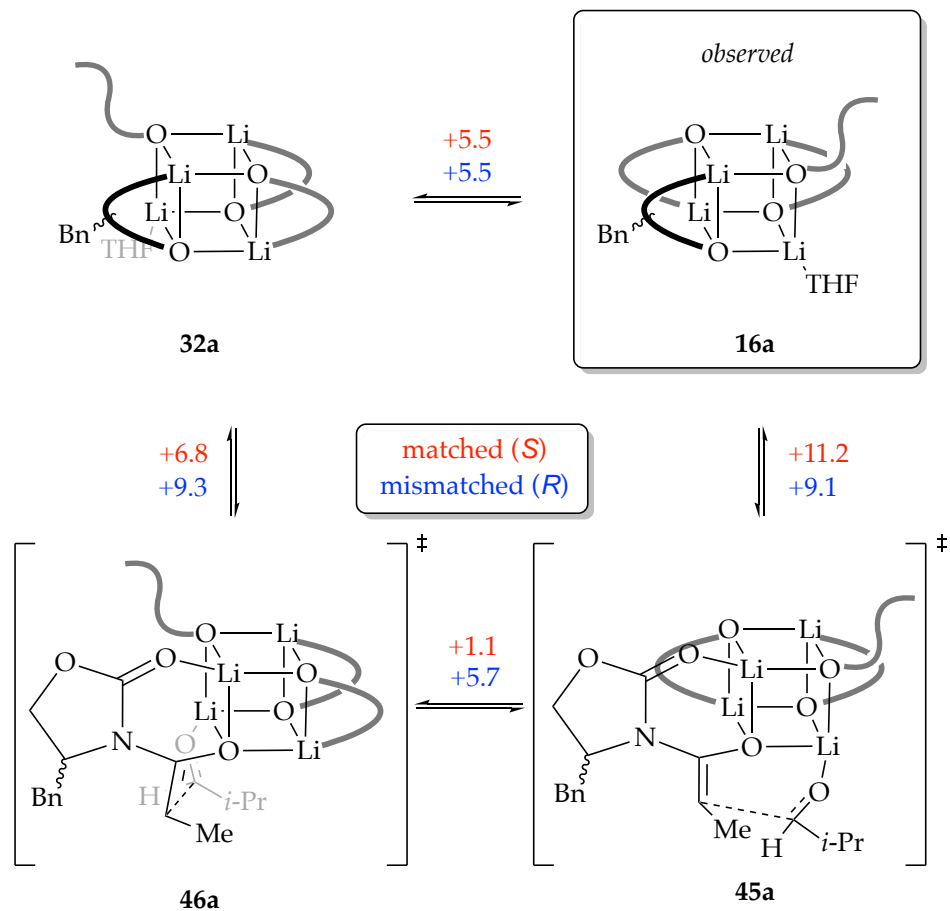
* Relative energies are given in kcal/mol

Figure 176. Computational overview of transition states



* Relative energies are given in kcal/mol

Figure 177. Computational overview of transition states



* Relative energies are given in kcal/mol

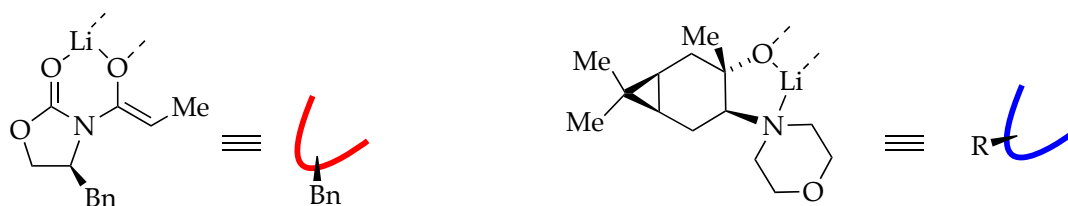
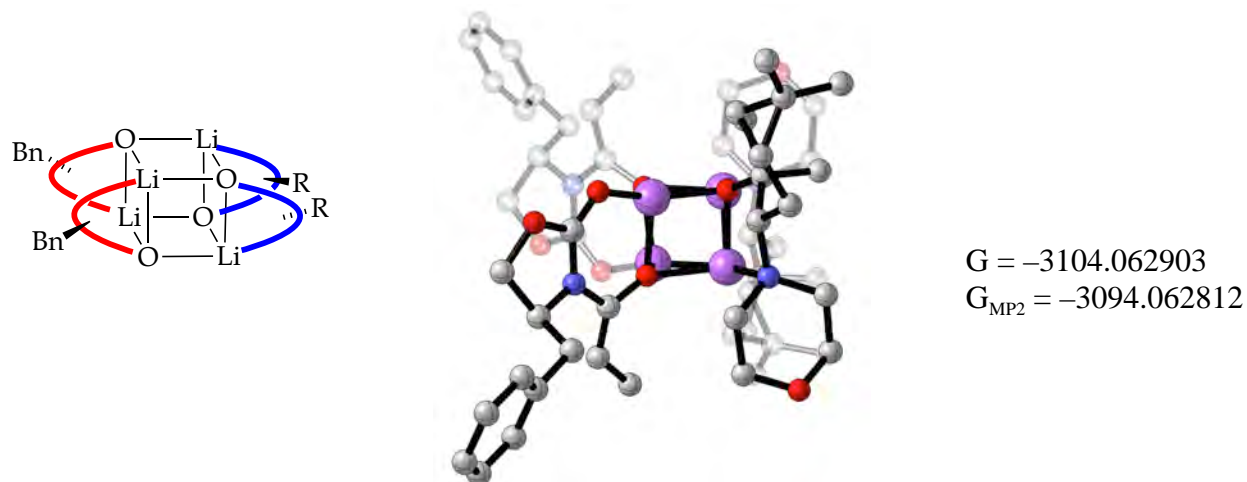


Table 15. Geometric coordinates and thermally corrected MP2 energies for (*S*)-22a

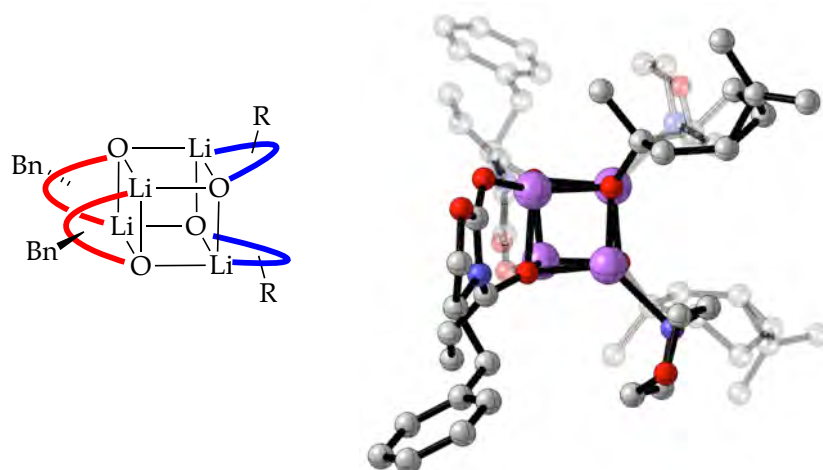


Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	Li	-1.76604800	1.83368100	0.57818800
Li	-0.48377500	1.84059100	-1.74318900	Li	-2.23341700	-0.01060700	-1.16735300
O	0.67538500	3.17716900	-2.39967400	O	-2.41746500	2.01264300	-1.27154800
C	1.41968900	3.84382900	-1.68918600	C	-3.10875200	2.99632500	-1.79386600
O	2.25798000	4.75058000	-2.26065900	N	-3.83374600	3.83193700	-0.83965800
C	2.83714500	5.56608700	-1.22853700	C	-3.67182300	3.83520300	0.51894000
H	2.27344000	6.50396300	-1.17058600	O	-2.93378800	3.16444700	1.23206100
H	3.87226800	5.78255200	-1.49677200	O	-4.50575300	4.74781200	1.08746100
C	2.69794400	4.72568600	0.04842900	C	-5.07828000	5.56494800	0.05287400
H	2.40695900	5.36344100	0.88585700	H	-4.50804000	6.49876400	-0.00685900
N	1.58480200	3.84073800	-0.33108300	H	-6.11216400	5.78903200	0.31957400
C	0.85500700	3.01161600	0.62539600	C	-4.94348100	4.72023200	-1.22152100
C	0.96251500	3.31252000	1.94422000	H	-4.65034600	5.35388500	-2.06129300
H	1.51992300	4.18810100	2.25601700	C	-6.22027900	3.92690300	-1.58819700
C	0.27993800	2.52670400	3.02887300	H	-5.94069000	3.20182800	-2.36001100
H	0.95263100	2.34745500	3.87881100	H	-6.54041100	3.36033800	-0.70501800
H	-0.60392100	3.04698400	3.42705200	C	-7.34280900	4.81551700	-2.07711600
H	-0.05700700	1.55162500	2.66234200	C	-8.44333700	5.11086900	-1.26139000
O	0.16599700	2.02472500	0.10616300	C	-9.46270500	5.95451100	-1.70816600

C	-9.39579600	6.51855800	-2.98229000	H	-5.21113000	-3.46290200	4.49913800
C	-8.30648700	6.22972400	-3.80778900	C	-5.67612200	-0.89025200	5.51457400
C	-7.29162100	5.38564200	-3.35839500	H	-6.55909300	-1.52728400	5.65962500
H	-6.45355700	5.15591700	-4.01336600	H	-5.07131800	-0.94767100	6.42931600
H	-8.25034000	6.65751800	-4.80532100	H	-6.02482400	0.14364800	5.41188600
H	-10.1885430	7.17376900	-3.33288800	H	-4.09381700	0.71842300	4.08736500
H	-10.3097590	6.16638200	-1.06102400	C	-2.09175200	-2.36181500	1.28238500
H	-8.50893600	4.66557200	-0.27075800	H	-1.14949300	-2.42916500	1.83850300
C	-3.22157800	3.28867100	-3.11421900	H	-2.76365000	-3.13147400	1.68082700
C	-2.54736600	2.49300300	-4.19695000	H	-1.86929200	-2.60400000	0.23946200
H	-2.21523300	1.51742500	-3.82719200	O	-0.47237400	-0.05678100	-1.89174800
H	-3.22386300	2.31355700	-5.04380000	C	0.41187900	-0.90361500	-2.57856900
H	-1.66157800	3.00553700	-4.60107400	C	0.46015400	-0.49140300	-4.11062300
H	-3.77965600	4.16256400	-3.42940500	H	-0.13433600	-1.21047800	-4.69069700
O	-1.75987000	-0.06351400	0.72521700	H	-0.08887200	0.45212400	-4.15901700
C	-2.63764000	-0.92049000	1.40789000	C	1.81276100	-0.25583700	-4.79136100
C	-2.68175400	-0.52863600	2.94583700	C	3.08878900	-0.75526600	-4.13526300
H	-2.11732000	-1.27666100	3.51881800	H	3.94599400	-0.08509200	-4.19175400
H	-2.10004700	0.39379900	3.01345200	C	2.94049800	-1.44833300	-2.78660900
C	-4.03160300	-0.26290000	3.62006400	H	3.89919300	-1.40690300	-2.25606100
C	-5.31199300	-0.75549800	2.96714200	H	2.70510400	-2.51286600	-2.89829400
H	-6.16194500	-0.07549900	3.01572200	C	1.84596000	-0.72569900	-1.97076500
C	-5.16718100	-1.46040600	1.62445200	H	2.03765800	0.34897600	-2.07792600
H	-6.12655100	-1.42314700	1.09484200	N	1.89732400	-0.95319800	-0.48671100
H	-4.93133600	-2.52397200	1.74433100	C	2.92687000	-0.09258400	0.14003700
C	-4.07325100	-0.74319000	0.80328700	C	2.91684900	-0.26079100	1.65745700
H	-4.26303200	0.33208700	0.90702200	O	3.13926400	-1.61214500	2.03687500
N	-4.12745200	-0.97596000	-0.67995800	C	2.15901100	-2.45553600	1.45154500
C	-5.15733800	-0.11646200	-1.30811000	H	2.40244400	-3.47733600	1.75871200
H	-4.93694500	0.92611900	-1.06308800	H	1.15965000	-2.20244500	1.84442900
H	-6.16519900	-0.35662400	-0.92666600	C	2.16377900	-2.34782300	-0.07197300
C	-5.15128500	-0.29152900	-2.82485600	H	3.14556300	-2.69159500	-0.43631700
O	-5.37684500	-1.64413200	-3.19799900	H	1.40232400	-3.01016100	-0.48598400
C	-4.39668500	-2.48653400	-2.61111100	H	1.95767000	0.09556400	2.06781500
C	-4.39806400	-2.37178700	-1.08815900	H	3.72096200	0.32739200	2.10974500
H	-5.38011400	-2.71109600	-0.72036400	H	2.70859000	0.94922600	-0.11019000
H	-3.63786300	-3.03455000	-0.67275100	H	3.93533700	-0.33567800	-0.23796100
H	-4.64262000	-3.50929700	-2.91304900	C	2.64214900	-1.34030200	-5.46209700
H	-3.39760600	-2.23709400	-3.00723900	C	2.12678500	-2.76295000	-5.57154000
H	-4.19251100	0.06090000	-3.23937500	H	1.50339600	-3.06255200	-4.72682400
H	-5.95536400	0.29619400	-3.27778100	H	1.51938900	-2.87929700	-6.47868900
C	-4.87340000	-1.33290100	4.29951800	H	2.95942100	-3.47564900	-5.64090700
C	-4.37149600	-2.75956600	4.41988000	C	3.44792200	-0.91543900	-6.68164000
H	-3.75517400	-3.07333800	3.57474600	H	4.32405500	-1.56276000	-6.82255400
H	-3.76120900	-2.87423100	5.32531700	H	2.84145900	-0.97397000	-7.59521800

H 3.80750400 0.11556200 -6.58770500
H 1.88591000 0.71963500 -5.26940500
C -0.12979000 -2.34759000 -2.46500800
H -1.06868000 -2.41503200 -3.02686600
H 0.54600000 -3.11456200 -2.86111800
H -0.35783700 -2.59448900 -1.42439100
C 3.97078800 3.92822000 0.41933300
H 3.68689500 3.20781800 1.19397500
H 4.28905600 3.35642100 -0.46113100
C 5.09706600 4.81343200 0.90576300
C 5.04798200 5.38770300 2.18526900
C 6.06650600 6.22855700 2.63243800
C 7.15739400 6.50991500 1.80644300
C 7.22219900 5.94167600 0.53407100
C 6.19919900 5.10125800 0.08952400
H 6.26321600 4.65251100 -0.89965700
H 8.07045600 6.14769700 -0.11338300
H 7.95300100 7.16256900 2.15533100
H 6.01198500 6.65963000 3.62864700
H 4.20865300 5.16367600 2.84059400

Table 16. Geometric coordinates and thermally corrected MP2 energies for (*S*)-**21a**



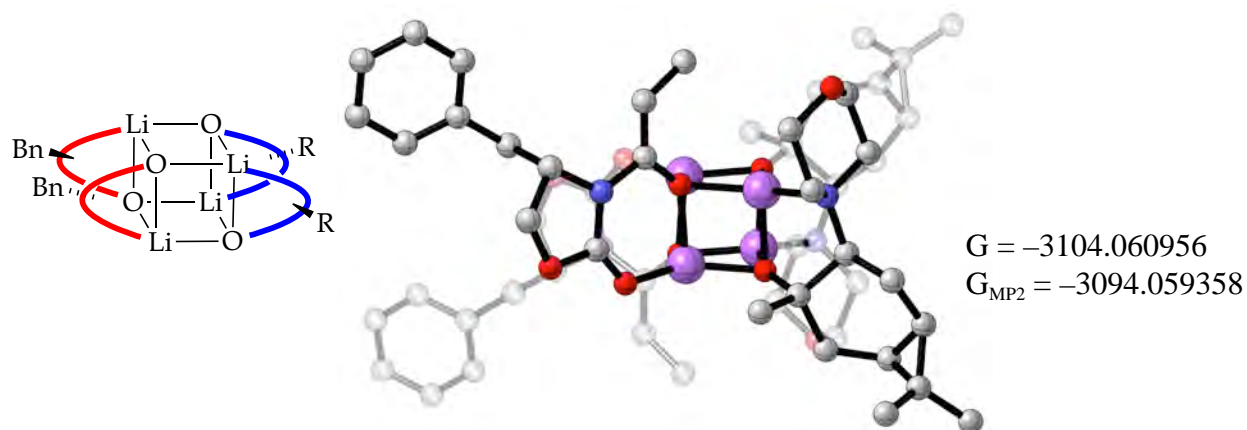
G = -3104.060559
G_{MP2} = -3094.062469

Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	O	0.48963200	-2.84020900	2.70149100
Li	-1.63898100	-1.80934300	-0.82410500	C	1.63298800	-2.95067100	2.27330400
O	-2.88905200	-2.83764500	-1.84415600	O	2.67563200	-3.15375700	3.11608000
C	-4.03235000	-2.94852200	-1.41591300	C	3.89881600	-3.13520900	2.35582300
N	-4.46201100	-2.90833800	-0.11877700	H	4.55652300	-3.91504800	2.74097400
C	-5.86111200	-3.35577000	-0.04097500	H	4.37539500	-2.15738200	2.49200600
C	-6.29819300	-3.13300900	-1.49815000	C	3.46204000	-3.35654700	0.89834900
H	-6.95596300	-3.91247700	-1.88394600	H	3.49329900	-4.42942400	0.65988700
H	-6.77480400	-2.15504900	-1.63327100	N	2.06289100	-2.90923900	0.97627500
O	-5.07515600	-3.15078800	-2.25868100	C	1.12086600	-2.90650600	-0.14452100
H	-5.89230500	-4.42888000	0.19645300	O	0.20082000	-1.96930900	-0.07553600
C	-6.71292000	-2.59255400	0.98445500	C	1.30071900	-3.82726500	-1.11875900
H	-6.23894500	-2.71019000	1.96503600	H	2.07359400	-4.57848400	-0.98265200
H	-6.68948900	-1.52414600	0.73951500	C	0.46703100	-3.93063000	-2.36433900
C	-8.14347400	-3.09082100	1.02132200	H	-0.29351600	-4.72166700	-2.29413600
C	-8.45039500	-4.34162800	1.57863700	H	-0.06514600	-2.99908900	-2.57715100
H	-7.65616900	-4.94342000	2.01570500	H	1.08847700	-4.16337900	-3.23952000
C	-9.76100900	-4.81789100	1.59107300	C	4.31415700	-2.59232300	-0.12608000
H	-9.97830700	-5.78808300	2.03019000	H	3.84073400	-2.70929100	-1.10700200
C	-10.7924300	-4.04781800	1.04862800	H	4.29037200	-1.52410700	0.11966100
C	-10.5026140	-2.79903300	0.49841200	C	5.74485500	-3.09021800	-0.16259800
C	-9.18853500	-2.32665000	0.48559200	C	6.05234500	-4.34067300	-0.72039000
H	-8.97288100	-1.34642000	0.06605300	H	5.25847300	-4.94247400	-1.15808700
H	-11.2990070	-2.18798200	0.08174200	C	7.36309200	-4.81657800	-0.73251200
H	-11.8144710	-4.41664900	1.06098400	H	7.58083200	-5.78650200	-1.17200300
C	-3.51975800	-2.90671400	1.00178800	C	8.39408400	-4.04648800	-0.18927600
O	-2.60002800	-1.96912000	0.93382500	C	8.10370600	-2.79804100	0.36140900
Li	-0.76026500	-1.81044600	1.68233900	C	6.78949200	-2.32602000	0.37392000

H	6.57340200	-1.34604200	0.79382200	O	-1.69983800	0.11434300	-0.92376300
H	8.89976200	-2.18696900	0.77869300	C	-1.54274200	0.87165500	-2.09511800
H	9.41622900	-4.41503900	-0.20138700	C	-2.93662800	1.48611500	-2.54488300
Li	-2.39879100	-0.00001500	0.85935400	H	-3.26493500	0.98258200	-3.46293100
O	-0.69884800	0.11328400	1.78309500	H	-3.64132800	1.16880600	-1.77267100
C	-0.85565300	0.86987900	2.95494300	C	-3.06949800	3.00312200	-2.71209200
C	0.53850100	1.48337700	3.40516700	C	-1.82386900	3.84770300	-2.92998400
H	0.86664800	0.97889300	4.32275200	H	-1.80366700	4.80954400	-2.41820600
H	1.24302000	1.16646700	2.63262600	C	-0.49153500	3.11063800	-2.90626600
C	0.67202500	3.00018800	3.57365400	H	0.31420800	3.82903000	-2.71333900
C	-0.57325300	3.84514000	3.79207900	H	-0.26271500	2.65273000	-3.87494800
H	-0.59299000	4.80739200	3.28105300	C	-0.53771100	2.04106400	-1.79341400
C	-1.90590900	3.10868000	3.76767700	H	-0.96531500	2.53054200	-0.90912000
H	-2.71131700	3.82759300	3.57529600	N	0.79807100	1.54837800	-1.32497400
H	-2.13497400	2.65010100	4.73598400	C	1.43383300	2.47398300	-0.36340200
C	-1.86013000	2.03995300	2.65399800	H	0.74299900	2.65727200	0.46610400
H	-1.43221400	2.52990400	1.77011700	H	1.67324100	3.44543200	-0.83123200
N	-3.19611100	1.54824500	2.18503900	C	2.72067900	1.85335500	0.18263700
C	-3.83120200	2.47499800	1.22412300	O	3.64460100	1.53553200	-0.84812300
C	-5.11851500	1.85580100	0.67758400	C	3.04540900	0.67880300	-1.81378800
O	-6.04267400	1.53791100	1.70810500	C	1.78117200	1.29480900	-2.40039300
C	-5.44414400	0.67984800	2.67297000	H	2.05453900	2.23198800	-2.91293100
H	-6.19368600	0.52588600	3.45520200	H	1.36103600	0.61700200	-3.14230600
H	-5.20420600	-0.29481100	2.21943800	H	3.79484100	0.52501700	-2.59616200
C	-4.17946300	1.29439400	3.26017700	H	2.80473200	-0.29608800	-1.36117000
H	-4.45219600	2.23129300	3.77356100	H	2.47516000	0.94420500	0.75771800
H	-3.75984900	0.61561000	4.00149400	H	3.22804600	2.55571200	0.85124900
H	-4.87373000	0.94690900	0.10178200	C	-2.85601200	3.72854900	-4.03382100
H	-5.62532200	2.55908700	0.00952500	C	-2.56852800	2.95435500	-5.30691200
H	-3.14020600	2.65838700	0.39477700	H	-2.02491900	3.58030300	-6.02677400
H	-4.06990900	3.44627600	1.69266400	H	-1.97674900	2.05140900	-5.14071100
C	0.45871900	3.72466200	4.89593100	H	-3.50623700	2.64297500	-5.78520900
C	0.17076800	2.94959800	6.16838700	C	-3.71860200	4.95857800	-4.27760100
H	-0.37268000	3.57520900	6.88866400	H	-3.22847100	5.65422400	-4.97185500
H	-0.42134500	2.04700400	6.00143600	H	-4.68704300	4.68117900	-4.71457400
H	1.10829300	2.63748300	6.64656500	H	-3.91747600	5.50363600	-3.34749500
C	1.32181900	4.95412300	5.14076000	H	-3.83545200	3.45242900	-2.08057700
H	0.83188200	5.64948000	5.83543900	C	-1.06094500	-0.07493300	-3.21951300
H	2.29006300	4.67597100	5.57769000	H	-1.85586900	-0.79717800	-3.43557700
H	1.52108800	5.49976800	4.21108500	H	-0.81656400	0.44037700	-4.15704000
H	1.43824400	3.44966400	2.94258000	H	-0.18431400	-0.64593400	-2.90013100
C	-1.33803900	-0.07728100	4.07859500	C	-3.69899800	-3.82876600	1.97490100
H	-0.54350100	-0.80005000	4.29432800	H	-4.47148900	-4.58022300	1.83797400
H	-1.58245800	0.43743800	5.01643400	C	-2.86471500	-3.93328700	3.22003400
H	-2.21483000	-0.64759600	3.75845400	H	-2.09994500	-4.71993500	3.14651500

H -2.33752300 -2.99983600 3.43704500
H -3.48507900 -4.17304900 4.09404200

Table 17. Geometric coordinates and thermally corrected MP2 energies for (*S*)-**15a**

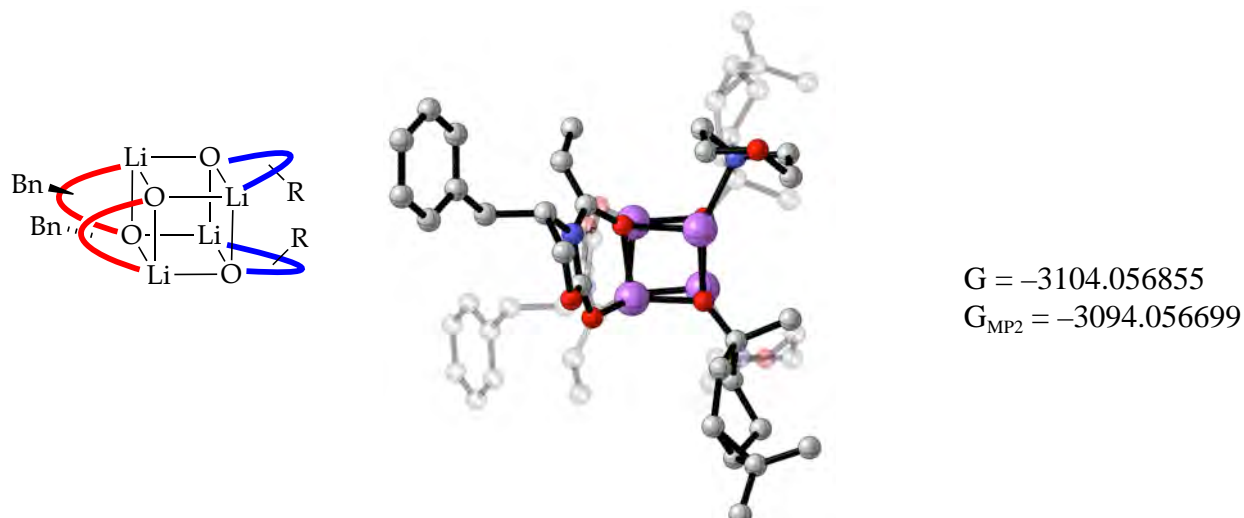


Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	H	4.79293400	3.12284700	-0.28577400
Li	0.00034300	-2.53122600	-0.15914300	N	3.87402300	1.28146200	-0.77649700
Li	1.83767900	-1.38134900	1.23158800	C	2.83478200	1.16350200	0.23857400
O	3.30879200	-2.12641200	2.16790200	C	2.84147900	2.04207200	1.27398000
C	3.99349900	-3.05385400	1.75171600	C	1.87390600	1.98067300	2.42280900
O	5.07804800	-3.45939100	2.46858200	H	1.22495900	1.10214900	2.35307200
C	5.58243900	-4.67906300	1.89700900	H	2.39934100	1.92334800	3.38693300
H	5.17491000	-5.52439500	2.46337100	H	1.22705100	2.86968800	2.47295500
H	6.67018400	-4.67672600	1.97849700	H	3.58699700	2.82720700	1.31326600
C	5.07401000	-4.64988400	0.45210900	O	1.97579700	0.19253500	0.04988900
H	4.79323600	-5.65355400	0.12640100	C	6.07930800	1.49547400	0.38784400
N	3.87430000	-3.81219300	0.61716900	H	5.53676700	1.28023100	1.31395800
C	2.83510200	-3.69422100	-0.39792500	H	6.41619400	0.53451300	-0.02051200
C	2.84187900	-4.57268200	-1.43342300	C	7.26561100	2.39326700	0.66276100
H	3.58742300	-5.35779000	-1.47276800	C	8.51383700	2.15104300	0.07336500
C	1.87428100	-4.51121200	-2.58223100	C	9.59771700	2.99914200	0.31108700
H	2.39970300	-4.45450900	-3.54639300	C	9.44900100	4.10760100	1.14487400
H	1.22697500	-5.39992000	-2.63199400	C	8.21175500	4.35917200	1.74261600
H	1.22575400	-3.63235800	-2.51277000	C	7.13263500	3.50908100	1.50323600
O	1.97603100	-2.72333400	-0.20917900	H	6.17653300	3.70510600	1.98445300
Li	1.83752200	-1.14942800	-1.39085000	H	8.08880000	5.21500900	2.40118600
O	3.30853200	-0.40430700	-2.32724200	H	10.2914000	4.76763100	1.33320200
C	3.99325900	0.52311000	-1.91102800	H	10.5582990	2.78958100	-0.15225700
O	5.07785300	0.92859800	-2.62784700	H	8.64210300	1.28100800	-0.56746400
C	5.58225700	2.14826400	-2.05627600	O	-0.08083400	-1.19237100	-1.53982100
H	5.17481000	2.99359500	-2.62269900	C	-0.84590800	-0.60424000	-2.56009200
H	6.67000800	2.14587500	-2.13768000	C	-1.52561600	-1.73962200	-3.43844700
C	5.07372400	2.11915700	-0.61140700	H	-0.97020700	-1.83991600	-4.38002700

H	-1.33074200	-2.66185700	-2.88652700	C	8.51410600	-4.68188200	-0.23233900
C	-3.03142400	-1.68728600	-3.72059400	H	8.64232500	-3.81195700	0.40864800
C	-3.79953100	-0.39545000	-3.49534100	H	10.5585000	-5.32056600	-0.00651800
H	-4.79036100	-0.49894400	-3.05380800	H	10.2917220	-7.29834500	-1.49236000
C	-3.00321300	0.78257400	-2.94847200	H	8.08926400	-7.74542000	-2.56076000
H	-3.69386600	1.49474900	-2.48266800	H	6.17700800	-6.23548800	-2.14405000
H	-2.49535800	1.33421400	-3.74687900	O	-0.08061600	-1.33875400	1.38072400
C	-1.98556400	0.25868100	-1.90983100	C	-0.84572700	-1.92688000	2.40096400
H	-2.52658000	-0.46075800	-1.28086800	C	-1.52547800	-0.79149400	3.27928200
N	-1.48777800	1.27885500	-0.92832000	H	-0.97007900	-0.69115800	4.22086300
C	-1.08790500	2.57489100	-1.52291000	H	-1.33062700	0.13073500	2.72734200
C	-0.56490400	3.51815800	-0.44326600	C	-3.03128700	-0.84386700	3.56141800
O	-1.55304500	3.76403000	0.55046200	C	-3.79935100	-2.13573500	3.33619400
C	-1.96624200	2.54334500	1.14482600	H	-4.79018600	-2.03227300	2.89466500
H	-1.12366300	2.08844800	1.68938900	C	-3.00300700	-3.31373900	2.78932500
H	-2.74760200	2.79478900	1.86882900	H	-3.69364200	-4.02592400	2.32350800
C	-2.50730800	1.55875200	0.10880300	H	-2.49514600	-3.86537800	3.58772900
H	-2.77307000	0.61930600	0.60620900	C	-1.98535500	-2.78982700	1.75069100
H	-3.42666500	1.98026100	-0.33314200	H	-2.52638400	-2.07041100	1.12171300
H	-0.32088700	4.49044700	-0.88253300	N	-1.48752800	-3.80999300	0.76920800
H	0.34744100	3.10380100	0.01529800	C	-2.50702000	-4.08997600	-0.26792500
H	-1.94280300	3.06003900	-2.02131000	C	-1.96585200	-5.07453000	-1.30393200
H	-0.31016200	2.41578000	-2.26898800	O	-1.55257300	-6.29518500	-0.70955600
C	-3.66069700	-0.95661000	-4.89762500	C	-0.56449100	-6.04924100	0.28420900
C	-2.79849100	-0.28032700	-5.94694400	H	-0.32041800	-7.02150900	0.72348900
H	-1.86061300	0.11170400	-5.54901600	H	0.34784100	-5.63481800	-0.17432200
H	-2.53928500	-0.99216400	-6.74139900	C	-1.08758900	-5.10599800	1.36382700
H	-3.33710500	0.55322600	-6.41694000	H	-1.94247000	-5.59119600	1.86220700
C	-4.91469800	-1.58565900	-5.48846900	H	-0.30987800	-4.94683100	2.10992600
H	-5.54073800	-0.83050900	-5.98238500	H	-1.12329600	-4.61956400	-1.84847400
H	-4.65849600	-2.34620700	-6.23784500	H	-2.74717100	-5.32604000	-2.02795500
H	-5.52519300	-2.07045500	-4.71795000	H	-2.77284700	-3.15055400	-0.76534000
H	-3.55594100	-2.59994000	-3.43846900	H	-3.42635000	-4.51155800	0.17400800
C	0.11186900	0.20908100	-3.46361400	C	-3.66053500	-1.57453400	4.73846400
H	0.76892300	-0.48436600	-4.00052000	C	-2.79828700	-2.25071100	5.78781500
H	-0.39512200	0.83005200	-4.21146800	H	-1.86054300	-2.64301600	5.38984400
H	0.76028000	0.85362500	-2.86424900	H	-2.53883300	-1.53872500	6.58205700
C	6.07964900	-4.02615000	-0.54705800	H	-3.33698300	-3.08405000	6.25809500
H	5.53714500	-3.81086500	-1.47318300	C	-4.91455500	-0.94550700	5.32929100
H	6.41651900	-3.06521000	-0.13864000	H	-5.54057300	-1.70066300	5.82322600
C	7.26595600	-4.92393900	-0.82196700	H	-4.65837500	-0.18493300	6.07864800
C	7.13305000	-6.03959700	-1.66265900	H	-5.52506300	-0.46074700	4.55876000
C	8.21216200	-6.88970300	-1.90202200	H	-3.55582900	0.06876400	3.27926900
C	9.44932900	-6.63830200	-1.30404500	C	0.11204500	-2.74016600	3.30453100
C	9.59797600	-5.52999700	-0.47004200	H	0.76904800	-2.04669200	3.84146300

H -0.39494500 -3.36116500 4.05236200
H 0.76051400 -3.38467300 2.70518600

Table 18. Geometric coordinates and thermally corrected MP2 energies for (*S*)-**23a**



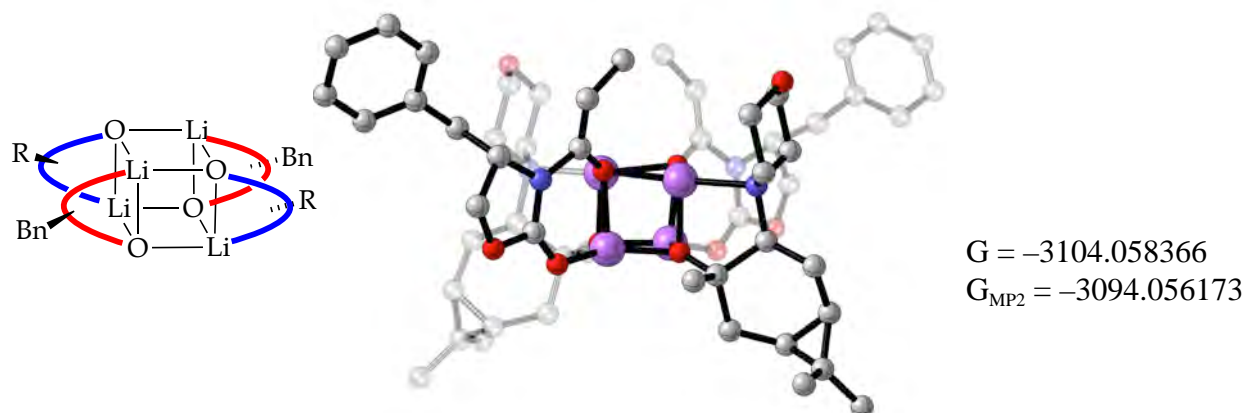
G = -3104.056855
G_{MP2} = -3094.056699

Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	N	-1.96399700	3.24443000	-0.94231100
Li	1.66699300	1.89199300	0.67660000	C	-1.06519700	2.99137900	0.17666600
O	2.99485300	2.93431800	1.56056600	C	-1.26888300	3.68162200	1.32724800
C	4.06253200	3.15311300	0.99982800	H	-2.04416000	4.43732600	1.35858900
O	5.19393100	3.36211200	1.72703400	C	-0.45257900	3.52485100	2.57925700
C	6.31233700	3.43394900	0.81566200	H	0.21895500	2.66344100	2.53110800
H	6.76746500	2.43986600	0.74198300	H	0.17683500	4.40541500	2.77296500
H	7.03549700	4.14410600	1.21770500	H	-1.08990400	3.39201200	3.46528900
C	5.66639600	3.88063600	-0.49981000	O	-0.16849900	2.05957800	-0.04319800
H	6.16483500	3.45263200	-1.37278900	C	-3.17167600	5.45695100	-0.89428100
N	4.34265500	3.25978300	-0.33435100	H	-2.45767300	5.78553700	-0.13366800
C	3.43568500	2.89462200	-1.41463000	H	-2.74839800	5.74176600	-1.86521000
C	3.62802000	3.46329600	-2.63122500	C	-4.51024800	6.13424800	-0.69069900
H	4.39575400	4.21922100	-2.74456000	C	-5.11292200	6.15561600	0.57652600
C	2.80293800	3.16793900	-3.85225000	C	-6.35628500	6.75678900	0.76896000
H	2.10769800	3.98560500	-4.09179700	C	-7.02162200	7.35182000	-0.30559000
H	3.43486400	3.01999900	-4.73911100	C	-6.43259900	7.34265700	-1.56997700
H	2.19663900	2.26556100	-3.73158300	C	-5.18781900	6.73797100	-1.75849700
O	2.54319500	1.98795500	-1.09364700	H	-4.72993000	6.74544600	-2.74542900
Li	0.70120800	1.74303300	-1.79212700	H	-6.93822900	7.80927600	-2.41127900
O	-0.62314900	2.68078400	-2.78711200	H	-7.98920600	7.82308400	-0.15600200
C	-1.68435700	2.98741200	-2.25626500	H	-6.80377200	6.76590800	1.75937100
O	-2.80858900	3.14712000	-3.00697700	H	-4.59857600	5.70524500	1.42325900
C	-3.92687700	3.34429900	-2.11525100	Li	2.36790100	-0.05277100	-0.87568900
H	-4.41028800	2.37637400	-1.94140800	O	0.66515600	-0.17069300	-1.78380200
H	-4.62881300	4.02903400	-2.59228500	C	0.73976600	-1.12104600	-2.81481600
C	-3.27374400	3.90841900	-0.84945800	C	-0.36441500	-0.80441400	-3.90770400
H	-3.78515200	3.58245300	0.05930100	H	-1.20393400	-1.50090500	-3.77436100

H	-0.74709600	0.18162400	-3.63360100	C	0.07374900	-1.27415700	4.09898200
C	0.03257400	-0.73326800	-5.38640000	H	-0.96485400	-1.23165300	4.44761900
C	1.37077800	-1.29091800	-5.84346800	H	0.33223800	-2.33788400	4.05158600
H	1.90478400	-0.69977300	-6.58682500	C	0.20178000	-0.61223900	2.70874200
C	2.27442100	-1.87862900	-4.76560600	N	-0.92874600	-0.88660800	1.75527700
H	3.30920100	-1.87586900	-5.12802900	C	-2.09217800	-0.02189400	2.06516000
H	2.03119200	-2.92615900	-4.55607700	C	-3.21119600	-0.24210500	1.05152300
C	2.15229400	-1.01974300	-3.48814200	O	-3.63406700	-1.59720000	1.01568100
N	3.29020500	-1.14775000	-2.51379800	C	-2.53590200	-2.44662600	0.71693300
C	4.44134300	-0.31833700	-2.94110400	H	-2.91971900	-3.47123100	0.73763900
H	4.11406000	0.71858500	-3.05385200	H	-2.16320400	-2.23484400	-0.29922300
H	4.84302900	-0.66287400	-3.90994900	C	-1.40517100	-2.28697900	1.73189000
C	5.55723900	-0.37445200	-1.90159800	H	-1.78473800	-2.59327300	2.71997700
O	5.99941600	-1.70353000	-1.66748300	H	-0.58485900	-2.95548800	1.46676000
C	4.91130200	-2.52108400	-1.26122000	H	-2.87611700	0.07569800	0.04822300
H	5.31153900	-3.53177800	-1.13535300	H	-4.08881000	0.35204600	1.32492200
H	4.52389900	-2.17582400	-0.28802500	H	-1.78039400	1.02547900	2.02871300
C	3.78856600	-2.52362600	-2.29735800	H	-2.48624100	-0.23098500	3.07483800
H	4.18363600	-2.95605300	-3.23098500	H	0.13710400	0.46809700	2.87945300
H	2.97719700	-3.16421700	-1.94846500	C	2.24684300	-1.05376900	5.67808800
H	5.20993000	0.08087200	-0.95719800	C	2.69934100	-2.48227600	5.44127900
H	6.42843100	0.18677500	-2.25380200	H	2.20021700	-3.17101100	6.13600700
H	2.20843100	0.02444900	-3.81632200	H	2.50287500	-2.83406200	4.42662600
C	0.08073300	-1.92450900	-6.33082000	H	3.78038100	-2.57240500	5.61072000
C	-0.35034800	-3.30550100	-5.87391700	C	2.59425400	-0.55483200	7.07361000
H	0.15040000	-4.08551900	-6.46294100	H	2.12004700	-1.17542800	7.84604000
H	-0.13798400	-3.49711800	-4.82051200	H	3.67872000	-0.58376400	7.24402100
H	-1.43182200	-3.43285300	-6.01417200	H	2.26207800	0.47836500	7.22704100
C	-0.29085900	-1.64750900	-7.78068800	H	2.58577400	0.97509500	4.88943900
H	0.17714500	-2.37573100	-8.45689500	C	1.91732000	-2.26666100	1.67316800
H	-1.37744700	-1.70866700	-7.92714100	H	2.96633400	-2.34292800	1.36454100
H	0.02984400	-0.64783400	-8.09510700	H	1.76090100	-2.99021100	2.48173200
H	-0.27194000	0.19695100	-5.86372100	H	1.30515300	-2.56834500	0.81938800
C	0.46171400	-2.51239400	-2.20169400	C	5.59857100	5.42742800	-0.61219400
H	-0.58060700	-2.54637100	-1.86473500	H	4.89830400	5.69298900	-1.40930600
H	0.60909200	-3.34805000	-2.89530400	H	5.17320900	5.81671000	0.32086200
H	1.09221800	-2.67945900	-1.32476200	C	6.95349900	6.05201500	-0.86826500
O	1.70186700	-0.01037800	0.91385900	C	7.56087300	5.94481300	-2.12884900
C	1.62197000	-0.80235000	2.07118600	C	8.82006000	6.49478700	-2.36658600
C	2.71448500	-0.32526600	3.11845800	C	9.49679000	7.16577200	-1.34524600
H	3.54741100	-1.04172300	3.11212700	C	8.90333800	7.28438300	-0.08843900
H	3.11324200	0.60164100	2.69997700	C	7.64257200	6.73102500	0.14561300
C	2.29657700	-0.02200600	4.56111900	H	7.18156300	6.83799800	1.12525600
C	0.95796400	-0.51834400	5.08374500	H	9.41795900	7.81091200	0.71099600
H	0.40984400	0.17467200	5.72113300	H	10.4769210	7.59670900	-1.53052600

H 9.27137700 6.40429500 -3.35115700
H 7.03799700 5.43328400 -2.93465400

Table 19. Geometric coordinates and thermally corrected MP2 energies for (*S*)-**24a**



Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	N	4.53251000	-2.70239600	-1.45066200
O	-1.66794200	0.83820500	0.14656200	C	3.34724800	-2.47275300	-2.28287600
C	-2.45277800	1.03030100	-0.77232600	C	3.32118900	-3.09128100	-3.49311500
O	-3.69183800	1.52302900	-0.50030700	H	4.13262900	-3.75164000	-3.77271400
C	-4.32544900	1.89881200	-1.73268200	C	2.23986700	-2.91511200	-4.51875300
H	-4.19671500	2.97775300	-1.87522700	H	1.36725300	-2.40789000	-4.10280500
H	-5.38945200	1.66832600	-1.66233700	H	2.57525600	-2.31961900	-5.38240500
C	-3.59135200	1.08151500	-2.80341600	H	1.90206400	-3.87951300	-4.92141600
H	-3.43265000	1.69564900	-3.69145200	O	2.43317100	-1.67655400	-1.78163100
N	-2.31191500	0.82057200	-2.11864400	Li	1.78570000	0.23821600	-1.90112900
C	-1.12035900	0.31893700	-2.81153200	O	1.77161000	0.64694900	-0.05935300
C	-1.09051300	0.46958800	-4.16210500	C	2.34738400	1.89494200	0.20905800
H	-1.90510200	0.97868500	-4.66195800	C	2.83146400	1.94181000	1.71845300
C	0.00430800	-0.04334400	-5.05121100	H	2.12125800	2.54309500	2.30173600
H	-0.29500300	-0.94169200	-5.61364900	H	2.71340800	0.91528500	2.07626600
H	0.29974800	0.70529900	-5.79819200	C	4.26910100	2.36777200	2.03578300
H	0.89638400	-0.30914200	-4.48029500	C	5.10175500	3.07688400	0.98063500
O	-0.20370600	-0.24133400	-2.05868600	H	6.14801700	2.77859100	0.92091300
Li	0.45183200	-2.07636200	-1.48401100	C	4.44870700	3.29695200	-0.37909700
Li	2.21497100	-1.17493400	0.22981400	H	5.23299800	3.44411200	-1.13131100
O	3.88155400	-1.91094600	0.66990200	H	3.83991100	4.20781700	-0.39526100
C	4.66821900	-2.41995600	-0.11705900	C	3.59274000	2.05974600	-0.72380300
O	5.90395800	-2.78816900	0.31811500	H	4.20609300	1.18119000	-0.48834200
C	6.54137200	-3.57841000	-0.69699400	N	3.25484300	1.88664300	-2.17809000
H	6.41502500	-4.63705200	-0.44381400	C	4.38525600	1.27890600	-2.91406900
H	7.60480200	-3.33494700	-0.71213100	H	4.64121200	0.32699600	-2.43835300
C	5.80993300	-3.20081400	-1.99200500	H	5.27840100	1.92751100	-2.88508500
H	5.64585600	-4.09498400	-2.59599500	C	4.00556500	1.02724400	-4.37192300

O	3.59716300	2.21934100	-5.02685500	C	-2.25495700	-4.38693900	0.97873600
C	2.51832600	2.83219000	-4.33159100	H	-3.02361800	-4.79564300	0.31188300
C	2.88585200	3.13499500	-2.88269100	H	-1.65367700	-5.24238700	1.30599400
H	3.72229100	3.85236800	-2.88016600	C	-1.38060400	-3.35730700	0.23138600
H	2.03778500	3.60641400	-2.38491500	H	-1.98990600	-2.45167900	0.12064900
H	2.29572000	3.76070700	-4.86643500	N	-1.01153500	-3.72013600	-1.17935500
H	1.62493400	2.18905700	-4.36567600	C	-2.12210500	-3.41933300	-2.10932600
H	3.20567000	0.27034000	-4.42415400	H	-2.38094700	-2.36020100	-2.01406500
H	4.86876500	0.64732300	-4.92739000	H	-3.02028300	-4.01487600	-1.86840200
C	4.71317200	3.80612500	2.25344800	C	-1.70851600	-3.70941800	-3.55050600
C	3.70878900	4.94317000	2.24176900	O	-1.29426900	-5.05678000	-3.72318300
H	3.28579100	5.08810000	3.24446700	C	-0.23608000	-5.37899000	-2.82862500
H	4.18947500	5.88635700	1.94924500	C	-0.63822900	-5.13832700	-1.37728100
H	2.87156000	4.77205900	1.56224900	H	-1.48166700	-5.80522300	-1.13651500
C	5.82940300	4.02140500	3.26552500	H	0.19345000	-5.39818500	-0.72158600
H	6.38653300	4.94379800	3.05223600	H	-0.01156200	-6.43831100	-2.98735400
H	5.42731900	4.10446600	4.28399000	H	0.66431200	-4.79287900	-3.07133400
H	6.54502500	3.19130400	3.25831400	H	-0.90225300	-3.02124700	-3.85257500
H	4.80700200	1.64079300	2.64236100	H	-2.55621200	-3.55587400	-4.22566300
C	1.26034100	2.97425900	-0.00904800	C	-2.57801700	-3.91498100	3.61115900
H	0.48315000	2.85191400	0.75357900	C	-1.58276500	-4.97940700	4.03341000
H	1.63150300	4.00417300	0.05542400	H	-1.18000200	-4.75016800	5.02867500
H	0.77310700	2.84216800	-0.98024900	H	-2.06566600	-5.96399000	4.09398100
C	6.54140600	-2.13015900	-2.83506000	H	-0.73143000	-5.06835700	3.35577200
H	5.83688500	-1.77453200	-3.59458300	C	-3.71756000	-3.75277800	4.60713800
H	6.77839500	-1.28045900	-2.18299500	H	-4.27820700	-4.69012600	4.72421300
C	7.80006400	-2.65594000	-3.49034200	H	-3.33829800	-3.46682200	5.59721600
C	7.71920700	-3.51157000	-4.59965800	H	-4.42533700	-2.97948200	4.28729700
C	8.87151700	-4.02378400	-5.19469300	H	-2.66499700	-1.75545600	3.19358100
C	10.13015300	-3.68670500	-4.69108100	C	0.92669600	-3.95550800	1.28553100
C	10.22593600	-2.83267100	-3.59229000	H	1.68606600	-3.56687300	1.97324700
C	9.06918600	-2.32299100	-2.99837700	H	0.54448400	-4.89382600	1.70527700
H	9.15318200	-1.64776800	-2.14932900	H	1.43888900	-4.17968900	0.34459600
H	11.2005710	-2.55777700	-3.19779200	C	-4.31481000	-0.22766000	-3.19733900
H	11.0287430	-4.08278000	-5.15614500	H	-3.60838000	-0.82807700	-3.78042800
H	8.78754000	-4.68121100	-6.05606000	H	-4.54113800	-0.78506400	-2.28004200
H	6.74361600	-3.76887500	-5.00737800	C	-5.58025400	0.01426400	-3.99087100
O	0.44204600	-1.80489000	0.38371900	C	-5.51060300	0.39843900	-5.33872100
C	-0.15388500	-2.86902000	1.07179600	C	-6.66925800	0.65176900	-6.07200000
C	-0.67292300	-2.36318600	2.48263200	C	-7.92284700	0.52337900	-5.46921100
H	0.02190600	-2.70487900	3.26153700	C	-8.00747700	0.13686000	-4.13151000
H	-0.56126400	-1.27616400	2.44249400	C	-6.84449600	-0.11505400	-3.40041500
C	-2.11898500	-2.65092500	2.90079900	H	-6.91953900	-0.42868600	-2.36127100
C	-2.93439600	-3.69257200	2.15277400	H	-8.97821100	0.02607800	-3.65556900
H	-3.97708000	-3.43650100	1.96681300	H	-8.82635000	0.71777400	-6.04063900

H -6.59421200 0.94373800 -7.11618600
H -4.53880800 0.48866200 -5.82015900

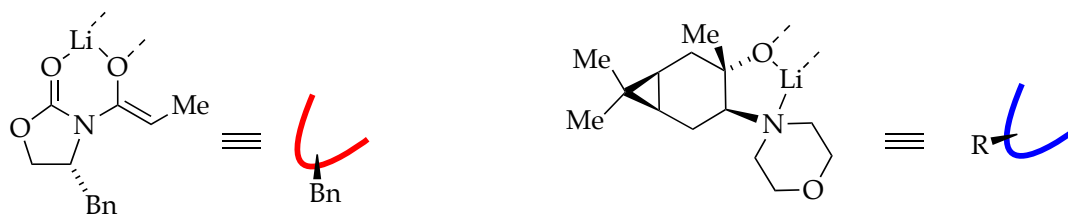
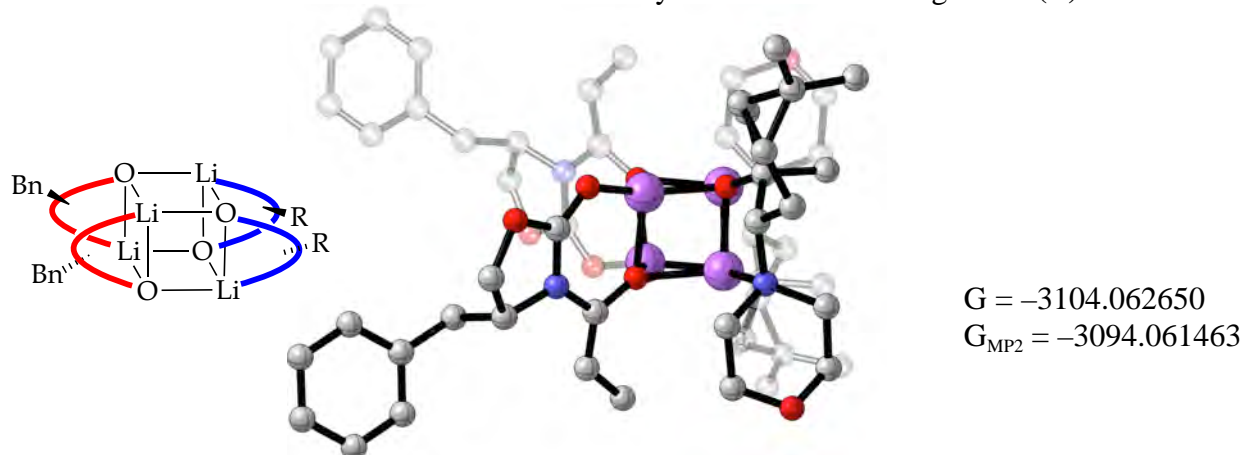


Table 20. Geometric coordinates and thermally corrected MP2 energies for (*R*)-22a

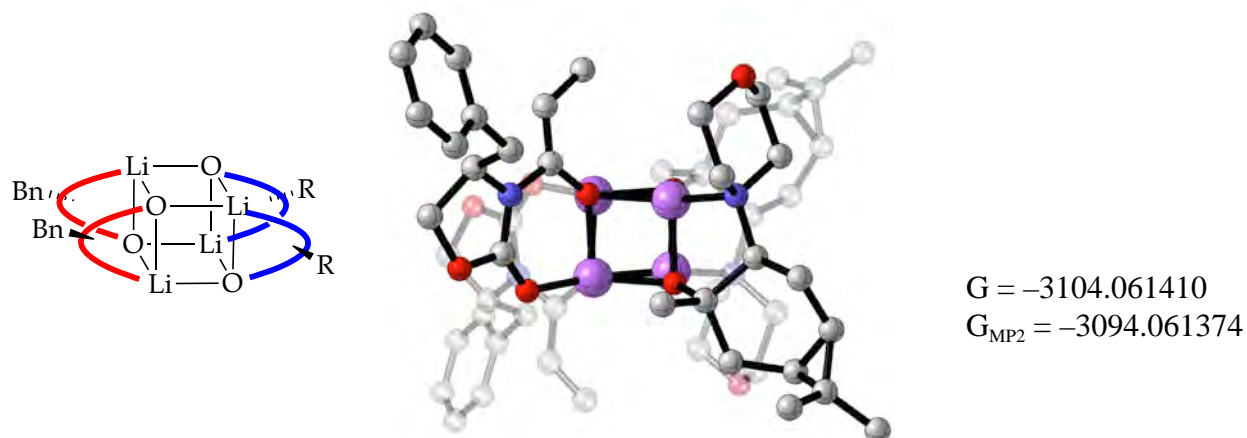


Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	C	-8.48556800	-4.49745600	-2.21551300
Li	-1.83734000	-0.17274200	-1.79249700	C	-9.55096200	-5.17722900	-2.80988000
O	-2.02575800	0.12139400	0.14751300	C	-9.49311200	-5.52474500	-4.15965500
Li	-1.83647700	-1.84734200	0.26822500	C	-8.36581300	-5.18452300	-4.91124800
Li	0.00101800	-2.01838600	-1.52441800	C	-7.30495800	-4.50456300	-4.31399400
O	-2.02495500	-2.14174400	-1.67172400	H	-6.43727800	-4.23246500	-4.91171000
C	-2.94663000	-2.79881800	-2.33085200	H	-8.31537300	-5.44364400	-5.96555500
C	-3.14740600	-2.77716400	-3.67366700	H	-10.3215760	-6.05176600	-4.62506100
C	-2.33632600	-1.93645700	-4.61992700	H	-10.4266230	-5.43039200	-2.21796100
H	-1.98405000	-2.52215800	-5.48060400	H	-8.54360700	-4.21915700	-1.16525100
H	-1.45606500	-1.51331100	-4.12664800	C	-5.21136000	-5.37128000	-0.91060400
H	-2.91641100	-1.09549400	-5.02913300	O	-4.68928100	-4.69996000	0.25030600
H	-3.94466500	-3.36390200	-4.11320100	C	-3.78256500	-3.76755000	-0.15127700
N	-3.81216800	-3.64497200	-1.51536700	O	-3.10516300	-3.18395800	0.68762900
C	-4.97168300	-4.37646300	-2.05096500	H	-4.65805100	-6.30698500	-1.05101700
H	-4.69275100	-4.89906700	-2.96850400	H	-6.26514900	-5.59319200	-0.73747800
C	-6.17869300	-3.43976400	-2.31045900	O	0.06061600	-1.86461300	0.41694100
H	-5.83318600	-2.61526400	-2.94224000	C	0.92032400	-2.83750300	0.95130700
H	-6.48404200	-3.00422900	-1.35093900	C	0.51065000	-3.13259800	2.45392300
C	-7.34687300	-4.15258400	-2.95616100	H	1.18334800	-2.57631300	3.12138200

H	-0.47062400	-2.66490000	2.56686500	C	1.51789400	3.33476800	-2.27138800
C	0.36103500	-4.58039000	2.93467100	H	1.47564900	4.20215600	-1.60213000
C	0.87834400	-5.72391300	2.07906300	H	2.58119700	3.09624400	-2.38621000
H	0.23999300	-6.60517400	2.02568400	C	0.75294200	2.14387700	-1.65237600
C	1.52140500	-5.35193500	0.74839900	H	-0.31485700	2.37542800	-1.74903500
H	1.47976600	-6.21964100	0.07951400	N	0.94822500	1.95651400	-0.17308100
H	2.58453800	-5.11251400	0.86296600	C	0.07942000	2.88621100	0.58656700
C	0.75541700	-4.16194100	0.12892500	C	0.21709000	2.65084500	2.08843700
H	-0.31217100	-4.39450400	0.22544700	O	1.56240300	2.80471700	2.52231900
N	0.95084400	-3.97468600	-1.35033100	C	2.40899400	1.91166000	1.81584700
C	0.08276500	-4.90498100	-2.11005300	H	3.42643600	2.09367700	2.17565600
H	-0.95587000	-4.73437400	-1.81287500	H	2.13794500	0.86814500	2.05097000
H	0.33707900	-5.95646300	-1.89026100	C	2.33542700	2.14336300	0.30801500
C	0.22077300	-4.66985200	-3.61193600	H	2.69329600	3.16435500	0.10074000
O	1.56629100	-4.82298700	-4.04540400	H	3.00297100	1.44490600	-0.19908200
C	2.41211000	-3.92922600	-3.33889400	H	-0.15123300	1.64540400	2.34640200
C	2.33827700	-4.16072600	-1.83105300	H	-0.37687300	3.38366300	2.64248300
H	2.69675600	-5.18145600	-1.62353900	H	-0.95903500	2.71513500	0.28904100
H	3.00523700	-3.46176300	-1.32388200	H	0.33325900	3.93785700	0.36704500
H	3.42976600	-4.11063900	-3.69840200	C	1.49029200	3.44251300	-4.96419100
H	2.14042600	-2.88593400	-3.57429900	C	2.90046600	2.90366700	-5.11552500
H	-0.14803800	-3.66467300	-3.87024200	H	3.15571200	2.14485900	-4.37390000
H	-0.37260400	-5.40312800	-4.16600700	H	3.02722500	2.44373700	-6.10437100
C	1.49417500	-5.45824100	3.44129900	H	3.63906600	3.71238400	-5.03402800
C	2.90372200	-4.91771500	3.59242700	C	1.12725000	4.43605500	-6.05925300
H	3.15818900	-4.15899700	2.85046100	H	1.80812900	5.29801900	-6.05448400
H	3.02985900	-4.45713800	4.58105200	H	1.18954100	3.96939900	-7.05134900
H	3.64324900	-5.72563600	3.51142300	H	0.10723500	4.81748300	-5.93573600
C	1.13235000	-6.45172500	4.53683500	H	-0.59522400	2.74522500	-4.95109200
H	1.81416300	-7.31295200	4.53231800	C	2.35625400	0.25346300	-2.43365900
H	1.19428400	-5.98459300	5.52873000	H	2.42193100	-0.59293400	-3.12748300
H	0.11273300	-6.83430900	4.41362000	H	3.13414300	0.97138300	-2.71659400
H	-0.59213600	-4.76367800	3.42817100	H	2.58823200	-0.12649800	-1.43521400
C	2.35709100	-2.27024900	0.91025200	C	-2.94719200	0.77846600	0.80695700
H	2.58899400	-1.89018600	-0.08817000	C	-3.14727000	0.75703000	2.14988400
H	2.42211200	-1.42379300	1.60406000	C	-2.33593500	-0.08392700	3.09570800
H	3.13540600	-2.98764800	1.19329100	H	-2.91583800	-0.92512100	3.50469800
O	0.05972800	-0.15381700	-1.94173100	H	-1.98342000	0.50141400	3.95653700
C	0.91914800	0.81982500	-2.47513400	H	-1.45573000	-0.50677100	2.60206700
C	0.51036400	1.11516700	-3.97805100	H	-3.94433500	1.34378400	2.58974900
H	1.18504000	0.56089500	-4.64518200	N	-3.81307100	1.62445300	-0.00828000
H	-0.46968100	0.64524200	-4.09228400	C	-4.97252500	2.35581600	0.52763200
C	0.35829300	2.56297400	-4.45788200	H	-4.69332800	2.87869800	1.44493300
C	0.87428500	3.70672500	-3.60177500	C	-6.17922900	1.41892300	0.78785100
H	0.23481500	4.58714300	-3.54784700	H	-5.83323900	0.59460300	1.41959700

H -6.48496300 0.98317300 -0.17144800
C -7.34722900 2.13160100 1.43403300
C -8.48632300 2.47624000 0.69388900
C -9.55155300 3.15587200 1.28870900
C -9.49313700 3.50348200 2.63843500
C -8.36543400 3.16349400 3.38952800
C -7.30474600 2.48367000 2.79182500
H -6.43674400 2.21174700 3.38915700
H -8.31454900 3.42268500 4.44379700
H -10.3214730 4.03039200 3.10419300
H -10.4275320 3.40885000 0.69718200
H -8.54480800 2.19785900 -0.35632700
C -5.21284900 3.35029100 -0.61288200
O -4.69126100 2.67869100 -1.77385200
C -3.78415500 1.74658000 -1.37243300
O -3.10701200 1.16288400 -2.21145900
H -4.65954600 4.28607700 -0.47298300
H -6.26673900 3.57206800 -0.78556500

Table 21. Geometric coordinates and thermally corrected MP2 energies for (*R*)-**15a**

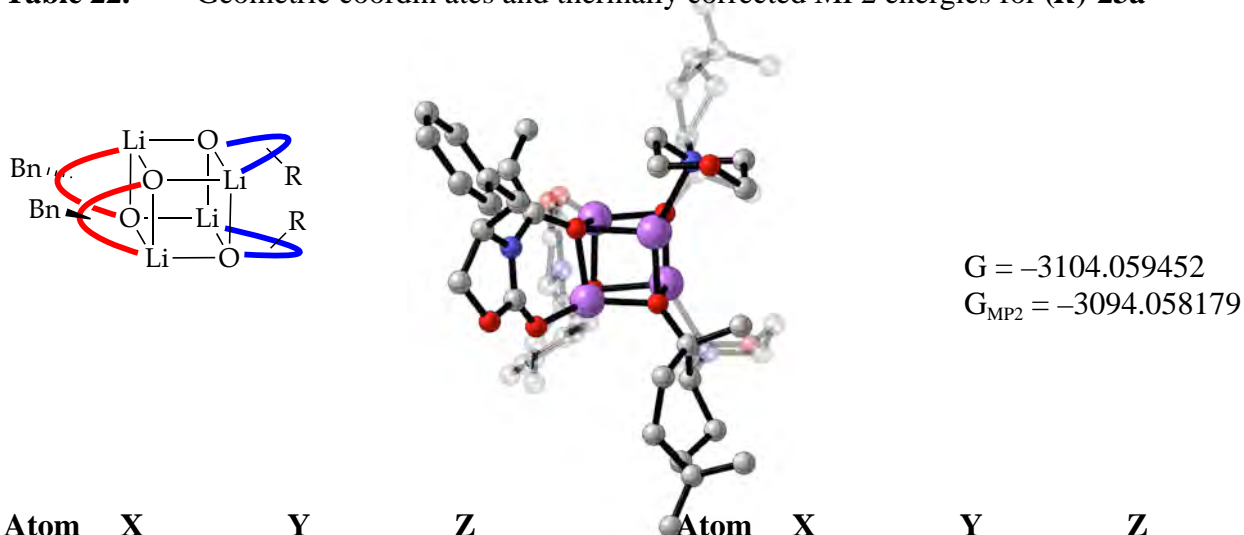


Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	H	8.08989700	-5.82092900	-1.47394300
Li	-2.32577700	-0.00130800	-0.96840200	H	6.05497000	-4.51333400	-1.99331400
Li	-1.65266700	-1.85674800	0.72388200	C	2.73362800	-5.54806600	-1.37706100
O	-2.53033900	-1.96175400	-1.04471500	O	1.90012600	-4.89394600	-2.34829800
Li	-0.67147000	-1.85609800	-1.69279100	C	1.16156900	-3.93553800	-1.72414000
O	0.20634300	-1.96051600	0.07589700	O	0.25388700	-3.38046500	-2.33208300
C	1.05942600	-2.83875800	0.54411900	H	2.24461700	-6.47968500	-1.07088900
C	1.46497100	-2.95906100	1.83353800	H	3.69335600	-5.77851300	-1.84191200
C	0.95491000	-2.09124100	2.94998000	O	-0.62647300	0.07394500	-1.85034600
H	1.77441300	-1.61063900	3.50442500	C	0.31732100	0.78672500	-2.60688500
H	0.37757200	-2.67154700	3.68465000	C	-0.37029100	1.39328800	-3.90393400
H	0.29812800	-1.29979400	2.57566300	H	-0.02263000	0.83502900	-4.78273800
H	2.15059300	-3.75077100	2.11241200	H	-1.42749800	1.13965500	-3.79844000
N	1.61622600	-3.75290500	-0.44594200	C	-0.27499400	2.89823600	-4.17495500
C	2.83671700	-4.54241100	-0.22253200	C	0.82039800	3.71464400	-3.50743500
H	2.78206300	-5.06441200	0.73512000	H	0.53247700	4.70543300	-3.15661300
C	4.10563800	-3.65749000	-0.26591800	C	1.73150400	2.96315400	-2.54570500
H	3.95873800	-2.84611500	0.45512500	H	2.22015800	3.68254200	-1.87836200
H	4.17315200	-3.20261100	-1.26200800	H	2.53849400	2.44263100	-3.07249700
C	5.37097200	-4.42453400	0.04868700	C	0.87605500	1.96630200	-1.73424300
C	6.26004600	-4.80553800	-0.96545500	H	-0.02706600	2.51032500	-1.42900500
C	7.41150000	-5.53954200	-0.67278800	N	1.47503900	1.51788300	-0.43246700
C	7.69235100	-5.90502100	0.64389900	C	2.91331900	1.17029000	-0.48914000
C	6.81745700	-5.52804500	1.66558900	C	3.39472600	0.68401900	0.87536000
C	5.66929500	-4.79429700	1.36906000	O	3.21518900	1.68363500	1.87042900
H	5.00021100	-4.49381100	2.17288400	C	1.84660500	2.05021300	1.95506100
H	7.03264400	-5.80065300	2.69545300	H	1.25007100	1.19080600	2.30150900
H	8.58878200	-6.47427900	0.87428800	H	1.77918600	2.84153400	2.70807900

C	1.30607600	2.55002900	0.61587400	C	-5.05719200	-5.54918900	0.40945200
H	0.23951000	2.77693100	0.72019100	O	-4.22343800	-4.89485600	1.38033600
H	1.82922700	3.48458700	0.34848800	C	-3.48471600	-3.93688100	0.75572600
H	4.46763400	0.47069700	0.84115200	O	-2.57678800	-3.38179300	1.36328900
H	2.86232400	-0.23902000	1.15913700	H	-4.56851700	-6.48114200	0.10376600
H	3.51980500	2.04422500	-0.77715100	H	-6.01698400	-5.77906900	0.87445100
H	3.07849000	0.38842400	-1.23007300	O	-1.69942700	0.07323500	0.88187600
C	0.82164000	3.53992100	-5.01343800	C	-2.64351300	0.78554500	1.63849700
C	1.86485900	2.68753300	-5.71199400	C	-1.95592800	1.39265700	2.93528100
H	2.13328100	1.78775000	-5.15410400	H	-2.30230700	0.83371500	3.81416200
H	1.49668400	2.36162200	-6.69350600	H	-0.89846100	1.14043900	2.82903000
H	2.78557100	3.26145900	-5.88069100	C	-2.05285000	2.89743300	3.20672700
C	0.42174700	4.76206500	-5.82750300	C	-3.14889000	3.71298900	2.53924600
H	1.28705100	5.41068600	-6.01873400	H	-2.86183200	4.70412100	2.18868700
H	0.00475100	4.46925800	-6.80014700	C	-4.05927800	2.96093000	1.57728600
H	-0.33504900	5.36203800	-5.30905800	H	-4.54835000	3.68004100	0.90995000
H	-1.24288000	3.39124000	-4.26013700	H	-4.86596800	2.43974400	2.10387600
C	1.41130000	-0.20678900	-3.06685000	C	-3.20302900	1.96474500	0.76583200
H	0.96716700	-0.92450600	-3.76585700	H	-2.30028300	2.50944500	0.46067800
H	2.25808200	0.26893800	-3.57695100	N	-3.80159600	1.51594100	-0.53597600
H	1.79424300	-0.78325200	-2.22030100	C	-3.63321100	2.54813900	-1.58434000
C	-3.38248800	-2.84096200	-1.51287100	C	-4.17328100	2.04787300	-2.92353700
C	-3.78705200	-2.96250200	-2.80246400	O	-5.54165100	1.68047400	-2.83900300
C	-3.27665000	-2.09533100	-3.91925900	C	-5.72072500	0.68082800	-1.84389200
H	-4.09630700	-1.61926800	-4.47732500	H	-6.79354400	0.46704400	-1.80968800
H	-2.69470300	-2.67501300	-4.65080700	H	-5.18799200	-0.24203000	-2.12769200
H	-2.62418000	-1.30038800	-3.54477700	C	-5.23963700	1.16737900	-0.47938200
H	-4.47166900	-3.75511700	-3.08126100	H	-5.84671500	2.04090000	-0.19137100
N	-3.93946300	-3.75462400	-0.52248300	H	-5.40431600	0.38538200	0.26153000
C	-5.15999300	-4.54412900	-0.74564200	H	-3.57617300	1.18880200	-3.26984400
H	-5.10526600	-5.06667700	-1.70299400	H	-4.10627900	2.83916100	-3.67662500
C	-6.42882200	-3.65905600	-0.70303400	H	-2.56679000	2.77573400	-1.68856900
H	-6.28165200	-2.84813500	-1.42453600	H	-4.15701600	3.48236600	-1.31706700
H	-6.49653300	-3.20358300	0.29277100	C	-3.15014600	3.53793000	4.04521800
C	-7.69414500	-4.42616300	-1.01752400	C	-4.19267900	2.68447200	4.74349100
C	-8.58341300	-4.80670700	-0.00338000	H	-4.46003200	1.78442500	4.18552000
C	-9.73483000	-5.54081200	-0.29594400	H	-3.82441700	2.35891500	5.72508800
C	-10.0154470	-5.90684700	-1.61252700	H	-5.11401500	3.25745900	4.91197600
C	-9.14036000	-5.53032500	-2.63421900	C	-2.75143100	4.76026600	4.85957600
C	-7.99223700	-4.79647800	-2.33779400	H	-3.61734000	5.40806100	5.05086600
H	-7.32298900	-4.49635000	-3.14161600	H	-2.33424500	4.46763900	5.83219200
H	-9.35537000	-5.80336400	-3.66400500	H	-1.99514400	5.36102700	4.34130300
H	-10.9118490	-6.47618300	-1.84283700	H	-1.08544100	3.39133400	3.29217900
H	-10.4133820	-5.82183900	0.50520700	C	-3.73680600	-0.20861300	2.09868700
H	-8.37852700	-4.51405900	1.02439000	H	-3.29210500	-0.92600700	2.79766300

H -4.58387000 0.26654200 2.60885300
H -4.11947100 -0.78537100 1.25221000

Table 22. Geometric coordinates and thermally corrected MP2 energies for (*R*)-**23a**

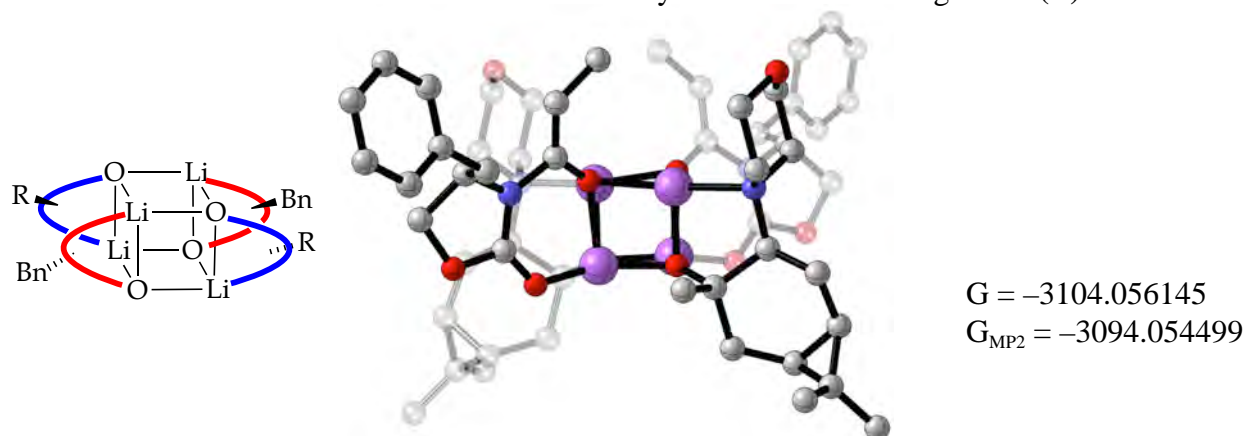


Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	H	-6.22235300	-2.29197300	-2.57391200
Li	1.62731000	0.82332100	-1.87577200	C	-1.16769800	1.20292100	-3.84018300
O	2.70721000	-0.85244600	-1.91103800	C	-0.55005000	2.54703300	-3.57865700
Li	0.90390700	-1.69801700	-1.76473800	H	-1.29441400	3.35141200	-3.66072000
O	-0.15606400	-0.04386000	-2.06159200	H	0.25436400	2.78058000	-4.28963900
C	-0.94237900	0.08652400	-3.10548500	H	-0.11125700	2.60792600	-2.57814600
N	-1.68225900	-1.11561800	-3.49153900	H	-1.79691800	1.12476600	-4.72119100
C	-3.04999600	-1.10043100	-4.02732100	Li	2.43103500	-0.67873100	0.10196300
H	-3.10913000	-0.44977000	-4.90331600	O	0.80257000	-1.72304900	0.14366200
C	-3.20905100	-2.57192300	-4.45870600	C	0.92370200	-2.81025000	1.02243500
H	-3.06937300	-2.70529700	-5.53662900	C	-0.04980800	-3.97870500	0.56582100
H	-4.16667100	-3.00577500	-4.16578200	H	-0.90972700	-4.01083200	1.24857000
O	-2.15956200	-3.28059900	-3.77672400	H	-0.44573500	-3.65040100	-0.39816900
C	-1.22804400	-2.39096300	-3.34448100	C	0.50824000	-5.39130400	0.36404500
O	-0.15463300	-2.78760200	-2.90204100	C	1.85079200	-5.76909700	0.96746200
C	-4.08131900	-0.62576600	-2.98012800	H	2.49534700	-6.38891600	0.34489900
H	-3.74017100	0.34969700	-2.61629400	C	2.59527000	-4.67071500	1.71615700
H	-4.06254300	-1.31853500	-2.13020000	H	3.65938000	-4.93025500	1.76475600
C	-5.48087500	-0.51613900	-3.54461500	H	2.25896400	-4.58436000	2.75555200
C	-6.46060600	-1.47371100	-3.25025200	C	2.39995500	-3.33718200	0.96067700
C	-7.74156500	-1.38202100	-3.79916200	N	3.42693000	-2.27776500	1.24392700
C	-8.06291100	-0.32731800	-4.65380800	C	4.67415600	-2.54016000	0.48783500
C	-7.09737500	0.63708800	-4.95213400	H	4.43872200	-2.58842900	-0.57975000
C	-5.81992600	0.54250900	-4.40119800	H	5.12734600	-3.50133300	0.78573600
H	-5.07731700	1.30461100	-4.62935300	C	5.69092700	-1.42678200	0.72797800
H	-7.34140600	1.46723400	-5.60984500	O	5.99958000	-1.27514000	2.10537600
H	-9.05962800	-0.25284800	-5.08006100	C	4.81706400	-1.01676800	2.84818800
H	-8.48815900	-2.13272000	-3.55383200	H	5.11791400	-0.94315500	3.89777200

H	4.38297400	-0.05121700	2.54064400	H	-1.97770500	1.83046300	-0.89744400
C	3.78980100	-2.13135900	2.67079100	H	-2.73180600	2.83430600	0.36511400
H	4.22518200	-3.06319900	3.06657400	H	-0.12709400	2.87717100	-0.40521000
H	2.90110600	-1.90122300	3.25948400	C	1.78001800	5.84827800	1.06228300
H	5.30569200	-0.47507900	0.32081000	C	2.29358900	5.64636200	2.47541200
H	6.63212500	-1.66216100	0.22237600	H	1.75110900	6.28612600	3.18425300
H	2.54821400	-3.56381000	-0.10178100	H	2.20381800	4.61519700	2.82224600
C	0.58509200	-6.44589200	1.45834500	H	3.35593300	5.91691600	2.53697500
C	0.02576500	-6.17402400	2.84217500	C	1.99158100	7.26923200	0.55975200
H	0.53462000	-6.78831100	3.59699100	H	1.47536800	7.99745200	1.19985200
H	0.11864500	-5.12963800	3.14676600	H	3.05818000	7.53037000	0.55298500
H	-1.04192000	-6.42772500	2.87862400	H	1.61302600	7.39652900	-0.46089000
C	0.38660500	-7.88939600	1.01907600	H	2.12172700	5.09657700	-0.97969600
H	0.87986400	-8.58632400	1.71011900	C	1.83944500	1.82341300	2.26745100
H	-0.67988900	-8.14941600	0.99007800	H	2.91596900	1.62218400	2.30969200
H	0.79780300	-8.06584900	0.01863900	H	1.62343800	2.60446200	3.00578600
H	0.31166700	-5.79260100	-0.62890500	H	1.32562900	0.90723600	2.57309400
C	0.50163000	-2.33610100	2.43201000	C	3.60196100	-1.00973400	-2.85868600
H	-0.57386400	-2.12619900	2.42334700	C	3.85709600	-2.12989200	-3.57681300
H	0.68471800	-3.07097900	3.22499600	C	3.15155200	-3.44385400	-3.38645200
H	1.01165800	-1.40533400	2.69750500	H	2.32024100	-3.58572700	-4.09072800
O	1.62094300	1.05533500	0.01942400	H	2.72714100	-3.53461700	-2.38092400
C	1.46312100	2.19971700	0.81558200	H	3.84185100	-4.28582000	-3.52848000
C	2.44324700	3.33991900	0.30654900	H	4.58700500	-2.07889300	-4.37878600
H	3.29926800	3.40354100	0.99230300	N	4.42804000	0.16957300	-3.12390900
H	2.84388000	2.95991200	-0.63644100	C	5.78137600	0.12680900	-3.70129600
C	1.89304700	4.74200000	0.02410100	H	5.73437600	-0.28487100	-4.71940500
C	0.53100700	5.14600500	0.56342800	C	6.10724900	1.62892900	-3.75763100
H	-0.09242600	5.73391300	-0.10948700	H	6.63089200	1.93054100	-4.66544300
C	-0.23829700	4.08644400	1.34280700	H	6.68291600	1.95241700	-2.88283000
H	-1.30420600	4.34300200	1.33680200	O	4.82956000	2.28935800	-3.72658600
H	0.05931400	4.06041900	2.39714500	C	3.89109900	1.41713000	-3.28296300
C	-0.01239600	2.71262600	0.67227700	O	2.73928400	1.78855900	-3.08719400
N	-1.04277100	1.66435600	0.98441300	C	6.79343200	-0.68515000	-2.87674500
C	-2.25898400	1.85801600	0.16013100	H	6.40455000	-1.70348400	-2.77460500
C	-3.27686000	0.75447900	0.43996500	H	6.84351500	-0.25391600	-1.87032300
O	-3.64336500	0.70653100	1.81047600	C	8.16873800	-0.70185800	-3.51165700
C	-2.49211300	0.50837700	2.61790300	C	9.21247500	0.08088900	-3.00033700
H	-2.83529500	0.50953500	3.65702700	C	10.4720760	0.08000300	-3.60318300
H	-2.04406500	-0.47464900	2.39925100	C	10.7078090	-0.70651000	-4.73103800
C	-1.46122900	1.61277300	2.40273500	C	9.67781600	-1.49518700	-5.24879000
H	-1.91369300	2.56721200	2.71661000	C	8.42181600	-1.49276300	-4.64278700
H	-0.59486400	1.42801900	3.03922700	H	7.62976000	-2.12072700	-5.04559500
H	-2.86569800	-0.22122700	0.12650200	H	9.85445400	-2.11817600	-6.12165600
H	-4.19708000	0.93639200	-0.12305700	H	11.6879310	-0.71056100	-5.20009300

H 11.2690300 0.69086500 -3.18741600
H 9.04111000 0.68882300 -2.11456100

Table 23. Geometric coordinates and thermally corrected MP2 energies for (*R*)-**24a**

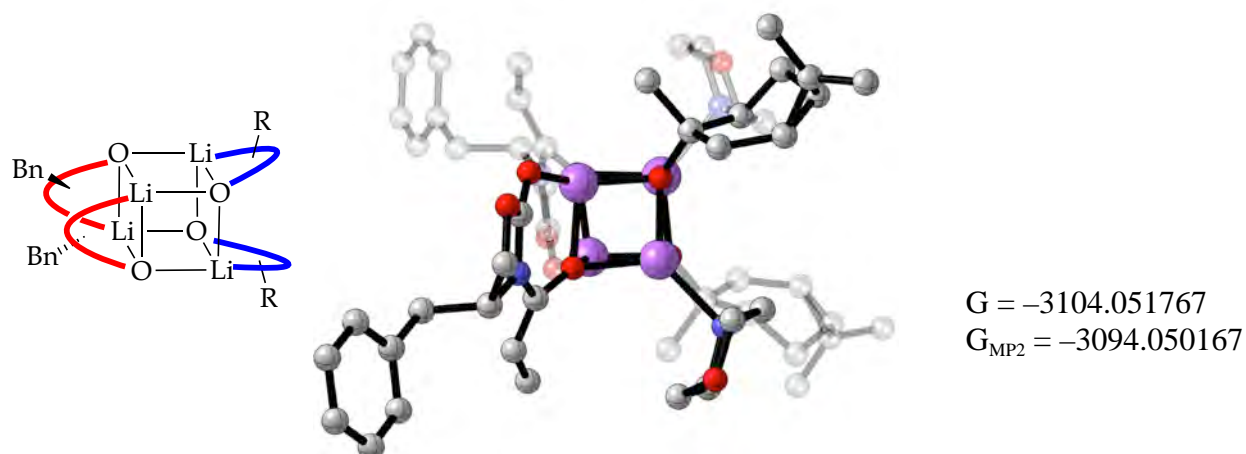


Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	H	-0.12115400	4.40836200	-1.98180400
O	-0.22851100	-0.04911400	-2.06713000	H	-0.05806400	4.94650300	-4.42337100
Li	1.28793500	-1.37166400	-1.77704100	H	0.12069400	3.20021700	-4.12530700
O	2.78155500	-0.02598900	-2.03351900	H	2.41147000	2.28625900	-4.35903300
Li	2.51677800	0.08285600	0.02495300	H	3.67909000	3.45425900	-4.79037100
Li	1.26963400	1.31991200	-1.87656100	C	2.27667000	5.40531500	2.68910100
O	1.19866700	1.45043800	0.00672200	C	0.83947200	5.88102300	2.78858000
C	1.09393800	2.78553300	0.41753200	H	0.44430100	5.68831400	3.79456200
C	1.55451700	2.91365500	1.92931000	H	0.77169500	6.96276300	2.61131100
H	0.66461400	3.01650700	2.56507000	H	0.17147800	5.38560200	2.08143000
H	1.98063900	1.93582600	2.16986400	C	3.17879000	6.04783300	3.73322500
C	2.59980900	3.96765500	2.31116800	H	3.19761300	7.14058300	3.62266900
C	2.92396400	5.09969000	1.35092500	H	2.82833400	5.82297800	4.74934100
H	3.97641600	5.37118500	1.27485300	H	4.21063200	5.68747300	3.65116600
C	2.19384300	5.09921100	0.01321700	H	3.45331000	3.55040200	2.84310300
H	2.77020100	5.69194400	-0.70716500	C	-0.39360400	3.19543800	0.30020300
H	1.21255800	5.58166300	0.08457600	H	-0.97563900	2.61754400	1.02730300
C	2.05148200	3.64187700	-0.47578500	H	-0.58380800	4.25848900	0.49008800
H	3.02932400	3.16685300	-0.33085700	H	-0.78449900	2.94479200	-0.69122300
N	1.77839700	3.47613700	-1.94601900	O	1.31357300	-1.36787700	0.11150700
C	3.03297100	3.56419900	-2.72750800	C	1.37369800	-2.66915200	0.62538800
H	3.73099100	2.80520700	-2.36042400	C	0.82689900	-2.68117500	2.11443000
H	3.50880400	4.55345500	-2.60912800	H	1.67484400	-2.78614700	2.80432100
C	2.76111800	3.32054200	-4.20993000	H	0.43880800	-1.67136800	2.27263800
O	1.81400500	4.24154500	-4.73246000	C	-0.28514200	-3.66284300	2.49841200
C	0.59964500	4.18362800	-3.99532700	C	-0.57816800	-4.86108200	1.61065500
C	0.83026800	4.46152300	-2.51307800	H	-1.63113700	-5.10769200	1.47726800
H	1.21838200	5.48752200	-2.41174100	C	0.24722800	-4.98849000	0.33578100

H	-0.28773200	-5.63074300	-0.37399400	H	5.09203500	-0.46230200	-4.40763300
H	1.20968000	-5.47862000	0.52111100	C	7.03684900	-1.26486100	-2.55658200
C	0.45389900	-3.57801500	-0.25711300	H	6.31283000	-1.87156400	-3.10916100
H	-0.51959900	-3.07524300	-0.20832700	H	7.08868000	-1.67412000	-1.54017500
N	0.81099100	-3.53149200	-1.71707800	C	8.39761600	-1.32959500	-3.21612900
C	-0.39506600	-3.69476700	-2.56019000	C	9.56013400	-1.54004300	-2.46220700
H	-1.11884700	-2.91755100	-2.29497500	C	10.8161870	-1.57290200	-3.07197000
H	-0.87044800	-4.67709500	-2.39248100	C	10.9294430	-1.39400600	-4.45074900
C	-0.03895700	-3.56629100	-4.03956200	C	9.77897800	-1.18745500	-5.21566300
O	0.94481000	-4.51350600	-4.43101200	C	8.52671400	-1.15714500	-4.60287900
C	2.11252100	-4.38519400	-3.63020000	H	7.63624200	-1.00895300	-5.21068200
C	1.79514800	-4.55018900	-2.14704000	H	9.85650800	-1.05584600	-6.29172900
H	1.40444100	-5.56813900	-1.98829700	H	11.9053430	-1.42071800	-4.92777300
H	2.71243000	-4.44866600	-1.56587100	H	11.7040820	-1.74226500	-2.46857200
H	2.79935100	-5.17155100	-3.95838100	H	9.47971100	-1.69193800	-1.38784300
H	2.59266800	-3.40917000	-3.80597900	H	7.20493600	2.10214300	-1.68957600
H	0.31120500	-2.54349200	-4.25199200	H	8.24715500	0.71769400	-1.25407200
H	-0.92035300	-3.75813600	-4.65913000	C	-1.36162000	-0.03055900	-2.72737500
C	-0.03981900	-5.07334000	3.01311400	N	-2.55903000	-0.35701100	-1.95144100
C	1.37070400	-5.57958800	3.25022300	C	-3.91185200	-0.43334300	-2.53368100
H	1.70706000	-5.31417400	4.26109800	H	-3.88009100	-0.96947500	-3.48425900
H	1.41187100	-6.67393300	3.16754100	C	-4.61593700	-1.26274700	-1.45809400
H	2.09970600	-5.16592400	2.55017200	H	-4.52336400	-2.34057500	-1.63563400
C	-1.03358500	-5.60242700	4.03704200	H	-5.66621200	-1.00304100	-1.32026400
H	-1.07425100	-6.70003500	4.02020400	O	-3.90132000	-0.93076400	-0.25453400
H	-0.75354400	-5.29599200	5.05365500	C	-2.65225900	-0.50448500	-0.59062600
H	-2.04597700	-5.22905800	3.84525100	O	-1.82796300	-0.30328600	0.29054500
H	-1.15969600	-3.17659400	2.92754400	C	-4.54600900	0.96906200	-2.71990800
C	2.85896600	-3.10303600	0.63300400	H	-3.85063700	1.58203800	-3.30147700
H	3.40148000	-2.47999300	1.35336200	H	-4.63322700	1.43541600	-1.73089700
H	3.02055400	-4.15163000	0.91194600	C	-5.90076800	0.91771100	-3.39266000
H	3.31820100	-2.92926700	-0.34531400	C	-7.08020300	1.11310800	-2.66123500
O	4.34460100	0.39005000	0.31726400	C	-8.33009200	1.04210300	-3.28013800
C	5.19612700	0.46721900	-0.55753100	C	-8.42002100	0.77253900	-4.64585100
O	6.46276900	0.84180200	-0.22665400	C	-7.25278600	0.57933500	-5.38853300
C	7.21963400	1.03620600	-1.43394900	C	-6.00674500	0.65271200	-4.76673100
C	6.48210700	0.17961800	-2.46559600	H	-5.10372200	0.51356300	-5.35792700
H	6.49504500	0.65621000	-3.44776100	H	-7.31270500	0.37722900	-6.45475000
N	5.11906000	0.21695600	-1.90444200	H	-9.39112900	0.71856500	-5.13030400
C	3.92085700	-0.11022800	-2.67767600	H	-9.23156700	1.20183400	-2.69451100
C	4.09580100	-0.43926700	-3.98547600	H	-7.01831000	1.33577300	-1.59803600
C	2.97693600	-0.75880800	-4.93250400	C	-1.53285900	0.22387500	-4.05210600
H	3.17763000	-1.67698500	-5.50150900	C	-0.41769200	0.52279900	-5.01048700
H	2.81290300	0.03678500	-5.67565000	H	-0.20686000	-0.31796400	-5.68933700
H	2.03266300	-0.89766000	-4.40226400	H	0.51378500	0.74840800	-4.48714200

H -0.65670300 1.38378000 -5.64952100
H -2.52597300 0.19631900 -4.48104400

Table 24. Geometric coordinates and thermally corrected MP2 energies for (*R*)-21a



Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	C	-6.76308400	6.15436400	-1.23351200
Li	1.66210500	1.85089800	-0.64653800	C	-5.48592100	5.64749400	-0.99621400
O	2.44467200	2.07172700	1.15310300	H	-4.94103400	5.16648200	-1.80619000
Li	0.55736800	1.82129600	1.75119900	H	-7.20588300	6.06054100	-2.22165300
O	-0.23857700	2.01176800	-0.04596800	H	-8.46299000	7.18444000	-0.39211800
C	-1.23242600	2.81850600	-0.33983200	H	-7.42373300	7.40626100	1.85791200
C	-1.49924300	3.38414100	-1.54318800	H	-5.15552000	6.50967500	2.27138700
C	-0.65100700	3.20867200	-2.77176300	Li	2.30417400	0.05201700	1.09661800
H	-0.96745800	2.36189400	-3.40154000	O	0.52801200	-0.10617900	1.83677200
H	0.40567000	3.05793000	-2.53047700	C	0.54478100	-0.88432800	3.00498600
H	-0.70735500	4.10276300	-3.40463700	C	-0.84605500	-1.63049200	3.17371500
H	-2.36944800	4.01946600	-1.64734600	H	-1.43765300	-1.10656300	3.93581100
N	-2.16187900	3.07225800	0.75470500	H	-1.36639000	-1.45244700	2.22985200
C	-3.51365900	3.63497600	0.60093700	C	-0.87280200	-3.14150000	3.43260400
H	-3.99388900	3.20333800	-0.28009300	C	0.39055400	-3.85704000	3.88322300
C	-4.14014100	3.13057600	1.90350200	H	0.56997600	-4.83569200	3.43859700
H	-4.54761500	2.11785900	1.80681100	C	1.64644100	-3.00434800	4.01759700
H	-4.89730200	3.79763500	2.31688500	H	2.52746900	-3.65477700	3.96710000
O	-3.02177100	3.09293700	2.81584400	H	1.69611800	-2.50450800	4.99094300
C	-1.87970900	2.95517200	2.08759100	C	1.67245400	-1.96952100	2.87112700
O	-0.80538200	2.78012900	2.65112700	H	1.40418500	-2.51230900	1.95494600
C	-3.51152900	5.18548200	0.52312100	N	3.02176700	-1.39349700	2.55661900
H	-2.81578600	5.49608400	-0.26149600	C	3.84891500	-2.34062800	1.77727700
H	-3.11070200	5.57099400	1.46854100	C	5.16975200	-1.68351300	1.37595200
C	-4.88871800	5.75985800	0.26889500	O	5.90691600	-1.24275100	2.50513700
C	-5.60749000	6.39917000	1.28794100	C	5.13079200	-0.34085500	3.28494300
C	-6.88630600	6.90961800	1.05433500	H	5.74053900	-0.08415300	4.15664500
C	-7.46882300	6.78674400	-0.20716300	H	4.92745700	0.58332300	2.71856600

C	3.81811200	-0.97714800	3.73268900	H	-2.63303100	0.42238600	-1.62610200
H	4.05308300	-1.84242700	4.37445200	H	-2.62260600	-0.99515500	0.38928200
H	3.25679100	-0.25923200	4.32916300	H	-3.38649300	-2.59736800	0.24135500
H	4.97219700	-0.83238700	0.70124700	C	3.28946700	-3.69232400	-3.70395100
H	5.80476600	-2.40027200	0.84602300	C	3.24181000	-2.84719700	-4.96303100
H	3.29966600	-2.63481100	0.87645800	H	2.78487400	-3.40675500	-5.78995800
H	4.07094800	-3.25601800	2.35340200	H	2.68041600	-1.91961100	-4.83949600
C	-0.80759000	-3.78236200	4.81098400	H	4.25753000	-2.57176400	-5.27541000
C	-0.79146300	-2.93353900	6.06848800	C	4.13051100	-4.94952500	-3.87614700
H	-0.31011700	-3.47265600	6.89515100	H	3.73280900	-5.58525600	-4.67852200
H	-0.26876500	-1.98375300	5.94261300	H	5.16739100	-4.69777400	-4.13559800
H	-1.81682600	-2.69928700	6.38293700	H	4.15418100	-5.54917800	-2.95880000
C	-1.59192100	-5.07481100	4.98937500	H	3.96082800	-3.56808100	-1.61435900
H	-1.16154400	-5.69137000	5.78981500	C	1.58146800	0.08752500	-3.11524800
H	-2.63717500	-4.86837800	5.25508400	H	2.44047000	0.76105300	-3.20058500
H	-1.59470000	-5.67590700	4.07273900	H	1.46596800	-0.43228600	-4.07343700
H	-1.49263900	-3.69039700	2.72385600	H	0.70133200	0.71462100	-2.96093900
C	0.73675100	0.06734500	4.20823200	C	3.40920800	2.91394000	1.44566000
H	-0.15024800	0.70272800	4.29955000	N	4.33698500	3.18510000	0.35359000
H	0.88397700	-0.44329500	5.16710400	C	5.68026800	3.76748200	0.50787100
H	1.58742200	0.73145000	4.04271400	H	6.16451800	3.34588100	1.39158300
O	1.78380500	-0.07190900	-0.74119700	C	6.31529300	3.26736500	-0.79237600
C	1.80609300	-0.85204200	-1.90781200	H	6.73469300	2.25986300	-0.69226600
C	3.22861800	-1.53830800	-2.07010200	H	7.06486600	3.94239000	-1.20658700
H	3.79979200	-0.99124400	-2.83146000	O	5.19871000	3.21377500	-1.70652000
H	3.73777700	-1.33598500	-1.12511700	C	4.05782600	3.06152600	-0.97923200
C	3.32084300	-3.04709000	-2.32629000	O	2.98607100	2.86983600	-1.54236900
C	2.09168100	-3.81737300	-2.78123600	C	5.65850500	5.31830100	0.57911300
H	1.95292200	-4.80228200	-2.33588300	H	4.95828500	5.62446200	1.36142900
C	0.80066000	-3.01948300	-2.92120700	H	5.25416900	5.69495900	-0.36836100
H	-0.05162900	-3.70730500	-2.87205600	C	7.02856900	5.90998600	0.83226200
H	0.73203300	-2.52363000	-3.89552600	C	7.74066100	6.55361100	-0.18876300
C	0.72688300	-1.98574800	-1.77620600	C	9.01347400	7.07940300	0.04365100
H	1.01716700	-2.51542100	-0.85901600	C	9.59651300	6.96787400	1.30595200
N	-0.64696800	-1.46979900	-1.46401700	C	8.89728800	6.33150400	2.33428700
C	-1.43347000	-2.45258500	-0.68658200	C	7.62609500	5.80927600	2.09818000
H	-0.87352700	-2.72336600	0.21504300	H	7.08621800	5.32503400	2.90958500
H	-1.61446700	-3.37602200	-1.26401800	H	9.34052100	6.24645500	3.32302400
C	-2.78209900	-1.85326400	-0.28669800	H	10.5860380	7.37740500	1.48997100
O	-3.53557000	-1.44340300	-1.41671500	H	9.54577300	7.57899800	-0.76150800
C	-2.79732200	-0.50830300	-2.19445600	H	7.28813900	6.65509300	-1.17292800
C	-1.45829800	-1.08802700	-2.64129100	C	3.64978600	3.50082500	2.64407900
H	-1.65420500	-1.96275300	-3.28326500	C	2.80224500	3.31387200	3.87166200
H	-0.92708700	-0.34646100	-3.23661500	H	3.15255600	2.49541700	4.52074400
H	-3.41660600	-0.27603200	-3.06625800	H	1.75452900	3.11119500	3.62932700

H 2.81577400 4.22273700 4.48569200
H 4.49795900 4.16607100 2.74411800

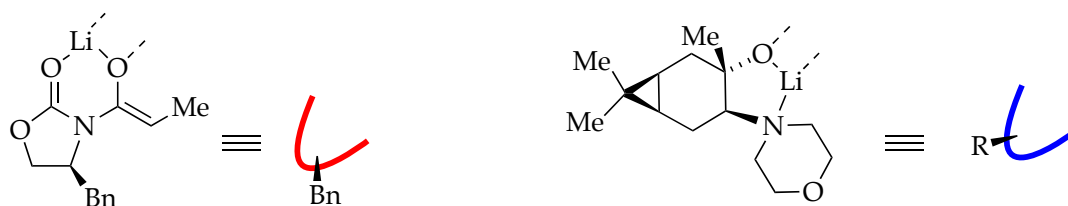
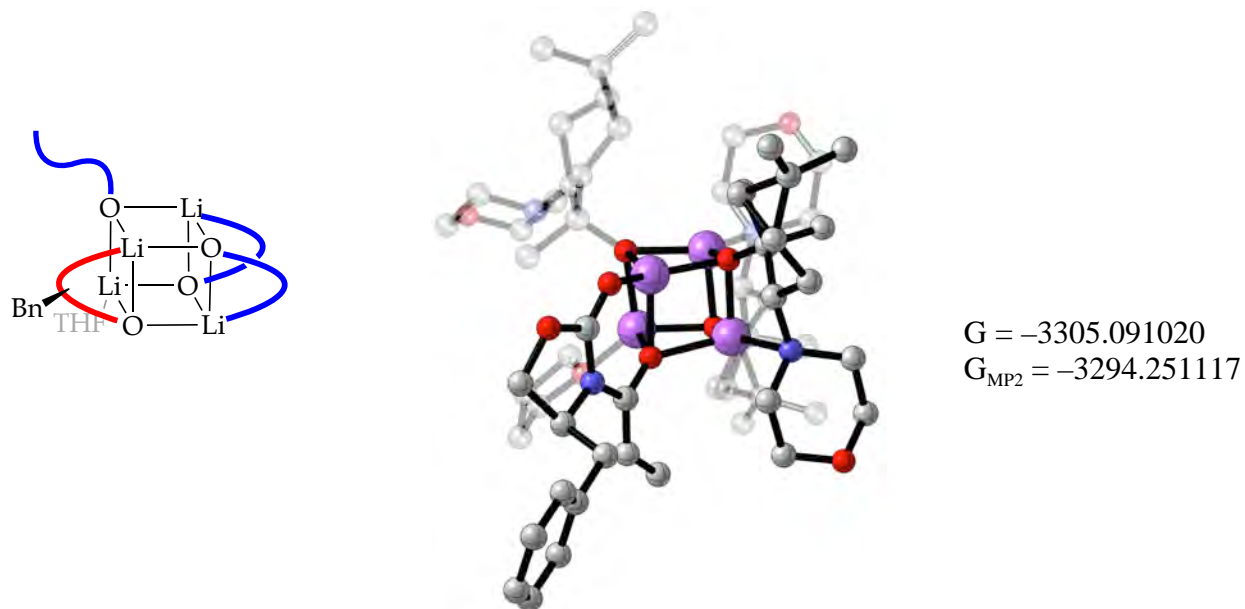


Table 25. Geometric coordinates and thermally corrected MP2 energies for (*S*)-32a



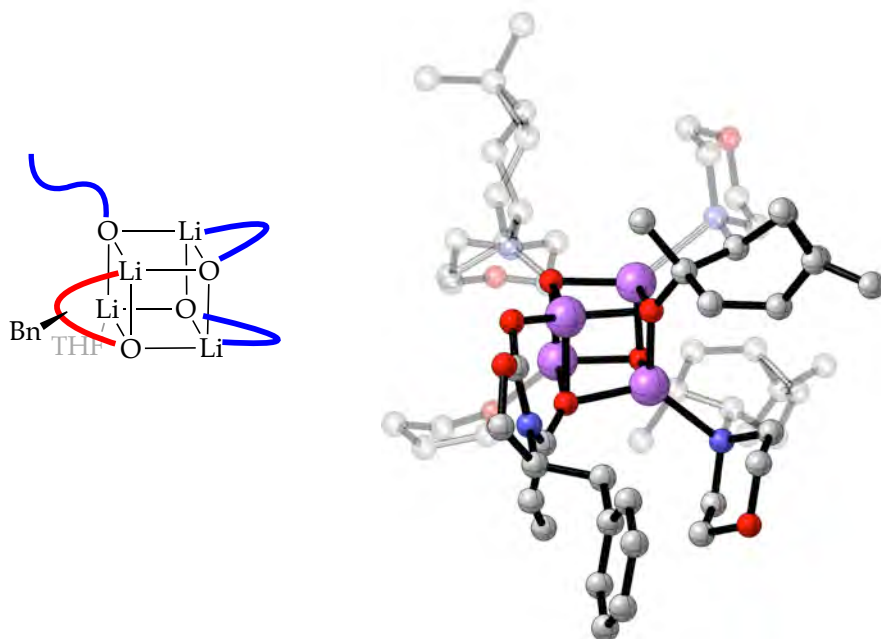
G = -3305.091020
G_{MP2} = -3294.251117

Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	Li	0.01073900	-0.62085400	2.46216000
O	-1.60543600	0.07767800	-1.05760200	Li	2.14644200	0.26517100	1.34941600
C	-2.39891100	-0.84661100	-1.18272200	O	1.78894100	-1.37526300	2.36848000
O	-3.35609100	-0.78672400	-2.14937500	Li	1.37670900	-2.08215500	0.61481700
C	-4.00748700	-2.06660900	-2.23645400	C	-4.91886000	-2.43814600	0.14169100
H	-3.54080200	-2.64059300	-3.04500300	H	-4.56406100	-2.71890700	1.13847400
H	-5.06142400	-1.90432100	-2.46529600	H	-5.11742300	-1.35946200	0.16111600
C	-3.76713100	-2.69920500	-0.86152600	C	-6.18276300	-3.19534400	-0.20365200
H	-3.58634700	-3.77234900	-0.95578900	C	-6.27129000	-4.57731500	0.02333300
N	-2.52457500	-2.01217000	-0.47273100	C	-7.42242000	-5.28723200	-0.31661500
C	-1.63277500	-2.47217400	0.58882400	C	-8.51091000	-4.62565400	-0.88992900
C	-1.92564600	-3.65212800	1.20221300	C	-8.43938000	-3.25100600	-1.11647700
H	-2.79894500	-4.21803000	0.90032900	C	-7.28407100	-2.54427500	-0.77585300
C	-1.08515500	-4.24712700	2.29789400	H	-7.24113600	-1.47024300	-0.94458500
H	-0.24538200	-3.59435400	2.55164700	H	-9.28360900	-2.72514700	-1.55449300
H	-1.66784100	-4.42234000	3.21392600	H	-9.40952000	-5.17737400	-1.15208100
H	-0.66343200	-5.22387400	2.01499600	H	-7.47243900	-6.35642200	-0.12805900
O	-0.61855400	-1.69214100	0.84303700	H	-5.43446300	-5.10033600	0.48213300

O	1.85848800	-0.51534200	-0.45420900	C	-3.61188300	5.67917400	0.33248200
O	0.37054400	1.03134600	1.56141100	H	-4.37574000	6.19108200	0.93341400
C	0.95390100	-4.86400700	-0.70885200	H	-3.06072400	6.44632800	-0.22755400
H	-0.03999200	-4.83818200	-0.25966800	H	-4.13034600	5.04567800	-0.39616300
H	0.88456400	-4.52147800	-1.75241000	H	-2.26263000	3.52912000	-0.49151300
C	1.68052200	-6.20248500	-0.61799000	C	0.41181600	2.76765400	3.19984200
H	1.37094100	-6.90802600	-1.39527000	H	1.29941100	3.25172600	2.77875700
H	1.49274100	-6.66267200	0.35857800	H	-0.14658400	3.53317600	3.75223000
C	3.15658700	-5.77387600	-0.74852800	H	0.76086700	2.01273900	3.91017900
H	3.83383000	-6.43447100	-0.19943100	C	2.12308000	-0.37011200	-1.83645400
H	3.46741300	-5.78400200	-1.79894500	C	1.48874600	0.95665200	-2.37544100
C	3.17182700	-4.32928400	-0.19622000	H	1.44037500	0.90021300	-3.46896000
H	3.60018000	-3.61535000	-0.90685100	H	0.44354700	1.00340300	-2.05066500
H	3.69234000	-4.24253800	0.76126300	C	2.24005600	2.20829400	-1.95695100
O	1.78863500	-3.96629600	0.04280600	C	3.71604800	2.18028400	-2.31450500
C	-0.38304500	2.10767600	2.05013200	H	4.42109400	2.58047200	-1.58752600
C	-0.58968700	3.18190000	0.89676600	C	4.15905600	0.87939100	-2.96256700
H	0.06843700	4.04017100	1.08906800	H	5.25084300	0.86618400	-3.07170800
H	-0.19257100	2.70313900	-0.00136700	H	3.75581700	0.78517700	-3.97611300
C	-2.00041000	3.67057300	0.55545400	C	3.70442300	-0.32087800	-2.08412600
C	-3.13225200	3.45639500	1.54505500	H	4.08848800	-0.12675300	-1.07967100
H	-4.09190400	3.16866300	1.11646400	N	4.34254500	-1.60937700	-2.48475700
C	-2.78288900	2.71277900	2.82709400	C	5.69769700	-1.74634400	-1.93518900
H	-3.70117200	2.30431100	3.26488400	H	5.65192900	-1.64712700	-0.84453800
H	-2.36346100	3.38557200	3.58303400	H	6.38461700	-0.96513700	-2.31421300
C	-1.79074900	1.57584700	2.49133400	C	6.29454400	-3.11266700	-2.27681200
H	-2.17377200	1.08716600	1.58751100	O	6.30038200	-3.35755400	-3.67487100
N	-1.72633900	0.46372900	3.50151900	C	4.98546100	-3.24538700	-4.20248100
C	-2.89214000	-0.43623700	3.34675800	C	4.39849400	-1.86309700	-3.93169700
H	-2.89714200	-0.83455600	2.32879800	H	5.02812600	-1.12498100	-4.45921500
H	-3.84090100	0.10442600	3.50957400	H	3.39380600	-1.80676800	-4.35702000
C	-2.81972200	-1.59314700	4.33886500	H	5.06921200	-3.42252100	-5.27935100
O	-2.77983500	-1.12954000	5.68148500	H	4.33367800	-4.02232000	-3.76729300
C	-1.66085500	-0.27527200	5.86493400	H	5.72938000	-3.90697600	-1.76154700
C	-1.70033200	0.91636200	4.91119300	H	7.33763000	-3.16354400	-1.94812000
H	-2.59656200	1.51064400	5.15119100	C	2.80088400	3.20494100	-2.96214100
H	-0.82683000	1.54576300	5.08427300	C	2.45111500	3.16413500	-4.44011600
H	-1.70011300	0.07339900	6.90170000	H	1.49640700	3.67409900	-4.62374900
H	-0.72686900	-0.84268900	5.72385700	H	3.22025900	3.68332500	-5.02711200
H	-1.93363300	-2.21240600	4.12805500	H	2.36168500	2.15287300	-4.84492600
H	-3.70867300	-2.22511700	4.25058900	C	2.95649600	4.63015100	-2.44940400
C	-2.67493300	4.86465800	1.21284300	H	3.75109200	5.16193400	-2.98987000
C	-1.93429800	5.71919700	2.22478000	H	2.02624300	5.19845400	-2.58092200
H	-1.35439300	6.49920600	1.71395200	H	3.20885300	4.64989200	-1.38293800
H	-2.63873400	6.22374400	2.89955200	H	1.96057400	2.61949900	-0.98879300
H	-1.23484100	5.15102300	2.84215800	C	1.44136800	-1.53110200	-2.59064900

H 1.89607200 -2.48570800 -2.31701300
H 0.38177200 -1.55506300 -2.31185200
H 1.48715200 -1.42165300 -3.68116300
C 2.69562000 -1.65502800 3.39709100
C 2.77691500 -3.22943300 3.60842800
H 2.14984100 -3.50460300 4.46751700
H 2.27275000 -3.64416500 2.73201800
C 4.14016600 -3.92225700 3.71116700
C 5.39779800 -3.09327900 3.91217300
H 6.27374500 -3.40234700 3.34237600
C 5.21495100 -1.58345600 3.99341500
H 6.16867900 -1.09807500 3.75689300
H 4.96150100 -1.26374200 5.00998800
C 4.12045000 -1.14152700 2.99250200
H 4.32607700 -1.66866700 2.05142300
N 4.16289300 0.30649800 2.60390100
C 5.26911000 0.55034300 1.65393800
H 5.12746400 -0.09257400 0.78027700
H 6.24932200 0.30547100 2.09945700
C 5.29672600 2.01034500 1.21175700
O 5.45373700 2.88512300 2.31836000
C 4.38948000 2.68894900 3.23749800
C 4.33314700 1.24661800 3.73475400
H 5.26567300 1.04062700 4.28520300
H 3.50255500 1.14311700 4.43274600
H 4.57059300 3.36793200 4.07648100
H 3.43251800 2.96241300 2.76654200
H 4.36940100 2.25293300 0.66734400
H 6.14647800 2.18883800 0.54549000
C 4.95419900 -4.06839600 4.98748300
C 4.40975400 -3.59319500 6.32122800
H 3.82922100 -4.39199200 6.80095200
H 5.22638400 -3.32560100 7.00489600
H 3.75204800 -2.72700200 6.23264100
C 5.78324400 -5.33884100 5.11475100
H 6.64175400 -5.18512200 5.78223400
H 5.18479700 -6.16148300 5.52832400
H 6.17296600 -5.66667600 4.14394500
H 4.24054400 -4.76977300 3.03333000
C 2.15176800 -1.00440800 4.69260100
H 1.25692800 -1.55264800 5.00910000
H 2.85066300 -1.00589600 5.53673000
H 1.84954700 0.02888800 4.50048400

Table 26. Geometric coordinates and thermally corrected MP2 energies for (*S*)-33a



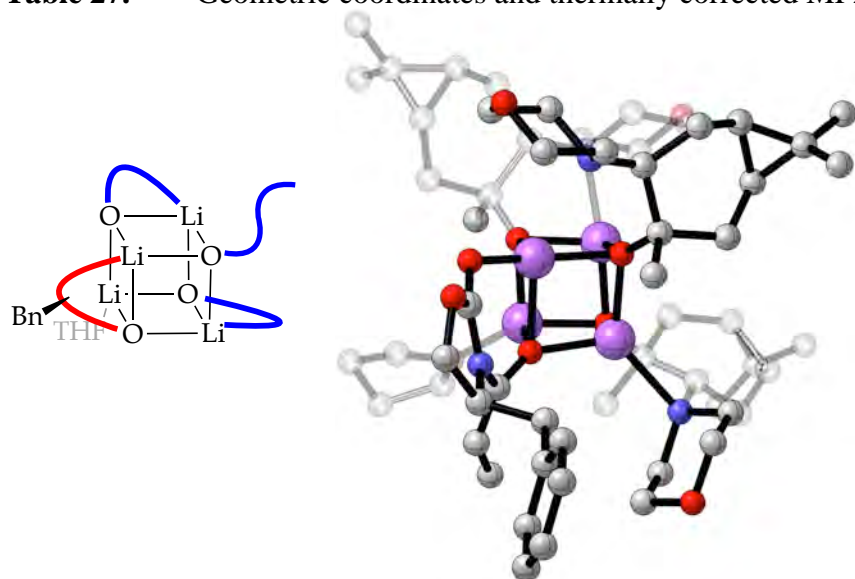
G = -3305.088249
G_{MP2} = -3294.251937

Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	C	6.88763700	-1.11887800	-2.29509600
O	1.03582000	-1.26758100	0.96966200	C	8.26805200	-1.30154200	-2.37038400
C	2.15960000	-1.50204400	0.53757800	C	9.08818700	-0.89427100	-1.31547500
O	3.17626000	-1.78240200	1.39828900	C	8.51752800	-0.30074100	-0.18938000
C	4.31091900	-2.23768400	0.64088200	C	7.13451100	-0.12061100	-0.11762100
H	4.32748000	-3.33320100	0.66714400	H	6.69824100	0.35466200	0.75850800
H	5.21789900	-1.85084400	1.10735000	H	9.14753800	0.02755600	0.63316500
C	4.06932000	-1.69735400	-0.77673400	H	10.1642800	-1.03315000	-1.37470600
H	4.36171500	-2.44551200	-1.51564800	H	8.70490900	-1.75597100	-3.25581100
N	2.60740800	-1.52968300	-0.75039400	H	6.25743400	-1.42699000	-3.12703900
C	1.78762100	-1.27852200	-1.94594900	O	-1.91509400	0.00871600	-0.26239900
C	2.21486200	-1.87395600	-3.09090500	O	0.37651200	1.90107400	-0.21516100
H	3.07169100	-2.53756200	-3.04720900	C	-1.15269900	-3.29903700	-2.88447600
C	1.56630900	-1.70654600	-4.43414400	H	-0.24600800	-3.47711100	-3.47471800
H	0.58810900	-1.22959800	-4.33938000	H	-0.87914600	-3.22913700	-1.83195800
H	2.17303400	-1.10346700	-5.12798100	C	-2.23978500	-4.32295700	-3.19649600
H	1.41818700	-2.67622300	-4.93100500	H	-2.98847200	-4.32592300	-2.39735500
O	0.75747900	-0.49369000	-1.77976500	H	-1.84572000	-5.33852200	-3.30113100
Li	0.57526600	1.47357400	-2.06029400	C	-2.83841100	-3.77344600	-4.50764300
Li	-1.51545100	1.88021500	-0.65786400	H	-2.34071900	-4.21772500	-5.37597500
O	-1.28611200	1.57869800	-2.60224200	H	-3.90816800	-3.98285700	-4.59843000
Li	-1.44542400	-0.30665800	-2.13287600	C	-2.54761000	-2.25500700	-4.43810100
C	4.79726900	-0.36673900	-1.07956100	H	-3.45047400	-1.64996200	-4.32374400
H	4.40183100	0.01710800	-2.02630600	H	-2.00086400	-1.90638800	-5.32244200
H	4.53451800	0.35827500	-0.29950600	O	-1.74064300	-2.03772200	-3.26176300
C	6.29922200	-0.52850000	-1.16636700	C	0.69882200	2.78827700	0.81829500

C	2.26840800	3.03910300	0.85557800	C	-5.23148300	-0.36263700	1.47368800
H	2.67194700	2.61324400	1.78308900	H	-6.24835400	-0.03765600	1.22267200
H	2.66560800	2.41395200	0.05090500	H	-5.30689100	-1.42517500	1.73283800
C	2.80499700	4.46073800	0.67068600	C	-4.28968800	-0.16270200	0.25672500
C	1.90253900	5.64063900	0.99415700	H	-4.11910800	0.91766300	0.18614500
H	1.96496200	6.49313500	0.31790000	N	-4.88709900	-0.53778800	-1.05282800
C	0.48341200	5.30324900	1.42971100	C	-5.57909600	0.58462000	-1.69396500
H	-0.14769400	6.19212400	1.31394100	H	-4.88836300	1.43077900	-1.77358000
H	0.43810000	5.03620500	2.49112500	H	-6.46133400	0.91883000	-1.11210000
C	-0.04105100	4.14440900	0.55169500	C	-6.04127300	0.19685900	-3.09641200
H	0.24020400	4.39028600	-0.47950900	O	-6.88342500	-0.94801400	-3.07974200
N	-1.53464800	4.00851000	0.49460900	C	-6.22755100	-2.04246600	-2.45568700
C	-2.10736100	4.98601500	-0.45645100	C	-5.78620600	-1.69783300	-1.03524000
H	-1.67236500	4.81627800	-1.44644500	H	-6.69724300	-1.51176200	-0.43819600
H	-1.87311600	6.02349400	-0.15771700	H	-5.27459200	-2.55966900	-0.59945200
C	-3.62506600	4.84068100	-0.54414700	H	-6.94836000	-2.86654100	-2.44308400
O	-4.24629100	5.00544400	0.71972100	H	-5.35259200	-2.34957500	-3.05305400
C	-3.72228100	4.05937700	1.64186800	H	-5.15874700	0.00747300	-3.73122300
C	-2.21241100	4.20977600	1.79512800	H	-6.62686400	1.00473100	-3.54666700
H	-2.01294000	5.21704200	2.19580100	C	-4.22630900	-0.08365700	3.96216400
H	-1.84706000	3.48309300	2.52098500	C	-4.45460900	-1.53125600	4.36001500
H	-4.22020500	4.24769500	2.59818000	H	-3.69262400	-1.86013600	5.07870900
H	-3.96751000	3.03735700	1.31500000	H	-5.43394200	-1.64148000	4.84395600
H	-3.88143300	3.85172100	-0.96047400	H	-4.42915800	-2.22594800	3.51700200
H	-4.04151200	5.60981600	-1.20196200	C	-4.33884700	0.86537200	5.14701900
C	3.14046100	5.38860700	1.83137700	H	-5.33378500	0.80788400	5.60848100
C	3.03879900	4.90616000	3.26682500	H	-3.59868200	0.62048300	5.92031600
H	3.97176500	4.41498500	3.57288000	H	-4.17236800	1.90665600	4.84693500
H	2.87402000	5.75111500	3.94825500	H	-2.65337100	1.21944600	3.10714900
H	2.22964900	4.18971500	3.42675500	C	-2.74671900	-2.22288300	0.06360900
C	4.30111700	6.34886900	1.61520800	H	-2.94958200	-2.32285300	-1.00426200
H	4.19758200	7.24321000	2.24409200	H	-1.73067200	-2.58050500	0.26962000
H	5.25876700	5.87462200	1.86771300	H	-3.44067300	-2.86941100	0.61721800
H	4.36048800	6.68185600	0.57253400	C	-1.40688100	2.23900000	-3.83385500
H	3.45252600	4.58453000	-0.19624400	C	-2.80616900	2.98856000	-3.89340000
C	0.30471600	2.13591700	2.16380200	H	-3.51542800	2.37025000	-4.46043200
H	0.92533500	1.24647500	2.32201100	H	-3.16267900	2.96781100	-2.86056100
H	0.44502200	2.79491100	3.03038800	C	-2.88141400	4.44523100	-4.36427600
H	-0.73527500	1.80213100	2.14341300	C	-1.68458800	5.08589100	-5.04763600
C	-2.84260800	-0.74467400	0.48986400	H	-1.46427300	6.11471800	-4.76417100
C	-2.49303200	-0.71788500	2.03101100	C	-0.44542500	4.21514100	-5.21547100
H	-2.68236200	-1.71565900	2.44145700	H	0.42937500	4.86357500	-5.34090700
H	-1.41065300	-0.57927800	2.11095600	H	-0.49879900	3.60673800	-6.12461000
C	-3.21495300	0.31248800	2.89052200	C	-0.27448600	3.31949300	-3.96624600
C	-4.70379300	0.46762600	2.63311000	H	-0.43031500	3.96904800	-3.09564900
H	-5.11086700	1.47760400	2.66887700	N	1.10891900	2.77913600	-3.75467200

C 2.00934600 3.82353100 -3.21633300
H 1.58411900 4.21693000 -2.28763100
H 2.11955600 4.66387500 -3.92359300
C 3.39305600 3.24476600 -2.92955500
O 3.98067000 2.67568200 -4.08893900
C 3.13277100 1.66769500 -4.62499900
C 1.75205900 2.22151900 -4.96496300
H 1.87091700 2.99520000 -5.74120300
H 1.13687300 1.42283400 -5.37730200
H 3.62401200 1.29999200 -5.53125000
H 3.03807200 0.83081100 -3.91453700
H 3.32019400 2.48637400 -2.13248400
H 4.07037000 4.03500800 -2.59181300
C -2.98150400 4.89505100 -5.81336700
C -3.10665400 3.89077500 -6.94362200
H -4.16109900 3.63219400 -7.10638700
H -2.72443300 4.31201500 -7.88289900
H -2.57193300 2.95851700 -6.75603900
C -3.79281000 6.15823300 -6.06731200
H -3.46361700 6.66054900 -6.98666500
H -4.86006700 5.92593300 -6.17979000
H -3.69405000 6.87489100 -5.24386300
H -3.42477200 5.08814500 -3.67251100
C -1.37194300 1.17211600 -4.95288500
H -2.29030700 0.57812200 -4.89605700
H -1.30715800 1.57960500 -5.96800900
H -0.53471700 0.48731600 -4.80537900

Table 27. Geometric coordinates and thermally corrected MP2 energies for (*S*)-**34a**



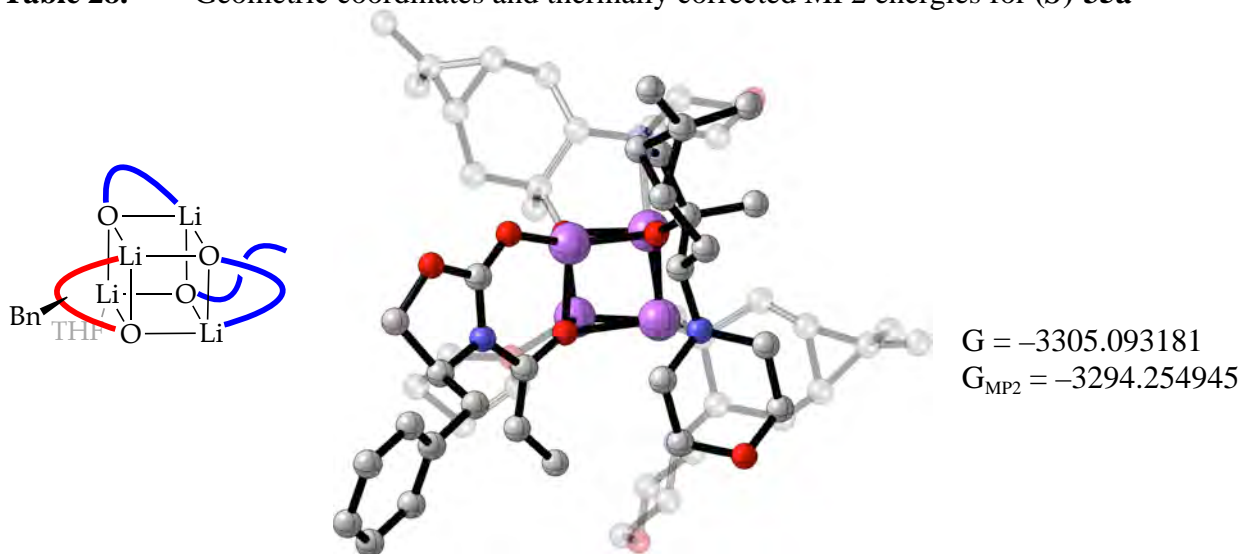
G = -3305.090159
 G_{MP2} = -3294.252259

Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	C	8.97335400	2.12135800	1.00956300
O	1.40997800	-1.23412200	-0.50778000	C	8.23849800	1.34301900	1.90406100
C	2.55703500	-0.80454300	-0.55449500	C	6.86720300	1.16158100	1.71150300
O	3.59947200	-1.55620900	-0.10298300	H	6.29853200	0.56379500	2.42077100
C	4.83387100	-0.91220400	-0.46926800	H	8.72964700	0.87946400	2.75560200
H	5.23669700	-1.41875200	-1.35314500	H	10.0399540	2.26604500	1.15852200
H	5.53746300	-1.01669000	0.35789000	H	8.89056600	3.33716500	-0.77068700
C	4.44584500	0.54815100	-0.76412400	H	6.46032900	3.02001400	-1.10139600
H	4.96006800	0.89732700	-1.66221100	O	-1.63629600	0.08467700	-0.97340400
N	3.00659900	0.39466400	-1.01631400	O	-0.54458900	1.12883900	1.51781900
C	2.14944600	1.43990800	-1.58312800	C	-0.01372000	0.48987500	-4.42079400
C	2.69821900	2.16949100	-2.58918800	H	1.05031700	0.74666700	-4.37774600
H	3.68058700	1.88526700	-2.95418700	H	-0.18960900	-0.38702800	-3.79340200
C	2.04235100	3.33434500	-3.26946400	C	-0.51660100	0.33766600	-5.85655900
H	1.07523200	3.55850800	-2.81520600	H	-1.40794400	-0.30022800	-5.88793500
H	2.66262600	4.24178300	-3.22045900	H	0.23771100	-0.10001200	-6.51730000
H	1.86338300	3.14210600	-4.33821300	C	-0.88053900	1.78463900	-6.22443900
O	0.96769500	1.55624500	-1.03772300	H	0.01937500	2.34491200	-6.50422100
Li	0.05522300	2.63318600	0.34498300	H	-1.59595200	1.85765100	-7.04908100
Li	-2.15829300	1.31762000	0.38781300	C	-1.45288500	2.31645000	-4.90733800
O	-1.61829100	2.93948500	-0.53172400	H	-2.53020300	2.11986200	-4.82643200
Li	-0.92518100	1.65176500	-1.84744400	H	-1.27898300	3.38565200	-4.75790000
C	4.72843900	1.53252300	0.39402900	O	-0.77255400	1.59273300	-3.86072000
H	4.23740800	2.47988300	0.14322800	C	-2.01410500	4.28183400	-0.55329800
H	4.24961200	1.14982000	1.30309300	C	-3.55984700	4.36003100	-0.20531900
C	6.20742700	1.75289500	0.62575500	H	-4.13579500	4.32244800	-1.14058900
C	6.95815800	2.53791100	-0.26244400	H	-3.75883800	3.41082000	0.29994800
C	8.32773100	2.72076400	-0.07457400	C	-4.10008400	5.45403000	0.72185300

C	-3.18760000	6.57993100	1.17730100	H	-1.49135000	-0.67894600	2.80306700
H	-3.26654500	6.86733700	2.22524400	N	0.34571900	-1.59520700	2.89764000
C	-1.75589600	6.55631400	0.65333400	C	-0.37688200	-2.79418000	2.45860200
H	-1.12290200	7.13485700	1.33491500	H	-1.11134600	-2.51134200	1.69737500
H	-1.67408200	7.05175400	-0.31997100	H	-0.92227400	-3.28038900	3.29322100
C	-1.26271700	5.09005900	0.56921300	C	0.59287500	-3.80619600	1.85084900
H	-1.58469900	4.60118000	1.49912300	O	1.61108400	-4.17363500	2.77672300
N	0.22424800	4.90557600	0.57995700	C	2.32633600	-3.01908600	3.19514400
C	0.79366800	5.22259100	1.90982100	C	1.39286800	-1.99889700	3.84524500
H	0.30690200	4.59966900	2.66634100	H	0.97102900	-2.46238000	4.75641100
H	0.62251000	6.27756700	2.18262300	H	1.97406800	-1.12740400	4.15670100
C	2.29936300	4.96765300	1.92993200	H	3.07195800	-3.36394700	3.91991000
O	2.97553300	5.73837600	0.94940300	H	2.84538200	-2.56293900	2.33805300
C	2.45365800	5.44824000	-0.34109100	H	1.04172000	-3.37742900	0.94338000
C	0.95416700	5.72179800	-0.41472400	H	0.06557800	-4.73054600	1.59156300
H	0.78954000	6.79763000	-0.23672100	C	-2.19122100	1.54262000	5.97469700
H	0.60008200	5.48870500	-1.41717600	C	-1.05785400	1.88160700	6.92728700
H	2.98733400	6.09587300	-1.04367700	H	-1.04956300	2.95666800	7.15045100
H	2.65805600	4.39922100	-0.60873100	H	-1.18861500	1.34918100	7.87833200
H	2.50250900	3.89639800	1.76814700	H	-0.06883100	1.62024200	6.54302000
H	2.71717000	5.25431700	2.90004800	C	-3.55490600	1.88888800	6.55590600
C	-4.41257500	6.88976900	0.33390600	H	-3.73840600	1.34144600	7.49006800
C	-4.30844600	7.37051000	-1.10103900	H	-3.62752900	2.96148100	6.77973800
H	-5.25449200	7.19271600	-1.62921500	H	-4.36613100	1.64056400	5.86167500
H	-4.11290200	8.45065200	-1.13785600	H	-2.94322200	2.08657900	3.96265800
H	-3.52406300	6.87111900	-1.67043600	C	1.41435300	1.10568000	2.90173300
C	-5.57358400	7.53849500	1.07623800	H	1.90109200	0.38489100	2.23942400
H	-5.46408800	8.63098500	1.10281400	H	1.67440400	2.11584200	2.56455000
H	-6.53036600	7.31253600	0.58702100	H	1.82328100	0.98908100	3.91361000
H	-5.63917900	7.18553200	2.11171500	C	-2.63094500	-0.80369800	-1.40017900
H	-4.76935700	5.05748400	1.48489000	C	-1.97685200	-2.12472200	-1.99319000
C	-1.78105900	4.81299800	-1.99000000	H	-2.34286400	-2.27133600	-3.01714800
H	-2.53380500	4.37189000	-2.65364300	H	-0.91036100	-1.89921500	-2.08046200
H	-1.83961200	5.90059200	-2.09944700	C	-2.12994800	-3.43039400	-1.21395300
H	-0.80378400	4.49068500	-2.35644800	C	-3.40600700	-3.63773200	-0.41375800
C	-0.11855600	0.93242100	2.84602700	H	-3.29505200	-4.12244800	0.55624400
C	-0.73256100	2.03639700	3.78878400	C	-4.36584800	-2.45732500	-0.40210300
H	0.00792300	2.30205400	4.55253200	H	-5.10376700	-2.59519800	0.39687500
H	-0.85980500	2.92843500	3.16746700	H	-4.93915800	-2.38576900	-1.33339500
C	-2.05608700	1.70351000	4.46328600	C	-3.53311800	-1.17390600	-0.16862600
C	-2.14778300	0.31912500	5.08062900	H	-2.80349600	-1.42394700	0.61077100
H	-3.09302600	-0.21327700	4.97046700	N	-4.28431900	-0.01103200	0.40504100
C	-0.92141300	-0.55044300	4.85068400	C	-4.51191600	-0.19096000	1.85421700
H	-1.13652000	-1.58249700	5.15213200	H	-3.54678300	-0.30972700	2.35587300
H	-0.07296600	-0.22558300	5.46389000	H	-5.11556200	-1.09279400	2.06285200
C	-0.55509200	-0.50603400	3.34365700	C	-5.23789200	1.01712300	2.44237400

O -6.49003000 1.23839000 1.81402900
C -6.30500900 1.42523100 0.41726200
C -5.60477200 0.22833100 -0.21915600
H -6.26229700 -0.64871900 -0.09744200
H -5.48733700 0.41035300 -1.28663500
H -7.30332900 1.54845700 -0.01422500
H -5.72821400 2.34472000 0.23249000
H -4.60590100 1.91653500 2.34513600
H -5.44434300 0.85430000 3.50480500
C -3.12347000 -4.51677700 -1.61425800
C -3.94056900 -4.40306200 -2.88905500
H -3.36925200 -4.78142900 -3.74712800
H -4.85632600 -5.00410300 -2.81385300
H -4.23962200 -3.37835900 -3.12500600
C -2.71124500 -5.94950900 -1.30980600
H -3.58951600 -6.59755500 -1.18671600
H -2.10169300 -6.36616500 -2.12254300
H -2.12132700 -6.01146300 -0.38823700
H -1.21080300 -3.79865500 -0.76177500
C -3.42389000 -0.13504200 -2.54803700
H -2.75829200 -0.01771800 -3.40897700
H -4.29330000 -0.71946900 -2.87738300
H -3.75461500 0.86618200 -2.25520800

Table 28. Geometric coordinates and thermally corrected MP2 energies for (*S*)-35a

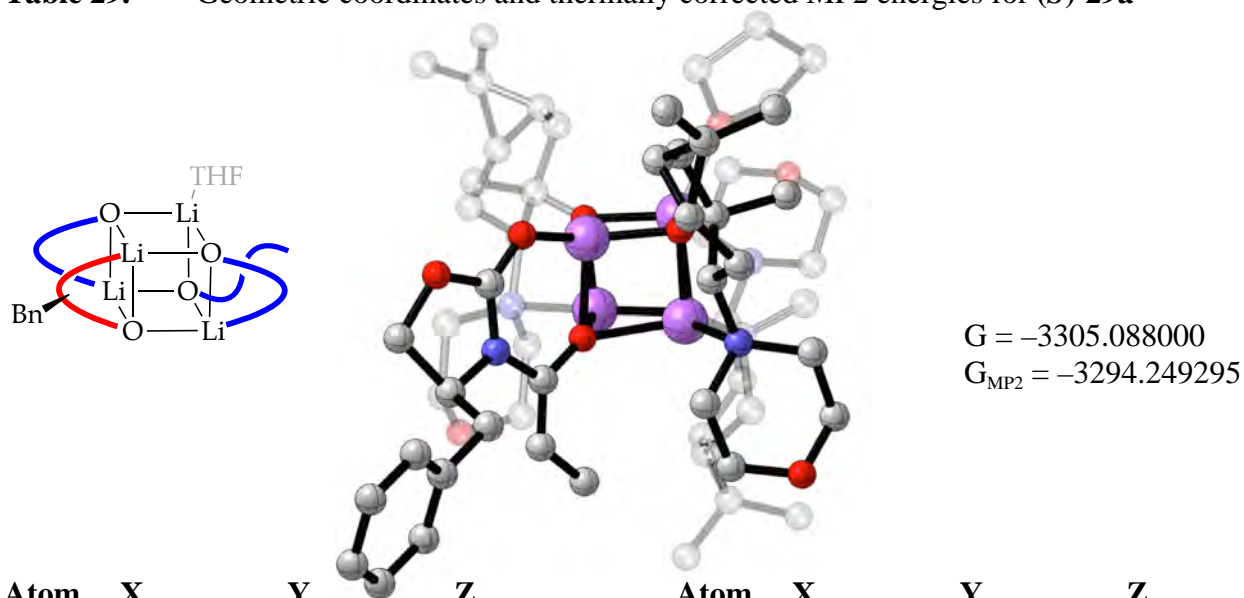


Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	C	-8.65323500	-4.20755300	-0.64490800
O	-1.78057800	0.58868500	-0.22749100	C	-8.50305300	-3.05050600	0.11968000
C	-2.69091400	-0.14727900	-0.58786900	C	-7.22747900	-2.54971100	0.38899000
O	-3.93042700	0.37628700	-0.79663300	H	-7.11861900	-1.65347900	0.99623200
C	-4.75453400	-0.61571800	-1.43060700	H	-9.37744700	-2.53776600	0.51165500
H	-4.75786400	-0.42745400	-2.51031600	H	-9.64447300	-4.60036500	-0.85411600
H	-5.77035900	-0.52303700	-1.04398600	H	-7.62735400	-5.76978600	-1.72267800
C	-4.08306700	-1.94727800	-1.07451500	H	-5.37184900	-4.88518300	-1.23487600
H	-4.11063800	-2.62457900	-1.93063700	O	1.46984100	0.11444500	-1.20069100
N	-2.70257800	-1.49557600	-0.82874100	O	0.99558400	-0.18191800	1.64136100
C	-1.55272800	-2.40427400	-0.77129200	C	0.04342400	-2.10673300	-4.04902100
C	-1.75017200	-3.68550600	-1.18686900	H	-0.85017500	-2.52108100	-3.57148700
H	-2.72145800	-3.99926300	-1.54913300	H	-0.03829300	-1.01560200	-4.07271100
C	-0.66331000	-4.72015100	-1.19978900	C	0.31034100	-2.72220100	-5.43075200
H	-0.91754400	-5.59695200	-0.58487100	H	0.79406400	-1.99397700	-6.09237500
H	-0.46961500	-5.10007900	-2.21436300	H	-0.60996200	-3.05790300	-5.91816500
H	0.27612000	-4.30512000	-0.82555800	C	1.28117300	-3.87050300	-5.10919200
O	-0.44137100	-1.89221700	-0.32218900	H	0.73472200	-4.74916900	-4.74622500
Li	0.91702700	-2.07063900	1.28246100	H	1.89010900	-4.17532700	-5.96574200
Li	2.46244900	-0.23110300	0.38644500	C	2.11051400	-3.26311000	-3.98092100
O	2.48965400	-2.31377400	0.20553800	H	2.90699300	-2.61616200	-4.37780500
Li	1.37615800	-1.79615400	-1.34704400	H	2.54880900	-3.98979800	-3.29393600
C	-4.69909700	-2.63953200	0.16545700	O	1.18007100	-2.46604000	-3.22347900
H	-4.01725000	-3.44051600	0.46916100	C	0.52135300	0.13844800	2.92097500
H	-4.73116900	-1.91083400	0.98484300	C	-0.04112600	1.62635100	2.92667300
C	-6.08227300	-3.19396900	-0.09818700	H	0.68137700	2.27728800	3.43802700
C	-6.24858900	-4.35993500	-0.86110200	H	-0.02776100	1.93274600	1.87724300
C	-7.52038600	-4.86259600	-1.13376300	C	-1.45276000	1.90406400	3.45276000

C	-2.15347900	0.86964600	4.31684700	H	1.67393800	2.48533100	-0.32328500
H	-3.21662800	0.72981900	4.12284200	N	3.59252900	1.77027000	-0.11471500
C	-1.40002600	-0.42954200	4.57069400	C	3.58877200	2.50616900	1.16997500
H	-2.11702200	-1.20705100	4.85998900	H	2.60683700	2.38673600	1.63786200
H	-0.70129900	-0.33878600	5.40998500	H	3.76638600	3.58535200	1.01617000
C	-0.65758000	-0.83336100	3.27654900	C	4.66748000	1.96985700	2.10735700
H	-1.36733400	-0.68457300	2.45411600	O	5.96147200	2.05426400	1.52762600
N	-0.29104300	-2.28530100	3.17234900	C	5.99445000	1.34210900	0.29882000
C	-1.47109400	-3.09164800	2.78628500	C	4.95428400	1.87266000	-0.68431700
H	-1.86829500	-2.70515200	1.84497900	H	5.21006800	2.92012700	-0.91324100
H	-2.26567200	-3.02807400	3.55017000	H	5.01242700	1.30470600	-1.61365400
C	-1.08791200	-4.55711400	2.60421600	H	7.00049800	1.47605800	-0.11101700
O	-0.52030500	-5.10226800	3.78721100	H	5.83276700	0.26752600	0.48031500
C	0.61616600	-4.34504500	4.17662100	H	4.44399200	0.92459000	2.37748000
C	0.26390800	-2.87800600	4.40846200	H	4.69783400	2.56236800	3.02716300
H	-0.46228000	-2.82432800	5.23598500	C	1.00586400	4.37505200	-3.58218300
H	1.15885000	-2.33422800	4.71345900	C	1.88339100	3.97594500	-4.75386100
H	0.98949600	-4.79606900	5.10157500	H	1.26794100	3.78110400	-5.64220800
H	1.40178700	-4.42016500	3.40794400	H	2.58272800	4.78267000	-5.01103200
H	-0.38023000	-4.65817900	1.76513200	H	2.47094400	3.07500400	-4.56550700
H	-1.97506700	-5.15593500	2.37674800	C	0.12699000	5.57834800	-3.89257600
C	-1.77931800	2.21664400	4.90556100	H	0.73371500	6.45649800	-4.15212700
C	-0.67879200	2.35187800	5.94128900	H	-0.53865400	5.37257000	-4.74158000
H	-0.30137600	3.38270900	5.96458700	H	-0.50159200	5.84971000	-3.03674200
H	-1.05706400	2.11926200	6.94568200	H	-0.60128600	3.54886200	-2.31990100
H	0.17624300	1.70010800	5.75020700	C	2.94238900	0.65344200	-3.00002300
C	-2.93090700	3.18267600	5.14462900	H	2.42129800	-0.01322400	-3.69552400
H	-3.39191100	3.01517300	6.12750900	H	3.43712900	1.43474900	-3.58989000
H	-2.58536200	4.22460000	5.11348600	H	3.70841500	0.05443500	-2.50157600
H	-3.71399200	3.07055500	4.38608100	C	3.75692100	-2.93098600	0.26799900
H	-2.08623500	2.41634200	2.73087200	C	4.55149400	-2.40718100	1.51920600
C	1.70749000	0.05345800	3.90883000	H	5.62527600	-2.49161800	1.31645100
H	2.41394900	0.86023200	3.68679100	H	4.35499800	-1.33180500	1.60428900
H	1.42266800	0.14913600	4.96347700	C	4.23014800	-3.09645100	2.83469100
H	2.24825300	-0.88710500	3.77870300	C	4.29933500	-4.61206400	2.78026600
C	1.91723900	1.19037300	-1.97415100	H	3.53578800	-5.17114100	3.32004700
C	0.69070300	1.82114100	-2.76672700	C	4.59456100	-5.15506700	1.39319200
H	0.76451700	1.53032600	-3.82410600	H	4.48078300	-6.24562900	1.38831200
H	-0.18694400	1.30159100	-2.37339100	H	5.63037000	-4.95731500	1.09625400
C	0.40869700	3.32299800	-2.65865000	C	3.60487800	-4.51443800	0.37898500
C	1.49248400	4.25858200	-2.15059200	H	2.60674900	-4.63027500	0.81506400
H	1.16069200	5.05351100	-1.48339600	N	3.53529900	-5.25063900	-0.91534700
C	2.80813000	3.61531100	-1.73167200	C	2.63793600	-6.41179100	-0.83085400
H	3.34133700	4.29982700	-1.06175300	H	1.65633300	-6.08133000	-0.47970500
H	3.47243500	3.45455100	-2.58821000	H	3.01131300	-7.17322200	-0.11899000
C	2.50308800	2.28126400	-1.01237800	C	2.48239800	-7.07395000	-2.19798800

O 3.73400900 -7.48042500 -2.73417600
C 4.62403300 -6.37648400 -2.81520700
C 4.82426000 -5.71262700 -1.45389300
H 5.30914300 -6.45143600 -0.79130900
H 5.50819800 -4.86871500 -1.56665300
H 5.57416000 -6.77363500 -3.18685800
H 4.24725200 -5.63815800 -3.54266300
H 1.98222300 -6.37720700 -2.89160300
H 1.87249300 -7.97937500 -2.11677400
C 5.28127100 -3.84570300 3.64612200
C 6.76410300 -3.77595300 3.32339200
H 7.21155700 -2.87045400 3.75361700
H 7.28629900 -4.63941000 3.75572400
H 6.98100700 -3.77036800 2.25252500
C 5.02324000 -3.91430700 5.14506600
H 5.49974100 -4.79830500 5.58921800
H 5.42431400 -3.02824200 5.65464200
H 3.95137100 -3.96873500 5.36852300
H 3.42389900 -2.65114800 3.41377700
C 4.57017200 -2.50511900 -0.97194300
H 4.63573800 -1.41128700 -0.99286200
H 5.59691500 -2.89149000 -0.96776500
H 4.07750400 -2.83331500 -1.89049600

Table 29. Geometric coordinates and thermally corrected MP2 energies for (*S*)-**29a**

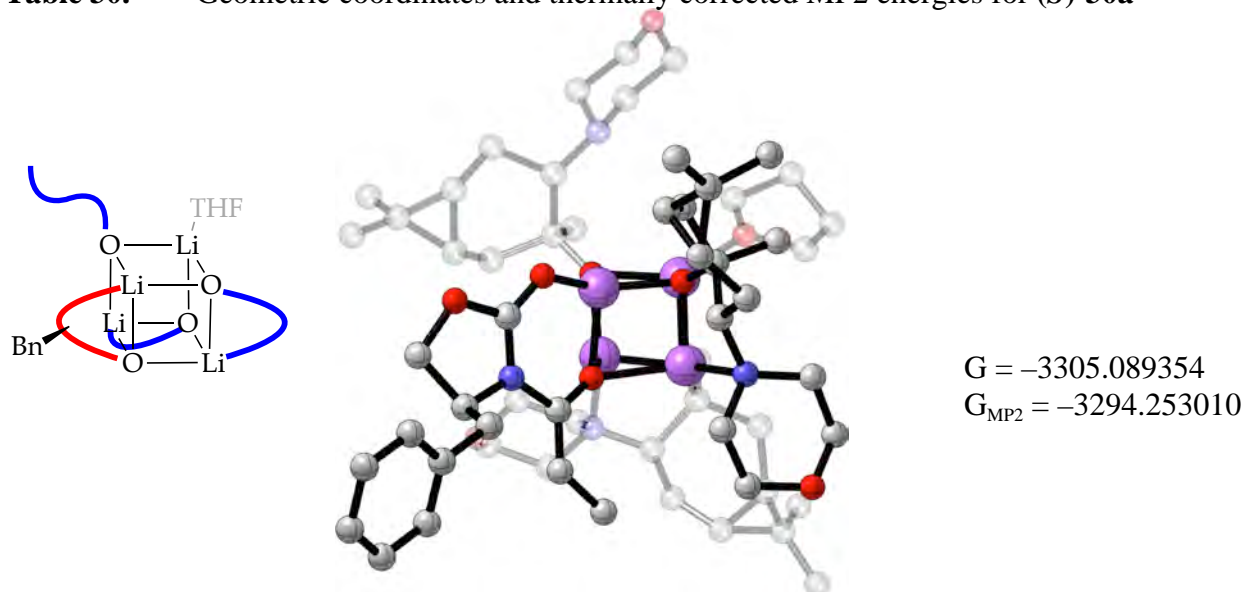


Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	C	8.83252900	-3.94280600	-0.19006600
O	1.60135600	0.09146200	1.00277200	C	8.67508100	-2.60776600	0.18250400
C	2.48096800	-0.75881100	0.97050800	C	7.44250700	-1.97369100	0.01157300
O	3.51295200	-0.68809000	1.85694000	H	7.33166700	-0.92851000	0.29291200
C	4.27992100	-1.90099300	1.77266000	H	9.51178400	-2.05578100	0.60247500
H	3.94224900	-2.58333600	2.56121500	H	9.79104600	-4.43779200	-0.06013900
H	5.33201500	-1.65857200	1.92772700	H	7.86766700	-5.67520800	-1.04011000
C	3.97296900	-2.43662300	0.37088500	H	5.69184000	-4.54654900	-1.34929800
H	3.89809800	-3.52571900	0.38643400	O	-1.78349700	-0.59878600	0.39815600
N	2.64318000	-1.84176700	0.14640600	O	-0.40181600	1.13038100	-1.47190700
C	1.71695200	-2.30344700	-0.89058700	C	-4.63911100	2.63623000	-1.43732400
C	2.07459800	-3.41299800	-1.59380000	H	-4.81776400	2.06824100	-2.35086800
H	2.99755600	-3.93071700	-1.36597000	H	-5.50416800	2.50796800	-0.76805900
C	1.22635600	-4.01332400	-2.67591600	C	-4.31734300	4.11771100	-1.64422500
H	1.80617900	-4.21155300	-3.58815700	H	-5.21776100	4.73524200	-1.71669700
H	0.78411100	-4.97617500	-2.37617100	H	-3.74184900	4.24728500	-2.56623900
H	0.40412100	-3.34476400	-2.94299000	C	-3.44987300	4.45672100	-0.40625700
O	0.62551200	-1.60236700	-1.04190400	H	-2.58557500	5.06949400	-0.67763300
Li	-0.20956700	-0.41015500	-2.55840900	H	-4.02187500	5.01140900	0.34411300
Li	-2.21754600	0.45957000	-1.17811000	C	-3.02255700	3.07447400	0.14585100
O	-2.01663000	-1.15520100	-2.46256600	H	-3.50067000	2.86540400	1.11109900
Li	-1.38470400	-2.01207800	-0.81638700	H	-1.94505600	2.94756700	0.25055800
C	5.00258200	-1.98625300	-0.69550100	O	-3.46541500	2.09790200	-0.81825600
H	4.58139700	-2.20750000	-1.68124700	C	0.34168000	2.21638700	-1.94951400
H	5.11157000	-0.89689600	-0.62662200	C	0.78314200	3.14205500	-0.73144700
C	6.34838400	-2.65919600	-0.53343800	H	0.17766300	4.05893200	-0.74665100
C	6.52333800	-4.00003500	-0.90866100	H	0.47462600	2.59313500	0.16186800
C	7.75187200	-4.63746200	-0.73865000	C	2.25981400	3.50126800	-0.54290000

C	3.22324800	3.35086100	-1.70668200	H	-3.95268900	-2.49027800	-2.17092300
H	4.20965300	2.95762300	-1.46149800	N	-5.30908600	-1.07576300	-2.80043500
C	2.64344400	2.79576100	-2.99995400	C	-6.08670200	-1.51926200	-1.63609000
H	3.45956500	2.40381500	-3.61795500	H	-5.40828700	-1.65649800	-0.78726000
H	2.16451700	3.57859400	-3.59815900	H	-6.59909300	-2.48418600	-1.82109500
C	1.63711900	1.67440200	-2.65354600	C	-7.14111900	-0.48235200	-1.25554300
H	2.11123700	1.05881100	-1.87951100	O	-8.01313600	-0.19051400	-2.33901900
N	1.35817400	0.69995800	-3.76390300	C	-7.27220400	0.25706300	-3.46529400
C	2.48076200	-0.25692000	-3.90902300	C	-6.23832700	-0.77906700	-3.90053900
H	2.61640400	-0.79289700	-2.96506400	H	-6.79106400	-1.67598300	-4.23167600
H	3.42312900	0.26587200	-4.14794200	H	-5.68492500	-0.39454400	-4.76152200
C	2.19716100	-1.26862100	-5.01675200	H	-7.99959700	0.42585700	-4.26586900
O	1.96335500	-0.63551300	-6.26664600	H	-6.77723500	1.21523900	-3.23709700
C	0.87801400	0.27397800	-6.15605900	H	-6.64472500	0.43957000	-0.91217900
C	1.14038000	1.32979000	-5.08661700	H	-7.77135600	-0.86049000	-0.44425100
H	2.02459600	1.91072000	-5.39511600	C	-2.88998400	-4.79921600	-5.25837500
H	0.29265700	2.01304100	-5.03856300	C	-3.31702900	-4.42534000	-6.66730600
H	0.77046700	0.75131800	-7.13511000	H	-2.46808700	-4.50024600	-7.35927400
H	-0.05234300	-0.27223700	-5.93142300	H	-4.09469400	-5.11325600	-7.02416400
H	1.33153500	-1.89260400	-4.74400900	H	-3.71712600	-3.41198800	-6.75174500
H	3.06103100	-1.92596300	-5.15465100	C	-2.37154500	-6.22837300	-5.17529700
C	2.92215400	4.72939400	-1.14967800	H	-3.14144800	-6.94756700	-5.48537500
C	2.11322800	5.74211800	-1.93897200	H	-1.50158500	-6.36993700	-5.83005100
H	1.68073300	6.49422900	-1.26574900	H	-2.06415700	-6.48875000	-4.15598300
H	2.74996500	6.27430900	-2.65816600	H	-1.42103100	-4.21384600	-3.70835700
H	1.28715600	5.29490900	-2.49651000	C	-3.05672000	-0.02442100	-4.30656600
C	4.02913200	5.37483500	-0.32872800	H	-2.08140000	0.39178700	-4.58541500
H	4.73167600	5.92279900	-0.97125000	H	-3.64757500	-0.11736200	-5.22624500
H	3.61779900	6.08832300	0.39771100	H	-3.55643600	0.68936900	-3.64604100
H	4.60333700	4.62727000	0.23041100	C	-2.31634800	-1.02510000	1.62160300
H	2.65189200	3.21403900	0.43095600	C	-3.46775100	-0.02500800	2.05450900
C	-0.56683700	3.04429500	-2.88922400	H	-3.03403500	0.76056400	2.68906300
H	-1.35932000	3.50540700	-2.29255600	H	-3.74886300	0.46393200	1.11865900
H	-0.04456900	3.84640100	-3.42535600	C	-4.77093400	-0.55501500	2.66599900
H	-1.05825000	2.39603000	-3.61908400	C	-4.90358300	-2.02765100	3.01617500
C	-2.84028800	-1.37272400	-3.58783500	H	-5.85289200	-2.49852300	2.76209000
C	-2.12492600	-2.31802800	-4.61751900	C	-3.68965900	-2.90926400	2.74416700
H	-2.52571900	-2.11907100	-5.61860700	H	-4.02408100	-3.94768500	2.64095500
H	-1.07281200	-2.01174300	-4.65633400	H	-2.98945200	-2.90388500	3.58627600
C	-2.22361800	-3.80434500	-4.31514800	C	-2.99255800	-2.43179900	1.44601300
C	-3.62963000	-4.29908900	-4.03151100	H	-3.79188600	-2.24393500	0.71676800
H	-3.75376200	-5.02593400	-3.22856900	N	-2.13437800	-3.44918900	0.75921500
C	-4.67980700	-3.20261300	-4.04467600	C	-2.96373700	-4.48856200	0.11034500
H	-5.63717500	-3.59913800	-3.68453400	H	-3.65789400	-4.00655100	-0.58604100
H	-4.86613800	-2.84193000	-5.06196500	H	-3.56214700	-5.04911000	0.84890200
C	-4.21686100	-2.03494400	-3.13010700	C	-2.08691100	-5.47977500	-0.65059200

O -1.14877200 -6.11348600 0.20491000
C -0.33211300 -5.14065900 0.84749300
C -1.16817700 -4.14045900 1.64128900
H -1.69098400 -4.68313500 2.44640700
H -0.50592000 -3.40981200 2.10486000
H 0.32779800 -5.69315600 1.52417100
H 0.29009300 -4.61349900 0.10811000
H -1.56447700 -4.96239200 -1.47101100
H -2.70380700 -6.27477000 -1.08145000
C -4.98549700 -0.97683600 4.11028800
C -3.90346300 -0.81165200 5.16053800
H -3.98019500 0.17855200 5.62853900
H -4.01429000 -1.55897900 5.95772900
H -2.89372900 -0.89833600 4.75931200
C -6.37806700 -0.72708400 4.67485200
H -6.60334300 -1.42363000 5.49360700
H -6.46497100 0.29238900 5.07382100
H -7.15371100 -0.85171600 3.91045100
H -5.65400600 -0.10326900 2.21387600
C -1.17123500 -0.99743900 2.66392800
H -0.90805100 0.04536300 2.87507600
H -1.40189400 -1.48185400 3.61797400
H -0.27388500 -1.46782000 2.25539700

Table 30. Geometric coordinates and thermally corrected MP2 energies for (*S*)-**30a**

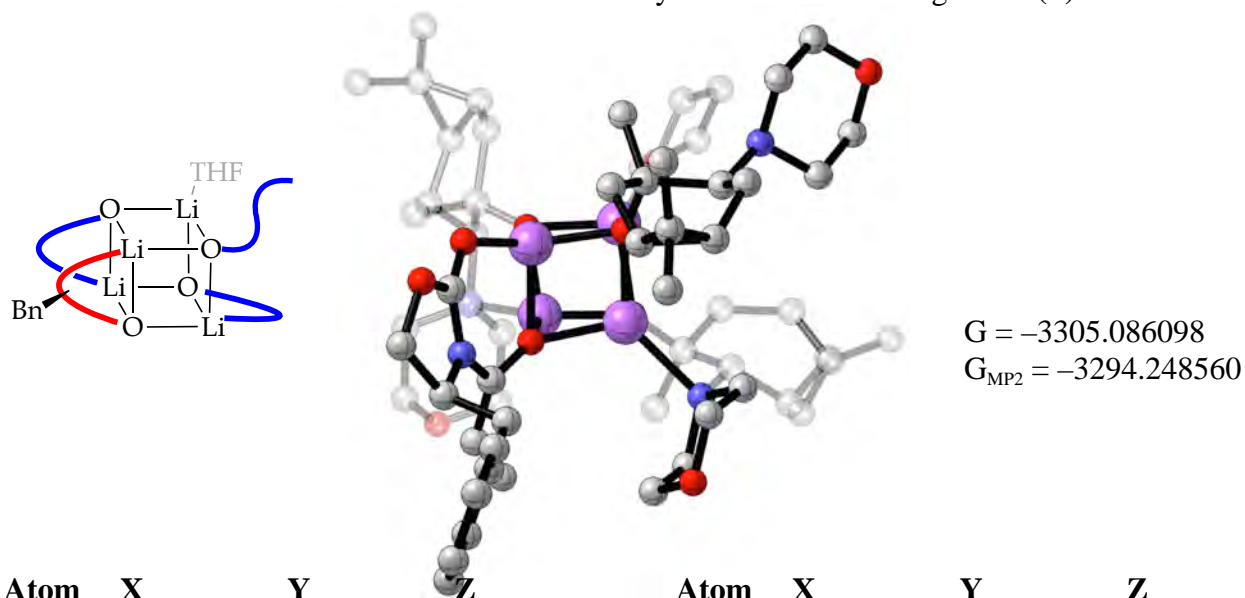


Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	C	8.21965500	3.55861600	-1.35696700
O	1.74667900	-0.74249300	0.04093700	C	9.24678600	2.69109000	-0.97791800
C	2.69771200	-0.19251600	-0.49776500	C	8.94192500	1.53994100	-0.25148700
O	3.80012100	-0.92390800	-0.83288100	C	7.61744500	1.25678100	0.08932500
C	4.68727100	-0.08881600	-1.60305200	H	7.38984000	0.36245600	0.66564400
H	4.49427400	-0.26252500	-2.66738000	H	9.73406900	0.86183300	0.05483400
H	5.71485200	-0.36560900	-1.36461800	H	10.2765940	2.91443100	-1.24297300
C	4.31178000	1.32716900	-1.16405300	H	8.44807400	4.46195500	-1.91649700
H	4.40462100	2.03628400	-1.98911000	H	6.10885600	3.96245200	-1.30397700
N	2.88887200	1.11985800	-0.83711700	O	-1.44961200	-0.26971400	-1.26248100
C	1.90204600	2.19902900	-0.73065300	O	-1.00979800	0.49084200	1.52757100
C	2.37628100	3.46946400	-0.87091600	C	-5.10804300	0.89860200	1.99035600
H	3.43246200	3.62730400	-1.04523800	H	-4.74258400	0.56480200	2.96669000
C	1.54541300	4.71640500	-0.79000400	H	-4.83733900	1.94992800	1.85408800
H	1.93497900	5.41175500	-0.03281600	C	-6.60772100	0.62613600	1.82747300
H	1.52995900	5.27860000	-1.73599500	H	-7.06035500	1.34760100	1.13688500
H	0.50899700	4.48968700	-0.52825800	H	-7.14473200	0.68652700	2.77885400
O	0.66709700	1.82541600	-0.53262500	C	-6.61648000	-0.77930400	1.20661100
Li	-0.80451200	2.29008500	0.95643700	H	-6.46276100	-1.54358400	1.97790600
Li	-2.51277100	0.48556400	0.28625000	H	-7.54300600	-1.01281500	0.67338800
O	-2.23615000	2.41177600	-0.27310800	C	-5.40734000	-0.70680600	0.27758200
Li	-1.17001500	1.57546700	-1.63734600	H	-5.67028800	-0.22793600	-0.67586300
C	5.13688500	1.80200800	0.06109300	H	-4.92822200	-1.66555000	0.07338100
H	4.64520800	2.68151400	0.48740900	O	-4.44265900	0.11663900	0.96883500
H	5.09693700	1.01406400	0.82317800	C	-0.66452200	0.29242700	2.86938200
C	6.57622400	2.11610900	-0.28661400	C	0.00479900	-1.13978500	3.05772200
C	6.89887400	3.27274700	-1.01310600	H	-0.70055600	-1.78967600	3.59262800

H	0.08101300	-1.55169700	2.04913300	H	-3.97392500	5.20554200	-2.79826700
C	1.39244100	-1.24934000	3.69508400	C	-2.26356800	4.07881000	-2.01760600
C	1.91308700	-0.10977700	4.55426300	H	-1.35018700	4.38595000	-1.49931600
H	2.96949800	0.13161300	4.43819900	N	-1.77021400	3.16158000	-3.10026100
C	1.01385500	1.11366900	4.67038300	C	-0.47075600	3.63270500	-3.63658100
H	1.61331300	1.96999800	5.00092000	H	0.25536800	3.67452400	-2.82153200
H	0.23735400	0.97812600	5.43121500	H	-0.56080200	4.64427600	-4.07006200
C	0.38251600	1.38838200	3.28603900	C	0.05391900	2.68501700	-4.71153600
H	1.18672200	1.26700400	2.54941900	O	-0.86517500	2.53404800	-5.78319800
N	-0.09614900	2.79385600	3.06164200	C	-2.11712400	2.07022200	-5.29674400
C	1.03919000	3.71557100	2.82392800	C	-2.69627600	3.01384500	-4.24659600
H	1.61268700	3.36603600	1.95796200	H	-2.87896500	3.98744200	-4.72948600
H	1.72002600	3.74787400	3.69213500	H	-3.65553200	2.62551900	-3.90408900
C	0.53330100	5.13304400	2.55541100	H	-2.78585300	2.01850600	-6.16162600
O	-0.25161800	5.63320200	3.62765700	H	-2.01091300	1.05740700	-4.87871100
C	-1.35331700	4.76926000	3.86297600	H	0.28107100	1.70203200	-4.26593900
C	-0.88958000	3.35174600	4.17930900	H	0.97636300	3.08451200	-5.14415800
H	-0.29130600	3.38853600	5.10453200	C	-4.01096500	6.95096700	-0.57728500
H	-1.75870000	2.72423000	4.36973300	C	-5.44301200	6.68074900	-1.00282200
H	-1.90128200	5.18617000	4.71375700	H	-6.12436200	6.77813800	-0.14730800
H	-2.02260300	4.76024800	2.98602300	H	-5.76176500	7.40834100	-1.76056600
H	-0.05698300	5.15188600	1.62543300	H	-5.59054000	5.68305700	-1.42407600
H	1.37799600	5.81879000	2.43948900	C	-3.82520800	8.34549000	0.00307000
C	1.62528000	-1.45806000	5.18514500	H	-4.09010100	9.11872600	-0.73047800
C	0.45837400	-1.65302700	6.13567100	H	-4.46177600	8.49286000	0.88551900
H	0.18165800	-2.71427300	6.18857500	H	-2.78762700	8.51928300	0.31015600
H	0.72528700	-1.33278200	7.15161800	H	-2.49006500	6.17647300	0.83209700
H	-0.43649400	-1.10153800	5.83856500	C	-4.31073100	2.58383600	-1.46255600
C	2.84087400	-2.28895200	5.56965600	H	-4.88639900	2.18083100	-0.62372000
H	3.19981600	-2.02686700	6.57425400	H	-4.98133200	3.22521800	-2.05006500
H	2.60200300	-3.36077500	5.57159100	H	-4.00217100	1.73364000	-2.07707400
H	3.67009300	-2.13578900	4.86952200	C	-1.66016800	-1.38331800	-2.10476800
H	2.12808800	-1.72749300	3.05096800	C	-0.69325600	-1.33160100	-3.33811200
C	-1.96564200	0.31593300	3.70264900	H	-1.13838200	-1.90715300	-4.15826700
H	-2.56644500	-0.55731300	3.42402700	H	-0.67350600	-0.29239400	-3.68481400
H	-1.80638100	0.27954800	4.78775300	C	0.71827300	-1.82448900	-3.07385300
H	-2.55908200	1.20135000	3.46368400	C	0.79344100	-3.17711900	-2.39161100
C	-3.08253400	3.33746900	-0.90146500	H	1.53814400	-3.28906700	-1.60526600
C	-3.62674100	4.40017600	0.14423100	C	-0.56411100	-3.77391000	-2.05548400
H	-4.72373000	4.37854400	0.13238300	H	-0.43335700	-4.67091300	-1.43778300
H	-3.33402600	4.00824400	1.12337200	H	-1.09369700	-4.09984800	-2.95753500
C	-3.14930200	5.84795900	0.02963000	C	-1.40042400	-2.72062400	-1.27919900
C	-2.83841200	6.39257200	-1.35567700	H	-0.75607200	-2.38439700	-0.46191000
H	-1.97266900	7.05051200	-1.42846800	N	-2.60161800	-3.28356300	-0.60061800
C	-2.93655300	5.38645300	-2.49490200	C	-2.28477100	-3.79330200	0.73981000
H	-2.42688000	5.78848500	-3.37830800	H	-1.81880300	-2.99229800	1.32293000

H -1.57508900 -4.64321000 0.70417400
C -3.55225900 -4.25573900 1.45478800
O -4.25257400 -5.24341300 0.70968000
C -4.57093200 -4.75797500 -0.58655900
C -3.31851200 -4.32551400 -1.34684900
H -2.69842400 -5.22580200 -1.50532600
H -3.60897800 -3.94540700 -2.33040500
H -5.06916900 -5.58057900 -1.10989400
H -5.27822100 -3.91449300 -0.51202300
H -4.20942500 -3.38914700 1.64079000
H -3.30302700 -4.71399300 2.41720300
C 1.33466300 -3.01456200 -3.80025300
C 0.67473200 -3.66358800 -5.00443500
H 0.92836500 -3.11867300 -5.92347900
H 1.03123900 -4.69512600 -5.12461000
H -0.41550300 -3.70268500 -4.94018500
C 2.85261600 -2.99553800 -3.91596800
H 3.25341100 -4.01216600 -4.02686100
H 3.17492600 -2.41621100 -4.79248800
H 3.31383200 -2.55372000 -3.02588000
H 1.42332200 -1.06366400 -2.74762900
C -3.08968500 -1.31020500 -2.67730700
H -3.20609700 -0.36232200 -3.21683000
H -3.30891000 -2.11825300 -3.38679100
H -3.82971700 -1.34460900 -1.87698200

Table 31. Geometric coordinates and thermally corrected MP2 energies for (*S*)-**31a**

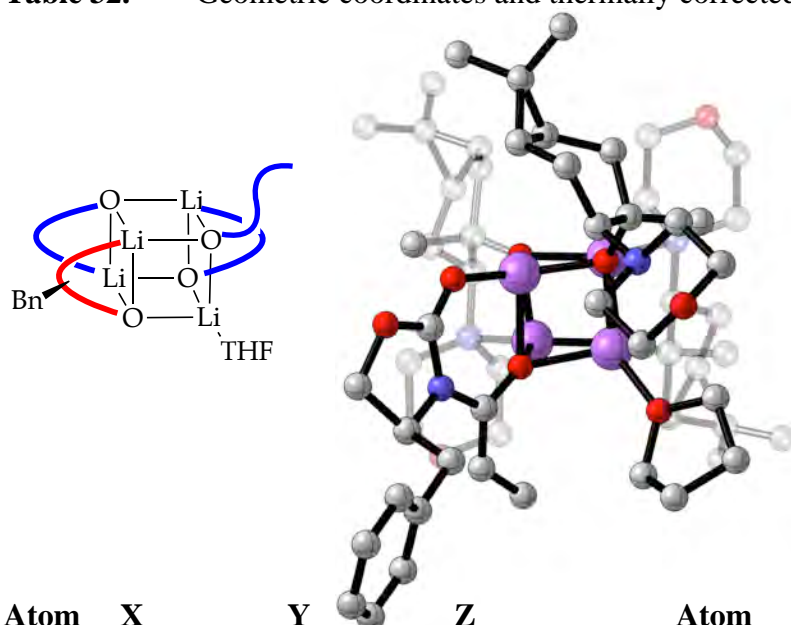


Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	C	9.27981400	0.25756800	1.83991000
O	1.37243100	0.90702500	-0.97551300	C	8.75996400	-0.43195900	0.74442700
C	2.49140800	1.08098500	-0.50662700	C	7.37783100	-0.55327100	0.58457300
O	3.55963600	1.23286900	-1.33419800	H	6.98044100	-1.10422500	-0.26535600
C	4.69769100	1.64593000	-0.55830000	H	9.42856500	-0.88076300	0.01449600
H	4.81459500	2.72994100	-0.66675500	H	10.3548230	0.35150000	1.96752800
H	5.58447000	1.14590400	-0.95059700	H	8.80531800	1.35024100	3.63878900
C	4.35496500	1.23956800	0.88439100	H	6.35970900	1.12267800	3.35707700
H	4.65223100	2.03240200	1.57334800	O	-1.73526500	0.58027100	0.48020800
N	2.88804600	1.14884400	0.79747700	O	-0.26471200	-1.94616700	0.17205400
C	2.00779900	1.03506600	1.96306900	C	-4.61710300	-2.64518600	-0.49009600
C	2.43291100	1.64491000	3.10050300	H	-4.73071700	-2.01258800	-1.38230700
H	3.33709000	2.24300400	3.07014700	H	-3.91251100	-3.44795900	-0.70865500
C	1.73669200	1.56041100	4.42684800	C	-5.99011500	-3.12346600	0.03288700
H	2.35454600	1.05924000	5.18826600	H	-5.96506500	-4.18195800	0.30812900
H	1.49817700	2.55256500	4.83436300	H	-6.76303100	-3.00331400	-0.73225200
H	0.80015400	1.00205600	4.34597700	C	-6.25267100	-2.23044700	1.27488000
O	0.91599000	0.33499100	1.79017100	H	-7.24676600	-1.77335800	1.26743500
Li	0.30049600	-1.56300700	1.99576000	H	-6.15926900	-2.81359900	2.19631800
Li	-2.03213600	-1.30732800	0.87277600	C	-5.13709000	-1.18102500	1.19923800
O	-1.44192900	-1.19221200	2.77013400	H	-4.78720700	-0.82444200	2.16892700
Li	-1.08532100	0.66835900	2.25712400	H	-5.43433100	-0.32012000	0.58517700
C	4.99422500	-0.09464900	1.33204100	O	-4.04098500	-1.86308000	0.57015400
H	4.51754100	-0.39256600	2.27202400	C	-0.06802200	-2.74536800	-0.97824700
H	4.75294000	-0.86263300	0.58728800	C	1.32195200	-2.44968700	-1.63386600
C	6.49297300	0.00896600	1.51420700	H	1.30210400	-2.81808500	-2.66577600
C	7.03008100	0.69448200	2.61448300	H	1.43517000	-1.36463900	-1.71036800
C	8.40926300	0.81970400	2.77680800	C	2.50007100	-3.06139300	-0.89766800

C	2.35873700	-4.55012400	-0.63538400	H	-0.91974400	-3.76064300	3.06208600
H	2.69157600	-4.92910800	0.33059700	N	0.76752000	-2.82536400	3.75745400
C	1.03978300	-5.13599900	-1.11453400	C	1.54956500	-3.98264500	3.26974000
H	0.94312400	-6.17247500	-0.76718800	H	1.08308100	-4.37052300	2.35889100
H	1.00187500	-5.18021200	-2.20792400	H	1.57523500	-4.79888700	4.01181000
C	-0.13813800	-4.28520300	-0.56235900	C	2.98702800	-3.56510800	2.96791100
H	0.00596200	-4.23772200	0.52043900	O	3.63001100	-3.03080900	4.11396000
N	-1.46817400	-4.93790500	-0.72973100	C	2.89670900	-1.92049600	4.61684100
C	-1.76561600	-5.86592500	0.36830100	C	1.45835300	-2.30058600	4.95476300
H	-1.69623700	-5.32619400	1.31956400	H	1.47371000	-3.05349600	5.76048600
H	-1.05095600	-6.71188800	0.40684800	H	0.93910900	-1.41936300	5.32693900
C	-3.17556500	-6.43693300	0.22986500	H	3.41952800	-1.58848100	5.51919000
O	-3.36585800	-7.08369600	-1.02002300	H	2.90001800	-1.09655100	3.88642800
C	-3.09374900	-6.18969000	-2.09081300	H	2.99643600	-2.82677300	2.14985500
C	-1.67341900	-5.63527100	-2.00726200	H	3.57539200	-4.43366700	2.65643800
H	-0.97885200	-6.48451100	-2.13382500	C	-3.55324500	-4.50824800	5.73903700
H	-1.50715200	-4.94321700	-2.83747100	C	-3.57110700	-3.54695600	6.91226500
H	-3.22377800	-6.76524600	-3.01279500	H	-4.59496200	-3.19673600	7.09814000
H	-3.82463600	-5.36391300	-2.09040000	H	-3.22490700	-4.04301900	7.82889200
H	-3.91512200	-5.62745600	0.35174100	H	-2.95233900	-2.66336900	6.75732100
H	-3.35928200	-7.19227200	1.00071200	C	-4.51195800	-5.67525800	5.93718500
C	3.46191800	-4.04604800	-1.55035200	H	-4.25729000	-6.24718300	6.83948000
C	3.46406100	-4.31651600	-3.04528000	H	-5.54583700	-5.32227000	6.04942600
H	4.05742900	-3.55768100	-3.57184100	H	-4.48812700	-6.36816000	5.08817900
H	3.91732600	-5.29438000	-3.25513900	H	-3.99998600	-4.58100000	3.59470700
H	2.46783700	-4.31701600	-3.49373000	C	-1.56050200	-1.02763500	5.14529300
C	4.86488200	-4.08427700	-0.96036500	H	-2.45060200	-0.38978900	5.18003800
H	5.33372400	-5.06585700	-1.11157600	H	-1.48018700	-1.53109300	6.11359200
H	5.51151500	-3.33384900	-1.43588600	H	-0.69594700	-0.36884000	5.04072900
H	4.85751700	-3.88282300	0.11688800	C	-2.39431800	1.73346100	0.03315300
H	2.92403200	-2.44814000	-0.10393200	C	-3.34844200	1.34680600	-1.17417100
C	-1.12647700	-2.36358800	-2.03374800	H	-2.85901100	1.62779500	-2.11633100
H	-1.03798400	-1.29363900	-2.25687900	H	-3.36313100	0.25424900	-1.16088500
H	-1.00103100	-2.90393200	-2.98031900	C	-4.80731400	1.81493600	-1.17793400
H	-2.13507700	-2.55445300	-1.66319900	C	-5.26902400	2.87112400	-0.18744600
C	-1.66365300	-1.96762600	3.92004000	H	-6.24420000	2.70948600	0.27154700
C	-3.11918400	-2.59095700	3.84189900	C	-4.22009200	3.42697100	0.76784900
H	-3.82597900	-1.89306300	4.31399400	H	-4.72753300	3.85849500	1.63885300
H	-3.34727000	-2.58098200	2.77459800	H	-3.66002200	4.24875000	0.30923100
C	-3.38707700	-4.02784800	4.30679600	C	-3.26115600	2.29705500	1.20960100
C	-2.28216300	-4.83085900	4.97160200	H	-3.88901100	1.44735000	1.50229500
H	-2.18655700	-5.87035100	4.65922100	N	-2.45335300	2.59518800	2.44051700
C	-0.94674300	-4.12247900	5.16898500	C	-3.25509100	2.37870500	3.66402200
H	-0.15746000	-4.87758600	5.25219500	H	-3.60248900	1.33941700	3.67892800
H	-0.92214300	-3.56282400	6.10995900	H	-4.14436600	3.03374800	3.68679500
C	-0.66940700	-3.18719400	3.96529800	C	-2.42022200	2.64925100	4.91517200

O -1.89409700 3.96728400 4.92801500
C -1.10700500 4.19141600 3.76486400
C -1.92084200 3.97631900 2.49497200
H -2.73818900 4.71537000 2.48760900
H -1.29044800 4.16471700 1.62602300
H -0.76224700 5.22867000 3.81951600
H -0.22683500 3.53038700 3.76465100
H -1.59952600 1.91794100 4.98149500
H -3.04069100 2.55004300 5.81157400
C -5.29952500 3.16433200 -1.67683400
C -4.35062700 4.16104600 -2.31574900
H -4.28529400 3.98243400 -3.39689500
H -4.71018500 5.18918200 -2.17510100
H -3.33531900 4.10542600 -1.92001100
C -6.67835500 3.17713900 -2.32221500
H -7.14295900 4.16929000 -2.24409500
H -6.61727200 2.92272400 -3.38871100
H -7.35402100 2.45658700 -1.84670600
H -5.51415700 1.00617700 -1.36294700
C -1.32710200 2.73586200 -0.46665400
H -0.85221800 2.33717200 -1.36879500
H -1.72587700 3.72742100 -0.71106200
H -0.53419400 2.85438600 0.27706000

Table 32. Geometric coordinates and thermally corrected MP2 energies for (*S*)-**16a***



G = -3305.096039
G_{MP2} = -3294.259156

Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	C	-7.48770800	-4.92555300	-1.43399300
O	-1.47719900	0.30818500	-1.19032800	C	-8.60863200	-4.11007100	-1.60721000
C	-2.36168200	-0.48915900	-1.47154600	C	-8.50465900	-2.73846800	-1.37483700
O	-3.42053700	-0.07999300	-2.22509100	C	-7.28555900	-2.18603000	-0.97600700
C	-4.18908800	-1.23041900	-2.61343000	H	-7.21645500	-1.11709900	-0.78487900
H	-3.89449000	-1.51951900	-3.62863900	H	-9.37262100	-2.09634900	-1.49902600
H	-5.24629000	-0.96137300	-2.60615800	H	-9.55660600	-4.54242800	-1.91548100
C	-3.82201200	-2.30006200	-1.57656700	H	-7.56135300	-5.99640000	-1.60464200
H	-3.72655500	-3.27408700	-2.06086600	H	-5.40816400	-5.01492700	-0.88992000
N	-2.50327900	-1.81077100	-1.14289300	O	1.86928000	-0.39011100	-0.33482100
C	-1.56449800	-2.60360500	-0.35075400	O	0.14385700	0.47641600	1.86949300
C	-1.77212900	-3.94916500	-0.29615900	C	-1.92868800	-1.48162600	4.76042700
H	-2.57322900	-4.39349400	-0.87507900	H	-1.02233000	-1.36950700	5.36416200
C	-0.93058900	-4.89577000	0.51363700	H	-2.31765500	-0.48954100	4.51641800
H	-1.54727000	-5.52974500	1.16762700	C	-2.97700600	-2.38556000	5.42698600
H	-0.34901000	-5.58500300	-0.11604300	H	-3.73455700	-1.80856100	5.96577200
H	-0.22618500	-4.35275500	1.15137700	H	-2.50264900	-3.06721000	6.14251900
O	-0.61582800	-1.93207200	0.24012100	C	-3.54794000	-3.17820400	4.24036300
Li	-0.22222100	-1.40838000	2.17963500	H	-3.99977900	-4.13077600	4.53354700
Li	1.97302800	-0.20800900	1.60838900	H	-4.30447000	-2.58785200	3.70974500
O	1.62593800	-2.07903700	2.03798800	C	-2.30985900	-3.35671400	3.36644900
Li	1.36659500	-2.19317300	0.13252900	H	-2.51846200	-3.49532900	2.30392100
C	-4.82089700	-2.39591700	-0.39812900	H	-1.69067400	-4.19367100	3.72011900
H	-4.35020200	-3.00498200	0.38081600	O	-1.57578600	-2.12337000	3.50687200
H	-4.96283200	-1.38967500	0.01535900	C	2.44498600	-2.51915800	3.08555800
C	-6.15182900	-2.99121800	-0.80228200	C	2.52449200	-4.10740400	3.07775400
C	-6.27269200	-4.36992100	-1.03453500	H	1.97759800	-4.49447200	3.94792600

H	1.93475300	-4.40656200	2.20789000	H	-1.67841000	4.25134600	1.91397000
C	3.88848200	-4.79490600	2.97953200	C	-1.73634600	2.05839200	1.94705600
C	5.14021200	-4.03122500	3.37748000	H	-1.93494000	1.30114600	1.18492400
H	6.01886100	-4.19005600	2.75265900	N	-2.76629700	1.80811400	2.99339300
C	4.94143600	-2.58368600	3.80486400	C	-4.01365600	1.28549800	2.42453800
H	5.89852600	-2.05493000	3.72765400	H	-3.78591700	0.38764600	1.83773600
H	4.64106300	-2.50909700	4.85564300	H	-4.50244300	2.01396900	1.74853500
C	3.88407900	-1.92828600	2.88630500	C	-5.00210000	0.92054200	3.53183900
H	4.14336900	-2.22101700	1.86123500	O	-5.27195300	2.02019600	4.38811200
N	3.91536800	-0.42598300	2.85084300	C	-4.06575400	2.52406800	4.94817800
C	4.99458600	0.04485300	1.95251800	C	-3.08568000	2.95078900	3.85829900
H	4.81042600	-0.34610800	0.94713100	H	-3.54851400	3.78199800	3.29687600
H	5.98223800	-0.32008200	2.28575900	H	-2.17221900	3.33217400	4.32245800
C	5.03750800	1.56997400	1.89558200	H	-4.34948800	3.38007600	5.56860400
O	5.22395500	2.14143300	3.18130000	H	-3.59956000	1.76023000	5.59346700
C	4.17942300	1.72747300	4.05071700	H	-4.60372000	0.07701800	4.12117400
C	4.12645300	0.20727400	4.17341200	H	-5.96367400	0.61912800	3.10307600
H	5.07580400	-0.12528600	4.62220700	C	0.08906200	4.49925000	-0.22286700
H	3.32017100	-0.07233100	4.85236900	C	0.20278600	5.75778800	0.61983200
H	4.39134500	2.17359600	5.02738300	H	1.22651900	6.15336900	0.58451200
H	3.21375500	2.11663700	3.69245400	H	-0.46529900	6.53866900	0.23283600
H	4.10859900	1.95566200	1.44415100	H	-0.05047900	5.60545700	1.67185200
H	5.88058000	1.89977300	1.28081500	C	0.44972600	4.74865200	-1.68101200
C	4.70141200	-5.23408200	4.18965500	H	-0.20881200	5.50640900	-2.12661600
C	4.14661300	-5.08218000	5.59379000	H	1.48315900	5.10781700	-1.77741900
H	3.53002000	-5.95156400	5.85729100	H	0.35612900	3.83498200	-2.27900400
H	4.96029000	-5.02215200	6.32852200	H	0.97624700	2.46948000	-0.38405800
H	3.52275900	-4.19411700	5.71784500	C	-0.02181400	1.74620700	3.90306700
C	5.53512700	-6.49590000	4.02077600	H	1.00713700	1.43459100	4.11628000
H	6.39324000	-6.49936600	4.70619300	H	-0.16386700	2.73642900	4.35372900
H	4.93904600	-7.39394500	4.23055600	H	-0.70182800	1.04614500	4.39108500
H	5.92527100	-6.58753800	3.00054300	C	2.52886700	-0.34361500	-1.57149100
H	3.99094700	-5.45216800	2.11682800	C	3.43342600	0.96120300	-1.65434700
C	1.79575500	-2.08672000	4.42160100	H	2.96827400	1.67094400	-2.35056100
H	0.84828800	-2.62474400	4.53216800	H	3.34298000	1.42147300	-0.66757500
H	2.40845300	-2.30439500	5.30570400	C	4.92581500	0.82876300	-1.97290900
H	1.56256100	-1.01820200	4.41058900	C	5.44371300	-0.43712500	-2.63531500
C	-0.22706000	1.74160400	2.37579100	H	6.40271000	-0.80934800	-2.27529500
C	0.71970100	2.83585700	1.78170200	C	4.41888800	-1.53128600	-2.90028500
H	0.62783900	3.75411800	2.37412200	H	4.94096900	-2.48574200	-3.03446800
H	1.75185500	2.49164700	1.92485700	H	3.86879300	-1.35492900	-3.83085900
C	0.45477000	3.12152500	0.31407000	C	3.44885600	-1.60866700	-1.69947800
C	-0.99452800	3.46281000	0.00815600	H	4.07068500	-1.56971700	-0.79650400
H	-1.42872800	3.01514200	-0.88351100	N	2.70317500	-2.90314800	-1.56172900
C	-1.90048500	3.42654700	1.22861300	C	3.56762500	-3.95439000	-0.98036800
H	-2.94594300	3.55930600	0.92286700	H	3.95003200	-3.60917100	-0.01396300

H 4.43399100 -4.16851200 -1.63101200
C 2.77884600 -5.24575100 -0.77252100
O 2.20307600 -5.72264000 -1.97978600
C 1.38231900 -4.72387200 -2.57638500
C 2.16216900 -3.43920200 -2.83159600
H 2.97558300 -3.66226100 -3.54150400
H 1.50379300 -2.70583500 -3.29619800
H 1.03033300 -5.14390800 -3.52395100
H 0.50772200 -4.51153800 -1.94278500
H 1.99271100 -5.08391000 -0.01877000
H 3.44243900 -6.03783800 -0.41150000
C 5.50322300 0.88228800 -3.38044100
C 4.61209400 1.15785700 -4.57737200
H 4.51513400 2.23926600 -4.73954600
H 5.04302700 0.72639100 -5.49053700
H 3.60229300 0.75737400 -4.46611700
C 6.88347200 1.50809100 -3.52048000
H 7.40551100 1.12142100 -4.40598200
H 6.81349600 2.59878500 -3.62600900
H 7.51158100 1.29854400 -2.64699700
H 5.57664100 1.26195300 -1.21427300
C 1.46134500 -0.25271100 -2.68847300
H 0.94392300 0.70927700 -2.60879700
H 1.87398200 -0.32231500 -3.70272600
H 0.70085200 -1.02844100 -2.56629700

Table 33. Geometric coordinates and thermally corrected MP2 energies for (*S*)-**26a**

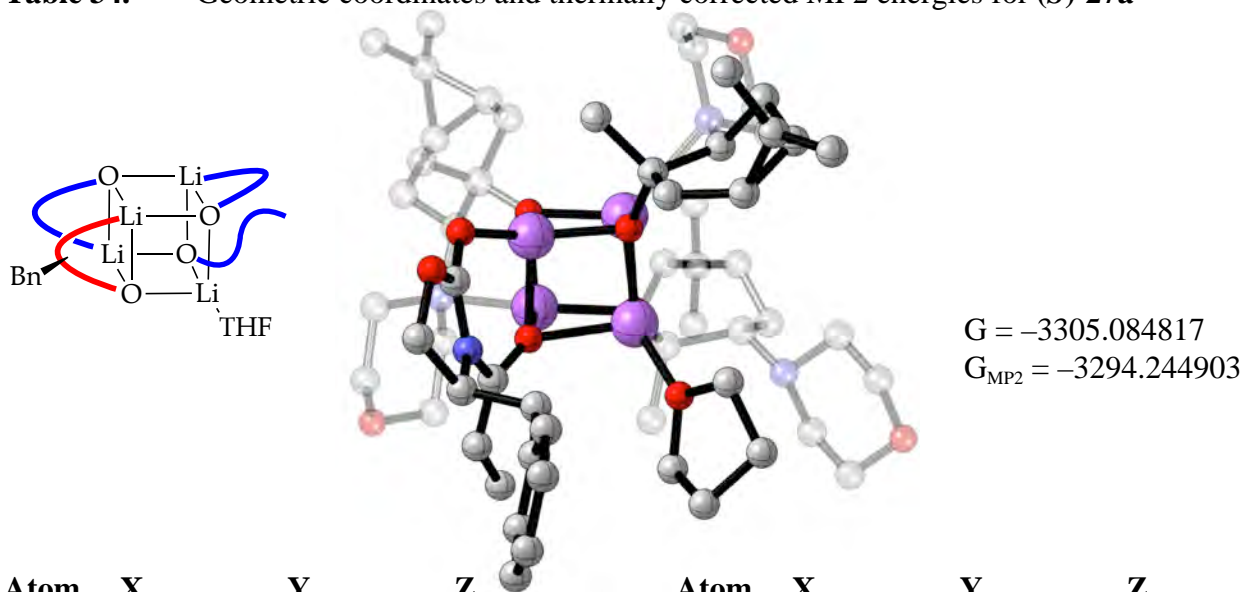


Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	C	-7.57007900	-5.03113700	0.52217000
O	-1.87065000	0.41556800	0.18831300	C	-8.68575500	-4.26474600	0.86727100
C	-2.76198000	-0.36351000	-0.11948600	C	-8.51013500	-2.95237100	1.30630700
O	-4.00771200	0.10690700	-0.40868400	C	-7.22651800	-2.40944500	1.39488300
C	-4.80906500	-0.98951300	-0.89171700	H	-7.09741900	-1.38933700	1.75044100
H	-4.77381600	-0.99425200	-1.98709500	H	-9.37077000	-2.34993800	1.58471500
H	-5.83589200	-0.83898700	-0.55669100	H	-9.68325900	-4.69020900	0.79918300
C	-4.13261500	-2.21938300	-0.28048600	H	-7.69666000	-6.05717400	0.18673700
H	-4.18657400	-3.08250300	-0.94753100	H	-5.42739600	-5.09524800	0.35256500
N	-2.74564900	-1.72815100	-0.21076600	O	0.64162500	0.37808200	-1.81058200
C	-1.56069500	-2.58128200	-0.12791700	O	1.72282600	-0.20630000	0.88195400
C	-1.77933000	-3.91158000	0.06332700	C	3.86485300	-3.41638800	2.19480200
H	-2.79155000	-4.27155000	0.19612500	H	4.46059800	-3.10886500	1.33213200
C	-0.70322300	-4.95466700	0.11618000	H	3.89801700	-2.62674100	2.95267700
H	-0.71485400	-5.50435100	1.06829900	C	4.27551500	-4.77336800	2.76713500
H	-0.81461700	-5.71201200	-0.67535300	H	5.06262700	-4.68228700	3.52185700
H	0.28722500	-4.50764000	0.00296600	H	4.64046900	-5.43621900	1.97408200
O	-0.41603000	-1.97643500	-0.30718800	C	2.94733900	-5.29404300	3.33568200
Li	1.64703600	-2.10386800	0.41342000	H	2.91796800	-6.38229200	3.44611900
Li	2.33518200	-0.06455900	-1.02601300	H	2.75201500	-4.84952900	4.31783300
O	2.34684800	-1.98243400	-1.36533700	C	1.93782000	-4.79132800	2.30119400
Li	0.57726200	-1.51237100	-2.04437400	H	0.95272200	-4.56862100	2.72096000
C	-4.70719500	-2.57188400	1.11742700	H	1.81368400	-5.51417200	1.48684300
H	-4.01875700	-3.26528100	1.60962600	O	2.48823100	-3.56936500	1.75595900
H	-4.71754500	-1.65527200	1.71992200	C	0.57545500	1.51905500	-2.62504300
C	-6.09811000	-3.16482500	1.04812900	C	-0.85586800	2.20172000	-2.54020000
C	-6.29015500	-4.48521100	0.61313000	H	-1.22833500	2.35626100	-3.55973900

H	-1.50927300	1.45041900	-2.09141600	H	0.73601400	0.98204700	4.78045200
C	-0.98753400	3.50493300	-1.75719200	C	1.66398900	-0.34165800	3.32532300
C	0.16460500	4.49183700	-1.85641900	H	1.34835200	-1.30942800	2.92629300
H	0.43375000	5.01821500	-0.94046600	N	2.66488200	-0.69864100	4.37103100
C	1.36591800	3.98696100	-2.64366800	C	2.21592900	-1.78440600	5.24697900
H	2.22354700	4.64864700	-2.47569900	H	1.84544600	-2.61089100	4.62923900
H	1.18283500	3.99339300	-3.72410900	H	1.39199300	-1.47533600	5.91772400
C	1.66125800	2.54957300	-2.14337200	C	3.37950900	-2.27162700	6.11143800
H	1.50962700	2.57669500	-1.05770900	O	3.93650600	-1.21833300	6.88330600
N	3.07485400	2.08060900	-2.28535400	C	4.35115800	-0.14377400	6.04839000
C	3.95601200	2.74861500	-1.30547200	C	3.18774000	0.38452300	5.21030900
H	3.56466300	2.58120900	-0.29871400	H	2.43060300	0.78908300	5.90642100
H	3.99582100	3.84021900	-1.47048200	H	3.53499400	1.21161800	4.58582900
C	5.37901800	2.20329800	-1.39219300	H	4.73165900	0.63420700	6.71774800
O	5.93131200	2.39365500	-2.68562900	H	5.16719900	-0.47221700	5.38358200
C	5.10825500	1.77304800	-3.66299400	H	4.15772200	-2.71590600	5.46680100
C	3.67467000	2.29853200	-3.61876400	H	3.04120800	-3.03049600	6.82503500
H	3.69629700	3.37297700	-3.87020500	C	-0.52135100	2.70276300	3.10125200
H	3.08970500	1.78981100	-4.38345800	C	0.07476200	3.46215400	4.27364000
H	5.55957200	1.99627000	-4.63497700	H	0.21221900	4.51923000	4.01058900
H	5.11131000	0.68110800	-3.51850300	H	-0.59791900	3.42533600	5.14107800
H	5.38688600	1.13044900	-1.13158600	H	1.04731600	3.08208700	4.59719900
H	6.03179000	2.73334800	-0.69149600	C	-1.82537700	3.31883600	2.61295800
C	-1.18264400	4.85373000	-2.44472900	H	-2.57427800	3.34200800	3.41656200
C	-1.39421000	4.95815000	-3.94465300	H	-1.67136400	4.35321700	2.27578600
H	-2.44694700	4.77901500	-4.20050300	H	-2.24648100	2.74988600	1.77771700
H	-1.13704900	5.96553500	-4.29771300	H	-0.05573300	2.15919500	1.01950800
H	-0.79434100	4.24825600	-4.51984200	C	3.79257200	0.30909900	1.95958400
C	-1.99042600	5.88470900	-1.66943300	H	4.10859600	0.76449900	1.01351300
H	-1.71382800	6.90714100	-1.96062400	H	4.32176500	0.82862200	2.76468200
H	-3.06564300	5.76451800	-1.85716500	H	4.12489900	-0.72973700	1.95526900
H	-1.83078300	5.79083900	-0.58922800	C	2.94421900	-2.81904800	-2.32158700
H	-1.46760000	3.40931900	-0.78552000	C	4.14647600	-3.64510600	-1.70570900
C	0.73929200	1.08375900	-4.09794000	H	5.00227000	-3.57733900	-2.38706200
H	-0.14989400	0.51057600	-4.38461300	H	4.44364500	-3.09603300	-0.80755000
H	0.82022500	1.92750000	-4.79579900	C	3.89656300	-5.11082200	-1.36483800
H	1.60641500	0.43131700	-4.22713200	C	3.05438500	-5.90745000	-2.34889500
C	2.25539400	0.40037500	2.04433100	H	2.34690900	-6.61643700	-1.91855000
C	1.84965600	1.90330700	2.09710000	C	2.46948100	-5.08727000	-3.49151400
H	2.26199900	2.36043000	3.00600800	H	1.70934100	-5.67634700	-4.01732000
H	2.31755000	2.42945100	1.25779500	H	3.22516300	-4.82245100	-4.23975600
C	0.34305200	2.06517800	2.02736100	C	1.85442700	-3.81837700	-2.85154900
C	-0.43260700	1.18615500	2.99105200	H	1.36476700	-4.15905600	-1.93406200
H	-1.31705200	0.69435400	2.59502300	N	0.74538600	-3.15666300	-3.61437900
C	0.40649600	0.35290300	3.94833700	C	-0.52029100	-3.91046300	-3.45037300
H	-0.22716400	-0.41593700	4.40572700	H	-0.77136400	-3.96630000	-2.38820300

H -0.42507300 -4.94027300 -3.83727900
C -1.66202600 -3.22330900 -4.19252500
O -1.38979000 -3.10196000 -5.58006600
C -0.18844900 -2.36879600 -5.77404100
C 0.99713900 -3.02309600 -5.06743400
H 1.16258500 -4.01162700 -5.52583500
H 1.89045000 -2.42182700 -5.23802900
H -0.01025300 -2.34247200 -6.85356700
H -0.31806100 -1.33625000 -5.41677900
H -1.84770200 -2.22615600 -3.75526600
H -2.57821900 -3.81526000 -4.10239100
C 4.51646500 -6.25382400 -2.16487200
C 5.53919800 -5.99969900 -3.25830100
H 6.54359600 -5.88292800 -2.83065700
H 5.57313600 -6.85045300 -3.95112100
H 5.33129000 -5.10571400 -3.85151100
C 4.80138500 -7.53150300 -1.38795500
H 4.79221400 -8.40846600 -2.04873600
H 5.78772300 -7.48915600 -0.90690300
H 4.05488000 -7.70019300 -0.60294900
H 3.73249900 -5.32092700 -0.30988300
C 3.56625500 -1.93786300 -3.42640400
H 4.39469800 -1.37093300 -2.98618000
H 3.97385400 -2.51596100 -4.26631800
H 2.84361300 -1.21340600 -3.80972600

Table 34. Geometric coordinates and thermally corrected MP2 energies for (*S*)-**27a**

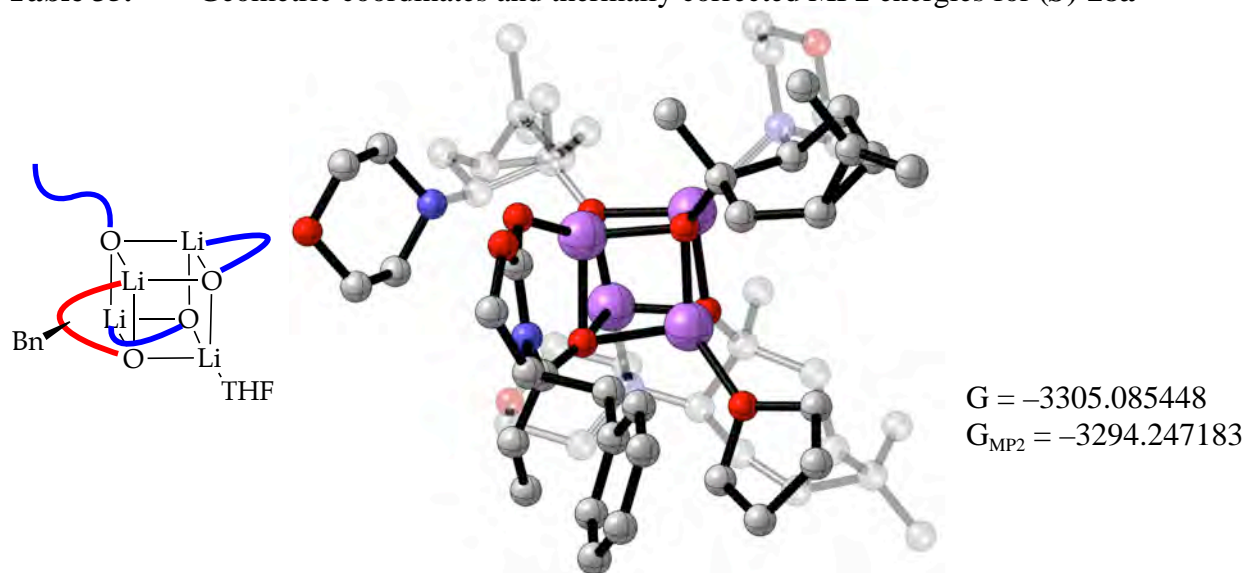


Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	C	9.03401000	-0.88300000	-1.92966000
O	1.09145100	-1.35475500	0.80530300	C	8.57502800	-0.42572000	-0.69406000
C	2.19166900	-1.58574500	0.31606600	C	7.20681400	-0.24928300	-0.47639900
O	3.22534400	-1.97612100	1.11196700	H	6.85778100	0.11820600	0.48640100
C	4.31870500	-2.39472200	0.27588600	H	9.28087100	-0.20189900	0.10147000
H	4.29528600	-3.48735300	0.19485600	H	10.09821500	-1.01916500	-2.10159500
H	5.25368100	-2.08549500	0.74562200	H	8.46612900	-1.51006100	-3.91432500
C	4.05144900	-1.70809500	-1.07094100	H	6.04406300	-1.19288600	-3.52500300
H	4.30648000	-2.37787700	-1.89372000	O	-1.89405100	0.03157000	-0.40043800
N	2.59652300	-1.51174500	-0.98352800	O	0.29695200	1.91768200	0.02619900
C	1.75737500	-1.10962200	-2.11893200	C	3.41016900	3.37194100	-2.00051300
C	2.13063200	-1.59333200	-3.33340000	H	2.82661500	4.19367800	-1.57600600
H	2.93722300	-2.31759000	-3.38182800	H	3.92711100	2.85445100	-1.18350600
C	1.46190600	-1.24896200	-4.63297100	C	4.38857200	3.81654500	-3.09221400
H	2.19207300	-0.95337700	-5.40088000	H	5.37468100	4.06331100	-2.68757800
H	0.90244100	-2.09766200	-5.05352600	H	4.00757600	4.69949100	-3.61730000
H	0.76087100	-0.42004200	-4.50685700	C	4.40360900	2.60256500	-4.03372600
O	0.76164000	-0.31120600	-1.84116000	H	4.71253500	2.85256800	-5.05322400
Li	0.70945900	1.79639200	-1.84787400	H	5.08221000	1.83003800	-3.65410000
Li	-1.52786500	1.91721100	-0.57123700	C	2.95082500	2.13028400	-3.96674000
O	-1.13851500	1.88841000	-2.52265000	H	2.82653400	1.05624500	-4.11659400
Li	-1.20687300	-0.10184000	-2.17694700	H	2.32021500	2.67217100	-4.68207900
C	4.78996200	-0.36251500	-1.25041300	O	2.50047000	2.43963100	-2.62664600
H	4.31934100	0.14661100	-2.09734800	C	0.54564100	2.50600100	1.27511600
H	4.60751600	0.25365300	-0.36141800	C	2.10914700	2.69021000	1.49642400
C	6.27515200	-0.52563700	-1.48616700	H	2.41124700	2.11193900	2.37832400
C	6.75157900	-0.98154200	-2.72543100	H	2.57047500	2.18438100	0.64340100
C	8.11710100	-1.15944400	-2.94658000	C	2.68149700	4.10434300	1.60066500

C	1.78939100	5.21240500	2.13363400	H	-1.79253700	4.19191900	-2.49643200
H	1.87993900	6.18180500	1.64348600	N	-0.50143500	4.69721000	-4.01561200
C	0.35610900	4.81412600	2.45092500	C	-0.16738800	5.84139400	-3.16177900
H	-0.25935500	5.71743500	2.53577500	H	-0.10772400	5.50285300	-2.12134800
H	0.28077500	4.30671600	3.41875600	H	-0.93256600	6.64158000	-3.21522400
C	-0.16654600	3.90199000	1.31624600	C	1.18255700	6.43591500	-3.55643900
H	0.14292600	4.37079600	0.37341400	O	1.22047800	6.81673900	-4.92380000
N	-1.65838300	3.81448100	1.21006300	C	0.90362800	5.70994600	-5.75681900
C	-2.20364100	5.00196100	0.52362400	C	-0.46798800	5.13215600	-5.41801900
H	-1.74446500	5.08226400	-0.46678500	H	-1.22119000	5.91210300	-5.63186000
H	-1.97698400	5.93234600	1.07578500	H	-0.67193700	4.28493400	-6.07672100
C	-3.71817500	4.89154200	0.36716600	H	0.91860800	6.08428900	-6.78535800
O	-4.36925200	4.75228600	1.61928500	H	1.67436300	4.92675100	-5.65595000
C	-3.87048900	3.60853200	2.30049800	H	1.97570000	5.69896600	-3.35039200
C	-2.36157700	3.69566600	2.50722400	H	1.38762800	7.34163500	-2.97646700
H	-2.16009000	4.56932700	3.14903600	C	-5.41572200	3.40237600	-3.81647800
H	-2.02139100	2.80654800	3.03740900	C	-5.68491400	3.20654500	-5.29861500
H	-4.38119800	3.57609200	3.26788200	H	-6.27083800	2.29370800	-5.46879400
H	-4.12283900	2.69465500	1.74069400	H	-6.26877600	4.04950600	-5.69054700
H	-3.96012600	4.03386600	-0.28194900	H	-4.77869300	3.13213600	-5.90478300
H	-4.11836100	5.79985500	-0.09458300	C	-6.69973700	3.56668300	-3.01480700
C	3.00056300	4.77504500	2.93230600	H	-7.27354900	4.43712500	-3.35965300
C	2.85475900	4.02097100	4.24163000	H	-7.34306000	2.68277400	-3.11750600
H	3.76808200	3.45259100	4.46146100	H	-6.49483000	3.70549400	-1.94721100
H	2.69415700	4.71915600	5.07354400	H	-4.50924800	2.33524200	-2.08900300
H	2.02459100	3.31026000	4.24304200	C	-0.96278600	1.94462500	-4.91933000
C	4.18066900	5.73575000	2.93630200	H	-1.01815600	0.84995200	-4.96165800
H	4.07932200	6.48596600	3.73196400	H	-1.38228100	2.32146800	-5.86095100
H	5.12527700	5.20102200	3.10347800	H	0.08959800	2.23247400	-4.86371500
H	4.26656600	6.27246400	1.98426000	C	-2.88410200	-0.89246000	-0.03544700
H	3.35184100	4.38504300	0.78989400	C	-4.02099700	-0.12246700	0.75210100
C	0.04821900	1.54550500	2.38389000	H	-3.76367000	-0.10544500	1.82026100
H	0.66271600	0.63789300	2.37517000	H	-3.91984800	0.91007700	0.40197600
H	0.12047900	1.97421400	3.39219400	C	-5.49703000	-0.48776600	0.54976000
H	-0.98661400	1.23997900	2.20341900	C	-5.87293200	-1.66446400	-0.33476600
C	-1.72954500	2.43901700	-3.67655500	H	-6.71349800	-1.50649400	-1.00985600
C	-3.20359100	1.91347300	-3.83444200	C	-4.72478800	-2.45175800	-0.95858700
H	-3.45294500	1.87576300	-4.90115300	H	-5.09494300	-2.95886900	-1.85629600
H	-3.20036200	0.87484500	-3.49169200	H	-4.37001800	-3.24594200	-0.29367100
C	-4.27590900	2.69347900	-3.09133000	C	-3.57201900	-1.48133300	-1.32027100
C	-4.22668200	4.19570500	-3.31113800	H	-4.04110200	-0.60590500	-1.79032400
H	-4.42658400	4.83315800	-2.45123300	N	-2.61969900	-1.96416500	-2.36759500
C	-3.04780700	4.65435800	-4.15478500	C	-3.27267300	-2.04276700	-3.69209800
H	-2.97661500	5.74857200	-4.12883200	H	-3.71905800	-1.07308500	-3.93391900
H	-3.17251100	4.38361000	-5.20941100	H	-4.07979000	-2.79487500	-3.70261500
C	-1.75124400	4.02168700	-3.57681600	C	-2.25489900	-2.42021700	-4.76435000

O -1.64252200 -3.67077700 -4.48839600
C -1.03438100 -3.66457900 -3.19910800
C -2.02404800 -3.29140400 -2.09993000
H -2.80639200 -4.06740500 -2.04500200
H -1.49826000 -3.27307800 -1.14656600
H -0.65957200 -4.67992400 -3.03519800
H -0.18039800 -2.97303600 -3.18020900
H -1.48914800 -1.63189100 -4.84794600
H -2.74914800 -2.52362200 -5.73572600
C -6.23369000 -1.67777300 1.14169300
C -5.57854800 -2.62098900 2.13269100
H -5.72882800 -2.25496700 3.15688200
H -6.02740700 -3.62179700 2.07520100
H -4.50438400 -2.72760400 1.98513000
C -7.70730000 -1.45096200 1.45478900
H -8.26405100 -2.39753000 1.43702200
H -7.83542300 -1.00927100 2.45197400
H -8.17650800 -0.77620500 0.72970000
H -6.12596300 0.39580700 0.44204500
C -2.21898900 -1.95042200 0.88296700
H -2.03374600 -1.50432900 1.86699900
H -2.80340300 -2.86224300 1.03760900
H -1.24361400 -2.24171500 0.48928300

Table 35. Geometric coordinates and thermally corrected MP2 energies for (*S*)-28a

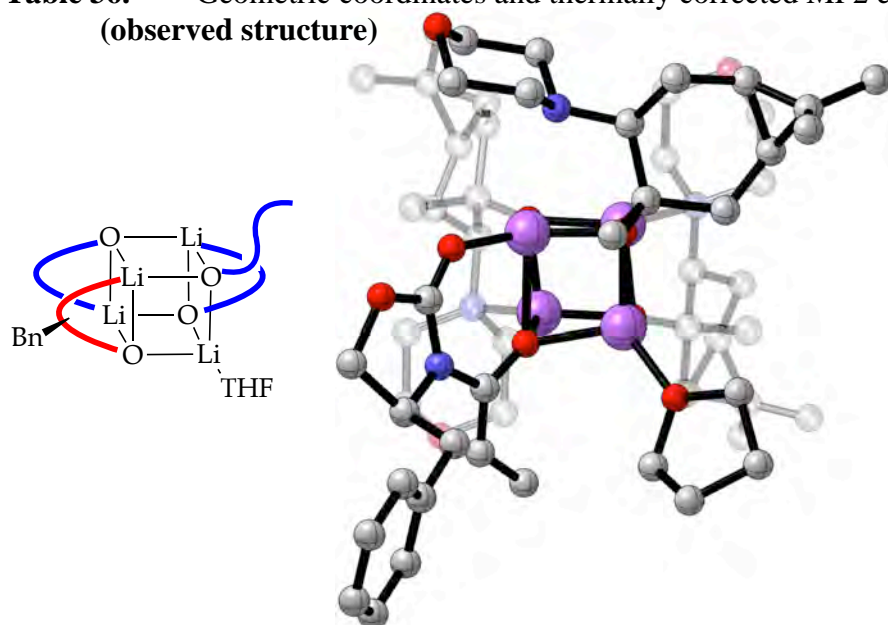


Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	C	6.44664800	-0.07159000	-3.36665200
O	1.00099200	-1.62585600	0.17943400	C	7.77909200	-0.17985800	-3.76397000
C	2.06786600	-1.66309800	-0.42048700	C	8.78859700	-0.30421600	-2.80629700
O	3.12431300	-2.35973500	0.08663900	C	8.45486800	-0.31757500	-1.45179800
C	4.15125700	-2.43569100	-0.91895800	C	7.11919300	-0.20928800	-1.05798500
H	4.07886500	-3.40998200	-1.41506400	H	6.86746100	-0.21053000	0.00043000
H	5.12283500	-2.34950500	-0.42937800	H	9.23335200	-0.40926500	-0.69892300
C	3.83962200	-1.27384600	-1.87558400	H	9.82717200	-0.38713800	-3.11483900
H	4.00061100	-1.58025800	-2.91079700	H	8.03045200	-0.16453400	-4.82133700
N	2.40833100	-1.08387500	-1.60451600	H	5.66589400	0.02805800	-4.11854400
C	1.52238200	-0.24959900	-2.43485000	O	-1.87082200	0.62227200	0.05688500
C	1.71175700	-0.37458600	-3.77491300	O	0.86067000	1.53702400	0.91842300
H	2.37579400	-1.15177500	-4.13837700	C	3.40375500	4.33304100	-1.02548500
C	0.99004700	0.44280200	-4.80465700	H	2.92662300	5.30459700	-1.22554100
H	1.60385300	0.58416500	-5.70379600	H	3.42809600	4.16598300	0.05253800
H	0.04729400	-0.01957800	-5.13910500	C	4.76285200	4.22652400	-1.72133400
H	0.74175800	1.43450700	-4.41207500	H	5.38394300	3.47844700	-1.21857500
O	0.69377800	0.53549800	-1.80497300	H	5.30744100	5.17536000	-1.71611000
Li	1.01128700	2.27356700	-0.83512200	C	4.38923800	3.75309500	-3.14993900
Li	-0.92670000	2.17823700	0.88065600	H	4.47717900	4.56310600	-3.88046600
O	-0.75847300	3.12930500	-0.86736700	H	5.04344100	2.94104500	-3.47956400
Li	-1.60397300	1.57819200	-1.52984900	C	2.91758600	3.28878400	-3.02225200
C	4.64549000	0.01275400	-1.58871400	H	2.73434000	2.27852800	-3.39179600
H	4.14833600	0.82782500	-2.12413500	H	2.23362600	3.98500400	-3.52631600
H	4.56786900	0.24049400	-0.51946700	O	2.62222700	3.28119600	-1.61080100
C	6.09575200	-0.08544200	-2.00717100	C	1.51362700	1.62554200	2.15245100

C	3.08478700	1.70939700	1.91292700	C	-2.04005400	5.31077100	-3.69938800
H	3.52496800	0.72493300	2.12234000	H	-2.37329600	5.06759800	-4.71460700
H	3.18491000	1.85482000	0.83377100	H	-2.89180500	5.79816600	-3.21318700
C	3.90729100	2.80826300	2.59602200	C	-1.63684700	4.02587800	-2.94093400
C	3.30562100	3.60422800	3.74180000	H	-0.66856700	3.71166200	-3.35123100
H	3.51597300	4.67352900	3.74648800	N	-2.52783300	2.83939800	-3.18028100
C	1.87866100	3.25349300	4.14164200	C	-2.24357000	2.24263200	-4.50616800
H	1.44396400	4.10167400	4.68345100	H	-1.18616700	1.98124200	-4.55695600
H	1.85443000	2.40859600	4.83796000	H	-2.45777100	2.95811500	-5.31878700
C	1.05132100	2.94020100	2.87326700	C	-3.08719700	0.99270500	-4.73370600
H	1.28252300	3.73096600	2.14739400	O	-4.47509800	1.27995200	-4.65866800
N	-0.43745200	3.03651700	3.04751600	C	-4.78669100	1.86168000	-3.40043200
C	-0.87180100	4.45033700	3.03004700	C	-3.98041000	3.13296400	-3.14742900
H	-0.57168000	4.89899400	2.07636400	H	-4.24954100	3.87128400	-3.91975800
H	-0.39432900	5.03035300	3.83954500	H	-4.25904600	3.54514600	-2.17798300
C	-2.38751900	4.55968000	3.19179900	H	-5.85595900	2.09504000	-3.42231900
O	-2.83481800	3.95568100	4.39486200	H	-4.60627500	1.13709700	-2.59266600
C	-2.45543100	2.58597400	4.41319300	H	-2.81928500	0.21867000	-3.99449900
C	-0.94235900	2.42880300	4.30052800	H	-2.90299600	0.58874500	-5.73383400
H	-0.49011700	2.90921200	5.18330400	C	-0.70221900	7.54262100	-3.01901000
H	-0.68497200	1.37024700	4.32752400	C	-1.84994000	8.10637700	-2.20171600
H	-2.80471300	2.17846900	5.36690600	H	-1.47084300	8.79866900	-1.43856900
H	-2.95851700	2.04398600	3.59653000	H	-2.54218000	8.67037000	-2.84059000
H	-2.89165500	4.09061200	2.33138200	H	-2.42908600	7.33967100	-1.68285100
H	-2.68782200	5.61149100	3.23580200	C	0.12737600	8.62762500	-3.69058400
C	4.50692700	2.71184900	3.99127400	H	-0.48633800	9.23045800	-4.37308900
C	4.40117400	1.43472500	4.80349800	H	0.56352200	9.30857400	-2.94769700
H	5.24092500	0.76653600	4.57154300	H	0.95128300	8.20156700	-4.27472200
H	4.44355900	1.65175000	5.87912500	H	1.12490500	6.34524400	-2.75268300
H	3.48398400	0.87483600	4.61304200	C	-2.59847800	4.63492400	-0.60906400
C	5.83351900	3.42836500	4.20239800	H	-2.29476200	4.98598500	0.38148000
H	5.97109500	3.70312200	5.25677100	H	-3.21454200	5.42419900	-1.05620500
H	6.67865000	2.78892900	3.91412800	H	-3.22247400	3.74870700	-0.46098600
H	5.89512500	4.34827000	3.60943500	C	-2.87088100	-0.22237200	0.58494500
H	4.52359000	3.38015000	1.90209200	C	-4.10064200	0.63389300	1.09210800
C	1.21006700	0.34211400	2.96034600	H	-4.40734100	0.25995500	2.07609000
H	1.67076000	-0.51305500	2.45720200	H	-3.71403200	1.64329800	1.26927600
H	1.57885800	0.36614600	3.99274900	C	-5.32661800	0.71813100	0.18902100
H	0.13611700	0.14697200	2.98348100	C	-5.73484000	-0.56101000	-0.52346900
C	-1.33114900	4.28234300	-1.42425300	H	-6.08845000	-0.45900700	-1.54945000
C	-0.30797400	5.49291600	-1.30794300	C	-4.78962600	-1.73534100	-0.31715300
H	-0.64527500	6.16776200	-0.50939300	H	-5.02266000	-2.52608400	-1.03960100
H	0.61022800	5.03151100	-0.93916100	H	-4.90496100	-2.18568100	0.67557500
C	0.05412600	6.30653500	-2.55354600	C	-3.33603200	-1.23682700	-0.52540900
C	-0.83611300	6.23924800	-3.78307100	H	-3.36274500	-0.62660300	-1.43666400
H	-0.32400500	6.21212200	-4.74463100	N	-2.34189200	-2.29563000	-0.80460500

C -2.16195500 -2.55805000 -2.23397600
H -1.94033200 -1.61415600 -2.74472800
H -3.07137700 -2.99190400 -2.69838400
C -0.99177000 -3.51488500 -2.45993900
O -1.16286200 -4.73486700 -1.75027300
C -1.32241000 -4.47717000 -0.35886800
C -2.52494500 -3.57075400 -0.10301700
H -3.43310000 -4.10605400 -0.43927000
H -2.61969900 -3.39792400 0.97158000
H -1.46969500 -5.45162300 0.11843900
H -0.41426100 -4.00818800 0.04858900
H -0.05772000 -3.02260900 -2.15092600
H -0.91651000 -3.78035100 -3.51970900
C -6.64429500 0.02993700 0.53466300
C -6.86019800 -0.65155700 1.87425400
H -7.14407200 0.08193000 2.64042800
H -7.67476300 -1.38387100 1.80146100
H -5.97839300 -1.18304200 2.24079700
C -7.90359800 0.71225000 0.01971200
H -8.71900300 -0.01048700 -0.11672700
H -8.25332900 1.47937000 0.72343700
H -7.73009600 1.20151000 -0.94581500
H -5.43081300 1.64789400 -0.36920100
C -2.30392100 -0.95150200 1.82044600
H -2.04087900 -0.20773300 2.58179300
H -3.03003700 -1.63762500 2.27562500
H -1.40325500 -1.51600800 1.56503700

Table 36. Geometric coordinates and thermally corrected MP2 energies for (*S*)-**16a** (observed structure)



$G = -3305.095693$
 $G_{\text{MP2}} = -3294.259925$

Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	C	7.19467600	-2.67365100	-1.78290100
O	1.72217900	0.11054000	0.87466200	C	8.54694200	-3.01388200	-1.78920200
C	2.77220000	-0.48694900	0.69128600	C	9.50448800	-2.09038500	-1.36295000
O	3.85906800	-0.18151600	1.45805700	C	9.09850400	-0.82643000	-0.93439100
C	4.88427900	-1.15996700	1.22359300	C	7.74293200	-0.49045800	-0.92843300
H	4.83385400	-1.91562500	2.01595200	H	7.43615800	0.50153700	-0.60355800
H	5.85493200	-0.66305100	1.25829300	H	9.83589100	-0.09798700	-0.60750700
C	4.54185900	-1.74112100	-0.15335700	H	10.5587540	-2.35334700	-1.36996300
H	4.72845700	-2.81695400	-0.16572600	H	8.85416800	-3.99839200	-2.13222600
N	3.09571900	-1.47182100	-0.20384600	H	6.45741000	-3.39584200	-2.12829700
C	2.19030800	-2.07603900	-1.18038800	O	-1.48912200	-1.21820600	0.36118200
C	2.66073100	-3.13889700	-1.89497400	O	-0.77352300	0.92154300	-1.52941000
H	3.65285200	-3.52643000	-1.69597000	C	0.90168700	0.98570500	-5.37043300
C	1.86942300	-3.85192700	-2.95599600	H	-0.11580200	0.94963600	-5.77202600
H	2.41740300	-3.90297700	-3.90856800	H	1.03916100	1.94206600	-4.85763500
H	1.64262900	-4.89250000	-2.68075300	C	1.97748700	0.74803800	-6.44073100
H	0.91862700	-3.34546300	-3.14881100	H	2.36690000	1.68576300	-6.84803000
O	1.01339300	-1.52790000	-1.27088500	H	1.57185900	0.16226900	-7.27386500
Li	-0.03074300	-0.49235100	-2.65005200	C	3.03022500	-0.07288500	-5.67991800
Li	-2.20239400	-0.36307500	-1.25622700	H	3.67245500	-0.66778100	-6.33649900
O	-1.57511700	-1.70445900	-2.54678400	H	3.66866900	0.58134900	-5.07420300
Li	-0.74518400	-2.40967800	-0.95850200	C	2.14789400	-0.93398900	-4.78246700
C	5.29852100	-1.06075700	-1.32004900	H	2.63044200	-1.29244800	-3.87139100
H	4.81333800	-1.37337800	-2.25035900	H	1.74744800	-1.79598500	-5.33341300
H	5.16390200	0.02419300	-1.23071900	O	1.05753000	-0.07045700	-4.39015000
C	6.77090800	-1.40772300	-1.34995900	C	-2.55242600	-1.91286400	-3.52736100

C	-2.29149700	-3.29182600	-4.27557400	C	-1.49017800	4.51777900	-0.65725500
H	-1.96741000	-3.08106900	-5.30330000	H	-1.84002000	5.01075700	0.25720300
H	-1.41706800	-3.71491500	-3.77561700	H	-0.57394800	5.04161000	-0.95356100
C	-3.38819500	-4.36009600	-4.29452300	C	-1.19973000	3.01914300	-0.38714300
C	-4.83354600	-3.94843200	-4.06773700	H	-2.17942800	2.52812400	-0.33904200
H	-5.43533800	-4.62305400	-3.45910900	N	-0.57260400	2.72545000	0.92611300
C	-5.07670800	-2.47394400	-3.77675900	C	-1.57393800	2.64486700	1.99964400
H	-6.05986200	-2.35953700	-3.30586000	H	-2.32250600	1.89252400	1.72992300
H	-5.11175500	-1.87954400	-4.69624800	H	-2.09893500	3.60892600	2.14777000
C	-3.96193200	-1.95978300	-2.83789800	C	-0.92174500	2.24303900	3.32179900
H	-3.83977600	-2.72014900	-2.05702200	O	0.11158700	3.14125700	3.69640100
N	-4.29864000	-0.71295100	-2.07202100	C	1.09669200	3.20229900	2.66934600
C	-5.15468400	-1.03575600	-0.90812600	C	0.48263200	3.66200800	1.34933100
H	-4.62490400	-1.74724300	-0.26765800	H	0.08709900	4.68329800	1.49675800
H	-6.10438800	-1.50241000	-1.22449800	H	1.26393200	3.71351100	0.58978600
C	-5.47893200	0.21821800	-0.09936400	H	1.84918200	3.92187000	3.00835100
O	-6.12074800	1.20629100	-0.88994200	H	1.57204900	2.21965500	2.53565600
C	-5.29510600	1.54771800	-1.99405900	H	-0.51846200	1.22166800	3.23672900
C	-4.99432300	0.32874900	-2.86158800	H	-1.66093000	2.26119700	4.12964700
H	-5.95071200	-0.04648900	-3.26048300	C	-2.37946400	5.22616200	-3.09822600
H	-4.37520600	0.63048300	-3.70672300	C	-1.13565000	6.02261500	-3.45015000
H	-5.84413700	2.29578300	-2.57477600	H	-0.97022000	6.02231900	-4.53587200
H	-4.35651300	2.00133700	-1.63917600	H	-1.25023200	7.06826200	-3.13594400
H	-4.55409900	0.63100000	0.33658200	H	-0.22568200	5.63995900	-2.98098900
H	-6.16540400	-0.02659700	0.71684600	C	-3.63450900	5.78951100	-3.74934800
C	-4.41014600	-4.49904800	-5.41510600	H	-3.81335800	6.82634100	-3.43458400
C	-4.33928900	-3.61179900	-6.64441800	H	-3.54831700	5.78537900	-4.84430600
H	-3.67181800	-4.05279700	-7.39639200	H	-4.52310000	5.20514300	-3.48383100
H	-5.33008300	-3.50735200	-7.10589400	H	-3.21028300	3.18914500	-3.32631900
H	-3.96596900	-2.60765600	-6.43069900	C	1.03178100	2.49638800	-1.61220700
C	-4.87234600	-5.91258900	-5.73743200	H	1.43804200	2.00954200	-2.50742300
H	-5.87216200	-5.90869800	-6.19196300	H	1.32833900	3.55355900	-1.64632200
H	-4.18814900	-6.40007100	-6.44458200	H	1.49592500	2.02670900	-0.74170100
H	-4.91987200	-6.53699100	-4.83784100	C	-1.73223600	-1.90949300	1.55895000
H	-3.09116000	-5.30762100	-3.84682000	C	-2.82455300	-1.13328900	2.41246100
C	-2.43524100	-0.78408400	-4.57986100	H	-2.32774800	-0.63279000	3.25349900
H	-1.47472400	-0.89299200	-5.09539100	H	-3.16228000	-0.33107600	1.75272600
H	-3.22573200	-0.80409200	-5.34067900	C	-4.07086900	-1.87128200	2.91113300
H	-2.43555000	0.19735800	-4.09797900	C	-4.07727300	-3.38939200	2.96234400
C	-0.50295700	2.30043200	-1.59920200	H	-5.00357700	-3.87676700	2.65888400
C	-1.03956900	2.91092200	-2.96107400	C	-2.82004600	-4.08911700	2.46582600
H	-0.24999800	3.53340500	-3.39969200	H	-3.06605000	-5.12678000	2.21149400
H	-1.15912300	2.06189000	-3.63904100	H	-2.05398400	-4.14379800	3.24630300
C	-2.33892500	3.70906000	-2.93181000	C	-2.27761600	-3.34313900	1.22477800
C	-2.56635000	4.60711900	-1.72842800	H	-3.14117700	-3.15186800	0.57590200
H	-3.58098600	4.64448700	-1.33123200	N	-1.34867300	-4.14586200	0.36065200

C -2.10709500 -5.07230000 -0.50893700
H -2.81215400 -4.49468100 -1.11539700
H -2.68697400 -5.79879900 0.08734000
C -1.16312500 -5.83587900 -1.43462600
O -0.18075900 -6.56564400 -0.71448500
C 0.55585700 -5.70220000 0.14569200
C -0.36297600 -4.95978300 1.10907800
H -0.87100000 -5.70266100 1.74460600
H 0.23619000 -4.31865400 1.75507000
H 1.24537300 -6.34302700 0.70449200
H 1.14575000 -4.98153600 -0.44053900
H -0.67726500 -5.13290200 -2.12820000
H -1.72406900 -6.56861200 -2.02329500
C -4.16145800 -2.59037600 4.24901500
C -3.00989700 -2.54722600 5.23619400
H -3.08126200 -1.65130600 5.86665800
H -3.03602200 -3.41961800 5.90251100
H -2.02887400 -2.52562400 4.75714500
C -5.52072100 -2.56957900 4.93379200
H -5.64014500 -3.43168500 5.60360800
H -5.64485400 -1.66069700 5.53730200
H -6.33974000 -2.59895200 4.20576400
H -5.00609600 -1.40774700 2.59880700
C -0.41668600 -1.94961800 2.37226700
H -0.15218500 -0.93276400 2.67868200
H -0.47515300 -2.56410600 3.27924600
H 0.40772400 -2.31448300 1.75447200

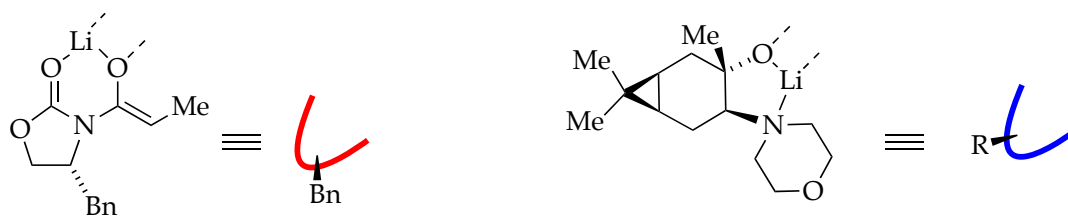
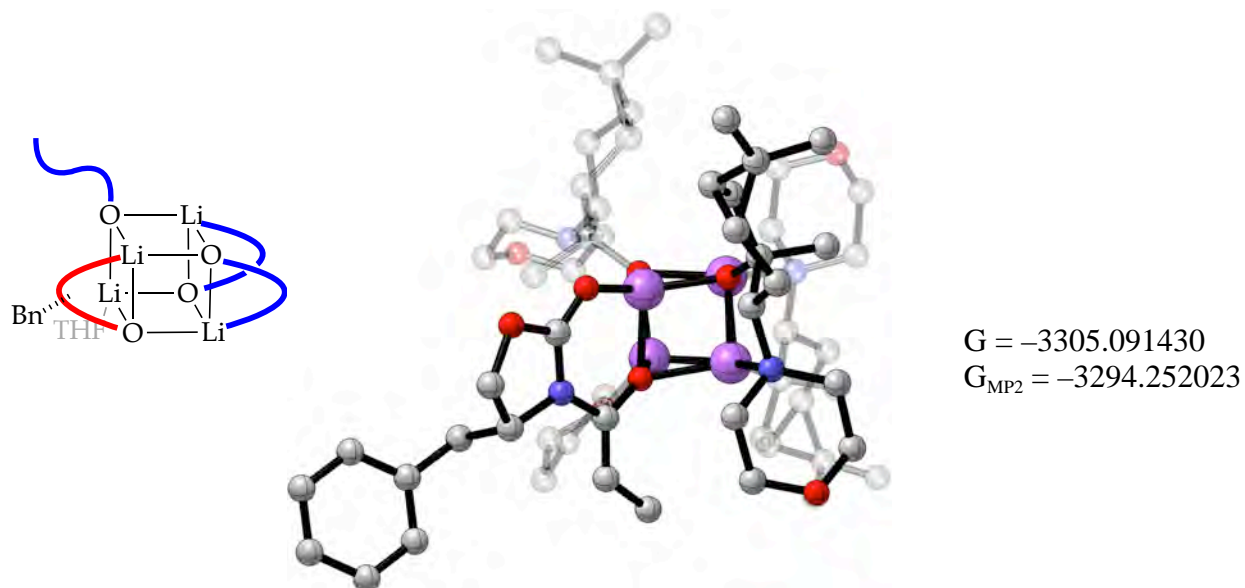


Table 37. Geometric coordinates and thermally corrected MP2 energies for (*R*)-**32a**

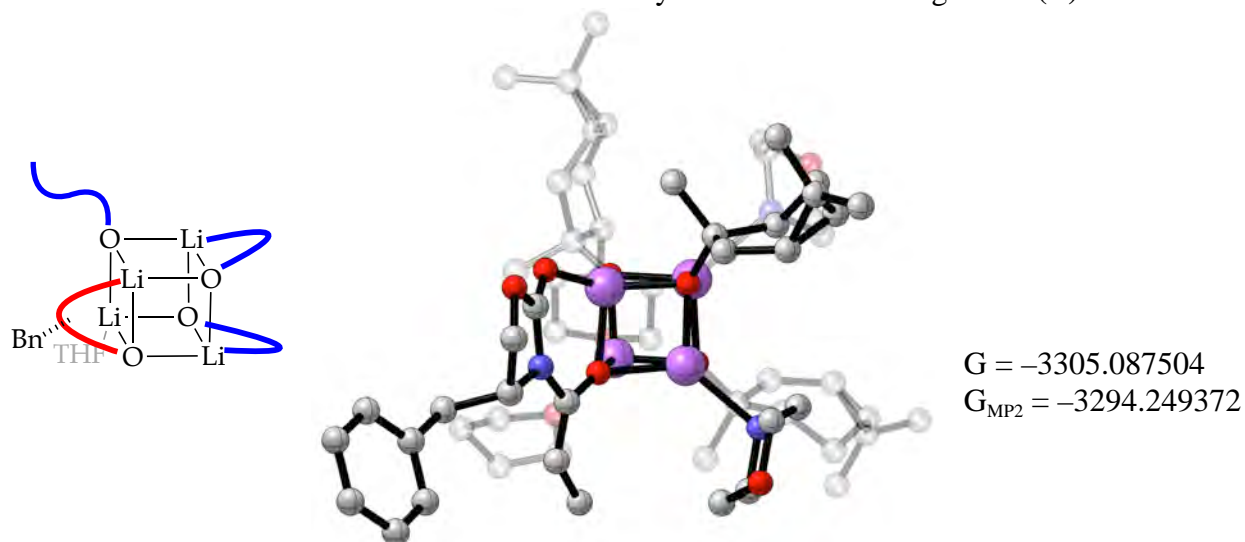


Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	O	-2.06836000	-0.78871800	-2.41497100
O	1.79702000	0.22524500	0.64372500	Li	-1.05906700	-1.97794600	-1.27278000
C	2.78695900	-0.31514300	0.16650200	O	-1.50807100	-1.20499500	0.46905100
O	3.98855900	-0.19254800	0.79417300	O	-1.00434400	1.39549100	-0.82496900
C	5.01789600	-0.71840300	-0.06102400	C	0.20709300	-4.79885000	-1.51863600
H	5.76354500	-1.21712800	0.55955600	H	1.03046500	-4.28246400	-2.01422600
H	5.48669900	0.11584800	-0.59514500	H	0.46399000	-4.95338000	-0.45974400
N	2.92284300	-1.08333700	-0.96009100	C	-0.23643600	-6.10409000	-2.17561600
C	1.86625300	-1.38870600	-1.92415000	H	0.37827900	-6.95856400	-1.87638500
C	2.21191800	-2.07316700	-3.04926900	H	-0.18056400	-6.00782400	-3.26526700
H	3.24452200	-2.35893600	-3.21242900	C	-1.70617900	-6.22781200	-1.71079100
C	1.23352400	-2.44969100	-4.12741400	H	-2.34711500	-6.64754700	-2.49145900
H	0.22481600	-2.10161500	-3.88895200	H	-1.78684500	-6.88018700	-0.83500900
H	1.51423600	-2.02578300	-5.10260500	C	-2.10688500	-4.77741700	-1.34328400
H	1.17762000	-3.53914900	-4.27620500	H	-2.36200700	-4.67320600	-0.28339300
O	0.67794200	-0.95452900	-1.60687900	H	-2.92635800	-4.38501100	-1.95017400
Li	-0.57229400	0.43486900	-2.42873300	O	-0.94994000	-3.95409800	-1.61859400
Li	-2.44866700	0.10425500	-0.70462500	C	-0.67951800	2.75793000	-0.88093100

C	-0.41280900	3.29757200	0.58905100	C	-3.12935600	-1.74445400	3.72895100
H	-1.29807900	3.85216400	0.92956300	H	-4.10044400	-2.15739900	4.02992600
H	-0.37340700	2.39802400	1.20768200	H	-2.41142900	-2.08880300	4.48046900
C	0.85851500	4.09646500	0.89131200	C	-2.74255000	-2.28232000	2.32070700
C	1.68261100	4.66555300	-0.24982100	H	-3.45777300	-1.84306600	1.62087300
H	2.76409000	4.59551400	-0.13750400	N	-2.94120500	-3.75463700	2.18422500
C	1.19138700	4.37294600	-1.66163200	C	-4.34147200	-4.09807400	1.90498800
H	2.02970300	4.48705400	-2.35895600	H	-4.66542000	-3.56786500	1.00188900
H	0.43373300	5.09549600	-1.98455600	H	-5.01817400	-3.79951700	2.72883000
C	0.63584100	2.93104400	-1.71640900	C	-4.50452500	-5.60154500	1.67512700
H	1.36015700	2.29887600	-1.18932600	O	-4.01664300	-6.36428500	2.76809100
N	0.56051200	2.32434100	-3.08982700	C	-2.65492700	-6.04716200	3.02327900
C	1.90158900	1.86528600	-3.51968300	C	-2.48155700	-4.56118900	3.32419900
H	2.27663200	1.14080000	-2.79179300	H	-3.04823000	-4.33985000	4.24600100
H	2.61595500	2.70572500	-3.56699300	H	-1.42795600	-4.35336100	3.52483100
C	1.83624700	1.20856100	-4.89484300	H	-2.35422700	-6.65078700	3.88543500
O	1.32424900	2.09995900	-5.87638900	H	-2.03020100	-6.33174400	2.15924800
C	0.02952400	2.54199000	-5.49874600	H	-3.98112700	-5.89789300	0.75087600
C	0.04552100	3.23449800	-4.13798500	H	-5.56401700	-5.85557700	1.56723700
H	0.67511600	4.13459000	-4.22399100	C	-2.35843500	0.70390700	4.54712100
H	-0.96535700	3.55732800	-3.88630600	C	-1.55507200	0.21000200	5.73844700
H	-0.30004900	3.24305300	-6.27200100	H	-0.72173700	0.89271800	5.94974700
H	-0.66941200	1.68943500	-5.48199400	H	-2.18787600	0.17482000	6.63510600
H	1.21310300	0.30183300	-4.84799300	H	-1.13119900	-0.78783400	5.60145100
H	2.83843400	0.91885000	-5.22478100	C	-2.96428700	2.07862200	4.79545000
C	0.99336100	5.60205600	0.72623400	H	-3.64030000	2.06355600	5.66095800
C	-0.19142400	6.45444500	0.31171100	H	-2.18213100	2.82244000	4.99683000
H	-0.76937900	6.75822200	1.19447700	H	-3.53934000	2.42865500	3.93045700
H	0.14377700	7.37153100	-0.19113300	H	-2.08724200	1.23996300	2.40464200
H	-0.87965000	5.93946400	-0.36116900	C	-0.23754900	-2.78379500	1.75785700
C	1.90024300	6.30883500	1.72367400	H	-0.55297400	-3.64796400	1.16867300
H	2.30320400	7.24047200	1.30362900	H	0.65782800	-2.35278800	1.29551500
H	1.35285500	6.56775600	2.63985600	H	0.04837600	-3.12984600	2.75891100
H	2.74965500	5.67912100	2.01209400	C	-3.16461000	-0.89593100	-3.27891400
H	1.43224400	3.68681300	1.72097200	C	-2.98060300	-2.17728200	-4.20178900
C	-1.88758400	3.51333500	-1.48113000	H	-2.59736500	-1.85724800	-5.18045800
H	-2.71434000	3.47956800	-0.76392700	H	-2.16330800	-2.73048300	-3.73288300
H	-1.69275200	4.56781100	-1.70854400	C	-4.13826700	-3.16425200	-4.38752300
H	-2.23188600	3.02138000	-2.39498800	C	-5.54022400	-2.78127000	-3.94278300
C	-1.34709100	-1.71130700	1.77996500	H	-6.11857600	-3.56173100	-3.44881000
C	-0.86479700	-0.57586400	2.74540400	C	-5.70526200	-1.40192400	-3.31729100
H	-0.46657800	-1.03930300	3.65524700	H	-6.61966100	-1.39425900	-2.71298700
H	-0.00639800	-0.06738900	2.29260500	H	-5.84574000	-0.62883500	-4.08047700
C	-1.95268500	0.41966000	3.10715500	C	-4.47386900	-1.08338800	-2.43720200
C	-3.19715700	-0.22689200	3.68929800	H	-4.27105100	-1.98556200	-1.84509000
H	-4.16383400	0.16901700	3.38182500	N	-4.69146600	-0.02252100	-1.40040400

C -5.46478200 -0.56823800 -0.26437900
H -4.92293900 -1.42546100 0.14576300
H -6.46262400 -0.91800500 -0.58279000
C -5.64986800 0.48421300 0.82447200
O -6.32179500 1.63273600 0.33011200
C -5.58644100 2.19045900 -0.74881100
C -5.40171600 1.18406100 -1.88198900
H -6.40042600 0.92883300 -2.27296600
H -4.83616800 1.65214800 -2.68751900
H -6.15648700 3.05470800 -1.10342700
H -4.60516600 2.54072100 -0.39205100
H -4.66858700 0.76928800 1.23715400
H -6.26465500 0.08494300 1.63712700
C -5.25342600 -3.02665000 -5.41265600
C -5.25244700 -1.89835900 -6.42700900
H -4.70621900 -2.20118400 -7.32983900
H -6.27643900 -1.64594900 -6.73292900
H -4.78063700 -0.98647900 -6.05757500
C -5.79950800 -4.32611600 -5.98777500
H -6.83201400 -4.20007700 -6.34019700
H -5.19655800 -4.66361000 -6.84124600
H -5.79951700 -5.12974500 -5.24230700
H -3.85153400 -4.19831500 -4.19624900
C -3.18725400 0.36669200 -4.17405000
H -2.33299700 0.32569500 -4.86009400
H -4.08974600 0.47851000 -4.78556200
H -3.07304000 1.26767100 -3.56517100
C 4.27281600 -1.66797100 -1.00728300
H 4.68169800 -1.59421600 -2.01729300
C 4.28103400 -3.14370400 -0.53909700
H 3.92927100 -3.17592400 0.49936800
H 3.54827200 -3.68600700 -1.14543600
C 5.64443800 -3.79037900 -0.65135000
C 6.43564100 -4.01435200 0.48343300
C 6.15643900 -4.16305500 -1.90367200
C 7.70342300 -4.58964500 0.37321300
H 6.04928900 -3.74718900 1.46482100
C 7.42239900 -4.73657200 -2.01849500
H 5.55221700 -4.01220500 -2.79617400
C 8.20145200 -4.95046100 -0.87891300
H 8.29836600 -4.75886300 1.26682000
H 7.79888700 -5.02204800 -2.99727300
H 9.18678100 -5.39990100 -0.96709400

Table 38. Geometric coordinates and thermally corrected MP2 energies for (*R*)-**33a**



Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	C	-1.39446700	5.76044600	1.05776600
O	0.92135300	-0.05933100	-1.75380800	H	-1.78931700	6.54107600	0.40783900
Li	-0.27643200	1.51835200	-2.06977600	C	-2.42497300	4.71615600	1.46262200
Li	-2.28647400	0.75590200	-0.68374300	H	-3.42875500	5.14284500	1.35156500
O	-1.90924900	0.61340700	-2.62061600	H	-2.32953000	4.44222100	2.51883100
Li	-1.07332200	-1.06781700	-2.13617000	C	-2.25907900	3.47160900	0.55993400
O	-1.61183500	-1.03654200	-0.26541600	H	-2.15710900	3.84542800	-0.46589900
O	-0.72280600	1.79718400	-0.23693000	N	-3.45490500	2.56623300	0.49528100
C	0.80835900	-3.38804400	-2.90073100	C	-4.46542600	3.10772300	-0.43857100
H	1.66289100	-3.01112700	-3.47531500	H	-4.01443600	3.21439700	-1.43029200
H	0.98780400	-3.20409000	-1.84174100	H	-4.81661200	4.10540900	-0.11897400
C	0.48186200	-4.83687600	-3.25349100	C	-5.67566000	2.18143900	-0.53671400
H	-0.12917300	-5.28377900	-2.46222100	O	-6.27948400	1.96168200	0.72716800
H	1.37811100	-5.45169900	-3.38099700	C	-5.32584500	1.42207000	1.63204000
C	-0.33246000	-4.68696700	-4.55679900	C	-4.12760600	2.35121300	1.79583400
H	0.31150000	-4.79978700	-5.43496600	H	-4.49288300	3.30214600	2.21654100
H	-1.12791400	-5.43364600	-4.63497600	H	-3.42692400	1.91809900	2.50931300
C	-0.89493900	-3.24663000	-4.48138600	H	-5.84153300	1.29731800	2.58940400
H	-1.98494000	-3.21074300	-4.41840800	H	-4.99106600	0.43232800	1.28396000
H	-0.57186800	-2.64239700	-5.33796700	H	-5.37337000	1.21704600	-0.97935600
O	-0.38239600	-2.66301000	-3.26706000	H	-6.44239200	2.62832000	-1.17715000
C	-0.91235900	2.70871100	0.80901200	C	-0.20825000	6.16991900	1.90837100
C	0.28984800	3.74823500	0.84594700	C	-0.03568900	5.65941800	3.32710500
H	0.88534000	3.56707300	1.74993000	H	1.01676300	5.72714000	3.63200700
H	0.93156200	3.45416300	0.01111300	H	-0.62113300	6.26508900	4.03135700
C	-0.00653700	5.24433900	0.71606600	H	-0.34023900	4.61791700	3.45393200

C	0.27143000	7.60438600	1.73915600	H	-1.21790100	-3.56221100	-0.98774800
H	-0.28594300	8.28814200	2.39337800	H	-0.06998300	-3.12400800	0.30203600
H	1.33599500	7.69758100	1.99209600	H	-1.36712000	-4.27930100	0.63474800
H	0.14314600	7.95366000	0.70803900	C	-2.38272700	1.13851100	-3.83170400
H	0.47695400	5.72102500	-0.13578400	C	-3.96739200	1.02423900	-3.86585800
C	-0.89850400	1.93213200	2.14598900	H	-4.24601900	0.13412300	-4.44646600
H	0.09856200	1.50462600	2.29784200	H	-4.23861000	0.79487500	-2.83207500
H	-1.12928500	2.55510500	3.01967800	C	-4.81950400	2.22374800	-4.29478000
H	-1.60529100	1.09978200	2.11614400	C	-4.16177300	3.42170300	-4.95939500
C	-1.99671800	-2.16488000	0.48974100	H	-4.52185400	4.40158700	-4.64712300
C	-1.73347400	-1.94041600	2.03245400	C	-2.65210100	3.35380900	-5.15341300
H	-1.33171700	-2.86961900	2.45171700	H	-2.26306400	4.37242700	-5.26306600
H	-0.91688600	-1.21667900	2.11347800	H	-2.38747800	2.83144700	-6.07903100
C	-2.91264800	-1.48549800	2.88363700	C	-2.00713600	2.66104300	-3.93053600
C	-4.24105900	-2.16927400	2.60977100	H	-2.47304800	3.10362900	-3.04119200
H	-5.13461100	-1.54653000	2.64330100	N	-0.54602100	2.94453000	-3.73427900
C	-4.21952500	-3.14462100	1.44356800	C	-0.34539900	4.29708700	-3.16534600
H	-5.24627500	-3.42443200	1.17890100	H	-0.88963900	4.36745900	-2.21875600
H	-3.70548300	-4.07760200	1.70294400	H	-0.73272500	5.07927600	-3.84110600
C	-3.52581100	-2.45463200	0.24017400	C	1.13652600	4.56790400	-2.91289600
H	-3.96606300	-1.45271500	0.17705400	O	1.90627000	4.44233400	-4.09770200
N	-3.80993800	-3.07798300	-1.07891300	C	1.74296000	3.13984200	-4.64419000
C	-4.97923800	-2.48959300	-1.73823200	C	0.27751900	2.85091100	-4.96102900
H	-4.84322000	-1.40487700	-1.80155200	H	-0.05796300	3.57799900	-5.71865400
H	-5.91696900	-2.68368900	-1.17952000	H	0.19119400	1.85359600	-5.39107000
C	-5.13130500	-3.04559500	-3.15188000	H	2.33685800	3.11243200	-5.56319900
O	-5.23023500	-4.46353500	-3.15741800	H	2.13960800	2.38341900	-3.94783600
C	-4.10569000	-5.04673400	-2.51514600	H	1.51691000	3.87676500	-2.14196300
C	-3.94926800	-4.53865200	-1.08354900	H	1.27543200	5.59272100	-2.55515500
H	-4.83191000	-4.87762400	-0.51078800	C	-5.16674100	2.58581900	-5.73038200
H	-3.06567800	-4.99919000	-0.63452400	C	-4.75187600	1.69767800	-6.88820500
H	-4.27517500	-6.12844400	-2.52058700	H	-5.52060500	0.93684400	-7.07634500
H	-3.18815800	-4.83177700	-3.08861300	H	-4.63919200	2.28400000	-7.80979400
H	-4.27037200	-2.72455800	-3.76285100	H	-3.81367300	1.16919300	-6.71251300
H	-6.04804400	-2.67001700	-3.61746000	C	-6.53117900	3.22577900	-5.94775100
C	-3.54945000	-2.38216200	3.94158900	H	-6.53757700	3.84416600	-6.85526300
C	-2.94706300	-3.72203600	4.32772900	H	-7.31228800	2.46245200	-6.06090100
H	-2.13199900	-3.58629600	5.05063100	H	-6.81428800	3.86877800	-5.10644200
H	-3.70662500	-4.35696100	4.80247300	H	-5.61238400	2.45812700	-3.58538500
H	-2.54138200	-4.28046400	3.48039000	C	-1.79995700	0.28808000	-4.98418800
C	-4.17197000	-1.66456400	5.13090100	H	-2.26057900	-0.70537000	-4.95393800
H	-4.97909600	-2.26149700	5.57629100	H	-1.97241400	0.69955100	-5.98498300
H	-3.42519200	-1.47785500	5.91403500	H	-0.72554300	0.15048800	-4.85215200
H	-4.59692600	-0.69647200	4.84093500	C	4.51976600	0.22884100	-0.83826900
H	-2.94399500	-0.42133700	3.11074400	H	4.79692200	0.87955800	-1.67039500
C	-1.11741300	-3.36418200	0.08127500	C	4.74909700	0.91368500	0.51117000

H 4.65568600 2.00372600 0.44730400
H 5.69706000 0.65138800 0.98241600
O 3.67768000 0.40599200 1.33003900
C 2.65329800 0.02710200 0.51529800
N 3.05594000 0.07246900 -0.79219100
C 2.13953200 -0.53679700 -4.46933000
H 2.56700400 -1.39154000 -5.01397100
H 2.22494200 0.32446800 -5.14987100
H 1.07746800 -0.73901700 -4.31593900
C 5.25535300 -1.13365900 -0.93883900
H 4.83783400 -1.68645200 -1.78575000
H 5.02296300 -1.71191200 -0.03604700
C 6.75382400 -0.98202100 -1.08879200
C 7.62117700 -1.25736800 -0.02301300
C 9.00139300 -1.09236000 -0.15830100
C 9.53766900 -0.64657200 -1.36642900
C 8.68563300 -0.37133000 -2.43864800
C 7.30828200 -0.53884900 -2.29945000
H 6.65484400 -0.33141800 -3.14459900
H 9.09474100 -0.03016000 -3.38602500
H 10.6112750 -0.51857700 -1.47457500
H 9.65584600 -1.31593200 0.68010400
H 7.21191500 -1.61561900 0.91926900
C 2.84067000 -0.32204100 -3.15938900
H 3.92248300 -0.33594600 -3.19214500
C 2.20642800 -0.12723800 -1.96914700
O 1.58000000 -0.30816700 1.00131000

Table 39. Geometric coordinates and thermally corrected MP2 energies for (*R*)-**34a**

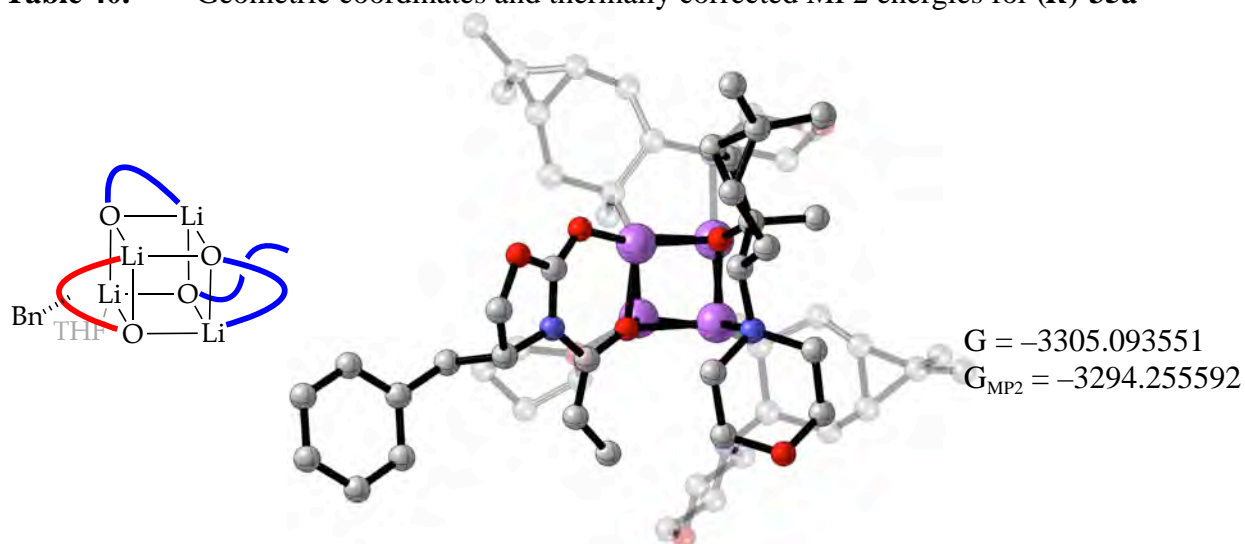


Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	C	-3.69859100	-5.65372200	-0.73852600
O	0.78036500	-1.88235200	0.43471400	H	-3.52333200	-6.20211600	-1.67022100
Li	-0.80983400	-2.43190900	-0.64954900	H	-3.45279700	-6.35261800	0.06761500
Li	-2.42326300	-0.68291900	0.29484700	C	-2.79841000	-4.39505100	-0.67006300
O	-2.11049600	-2.53140400	0.75499000	H	-3.25345900	-3.65282500	-1.34009800
Li	-0.68871300	-1.73792600	1.86706900	N	-1.41531200	-4.55368000	-1.22677500
O	-1.16355500	0.09693400	1.50097600	C	-1.45314300	-4.70558500	-2.70015600
O	-1.31706200	-0.61419800	-1.32326200	H	-1.96424200	-3.84284500	-3.13688200
C	1.34550700	-1.51553900	4.04514100	H	-2.00781600	-5.61098900	-2.99889400
H	2.15725500	-1.96351500	3.46246000	C	-0.04280100	-4.81049500	-3.27617800
H	1.25569300	-0.46104200	3.77132700	O	0.66426300	-5.91095800	-2.72800500
C	1.50858800	-1.74565800	5.55002500	C	0.73279800	-5.78013200	-1.31364000
H	1.00703500	-0.95373400	6.11888400	C	-0.65841900	-5.70565000	-0.68818700
H	2.55920400	-1.76720600	5.85444400	H	-1.18331000	-6.65282100	-0.89769000
C	0.78821800	-3.08724600	5.75612800	H	-0.55770800	-5.60799300	0.39102200
H	1.44011000	-3.91999700	5.46727300	H	1.25979100	-6.66601900	-0.94562500
H	0.46030400	-3.25138100	6.78701700	H	1.31894400	-4.88700200	-1.04338800
C	-0.38371600	-2.96818400	4.78139000	H	0.51450100	-3.87765200	-3.08883800
H	-1.23681400	-2.44740100	5.23776600	H	-0.09045300	-4.97159000	-4.35776500
H	-0.72786100	-3.92829800	4.38899700	C	-6.08215800	-5.41927700	0.50443000
O	0.10844900	-2.18136900	3.67762000	C	-5.66934900	-6.21352900	1.72929000
C	-2.86735700	-3.70888300	0.74584300	H	-6.31555400	-5.95879600	2.57955200
C	-4.39082500	-3.33564000	0.98529500	H	-5.77602300	-7.29186100	1.55023700
H	-4.59558900	-3.36051000	2.06477300	H	-4.64154900	-6.02727500	2.04096300
H	-4.45085400	-2.28066400	0.70125200	C	-7.55776000	-5.60015700	0.17219900
C	-5.50138200	-4.04726800	0.20326900	H	-7.79252000	-6.65550000	-0.02117100
C	-5.16235600	-5.22909700	-0.68943500	H	-8.19292700	-5.26528500	1.00293400
H	-5.65851800	-5.25456400	-1.65902700	H	-7.84529400	-5.02758300	-0.71694100

H	-6.23249100	-3.34908300	-0.20342700	C	-0.48413200	2.02376600	2.87031300
C	-2.36190400	-4.59504100	1.91186200	H	-0.53227900	2.12057700	3.96177700
H	-2.68800000	-4.14688200	2.85757800	H	0.44425300	1.48585600	2.65437200
H	-2.71473000	-5.63086100	1.89806100	C	-0.40922500	3.41387100	2.24469100
H	-1.27019800	-4.61377400	1.92467400	C	-1.72897700	4.12679100	1.99363100
C	-1.34876200	-0.23329900	-2.68092600	H	-1.80603100	4.69591900	1.06699400
C	-2.54087300	-0.94476300	-3.41979900	C	-2.96870700	3.29825900	2.30209800
H	-2.25185600	-1.13336800	-4.46048700	H	-3.85555400	3.79114100	1.88673200
H	-2.65046200	-1.92836500	-2.95309200	H	-3.14624000	3.20786000	3.38008900
C	-3.87996000	-0.22298300	-3.39102200	C	-2.75494400	1.90555400	1.65844900
C	-3.82591000	1.25506600	-3.73735500	H	-2.30783700	2.09806500	0.67581200
H	-4.46281600	1.92650200	-3.16110600	N	-3.99197700	1.13150100	1.34124600
C	-2.42095800	1.78635000	-3.97238600	C	-4.64351200	1.63179900	0.11536400
H	-2.44155600	2.88126200	-4.03119300	H	-3.92737500	1.59875700	-0.71134100
H	-2.01295100	1.43988000	-4.92865300	H	-4.98062700	2.67875800	0.22867300
C	-1.51069700	1.34188500	-2.79549300	C	-5.85485000	0.77173000	-0.23858100
H	-2.05792800	1.59709600	-1.88208700	O	-6.81195600	0.74647900	0.80803900
N	-0.23742600	2.09018100	-2.69539900	C	-6.21274800	0.27433600	2.00750500
C	-0.33816400	3.29678500	-1.86993000	C	-5.01402400	1.12878000	2.40884700
H	-0.75527300	3.02854600	-0.89337600	H	-5.37729800	2.15129000	2.61019800
H	-1.00241000	4.06006300	-2.32522200	H	-4.59196700	0.73767900	3.33353100
C	1.04437500	3.91329700	-1.65946700	H	-6.98669600	0.32400100	2.77988500
O	1.67199200	4.22568800	-2.89886600	H	-5.90302600	-0.77623900	1.88844200
C	1.78738400	3.05275900	-3.69391600	H	-5.52599100	-0.25598700	-0.47078300
C	0.41606400	2.43456700	-3.96305400	H	-6.36458400	1.17783900	-1.11783300
H	-0.17320800	3.16305400	-4.55091600	C	-0.76197800	4.68111600	3.01859800
H	0.54060700	1.53877400	-4.57676400	C	-1.07063300	4.64696500	4.50506600
H	2.25483500	3.36287300	-4.63480700	H	-0.14328100	4.66202600	5.09292100
H	2.43829600	2.31827100	-3.19487500	H	-1.65659300	5.52948000	4.79335300
H	1.66808700	3.21380000	-1.08433000	H	-1.63814800	3.76495500	4.81291900
H	0.96104000	4.85781000	-1.11075100	C	-0.01167900	5.94057200	2.60951400
C	-4.55860900	0.29543800	-4.65537300	H	-0.59518100	6.84233800	2.83866000
C	-4.04490100	-0.03738100	-6.04569700	H	0.94553000	6.01916800	3.14168600
H	-4.41374300	-1.01955100	-6.36971500	H	0.20536400	5.94898100	1.53523400
H	-4.40545100	0.70454900	-6.77004000	H	0.36462100	3.53550400	1.48889200
H	-2.95487700	-0.05720500	-6.11895100	C	-2.17467700	0.34488200	3.65722400
C	-6.07843000	0.36560200	-4.60761500	H	-1.32796100	-0.12837400	4.16513300
H	-6.46110800	1.13755200	-5.28843400	H	-2.65415800	1.02493400	4.37391800
H	-6.52683500	-0.59174800	-4.90480500	H	-2.87952600	-0.44776400	3.38786400
H	-6.44158900	0.60154500	-3.60085600	C	4.28247200	-1.66695600	-0.75873300
H	-4.55765700	-0.52587000	-2.59463200	H	4.30215000	-2.69964200	-1.11430000
C	-0.05011000	-0.72015300	-3.35769400	C	4.40498000	-0.65962800	-1.90507500
H	0.82123900	-0.26355800	-2.88170900	H	3.98156300	-1.03993200	-2.84140500
H	0.02357000	-1.80890400	-3.24998600	H	5.42149600	-0.30281800	-2.07401200
H	-0.01751300	-0.50112100	-4.43262400	O	3.60272800	0.45258200	-1.45472000
C	-1.64881700	1.06256400	2.39231500	C	2.66558800	-0.02018400	-0.58245300

N 2.92889600 -1.32991400 -0.28882300
C 1.86109800 -4.37140000 1.79056200
H 1.98445100 -5.37070900 1.34722500
H 0.79410200 -4.14584300 1.82875000
H 2.21412500 -4.45392800 2.82998800
C 5.37011400 -1.43889000 0.32568800
H 5.08096900 -1.97911600 1.23178500
H 5.37333600 -0.37270800 0.58324900
C 6.74855400 -1.86838100 -0.12957900
C 7.72941000 -0.92375500 -0.46042500
C 8.99206000 -1.32381200 -0.90330800
C 9.29383200 -2.68035300 -1.02372800
C 8.32712900 -3.63335100 -0.69411900
C 7.06827300 -3.22949100 -0.25068800
H 6.32634100 -3.98087100 0.01256500
H 8.55538700 -4.69263200 -0.77817800
H 10.2757730 -2.99415300 -1.36724800
H 9.73905600 -0.57417400 -1.15067000
H 7.50515900 0.13613900 -0.36010800
C 2.60906200 -3.31641600 1.03010600
H 3.68022300 -3.45674000 0.95376900
C 2.04208400 -2.22259900 0.45126400
O 1.77862400 0.71235000 -0.16581300

Table 40. Geometric coordinates and thermally corrected MP2 energies for (*R*)-**35a**

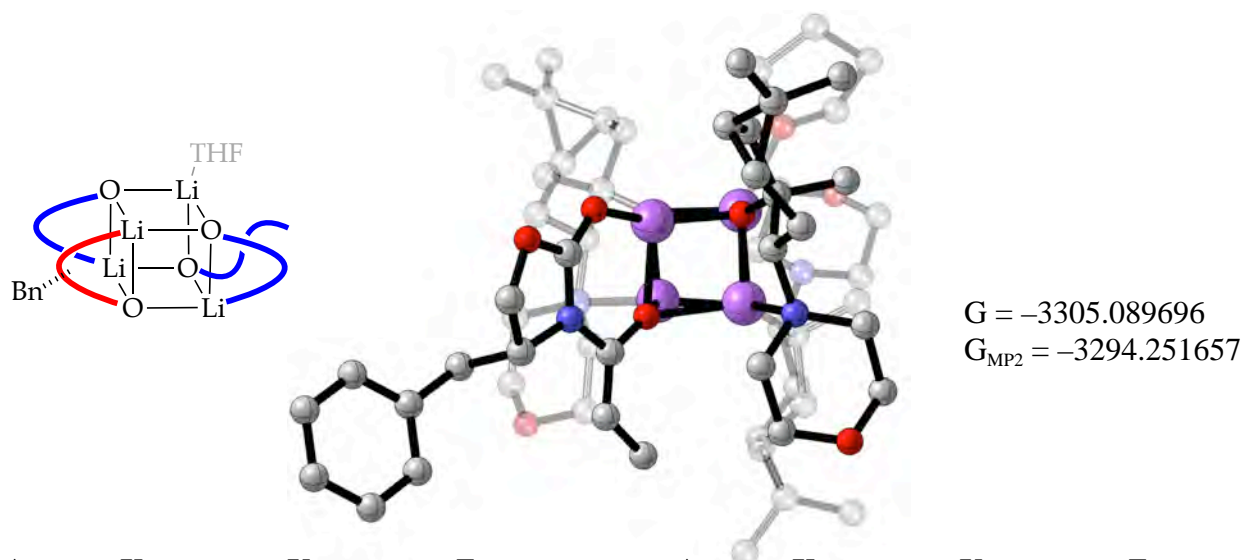


Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	C	-0.42405800	5.31457000	3.79888800
O	-1.75939200	-0.57503400	-0.39769000	H	-0.71329000	6.07967700	3.06849600
C	-2.61486600	0.16579500	-0.86575500	H	-0.15330200	5.81728500	4.73230000
O	-3.79742500	-0.35913800	-1.29227200	C	0.70780900	4.45328100	3.24310500
C	-4.53915900	0.66748400	-1.97529800	H	1.24158300	3.93006900	4.04995300
H	-5.60064100	0.52216300	-1.77100000	H	1.43104800	4.99046200	2.62668700
H	-4.35569200	0.57378200	-3.05184200	O	0.05983500	3.48540300	2.39513000
N	-2.61558800	1.52468500	-1.04343700	C	1.64526700	-1.09795200	-2.24082500
C	-1.49247700	2.43725300	-0.81535200	C	1.05151600	-2.54661800	-1.96608300
C	-1.73032600	3.77046300	-0.95166600	H	1.88413100	-3.25306300	-1.84195400
H	-2.72231000	4.12517200	-1.20203100	H	0.57685700	-2.46851900	-0.98415500
C	-0.66797400	4.81595500	-0.77720000	C	0.00321700	-3.13573700	-2.91565800
H	-0.56297300	5.44759800	-1.67215900	C	-0.21862600	-2.51024300	-4.28188500
H	-0.88883700	5.49737000	0.05846100	H	-1.25550600	-2.43833900	-4.60876200
H	0.30201600	4.35601800	-0.57189100	C	0.61765500	-1.28160200	-4.61743100
O	-0.35252400	1.87057700	-0.53241200	H	0.11527300	-0.71360900	-5.40939400
Li	1.49929300	1.56023700	-1.43313800	H	1.59822000	-1.55582000	-5.02202900
Li	2.42988400	0.22862800	0.55849800	C	0.77061200	-0.41349000	-3.34779900
O	2.56361300	2.24678300	0.02332500	H	-0.22347800	-0.35566700	-2.88870200
Li	0.89694200	2.22814300	1.08535400	N	1.13427800	1.02196200	-3.59422000
O	0.87081000	0.38847500	1.64248300	C	-0.05487700	1.79756100	-4.01274500
O	1.56974000	-0.33253000	-1.06920300	H	-0.83254500	1.69093900	-3.25315600
C	-1.33666100	3.35507000	2.76070900	H	-0.45626500	1.42682900	-4.97240000
H	-1.93308200	3.66006800	1.89463900	C	0.29602700	3.27400700	-4.16870300
H	-1.54085300	2.30247600	2.97869500	O	1.33326000	3.46871000	-5.12113100
C	-1.54582400	4.27673600	3.96952300	C	2.48600000	2.72757600	-4.74948600
H	-1.40868900	3.72366600	4.90622200	C	2.17950000	1.23743500	-4.61810400
H	-2.54659700	4.71883800	3.98447900	H	1.85486900	0.86412800	-5.60324400

H	3.08882800	0.70221200	-4.34230500	C	-0.46284500	-1.95379600	6.15390900
H	3.22954500	2.89323700	-5.53573400	H	-1.35970500	-1.49659100	6.59269900
H	2.89183800	3.10966700	-3.79860700	H	0.00651300	-2.56758700	6.93430800
H	0.59413700	3.69090400	-3.19319400	H	0.22619000	-1.14262200	5.91048900
H	-0.57079000	3.83541300	-4.52982900	C	-1.86049700	-3.87616700	5.29047500
C	0.32463600	-3.92364300	-4.17608600	H	-1.47856900	-4.55957900	6.06100900
C	1.75739300	-4.25772100	-4.54699700	H	-2.78923000	-3.43152100	5.67254100
H	2.06786600	-5.19202200	-4.06094200	H	-2.11813700	-4.47767800	4.41128600
H	1.85616400	-4.40437300	-5.63086200	H	-1.74808100	-2.58824800	2.95700500
H	2.47215600	-3.48774800	-4.25024100	C	1.46004100	0.59393600	3.94554300
C	-0.64659300	-5.03855800	-4.53770800	H	0.75461200	1.41423900	4.11428700
H	-0.63188200	-5.24283000	-5.61692300	H	1.62933500	0.09434000	4.90703200
H	-0.38677800	-5.97145300	-4.01984200	H	2.39921000	1.04609700	3.61748700
H	-1.67569400	-4.78195200	-4.26163000	C	3.81147500	2.86079000	0.25533000
H	-0.89846900	-3.46527900	-2.40240300	C	4.96201600	2.00257100	-0.38983600
C	3.13478400	-1.22856600	-2.63373400	H	5.88549700	2.16221300	0.17856400
H	3.64619500	-1.85693800	-1.89690900	H	4.70314400	0.94807500	-0.23675700
H	3.30416500	-1.67778000	-3.61913700	C	5.22599700	2.25623000	-1.86523900
H	3.62225100	-0.25089800	-2.61157800	C	5.39666400	3.71899800	-2.23318100
C	0.88570500	-0.32759300	2.84327400	H	4.94265600	4.05905200	-3.16371800
C	-0.60257600	-0.72763900	3.23900000	C	5.19030800	4.66604200	-1.06446200
H	-0.93826500	-0.07661000	4.05844100	H	5.17573800	5.70203000	-1.42357800
H	-1.20297700	-0.44797000	2.36910900	H	6.01652600	4.60603100	-0.34745100
C	-0.93771100	-2.18693400	3.56383100	C	3.84194500	4.32555700	-0.37091900
C	0.18052200	-3.16290100	3.88775100	H	3.09634000	4.26179700	-1.17094000
H	0.07586300	-4.16341800	3.46914100	N	3.34714800	5.41816100	0.51494100
C	1.60128500	-2.61700900	3.82699700	C	2.65224500	6.46193500	-0.25258500
H	2.29915900	-3.45369500	3.70786100	H	1.85332300	6.00169600	-0.84073900
H	1.88535200	-2.11910200	4.76071000	H	3.33266000	6.98039700	-0.95553900
C	1.71240600	-1.64275100	2.63136400	C	2.04724800	7.50787800	0.68093200
H	1.20865500	-2.13008300	1.78693100	O	3.03289100	8.10829600	1.51053600
N	3.10582200	-1.40383500	2.12427100	C	3.72736200	7.11900200	2.25592600
C	3.55182700	-2.54420300	1.29212800	C	4.37041400	6.07460300	1.34486500
H	2.85268900	-2.66247100	0.45888500	H	5.13022600	6.59195500	0.73278000
H	3.55873300	-3.48525300	1.86985600	H	4.88728200	5.33563700	1.96064800
C	4.95721200	-2.30568000	0.74571100	H	4.49680300	7.64796600	2.82763100
O	5.90026200	-2.09245200	1.78627800	H	3.04159100	6.62901300	2.96706400
C	5.50169500	-0.98799800	2.58539400	H	1.26344600	7.04156600	1.30124500
C	4.11579300	-1.20388600	3.18721400	H	1.59430400	8.31952100	0.10266800
H	4.16955800	-2.08127100	3.85200600	C	6.56603600	2.76476600	-2.38537400
H	3.84831800	-0.34010300	3.79700600	C	7.80147800	2.84977500	-1.50518800
H	6.24622000	-0.89592400	3.38244700	H	8.29744100	1.87249000	-1.44056800
H	5.51680500	-0.06322000	1.98656100	H	8.52290200	3.55804300	-1.93301100
H	4.95277600	-1.44165200	0.06084800	H	7.59317700	3.17829600	-0.48402900
H	5.29934500	-3.18321000	0.18813500	C	6.90705800	2.36887700	-3.81523900
C	-0.83741300	-2.80123400	4.95249300	H	7.58551100	3.09854200	-4.27686600

H 7.40152500 1.38892300 -3.84579000
H 6.01052800 2.30753000 -4.44311900
H 4.66816700 1.62841000 -2.55675400
C 4.07636300 2.86936600 1.77612600
H 4.03473100 1.83919300 2.14807300
H 5.06356000 3.26936700 2.03964400
H 3.31295600 3.45025900 2.30003600
C -3.97371700 1.96932200 -1.40073000
H -3.92181600 2.74480500 -2.16792900
C -4.76498500 2.48107900 -0.17032700
H -4.87281400 1.64868100 0.53585500
H -4.15905400 3.24613800 0.32506800
C -6.12456100 3.03724500 -0.53499700
C -6.23750200 4.28612600 -1.16522700
C -7.29778900 2.31646400 -0.27432300
C -7.48345800 4.79554200 -1.52917500
H -5.34079400 4.87004100 -1.36355000
C -8.54792000 2.82340300 -0.63604300
H -7.23266400 1.35382500 0.22859600
C -8.64410800 4.06384900 -1.26695000
H -7.54917800 5.76666800 -2.01274000
H -9.44532000 2.24962700 -0.42022600
H -9.61566800 4.46115300 -1.54772800

Table 41. Geometric coordinates and thermally corrected MP2 energies for (*R*)-**29a**

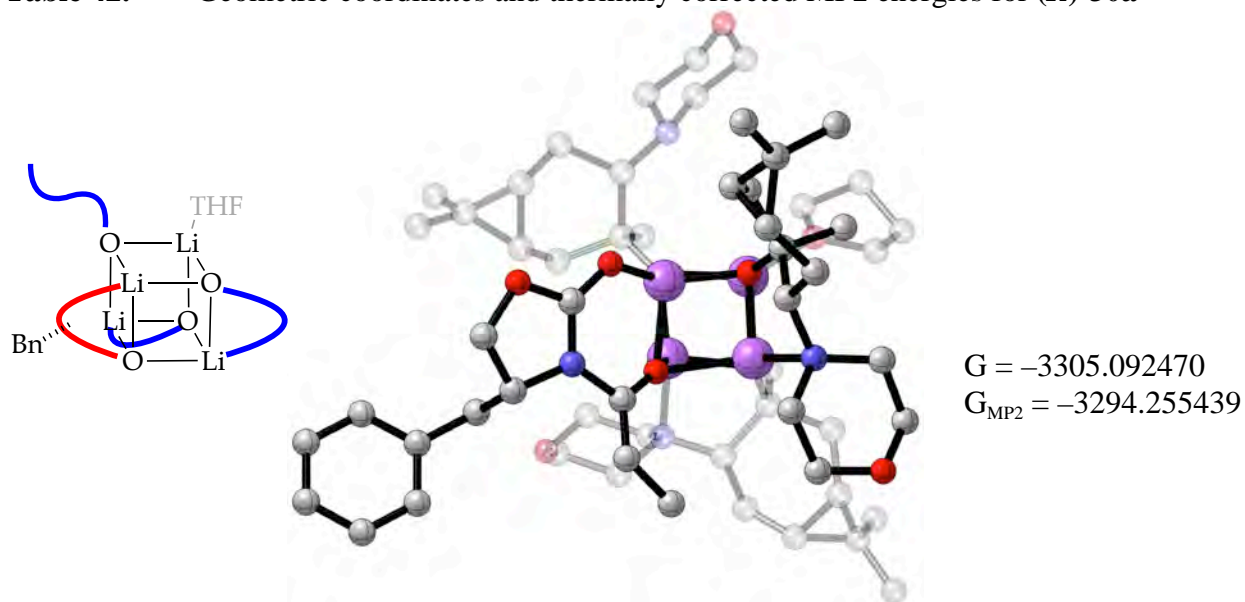


Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	C	-1.43908400	4.18680900	2.07288500
O	-0.69437500	-0.98436500	1.60635800	H	-2.19517600	4.22571500	2.86568700
Li	0.59623000	0.39759700	2.49344900	H	-0.71032900	4.96799700	2.31528500
Li	2.45156400	0.28682100	0.68121000	C	-0.76206500	2.79717200	2.03437700
O	2.18815300	-0.73840000	2.47693600	H	-1.48104700	2.11379400	1.56629500
Li	1.12502100	-1.90205900	1.32148100	N	-0.50150300	2.17502800	3.37812600
O	1.54579000	-1.09684700	-0.35572700	C	-1.75454000	1.62240500	3.94419900
O	0.87516600	1.41547500	0.91724200	H	-2.16079400	0.87714500	3.25475000
C	5.19184900	1.93362900	-0.12056000	H	-2.51221900	2.41318700	4.08459800
H	5.39692700	1.77529800	0.93891500	C	-1.49463000	0.95617600	5.29266000
H	5.93045500	1.37026800	-0.71078600	O	-0.92630200	1.86035600	6.22950600
C	5.14754800	3.40531300	-0.54707200	C	0.28480200	2.39560800	5.71598100
H	6.13209000	3.77619600	-0.84771900	C	0.06218700	3.10549800	4.38342200
H	4.79409000	4.02595500	0.28189100	H	-0.62092300	3.95168000	4.56078800
C	4.12081300	3.40839000	-1.70886300	H	1.00911200	3.51067100	4.02680600
H	3.38151800	4.20429100	-1.58227700	H	0.65238900	3.10678600	6.46238300
H	4.60432800	3.56147900	-2.67857300	H	1.03349000	1.59514200	5.59991300
C	3.46432800	2.01029900	-1.63917900	H	-0.83146500	0.08703600	5.15914400
H	3.80798500	1.36868100	-2.46074700	H	-2.43557700	0.60447400	5.72650000
H	2.37437900	2.02807700	-1.63587800	C	-1.64322100	5.45047700	-0.29636600
O	3.87710600	1.43147600	-0.38611500	C	-0.52127000	6.42580600	0.00781600
C	0.47211900	2.74792100	1.06625600	H	-0.07806200	6.80061200	-0.92441300
C	0.02738700	3.33657300	-0.34433900	H	-0.89941100	7.29477700	0.56265400
H	0.79766200	4.03760300	-0.69449400	H	0.28781200	5.98465100	0.59435300
H	0.06602300	2.48320500	-1.02612000	C	-2.72587900	6.05803800	-1.17654400
C	-1.35788300	3.96981300	-0.50186700	H	-3.18388100	6.93316600	-0.69585500
C	-2.11216800	4.43765700	0.73057800	H	-2.31375200	6.38631400	-2.14008600
H	-3.18484600	4.24534700	0.73361500	H	-3.52451600	5.33743900	-1.38628100

H	-1.96447700	3.49610700	-1.27145300	C	2.90793000	-1.52023300	-2.32382100
C	1.68369600	3.56368700	1.57537000	H	2.49937500	-0.89328400	-3.12868400
H	2.44226600	3.58719700	0.78804000	H	3.47323400	-0.84779400	-1.67398100
H	1.44523400	4.60105800	1.84170500	C	3.92524700	-2.52350800	-2.88206400
H	2.14272500	3.07593100	2.43920400	C	3.70694100	-4.01470700	-2.69025400
C	3.15315800	-0.78385100	3.50463900	H	4.58598700	-4.59901300	-2.41939000
C	2.48360800	-1.15122500	4.87910400	C	2.44017000	-4.43294200	-1.95200300
H	3.06836800	-0.69771000	5.68810600	H	2.59109500	-5.43270700	-1.52933100
H	1.51035300	-0.64716500	4.90146100	H	1.58715800	-4.52214400	-2.63299700
C	2.30382600	-2.63547700	5.15637300	C	2.14034600	-3.40900700	-0.82917200
C	3.53676100	-3.48642500	4.91142800	H	3.09824300	-3.20109000	-0.33475400
H	3.38719700	-4.45884300	4.44164900	N	1.27897100	-3.90905200	0.28921200
C	4.72401700	-2.71076200	4.36751900	C	2.02976100	-4.85052000	1.14910900
H	5.51312100	-3.40742400	4.05912500	H	2.92925200	-4.35049200	1.52304800
H	5.17049000	-2.06947600	5.13548700	H	2.35035800	-5.74453900	0.58720400
C	4.26466000	-1.86509600	3.14964500	C	1.17417500	-5.30335400	2.32871300
H	3.72310000	-2.55435300	2.49462200	O	-0.02143400	-5.93386400	1.89571800
N	5.39086400	-1.35814000	2.31831800	C	-0.77063400	-5.05384100	1.06542600
C	5.80226100	-2.32674700	1.29543900	C	0.03959700	-4.59224800	-0.14280800
H	4.93161600	-2.59251900	0.68712300	H	0.27157000	-5.47285700	-0.76470900
H	6.20438900	-3.25889900	1.74074300	H	-0.56665800	-3.91052600	-0.73889200
C	6.87063000	-1.72857200	0.38370900	H	-1.64710000	-5.61870500	0.73170400
O	8.00732500	-1.29130500	1.11663000	H	-1.11605900	-4.18309900	1.64291400
C	7.62641100	-0.34944500	2.10999400	H	0.93820200	-4.44093600	2.97211300
C	6.58374100	-0.92969500	3.06265200	H	1.71762000	-6.04143500	2.92716300
H	7.05908900	-1.76697700	3.60438000	C	3.73707000	-3.42603600	-4.09030400
H	6.31030100	-0.17051800	3.80024300	C	2.49817700	-3.34592400	-4.96183400
H	8.53918500	-0.09248600	2.65714400	H	2.65551300	-2.62561800	-5.77536600
H	7.23478000	0.56389900	1.63456000	H	2.28040800	-4.31803500	-5.42429100
H	6.43885100	-0.88692500	-0.18193800	H	1.60841400	-3.02608700	-4.41944400
H	7.23092500	-2.47911500	-0.32710600	C	4.99286300	-3.72443000	-4.89890900
C	2.98674800	-3.34809200	6.31851000	H	4.89921700	-4.67775700	-5.43620800
C	3.73544400	-2.59773500	7.40642700	H	5.17777900	-2.94025900	-5.64517500
H	3.03928400	-2.23651800	8.17461200	H	5.88030800	-3.79026000	-4.25898400
H	4.45496100	-3.26351500	7.90062800	H	4.95318200	-2.18349300	-2.75504200
H	4.29321700	-1.73221700	7.04003600	C	0.39342800	-2.03894600	-2.21445700
C	2.25353400	-4.56729500	6.86056900	H	0.28885500	-1.09387100	-2.75969100
H	2.95258300	-5.27678200	7.32331300	H	0.31429500	-2.85299500	-2.94192500
H	1.51992100	-4.27770900	7.62453100	H	-0.46373700	-2.10567200	-1.54012700
H	1.71405900	-5.09986000	6.06887100	C	-4.34366500	-1.41490400	0.99365200
H	1.34528600	-3.05612200	4.86429400	H	-4.71063100	-1.31788100	2.01742900
C	3.75524900	0.62679200	3.67734500	C	-5.01125600	-0.37837800	0.08433800
H	2.95137300	1.33206500	3.91972600	H	-5.35728500	0.50080800	0.63988500
H	4.49310500	0.68314000	4.48769200	H	-5.83419100	-0.78170600	-0.50717100
H	4.23295300	0.95645400	2.75071400	O	-3.96085500	0.02815400	-0.80939700
C	1.71363900	-2.01108000	-1.40406200	C	-2.75889500	-0.22628500	-0.22115400

O -1.73347800 0.19327900 -0.74081300
N -2.94119600 -0.97083500 0.91512800
C -1.37720100 -2.57172400 4.02746900
H -1.70812800 -2.26784100 5.03057700
H -0.37416000 -2.16617500 3.87265300
H -1.29188300 -3.66914300 4.05005200
C -4.52016300 -2.87150100 0.49735700
H -3.82089700 -3.50098700 1.05682500
H -4.21999300 -2.91192200 -0.55714100
C -5.93656600 -3.38000300 0.65708500
C -6.79908600 -3.48222900 -0.44277700
C -8.11347600 -3.92731000 -0.28609700
C -8.58734600 -4.27789400 0.97823300
C -7.73764100 -4.18489300 2.08307100
C -6.42556000 -3.74107400 1.92183600
H -5.76772300 -3.68534200 2.78691400
H -8.09520900 -4.46442000 3.07058200
H -9.60889300 -4.62675100 1.10224900
H -8.76385900 -4.00392900 -1.15345700
H -6.43346100 -3.22333800 -1.43429700
C -2.31513400 -2.09527700 2.95719800
H -3.35706300 -2.36350900 3.07683900
C -1.91108400 -1.37663600 1.87368500

Table 42. Geometric coordinates and thermally corrected MP2 energies for (*R*)-**30a**

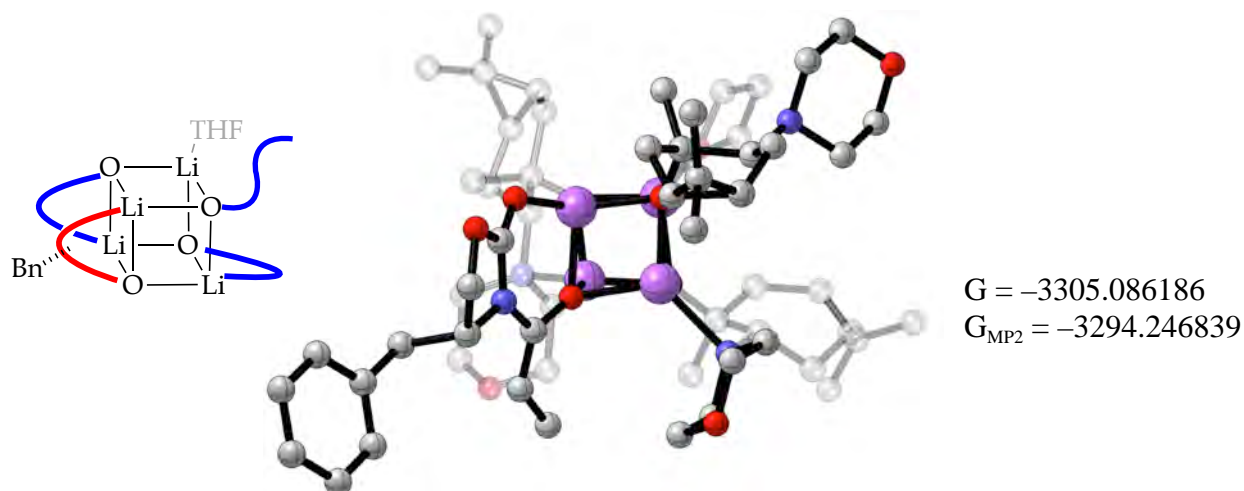


Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	H	-0.42016400	-0.97600700	5.29496100
O	0.62365100	1.90691200	0.26903100	C	-2.20648500	-0.03799100	4.41681100
Li	-1.51884600	2.01060700	0.68870600	H	-2.06098000	0.70695500	5.20787700
Li	-2.24022600	0.44055700	-1.21536400	H	-3.25986800	-0.33328900	4.47169300
O	-1.94737600	2.42998300	-1.09927600	C	-1.87805300	0.56365500	3.03031900
Li	-0.17673400	1.92701600	-1.67207500	H	-0.78356900	0.60120500	2.95935900
O	-0.37527800	0.04255800	-1.91303300	N	-2.29757300	1.99249100	2.83170700
O	-1.77022800	0.13184700	0.65506500	C	-1.38454500	2.91619300	3.54516500
C	-5.38719900	0.48591200	-1.41785900	H	-0.36382400	2.76879500	3.17411500
H	-5.65127600	-0.08120200	-0.51937400	H	-1.38230000	2.72079200	4.63153300
H	-5.22944800	1.53226800	-1.13971300	C	-1.80084300	4.36936100	3.31965800
C	-6.42749600	0.29732300	-2.52790700	O	-3.13307900	4.61567300	3.74483500
H	-6.45081400	1.17170400	-3.18910700	C	-4.02533200	3.75392700	3.05473200
H	-7.43535700	0.14765400	-2.12921700	C	-3.67474400	2.28870400	3.28744100
C	-5.87802300	-0.92291700	-3.28229200	H	-3.78326400	2.08070600	4.36426600
H	-6.13062500	-1.85033100	-2.75421700	H	-4.38702800	1.66080100	2.75396700
H	-6.24923900	-1.00224400	-4.30857700	H	-5.02719000	3.96706400	3.44051500
C	-4.37479100	-0.66448500	-3.22134300	H	-4.01144400	3.98007400	1.97522400
H	-4.06092700	0.02776300	-4.01488000	H	-1.69934100	4.63004300	2.25404900
H	-3.75334300	-1.56028300	-3.26521700	H	-1.15853000	5.03932100	3.89916300
O	-4.14340300	-0.04393700	-1.93733100	C	-1.70952700	-2.66968800	4.69207900
C	-2.28862300	-0.38631200	1.84858800	C	-3.17382700	-3.06227100	4.62463300
C	-1.67821900	-1.82903400	2.13165100	H	-3.27643800	-4.09415700	4.26347700
H	-2.45525400	-2.58249900	1.94527400	H	-3.63613600	-3.01649000	5.61979800
H	-0.92706800	-1.97768000	1.35364100	H	-3.76191000	-2.42779600	3.95763400
C	-0.99195700	-2.11235700	3.47108000	C	-0.89719200	-3.59207500	5.58965000
C	-1.27585400	-1.21655900	4.66455100	H	-1.27721900	-3.57966100	6.62028200

H	-0.94089500	-4.62953100	5.23221400	H	-2.18788600	2.23362600	-3.68793000
H	0.15782000	-3.29675400	5.62023000	C	0.08141600	-0.85945700	-2.89742200
H	0.04053400	-2.43950400	3.36466500	C	1.58136200	-0.57211100	-3.25201300
C	-3.81542100	-0.54196900	1.67079700	H	1.78871400	-0.96610900	-4.25373800
H	-3.99769000	-1.31360800	0.91422600	H	1.68930300	0.51569300	-3.33337600
H	-4.34730700	-0.83681900	2.58371600	C	2.58777500	-1.13043400	-2.26214400
H	-4.25147300	0.38562800	1.29339300	C	2.39216700	-2.59788600	-1.92984400
C	-2.37226900	3.49462700	-1.90695300	H	2.51445800	-2.88654200	-0.88695800
C	-3.56869500	4.27751900	-1.21690500	C	1.19075300	-3.22957900	-2.61436300
H	-4.43560000	4.26628700	-1.88939900	H	1.02432900	-4.23892300	-2.21831500
H	-3.85185100	3.65780600	-0.36041600	H	1.35893200	-3.34872000	-3.69037600
C	-3.32331300	5.70657500	-0.73112900	C	-0.05973500	-2.34839800	-2.34673700
C	-2.32910800	6.56562800	-1.49688100	H	-0.08673300	-2.20713100	-1.26218600
H	-1.68978800	7.21092800	-0.89470400	N	-1.35095500	-3.01910300	-2.66804500
C	-1.59414800	5.86495300	-2.63111100	C	-1.85804600	-3.80062200	-1.53259200
H	-0.72218800	6.46159300	-2.92355400	H	-1.94157600	-3.14348600	-0.66088600
H	-2.21516600	5.77275000	-3.52908800	H	-1.17869500	-4.63395400	-1.26511300
C	-1.16229800	4.47365800	-2.11482400	C	-3.23287500	-4.38457200	-1.84880100
H	-0.78721500	4.63421900	-1.09879900	O	-3.21298600	-5.18456200	-3.02390200
N	-0.00385100	3.83907300	-2.82876000	C	-2.73400300	-4.43438000	-4.13070700
C	1.28146200	4.40611900	-2.35777600	C	-1.33961000	-3.87026800	-3.86501500
H	1.36465200	4.24947900	-1.27953100	H	-0.64899600	-4.72573800	-3.76018500
H	1.33637800	5.49142300	-2.55380000	H	-1.01703800	-3.28752800	-4.73279300
C	2.45991100	3.72305500	-3.04687700	H	-2.70969800	-5.12264500	-4.98185700
O	2.39100700	3.83788200	-4.46023000	H	-3.43554900	-3.61593900	-4.36617400
C	1.16827600	3.29611900	-4.94029200	H	-3.96552800	-3.56753200	-1.96286200
C	-0.03719700	3.98069700	-4.30242600	H	-3.56679400	-5.03759000	-1.03619700
H	-0.01865800	5.04324800	-4.59459900	C	3.65465300	-2.15054200	-2.64391200
H	-0.95180400	3.54076000	-4.69995400	C	3.94596200	-2.51972600	-4.08855800
H	1.16134800	3.45778200	-6.02270300	H	4.62626100	-1.78800400	-4.54436900
H	1.13250700	2.21195700	-4.75040500	H	4.43696700	-3.50061600	-4.13832900
H	2.49692100	2.65997600	-2.75469900	H	3.05483800	-2.57213100	-4.71895300
H	3.39908400	4.19467000	-2.74113400	C	4.91488900	-2.13697300	-1.78988000
C	-3.79792100	6.93331700	-1.50364400	H	5.40336800	-3.12064500	-1.79131700
C	-4.64397200	6.79213300	-2.75630300	H	5.64262300	-1.40800000	-2.17483100
H	-5.70479300	6.68332000	-2.49449500	H	4.68871000	-1.87984300	-0.74952500
H	-4.55147000	7.68790200	-3.38417800	H	2.84457000	-0.46736300	-1.43947400
H	-4.37167500	5.93133500	-3.37281100	C	-0.71850200	-0.63209800	-4.19473000
C	-4.18736500	8.14390600	-0.66763700	H	-0.58991200	0.41016500	-4.51187300
H	-4.07103500	9.07432800	-1.23935000	H	-0.38106300	-1.26969600	-5.02171600
H	-5.23526600	8.08015300	-0.34602400	H	-1.78087600	-0.81463900	-4.03081500
H	-3.56863500	8.22685700	0.23302500	C	4.11950200	1.50863800	1.32740300
H	-3.32308900	5.82627900	0.35150200	H	4.29286600	2.26432700	2.09612300
C	-2.91087900	2.91980300	-3.23776900	C	4.64065400	0.14664100	1.82012300
H	-3.81407200	2.33894300	-3.02748900	H	4.77547100	0.12306200	2.90672300
H	-3.17513600	3.69347400	-3.97130300	H	5.56783400	-0.16274700	1.33542700

O 3.60890900 -0.79358400 1.47294200
C 2.45077800 -0.11940900 1.22842800
O 1.40485800 -0.73698400 1.06847400
N 2.68211900 1.22384700 1.19483700
C 1.08900000 4.70511800 1.36534000
H 0.83341300 5.14940500 2.33705800
H 0.15353800 4.48213900 0.84553500
H 1.60049800 5.49696400 0.79628300
C 4.73851700 1.99127900 -0.00404100
H 4.14881300 2.85273300 -0.33717200
H 4.61678900 1.20218500 -0.75516400
C 6.19687800 2.37063300 0.13347300
C 7.21261800 1.53391700 -0.34808600
C 8.55771700 1.87536100 -0.19146800
C 8.90836000 3.06269200 0.45156000
C 7.90596100 3.90834900 0.93264300
C 6.56403000 3.56427200 0.77347900
H 5.78901600 4.23431000 1.14064200
H 8.16972100 4.83965700 1.42703800
H 9.95432100 3.33120400 0.57229000
H 9.32986700 1.21472700 -0.57686100
H 6.94705700 0.61244700 -0.86195600
C 1.93469300 3.47580600 1.52350200
H 2.82471800 3.58861400 2.13234600
C 1.66249300 2.25981800 0.97680900

Table 43. Geometric coordinates and thermally corrected MP2 energies for (*R*)-**31a**

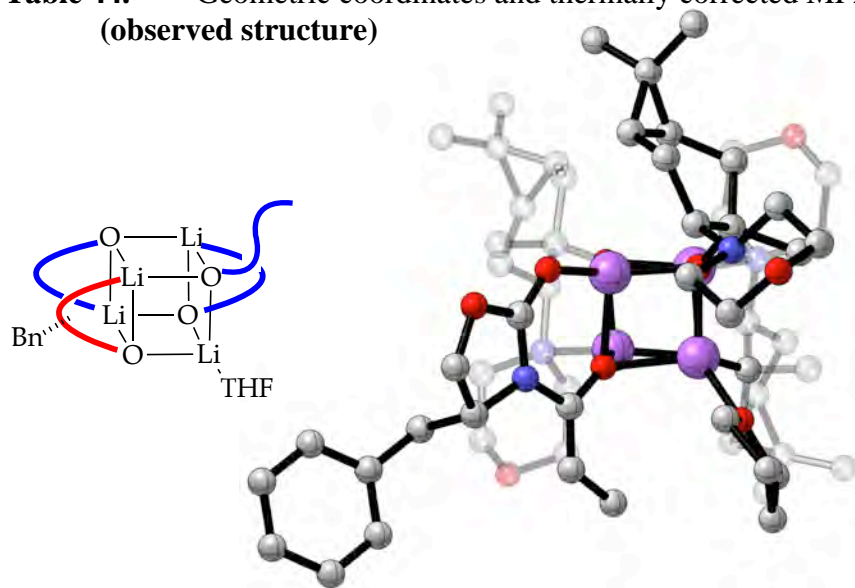


Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	C	-2.06312000	-4.80441200	-1.20158300
O	0.88454100	-0.19912600	1.81434400	H	-2.75881300	-5.59468400	-0.89264200
Li	-0.70400600	-1.44939800	1.97803500	H	-2.07725300	-4.80000100	-2.29643900
Li	-2.44149600	0.08608800	0.77621200	C	-2.54124600	-3.43437100	-0.64577200
O	-1.95706700	-0.15519900	2.70201100	H	-2.41876000	-3.49168800	0.43891500
Li	-0.59611600	1.17942100	2.22263100	N	-3.99905300	-3.18966700	-0.84210900
O	-1.11922300	1.46739900	0.42320500	C	-4.80452200	-3.77981100	0.23417500
O	-1.32689200	-1.44863300	0.13052800	H	-4.45339900	-3.39052800	1.19637700
C	-5.26501600	0.52466200	-0.69361100	H	-4.71804400	-4.88406600	0.26335000
H	-4.93887400	1.11734200	-1.56038700	C	-6.27950800	-3.41995100	0.06796500
H	-5.15827300	-0.53508700	-0.92600900	O	-6.78491600	-3.82465300	-1.19607600
C	-6.68103900	0.93909100	-0.23413900	C	-6.01910900	-3.25080700	-2.24693500
H	-7.30068500	0.06485500	-0.01402800	C	-4.54408100	-3.62895700	-2.13439800
H	-7.19144900	1.51388400	-1.01282400	H	-4.47231800	-4.72321400	-2.26650400
C	-6.43023200	1.78299600	1.04390900	H	-3.98771500	-3.15859400	-2.94963100
H	-6.96816900	2.73580600	1.03661800	H	-6.44085800	-3.63614600	-3.18069900
H	-6.73807100	1.23135800	1.93769200	H	-6.13092600	-2.15387800	-2.24128600
C	-4.90989700	1.98035500	1.04471200	H	-6.41038200	-2.33193600	0.19593100
H	-4.46441600	2.04622600	2.03818600	H	-6.88535500	-3.93234900	0.82224300
H	-4.61693800	2.86325300	0.46029300	C	0.55535500	-5.32800000	-1.54383200
O	-4.39290700	0.79672800	0.41690500	C	0.45703900	-5.53739100	-3.04521500
C	-1.58177500	-2.21991900	-1.02825800	H	1.39692400	-5.25196200	-3.53536800
C	-0.25260000	-2.78289800	-1.63438600	H	0.27521600	-6.59650600	-3.27065500
H	-0.44046900	-3.05888600	-2.67847000	H	-0.34286300	-4.96245200	-3.51751600
H	0.47198300	-1.96570700	-1.67188900	C	1.65320500	-6.17764400	-0.91816500
C	0.32228800	-3.97369800	-0.88783900	H	1.47345900	-7.24767700	-1.08835200
C	-0.66889100	-5.10443100	-0.67244600	H	2.63321500	-5.93405700	-1.35020300
H	-0.65618600	-5.61565600	0.28996500	H	1.71932600	-6.02037400	0.16466400

H	0.99909100	-3.72931800	-0.06985900	C	-1.95464200	3.02402900	-1.24974900
C	-2.18366400	-1.29910500	-2.11074900	H	-1.38291300	2.93554200	-2.18356200
H	-1.48291200	-0.47969300	-2.31059700	H	-2.62075300	2.15833400	-1.22538900
H	-2.35892000	-1.81435800	-3.06342700	C	-2.84639000	4.26951800	-1.28848500
H	-3.12899100	-0.86782000	-1.77639600	C	-2.61686400	5.40087600	-0.29970000
C	-2.62754500	-0.67692700	3.82062100	H	-3.51006400	5.85262400	0.13122900
C	-4.17613200	-0.36644700	3.67751600	C	-1.47144300	5.23227900	0.69166300
H	-4.38462800	0.60747000	4.14394600	H	-1.65504400	5.87953800	1.55757200
H	-4.31353500	-0.22629400	2.60378400	H	-0.52037000	5.56741100	0.26395200
C	-5.23019800	-1.39988800	4.09416900	C	-1.37711100	3.75521500	1.13839500
C	-4.80334200	-2.68903900	4.77502800	H	-2.39384900	3.43968000	1.40041100
H	-5.29980100	-3.59886400	4.43870200	N	-0.58847000	3.52071300	2.39554100
C	-3.31106300	-2.86289100	5.03234000	C	-1.40556600	3.81592500	3.59259300
H	-3.09354500	-3.93270600	5.12186600	H	-2.29745100	3.17906000	3.57640000
H	-3.01108400	-2.41958800	5.98732000	H	-1.73970400	4.86878300	3.60460100
C	-2.50610600	-2.24701400	3.85998700	C	-0.61370900	3.54017700	4.87001400
H	-3.00715700	-2.56769500	2.93632300	O	0.58660500	4.29536200	4.92460600
N	-1.11467000	-2.77462500	3.69516600	C	1.39420800	4.01621200	3.78736700
C	-1.12710700	-4.17356400	3.21303000	C	0.65237700	4.32344700	2.49216900
H	-1.69558700	-4.22389100	2.27964800	H	0.42656400	5.40185800	2.47831700
H	-1.60848100	-4.84941800	3.94011300	H	1.30075600	4.10508700	1.64339700
C	0.29599800	-4.67075300	2.97063800	H	2.27991700	4.65332400	3.87316000
O	1.08036300	-4.60513700	4.15034900	H	1.71830600	2.96444300	3.79603600
C	1.11854600	-3.26801400	4.63379700	H	-0.38408400	2.46566500	4.94043600
C	-0.28344700	-2.73383900	4.91775400	H	-1.20287900	3.82316500	5.74813500
H	-0.73283000	-3.34469700	5.71852800	C	-2.42912600	5.64326200	-1.78713800
H	-0.20778600	-1.70941800	5.27731300	C	-1.05888600	5.87835300	-2.39471900
H	1.70367200	-3.29030400	5.55857000	H	-1.08653100	5.68733200	-3.47538700
H	1.63300200	-2.61571300	3.91033600	H	-0.74225400	6.92049700	-2.25428000
H	0.76649300	-4.07761600	2.16934900	H	-0.28412300	5.23465100	-1.97577700
H	0.28117200	-5.72049900	2.66166200	C	-3.51467800	6.46677700	-2.46661800
C	-5.70132800	-1.70542400	5.50638900	H	-3.30105500	7.54145600	-2.39172400
C	-5.22744400	-0.90239900	6.70298900	H	-3.58961900	6.21723000	-3.53339700
H	-5.88400300	-0.03633800	6.85916300	H	-4.49806100	6.29196400	-2.01479600
H	-5.26312200	-1.50743100	7.61883400	H	-3.89067500	4.03650400	-1.49669000
H	-4.21261300	-0.52024500	6.59489800	C	0.48737800	2.97681900	-0.49305600
C	-7.15927300	-2.12629400	5.64022600	H	0.65949700	2.37288100	-1.39012800
H	-7.31095200	-2.74446400	6.53518000	H	0.75032000	4.01330200	-0.73404700
H	-7.81616500	-1.25049700	5.72744300	H	1.18187100	2.61215700	0.26900500
H	-7.49492000	-2.70844600	4.77434900	C	4.43358500	-1.02208200	1.06383300
H	-6.01602500	-1.50731300	3.34614300	H	4.57713900	-1.65196200	1.94433000
C	-2.06615700	0.02945600	5.07884900	C	4.58551000	-1.81822800	-0.23458700
H	-2.43712000	1.06027500	5.10396400	H	4.30693400	-2.87123100	-0.11422900
H	-2.33232000	-0.43679800	6.03224000	H	5.57716600	-1.74679300	-0.68272600
H	-0.97691500	0.07956800	5.02937300	O	3.63872900	-1.19064300	-1.12291800
C	-0.97514800	2.78720300	-0.02438200	C	2.66594800	-0.60508300	-0.37113100

O 1.67497900 -0.13145800 -0.91253000
N 3.01544200 -0.63957700 0.95157200
C 2.05577800 0.24515100 4.55640100
H 2.16518500 -0.55263800 5.30705900
H 0.98623700 0.38585700 4.38217200
H 2.43836100 1.16110600 5.02811700
C 5.37683700 0.20925400 1.10933100
H 5.04053500 0.87444200 1.91027100
H 5.25795300 0.76082600 0.16870500
C 6.82827600 -0.17052700 1.31084600
C 7.74563100 -0.11558500 0.25284100
C 9.07898000 -0.48781800 0.43747300
C 9.51681200 -0.92395400 1.68805900
C 8.61429800 -0.98116600 2.75271300
C 7.28428500 -0.60702800 2.56417300
H 6.59271600 -0.64550700 3.40357500
H 8.94780300 -1.31270400 3.73255300
H 10.5540160 -1.21268700 1.83471600
H 9.77444300 -0.43276000 -0.39588900
H 7.41464800 0.23396800 -0.72287600
C 2.77393700 -0.07310900 3.27836100
H 3.85092100 -0.15733500 3.34944600
C 2.16432500 -0.26656600 2.07736600

Table 44. Geometric coordinates and thermally corrected MP2 energies for **(R)-16a** (observed structure)



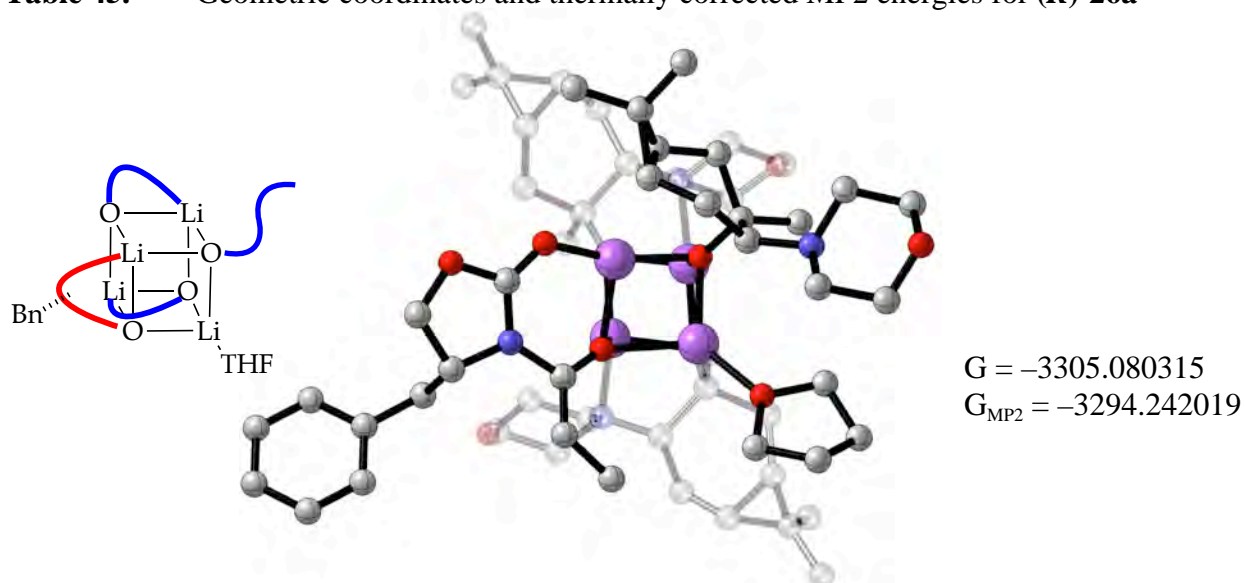
G = -3305.095949
G_{MP2} = -3294.260834

Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	C	-5.63225100	-2.36641800	-4.00558300
O	0.64749000	-1.06656600	-1.59806100	H	-6.14231900	-3.15435500	-3.45150000
Li	-0.42351500	0.40046100	-2.56696500	C	-5.75274200	-0.98887900	-3.37056200
Li	-2.36204200	0.31572800	-0.89991600	H	-6.64470300	-0.96369900	-2.73386000
O	-2.06537700	-0.65782500	-2.58093100	H	-5.89770600	-0.20692700	-4.12399400
Li	-1.15871200	-1.86606900	-1.38773100	C	-4.48185500	-0.71225400	-2.53505700
O	-1.61934300	-1.03953100	0.29735200	H	-4.28802500	-1.62469300	-1.95844700
O	-0.76152900	1.47091600	-0.97066600	N	-4.62859300	0.35378100	-1.48786400
C	0.34392400	0.86565000	-5.60308300	C	-5.30053700	-0.18552800	-0.28410700
H	-0.04170000	-0.14662300	-5.75077800	H	-4.71311900	-1.02365700	0.10167000
H	-0.40879500	1.58596500	-5.94790200	H	-6.31321300	-0.55768500	-0.52127000
C	1.69619300	1.10837500	-6.27753500	C	-5.42002100	0.88557700	0.79748800
H	1.58898900	1.46450900	-7.30661100	O	-6.14705900	2.01665000	0.34093100
H	2.28705500	0.18512900	-6.29541000	C	-5.52142600	2.56667100	-0.80907200
C	2.34157700	2.13746800	-5.33734300	C	-5.40287000	1.53821600	-1.92974000
H	3.43221700	2.17312400	-5.41855200	H	-6.42367300	1.25120900	-2.22911400
H	1.95155500	3.14174900	-5.54159300	H	-4.92017900	2.00091700	-2.79049600
C	1.87250600	1.65085900	-3.96595900	H	-6.14912800	3.40176900	-1.13548600
H	1.76004600	2.44753500	-3.22705400	H	-4.52750100	2.96121200	-0.54810100
H	2.53109000	0.86715900	-3.57018400	H	-4.41604300	1.19383900	1.13328500
O	0.56282900	1.07089300	-4.19022900	H	-5.96483100	0.49108200	1.66072400
C	-3.18996900	-0.54640600	-3.41252600	C	-5.48249700	-2.61341900	-5.49319100
C	-3.15654500	-1.67091500	-4.53581000	C	-5.60167200	-1.48165500	-6.49756500
H	-3.07758600	-1.18779400	-5.51826300	H	-5.09051800	-1.74438300	-7.43304000
H	-2.20401100	-2.18627700	-4.38735600	H	-6.65479700	-1.28996500	-6.74154400
C	-4.26936500	-2.71986500	-4.57719500	H	-5.16865700	-0.54235200	-6.14500000

C	-6.05030900	-3.92492100	-6.01573000	H	-2.04265800	3.33148700	-2.20850200
H	-7.11619600	-3.82573200	-6.26076600	H	-1.06842700	4.73335100	-1.75687300
H	-5.52846000	-4.24580100	-6.92698200	H	-0.36336400	3.45602600	-2.76384700
H	-5.95333400	-4.72874300	-5.27685100	C	-1.78811000	-2.01926800	1.28734200
H	-3.93202200	-3.74061700	-4.40512600	C	-2.74756100	-1.47189000	2.43051400
C	-3.13963600	0.82108000	-4.13216900	H	-2.14302700	-1.22854700	3.31405200
H	-2.28597400	0.82961300	-4.81656600	H	-3.10543600	-0.51233500	2.05048700
H	-4.03654900	1.03350400	-4.72873700	C	-3.97390900	-2.28862900	2.85051500
H	-2.98780700	1.63472600	-3.41863000	C	-4.05844100	-3.76337600	2.49295100
C	-0.61176500	2.84658100	-0.67836600	H	-5.03655300	-4.12409800	2.17568300
C	-1.57350200	3.21864000	0.48897400	C	-2.89999300	-4.33476200	1.68625500
H	-1.55571000	4.30377200	0.65257900	H	-3.23073100	-5.25416800	1.18932100
H	-2.59514800	2.97924500	0.17025100	H	-2.06217300	-4.62478000	2.32933100
C	-1.22448700	2.46167000	1.75858300	C	-2.45155600	-3.28782900	0.64157400
C	0.22759800	2.61441700	2.18052500	H	-3.36881100	-2.89693400	0.18321600
H	0.75153300	1.72200600	2.51717700	N	-1.68188500	-3.83744100	-0.52435900
C	1.04015200	3.52426200	1.27479600	C	-2.58474100	-4.49000100	-1.49855100
H	2.09810400	3.48793800	1.56145500	H	-3.34260400	-3.76865000	-1.82126700
H	0.72936900	4.56476100	1.40998800	H	-3.10586800	-5.35311300	-1.04871000
C	0.90346600	3.12893900	-0.22393000	C	-1.80041900	-4.97201400	-2.71777700
H	1.38176100	2.15340300	-0.33504800	O	-0.76430200	-5.87452800	-2.36141500
N	1.69158400	4.02200200	-1.11877700	C	0.11590400	-5.27147100	-1.42067400
C	3.12774600	3.72218200	-1.10822700	C	-0.63319500	-4.82067100	-0.17036400
H	3.27352600	2.65130600	-1.29448100	H	-1.07335800	-5.71078600	0.30819300
H	3.60084800	3.95654200	-0.13575900	H	0.07092200	-4.37683400	0.53260600
C	3.84201100	4.52641400	-2.19620700	H	0.85681000	-6.03384000	-1.15980700
O	3.63138000	5.92269800	-2.04726600	H	0.63856900	-4.41613500	-1.87827400
C	2.24060700	6.22225700	-2.03554300	H	-1.37888700	-4.10695700	-3.25504300
C	1.52587700	5.46654200	-0.91785100	H	-2.46175200	-5.51291700	-3.40170100
H	1.95155900	5.80714600	0.04311100	C	-3.96728200	-3.34343600	3.94748000
H	0.46428200	5.72703200	-0.92009600	C	-2.72037700	-3.60411500	4.77176700
H	2.16173400	7.30375000	-1.88573800	H	-2.68241700	-2.92413900	5.63277600
H	1.78776200	5.96305200	-3.00701800	H	-2.72062000	-4.62991800	5.16355900
H	3.48975700	4.20006700	-3.18953800	H	-1.79460900	-3.46374100	4.21011100
H	4.92460300	4.37014900	-2.14166200	C	-5.24648700	-3.47804400	4.76136400
C	-0.88537900	3.12040200	3.08530000	H	-5.34130600	-4.48685200	5.18504000
C	-1.11643200	4.59970800	3.34323100	H	-5.26095500	-2.76479300	5.59606800
H	-2.14659900	4.77193500	3.68204400	H	-6.13612200	-3.29055200	4.14903300
H	-0.44535300	4.96197400	4.13346500	H	-4.91008900	-1.73547200	2.78062100
H	-0.95591000	5.22985000	2.46493900	C	-0.40584100	-2.31070400	1.91979500
C	-1.15263500	2.27506100	4.32312800	H	-0.06663700	-1.42087900	2.46089500
H	-0.49790300	2.57265200	5.15333100	H	-0.40889700	-3.14699200	2.62935900
H	-2.19137400	2.38661200	4.66253500	H	0.34052700	-2.51183500	1.14725500
H	-0.97938700	1.21061600	4.12835300	C	4.16990800	-2.03183900	-0.93204900
H	-1.65344500	1.46417100	1.82547500	H	4.61446600	-1.93921100	-1.92519600
C	-1.03369200	3.65069100	-1.92286400	C	4.94452300	-1.18115200	0.08106100

H 5.47576400 -0.34941800 -0.39602000
H 5.64357200 -1.75508100 0.69077500
O 3.92516900 -0.64145500 0.93880800
C 2.73695100 -0.64925800 0.27080500
O 1.77105000 -0.07306100 0.75273100
N 2.86071700 -1.35977300 -0.89398600
C 1.18987100 -2.47851300 -4.16178100
H 1.56491800 -2.10417500 -5.12593200
H 0.22687700 -1.99615200 -3.97153300
H 1.00436900 -3.55453500 -4.30302400
C 4.06553000 -3.52522300 -0.53650600
H 3.30918000 -3.98459200 -1.18107100
H 3.69315400 -3.58070900 0.49392000
C 5.38314700 -4.25925900 -0.65753700
C 6.15034400 -4.56447200 0.47490600
C 7.38038800 -5.21496300 0.35561900
C 7.86376200 -5.57169800 -0.90342500
C 7.10751500 -5.27829300 -2.04064200
C 5.87937200 -4.62939400 -1.91688000
H 5.29157400 -4.41702200 -2.80777000
H 7.47180000 -5.56089500 -3.02487000
H 8.81940000 -6.07992200 -0.99887800
H 7.95691600 -5.44602000 1.24744700
H 5.77457600 -4.30112000 1.46149200
C 2.15859600 -2.20803600 -3.04540600
H 3.17200500 -2.56359300 -3.18809600
C 1.81850500 -1.55334500 -1.90131000

Table 45. Geometric coordinates and thermally corrected MP2 energies for (*R*)-26a

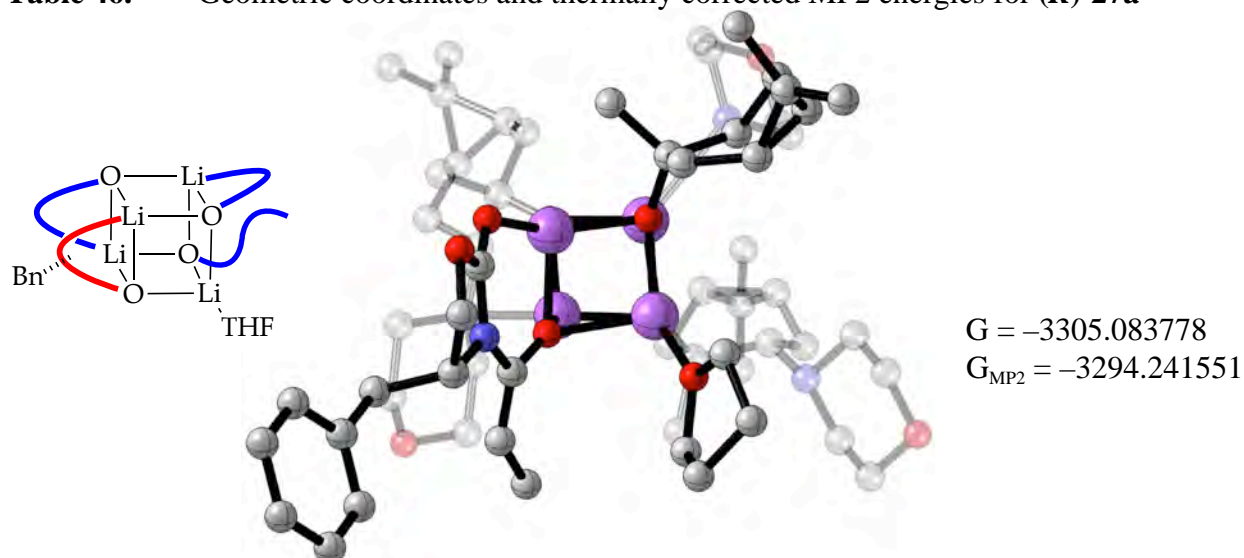


Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	H	0.37403700	-4.54669100	2.36206700
O	-0.78578900	1.83284800	-0.47354500	C	0.03670100	-3.05270200	3.93927300
Li	1.31827400	2.33608200	-0.08078900	H	0.89832900	-3.50719500	4.44211900
Li	1.33135800	0.81223100	2.00531900	H	-0.73294200	-2.92959100	4.71000300
O	0.94299800	2.69397400	1.76927400	C	0.41658900	-1.68564000	3.31517500
Li	-0.84416700	1.92307200	1.56802400	H	0.93595600	-1.92146800	2.37870400
O	-0.43635900	0.09157400	1.90320500	N	1.41509900	-0.87684000	4.07925800
O	1.87893300	0.47255100	0.11056100	C	2.77501300	-1.43484100	3.94483900
C	3.93194100	3.84867400	-0.82106900	H	3.02985300	-1.51299000	2.88479300
H	3.99227500	3.91856900	0.26768400	H	2.84805700	-2.44812000	4.38006500
H	4.47313500	2.95690500	-1.15273000	C	3.79737600	-0.54165200	4.64270400
C	4.41383800	5.11278900	-1.53526000	O	3.51025700	-0.40208600	6.02557400
H	5.48540000	5.07986700	-1.75428300	C	2.20016400	0.11797700	6.20397800
H	4.21983800	6.00241700	-0.92493000	C	1.14461100	-0.75402300	5.52670900
C	3.53638400	5.12667900	-2.79606200	H	1.15410300	-1.74374600	6.01582000
H	3.43854100	6.11919600	-3.24635800	H	0.16311400	-0.31196400	5.69180400
H	3.94360000	4.44960600	-3.55516000	H	2.02461200	0.14893100	7.28405900
C	2.20414500	4.60200700	-2.25943500	H	2.14545000	1.14532600	5.81097500
H	1.61164900	4.05706900	-2.99947400	H	3.81912900	0.45042000	4.15839200
H	1.59383400	5.41799000	-1.85540300	H	4.79703600	-0.98211000	4.57362600
O	2.53353800	3.69096300	-1.18560000	C	-1.82110300	-4.52206200	2.64420100
C	-0.84551100	-0.88221900	2.82705700	C	-2.85503600	-4.41881500	3.75121800
C	-1.87899300	-1.89221600	2.16802100	H	-3.87093400	-4.45347500	3.33579900
H	-2.76144400	-1.95897200	2.81519000	H	-2.75567300	-5.26174700	4.44775100
H	-2.21551300	-1.40463700	1.24985500	H	-2.77454000	-3.50017200	4.33797100
C	-1.39780500	-3.30099500	1.83203000	C	-1.92031000	-5.83125500	1.87450800
C	-0.42690400	-3.95322700	2.80319400	H	-1.76494500	-6.69426100	2.53611500

H	-2.90972400	-5.94106300	1.41100900	H	4.37575500	1.42857000	0.38995100
H	-1.17290800	-5.88521500	1.07475400	C	0.84284600	3.78893900	2.64220800
H	-1.22910200	-3.48740700	0.77342500	C	2.08345000	4.76067100	2.50700200
C	-1.61463200	-0.18405600	3.96968700	H	2.42880900	5.02758500	3.51230900
H	-2.55168400	0.21031500	3.55901300	H	2.88438100	4.15296000	2.07576500
H	-1.87914200	-0.86060900	4.79302600	C	1.89399100	6.03576400	1.69128200
H	-1.04983300	0.66111200	4.37151200	C	0.57456500	6.76922800	1.87330200
C	3.06251100	-0.16769300	-0.32857600	H	0.12841600	7.19632300	0.97493600
C	2.94469000	-1.70679600	-0.11989900	C	-0.42999700	6.05159400	2.76475400
H	3.87141200	-2.19211200	-0.45354600	H	-1.41360400	6.52588800	2.66834200
H	2.86601200	-1.91360500	0.95284500	H	-0.16183200	6.11601300	3.82546900
C	1.73103900	-2.26638900	-0.83765400	C	-0.46870500	4.57821700	2.28846200
C	1.60067900	-1.84077600	-2.28763000	H	-0.44150000	4.62211700	1.19515900
H	0.60704600	-1.55034400	-2.61755300	N	-1.72690400	3.81808300	2.58000400
C	2.74478200	-0.99916600	-2.83139500	C	-2.79975100	4.19668800	1.63058600
H	2.43899300	-0.54422200	-3.78094200	H	-2.46629000	3.98373000	0.61061100
H	3.58356900	-1.65335000	-3.08605600	H	-3.03213200	5.27427500	1.69630300
C	3.26653600	0.13015100	-1.88222000	C	-4.07782100	3.41077100	1.91242300
H	2.64876200	1.01740700	-2.04568800	O	-4.54744300	3.62179900	3.23406100
N	4.63771800	0.57163300	-2.26850400	C	-3.54664900	3.24166600	4.16765500
C	4.67050100	1.30323000	-3.53821400	C	-2.25169800	4.01947600	3.95048900
H	3.89890600	2.08190800	-3.52135000	H	-2.46428300	5.08539000	4.13360300
H	4.46549200	0.65118700	-4.40805400	H	-1.51245700	3.69600500	4.68297000
C	6.04472900	1.94587200	-3.73460500	H	-3.94895400	3.45856700	5.16209000
O	7.08537500	0.98085700	-3.69897300	H	-3.35657800	2.16036400	4.09604300
C	7.04755800	0.24070600	-2.48463100	H	-3.90055600	2.33423000	1.74322800
C	5.69472400	-0.44502600	-2.29970700	H	-4.87729700	3.73758300	1.24057500
H	5.57028500	-1.16497200	-3.12894200	C	1.86158900	7.42045800	2.33321400
H	5.69880600	-1.01576300	-1.36780200	C	2.17029300	7.62540500	3.80593700
H	7.85156300	-0.49893900	-2.55256100	H	3.25451500	7.66814800	3.97325300
H	7.24618400	0.90551200	-1.62774000	H	1.74566000	8.57594600	4.15390900
H	6.21232400	2.70670200	-2.95257500	H	1.77119900	6.83706400	4.44899100
H	6.10861400	2.43160800	-4.71413800	C	2.36984800	8.56538000	1.46827700
C	1.76983700	-3.31350300	-1.93718000	H	1.91485300	9.51962700	1.76524100
C	3.03456200	-4.08415000	-2.27341200	H	3.45876900	8.67458100	1.55911400
H	3.11418700	-4.97791000	-1.64064500	H	2.13841200	8.40349600	0.40888400
H	3.01570500	-4.42282100	-3.31805800	H	2.29407700	6.00406200	0.67979900
H	3.95245200	-3.50726100	-2.13337200	C	0.87982000	3.26257300	4.09331400
C	0.51614200	-4.16619100	-2.07693700	H	1.87309500	2.83655700	4.27803000
H	0.41530100	-4.55114300	-3.10103000	H	0.71392900	4.04560600	4.84503000
H	0.54895200	-5.03236300	-1.40140000	H	0.15016000	2.46261000	4.24281300
H	-0.38573900	-3.59016400	-1.84528300	C	-3.86735000	1.11252700	-2.37968500
H	0.81789700	-2.26977500	-0.24699500	H	-3.83966600	1.77694500	-3.24597600
C	4.22573700	0.35809300	0.53807000	C	-4.16325300	-0.32429300	-2.84109600
H	3.96523600	0.20025800	1.59206900	H	-3.95670300	-0.46758600	-3.90747200
H	5.18235800	-0.14430200	0.36309300	H	-5.18349900	-0.64650100	-2.62644000

O -3.25604800 -1.14550800 -2.08916400
C -2.23835700 -0.37194500 -1.62306200
O -1.25401900 -0.90184500 -1.12441100
N -2.51866600 0.95006700 -1.81057900
C -1.19264200 4.54532900 -1.76803700
H -0.72103300 4.96362500 -2.66817000
H -0.41304300 4.41754200 -1.01277500
H -1.88495300 5.31878800 -1.40013800
C -4.87254800 1.66379600 -1.34415700
H -4.45099200 2.59518500 -0.95239300
H -4.93587600 0.95608500 -0.50856700
C -6.24554400 1.91194000 -1.92966600
C -7.32019300 1.05846700 -1.64618000
C -8.57953900 1.27822700 -2.20835000
C -8.78378100 2.35849800 -3.06695200
C -7.72230400 3.21938400 -3.35604000
C -6.46690700 2.99743100 -2.79109300
H -5.64959400 3.68121600 -3.01185300
H -7.87412700 4.06861400 -4.01715500
H -9.76332400 2.53279900 -3.50370300
H -9.40048800 0.60694500 -1.97059800
H -7.17248900 0.22041700 -0.96831000
C -1.89037900 3.25014100 -2.05991600
H -2.62471300 3.27858600 -2.85652200
C -1.65686400 2.07357000 -1.41836000

Table 46. Geometric coordinates and thermally corrected MP2 energies for (*R*)-27a

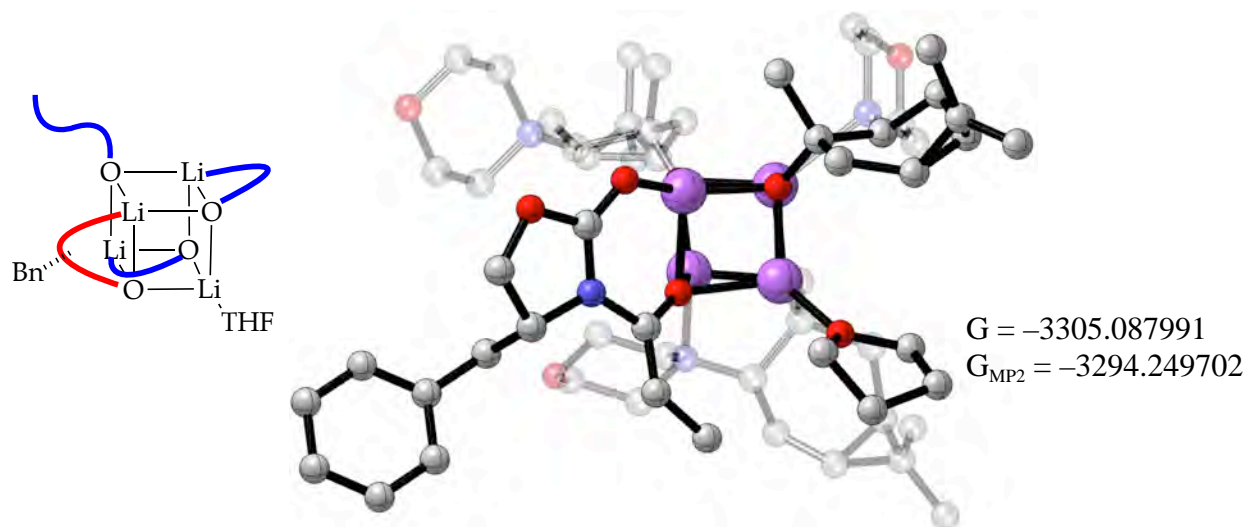


Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	C	2.64049500	-4.18463200	2.18315000
O	-0.89013200	-0.02504800	-1.80358100	H	3.66586300	-4.57188300	2.20031400
Li	0.34002100	-1.77663400	-1.92109000	H	2.46442900	-3.75341200	3.17487500
Li	2.33091700	-0.65986800	-0.72705000	C	2.47925200	-3.10797000	1.08408500
O	1.88026400	-0.77090700	-2.65004200	H	2.42663600	-3.64540700	0.12888400
Li	0.84626500	0.89301000	-2.18363700	N	3.65094600	-2.18744500	0.92058700
O	1.54782700	1.08158300	-0.42162000	C	4.72898700	-2.85528100	0.16365000
O	0.87280100	-1.73380200	-0.07915900	H	4.33937000	-3.16636600	-0.81090200
C	-1.40031700	-4.38420000	-1.91087400	H	5.09142500	-3.76020300	0.68429000
H	-0.54583600	-4.91875300	-1.48850300	C	5.91264900	-1.91441200	-0.04452800
H	-2.03483200	-4.03346700	-1.08716400	O	6.44441900	-1.45579900	1.18789800
C	-2.19922000	-5.20763800	-2.92345500	C	5.43191500	-0.79386800	1.93314000
H	-2.98983000	-5.79686000	-2.44900400	C	4.23882900	-1.70922400	2.19279100
H	-1.54007800	-5.89620200	-3.46459300	H	4.59385600	-2.55230500	2.80873900
C	-2.72877000	-4.12099100	-3.87091500	H	3.49058300	-1.16631000	2.76911300
H	-2.99945600	-4.50273200	-4.85991300	H	5.88846500	-0.49481900	2.88179100
H	-3.61219000	-3.63328200	-3.44121900	H	5.10534200	0.11407300	1.40210200
C	-1.55466900	-3.14266200	-3.92463200	H	5.59574500	-1.05775400	-0.66138100
H	-1.86134800	-2.10636300	-4.06702200	H	6.72459300	-2.43593000	-0.56117600
H	-0.82902100	-3.42219000	-4.69763300	C	0.49276300	-5.70267200	2.74763500
O	-0.90314500	-3.23850500	-2.63471800	C	0.27130800	-5.07432300	4.11174200
C	1.09932200	-2.36695400	1.15389200	H	-0.78796900	-5.13233600	4.39447000
C	-0.05613300	-3.41062200	1.46966000	H	0.84627100	-5.60896900	4.87914500
H	-0.51504400	-3.14569200	2.42955300	H	0.56076800	-4.02150800	4.15803700
H	-0.82425000	-3.21546200	0.71685700	C	0.07688900	-7.16596100	2.70345700
C	0.27808200	-4.90198400	1.46716300	H	0.64970000	-7.76268400	3.42590800
C	1.67716900	-5.32308700	1.88297300	H	-0.98751700	-7.28197300	2.94784600
H	2.12422100	-6.14138800	1.31840600	H	0.23953200	-7.60199100	1.71089200

H	-0.16930600	-5.47269200	0.65501100	C	3.17022000	2.37397600	0.83106300
C	1.04477700	-1.30427600	2.28004600	H	2.94269800	2.19113600	1.89055400
H	0.02193100	-0.91955300	2.35864500	H	3.67365400	1.47107600	0.47245500
H	1.31429100	-1.70933700	3.26437400	C	4.18789400	3.51004400	0.67841000
H	1.69927300	-0.45729000	2.05431100	C	3.84516200	4.72705300	-0.16385100
C	2.61883200	-0.90447700	-3.84274900	H	4.63568900	5.09631500	-0.81646100
C	3.61223400	0.30595300	-4.00844800	C	2.45945000	4.75666300	-0.80038900
H	3.71657700	0.53453300	-5.07534300	H	2.48664000	5.42244700	-1.67009500
H	3.11481200	1.17326700	-3.56418000	H	1.71452700	5.18379000	-0.12090000
C	4.99235500	0.14163700	-3.39120100	C	2.05849800	3.32310200	-1.22873600
C	5.68153600	-1.17514300	-3.70450400	H	2.94172900	2.88703300	-1.71553500
H	6.24967500	-1.64190400	-2.90127100	N	1.00206600	3.23361100	-2.28413300
C	4.82792000	-2.15053500	-4.49991200	C	1.51743900	3.68065600	-3.59643300
H	5.31261700	-3.13427900	-4.52085300	H	2.41757500	3.10941200	-3.84465500
H	4.72417400	-1.84136700	-5.54642100	H	1.79195600	4.74943900	-3.58219200
C	3.43605500	-2.25993000	-3.82055900	C	0.46428000	3.46900500	-4.67997500
H	3.63601700	-2.40484800	-2.75416600	O	-0.73252200	4.17842000	-4.39660700
N	2.65085000	-3.45345700	-4.22746500	C	-1.24681900	3.81826000	-3.11712900
C	2.90279300	-4.61412700	-3.36982100	C	-0.21827700	4.02405100	-2.00972300
H	2.72810200	-4.32974700	-2.32616300	H	0.01816300	5.09925800	-1.94055600
H	3.94632100	-4.98040500	-3.45301500	H	-0.65523600	3.71376100	-1.06161700
C	1.95665800	-5.75767500	-3.72899000	H	-2.11416300	4.46389600	-2.94600700
O	2.06752500	-6.13072600	-5.09557000	H	-1.58717400	2.77308700	-3.11885800
C	1.82402500	-5.01215000	-5.93692700	H	0.25156700	2.39339600	-4.78813700
C	2.78123200	-3.86277400	-5.63093400	H	0.82860100	3.84560800	-5.64116900
H	3.80375500	-4.20588600	-5.87318300	C	4.11800000	4.88434500	1.32289800
H	2.54962500	-3.02114300	-6.28854400	C	3.03025400	5.25130600	2.31453200
H	1.96354400	-5.36285700	-6.96454900	H	3.34969900	4.99990700	3.33444200
H	0.78138400	-4.67071100	-5.82066100	H	2.82850600	6.33077000	2.29317900
H	0.92194200	-5.44992700	-3.50669100	H	2.08887900	4.73161300	2.13711200
H	2.19335600	-6.65228000	-3.14384000	C	5.45749400	5.51682400	1.67809800
C	6.26329400	0.12057000	-4.23492300	H	5.38312800	6.61242900	1.69978400
C	6.25816100	0.45981300	-5.71550800	H	5.79914400	5.18801400	2.66860500
H	6.28348400	1.54743000	-5.86372900	H	6.23565400	5.25113900	0.95344300
H	7.14839100	0.04120400	-6.20268500	H	5.20632400	3.13828100	0.56732800
H	5.38618600	0.07644100	-6.25132300	C	0.64223300	2.82533800	0.92322300
C	7.52486600	0.60817100	-3.53569500	H	0.71195400	2.28983900	1.87698300
H	8.42217700	0.15303500	-3.97564100	H	0.60324500	3.89605600	1.14600200
H	7.62783400	1.69784700	-3.62421300	H	-0.31412900	2.54117300	0.47782000
H	7.51701600	0.36170800	-2.46782300	C	-4.52080100	-0.30443100	-1.04523800
H	5.10831800	0.54293800	-2.38483800	H	-4.75551700	-0.93795300	-1.90350900
C	1.65809100	-0.83933600	-5.04647800	C	-4.79512300	-1.02011700	0.28029600
H	1.15852900	0.13680500	-5.05618900	H	-4.68981000	-2.10811400	0.19749400
H	2.17600700	-0.94155000	-6.00894800	H	-5.76293900	-0.77669700	0.72006100
H	0.89438000	-1.61756200	-4.97547900	O	-3.76069700	-0.52195500	1.15064700
C	1.81609800	2.38777400	0.01033600	C	-2.71075600	-0.11270200	0.38394200

O -1.66139900 0.22684200 0.91530500
N -3.06265800 -0.13417600 -0.93784700
C -1.99145200 0.45980100 -4.57479500
H -2.39017400 -0.19071200 -5.36736200
H -0.93534900 0.21171000 -4.44967900
H -2.04896700 1.48661600 -4.96544600
C -5.27088400 1.05033800 -1.14591600
H -4.82931400 1.63015100 -1.96201600
H -5.08403700 1.61062200 -0.22154100
C -6.75962500 0.87920400 -1.35946100
C -7.67213200 1.10439100 -0.31990600
C -9.04276500 0.91897900 -0.51366700
C -9.52382100 0.50314900 -1.75525200
C -8.62646500 0.27898400 -2.80207300
C -7.25884400 0.46650100 -2.60443500
H -6.57013600 0.30101700 -3.43062900
H -8.99280900 -0.03640200 -3.77553000
H -10.5899030 0.36018000 -1.90921600
H -9.73293200 1.10411400 0.30519700
H -7.30627900 1.44036900 0.64808900
C -2.74434600 0.29102800 -3.28622800
H -3.82197900 0.37060000 -3.35301400
C -2.16385900 0.07139300 -2.07336700

Table 47. Geometric coordinates and thermally corrected MP2 energies for (*R*)-28a

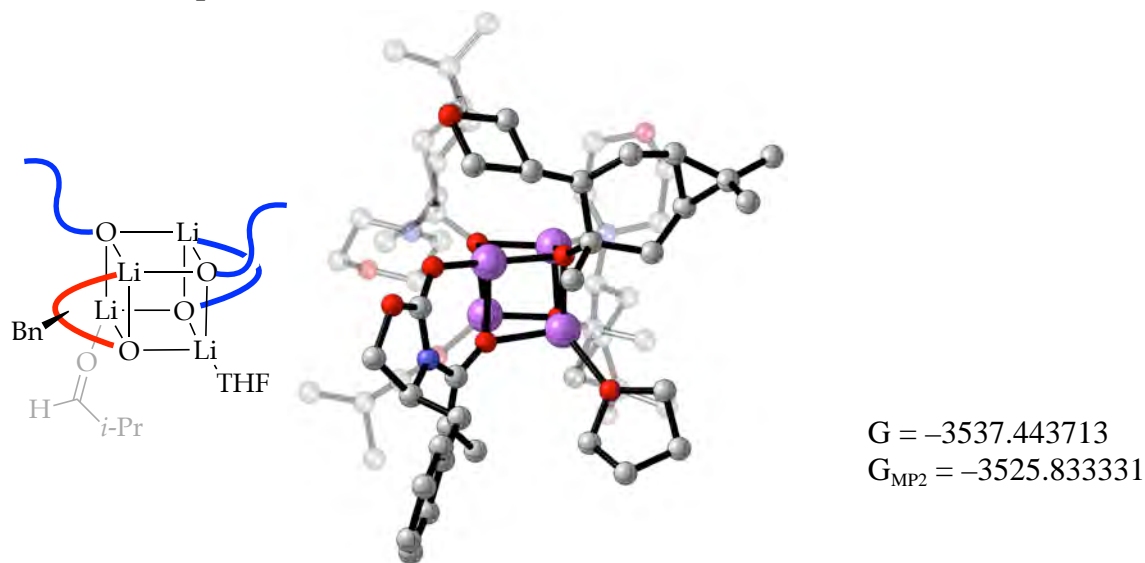


Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	C	-5.52183300	-2.15492400	-1.19567000
O	0.51767800	-1.04327900	1.69305300	H	-6.31106900	-2.40053400	-0.48487900
Li	-1.53403000	-1.24967600	1.77497000	C	-5.33043600	-0.66018500	-1.41044800
Li	-2.02669900	1.14414500	0.96058300	H	-6.25699300	-0.13671400	-1.14747400
O	-1.82608500	0.39913000	2.77457800	H	-5.13636900	-0.42438100	-2.46219000
Li	0.03323200	0.86479400	2.43420200	C	-4.15899300	-0.18635300	-0.52000800
O	-0.12724300	1.81478400	0.79887400	H	-4.30367800	-0.66340500	0.45761700
O	-1.84991300	-0.51654500	0.04191600	N	-4.14250400	1.28024600	-0.20313200
C	-3.69228200	-3.34150200	2.66541500	C	-5.10425500	1.58810600	0.87815100
H	-3.73709000	-2.91562000	3.67188700	H	-4.82941400	1.00992500	1.76740100
H	-4.41563800	-2.82103800	2.02894000	H	-6.13471300	1.30787300	0.59495700
C	-3.89914900	-4.86780600	2.67061600	C	-5.08721800	3.07726200	1.21808200
H	-4.47978700	-5.18025200	1.79545500	O	-5.38504100	3.88200400	0.08795700
H	-4.43257300	-5.20817400	3.56297500	C	-4.44878000	3.62240300	-0.94978900
C	-2.46407700	-5.41412900	2.57703800	C	-4.46496500	2.15186600	-1.35547100
H	-1.99365900	-5.44416000	3.56661300	H	-5.46817100	1.92711600	-1.75338000
H	-2.41438300	-6.41643700	2.14079900	H	-3.74409800	1.98832700	-2.15731200
C	-1.79234900	-4.35762500	1.70587900	H	-4.74280000	4.24859300	-1.79781900
H	-2.03186400	-4.51203100	0.64455700	H	-3.43798700	3.92062000	-0.62933400
H	-0.70927400	-4.28361000	1.81713500	H	-4.10153300	3.35738000	1.62428700
O	-2.35837500	-3.10718700	2.15323400	H	-5.84716500	3.30112500	1.97346800
C	-2.76972800	-0.73996000	-0.98971100	C	-5.23870700	-3.21918000	-2.23716100
C	-2.89762300	-2.29486000	-1.29630600	C	-4.88345700	-2.85467400	-3.66704700
H	-2.53491400	-2.48536800	-2.31386900	H	-4.32538700	-3.67155600	-4.14307100
H	-2.16841000	-2.76614000	-0.63485500	H	-5.79199300	-2.68775200	-4.26055700
C	-4.25005500	-2.98303400	-1.10204600	H	-4.26834800	-1.95514800	-3.74550600

C	-6.08050500	-4.48361900	-2.14650200	H	-3.34815400	2.49245600	3.50538900
H	-7.02685200	-4.37123500	-2.69234600	H	-2.57829700	2.74693300	5.07270900
H	-5.54971100	-5.34336400	-2.57689700	H	-1.62828600	2.86872700	3.57104800
H	-6.32573500	-4.73073000	-1.10683500	C	0.20866300	3.03919500	0.18325900
H	-4.25152200	-3.76554800	-0.34394200	C	-0.67498300	4.20746800	0.77216500
C	-2.23833100	-0.07703600	-2.28065300	H	-0.90826400	4.91063500	-0.03566300
H	-1.30840500	-0.57998500	-2.57014000	H	-1.63499500	3.76114300	1.05536300
H	-2.93348200	-0.14959000	-3.12767100	C	-0.10371100	4.98037000	1.95220500
H	-1.99669300	0.97370300	-2.11634800	C	1.34709800	5.40478400	1.80792100
C	-2.12820700	0.80277500	4.08443400	H	1.97506000	5.34225600	2.69598600
C	-3.43551000	0.05850600	4.59785500	C	2.01758700	4.89389600	0.54367000
H	-4.23723900	0.79733800	4.72689000	H	3.09776200	5.07365000	0.59910500
H	-3.74546800	-0.56519900	3.75548400	H	1.66648100	5.42836400	-0.34637800
C	-3.35387700	-0.82607700	5.84365800	C	1.73978900	3.37079400	0.40831300
C	-2.25591900	-0.57296800	6.86218300	H	1.94872100	2.93773600	1.39299600
H	-1.79763000	-1.45889000	7.30092700	N	2.66870700	2.67180800	-0.51521100
C	-1.26197600	0.52839100	6.52226000	C	3.90419000	2.25624500	0.15630500
H	-0.35877300	0.39414800	7.12876700	H	3.64519800	1.64467800	1.02899800
H	-1.65243400	1.52007500	6.77617300	H	4.49584700	3.12103200	0.51847800
C	-0.91990600	0.43855200	5.01820600	C	4.78355400	1.43253700	-0.78477600
H	-0.73976000	-0.62055300	4.80894800	O	5.09189800	2.14053900	-1.97636000
N	0.36010800	1.11503800	4.61328700	C	3.89071900	2.51703900	-2.64019200
C	1.52796100	0.24528600	4.88695300	C	3.02361400	3.39648600	-1.74354200
H	1.40710600	-0.69207600	4.34076700	H	3.59151900	4.32144500	-1.53292000
H	1.60935500	0.01235500	5.96350900	H	2.11960300	3.67753600	-2.28662800
C	2.82201700	0.91367100	4.43045200	H	4.19418800	3.06773800	-3.53640800
O	3.02076400	2.17229700	5.05466100	H	3.32777300	1.62047400	-2.94528900
C	1.91530400	3.02535900	4.79148300	H	4.27743500	0.48787900	-1.03574000
C	0.60654200	2.41273200	5.28067500	H	5.74221100	1.20782800	-0.30270700
H	0.67707800	2.28806500	6.37303400	C	0.25935100	6.45943100	1.85806800
H	-0.21379000	3.10109800	5.07499800	C	-0.09958900	7.30475600	0.64835700
H	2.11319700	3.96326500	5.31999000	H	-1.13796700	7.65524000	0.71480300
H	1.84887400	3.23863400	3.71412700	H	0.54536500	8.19185400	0.60068900
H	2.81046100	1.03451100	3.33323500	H	0.00715300	6.77610700	-0.30206400
H	3.68160000	0.29107700	4.69742000	C	0.16324800	7.24358600	3.15940500
C	-3.70378300	-0.33806500	7.24393200	H	0.84537200	8.10423900	3.15590800
C	-4.24592100	1.06231300	7.46505900	H	-0.85415500	7.62645300	3.31479500
H	-5.33706600	1.07437500	7.34388500	H	0.41925400	6.62145400	4.02514200
H	-4.02519000	1.40659400	8.48390900	H	-0.43034500	4.64826900	2.93609100
H	-3.83594500	1.80013700	6.77116500	C	-0.14279300	2.95197600	-1.31535100
C	-4.32375700	-1.36270200	8.18275000	H	-1.22002700	2.77991900	-1.41445400
H	-4.13180600	-1.10503200	9.23288500	H	0.08529500	3.87615100	-1.86127300
H	-5.41234200	-1.41475800	8.04778500	H	0.38600700	2.12141600	-1.79164200
H	-3.91857100	-2.36616500	8.00832300	C	3.69332600	-2.68193000	0.79828300
H	-3.59527900	-1.87380900	5.66662700	H	3.62060100	-3.69229500	1.20676600
C	-2.42818800	2.31872800	4.07307500	C	4.13917400	-2.75648200	-0.67330800

H 4.00539400 -3.75789900 -1.09622900
H 5.17105600 -2.43718500 -0.82891800
O 3.27129600 -1.85076200 -1.37264800
C 2.18385000 -1.57495000 -0.60011200
O 1.24414300 -0.95181300 -1.07255300
N 2.35806700 -2.08265900 0.65803800
C 0.60333800 -3.14623900 3.90642100
H 0.21965700 -4.17167400 4.00605300
H -0.26234700 -2.48058400 3.87055500
H 1.14746000 -2.93831900 4.84069400
C 4.61480100 -1.83601500 1.70648400
H 4.08882000 -1.69496200 2.65740000
H 4.73779400 -0.84626200 1.25183300
C 5.96263700 -2.48318500 1.93876400
C 7.11194600 -2.02299100 1.28219800
C 8.34735600 -2.64437400 1.47693300
C 8.45224300 -3.73966800 2.33449800
C 7.31562200 -4.20632000 2.99914100
C 6.08422100 -3.58217800 2.80273000
H 5.20616400 -3.94398900 3.33422000
H 7.38975000 -5.05350300 3.67601300
H 9.41290200 -4.22329600 2.48920200
H 9.22694600 -2.26832100 0.96121900
H 7.04151900 -1.16222900 0.62041000
C 1.47016500 -3.00825200 2.68598600
H 2.22430000 -3.77708100 2.56235900
C 1.37259900 -2.02855700 1.74324400

Table 48. Geometric coordinates and thermally corrected MP2 energies for precomplex pre-(*S*)-48a

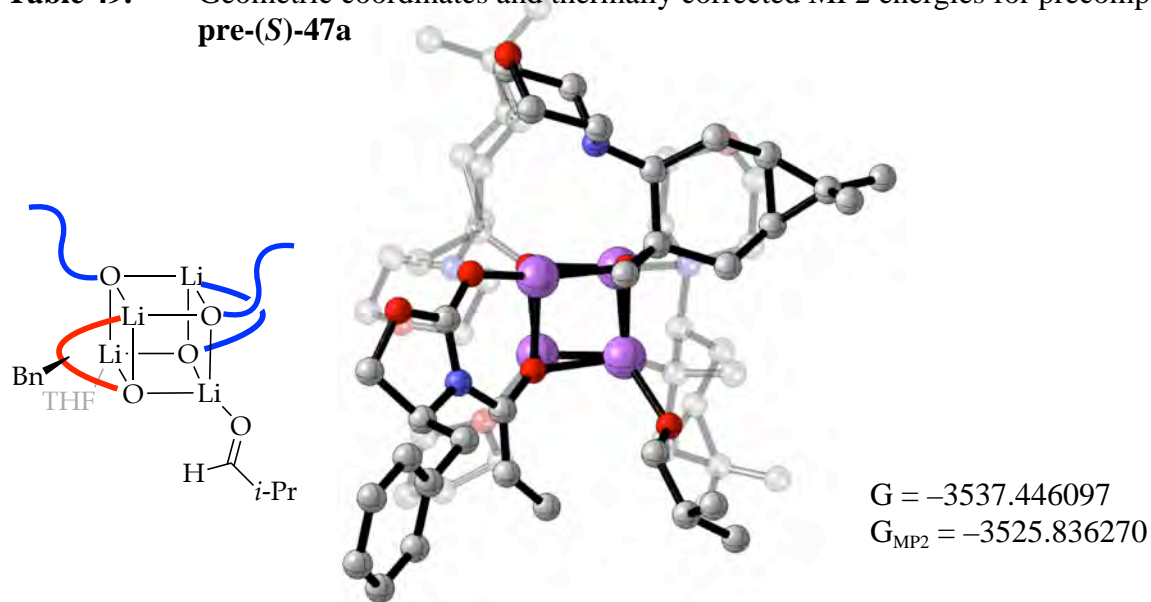


Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	H	2.25657100	-3.51833700	2.95927300
O	-0.64034500	-1.75668200	0.90262400	C	4.04436200	-3.72477400	4.07972200
Li	-0.11611200	-0.68678500	2.53304200	C	5.26668500	-2.85818200	4.32809100
Li	2.02723700	0.33578500	1.49525800	H	6.18269300	-3.16629300	3.82483000
O	1.71012900	-1.28233600	2.52387400	C	5.04604200	-1.35101000	4.33895400
Li	1.43306400	-2.06903200	0.78687100	H	6.00129000	-0.85175500	4.14167700
O	1.87864900	-0.54001000	-0.29580800	H	4.72362800	-0.99810200	5.32453900
O	0.17865700	1.05628100	1.61529600	C	4.00471400	-0.97521200	3.25658300
C	-1.71111800	-0.13703600	5.36739600	H	4.27306900	-1.53880600	2.35374800
H	-0.75557400	0.15892500	5.80972800	N	4.04632400	0.45520900	2.80518800
H	-2.23572700	0.76346500	5.03315300	C	5.21792500	0.67591400	1.92876000
C	-2.57427200	-0.98228200	6.31262100	H	5.15895200	-0.01034600	1.08030500
H	-3.27543600	-0.37055400	6.88794900	H	6.16362200	0.47319800	2.46116700
H	-1.94573500	-1.53278600	7.02242200	C	5.26305900	2.11207700	1.41690600
C	-3.26179700	-1.95827800	5.34679100	O	5.31775500	3.04387100	2.48640700
H	-3.61513300	-2.87315800	5.83215500	C	4.18673400	2.86764500	3.32535900
H	-4.11586600	-1.47820100	4.85421000	C	4.12400700	1.45221300	3.89617900
C	-2.14459500	-2.22136900	4.34131200	H	5.02252500	1.29585600	4.51590400
H	-2.48464700	-2.52282700	3.34894600	H	3.25187800	1.36551200	4.54426000
H	-1.44386600	-2.97859100	4.71822100	H	4.28121700	3.59630900	4.13691900
O	-1.45138500	-0.96101500	4.20278700	H	3.26598800	3.08716300	2.76192700
C	2.57028000	-1.50450300	3.60489900	H	4.38229900	2.31357300	0.78597400
C	2.67633400	-3.06950200	3.86312900	H	6.16434400	2.27002400	0.81666400
H	1.98989400	-3.34092000	4.67762600	C	4.77891300	-3.80653300	5.40880500

C	4.14415200	-3.30145800	6.69062100	H	1.13714900	5.45777800	6.11164800
H	3.54768500	-4.09628400	7.15783100	H	2.19291800	5.54177400	4.69136100
H	4.91232800	-3.00010200	7.41539300	H	1.50436800	3.34156500	3.98911900
H	3.48029300	-2.44945400	6.53581200	C	-2.14199100	1.62374700	1.80087400
C	5.62729900	-5.05086600	5.63019700	H	-2.28221400	0.77421200	2.47977100
H	6.44233700	-4.85393300	6.33972500	H	-2.88361100	2.38609100	2.07282600
H	5.02418900	-5.87323400	6.03803100	H	-2.34101700	1.28722400	0.78034300
H	6.07917300	-5.40227000	4.69552300	C	2.34690600	-0.52480000	-1.63097600
H	4.20704800	-4.58773600	3.43488800	C	2.05115600	0.86410600	-2.29004100
C	1.95085800	-0.82271200	4.84993100	H	1.98931800	0.73257900	-3.37619400
H	1.04598900	-1.36968200	5.13532200	H	1.04661100	1.16556700	-1.97704800
H	2.60923500	-0.78423500	5.72471300	C	3.06140200	1.95418000	-1.96872800
H	1.64562500	0.19909400	4.60676400	C	4.50779400	1.56277700	-2.21281400
C	-0.68521500	2.12923300	1.92252500	H	5.24457700	1.90046400	-1.48503000
C	-0.49415200	2.57471000	3.42380300	C	4.68881200	0.11624500	-2.64278700
H	-1.46905600	2.86955800	3.83065800	H	5.75424500	-0.14593500	-2.63462200
H	-0.19862500	1.67662800	3.97297300	H	4.34467800	-0.04692300	-3.67021900
C	0.51502600	3.68038600	3.69252100	C	3.91387200	-0.79590800	-1.65207400
C	0.44020500	4.87613800	2.76070500	H	4.22136100	-0.47905200	-0.65256000
H	1.38514300	5.30729200	2.42894500	N	4.29358400	-2.22823300	-1.73210400
C	-0.59687400	4.73243900	1.65907000	C	5.38656800	-2.58616800	-0.82700800
H	-0.48096800	5.54166400	0.92817700	H	5.12778800	-2.26740400	0.18836100
H	-1.61728000	4.82064500	2.04969100	H	6.34219900	-2.09618700	-1.10536900
C	-0.39804900	3.35898100	0.96427700	C	5.59749600	-4.09854100	-0.81989900
H	0.67702400	3.27223000	0.76805700	O	5.85830400	-4.60337000	-2.12457800
N	-1.03572600	3.26093000	-0.36963300	C	4.80646200	-4.25414800	-3.01295100
C	-0.20628800	3.82152200	-1.44174200	C	4.59567500	-2.74299300	-3.07036500
H	0.79412200	3.38486600	-1.39073400	H	5.51007700	-2.29181900	-3.49884300
H	-0.09796700	4.92147200	-1.35274500	H	3.76829400	-2.52293800	-3.75067500
C	-0.82085400	3.50729800	-2.80505000	H	5.09247600	-4.64050900	-3.99680000
O	-2.14128200	4.02623900	-2.91434200	H	3.86959100	-4.74397100	-2.69971000
C	-2.95834200	3.50316300	-1.87512600	H	4.70219000	-4.58214400	-0.39782000
C	-2.38289500	3.83315500	-0.49799900	H	6.46567800	-4.36460100	-0.20815100
H	-2.37625200	4.93403200	-0.38812400	C	3.87602300	2.65993500	-3.04826800
H	-3.04408600	3.42839200	0.26995700	C	3.58653000	2.48257000	-4.52900400
H	-3.94356500	3.96668900	-1.99611800	H	2.76730100	3.14193900	-4.84461000
H	-3.06002600	2.41199100	-1.98417000	H	4.47077900	2.74912100	-5.12273300
H	-0.83122500	2.41747300	-2.96023300	H	3.30755000	1.46212300	-4.80262800
H	-0.23717800	3.97538900	-3.60476000	C	4.32503500	4.07609000	-2.71498200
C	0.12045700	5.05189900	4.23260500	H	5.24466200	4.33778800	-3.25539300
C	-1.28551600	5.35570300	4.72011900	H	3.55652600	4.80918200	-2.99402200
H	-1.41750300	5.01871200	5.75711800	H	4.52390800	4.19616600	-1.64379000
H	-1.46920800	6.43789500	4.70069600	H	2.85056000	2.54656500	-1.07911100
H	-2.06797800	4.88427400	4.12042500	C	1.57520400	-1.57839300	-2.45414000
C	1.18378600	5.76330200	5.05757200	H	0.50450100	-1.35755900	-2.40541800
H	1.05033100	6.85273400	5.02161500	H	1.86428300	-1.57761800	-3.51325400

H 1.75470900 -2.57843500 -2.05230400
C -1.62516500 -2.53868200 0.57019200
N -2.59043000 -1.98649900 -0.38200600
C -3.99815400 -2.40725700 -0.45926000
C -4.41779500 -1.73914300 -1.77661000
H -4.32047100 -2.41651800 -2.63263100
H -5.42864100 -1.32921900 -1.75391500
O -3.48773100 -0.65693600 -1.94327400
C -2.37360800 -0.91054000 -1.20002600
O -1.38297000 -0.20679400 -1.32908100
H -4.07379700 -3.49243400 -0.55316100
C -4.80823400 -1.93733400 0.77202000
H -4.28449600 -2.30209800 1.66216400
H -4.78301400 -0.84142300 0.80645300
C -6.23677600 -2.43535000 0.76127900
C -6.52458200 -3.77578400 1.06084700
C -7.83451900 -4.25277400 1.02720300
C -8.88487500 -3.39437200 0.69351700
C -8.61439000 -2.05808300 0.39796300
C -7.30082100 -1.58486800 0.43191300
H -7.09975400 -0.53857000 0.21141700
H -9.42520400 -1.38035000 0.14419500
H -9.90631700 -3.76413700 0.66928400
H -8.03667400 -5.29352500 1.26670800
H -5.71354400 -4.44846500 1.33312900
C -1.86969000 -3.80236600 1.02359100
H -2.70988600 -4.35779900 0.62148500
C -1.04378100 -4.49889500 2.06751100
H -0.24498400 -3.85181300 2.44062600
H -1.65113600 -4.81580100 2.92822000
H -0.57167000 -5.41729800 1.68725800
O 1.89561200 -4.01723200 0.29534800
C 1.22436200 -4.82745000 -0.32541400
C 1.73418400 -6.16705700 -0.80118700
H 2.82796000 -6.14022900 -0.74170400
C 1.28637500 -6.41618300 -2.25178200
H 1.65796900 -7.38563000 -2.60032900
H 0.19233900 -6.42876800 -2.33085800
H 1.66550100 -5.64577400 -2.93160900
C 1.20947000 -7.27148900 0.14204900
H 0.11357400 -7.30834800 0.14235200
H 1.57667600 -8.24744400 -0.19369000
H 1.54849200 -7.11378100 1.17097500
H 0.16434400 -4.59747500 -0.55194800

Table 49. Geometric coordinates and thermally corrected MP2 energies for precomplex **pre-(S)-47a**

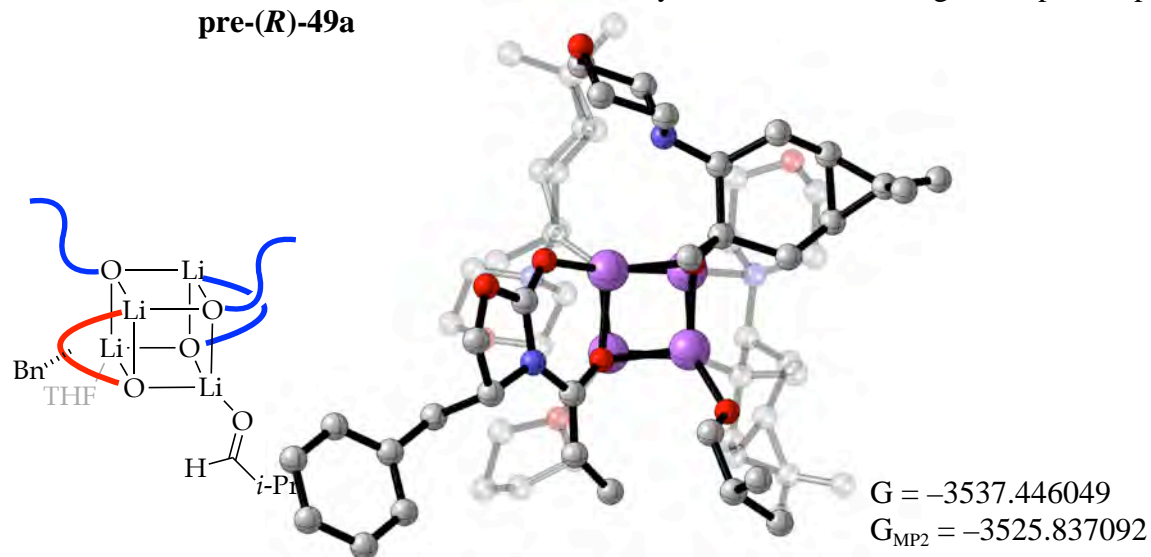


Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	H	1.65242000	-4.08304000	2.87330200
O	-0.81634900	-1.70497300	0.71066000	C	3.60587200	-4.63152500	3.54737700
Li	-0.00323400	-0.95915200	2.37718100	C	4.99094600	-4.02517400	3.68833800
Li	2.16490300	-0.14172100	1.31689500	H	5.76661600	-4.44658100	3.04922400
O	1.69502000	-1.82707000	2.19639400	C	5.05125700	-2.51015400	3.81566200
Li	1.15210800	-2.37750300	0.42103600	H	6.06490800	-2.17021800	3.57365300
O	1.75926400	-0.77042500	-0.51595600	H	4.86333800	-2.18325500	4.84418400
O	0.47216900	0.82135900	1.69492200	C	4.02136700	-1.88204800	2.84727100
C	1.63717700	-5.49667600	0.37061900	H	4.12760800	-2.41054600	1.89109100
H	2.69515200	-5.24333400	0.47956100	N	4.27790200	-0.44687800	2.49746900
H	1.22338500	-5.71242100	1.36421600	C	5.35820200	-0.34273800	1.49447700
C	1.37348000	-6.64984900	-0.59767400	H	5.07859800	-0.92509300	0.61241700
H	1.43553200	-7.62687500	-0.10868900	H	6.30966600	-0.74942000	1.88152800
H	2.09553900	-6.63376800	-1.42227200	C	5.58534200	1.11044000	1.08673500
C	-0.03449500	-6.31032900	-1.10864900	O	5.91337300	1.92625200	2.20079200
H	-0.26995100	-6.77512100	-2.07096000	C	4.88455800	1.84770500	3.17682900
H	-0.79146200	-6.62996700	-0.38294400	C	4.66579200	0.41024100	3.64000000
C	0.01453000	-4.78254600	-1.19875900	H	5.60292200	0.05704000	4.10127400
H	-0.94594700	-4.30269300	-0.99560600	H	3.89021000	0.39003200	4.40470400
H	0.38765500	-4.45154700	-2.17458400	H	5.20619900	2.47018100	4.01803700
O	0.95540600	-4.35303800	-0.18365000	H	3.94582800	2.26043500	2.77395300
C	2.53786200	-2.17182000	3.26262700	H	4.68449100	1.49944400	0.58585300
C	2.37993700	-3.71772700	3.60103000	H	6.42674700	1.18008100	0.39043800
H	1.89020400	-3.81736900	4.57851000	C	4.46522000	-4.95715600	4.76225800

C	4.08751300	-4.44632700	6.14048400	H	2.33075100	3.71970300	6.93695000
H	3.39413500	-5.14324600	6.62963300	H	3.38755100	3.80653300	5.51819900
H	4.97527500	-4.36337000	6.78135500	H	2.12255400	2.07841400	4.39878900
H	3.60071500	-3.46848100	6.12092100	C	-1.71410200	1.77188300	1.97415800
C	5.08227000	-6.34765100	4.80005300	H	-2.03272800	0.83439700	2.44287200
H	5.99811900	-6.35919400	5.40618400	H	-2.31669500	2.57433600	2.41798400
H	4.38703000	-7.07749500	5.23611100	H	-1.93064200	1.71588300	0.90505700
H	5.34550700	-6.69873700	3.79555500	C	2.08997000	-0.61547200	-1.88174200
H	3.52048600	-5.44995700	2.83358500	C	1.97413600	0.89176500	-2.30543000
C	2.09541900	-1.37608600	4.51390400	H	1.74200600	0.93898200	-3.37513100
H	1.10357000	-1.72202300	4.82314700	H	1.09510000	1.30868600	-1.80216400
H	2.76856100	-1.49481100	5.37295300	C	3.20110400	1.74283500	-2.01699000
H	2.00808600	-0.31108400	4.28495600	C	4.51012300	1.15779700	-2.51564900
C	-0.19775000	1.95260600	2.21257900	H	5.38093100	1.26530900	-1.86962300
C	-0.00338000	2.04777200	3.76952600	C	4.36873300	-0.22527400	-3.12874900
H	-0.86902200	2.56864700	4.19552400	H	5.36110800	-0.65612800	-3.31180400
H	-0.04702500	1.02789000	4.16678600	H	3.86920100	-0.18916500	-4.10349100
C	1.27178600	2.73543100	4.23088900	C	3.57505700	-1.12017300	-2.13759900
C	1.54513500	4.07598900	3.57324500	H	4.04638900	-0.97597600	-1.16196900
H	2.57643000	4.29671000	3.29709000	N	3.70542700	-2.57607400	-2.40782500
C	0.52612400	4.45974600	2.51227600	C	4.88526600	-3.16254500	-1.76694900
H	0.86827300	5.34930700	1.96952600	H	4.86019800	-2.93588700	-0.69502700
H	-0.43867500	4.72884300	2.95706700	H	5.83249500	-2.75636700	-2.17578800
C	0.35989900	3.27316000	1.52406500	C	4.89413600	-4.67976000	-1.94411600
H	1.37442400	2.98356100	1.22891700	O	4.84246000	-5.05839700	-3.31199800
N	-0.31572900	3.63759300	0.25652300	C	3.70296700	-4.49010800	-3.94386200
C	0.59740200	4.19220300	-0.74665400	C	3.69763200	-2.96861500	-3.82202400
H	1.44733100	3.51702700	-0.87244300	H	4.57969100	-2.58509500	-4.36683200
H	0.99409500	5.18388000	-0.44868700	H	2.80634100	-2.57360500	-4.31459100
C	-0.12017700	4.34191700	-2.08728100	H	3.75267600	-4.79134100	-4.99523000
O	-1.26928000	5.17359600	-1.97663900	H	2.77948300	-4.90221700	-3.50221600
C	-2.15784600	4.65738600	-0.99509600	H	4.03628900	-5.11200300	-1.40340600
C	-1.47264700	4.53412600	0.36525300	H	5.81626800	-5.10923500	-1.53889900
H	-1.18124300	5.54955100	0.69362700	C	3.98938500	2.44849800	-3.11688500
H	-2.18826100	4.14447200	1.09196700	C	3.49192100	2.52840100	-4.54992600
H	-2.99627900	5.35999700	-0.93930200	H	2.77726200	3.35372100	-4.66669800
H	-2.53788600	3.67108200	-1.30776600	H	4.33134700	2.72066300	-5.23096600
H	-0.41001400	3.34686700	-2.46085800	H	2.99710200	1.61718900	-4.89462200
H	0.53629900	4.81875400	-2.82274200	C	4.72718400	3.71110800	-2.69249600
C	1.26634100	4.01312400	5.06354100	H	5.60516800	3.88851500	-3.32794100
C	-0.00344200	4.58328900	5.67170500	H	4.07743400	4.59281800	-2.77150500
H	-0.23372000	4.08603100	6.62339900	H	5.07510100	3.64769100	-1.65511100
H	0.12367100	5.65335700	5.88195400	H	3.21711900	2.23318200	-1.04477200
H	-0.88100600	4.48189900	5.02873900	C	1.06931900	-1.39428800	-2.73651000
C	2.47481200	4.21495900	5.96722800	H	0.06379200	-1.02014500	-2.52292200
H	2.65044100	5.28147200	6.16181400	H	1.24073800	-1.27509700	-3.81413600

H 1.11268900 -2.45835600 -2.49372700
C -1.98246900 -2.25099200 0.53718600
N -2.85253200 -1.58393500 -0.42947400
C -4.25249300 -1.96077000 -0.67749200
C -4.48891100 -1.27073200 -2.02619900
H -4.27142800 -1.93184400 -2.87296100
H -5.49261900 -0.85804500 -2.13664200
O -3.54523900 -0.18750800 -2.03581600
C -2.52860800 -0.47858000 -1.17529700
O -1.53023200 0.22579200 -1.15932600
H -4.33843500 -3.04475800 -0.78195600
C -5.19586300 -1.46078800 0.44488300
H -4.80523100 -1.84135600 1.39462800
H -5.13245500 -0.36641100 0.48268200
C -6.63175700 -1.89620200 0.25075600
C -7.01243900 -3.22699400 0.48252500
C -8.32812900 -3.64193900 0.27877300
C -9.29129800 -2.73026400 -0.15993000
C -8.92868200 -1.40289800 -0.38949300
C -7.60964700 -0.99202400 -0.18556500
H -7.33743100 0.04738000 -0.35649500
H -9.67165100 -0.68394700 -0.72437100
H -10.3171610 -3.05227100 -0.31652100
H -8.60331500 -4.67640000 0.46719200
H -6.27240000 -3.94302300 0.83502600
C -2.46102000 -3.37329900 1.14985300
H -3.44913900 -3.74397800 0.90412800
C -1.65252800 -4.20145800 2.10943100
H -0.69001900 -3.73151400 2.32406900
H -2.17166300 -4.35637700 3.06774800
H -1.44716400 -5.20775600 1.71303700
O -1.28810900 -1.36263000 3.93094500
C -2.50348400 -1.44805000 3.99168800
H -3.12365700 -1.03591600 3.17373400
C -3.26574400 -2.07223700 5.13494500
H -3.84786900 -2.88595300 4.67022000
C -2.35311400 -2.64615800 6.21939300
H -2.94990100 -3.12976600 6.99996700
H -1.66030200 -3.38501800 5.80617100
H -1.75637500 -1.85539800 6.68622400
C -4.27905400 -1.04286300 5.68156300
H -4.91692400 -0.63825600 4.88745700
H -4.92779600 -1.51451900 6.42629300
H -3.76243600 -0.20568800 6.16470100

Table 50. Geometric coordinates and thermally corrected MP2 energies for precomplex **pre-(R)-49a**

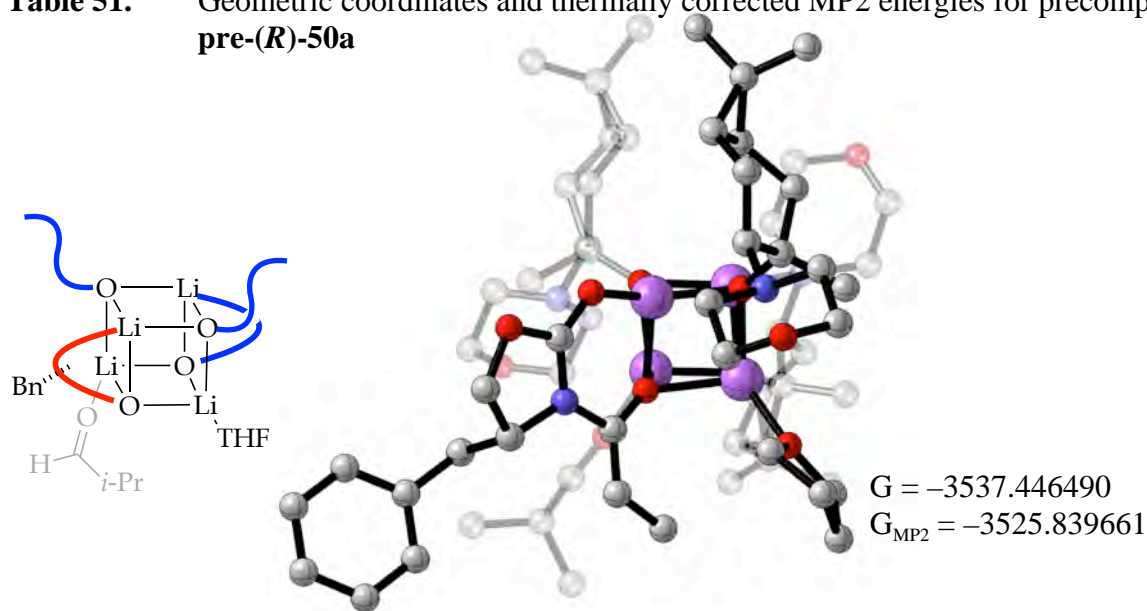


Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	C	2.55631200	5.52510600	-3.19334800
O	-1.13259100	1.18565400	-1.18252800	C	4.03466500	5.52200200	-2.84334100
Li	0.39741400	0.76506200	-2.40851000	H	4.35652100	6.26551400	-2.11436700
Li	2.24900200	0.97374500	-0.66510900	C	4.67998700	4.15656200	-2.65609700
O	1.48213800	2.26462300	-1.91757700	H	5.60812600	4.27513200	-2.08527300
Li	0.23320300	2.61947100	-0.47872700	H	4.97186500	3.71006600	-3.61295400
O	1.06046300	1.44568400	0.84904600	C	3.69405200	3.23316200	-1.90328100
O	1.26224900	-0.63393800	-1.33252400	H	3.28027300	3.82356800	-1.07564700
C	-0.45846500	5.68538500	-0.81302100	N	4.32498000	2.05439200	-1.22572100
H	0.59430600	5.85264200	-0.57034000	C	4.98289700	2.47098000	0.03049600
H	-0.57296700	5.69646600	-1.90494100	H	4.24160900	2.95242200	0.67411300
C	-1.41512100	6.67553400	-0.14995100	H	5.79181600	3.19891100	-0.16026500
H	-1.53797400	7.59267500	-0.73406300	C	5.57619700	1.26899900	0.76078600
H	-1.05326700	6.95009100	0.84755000	O	6.51435300	0.57099700	-0.04381100
C	-2.70049900	5.84060300	-0.04595700	C	5.89959300	0.15618400	-1.25527400
H	-3.39042700	6.20171400	0.72277900	C	5.34420300	1.34649700	-2.03185100
H	-3.23248900	5.83957800	-1.00453700	H	6.18833000	2.01106500	-2.28082200
C	-2.15670700	4.44418000	0.27257300	H	4.90669400	0.99964100	-2.96718500
H	-2.75147900	3.63423000	-0.15734100	H	6.67532000	-0.34825700	-1.84028800
H	-2.06150300	4.28757300	1.35289600	H	5.09387200	-0.56546000	-1.04580400
O	-0.83169700	4.38666100	-0.31113500	H	4.76692800	0.59020100	1.07324700
C	2.43170800	2.86637200	-2.75567800	H	6.11535700	1.59923600	1.65405900
C	1.82737600	4.19360200	-3.38816200	C	3.57725200	6.08306300	-4.17546200
H	1.64556700	4.02477900	-4.45763400	C	3.87270800	5.36917400	-5.48148700
H	0.83840700	4.28173500	-2.93383300	H	3.16591700	5.68763900	-6.25913200

H	4.88268900	5.61218600	-5.83709700	H	4.05960200	-1.20703600	-3.21324100
H	3.80063300	4.28169700	-5.40698200	C	-0.16350100	-2.43122100	-2.04342500
C	3.62365300	7.59814600	-4.31247400	H	-0.64630800	-1.73942500	-2.74220200
H	4.61509700	7.93627200	-4.64242000	H	-0.22355900	-3.43159000	-2.48993500
H	2.89066200	7.95105400	-5.05030000	H	-0.72230500	-2.42840400	-1.10544100
H	3.40332400	8.09602100	-3.36099300	C	0.95105800	1.48647200	2.25757000
H	1.95745800	6.28854400	-2.69789900	C	1.27512600	0.07781000	2.87268800
C	2.74227000	1.89265100	-3.91811400	H	0.72890200	-0.02660700	3.81675300
H	1.84883600	1.79162000	-4.54337200	H	0.84659200	-0.67893100	2.20688000
H	3.56253500	2.22393700	-4.56773300	C	2.75147700	-0.20288600	3.10934400
H	2.98198900	0.89657000	-3.53767900	C	3.48838700	0.88125200	3.87566900
C	1.29075600	-1.96346500	-1.81077000	H	4.49925700	1.12171700	3.54747800
C	2.00289500	-2.03603500	-3.21025000	C	2.63419700	2.10172900	4.17532800
H	1.59151100	-2.88796700	-3.76396600	H	3.25996300	2.90814400	4.57718300
H	1.70378500	-1.14545200	-3.77392800	H	1.88022300	1.89125200	4.94210700
C	3.51820600	-2.14995400	-3.17360100	C	1.96250900	2.55778400	2.85046700
C	4.05381800	-3.22256500	-2.24196600	H	2.76070800	2.57237300	2.10350000
H	4.94170100	-2.97961400	-1.65791300	N	1.45184600	3.95310100	2.88371300
C	2.97498000	-3.94736500	-1.45287200	C	2.48192000	4.93534000	2.53646900
H	3.43514700	-4.58572400	-0.68876000	H	2.91661500	4.67043000	1.56607600
H	2.38726400	-4.61613800	-2.09211700	H	3.30484800	4.96378100	3.27916900
C	2.05563400	-2.89634300	-0.77385800	C	1.87687600	6.33398100	2.43114900
H	2.72315000	-2.19443900	-0.26203600	O	1.21273800	6.72178500	3.62520200
N	1.19872600	-3.45653800	0.29816500	C	0.21592300	5.76971200	3.97357900
C	1.87707400	-3.54414800	1.59430300	C	0.81015400	4.37308400	4.13509700
H	2.31945700	-2.57496700	1.83665900	H	1.52307800	4.40719300	4.97939200
H	2.69227800	-4.29591600	1.58952700	H	0.01486200	3.67302800	4.40032400
C	0.87814500	-3.92291100	2.68713400	H	-0.22116400	6.11393000	4.91643900
O	0.23377100	-5.15883400	2.40316800	H	-0.57448100	5.74949200	3.20400000
C	-0.41525500	-5.09611300	1.14015000	H	1.17086400	6.35897000	1.58541700
C	0.57328700	-4.75613300	0.02551600	H	2.65946400	7.07962100	2.25631400
H	1.31891000	-5.57162100	-0.02814600	C	3.32050900	-0.49251600	4.49509900
H	0.04221500	-4.73009100	-0.92772700	C	2.43289000	-0.73176900	5.70423600
H	-0.85711600	-6.08418600	0.97218100	H	2.07540600	-1.76974800	5.72334300
H	-1.21999000	-4.34329700	1.16325000	H	3.00010200	-0.56205800	6.62882500
H	0.12816600	-3.12267400	2.79116400	H	1.55392100	-0.08354100	5.74037400
H	1.39058000	-4.05502800	3.64594300	C	4.57676400	-1.35263100	4.52390100
C	4.26987600	-3.35049300	-3.73855500	H	5.18209700	-1.13852300	5.41483800
C	3.58363000	-4.42501700	-4.56453600	H	4.32309200	-2.42080700	4.54428000
H	3.49494600	-4.10965500	-5.61271700	H	5.20650700	-1.17793600	3.64417900
H	4.17348400	-5.35087700	-4.54831600	H	3.28084100	-0.67068700	2.28060900
H	2.57985700	-4.67476900	-4.21228600	C	-0.50923400	1.80899500	2.63750500
C	5.68496500	-3.07116200	-4.22555000	H	-1.16955400	1.05221200	2.20271900
H	6.30745700	-3.97442100	-4.17378200	H	-0.67482000	1.80539900	3.72267800
H	5.68311800	-2.72800600	-5.26889000	H	-0.78921700	2.79036500	2.24744000
H	6.17462300	-2.29760900	-3.62268500	O	-0.41923700	0.55312700	-4.27433700

C -1.50256000 0.12047100 -4.63358200
H -2.08937400 -0.52620800 -3.95541200
C -2.12564200 0.37879600 -5.98402500
H -3.08056800 0.88126900 -5.75603600
C -1.26910800 1.28049300 -6.87378300
H -1.78770600 1.48791300 -7.81583800
H -1.05154400 2.23253800 -6.38106600
H -0.31243700 0.80194500 -7.10887100
C -2.46693700 -0.97369000 -6.64584800
H -3.07008200 -1.60894700 -5.98683800
H -3.03538200 -0.80940700 -7.56678600
H -1.55417400 -1.52197700 -6.90569000
C -4.65780700 0.06497600 -0.83781000
H -4.98156600 0.11088600 -1.88010600
C -4.86404400 -1.34291300 -0.26935300
H -4.84913700 -2.11191100 -1.05042700
H -5.77249400 -1.44633000 0.32541000
O -3.72938700 -1.53959000 0.59035400
C -2.72098600 -0.71604400 0.18538700
O -1.60787100 -0.83778300 0.67388300
N -3.19135100 0.16464200 -0.75732300
C -2.37165300 3.06823700 -3.13068900
H -2.56714600 3.00438200 -4.21158500
H -1.28923200 3.04430200 -2.98467900
H -2.72491800 4.06381800 -2.81980800
C -5.36586700 1.16736600 -0.01049100
H -4.97703900 2.13541500 -0.34208200
H -5.07528400 1.04505700 1.04007400
C -6.87258800 1.12818300 -0.14512400
C -7.67974700 0.62367600 0.88358200
C -9.06813600 0.56503400 0.74482100
C -9.67339700 1.01138300 -0.43011700
C -8.88201900 1.52097900 -1.46224900
C -7.49611100 1.57895500 -1.31869500
H -6.89001100 1.99056300 -2.12352900
H -9.34551400 1.87953800 -2.37765900
H -10.7535680 0.96858100 -0.53974400
H -9.67499500 0.17422700 1.55726800
H -7.21674000 0.28411300 1.80774100
C -3.04828200 1.96450500 -2.36586600
H -4.11536900 1.85266100 -2.51756700
C -2.39984400 1.16675200 -1.46606100

Table 51. Geometric coordinates and thermally corrected MP2 energies for precomplex **pre-(R)-50a**

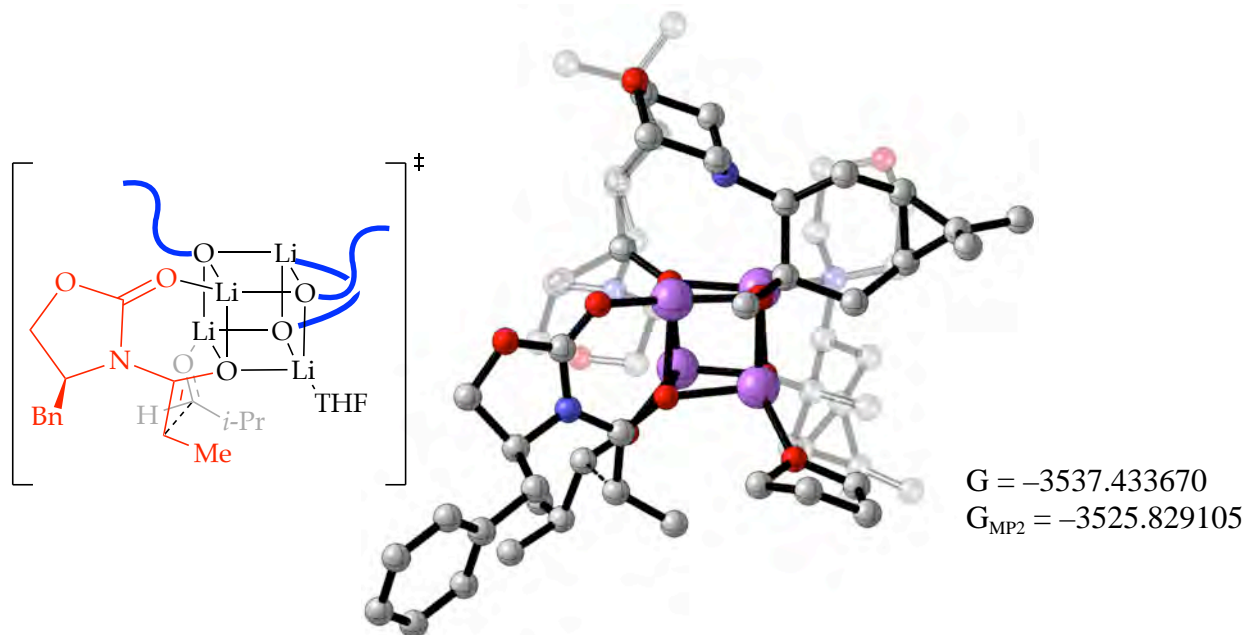


Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	H	5.55138700	-3.03457300	1.12767500
O	-1.29722100	-0.81350400	1.27581100	C	5.69318800	-1.06132500	0.29010400
Li	0.12651600	-0.09166100	2.60542500	O	6.64713300	-0.54504500	1.20595800
Li	2.08565600	-0.78422000	1.12195700	C	5.99580800	-0.08760100	2.38287200
O	1.17239800	-1.71884500	2.55444100	C	5.18546400	-1.19853600	3.04460600
Li	0.06024500	-2.38337000	1.14238700	H	5.88626000	-1.99239700	3.35363500
O	1.06714500	-1.65240300	-0.35147800	H	4.71084500	-0.80448500	3.94200400
O	1.11635600	0.93492900	1.24279600	H	6.78444500	0.25530700	3.06012900
C	2.05070300	-2.31294000	3.47086100	H	5.34240900	0.76726400	2.14715600
C	1.36572600	-3.53698100	4.20772100	H	5.02467800	-0.25457300	-0.05254600
H	1.56745300	-3.45516700	5.28243000	H	6.25675700	-1.43117800	-0.57214200
H	0.28884900	-3.37934000	4.09283100	C	2.57399300	-5.89129300	4.58413100
C	1.73089500	-4.94154900	3.73661900	C	2.97261800	-5.55171600	6.00936400
C	3.19287200	-5.18494200	3.39636000	H	2.16162400	-5.79708800	6.70791300
H	3.39281100	-5.81682100	2.53059700	H	3.85232500	-6.13654300	6.30818300
C	4.07139600	-3.94286200	3.45535600	H	3.21967900	-4.49691000	6.15348600
H	5.04272500	-4.15431400	2.99322300	C	2.29323000	-7.37553700	4.39735800
H	4.28482500	-3.63545700	4.48561800	H	3.17936100	-7.98047100	4.63171800
C	3.31736900	-2.82479000	2.69103000	H	1.48010500	-7.70937300	5.05585100
H	2.88282500	-3.30722700	1.80730400	H	1.99916000	-7.60263700	3.36607100
N	4.16332900	-1.73212800	2.11778900	H	0.99522500	-5.41793600	3.09172400
C	4.87178000	-2.19262800	0.90429000	C	2.38150300	-1.28268000	4.57332300
H	4.13574300	-2.53857700	0.17302800	H	1.47248400	-1.09385900	5.15309700

H	3.14858900	-1.63036500	5.27788600	C	-3.77004500	-6.09339100	0.68986100
H	2.69762000	-0.33022300	4.13854900	H	-4.19210800	-7.09079500	0.85223300
C	1.05914900	-2.17073900	-1.66655100	H	-4.58910000	-5.36756100	0.76607300
C	1.67762100	-1.13551000	-2.67170000	H	-3.37615200	-6.05717700	-0.33153900
H	1.24255000	-1.30782700	-3.66268900	C	-3.22482100	-5.91394700	3.16948200
H	1.32893300	-0.14175300	-2.36751100	H	-4.02719700	-5.18702900	3.34328000
C	3.19544300	-1.15627000	-2.77655700	H	-3.63886100	-6.91481700	3.33320300
C	3.79987100	-2.53251500	-2.99351400	H	-2.44010800	-5.74256400	3.91348100
H	4.71904600	-2.76660000	-2.45562900	H	-2.85824000	-3.60083300	1.45522500
C	2.77830600	-3.65682400	-2.98809100	C	-4.66394200	-0.29941100	-0.17296100
H	3.28940600	-4.62746600	-2.98747400	H	-5.28289100	-0.07301600	0.69749300
H	2.15879700	-3.64054000	-3.89163200	C	-4.83998400	0.79019400	-1.23900400
C	1.89750700	-3.52139300	-1.71679000	H	-5.19404500	1.73498900	-0.81105200
H	2.59252000	-3.40258300	-0.88103500	H	-5.49769400	0.49582300	-2.05818400
N	1.12830100	-4.74950000	-1.38863100	O	-3.51778900	0.99342500	-1.76298100
C	1.90330100	-5.69224400	-0.57610200	C	-2.60640000	0.55117300	-0.85243900
H	2.26820700	-5.17574600	0.31801000	O	-1.41807200	0.79218500	-1.02265500
H	2.78225500	-6.09019800	-1.12240200	N	-3.23811900	-0.13218500	0.15148800
C	1.03088300	-6.86583400	-0.13615000	C	-2.90144800	-1.78985700	3.59590000
O	0.44344900	-7.53948500	-1.24315400	H	-3.07691400	-1.15328300	4.47606800
C	-0.30671100	-6.63019700	-2.03509600	H	-1.82609500	-1.98045400	3.54066200
C	0.55851900	-5.47439800	-2.53036700	H	-3.40522400	-2.74506600	3.81043600
H	1.33863000	-5.89841000	-3.18856500	C	-4.97597800	-1.72707400	-0.68087700
H	-0.05485900	-4.80147500	-3.13400000	H	-4.59485600	-2.42820500	0.06910200
H	-0.69824500	-7.20673500	-2.87965600	H	-4.40820800	-1.89798600	-1.60356100
H	-1.15650700	-6.23183300	-1.45448000	C	-6.45178500	-1.96153600	-0.91763400
H	0.24563900	-6.49429600	0.53983000	C	-6.98060200	-2.01235200	-2.21435400
H	1.63160200	-7.61240300	0.39416900	C	-8.34734900	-2.20740600	-2.42537900
C	3.92890900	-1.47726100	-4.07516500	C	-9.20945900	-2.35420900	-1.33850800
C	3.20957300	-1.59506800	-5.40828700	C	-8.69589100	-2.30857800	-0.04016700
H	3.06226900	-0.60341500	-5.85575000	C	-7.33038600	-2.11514600	0.16593200
H	3.80923800	-2.18783800	-6.11154800	H	-6.93778800	-2.09230700	1.18077600
H	2.22767700	-2.07020800	-5.33965900	H	-9.35905700	-2.42912300	0.81247300
C	5.31088800	-0.85584900	-4.22220000	H	-10.2728530	-2.50766900	-1.50045700
H	5.94807400	-1.45928700	-4.88260500	H	-8.73578600	-2.24810500	-3.43954600
H	5.24615200	0.15237300	-4.65157000	H	-6.31339500	-1.91052000	-3.06767100
H	5.82061900	-0.77041300	-3.25569400	C	-3.40784900	-1.15789300	2.33031200
H	3.72446100	-0.48581900	-2.10286800	H	-4.47716700	-0.99260500	2.26665600
C	-0.40451200	-2.38974300	-2.10775800	C	-2.59299800	-0.73405700	1.32144000
H	-0.93255900	-1.43181700	-2.07745100	C	-0.71399200	0.46006900	5.64005900
H	-0.48380300	-2.77177500	-3.13335700	H	-0.79987500	-0.62100700	5.78663000
H	-0.90457100	-3.09309800	-1.43518900	H	0.25934300	0.79056300	6.02215000
O	-0.92539400	-4.16075200	1.43780200	C	-1.86566300	1.24605600	6.27703000
C	-2.11588400	-4.42080000	1.52103300	H	-1.63695600	1.55876500	7.30042100
C	-2.67333400	-5.80784900	1.73166300	H	-2.77729900	0.63754500	6.30526900
H	-1.84807600	-6.51801100	1.61029000	C	-2.04012100	2.41981400	5.30140000

H -3.03174000 2.87967300 5.35299800
H -1.29347800 3.19851300 5.49922500
C -1.77117100 1.75241200 3.95368200
H -1.36054100 2.42474300 3.19627100
H -2.66657500 1.25514400 3.55996500
O -0.76733000 0.74167600 4.22539900
C 1.61768500 2.25567800 1.30116300
C 2.99928200 2.32492000 0.57246800
H 3.53376900 3.22430400 0.90052500
H 3.59528500 1.47833000 0.93381700
C 2.89655000 2.29846800 -0.94191200
C 1.96032000 3.34652500 -1.51562200
H 1.30680800 3.03944900 -2.33197500
C 1.27820500 4.19309800 -0.45551100
H 0.52557000 4.84154900 -0.92062600
H 1.99089300 4.86221600 0.03806400
C 0.59629500 3.25569300 0.57947100
H -0.03563900 2.58177800 -0.00308700
N -0.36037300 3.97197300 1.47372600
C -1.66046600 4.17249500 0.81699600
H -2.04492000 3.20007200 0.49128800
H -1.57791200 4.81385100 -0.08111100
C -2.66410700 4.81698700 1.77270600
O -2.18451200 6.04480300 2.30168800
C -0.93414500 5.85144300 2.94977400
C 0.10241900 5.26625400 1.99398400
H 0.26696000 6.00415100 1.18885900
H 1.04893000 5.13741300 2.52467300
H -0.61554300 6.83717500 3.30364000
H -1.05788400 5.18816400 3.82266600
H -2.89880400 4.12205700 2.59606200
H -3.59440500 5.05096500 1.24436900
C 3.44229200 3.40261300 -1.83860600
C 4.34501700 4.50556600 -1.31274900
H 5.38900800 4.16679300 -1.28333500
H 4.30168400 5.38142400 -1.97366000
H 4.08454300 4.84496400 -0.30721000
C 3.81763900 2.97750300 -3.25144700
H 3.73095500 3.81864900 -3.95251300
H 4.85380900 2.61587400 -3.29269500
H 3.17059600 2.17124800 -3.61467700
H 2.85725900 1.30860000 -1.38645800
C 1.87886800 2.62132300 2.77643900
H 2.54644000 1.86629200 3.20899100
H 2.36807700 3.59594900 2.89607800
H 0.95023000 2.62410300 3.35120600

Table 52. Geometric coordinates and thermally corrected MP2 energies for transition state (*S*)-48a

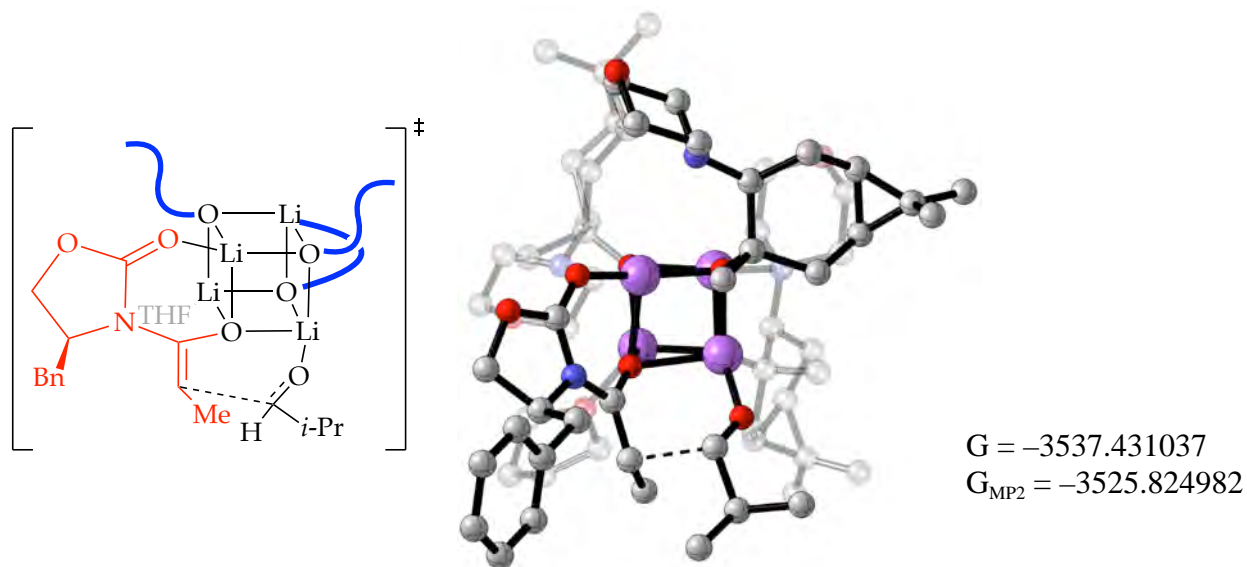


Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	H	0.98533800	3.96443400	-4.54260400
O	-1.31387000	0.93228400	-1.35221500	H	0.66025900	4.26769100	-2.85355200
Li	0.22059500	0.54565100	-2.59195100	C	2.27451100	5.43185900	-3.58853400
Li	2.15168600	0.95472900	-0.92970700	C	3.78402600	5.39900100	-3.41945700
O	1.30426700	2.09161600	-2.24491100	H	4.21184700	6.17605900	-2.78667500
Li	0.22834500	2.71640000	-0.74531000	C	4.42440600	4.02994700	-3.22722300
O	1.01861500	1.56261300	0.60036200	H	5.39152900	4.16009800	-2.72848200
O	1.16301100	-0.71136600	-1.36101800	H	4.64811900	3.54781800	-4.18516500
C	-0.21802000	-0.28828500	-5.73405700	C	3.49337000	3.13997300	-2.36953900
H	-0.30138200	0.68206500	-6.23747300	H	3.15278400	3.76388900	-1.53405700
H	0.84018700	-0.54142800	-5.63839500	N	4.16343800	1.98241300	-1.69326500
C	-1.03816200	-1.38474300	-6.45412500	C	4.95276900	2.44663500	-0.53142900
H	-0.39679800	-2.13571900	-6.92358600	H	4.29534100	2.99275800	0.14988100
H	-1.66061500	-0.94329300	-7.23953600	H	5.76147900	3.13166900	-0.84045700
C	-1.91771300	-1.97552500	-5.33488400	C	5.57888500	1.26795700	0.20724700
H	-2.88246500	-2.34245600	-5.69835400	O	6.42511800	0.50907000	-0.64279300
H	-1.40354100	-2.79798000	-4.82671400	C	5.68989100	0.04556100	-1.76581500
C	-2.05461300	-0.78805100	-4.38816700	C	5.07648000	1.20024500	-2.55415300
H	-2.28966800	-1.04772900	-3.35493700	H	5.89830600	1.82692200	-2.93880500
H	-2.80680900	-0.07369500	-4.75508300	H	4.53070000	0.80180100	-3.40954400
O	-0.75337200	-0.17627800	-4.39430900	H	6.39674000	-0.50640300	-2.39385400
C	2.16607900	2.77069600	-3.11767700	H	4.89770800	-0.64604600	-1.44018100
C	1.47312400	4.12523600	-3.57069500	H	4.78592100	0.62518200	0.62340600

H	6.20260000	1.62586900	1.03216200	C	5.39172300	-3.55655200	-4.27968000
C	3.17816200	5.89668700	-4.71964000	H	6.02922000	-4.44056500	-4.14614900
C	3.29063000	5.11113300	-6.01230800	H	5.27476600	-3.39120500	-5.35919600
H	2.52224100	5.44106900	-6.72399100	H	5.93042800	-2.69525900	-3.86832400
H	4.26736300	5.27472300	-6.48735000	H	3.85664000	-1.54435500	-3.40976100
H	3.16194600	4.03629400	-5.87721500	C	-0.19282100	-2.67658200	-1.62459100
C	3.24707400	7.40065800	-4.94666500	H	-0.77667400	-2.15197700	-2.38670200
H	4.19485900	7.68659200	-5.42263300	H	-0.21841100	-3.74502400	-1.87358600
H	2.43202700	7.73908900	-5.60019900	H	-0.67765900	-2.52825300	-0.65667300
H	3.16851600	7.95500400	-4.00458100	C	0.99516100	1.95226600	1.96134100
H	1.76327000	6.24473000	-3.07391900	C	1.45208700	0.76607900	2.88185700
C	2.39090300	1.86259800	-4.35104800	H	0.94364300	0.85792500	3.84829400
H	1.46501800	1.83165300	-4.93544800	H	1.06297900	-0.15498700	2.43431100
H	3.19106700	2.18807700	-5.02473200	C	2.95167100	0.64856000	3.11115500
H	2.61267300	0.83938700	-4.03199200	C	3.64514500	1.94023100	3.50706200
C	1.23867100	-2.09811100	-1.61975200	H	4.62578700	2.13115800	3.07005900
C	1.82379300	-2.35983200	-3.05803700	C	2.73046800	3.15419900	3.51829200
H	1.37132100	-3.27552500	-3.45691700	H	3.32362800	4.06901700	3.63811800
H	1.45914200	-1.54910200	-3.69597800	H	2.03377900	3.12957300	4.36388400
C	3.33723200	-2.46776700	-3.16104400	C	1.95803100	3.19450200	2.17249100
C	3.98552900	-3.37924900	-2.13424900	H	2.71104300	3.04962900	1.39295400
H	4.92844200	-3.04872900	-1.69914100	N	1.33625600	4.50189100	1.86065500
C	3.01134700	-3.96075300	-1.12241000	C	2.21361600	5.40609100	1.11528100
H	3.56356900	-4.46179500	-0.31828300	H	2.60362500	4.88353300	0.23561300
H	2.36924000	-4.72621800	-1.57289800	H	3.07981900	5.74753800	1.71854200
C	2.15452000	-2.80518200	-0.53580400	C	1.42861800	6.62994000	0.64752000
H	2.86303600	-2.01720400	-0.25618500	O	0.84519900	7.32610300	1.74232200
N	1.45294600	-3.15040200	0.72445300	C	-0.00044300	6.45922200	2.48827800
C	2.29296200	-2.96384500	1.91193400	C	0.75991100	5.23497100	2.99305900
H	2.70219700	-1.94990700	1.90392800	H	1.53581700	5.58191600	3.70062700
H	3.14557400	-3.67195700	1.93603000	H	0.07231300	4.59027000	3.54526300
C	1.46840100	-3.15850900	3.18385700	H	-0.37760700	7.04886900	3.33059700
O	0.86234400	-4.44408000	3.22498700	H	-0.85096500	6.13546700	1.86995700
C	0.04706500	-4.63768200	2.07746800	H	0.64749000	6.30627100	-0.05836500
C	0.85778800	-4.49213700	0.79107100	H	2.09050000	7.34374400	0.14592000
H	1.62722000	-5.28623200	0.78335900	C	3.58770900	0.78725800	4.49082200
H	0.20140400	-4.65810400	-0.06500300	C	2.75869900	0.85406800	5.76212800
H	-0.36338400	-5.64980400	2.15779400	H	2.48203000	-0.15429700	6.09690200
H	-0.78489400	-3.91429500	2.07522600	H	3.33884300	1.32139000	6.56853500
H	0.69376100	-2.37745800	3.24355200	H	1.83488300	1.42728500	5.65344600
H	2.10845500	-3.08825100	4.06926600	C	4.89458100	0.03325700	4.69407700
C	4.04054200	-3.74732700	-3.60458700	H	5.51660300	0.51864400	5.45798700
C	3.28177300	-4.93621200	-4.16876300	H	4.70871900	-0.99755300	5.02402900
H	3.07164600	-4.78952900	-5.23675200	H	5.48159100	-0.01590200	3.76975700
H	3.88358400	-5.84954800	-4.07519800	H	3.48452100	-0.00285500	2.42079200
H	2.32771300	-5.12562300	-3.67057000	C	-0.45934400	2.28473000	2.35830200

H -1.07150000 1.38538900 2.23663300
H -0.54924200 2.59529800 3.40716000
H -0.85662400 3.07814800 1.71918500
C -2.51860100 1.27833000 -1.23749600
N -3.28711400 0.65787300 -0.19884800
C -4.75511000 0.73444800 -0.07578700
C -4.93353300 0.18876000 1.34693100
H -4.93223800 0.98440300 2.09929200
H -5.82376800 -0.42902300 1.46783600
O -3.77351900 -0.63828400 1.55975200
C -2.78090200 -0.24208300 0.72685000
O -1.64945700 -0.67235300 0.85329000
H -5.08633800 1.77280300 -0.12937700
C -5.46814100 -0.11369300 -1.15656200
H -5.11688700 0.22609500 -2.13755500
H -5.14478200 -1.15588500 -1.04382400
C -6.97719000 -0.02148400 -1.07639100
C -7.64360200 1.14407500 -1.48392700
C -9.03108200 1.24545300 -1.38859600
C -9.77925500 0.17880900 -0.88488300
C -9.13024000 -0.98794000 -0.48074700
C -7.74032000 -1.08496200 -0.57623900
H -7.24280800 -2.00249600 -0.26903800
H -9.70375700 -1.82600800 -0.09401200
H -10.8605750 0.25616600 -0.81283800
H -9.52889600 2.15557800 -1.71227300
H -7.07234300 1.97764800 -1.88790600
C -3.11481900 2.34385100 -1.95879800
H -4.19567900 2.40031700 -1.91114100
C -2.50485600 2.74302100 -3.28488700
H -1.47920200 3.09467500 -3.14112500
H -2.47452700 1.91741900 -4.00410300
H -3.08305600 3.55447900 -3.73927000
O -1.21468200 3.92981100 -0.86509500
C -2.47700800 3.85996600 -0.72158600
C -3.32939400 5.06592100 -1.17570300
H -3.09336500 5.26571200 -2.22788200
C -2.87350900 6.29024000 -0.35708300
H -3.40480100 7.19206700 -0.68433600
H -3.08575700 6.14888400 0.71111900
H -1.79991900 6.45606300 -0.46961000
C -4.84218400 4.86678900 -1.01432100
H -5.08369200 4.48680200 -0.01167400
H -5.37103200 5.81951100 -1.13189100
H -5.26133700 4.17371700 -1.75132400
H -2.86970600 3.41938400 0.22074900

Table 53. Geometric coordinates and thermally corrected MP2 energies for transition state (S)-47a

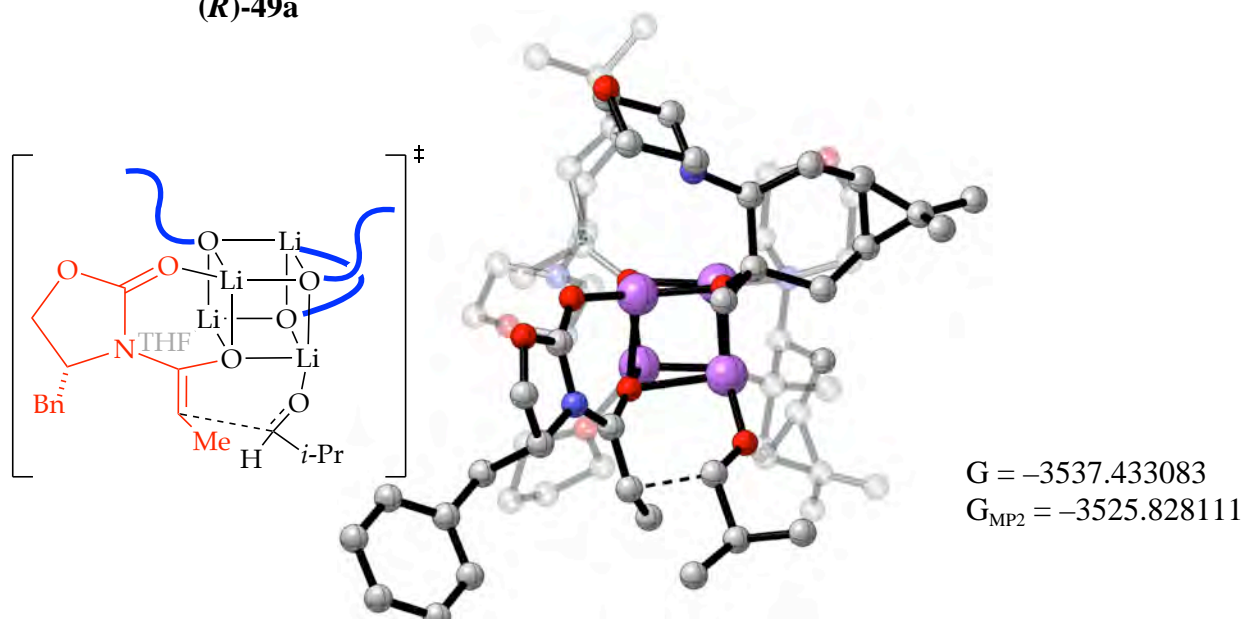


Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	H	1.74618600	-4.23941400	2.59388000
O	-0.84214000	-1.84923300	0.57285400	C	3.68916300	-4.78032200	3.30569400
Li	0.04449800	-1.11499500	2.40362500	C	5.05347700	-4.15104900	3.52876100
Li	2.15635000	-0.19920200	1.31342000	H	5.86062200	-4.51683100	2.89427400
O	1.75752500	-1.94440300	2.05010000	C	5.07202200	-2.64365100	3.74171700
Li	1.27330700	-2.41610500	0.27495100	H	6.08445300	-2.26805000	3.55326600
O	1.72817400	-0.73378800	-0.57710500	H	4.84019500	-2.37846000	4.77903200
O	0.44940600	0.69117900	1.72453100	C	4.05842200	-1.98993400	2.77328500
C	1.66758500	-5.53658600	0.06980800	H	4.20843100	-2.46817800	1.79662700
H	2.72870800	-5.32527100	0.22506900	N	4.28728200	-0.53373300	2.50079300
H	1.21192400	-5.78141900	1.03725900	C	5.37644300	-0.35637100	1.51810300
C	1.39950300	-6.63071900	-0.96338100	H	5.11689600	-0.89450700	0.60178800
H	1.40682900	-7.63147500	-0.52123000	H	6.33064600	-0.76802300	1.89347100
H	2.15264700	-6.60238000	-1.75913600	C	5.58188500	1.12056500	1.19188300
C	0.02473900	-6.21510000	-1.50831000	O	5.88050200	1.88046200	2.35217400
H	-0.19087300	-6.62474000	-2.49969300	C	4.83993700	1.73306300	3.30823200
H	-0.76933000	-6.53963500	-0.82561100	C	4.64196100	0.26930300	3.69210900
C	0.13569500	-4.68798300	-1.52308900	H	5.57933900	-0.08952900	4.14808100
H	-0.81420500	-4.17638100	-1.34381700	H	3.85602000	0.19236300	4.44304700
H	0.55864300	-4.32640000	-2.46683100	H	5.13931200	2.31573100	4.18524400
O	1.04388000	-4.34227700	-0.45183000	H	3.90009800	2.15134700	2.91405700
C	2.57140400	-2.33580200	3.12478300	H	4.67956800	1.51965700	0.70098900
C	2.43847600	-3.90046100	3.36711600	H	6.43000700	1.24296400	0.51101400
H	1.91586600	-4.06737900	4.31767200	C	4.51526700	-5.15422700	4.52973300

C	4.07923500	-4.72902200	5.91953800	H	2.26611800	3.37545300	7.11745100
H	3.38171400	-5.46319500	6.34370800	H	3.30769200	3.58435300	5.70003600
H	4.94224900	-4.66744800	6.59553400	H	2.10561600	1.86649900	4.49602900
H	3.57588800	-3.75974200	5.93564600	C	-1.75745600	1.55875600	2.11128800
C	5.16394200	-6.53058300	4.51212400	H	-2.03121900	0.59569100	2.55338000
H	6.05731100	-6.55670300	5.15041400	H	-2.36775800	2.32748900	2.60182500
H	4.47085000	-7.29870900	4.88045200	H	-1.99948400	1.54694700	1.04557400
H	5.47157000	-6.81834500	3.50002700	C	2.07698900	-0.47763200	-1.92326100
H	3.64877300	-5.55951400	2.54500400	C	1.95578300	1.05603500	-2.23833200
C	2.06455100	-1.62428800	4.40170100	H	1.71971100	1.17878200	-3.30116700
H	1.05668800	-1.98802700	4.63240000	H	1.07669000	1.43261200	-1.70381500
H	2.69187800	-1.80405300	5.28412800	C	3.17912400	1.89159200	-1.89464400
H	1.99207100	-0.54493100	4.24507600	C	4.49206700	1.34514000	-2.42724000
C	-0.24253300	1.77284000	2.32384600	H	5.36111500	1.41621100	-1.77374700
C	-0.02421400	1.78208900	3.88040800	C	4.35856100	0.00144700	-3.12527700
H	-0.90361900	2.23927900	4.34721700	H	5.35327900	-0.41249800	-3.33189500
H	-0.02980400	0.74036300	4.21738700	H	3.85961400	0.09428500	-4.09664800
C	1.22698600	2.49542500	4.36799800	C	3.56764500	-0.95267900	-2.18931300
C	1.43920900	3.88092800	3.78304600	H	4.02958900	-0.85166400	-1.20325000
H	2.45810100	4.15940300	3.51260100	N	3.71336300	-2.39238500	-2.52695500
C	0.39591300	4.27937000	2.75110500	C	4.89251700	-2.99802400	-1.90179500
H	0.69672800	5.21059100	2.25576900	H	4.85515900	-2.82154600	-0.82091000
H	-0.57553200	4.48243600	3.21579100	H	5.83965600	-2.56524300	-2.28205500
C	0.27265400	3.13995700	1.70404200	C	4.91644200	-4.50499900	-2.14852700
H	1.29754500	2.90039400	1.39909600	O	4.88168800	-4.82015100	-3.53299900
N	-0.40872200	3.54444000	0.44943500	C	3.74479800	-4.23258700	-4.15066900
C	0.49063200	4.20278400	-0.50332200	C	3.72330500	-2.71833800	-3.95820800
H	1.37186400	3.57538700	-0.66069300	H	4.60692600	-2.30200900	-4.47566300
H	0.83998300	5.18863200	-0.13596600	H	2.83309300	-2.30907100	-4.44112100
C	-0.21696500	4.41135200	-1.84137500	H	3.80866200	-4.48393500	-5.21426700
O	-1.40128800	5.18492800	-1.69357000	H	2.82002100	-4.67321700	-3.73955800
C	-2.27796700	4.57037200	-0.75894300	H	4.05676100	-4.96861600	-1.63737900
C	-1.60373900	4.38447700	0.59940200	H	5.83801100	-4.94520500	-1.75400600
H	-1.35735200	5.38639400	0.99765800	C	3.96506100	2.66749100	-2.94810000
H	-2.30983300	3.91831900	1.28872800	C	3.46789800	2.83150300	-4.37414600
H	-3.14491400	5.23354200	-0.66862500	H	2.74359100	3.65392100	-4.44019500
H	-2.61477100	3.59258400	-1.14129800	H	4.30533600	3.07566000	-5.04068600
H	-0.46032200	3.43238100	-2.28508700	H	2.98437500	1.93754500	-4.77564500
H	0.42756400	4.96238300	-2.53433000	C	4.69396400	3.90613500	-2.44507500
C	1.17574000	3.72484300	5.26922000	H	5.57074000	4.12952600	-3.06749900
C	-0.11204900	4.20615600	5.91509900	H	4.03783500	4.78626300	-2.46874300
H	-0.31682900	3.64364400	6.83557500	H	5.04216300	3.78005200	-1.41354600
H	-0.02643200	5.26608100	6.18858300	H	3.19050600	2.32205000	-0.89426000
H	-0.98894700	4.10763800	5.27087200	C	1.07154300	-1.19479500	-2.84723200
C	2.38185400	3.92837800	6.17556800	H	0.06193900	-0.83230000	-2.62941900
H	2.51372800	4.98927200	6.42723600	H	1.26370900	-1.00454200	-3.91105600

H 1.10539100 -2.27285900 -2.67520200
C -2.04949900 -2.21205200 0.61610400
N -2.97055500 -1.52136700 -0.24264900
C -4.37790100 -1.89624600 -0.48604700
C -4.55919600 -1.35323000 -1.90990500
H -4.32241500 -2.09916300 -2.67665800
H -5.55087100 -0.94033700 -2.09536900
O -3.59841100 -0.28392200 -2.00286900
C -2.61142200 -0.48848400 -1.09750600
O -1.60473200 0.19432500 -1.10767200
H -4.48005000 -2.98334300 -0.46878200
C -5.34589900 -1.25079600 0.53273500
H -5.02882500 -1.54395500 1.53790100
H -5.23379800 -0.16166600 0.47094500
C -6.78982300 -1.64305100 0.29800600
C -7.70191100 -0.73752400 -0.26072300
C -9.02727900 -1.10799600 -0.49829000
C -9.46116800 -2.39501300 -0.17990600
C -8.56405700 -3.30633800 0.38187100
C -7.24168300 -2.93209500 0.61908300
H -6.55593900 -3.64509500 1.07196100
H -8.89633900 -4.30782100 0.64207700
H -10.4923050 -2.68518000 -0.36177100
H -9.71946200 -0.38873100 -0.92771000
H -7.37397100 0.27179200 -0.50041400
C -2.55324400 -3.19492300 1.50589700
C -1.61761100 -4.31335000 1.91722700
H -1.25001600 -4.88730800 1.05757900
H -0.74701300 -3.91389000 2.44598600
H -2.13130200 -5.01405000 2.58358200
H -3.58398800 -3.49444300 1.34631600
O -1.37047600 -1.70905500 3.47904200
C -2.57650000 -2.04421600 3.27163200
H -3.27228800 -1.27589400 2.87666200
C -3.25012200 -2.96232700 4.30844700
H -2.59525800 -3.82966400 4.45353500
C -3.28604100 -2.18020200 5.63923000
H -3.70687200 -2.80150200 6.43893200
H -2.28014600 -1.86665300 5.92900900
H -3.91112700 -1.28165900 5.55091500
C -4.65923600 -3.43762000 3.93681500
H -4.65872600 -4.13691400 3.09423900
H -5.12589000 -3.95125400 4.78535900
H -5.30900200 -2.59111300 3.67807000

Table 54. Geometric coordinates and thermally corrected MP2 energies for transition state **(R)-49a**

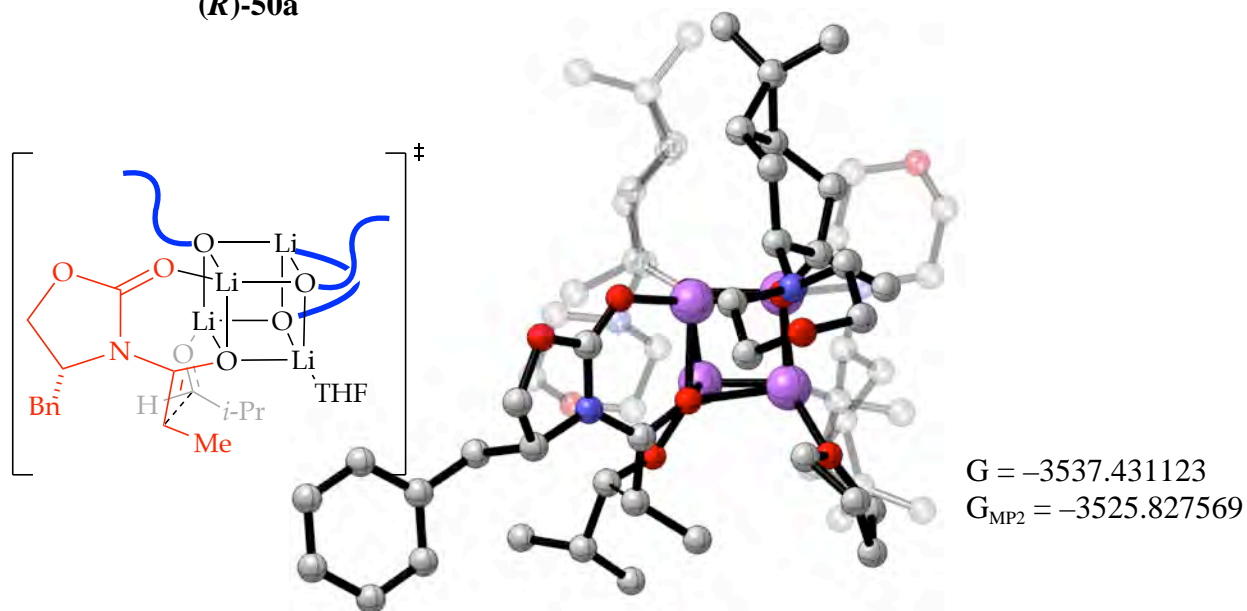


Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	H	-0.90391500	-4.28291200	-2.88986300
O	1.20416500	-1.41699000	-0.96338000	C	-2.68461100	-5.32998800	-3.43598400
Li	-0.16957200	-0.80269100	-2.53513200	C	-4.18971200	-5.14423800	-3.34719600
Li	-2.21175100	-0.71446100	-0.99729400	H	-4.71780200	-5.82005400	-2.67471400
O	-1.46721600	-2.15951400	-2.05427200	C	-4.69214400	-3.70815900	-3.29689200
Li	-0.54425700	-2.63547800	-0.45540600	H	-5.70987400	-3.69988400	-2.89004400
O	-1.30910800	-1.28220200	0.70182300	H	-4.76466200	-3.27015800	-4.29827000
O	-0.93705000	0.70493800	-1.51671000	C	-3.74475200	-2.87313700	-2.40493700
C	-0.04282100	-5.73972100	-0.61460500	H	-3.55095800	-3.47415700	-1.50696700
H	-1.13033800	-5.82485400	-0.54553300	N	-4.33380400	-1.60281500	-1.87008600
H	0.24544700	-5.76454000	-1.67305500	C	-5.20925900	-1.88557700	-0.71397200
C	0.71535900	-6.79433100	0.18972000	H	-4.62580500	-2.40512200	0.05164000
H	0.86463400	-7.72061000	-0.37312900	H	-6.05504300	-2.53852300	-0.99599900
H	0.17586300	-7.03650200	1.11252900	C	-5.77167800	-0.59372200	-0.12662300
C	2.02468900	-6.05736900	0.50936600	O	-6.50362100	0.14836300	-1.08931500
H	2.55245100	-6.46674400	1.37591900	C	-5.67553300	0.44173900	-2.20565800
H	2.70325000	-6.09654100	-0.35090000	C	-5.13609100	-0.83358700	-2.84687000
C	1.53752200	-4.62555600	0.75090900	H	-5.99800500	-1.42025800	-3.20579400
H	2.25794400	-3.86050400	0.44817900	H	-4.52466300	-0.57770600	-3.71183200
H	1.27247500	-4.46244500	1.80110200	H	-6.29962800	0.98792000	-2.92009700
O	0.34341200	-4.46681800	-0.05166800	H	-4.84171700	1.09343700	-1.89953400
C	-2.32205400	-2.68845400	-3.03341900	H	-4.94907600	0.01898900	0.27626000
C	-1.77735000	-4.09976900	-3.51871900	H	-6.46644900	-0.82026900	0.68809500
H	-1.38488700	-3.99642800	-4.53859600	C	-3.58273300	-5.79863700	-4.57296700

C	-3.56254700	-5.09632700	-5.91808700	H	-4.54901600	3.11920200	-6.06043100
H	-2.78228600	-5.52484300	-6.56066500	H	-5.28626000	2.84785400	-4.47299500
H	-4.52153500	-5.22283700	-6.43772500	H	-3.39563900	1.51964400	-3.75629000
H	-3.36472500	-4.02491500	-5.84275900	C	0.77928800	2.27208700	-2.12432800
C	-3.78683700	-7.30139900	-4.69805600	H	1.23769500	1.48667200	-2.73280500
H	-4.73997200	-7.53216100	-5.19244700	H	1.01755400	3.23268000	-2.59804000
H	-2.98544500	-7.76114600	-5.29177100	H	1.21710200	2.25946500	-1.12348900
H	-3.79597800	-7.79044900	-3.71697700	C	-1.43133600	-1.27662800	2.11127600
H	-2.27496000	-6.14108600	-2.83432300	C	-1.68089800	0.18228400	2.63239700
C	-2.30925500	-1.73477800	-4.25190400	H	-1.29754600	0.25943500	3.65591300
H	-1.30570800	-1.73899900	-4.69319100	H	-1.05512500	0.85918800	2.03975700
H	-3.01831000	-2.01551100	-5.04092700	C	-3.13000400	0.64331900	2.60131400
H	-2.52431000	-0.70769400	-3.94584600	C	-4.11338500	-0.31655300	3.24782700
C	-0.73908900	2.00236500	-2.05183100	H	-5.07519100	-0.44986700	2.75377100
C	-1.26227400	2.08313300	-3.53099400	C	-3.47940200	-1.61495700	3.71911600
H	-0.68095000	2.84647900	-4.05982700	H	-4.25992200	-2.32575500	4.01744900
H	-1.00673800	1.13811500	-4.02214900	H	-2.85256500	-1.46298800	4.60511100
C	-2.74305600	2.38737600	-3.68836000	C	-2.64496800	-2.20310100	2.54786100
C	-3.23968300	3.57039700	-2.87536200	H	-3.29713800	-2.16965100	1.67096600
H	-4.21519100	3.47451000	-2.39775600	N	-2.30681000	-3.64096300	2.71046900
C	-2.17620000	4.19574300	-1.98625300	C	-3.36079900	-4.52631500	2.20759900
H	-2.63464500	4.93100300	-1.31348000	H	-3.58249200	-4.26307500	1.16712900
H	-1.43142700	4.74435100	-2.57386000	H	-4.30095000	-4.43379000	2.78758000
C	-1.49982300	3.07063900	-1.15628900	C	-2.90588800	-5.98392600	2.25439800
H	-2.31867800	2.48782800	-0.71972700	O	-2.51498700	-6.38020100	3.56089900
N	-0.72263300	3.55968400	0.00739200	C	-1.49549900	-5.52365000	4.05788500
C	-1.54753100	3.79736400	1.19528300	C	-1.94700400	-4.06557000	4.06863100
H	-2.15197800	2.91008300	1.40004800	H	-2.79577600	-3.98128900	4.77180000
H	-2.23953100	4.65304600	1.06018300	H	-1.13605600	-3.44221700	4.45212100
C	-0.65740300	4.08303400	2.40382500	H	-1.27490000	-5.86595000	5.07404200
O	0.18671200	5.20564700	2.18046200	H	-0.58305600	-5.62493900	3.44536500
C	0.97878600	5.00431000	1.01734100	H	-2.06582700	-6.12371100	1.55442000
C	0.10784400	4.75028800	-0.21220000	H	-3.72227000	-6.65130600	1.95959400
H	-0.50449900	5.65427300	-0.38962100	C	-3.88694300	1.05174500	3.86137100
H	0.75022400	4.60931600	-1.08312200	C	-3.19402100	1.23251300	5.20099100
H	1.56991200	5.91699900	0.88651400	H	-2.71237300	2.21746900	5.25856300
H	1.66346400	4.15328300	1.16703700	H	-3.92719500	1.17660000	6.01616500
H	-0.04775400	3.19264100	2.62736200	H	-2.42689100	0.48133400	5.40373000
H	-1.26633100	4.32442000	3.28148900	C	-5.01386100	2.05468700	3.65498300
C	-3.25682200	3.63942100	-4.39117300	H	-5.78310200	1.95063300	4.43179200
C	-2.34026600	4.56936200	-5.16791000	H	-4.63717300	3.08521600	3.69736700
H	-2.17099000	4.18554300	-6.18260000	H	-5.50261000	1.92019500	2.68326900
H	-2.79926900	5.56219500	-5.26329500	H	-3.44834000	1.13727500	1.68438100
H	-1.36068800	4.70859700	-4.70453000	C	-0.09859300	-1.74559800	2.72953900
C	-4.62865000	3.51700200	-5.03981600	H	0.70941600	-1.09354800	2.38260400
H	-5.12571900	4.49431600	-5.10206300	H	-0.10334400	-1.70711700	3.82636700

H 0.11583200 -2.77064600 2.41977100
C 2.43035500 -1.38408400 -1.25696900
N 3.25379700 -0.43696700 -0.56402000
C 4.72805000 -0.39923700 -0.61851500
C 4.98133200 0.97990300 0.00285400
H 5.02008800 1.77335500 -0.75084500
H 5.87536600 1.02043400 0.62551500
O 3.83246200 1.20595600 0.84199200
C 2.79696300 0.45461000 0.39531100
O 1.67498100 0.60958300 0.83997900
H 5.07015900 -0.41925900 -1.65454400
C 5.36594400 -1.56040300 0.18216600
H 4.96162000 -2.50153700 -0.20710100
H 5.03846400 -1.47860300 1.22584500
C 6.87802100 -1.56488000 0.10686100
C 7.53317100 -1.96109000 -1.06887000
C 8.92492900 -1.94253600 -1.15358300
C 9.68860100 -1.52852800 -0.05969800
C 9.05061200 -1.13688800 1.11737300
C 7.65653000 -1.15537700 1.19770500
H 7.16696500 -0.85901300 2.12304300
H 9.63584200 -0.82004100 1.97642200
H 10.7730990 -1.51637500 -0.12403200
H 9.41371800 -2.25621500 -2.07206900
H 6.94918900 -2.29634000 -1.92385000
C 3.00880600 -2.10566700 -2.32984400
H 4.09131400 -2.11366800 -2.37478300
C 2.33457300 -3.37935800 -2.78765200
H 2.88282400 -3.82013300 -3.62717200
H 1.31150900 -3.17625100 -3.11721600
H 2.28445600 -4.13444100 -1.99395500
O 1.16482800 -0.81452900 -3.86958300
C 2.43264100 -0.75734500 -3.82574200
C 3.22781400 -1.21928900 -5.06144000
H 2.91526700 -2.24299400 -5.30084700
C 2.79965200 -0.31362000 -6.23576100
H 3.29454500 -0.62670300 -7.16296600
H 3.07595400 0.73214900 -6.04611900
H 1.71756600 -0.35660400 -6.38111800
C 4.75016400 -1.16981100 -4.88297000
H 5.12315300 -1.95341900 -4.21508800
H 5.06676300 -0.19797700 -4.47922800
H 5.25619500 -1.29796700 -5.84663300
H 2.90090000 0.12884600 -3.34628800

Table 55. Geometric coordinates and thermally corrected MP2 energies for transition state (*R*)-50a

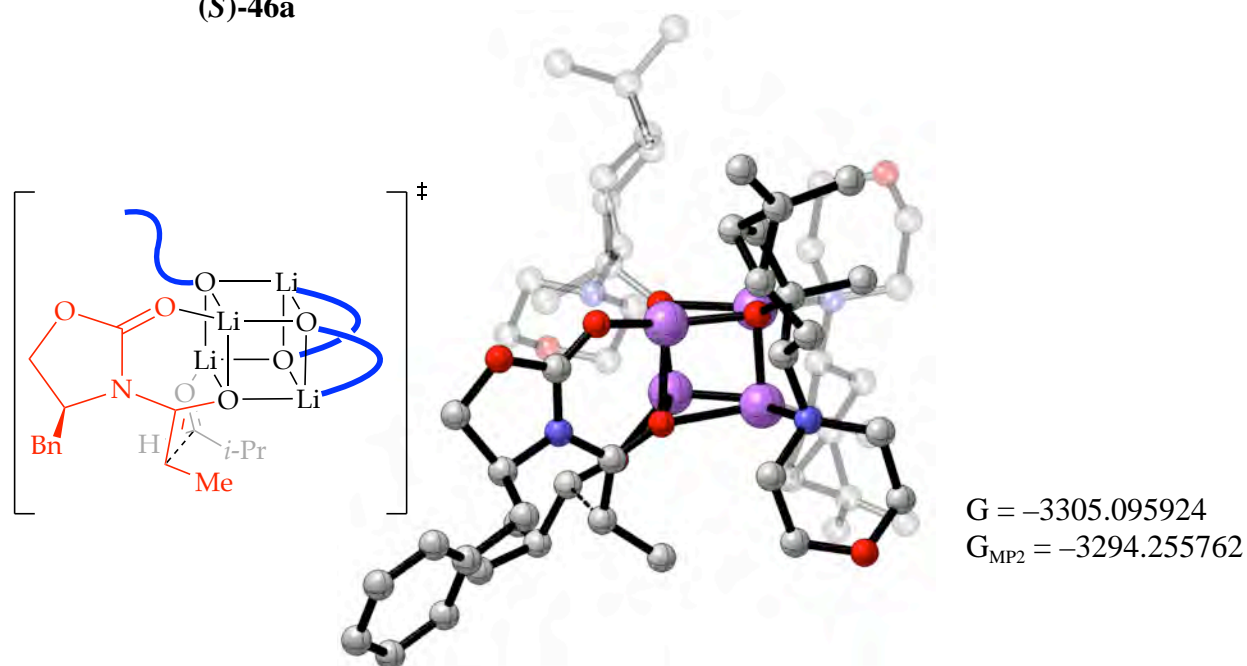


Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	C	-5.76665600	-0.26094000	0.13648300
O	1.16850800	-0.89339200	-1.43329600	O	-6.64617300	0.46617700	-0.70773500
Li	-0.38064500	-0.15321500	-2.63925500	C	-5.98077300	0.83153100	-1.90851600
Li	-2.26375100	-0.50584300	-0.95407500	C	-5.43277900	-0.38870200	-2.64348200
O	-1.63649900	-1.58180700	-2.40654200	H	-6.29024700	-1.01485300	-2.94084800
Li	-0.60428200	-2.50627600	-1.05176600	H	-4.93054800	-0.05946400	-3.55244300
O	-1.22400400	-1.44352700	0.46552100	H	-6.72347900	1.33878400	-2.53243300
O	-1.02589600	1.04390000	-1.21556500	H	-5.16806200	1.54155000	-1.69036800
C	-2.61368400	-2.10744400	-3.26637200	H	-4.93247500	0.38433600	0.45806800
C	-2.09502900	-3.47590500	-3.88979300	H	-6.34526600	-0.54195400	1.02192400
H	-1.93486200	-3.33460700	-4.96711200	C	-3.93100700	-5.29158300	-4.63829300
H	-1.10269500	-3.62453900	-3.45678500	C	-4.16410500	-4.60788000	-5.97311900
C	-2.89713100	-4.75762400	-3.65622800	H	-3.44938700	-4.97514700	-6.72149400
C	-4.37945800	-4.65770700	-3.33659100	H	-5.17284900	-4.82488300	-6.34858500
H	-4.75873700	-5.35309000	-2.58799000	H	-4.05550800	-3.52139900	-5.92886900
C	-4.94178300	-3.24963300	-3.20892300	C	-4.06067400	-6.80541000	-4.72497800
H	-5.89582800	-3.29044500	-2.67074500	H	-5.06349500	-7.09960800	-5.06301800
H	-5.16758300	-2.81074200	-4.18695100	H	-3.33485400	-7.22385400	-5.43494500
C	-3.92172800	-2.37596600	-2.44156400	H	-3.88462300	-7.28090800	-3.75325400
H	-3.57301700	-2.98199900	-1.59621500	H	-2.34647100	-5.52955000	-3.12087500
N	-4.49306300	-1.15151800	-1.78995700	C	-2.83057700	-1.10953900	-4.42678300
C	-5.22161300	-1.50853300	-0.55349500	H	-1.93156400	-1.09487100	-5.05022800
H	-4.53716300	-2.02346400	0.12646600	H	-3.67320700	-1.36792600	-5.08083500
H	-6.06792800	-2.18765700	-0.76162100	H	-2.97893100	-0.09529300	-4.04463200

C	-1.21838600	-1.98533600	1.77504600	C	1.98441700	1.87895700	-5.56035400
C	-1.60591900	-0.89038500	2.82776400	H	3.01553300	2.22618600	-5.67675200
H	-1.14251900	-1.14966000	3.78660400	H	1.31412500	2.71820100	-5.78173600
H	-1.12609400	0.04444800	2.51406100	C	1.70048700	1.32924500	-4.16476200
C	-3.09912000	-0.67922800	3.02871400	H	1.42849900	2.08504100	-3.42410200
C	-3.89875700	-1.95064000	3.25559600	H	2.55157600	0.74181700	-3.79052300
H	-4.87400600	-2.01771700	2.77288700	O	0.56256200	0.45324800	-4.33201100
C	-3.07647100	-3.22615600	3.16331100	C	-1.31359500	2.42731300	-1.26132600
H	-3.74038700	-4.09950100	3.15916000	C	-2.57694900	2.72747500	-0.39133100
H	-2.41964400	-3.34880500	4.03191400	H	-2.99084500	3.70044100	-0.68110500
C	-2.24979700	-3.19248900	1.85023100	H	-3.33850500	1.98832900	-0.66503200
H	-2.96412400	-2.95305500	1.05723600	C	-2.31257000	2.69134800	1.10311600
N	-1.67578800	-4.49983600	1.45947300	C	-1.16384400	3.57983700	1.54653600
C	-2.54184600	-5.29173800	0.58471900	H	-0.47911300	3.17745800	2.29302200
H	-2.86110400	-4.67536000	-0.26243500	C	-0.48074600	4.30163700	0.39819700
H	-3.45328100	-5.65044700	1.10590100	H	0.41070000	4.82677400	0.76249600
C	-1.77285400	-6.49769000	0.04801800	H	-1.13093800	5.07132900	-0.03098100
O	-1.27941300	-7.31635700	1.10366100	C	-0.07353600	3.25918600	-0.68007700
C	-0.45225700	-6.55921400	1.97637400	H	0.50481600	2.49969200	-0.14859500
C	-1.19646700	-5.35479700	2.54921800	N	0.88219600	3.80315500	-1.68909100
H	-2.02552300	-5.73277200	3.17629700	C	2.25851400	3.81687900	-1.17253900
H	-0.51949300	-4.79253300	3.19759400	H	2.52654900	2.80452700	-0.85009800
H	-0.14908200	-7.23919800	2.77964800	H	2.36691500	4.48150400	-0.29473700
H	0.44866100	-6.21414500	1.44496000	C	3.24333900	4.28118900	-2.24536300
H	-0.94071700	-6.13959100	-0.57735500	O	2.90143800	5.55649700	-2.76648200
H	-2.42750700	-7.13643700	-0.55425400	C	1.57516300	5.54542500	-3.27868300
C	-3.79440800	-0.92063800	4.36440900	C	0.56742400	5.14375100	-2.20499200
C	-3.02319800	-1.19202200	5.64435500	H	0.59895800	5.91190800	-1.41232100
H	-2.69316900	-0.25097800	6.10345900	H	-0.43722100	5.15094900	-2.63457800
H	-3.66442100	-1.70668400	6.37187400	H	1.37387800	6.56163400	-3.63197700
H	-2.13600600	-1.81277800	5.49837700	H	1.50526100	4.85539900	-4.13667900
C	-5.04875100	-0.09428500	4.61295600	H	3.28547400	3.54267500	-3.06363100
H	-5.73051700	-0.60788100	5.30407600	H	4.24758800	4.38060000	-1.81989100
H	-4.79816100	0.87926200	5.05452900	C	-2.57299300	3.87218000	2.02879900
H	-5.59886400	0.09605200	3.68407300	C	-3.34276500	5.10336700	1.58113900
H	-3.55518000	0.08643700	2.40459100	H	-4.42369600	4.93621000	1.67608800
C	0.21646200	-2.44146100	2.11347200	H	-3.08598800	5.96381700	2.21303000
H	0.88486500	-1.57486700	2.06981400	H	-3.14781500	5.39192800	0.54536100
H	0.29924500	-2.86281100	3.12334000	C	-2.85135500	3.51883100	3.48347300
H	0.55360800	-3.19161600	1.39337800	H	-2.56031200	4.34087400	4.15125500
C	0.44552300	0.05208400	-5.71737300	H	-3.91983900	3.32271200	3.64428700
H	0.42646800	-1.04082400	-5.76723500	H	-2.30007000	2.62447400	3.79466600
H	-0.50388900	0.43907200	-6.10411600	H	-2.38306100	1.70961600	1.56236500
C	1.64770700	0.66831400	-6.44460000	C	-1.67239800	2.80819700	-2.71166700
H	1.41244200	0.93523400	-7.47918000	H	-2.49204200	2.16147300	-3.04759500
H	2.48929100	-0.03413900	-6.46054400	H	-2.01437500	3.84565200	-2.81045100

H -0.82296000 2.65622100 -3.38184800
C 2.32591600 -1.37516800 -1.35012700
N 3.17324400 -0.87538400 -0.30379300
C 4.61636400 -1.15399500 -0.15409100
C 5.07124800 0.13937800 0.53638500
H 5.39623700 0.90335300 -0.17818700
H 5.84863600 -0.01624700 1.28435000
O 3.88791800 0.61899200 1.20575700
C 2.79122300 0.10259500 0.60269000
O 1.67583000 0.49802000 0.89153900
H 5.07705400 -1.24858100 -1.13953600
C 4.89345200 -2.42137000 0.68787600
H 4.37455700 -3.26470400 0.22160800
H 4.44288100 -2.28427000 1.67827700
C 6.37240200 -2.72057500 0.81930000
C 7.05918900 -2.46482400 2.01375900
C 8.42781500 -2.72044900 2.12303100
C 9.13177300 -3.23756700 1.03538300
C 8.45863900 -3.50224500 -0.15960100
C 7.09176000 -3.24661900 -0.26434500
H 6.57429500 -3.47099200 -1.19510300
H 8.99711400 -3.91503900 -1.00847600
H 10.1959420 -3.43995100 1.11908500
H 8.94042600 -2.52019800 3.06003000
H 6.51453300 -2.07515800 2.87126500
C 2.79952600 -2.44647300 -2.15859200
C 2.27664100 -2.51717800 -3.58047100
H 2.74303300 -3.35134300 -4.11304400
H 2.49076300 -1.60265900 -4.14710700
H 1.19368400 -2.67050200 -3.58215100
H 3.85635300 -2.68020100 -2.05722300
O 0.62549600 -3.87246400 -1.43588300
C 1.88182200 -3.99325400 -1.24695000
H 2.26319900 -3.76077200 -0.23202700
C 2.61606300 -5.23750300 -1.83135800
H 3.58658600 -4.92778500 -2.24228200
C 1.81128000 -5.93052300 -2.93746700
H 2.37055800 -6.78928000 -3.32840000
H 1.58790000 -5.26002600 -3.77054700
H 0.85588300 -6.29349100 -2.54692300
C 2.90367500 -6.22477900 -0.68391700
H 3.50792300 -5.76668300 0.10901800
H 3.45005000 -7.10070900 -1.05410100
H 1.97045300 -6.58031100 -0.23196400

Table 56. Geometric coordinates and thermally corrected MP2 energies for transition state (*S*)-46a

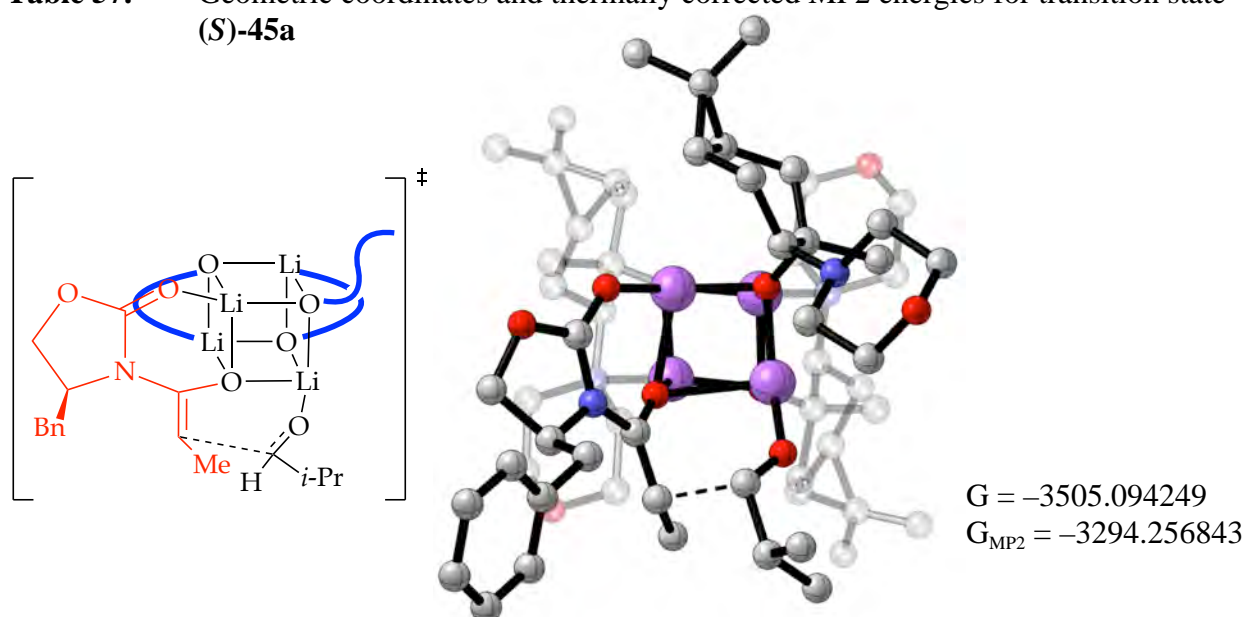


Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	C	0.89907800	1.71206100	-3.30598800
Li	-1.98968800	0.03680300	1.58607700	C	0.92822300	2.53526700	-2.02140500
O	-1.52799400	-1.13835400	0.10185400	H	1.64950200	3.35534600	-2.16355400
O	-1.20804900	-1.12982600	2.99803500	H	-0.05329900	2.97943200	-1.85549000
O	-0.42858700	1.19778800	1.42314500	H	0.67623300	2.35894200	-4.16005400
C	0.02383600	2.50844800	1.21582700	H	0.11941700	0.93597600	-3.24400300
C	0.26639200	3.21858700	2.61775500	H	1.81478500	-0.54661000	-2.38116800
H	-0.54265900	3.93992900	2.79367500	H	3.51373000	-0.13722500	-2.72737300
H	0.11859700	2.42954700	3.36017600	C	1.95347400	5.32220700	2.59720300
C	1.62013300	3.87133000	2.91261900	C	0.90336300	6.25551000	2.02402100
C	2.55980800	4.20657000	1.76717000	H	0.32571400	6.72185400	2.83280900
H	3.61768600	4.01768700	1.94812700	H	1.37218100	7.06426200	1.44769000
C	2.09674900	3.81826100	0.36910100	H	0.19015100	5.75161200	1.36828300
H	2.96817300	3.76604400	-0.29401000	C	2.89687800	6.02371900	3.56351200
H	1.43462700	4.57564100	-0.06435200	H	3.43498800	6.84321800	3.06810000
C	1.38645800	2.44700000	0.44209100	H	2.34608100	6.45243200	4.41114900
H	2.01296100	1.80664200	1.07481400	H	3.64428900	5.33256900	3.96970900
N	1.30506200	1.69642000	-0.85930200	H	2.09783200	3.48698900	3.81209600
C	2.60810100	1.06525100	-1.17122600	C	-1.07963400	3.28389100	0.46107000
H	2.87028000	0.38624600	-0.35404200	H	-1.93499700	3.41553300	1.13199500
H	3.40984700	1.81858700	-1.26121700	H	-0.77474600	4.28065500	0.12013300
C	2.53357800	0.28319100	-2.48068100	H	-1.43150700	2.71266100	-0.40296900
O	2.16051700	1.11428300	-3.56845700	C	-1.34983800	-1.52757200	4.34821400

C	-1.19181800	-0.29219600	5.30191100	C	-5.09374500	-1.69428600	-1.08268400
H	-0.84097500	-0.64795200	6.27730400	H	-6.06280800	-1.49720900	-0.61043000
H	-0.37682800	0.32943900	4.91187300	H	-5.07892300	-1.08864000	-1.99513500
C	-2.44811300	0.54331000	5.48831700	C	-3.93749700	-1.28729900	-0.13772500
C	-3.68812700	-0.25711800	5.85030100	H	-3.87788300	-2.06741100	0.63272500
H	-4.62802000	0.04438700	5.38823600	N	-4.16663300	-0.03222800	0.65347900
C	-3.47043300	-1.76352300	5.87615800	C	-5.13245900	-0.28589900	1.74602400
H	-4.43362800	-2.27970400	5.97403600	H	-4.75090400	-1.09387500	2.37617700
H	-2.87184100	-2.07260300	6.74048400	H	-6.11415800	-0.60098700	1.35197100
C	-2.78052900	-2.18234200	4.54945500	C	-5.33934900	0.96499900	2.59438000
H	-3.36842700	-1.71736500	3.75366800	O	-5.82121700	2.04768400	1.81344800
N	-2.82656700	-3.63315000	4.25672400	C	-4.90795700	2.32727700	0.76300600
C	-4.00574700	-4.04422600	3.49391200	C	-4.68533500	1.11005100	-0.13230300
H	-4.09229200	-3.41511700	2.60113600	H	-5.64624300	0.85772600	-0.61010700
H	-4.94379200	-3.93803400	4.07659700	H	-3.97873300	1.37148600	-0.91994600
C	-3.86669100	-5.50078200	3.05230400	H	-5.34121900	3.14671600	0.18114200
O	-3.67892100	-6.36917300	4.16247300	H	-3.94763600	2.66573000	1.18226600
C	-2.53604300	-5.97623000	4.91044300	H	-4.39362000	1.24479600	3.08796200
C	-2.66198800	-4.53510700	5.40056300	H	-6.09062700	0.77710100	3.36756800
H	-3.51954000	-4.48567700	6.09786500	C	-4.56622300	-3.75621700	-2.73306400
H	-1.76362300	-4.26770200	5.96224300	C	-4.34797700	-2.87653900	-3.94954200
H	-2.47145600	-6.66580200	5.75864300	H	-3.70846900	-3.39002500	-4.67946000
H	-1.62694300	-6.08035200	4.29610900	H	-5.30124500	-2.65532700	-4.44799700
H	-3.01719700	-5.58854000	2.35555600	H	-3.86736300	-1.92531700	-3.71521500
H	-4.77730000	-5.83841200	2.54662400	C	-5.16612800	-5.10831700	-3.09392900
C	-3.11209300	0.73012400	6.84798000	H	-6.14134500	-4.99072000	-3.58536400
C	-2.45588100	0.27981000	8.14191500	H	-4.51174800	-5.65918000	-3.78261600
H	-1.73857100	1.03297100	8.49346200	H	-5.31436600	-5.73368000	-2.20611600
H	-3.21273600	0.15349900	8.92714000	H	-3.42222000	-4.72893600	-1.12700400
H	-1.91810500	-0.66757500	8.05509400	C	-2.35992100	-0.32417300	-1.97628900
C	-3.90062500	2.02093800	7.02112700	H	-1.44958900	-0.57140200	-2.53575500
H	-4.69955200	1.90092300	7.76511900	H	-3.18357200	-0.28425900	-2.69740400
H	-3.24973100	2.83735500	7.36117600	H	-2.22431000	0.67780800	-1.55770100
H	-4.36668400	2.33867400	6.08131100	Li	-0.89276100	-2.31014600	1.51278700
H	-2.56740200	1.37345500	4.79291900	Li	0.35762500	-0.08457400	2.56672300
C	-0.21281400	-2.51018700	4.69727800	O	1.30109800	-1.20762100	1.13277200
H	-0.24935300	-3.38119200	4.03889900	C	2.25201500	-2.02030100	1.28574700
H	0.74793200	-2.00144400	4.56279100	N	3.12456700	-1.81812700	2.40828800
H	-0.25009100	-2.84995400	5.73998700	C	4.43494000	-2.47606500	2.58528400
C	-2.53921400	-1.36325700	-0.84345300	C	4.71994000	-2.11149400	4.04774700
C	-2.37229900	-2.82472400	-1.44331500	H	4.34922500	-2.87022000	4.74469700
H	-1.85266100	-2.75269900	-2.40916800	H	5.77176200	-1.90887400	4.25014500
H	-1.67042700	-3.32191200	-0.76836200	O	3.97359100	-0.89692700	4.26270500
C	-3.59011400	-3.74684500	-1.56727500	C	2.96114400	-0.83156700	3.36733700
C	-4.98986000	-3.18237300	-1.39310500	O	2.08278400	0.00673500	3.47496800
H	-5.68856500	-3.79891700	-0.82839300	H	4.33540700	-3.55711900	2.47522200

C 5.49320000 -1.92917200 1.59680900
H 5.10354700 -2.05367400 0.58024300
H 5.59987000 -0.85105500 1.76895000
C 6.83464800 -2.61751200 1.73476900
C 7.01949800 -3.92285800 1.25486800
C 8.24433700 -4.57260200 1.40362300
C 9.30937400 -3.92561600 2.03476500
C 9.14117500 -2.62567600 2.51192100
C 7.91262300 -1.97879900 2.36210600
H 7.79302900 -0.96020000 2.72525400
H 9.96599400 -2.11084900 2.99713100
H 10.2646850 -4.43048400 2.14829200
H 8.36917500 -5.58238500 1.02204300
H 6.20045000 -4.43242900 0.75096600
C 2.42532800 -3.19919500 0.51660400
H 3.37901200 -3.70130100 0.62693500
C 1.85040600 -3.22201300 -0.88192700
H 1.91808500 -4.22709500 -1.31053700
H 0.79639100 -2.93350100 -0.86774100
H 2.38806600 -2.54636500 -1.55956300
O -0.04944800 -3.96335000 1.29005800
C 1.11804400 -4.38983400 1.56483900
C 1.49447700 -5.81963900 1.11744400
H 1.38570200 -5.87767400 0.02751100
C 0.46041000 -6.78109300 1.73806700
H 0.65109300 -7.81198400 1.41620800
H 0.51227900 -6.75875700 2.83481700
H -0.55307500 -6.50042300 1.44252800
C 2.91220700 -6.24639300 1.51853000
H 3.08624000 -6.06843100 2.58878200
H 3.05603000 -7.31858500 1.34310900
H 3.69149800 -5.72152000 0.95534800
H 1.52905400 -4.16431200 2.57207100

Table 57. Geometric coordinates and thermally corrected MP2 energies for transition state (S)-45a

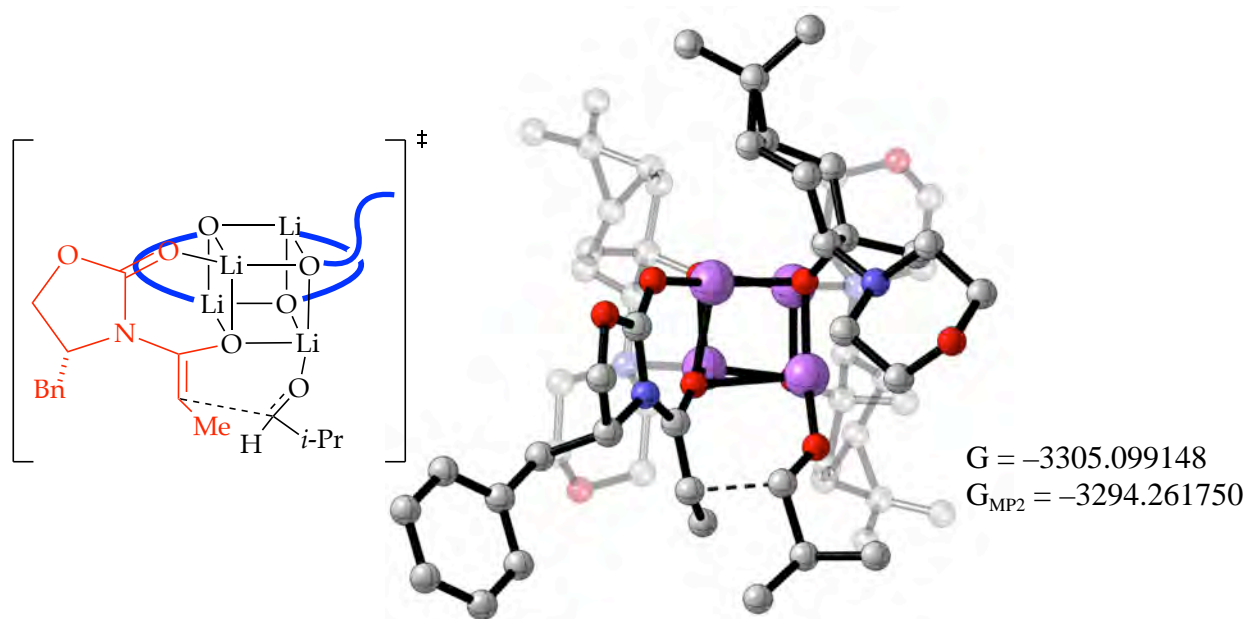


Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	H	-3.20540000	0.16111600	-2.89529800
O	0.37115700	-1.83151900	-0.52762300	H	-1.46054300	0.27383900	-3.18019400
Li	0.70347100	-2.04546100	1.31844400	H	-2.59239200	2.49924600	-3.17257300
O	0.24166400	-0.28080200	1.94029500	H	-1.36482500	2.38697200	-1.88781000
C	-0.44979900	-2.24437400	-1.58877300	H	-2.17374000	2.05403500	0.37735900
C	-0.47476500	-3.83044100	-1.67121000	H	-3.93755200	1.94632700	0.59779800
H	0.07237100	-4.14676000	-2.56845600	C	-2.63662500	-4.95731500	-2.81589900
H	0.13843500	-4.16062600	-0.82922200	C	-2.11757700	-4.70019300	-4.21864000
C	-1.81447700	-4.56800800	-1.59507200	H	-1.48304000	-5.53250100	-4.54994400
C	-3.09886200	-3.82391000	-1.92115900	H	-2.94953200	-4.61823900	-4.93046800
H	-3.95885900	-4.05229300	-1.29174300	H	-1.52136500	-3.78861900	-4.30073100
C	-2.95861800	-2.34591900	-2.25792300	C	-3.42580900	-6.25437000	-2.71114900
H	-3.93033700	-1.85620600	-2.12476500	H	-4.29847900	-6.24262300	-3.37778600
H	-2.68637900	-2.19284800	-3.30777800	H	-2.80635300	-7.11696000	-2.99021700
C	-1.90176700	-1.71627000	-1.32227300	H	-3.78995200	-6.42322500	-1.69111100
H	-2.12811500	-2.08304600	-0.31309500	H	-1.87964600	-5.28229000	-0.77479000
N	-1.97645200	-0.22099000	-1.18698800	C	0.16119500	-1.71306000	-2.90688500
C	-3.03724100	0.16041100	-0.22734100	H	1.13210900	-2.19704600	-3.06593400
H	-2.81422400	-0.29302800	0.74381600	H	-0.45598500	-1.91429300	-3.79148000
H	-4.02689700	-0.20503100	-0.55435800	H	0.34176200	-0.63616300	-2.85166900
C	-3.11067100	1.67736100	-0.06681700	C	2.16301600	1.97201100	-0.87357600
O	-3.35479100	2.32727200	-1.30379200	C	1.30488000	3.10351000	-0.23231400
C	-2.33374900	1.99664400	-2.23556100	H	1.45477300	4.03840700	-0.78657100
C	-2.24905500	0.48970700	-2.45867000	H	0.24639100	2.84322000	-0.36158400

C	1.62281400	3.28634400	1.24216300	C	-1.23588600	-1.63732900	3.29472600
C	3.10231700	3.49084500	1.53388000	H	-1.91197000	-1.55883000	2.43389300
H	3.51997900	2.96302000	2.38837600	N	-0.46004700	-2.89350100	3.02289300
C	3.98166400	3.49438300	0.29417600	C	-1.32134100	-3.93415900	2.41620200
H	5.04126600	3.51132600	0.58038400	H	-1.76810500	-3.53701800	1.49870400
H	3.81634100	4.40714400	-0.28659000	H	-2.14163800	-4.22582300	3.09531700
C	3.71770300	2.24883200	-0.59910300	C	-0.50147900	-5.17697100	2.07448800
H	4.02087300	1.37448800	-0.01683300	O	0.15078600	-5.71525400	3.21631100
N	4.57073900	2.21570000	-1.80863400	C	0.97753600	-4.73362200	3.82333600
C	5.84617800	1.52641200	-1.63284600	C	0.17980800	-3.49418700	4.21513100
H	5.66099600	0.54934700	-1.17380400	H	-0.57579600	-3.79563500	4.95845800
H	6.54622800	2.08692200	-0.97909700	H	0.84367800	-2.77043700	4.68764700
C	6.51225700	1.31573100	-2.99259300	H	1.41088300	-5.20066900	4.71337000
O	6.70113100	2.54510700	-3.68206700	H	1.79695300	-4.45129200	3.14164700
C	5.46036200	3.21843800	-3.85111300	H	0.24205000	-4.93112100	1.29947100
C	4.78953600	3.48326400	-2.50427600	H	-1.15339600	-5.96588300	1.68780000
H	5.43638500	4.17466700	-1.93156300	C	-3.26254400	0.66738100	5.24626900
H	3.83275700	3.98906800	-2.67076700	C	-2.30621500	0.91164400	6.39889400
H	5.68856200	4.15956800	-4.36215100	H	-2.24019500	1.98545300	6.61705400
H	4.78758000	2.62052500	-4.48771400	H	-2.65986200	0.41295800	7.31094100
H	5.88948400	0.63640900	-3.59769500	H	-1.29101000	0.56138000	6.20107500
H	7.50654100	0.87253100	-2.87451700	C	-4.65117800	1.23300500	5.50854800
C	2.10498800	4.59119900	1.85673700	H	-5.10099000	0.78072500	6.40252200
C	2.06936500	5.90700800	1.09856000	H	-4.61022100	2.31821700	5.67024400
H	1.08179300	6.37706800	1.19518200	H	-5.32846100	1.04832700	4.66675500
H	2.80897800	6.60710300	1.50931300	H	-3.48960400	1.16759500	3.11583600
H	2.27546000	5.80467100	0.03042500	C	0.75023200	-0.27066300	4.27507400
C	1.79244900	4.77229700	3.33587500	H	1.22298000	0.71719000	4.23933800
H	2.51381300	5.45034200	3.81156500	H	0.39566500	-0.42780900	5.30100100
H	0.79056200	5.19854800	3.48020200	H	1.53332700	-1.00285500	4.06069500
H	1.83010700	3.81797900	3.87390600	Li	2.04149100	0.25407300	1.53351200
H	1.06172200	2.63720900	1.91298300	O	1.79844200	0.73566700	-0.28504700
C	1.84642800	1.90797100	-2.37734200	Li	2.15310600	-1.07526700	-0.88179900
H	0.78452800	1.66627100	-2.50249000	O	2.71174900	-1.79490200	1.32488000
H	2.03247600	2.85374100	-2.89958600	C	3.86890800	-2.27992400	1.41211800
H	2.44459900	1.13284400	-2.86293000	N	4.79927000	-1.60369600	2.26160500
C	-0.36516500	-0.33451200	3.20390300	C	6.08094100	-2.14916400	2.75473400
C	-1.31467000	0.92450600	3.39744100	C	6.18023800	-1.41267200	4.09871300
H	-0.83309900	1.63086500	4.08617700	H	5.72275100	-1.97531200	4.91953800
H	-1.31086200	1.42016100	2.42350900	H	7.19856900	-1.13322800	4.36832500
C	-2.77679300	0.71635500	3.80504900	O	5.41810700	-0.20427200	3.89693400
C	-3.20786600	-0.60440600	4.42196100	C	4.52691300	-0.40003200	2.89799000
H	-4.17548700	-0.98952100	4.10116300	O	3.66169200	0.41939900	2.65386600
C	-2.13245700	-1.67509500	4.55198500	H	5.98595600	-3.22659100	2.90620900
H	-2.61346800	-2.65510900	4.65132700	C	7.26964700	-1.84616900	1.81263400
H	-1.53387800	-1.53971500	5.45927200	H	7.03600900	-2.24424900	0.82028700

H 7.35658500 -0.75843700 1.70296300
C 8.57216900 -2.43113100 2.31875500
C 9.55719400 -1.61723000 2.89399100
C 10.7461610 -2.16555900 3.37998700
C 10.9674930 -3.54036100 3.29745000
C 9.99627300 -4.36264300 2.72141900
C 8.81093800 -3.81123200 2.23625500
H 8.06736600 -4.45915000 1.77606500
H 10.1648320 -5.43337000 2.64384000
H 11.8928110 -3.96868400 3.67258600
H 11.4999260 -1.51637200 3.81721300
H 9.39876400 -0.54221700 2.94851300
C 4.32817800 -3.37823800 0.62893400
C 3.29821300 -4.42986800 0.26207600
H 3.76853700 -5.24223200 -0.29908500
H 2.82709400 -4.87723300 1.14733900
H 2.51194600 -3.99420700 -0.36113800
H 5.29731900 -3.77982100 0.91618400
O 3.61976100 -1.98636000 -1.55451500
C 4.71676700 -2.42677900 -1.06602500
H 5.40099500 -1.67771000 -0.61429800
C 5.53660900 -3.45779800 -1.89943900
H 5.98480100 -4.20070200 -1.22497400
C 4.67778700 -4.18516200 -2.94068100
H 5.28663000 -4.91279900 -3.49120200
H 3.83748900 -4.71673600 -2.48790500
H 4.26198400 -3.47092500 -3.65756000
C 6.69373100 -2.71199400 -2.59172800
H 7.35764500 -2.22509400 -1.86655300
H 7.30234200 -3.40379400 -3.18639500
H 6.30810100 -1.93849100 -3.26658200

Table 58. Geometric coordinates and thermally corrected MP2 energies for transition state **(R)-45a**

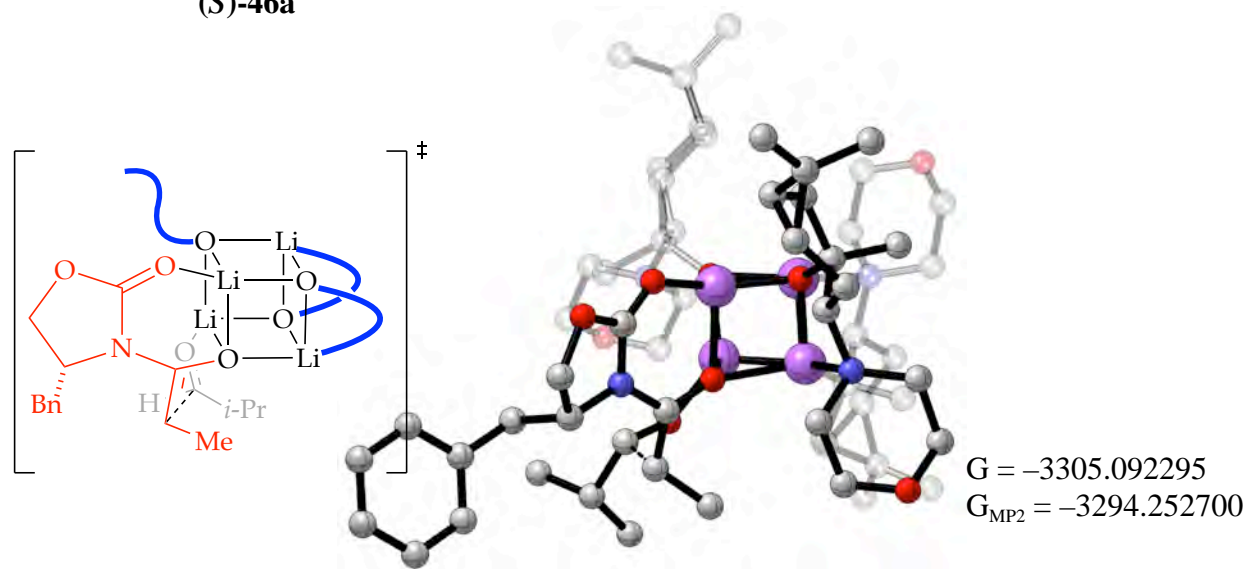


Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	H	6.18706700	-0.52706400	1.77022200
O	-0.87340400	-1.58500900	1.11493000	C	5.47804900	1.06229700	0.51041900
Li	0.00011400	-0.13826800	2.72720700	O	5.93696000	2.14294900	1.30610400
Li	2.16930800	0.10271800	1.35725800	C	4.98496300	2.43503500	2.32028100
O	1.63533800	-1.24052900	2.65497600	C	4.72774800	1.22185500	3.21033300
Li	1.07642600	-2.16094900	1.10132100	H	5.67405000	0.97101000	3.71555100
O	1.66436700	-0.91719600	-0.24642600	H	3.99831300	1.48347600	3.97778100
O	0.52930400	1.17637600	1.41138100	H	5.40326800	3.25288100	2.91489700
C	2.51284100	-1.28755400	3.74903900	H	4.04453700	2.78168600	1.86448100
C	2.34448400	-2.66742100	4.51886300	H	4.55566800	1.35170100	-0.02085500
H	1.84618700	-2.47882700	5.47843200	H	6.25649900	0.86711500	-0.23360400
H	1.62089600	-3.22954600	3.92364700	C	4.45552600	-3.50558500	5.96892000
C	3.56588400	-3.56563500	4.73558000	C	4.12243300	-2.58042900	7.12497900
C	4.96045600	-2.96910300	4.64365700	H	5.02836000	-2.32298100	7.68938500
H	5.71419600	-3.58441800	4.15270100	H	3.65143600	-1.64611100	6.81148300
C	5.04446200	-1.49148700	4.28682300	H	3.43112300	-3.07304300	7.82115000
H	6.04998500	-1.27274600	3.90891000	C	5.06165100	-4.82339700	6.43003600
H	4.90800300	-0.85332700	5.16640400	H	5.99189500	-4.65648800	6.98948000
C	3.98056500	-1.17264600	3.21212200	H	4.37141400	-5.36673900	7.08892900
H	4.04499200	-1.97675900	2.46845900	H	5.29702400	-5.47838500	5.58318200
N	4.23133400	0.07560900	2.41313800	H	3.45357500	-4.56750600	4.32220500
C	5.22433200	-0.18916900	1.34728100	C	2.12755600	-0.14862400	4.72290600
H	4.84314400	-0.98404900	0.69818700	H	1.12596600	-0.35111600	5.12091800

H	2.80711500	-0.04685900	5.57844300	C	4.51550000	-1.23914400	-2.54548000
H	2.08224100	0.81262300	4.20384700	C	4.73133700	-2.74384500	-2.55919800
C	0.39922700	2.58588100	1.39858000	H	5.68144900	-3.09552400	-2.15782900
C	1.27564900	3.16969900	0.24657000	C	3.53845900	-3.60217300	-2.15866600
H	1.39084500	4.25069500	0.39021800	H	3.89573300	-4.59461400	-1.85971900
H	2.28296000	2.74453000	0.34353700	H	2.85681800	-3.76825500	-3.00025900
C	0.70841800	2.87081900	-1.13083200	C	2.80404200	-2.91466700	-0.98598600
C	-0.74448100	3.28463300	-1.30494100	H	3.58149500	-2.58526200	-0.28531300
H	-1.39642100	2.58982200	-1.83100900	N	1.93624100	-3.81402800	-0.15534500
C	-1.36175500	3.90293300	-0.06006600	C	2.74973700	-4.62867900	0.77567500
H	-2.43908500	4.05268500	-0.20711800	H	3.34721200	-3.96013100	1.40460800
H	-0.94382300	4.89577800	0.13758300	H	3.44301100	-5.29195200	0.22966700
C	-1.13524400	2.96715800	1.15802700	C	1.85083600	-5.48336900	1.66669000
H	-1.58231700	2.00841100	0.88403200	O	1.00455000	-6.33690800	0.90856200
N	-1.86001900	3.38976300	2.37787700	C	0.22254300	-5.58363300	-0.00703800
C	-3.18464100	2.78990300	2.51518100	C	1.09639500	-4.74977600	-0.93725000
H	-3.08999700	1.70448200	2.40499500	H	1.71908300	-5.43894900	-1.53054400
H	-3.89856600	3.15687800	1.74804900	H	0.46093200	-4.19529100	-1.62744600
C	-3.75596100	3.09425900	3.89947600	H	-0.36051900	-6.30802900	-0.58423700
O	-3.81333500	4.49296800	4.14922100	H	-0.47595100	-4.92650000	0.53619200
C	-2.52015400	5.07108700	4.02628200	H	1.24450700	-4.83261700	2.31681600
C	-1.93739100	4.82794200	2.63545100	H	2.45816200	-6.13394000	2.30315000
H	-2.57505200	5.35521300	1.90088700	C	4.82926500	-1.95571700	-3.85097200
H	-0.93759800	5.27038000	2.58205300	C	3.77936100	-2.08483100	-4.93873700
H	-2.64307000	6.14306500	4.21216600	H	3.79455300	-1.20213500	-5.59123600
H	-1.84361800	4.65188900	4.78921700	H	3.97815900	-2.96196100	-5.56848100
H	-3.13446300	2.59956000	4.66292900	H	2.76356200	-2.17924700	-4.54872900
H	-4.78343800	2.72404000	3.98501300	C	6.23159400	-1.75770200	-4.40837800
C	0.33524800	3.94605600	-2.14231900	H	6.52643600	-2.60009500	-5.04828000
C	0.72529900	5.40291200	-1.96027700	H	6.28976400	-0.84400500	-5.01437200
H	1.74425000	5.57730600	-2.33034200	H	6.97537100	-1.67290000	-3.60771400
H	0.05102800	6.05313700	-2.53326300	H	5.34428200	-0.64838600	-2.15731600
H	0.69454500	5.73850500	-0.92097400	C	0.86464300	-1.79700700	-2.31861000
C	0.38449700	3.51534200	-3.60177700	H	0.51260400	-0.82295800	-2.67711600
H	-0.29506400	4.12135500	-4.21604500	H	1.06718200	-2.41765600	-3.20034600
H	1.39615200	3.62946900	-4.01381400	H	0.03854200	-2.24318900	-1.75841900
H	0.09206600	2.46564700	-3.72094000	C	-2.07985700	-1.88213200	1.32605600
H	1.01536700	1.91673000	-1.55809100	N	-3.06372600	-1.31849200	0.45234200
C	0.92945500	3.14594000	2.73045000	C	-4.46990100	-1.76055900	0.37082500
H	1.96648300	2.81839300	2.86655500	C	-5.05923100	-0.61414900	-0.45972700
H	0.92613800	4.24243200	2.76403400	H	-5.44061800	0.19969500	0.16576300
H	0.33005400	2.77938500	3.56739800	H	-5.83242800	-0.93426000	-1.15845400
C	2.09516900	-1.57929100	-1.40524800	O	-3.93933400	-0.11599400	-1.21882900
C	3.13680300	-0.67291400	-2.19180400	C	-2.78805400	-0.43965000	-0.58391500
H	2.65401100	-0.28323200	-3.09727100	O	-1.72133600	0.02051600	-0.94855500
H	3.28853100	0.19481400	-1.54490600	H	-4.92028200	-1.78294200	1.36446600

C -4.59603900 -3.14476300 -0.31029700
H -3.96622700 -3.85181600 0.24135200
H -4.17969900 -3.06805400 -1.32229700
C -6.02412000 -3.64406400 -0.36700600
C -6.65499000 -4.13223600 0.78711300
C -7.97882100 -4.56870000 0.74798800
C -8.69617000 -4.52655400 -0.44982700
C -8.07948000 -4.04867100 -1.60620600
C -6.75397600 -3.61115900 -1.56273100
H -6.27607400 -3.25181200 -2.47175600
H -8.62632900 -4.01947300 -2.54477500
H -9.72662500 -4.86940500 -0.48140000
H -8.44887800 -4.94720600 1.65166700
H -6.10210800 -4.18090800 1.72325400
C -2.53107100 -2.59760700 2.46288500
H -3.55033700 -2.96450700 2.42271900
C -1.54394800 -3.50666100 3.16069700
H -0.68380600 -2.93379900 3.52060500
H -1.17036200 -4.30340900 2.50459000
H -2.01320500 -3.99532700 4.02051400
O -1.50195500 -0.45146900 3.78866600
C -2.65846600 -0.97560800 3.72858200
C -3.25045000 -1.57129900 5.02262800
H -2.52444300 -2.29132100 5.41878800
C -3.36510300 -0.41950700 6.04270200
H -3.71991500 -0.79650000 7.00947900
H -4.07851300 0.34142000 5.70002700
H -2.39624800 0.06485700 6.18711000
C -4.61060300 -2.25517800 4.83820100
H -4.53542600 -3.20611100 4.30026800
H -5.30625000 -1.60597700 4.28815700
H -5.07015400 -2.46806200 5.81008000
H -3.43925900 -0.45267800 3.13251200

Table 59. Geometric coordinates and thermally corrected MP2 energies for transition state (S)-46a

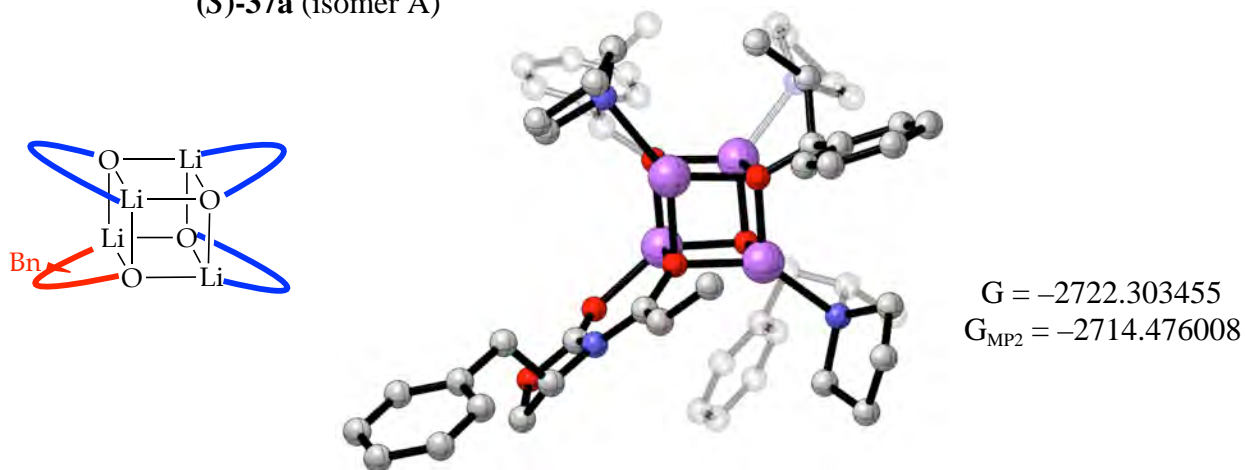


Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	C	-0.00171400	2.93331500	-1.78915200
Li	-1.59850800	-0.52975200	1.89277700	H	0.54031700	3.88256100	-1.92901600
O	-1.22198400	-1.43899900	0.21600600	H	-0.98020000	3.16722300	-1.37064800
O	-0.35538100	-1.63781100	2.98044800	H	-0.68022200	2.98904900	-3.84015700
O	-0.33726000	0.93761000	1.63040600	H	-0.80588600	1.38382100	-3.07634300
C	-0.19194300	2.32620700	1.50408200	H	1.24460600	0.13399800	-2.80669400
C	0.16856700	2.97987600	2.90889500	H	2.74439400	0.88864400	-3.40243600
H	-0.62251200	3.68922200	3.18210600	C	1.72554700	5.15973500	2.99472400
H	0.08843800	2.16260300	3.63193200	C	0.53922900	6.09116000	2.82307900
C	1.53240800	3.64993800	3.08238600	H	0.08592300	6.32072500	3.79630300
C	2.19675000	4.26922500	1.86341900	H	0.85752800	7.04217600	2.37614800
H	3.27675200	4.14069600	1.79026100	H	-0.24868500	5.67766100	2.18838400
C	1.46679200	4.07119700	0.54184300	C	2.81451900	5.75119900	3.87760600
H	2.15111900	4.28425400	-0.28778000	H	3.20581600	6.68598600	3.45385700
H	0.62752800	4.76609700	0.42748400	H	2.42935100	5.97649200	4.88083000
C	0.97693900	2.60519500	0.49517500	H	3.65651800	5.05932500	3.99385700
H	1.80019600	1.99742000	0.88864100	H	2.19730400	3.14235300	3.77826100
N	0.73932600	2.03439400	-0.87365600	C	-1.54685900	2.92252700	1.06372100
C	2.02465600	1.69963000	-1.52808100	H	-2.25505200	2.82324300	1.89322300
H	2.56088000	0.98342500	-0.89796600	H	-1.49680800	3.98838200	0.80489900
H	2.66030800	2.59398300	-1.64802900	H	-1.96206000	2.37035100	0.21523000
C	1.78858400	1.08803600	-2.90749400	C	-0.17129600	-2.21333700	4.26068000
O	1.06604100	1.96703000	-3.75444900	C	-0.10457900	-1.09791400	5.35904300
C	-0.18367500	2.28944200	-3.16080600	H	0.45251500	-1.48868300	6.21824100

H	0.50656400	-0.27564500	4.96676500	H	-5.04085000	-1.97844900	-1.24191100
C	-1.45577700	-0.57743900	5.82132700	C	-3.56233200	-2.05069600	0.37286700
C	-2.44323800	-1.66177100	6.22093200	H	-3.21252500	-2.85191400	1.03699200
H	-3.48347500	-1.52163300	5.92710100	N	-3.87212500	-0.92631600	1.31733100
C	-1.93033700	-3.07943500	6.01034800	C	-4.55506800	-1.44265800	2.52533000
H	-2.74563600	-3.79889300	6.15689000	H	-3.91809400	-2.19570300	2.99816300
H	-1.15726500	-3.34332900	6.74064800	H	-5.51543900	-1.92464200	2.27258300
C	-1.38550500	-3.19123700	4.56117200	C	-4.83689800	-0.31834500	3.51751600
H	-2.17641600	-2.78853300	3.92244400	O	-5.65086800	0.69058700	2.93963500
N	-1.17664300	-4.57556500	4.08069000	C	-5.01528700	1.21957500	1.78561200
C	-2.34181600	-5.15115400	3.40811100	C	-4.73151400	0.13576200	0.74807300
H	-2.68321100	-4.46153900	2.62819900	H	-5.69695000	-0.27628900	0.41169800
H	-3.18915800	-5.32352300	4.10326300	H	-4.24272800	0.58856900	-0.11446000
C	-1.96705800	-6.48077800	2.75523000	H	-5.69601900	1.96863300	1.36915300
O	-1.45328800	-7.40302900	3.70811100	H	-4.07750400	1.71995400	2.07154800
C	-0.32156300	-6.85366800	4.36932400	H	-3.88788500	0.11715500	3.87337500
C	-0.66569900	-5.53620900	5.06194600	H	-5.38476600	-0.70635600	4.38165800
H	-1.40312400	-5.75050100	5.85816700	C	-4.18865600	-4.43926900	-2.29745900
H	0.23289600	-5.13822800	5.54080100	C	-4.38479100	-3.46485500	-3.44370100
H	-0.00062400	-7.60059500	5.10288500	H	-3.82064700	-3.79697300	-4.32505300
H	0.49621700	-6.68896000	3.64864600	H	-5.44259200	-3.40988600	-3.73367600
H	-1.22211500	-6.29931200	1.96345600	H	-4.05081100	-2.45178000	-3.21201800
H	-2.84911500	-6.95457900	2.31196600	C	-4.57299900	-5.86401500	-2.67138500
C	-1.92976000	-0.68869000	7.26597400	H	-5.62851000	-5.92481000	-2.96921100
C	-1.00947200	-1.12659900	8.39245600	H	-3.96902400	-6.22715900	-3.51353700
H	-0.41183000	-0.27966500	8.75420500	H	-4.42344700	-6.55515700	-1.83403300
H	-1.59893500	-1.50023600	9.24001700	H	-2.58738700	-5.23656700	-1.01749600
H	-0.31343100	-1.91953400	8.10779300	C	-2.55950400	-0.65744200	-1.59341900
C	-2.92264600	0.37465800	7.71451400	H	-1.73465400	-0.67081500	-2.31610300
H	-3.56248500	0.00246000	8.52585700	H	-3.49244700	-0.73478000	-2.16290700
H	-2.40200000	1.26776800	8.08471800	H	-2.54252100	0.31752900	-1.09699000
H	-3.57658000	0.68933500	6.89311800	Li	0.86785400	-0.25430600	2.46244100
H	-1.84260600	0.27679700	5.26678500	Li	-0.11506400	-2.58094700	1.32003000
C	1.18387800	-2.94976600	4.28069200	O	1.74618600	-0.95764000	0.71063000
H	1.19747500	-3.73545700	3.52187600	C	2.84805400	-1.55369400	0.60615700
H	1.98180300	-2.23033000	4.06310800	N	3.88556600	-1.18082400	1.52123000
H	1.41012300	-3.39694600	5.25711900	C	5.31804700	-1.51806200	1.38883800
C	-2.33153000	-1.79213400	-0.56580200	C	5.94296600	-0.29860500	2.08267300
C	-2.01345700	-3.13930300	-1.34700200	H	6.16429500	0.51429300	1.38282800
H	-1.74473200	-2.89040300	-2.38306400	H	6.83474100	-0.53639900	2.66231000
H	-1.09538900	-3.51764100	-0.88935000	O	4.91971900	0.15352200	2.99383600
C	-3.02576800	-4.28940600	-1.32894800	C	3.71337700	-0.27533500	2.55988600
C	-4.44820700	-4.03984400	-0.85673400	O	2.68236200	0.11317400	3.07836000
H	-4.89084000	-4.81729700	-0.23457900	H	5.59163800	-1.54612600	0.33201700
C	-4.77539000	-2.62450400	-0.39805900	C	5.68774100	-2.85663900	2.06982300
H	-5.66182500	-2.65491500	0.24544700	H	5.05800700	-3.64596800	1.64784600

H 5.43323100 -2.78658900 3.13419400
C 7.15192500 -3.20511500 1.89868700
C 8.05710900 -3.07381900 2.96024800
C 9.41072700 -3.37235800 2.78944600
C 9.88001700 -3.80806300 1.55017700
C 8.98762400 -3.94861400 0.48478200
C 7.63664500 -3.65066000 0.65967100
H 6.94769800 -3.77775400 -0.17323000
H 9.34269900 -4.29704900 -0.48135300
H 10.9321460 -4.04335000 1.41581700
H 10.0952870 -3.26899800 3.62700600
H 7.69677800 -2.74819200 3.93386500
C 3.08245800 -2.63633400 -0.29181900
C 2.31725500 -2.59743000 -1.60083200
H 2.63873500 -3.41197000 -2.25552000
H 2.47846500 -1.65966700 -2.14722700
H 1.24464800 -2.70853200 -1.41612000
H 4.12044400 -2.94640000 -0.38404700
O 0.97770600 -3.95794300 0.71294200
C 2.24877200 -4.11011100 0.74831700
H 2.75382200 -3.87572000 1.70751600
C 2.85489000 -5.40948000 0.14380300
H 3.84610400 -5.18602300 -0.27549200
C 1.97735000 -6.03064800 -0.94898300
H 2.44289800 -6.94671700 -1.33255000
H 1.81721300 -5.35396100 -1.79161200
H 0.99364900 -6.28813400 -0.54557400
C 3.05967500 -6.41695900 1.29275300
H 3.72051200 -6.01856200 2.07237400
H 3.50561600 -7.34701300 0.92007500
H 2.10059100 -6.66721100 1.76143000

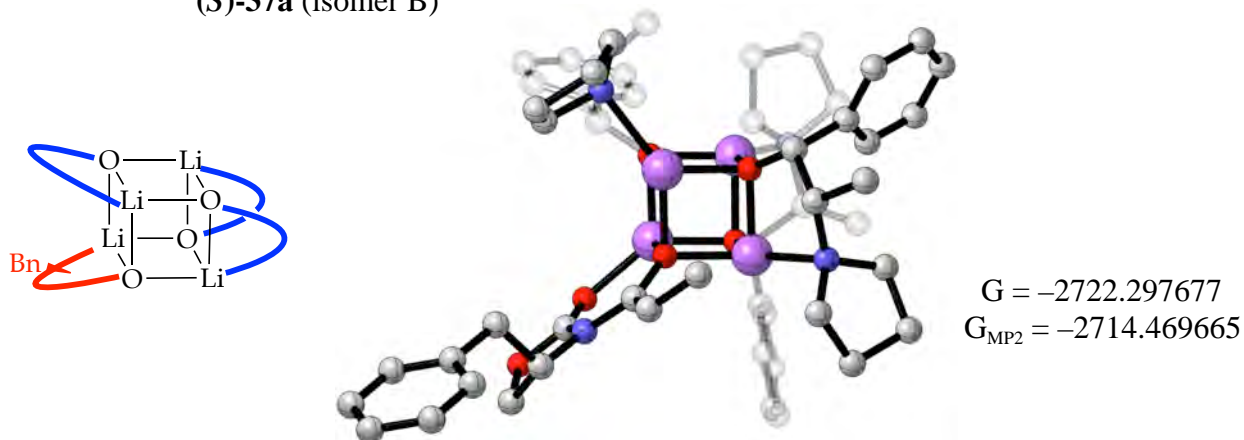
Table 60. Geometric coordinates and thermally corrected MP2 energies for transition state (*S*)-37a (isomer A)



Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	C	-1.54134500	0.08940700	3.13610500
Li	-0.79082400	-2.41405100	0.28357100	C	-0.15500800	0.26803500	3.22004500
O	0.92299100	-1.79306500	-0.47055200	C	0.40906800	1.10432900	4.18508700
Li	-0.24601600	-1.60307500	-2.14307700	C	-0.40609800	1.78456800	5.09139200
O	-0.75548000	0.22932900	-1.74313800	C	-1.79059200	1.62728500	5.01513700
Li	-2.23543000	-0.68473500	-1.00469100	C	-2.34639400	0.79360200	4.04331500
O	-1.56291500	-0.74299000	0.83435600	H	-3.42864800	0.69635800	3.98044400
C	-2.18949100	-0.80769000	2.07064200	H	-2.44019300	2.16398200	5.70246800
C	-2.40444900	-2.31227100	2.51325100	H	0.03202200	2.44068200	5.83910600
H	-3.17545200	-2.67687900	1.82071300	H	1.48817200	1.23241300	4.22013600
N	-1.23942100	-3.18891800	2.21465800	H	0.49025300	-0.23802500	2.51158300
C	-0.06168500	-3.10028600	3.13519500	O	-1.70980000	-2.58158800	-1.42761000
C	0.21601900	-4.53316300	3.61805800	C	-2.90663700	-3.28179800	-1.44165200
C	-0.34801400	-5.39503700	2.48013500	C	-4.00015900	-2.54701900	-2.29608200
C	-1.61316800	-4.62683500	2.09339700	H	-4.94135100	-3.12262900	-2.21791700
H	-1.95760800	-4.84784700	1.07702400	N	-4.23277000	-1.19438300	-1.71355600
H	-2.43038000	-4.89057200	2.78283400	C	-4.97583200	-0.25278800	-2.58150600
H	0.35295200	-5.42471600	1.63822300	C	-5.38896400	0.89208000	-1.64055800
H	-0.56361900	-6.42633900	2.77706800	C	-5.43662500	0.23768500	-0.23240700
H	1.27831500	-4.71030500	3.81491500	C	-5.06261900	-1.23141200	-0.48677200
H	-0.33292400	-4.73576600	4.54654000	H	-4.51717400	-1.68171300	0.34508900
H	-0.25002700	-2.41028500	3.96072000	H	-5.96960200	-1.83970900	-0.66237300
H	0.79846600	-2.70873200	2.57843200	H	-4.71095700	0.70819300	0.43890300
C	-2.97488200	-2.45321500	3.93413200	H	-6.41968100	0.32078200	0.24110900
H	-3.89152600	-1.86053800	4.03022500	H	-4.64987700	1.69836900	-1.67018100
H	-3.23459900	-3.49279900	4.16194500	H	-6.35021500	1.32127400	-1.93903700
H	-2.28054300	-2.09668500	4.70030500	H	-5.87196200	-0.74281100	-3.00412100
H	-3.23104500	-0.43282100	1.99902500	H	-4.35470000	0.08678400	-3.41260900

C	-3.60411300	-2.49983300	-3.77278800	H	-2.95055800	4.50389600	-1.17395500
H	-3.47494000	-3.52140600	-4.14105000	H	-2.18990500	2.13495300	-1.26981200
H	-4.36701100	-2.02042800	-4.39255000	C	2.13696400	-2.21444000	-0.22962600
H	-2.65758500	-1.97216900	-3.90916100	N	3.07149100	-1.19751000	0.24587300
H	-3.32985800	-3.33507700	-0.41742700	C	2.76849700	0.10577700	0.54316600
C	-2.77923400	-4.74337400	-1.88857800	O	1.71072100	0.71446900	0.45912900
C	-3.78200700	-5.67110500	-1.56994900	O	3.88178600	0.75036200	0.99187300
C	-3.69049000	-7.00129000	-1.98161200	C	4.91796500	-0.21744400	1.22681000
C	-2.58422900	-7.43121400	-2.71808800	H	4.92367600	-0.47095200	2.29312000
C	-1.57502900	-6.52008800	-3.03345500	H	5.87654700	0.22641700	0.95466900
C	-1.67362400	-5.18916600	-2.62071100	C	4.52437000	-1.41084800	0.34797400
H	-0.88763900	-4.47845600	-2.85368600	H	4.73146400	-2.34950500	0.86651200
H	-0.70578100	-6.84634100	-3.59968500	C	5.21107500	-1.40761200	-1.03965800
H	-2.50722200	-8.46770600	-3.03625900	H	4.68561800	-2.13152800	-1.67053600
H	-4.47871200	-7.70362700	-1.72127700	H	5.06683600	-0.41805800	-1.49094800
H	-4.64332900	-5.34871600	-0.98670000	C	6.68551400	-1.73958300	-0.96747700
C	-0.02744100	1.08373700	-2.55959000	C	7.66194700	-0.74296100	-1.09914900
C	0.00666300	0.54766800	-4.03201400	C	9.02083600	-1.05145300	-1.00638600
H	0.68499300	1.18864600	-4.62481400	C	9.42585000	-2.36693900	-0.77947100
N	0.57430000	-0.83221300	-4.01742200	C	8.46385700	-3.37162200	-0.65068400
C	0.41948800	-1.58804300	-5.27910900	C	7.10811700	-3.05918100	-0.74489400
C	1.36582400	-2.78580700	-5.11567600	H	6.36713100	-3.85127600	-0.65650300
C	2.49687800	-2.25683300	-4.19190900	H	8.77005300	-4.40082400	-0.48248500
C	2.04182500	-0.83719000	-3.80181400	H	10.4826210	-2.60974700	-0.70898200
H	2.28307600	-0.58238700	-2.76800900	H	9.76128300	-0.26348200	-1.11607200
H	2.51891100	-0.08319100	-4.45444800	H	7.35534400	0.28352200	-1.28926500
H	2.60881300	-2.88562800	-3.30382100	C	2.60310800	-3.48304700	-0.38384200
H	3.46736100	-2.23045800	-4.69742300	C	1.76365600	-4.62015200	-0.89321900
H	0.84058300	-3.62245800	-4.64249400	H	0.71674800	-4.32721700	-1.00926800
H	1.73558800	-3.14031800	-6.08269300	H	2.10890700	-4.98790900	-1.87267200
H	0.72722400	-0.97068400	-6.14330700	H	1.79430300	-5.48626400	-0.21697400
H	-0.62030200	-1.88540300	-5.43187200	H	3.63263400	-3.71503600	-0.13949000
C	-1.37800500	0.61221600	-4.67802200				
H	-2.10194700	0.02399900	-4.11043400				
H	-1.72010300	1.65094400	-4.68341200				
H	-1.37122900	0.26134800	-5.71403100				
H	1.02811000	1.11589400	-2.22554100				
C	-0.49738600	2.54351300	-2.51216900				
C	-1.64300200	2.90897700	-1.79796200				
C	-2.06118900	4.24135600	-1.74230000				
C	-1.33683700	5.23429200	-2.40196700				
H	-1.65925800	6.27144800	-2.35784800				
C	-0.18242100	4.88482800	-3.10697000				
H	0.40043800	5.65124400	-3.61238800				
C	0.23372300	3.55447900	-3.15463900				
H	1.14675500	3.30191200	-3.69043800				

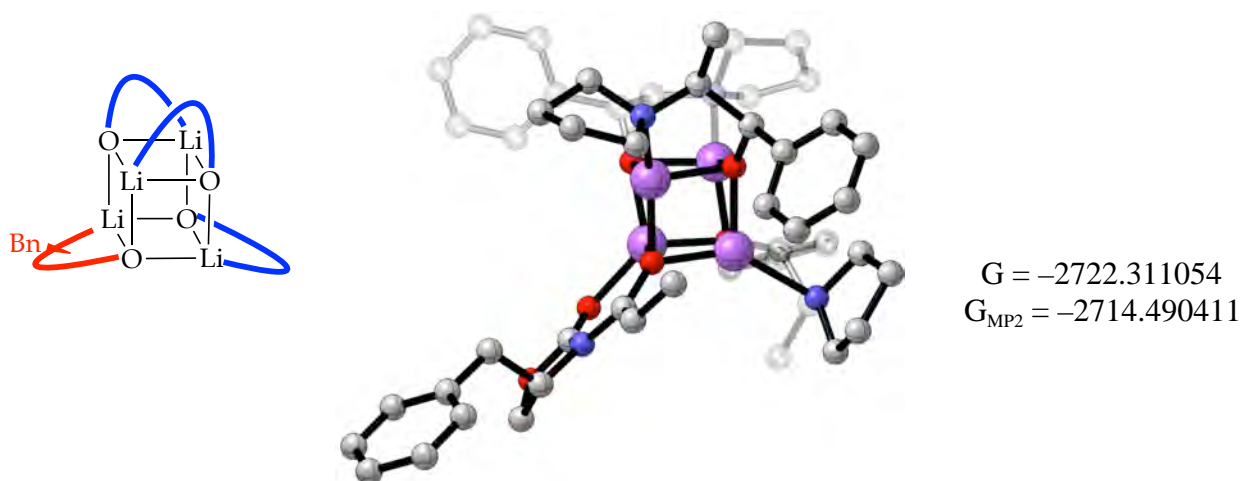
Table 61. Geometric coordinates and thermally corrected MP2 energies for transition state (*S*)-37a (isomer B)



Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	C	-2.82973200	-2.90911400	-0.76899100
Li	0.44971000	-2.28823400	1.17526600	C	-3.34193800	-3.37010000	0.44911100
O	1.78720900	-0.72411700	0.63622100	C	-4.61029700	-3.94886100	0.52812900
Li	1.02891000	0.02576300	2.33540100	C	-5.40462900	-4.06326800	-0.61428200
O	-0.46562000	0.96046500	1.63405600	C	-4.91962600	-3.58524500	-1.83225500
Li	-1.39048200	-0.75041200	2.01690400	C	-3.64865100	-3.01207800	-1.90296300
O	-1.05705800	-1.56278800	0.25269800	H	-3.28953700	-2.62970800	-2.85628700
C	-1.43479300	-2.27919700	-0.87555400	H	-5.53364200	-3.64948400	-2.72728600
C	-0.28128300	-3.27177700	-1.30805700	H	-6.39412300	-4.50876100	-0.55334400
H	0.51439900	-2.59656800	-1.63941400	H	-4.98207400	-4.30848800	1.48496700
N	0.33880300	-3.99339200	-0.15958600	H	-2.73760500	-3.25686800	1.34171000
C	-0.32758400	-5.22875200	0.30494000	O	0.14840200	-1.59226800	2.89335600
C	0.68704800	-5.84044900	1.28180200	C	-0.03898600	-1.75608300	4.25659300
C	2.06810800	-5.39403400	0.72589000	C	-1.44924000	-2.37466000	4.54817700
C	1.73133000	-4.42942400	-0.43026600	H	-1.58477800	-2.43665100	5.64432900
H	2.39543200	-3.56071600	-0.48241600	N	-2.49285000	-1.46469100	4.00274200
H	1.80103600	-4.96288100	-1.39296800	C	-3.85569000	-2.03790500	3.96954100
H	2.65519100	-4.89333200	1.50236300	C	-4.75678700	-0.82752600	3.70469000
H	2.66423000	-6.23905200	0.36778300	C	-4.02791000	0.34264400	4.41594700
H	0.53494900	-5.44183600	2.28923400	C	-2.67113500	-0.25529900	4.84343000
H	0.58563200	-6.92852300	1.34023100	H	-1.83313300	0.43309900	4.71975000
H	-0.50611400	-5.92193100	-0.53334400	H	-2.70330700	-0.54416600	5.91018600
H	-1.29293500	-5.00484600	0.76089000	H	-3.90004300	1.19485900	3.74250100
C	-0.65204200	-4.15554700	-2.50973900	H	-4.58078000	0.70391800	5.28871500
H	-0.94320000	-3.52307100	-3.35593200	H	-4.82671300	-0.64287900	2.62737800
H	0.19655300	-4.76418700	-2.84050600	H	-5.77353200	-0.98775200	4.07632700
H	-1.49204700	-4.82267600	-2.29870100	H	-4.10848700	-2.49930200	4.94299200
H	-1.50688500	-1.60835700	-1.75845900	H	-3.94306200	-2.80450200	3.19924400

C	-1.55072300	-3.79441100	3.98752800	H	-2.54007600	3.78257100	5.08483400
H	-1.40278800	-3.80052800	2.90465700	H	-1.86833100	2.02480300	3.45023100
H	-0.76865100	-4.41341700	4.43647200	O	2.68999600	0.52984900	3.05538300
H	-2.51183900	-4.26441600	4.21489200	C	3.66931500	-0.11919100	2.71187100
H	-0.02951400	-0.77152200	4.76480000	O	4.68913200	-0.33856100	3.58396400
C	1.06414300	-2.56778800	4.94975600	C	5.60652700	-1.27404000	2.98247200
C	1.12864500	-2.63629700	6.34957900	H	5.33160400	-2.28417000	3.30544300
C	2.12218800	-3.37626800	6.99082900	H	6.61409400	-1.03478900	3.32403200
C	3.08166300	-4.06170700	6.24199100	C	5.39099300	-1.05667100	1.48276100
C	3.03911400	-3.98856700	4.84942400	H	5.52753000	-1.97706600	0.91035600
C	2.04157700	-3.24426900	4.21314100	N	3.96474400	-0.68815400	1.49877300
H	2.01851000	-3.16869000	3.13096100	C	3.06411300	-0.79005100	0.35375800
H	3.78390300	-4.51380300	4.25461400	C	3.62629000	-0.99129800	-0.86867500
H	3.85719300	-4.63814000	6.73968300	C	2.85196300	-1.12770800	-2.14729500
H	2.15175800	-3.41212200	8.07712800	H	3.26831200	-0.48307400	-2.93401000
H	0.39846700	-2.09486600	6.94796000	H	2.86194500	-2.15193600	-2.55205000
C	-0.34338500	2.27759400	1.19657000	H	1.80531400	-0.84294000	-2.00919200
C	-1.13199400	2.48775900	-0.14120200	H	4.70388100	-1.03899000	-0.95864700
H	-1.08792300	3.55923000	-0.41026700	C	6.29754400	0.07523600	0.92773800
N	-0.45940500	1.70641400	-1.21818900	H	5.92000300	0.37924800	-0.05272700
C	-1.24896300	1.57540500	-2.46289900	H	6.19405700	0.94471600	1.58816300
C	-0.21765800	1.14317800	-3.50104300	C	7.75179500	-0.33388400	0.83125400
C	0.99808000	2.02075400	-3.14966600	C	8.70062500	0.14375500	1.74543100
C	0.85105300	2.29972800	-1.63280800	C	10.0375130	-0.25241100	1.66747200
H	1.66492800	1.85607000	-1.05130400	C	10.4479520	-1.13723400	0.67021900
H	0.85987900	3.38236800	-1.43465200	C	9.51407700	-1.61933900	-0.25000900
H	1.94887300	1.53915900	-3.39255100	C	8.18044900	-1.21980700	-0.16923100
H	0.95750500	2.96144400	-3.70960200	H	7.46392900	-1.59327200	-0.89833300
H	0.01936400	0.08043100	-3.37184500	H	9.82597000	-2.30323000	-1.03512400
H	-0.56879900	1.28557600	-4.52802000	H	11.4878710	-1.44582500	0.60626000
H	-1.69569400	2.54278400	-2.75675700	H	10.7570160	0.13416600	2.38446600
H	-2.06024100	0.85553700	-2.32892000	H	8.39077400	0.84268400	2.51942700
C	-2.60187100	2.08954300	0.01930300				
H	-2.70473900	1.00989800	0.16577900				
H	-3.01846100	2.59523300	0.89563800				
H	-3.20200000	2.38239000	-0.84762100				
H	0.71579800	2.49999000	0.95921200				
C	-0.74171700	3.34785300	2.21739400				
C	-1.54599100	3.04929800	3.31872500				
C	-1.91437000	4.03939100	4.23304200				
C	-1.47729100	5.35257100	4.05868100				
H	-1.75832700	6.12452100	4.77047500				
C	-0.66447400	5.66433500	2.96574400				
H	-0.30658300	6.68150400	2.82546100				
C	-0.30012800	4.66974900	2.05862300				
H	0.34744200	4.92122700	1.22017600				

Table 62. Geometric coordinates and thermally corrected MP2 energies for transition state (*S*)-37a (isomer C)



Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	H	-2.50552800	1.76054600	1.97257000
Li	-0.95127400	-1.93960900	-1.47086900	C	-1.72473400	3.21537800	0.65380000
O	-0.15524400	-0.08577000	-1.97419500	C	-1.12760100	3.50843200	-0.57938100
Li	-2.09035300	0.45103300	-1.55112100	C	-1.18510200	4.79344400	-1.12205500
O	-2.74140300	-1.36606100	-1.35242300	C	-1.85810600	5.81404100	-0.44601300
Li	-2.26035400	-1.08828700	0.47418200	C	-2.47307600	5.53464000	0.77529200
O	-1.74077900	0.79777700	0.31781200	C	-2.40617700	4.24758000	1.31444300
C	-1.65331600	1.80932400	1.26310000	H	-2.89942600	4.03903100	2.26176600
C	-0.40619700	1.58698200	2.20357200	H	-3.01219600	6.31548500	1.30620500
H	-0.62488400	0.62337800	2.68127500	H	-1.90887300	6.81333400	-0.87046400
N	0.85978400	1.32643200	1.46010600	H	-0.70579000	4.99628900	-2.07698700
C	1.59761100	2.51667800	0.92682100	H	-0.60790000	2.71808800	-1.11159200
C	2.98793500	2.49487200	1.57855900	O	-0.43356000	-1.82664300	0.38035400
C	3.21891800	0.99793800	1.82040300	C	-0.27866400	-2.53795200	1.56164100
C	1.83263500	0.52314300	2.26249900	C	-1.55681200	-3.38837700	1.88890700
H	1.67513900	-0.54618400	2.09442800	H	-1.38383500	-3.91182600	2.84794600
H	1.70600600	0.71209900	3.33954200	N	-2.70765600	-2.45293900	2.06278400
H	3.51901100	0.50254600	0.88948400	C	-4.04950000	-3.07659700	2.02309800
H	3.98669800	0.78677100	2.57127100	C	-4.98642500	-1.96327500	2.51841500
H	3.75412400	2.96148600	0.95088000	C	-4.09760600	-1.10122300	3.45757400
H	2.96904200	3.03029900	2.53632700	C	-2.70746200	-1.75715600	3.36798300
H	1.05373000	3.44246600	1.12098300	H	-1.89019500	-1.03516500	3.43231600
H	1.68643200	2.42350700	-0.16313400	H	-2.57001600	-2.48777700	4.18670100
C	-0.29411300	2.63435600	3.32418500	H	-4.06089700	-0.06178100	3.11488700
H	-1.22534200	2.66767000	3.90149400	H	-4.46257900	-1.08945700	4.48927700
H	0.51271700	2.38773800	4.02281400	H	-5.34680000	-1.36702700	1.67325800
H	-0.11645400	3.64267500	2.93909300	H	-5.86533700	-2.37372800	3.02475600

H	-4.09466800	-3.94591200	2.70442900	C	-5.74452800	-3.32785800	-2.18506300
H	-4.29082100	-3.42135000	1.01633700	H	-6.49019300	-2.60578600	-1.85524400
C	-1.83390100	-4.44124100	0.81349900	H	-3.10210400	-5.90826600	-3.32559500
H	-0.92978900	-5.03077100	0.63815400	H	-2.41107100	-3.61315100	-2.75047400
H	-2.62438300	-5.13310300	1.11983100	C	0.63408100	-0.05797700	-3.02181500
H	-2.13196200	-3.98373400	-0.13300700	N	1.55418800	-1.19258000	-3.15234400
H	-0.17208100	-1.84210600	2.41891200	C	1.18937400	-2.49024900	-3.00125900
C	0.98480800	-3.40514300	1.60870300	O	0.07532000	-2.94846900	-2.75911600
C	1.56589500	-3.74500200	2.83878500	O	2.26822300	-3.30624500	-3.14212200
C	2.71794500	-4.53099300	2.89988800	C	3.38997300	-2.51708900	-3.58913300
C	3.31458100	-4.99015800	1.72344000	H	3.50578800	-2.66545200	-4.66813500
C	2.74709100	-4.65629100	0.49191200	H	4.28506200	-2.87038600	-3.07522100
C	1.59376400	-3.86986700	0.43683700	C	3.01263100	-1.06519200	-3.24086000
H	1.14958100	-3.61814800	-0.51889300	H	3.28860300	-0.38841100	-4.05362000
H	3.19526600	-5.01120000	-0.43319500	C	3.61419100	-0.54848100	-1.91413600
H	4.21278700	-5.60114600	1.76760000	H	3.12947100	0.41048900	-1.69332100
H	3.15288300	-4.77941400	3.86516400	H	3.33577400	-1.24519300	-1.11432100
H	1.11541800	-3.38196800	3.76167600	C	5.11668400	-0.37877900	-1.96658200
C	-4.00767800	-1.49826300	-1.90619600	C	5.96753500	-1.28693000	-1.32142300
C	-4.17475500	-0.55114200	-3.14342500	C	7.35500800	-1.14396600	-1.39321300
H	-5.22665200	-0.62340200	-3.48281200	C	7.91401000	-0.08829900	-2.11393200
N	-3.91635600	0.85281900	-2.71640500	C	7.07731100	0.82603300	-2.75853500
C	-4.02720900	1.82560500	-3.82743900	C	5.69237800	0.68123800	-2.68354300
C	-4.13594500	3.18878600	-3.13808700	H	5.04816500	1.40494300	-3.17926200
C	-4.85326800	2.88439500	-1.79857500	H	7.50398900	1.65610400	-3.31560100
C	-4.90346600	1.34376200	-1.71881900	H	8.99323900	0.02553800	-2.16929700
H	-4.65583400	0.96976700	-0.72219700	H	7.99724200	-1.85598100	-0.88156000
H	-5.91236900	0.97581100	-1.97731600	H	5.53788300	-2.10557300	-0.74767500
H	-4.30174200	3.30975700	-0.95653100	C	0.73410400	0.87851800	-3.99384200
H	-5.86496200	3.30163200	-1.77036400	C	-0.04196200	2.16077200	-4.05160500
H	-3.14037700	3.59950800	-2.94725800	H	0.60302100	3.04549900	-3.93261900
H	-4.67645900	3.91134300	-3.75782700	H	-0.55136700	2.27709500	-5.01851100
H	-4.93480300	1.62011200	-4.42520000	H	-0.80550100	2.20509000	-3.27072400
H	-3.16445000	1.75591100	-4.49314500	H	1.42162000	0.68319200	-4.81255500
C	-3.26186300	-0.94558500	-4.30863600				
H	-2.20594300	-0.81940100	-4.04900000				
H	-3.42288200	-1.99478600	-4.56843800				
H	-3.47037100	-0.35252700	-5.20410200				
H	-4.77800200	-1.17145900	-1.18111100				
C	-4.40048500	-2.93653900	-2.26361700				
C	-3.45843600	-3.88788000	-2.67835300				
C	-3.85097700	-5.18731300	-3.00682500				
C	-5.19365700	-5.56195500	-2.92686800				
H	-5.49679400	-6.57489700	-3.17939000				
C	-6.14252500	-4.62502100	-2.51422600				
H	-7.19095300	-4.90442400	-2.44134200				

Part 6. Full reference (Gaussian)

Gaussian 09, Revision A.02, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, G. A. Petersson, H. Nakatsuji, X. Li, M. Caricato, A. Marenich, J. Bloino, B. G. Janesko, R. Gomperts, B. Mennucci, H. P. Hratchian, J. V. Ortiz, A. F. Izmaylov, J. L. Sonnenberg, D. Williams-Young, F. Ding, F. Lipparini, F. Egidi, J. Goings, B. Peng, A. Petrone, T. Henderson, D. Ranasinghe, V. G. Zakrzewski, J. Gao, N. Rega, G. Zheng, W. Liang, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, K. Throssell, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, T. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, J. M. Millam, M. Klene, C. Adamo, R. Cammi, J. W. Ochterski, R. L. Martin, K. Morokuma, O. Farkas, J. B. Foresman, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2016.