

SUPPLEMENTARY INFORMATION

Versatile Coordination of a Reactive P,N-Ligand toward Group 13 Metal Centers

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NMR spectra of all new compounds

NMR spectra of 1

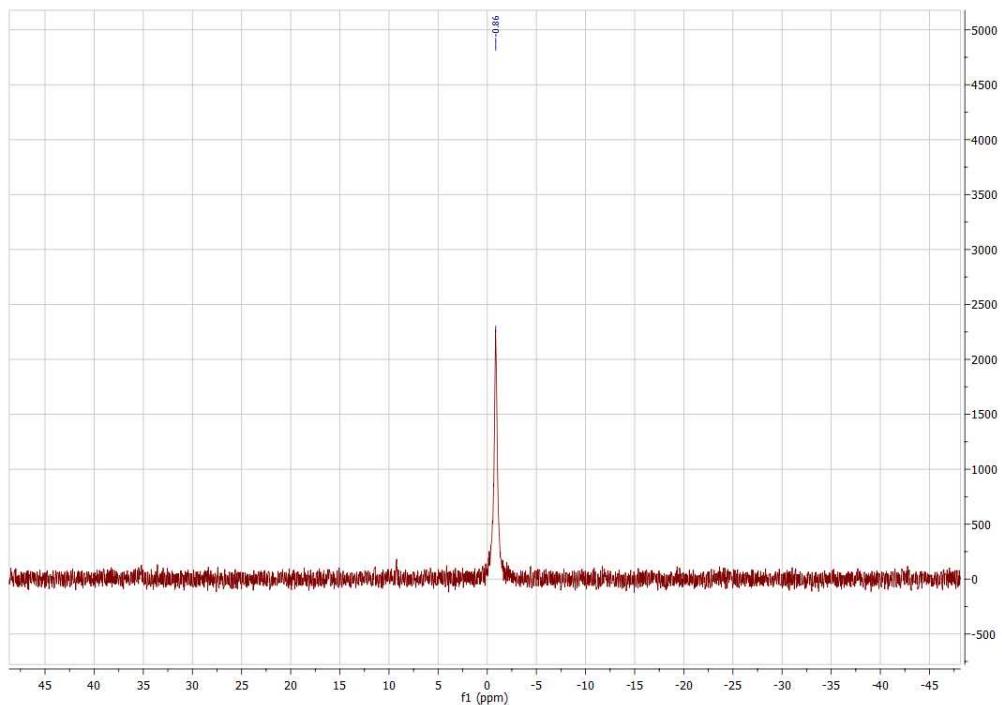


Figure 1. $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum of **1** (121 MHz, 20 °C) in CD_2Cl_2

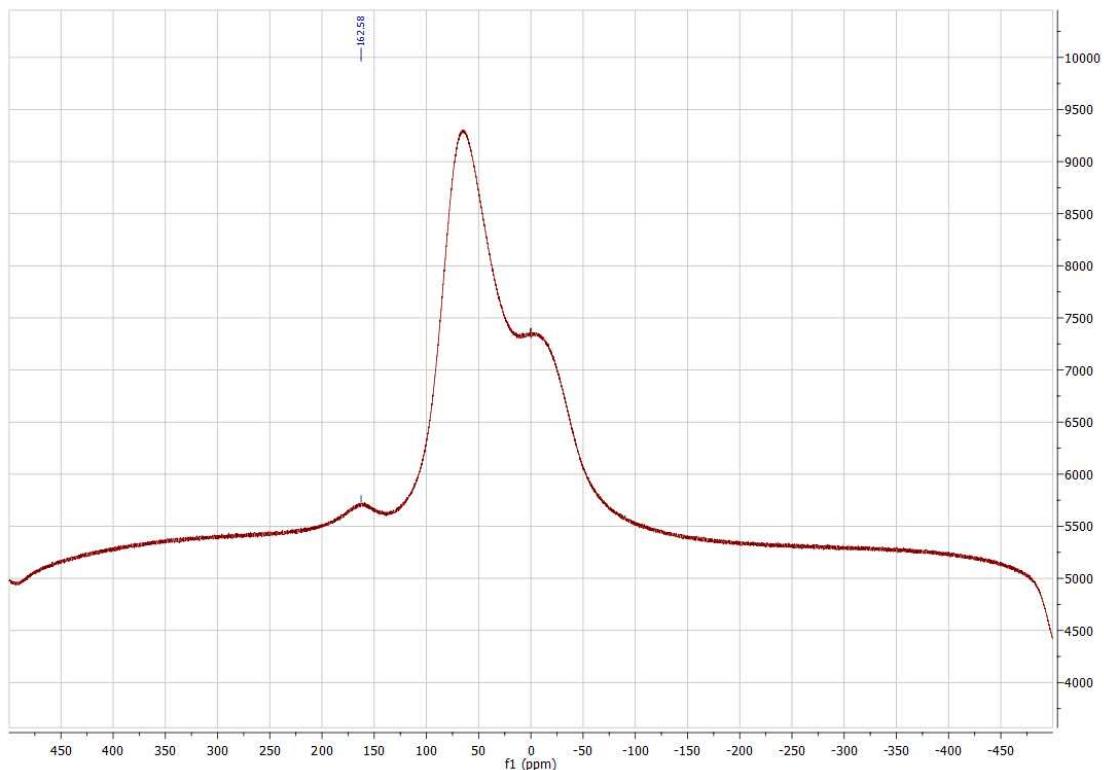


Figure 2. $^{27}\text{Al}\{^1\text{H}\}$ NMR spectrum of **1** (78 MHz, 20 °C) in CD_2Cl_2

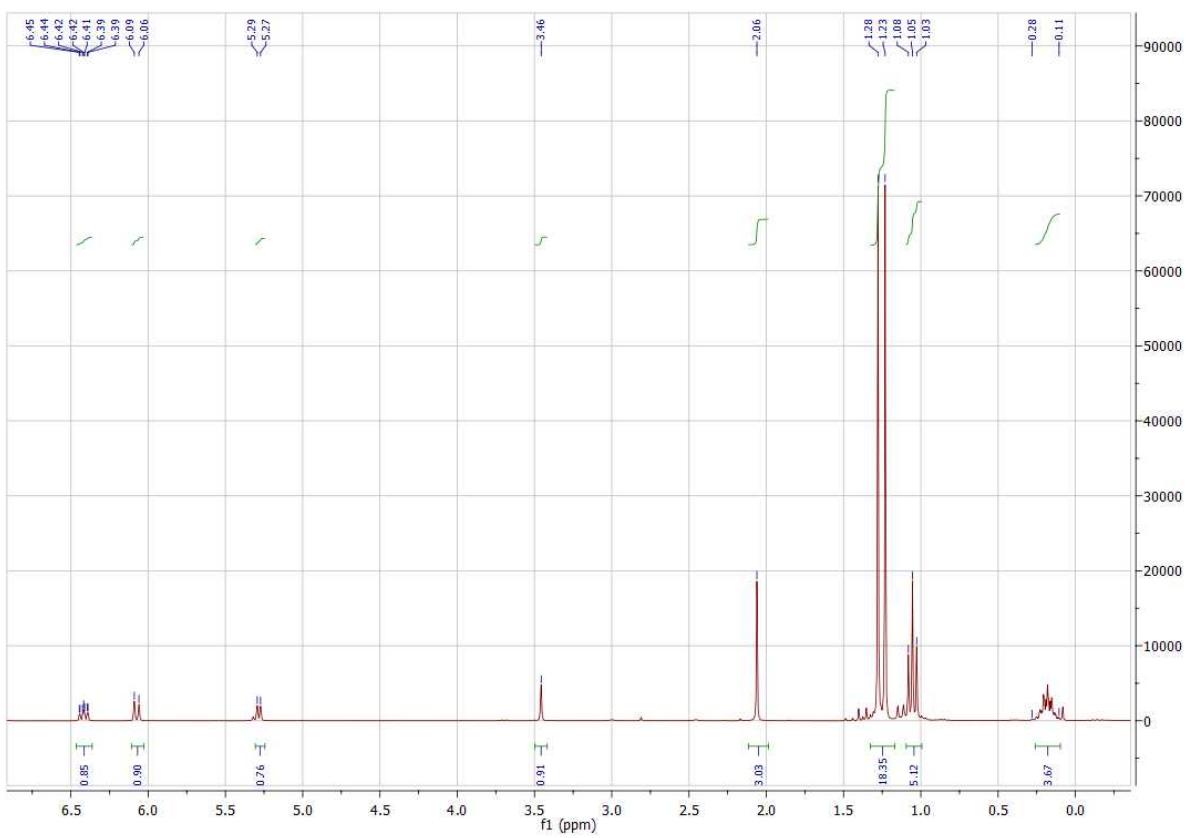


Figure 3. ¹H NMR spectrum of **1** (300 MHz, 20 °C) in CD₂Cl₂

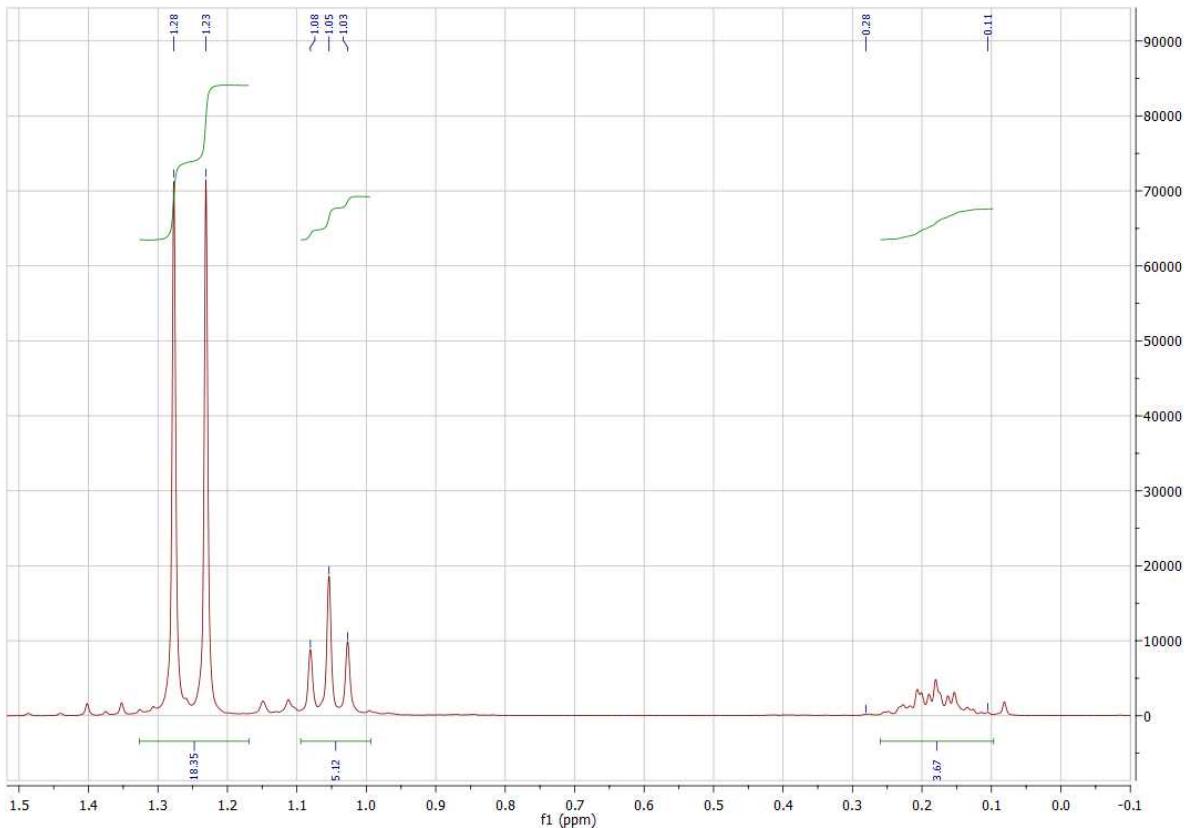


Figure 4. ^1H NMR spectrum of **1** (300 MHz, 20 °C) in CD_2Cl_2 : zoom 1

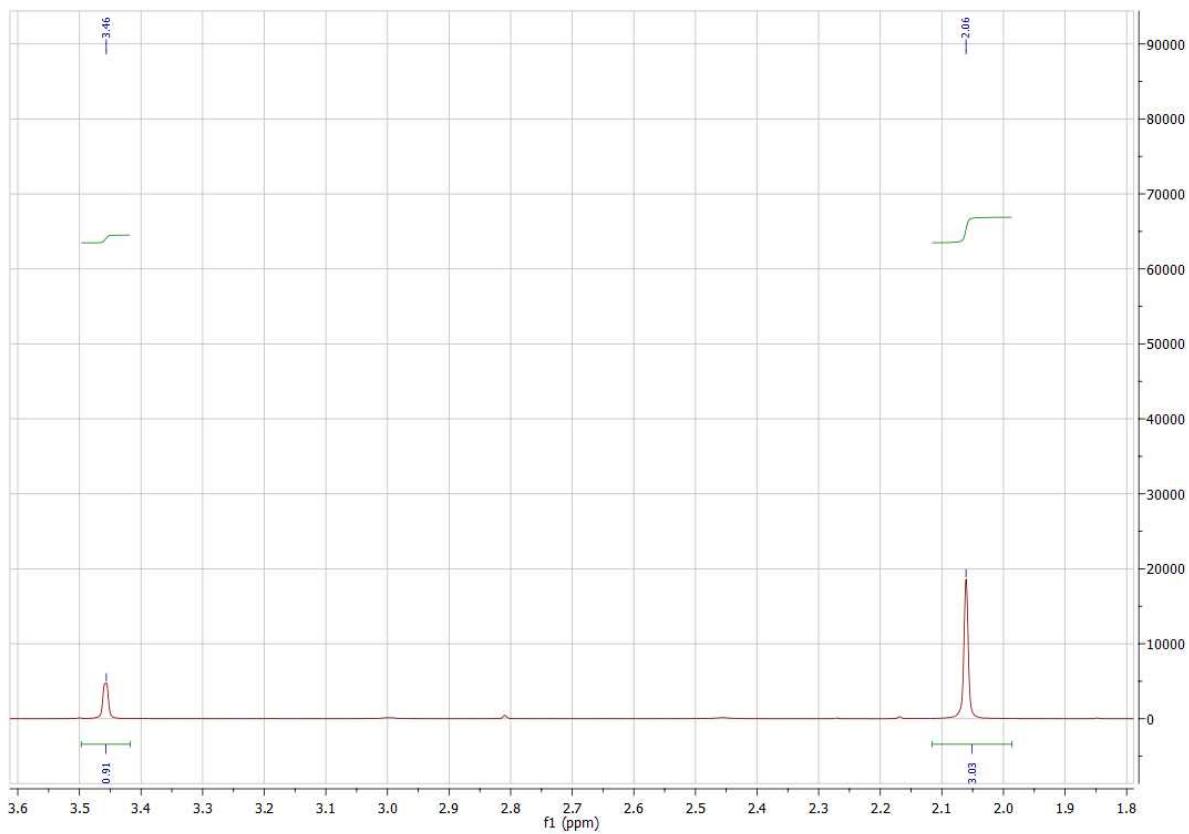


Figure 5. ^1H NMR spectrum of **1** (300 MHz, 20 °C) in CD_2Cl_2 : zoom 2

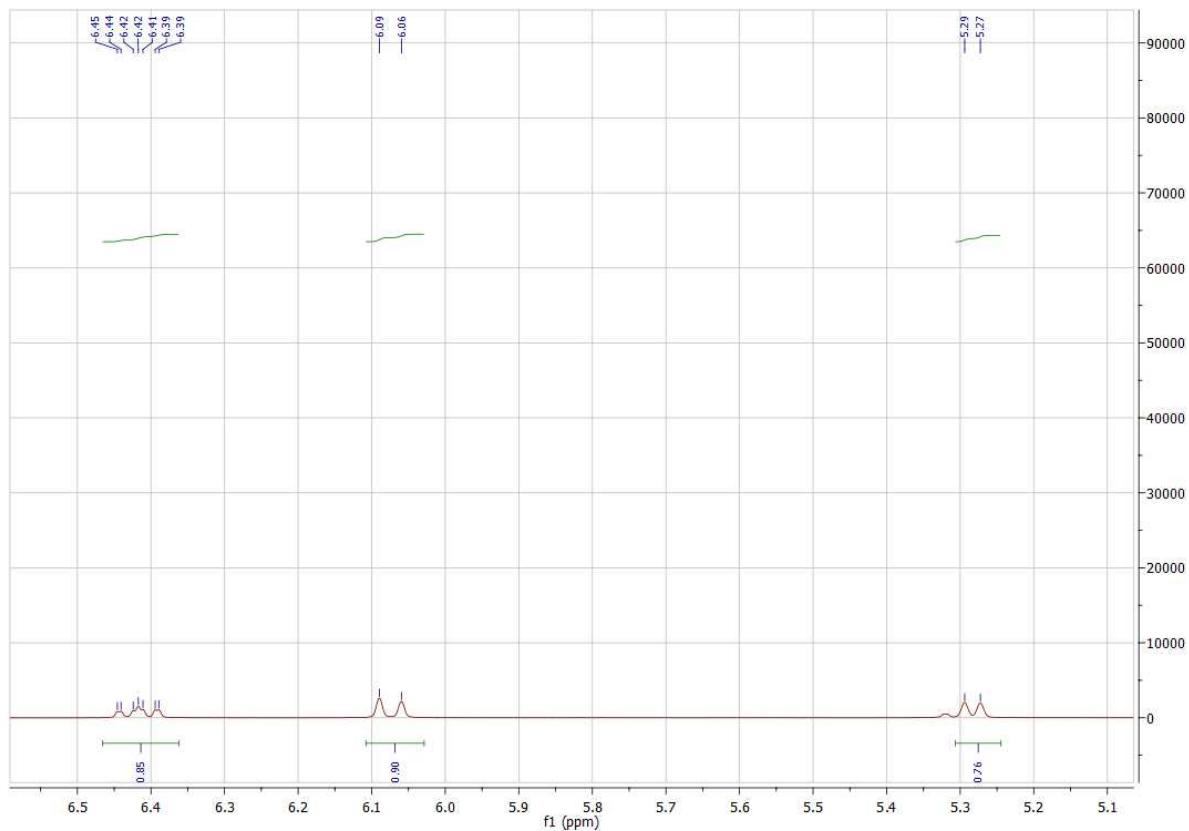


Figure 6. ^1H NMR spectrum of **1** (300 MHz, 20 °C) in CD_2Cl_2 : zoom 3

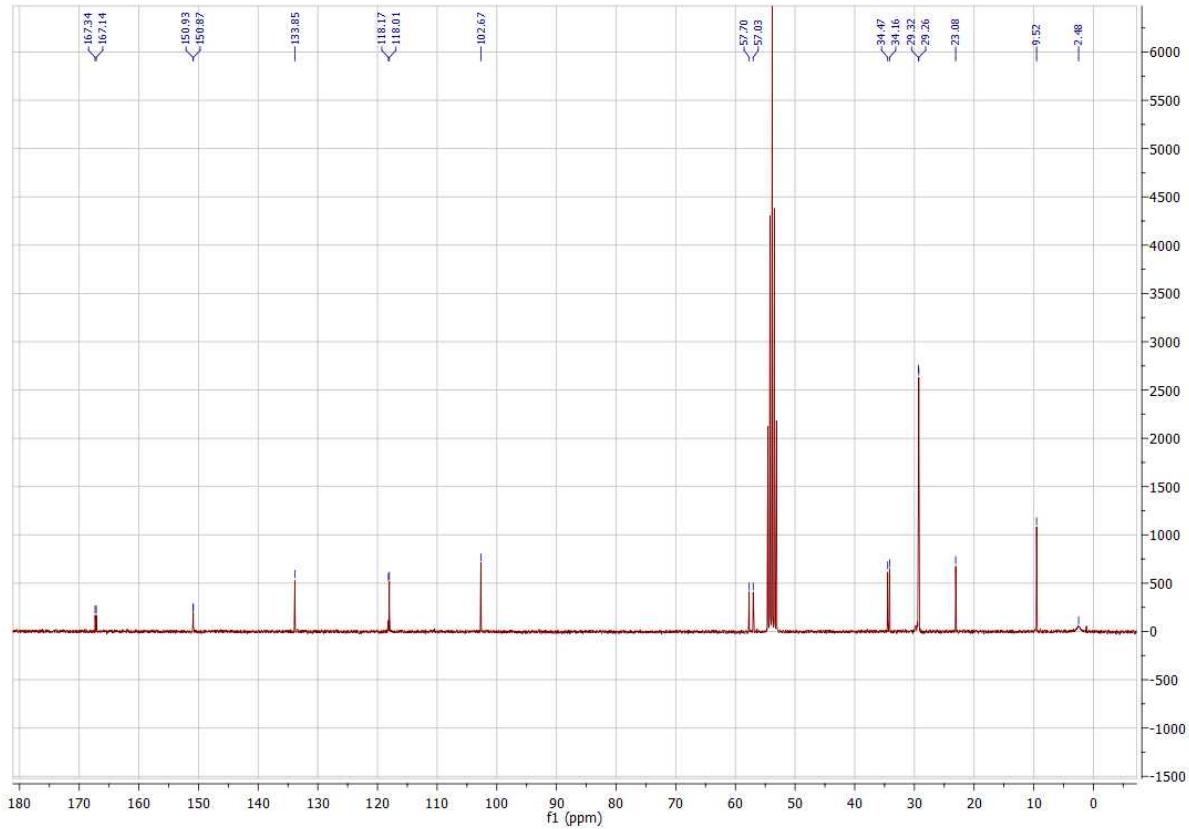


Figure 7. $^{13}\text{C}\{\text{H}\}$ NMR spectrum of **1** (75 MHz, 20 °C) in CD_2Cl_2

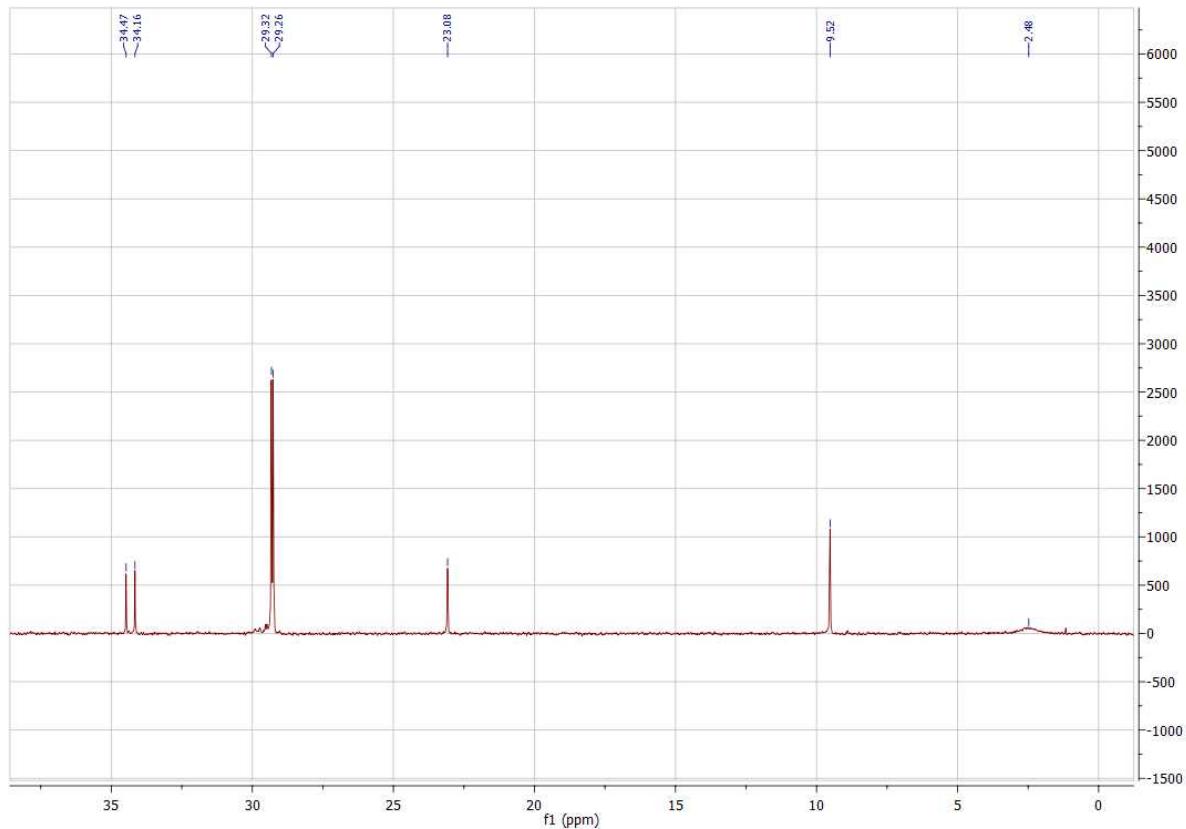


Figure 8. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **1** (75 MHz, 20 °C) in CD_2Cl_2 : zoom 1

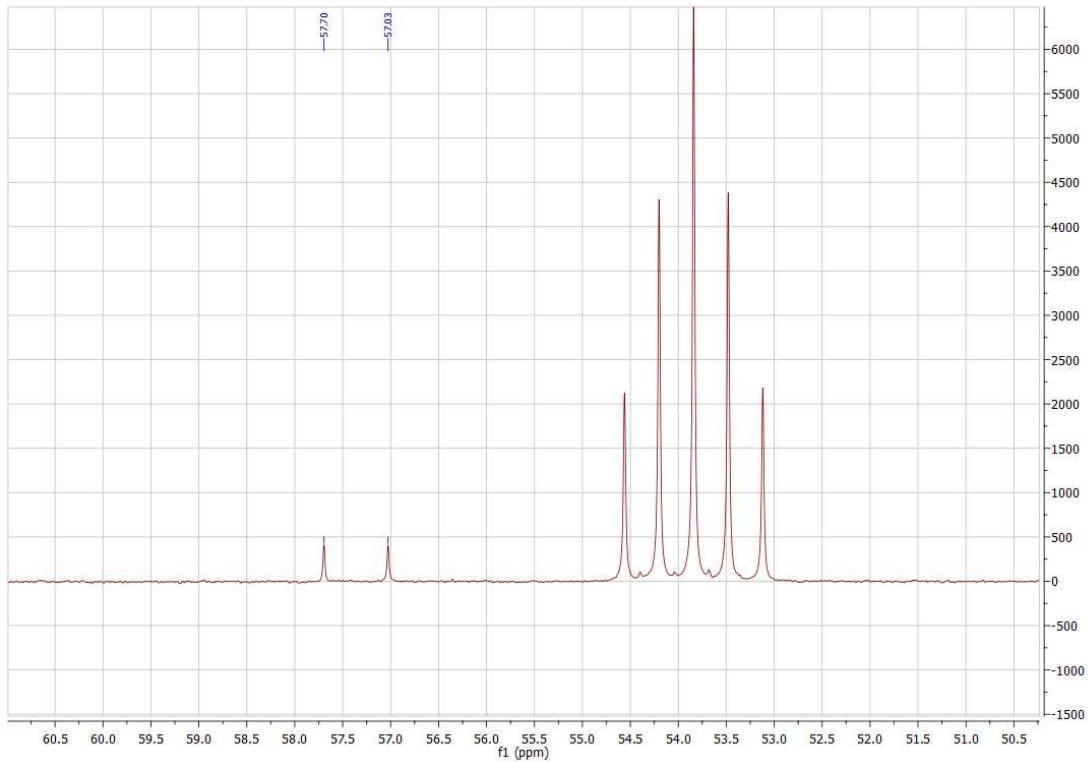


Figure 9. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **1** (75 MHz, 20 °C) in CD_2Cl_2 : zoom 2 (=CH-PPh₂ signal)

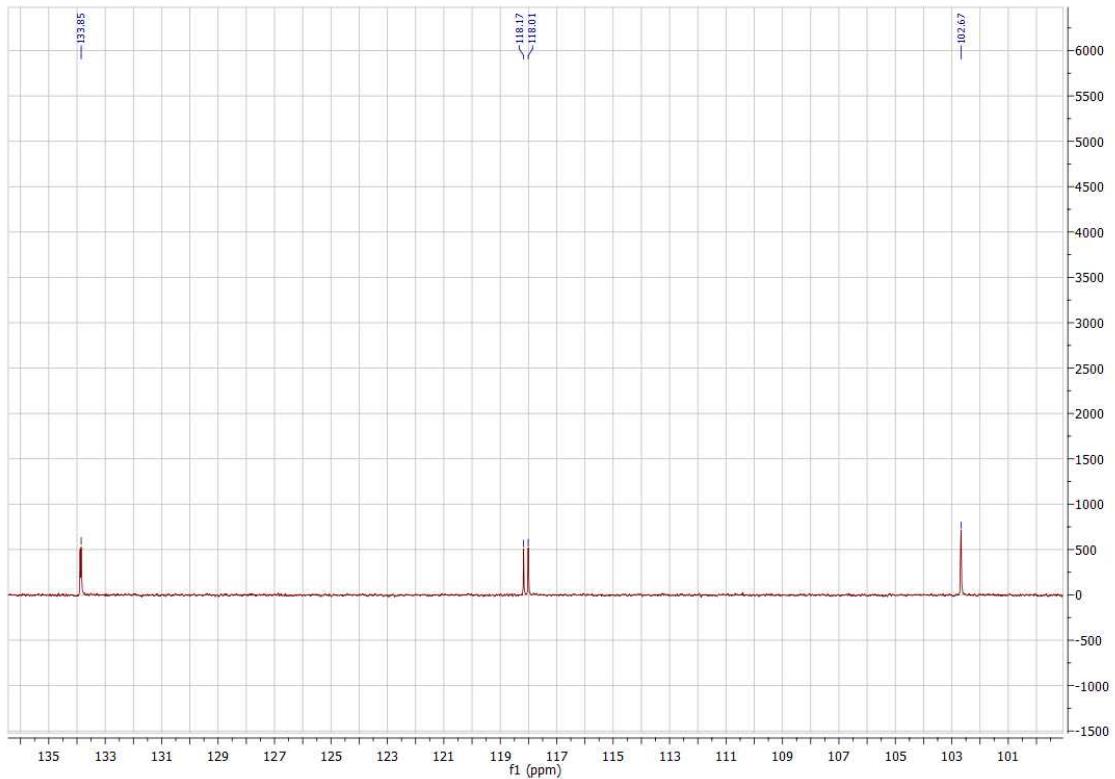


Figure 10. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **1** (75 MHz, 20 °C) in CD_2Cl_2 : zoom 3

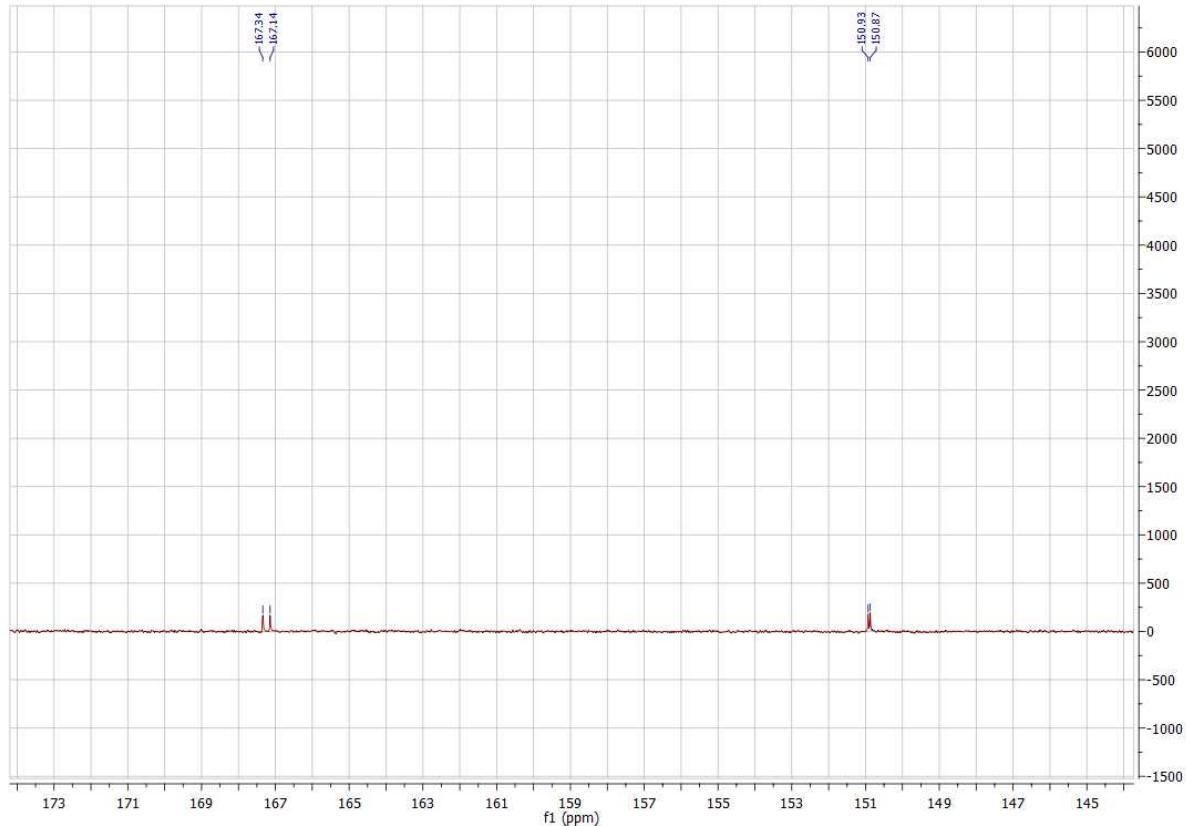


Figure 11. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **1** (75 MHz, 20 °C) in CD_2Cl_2 : zoom 4

NMR spectra of 2

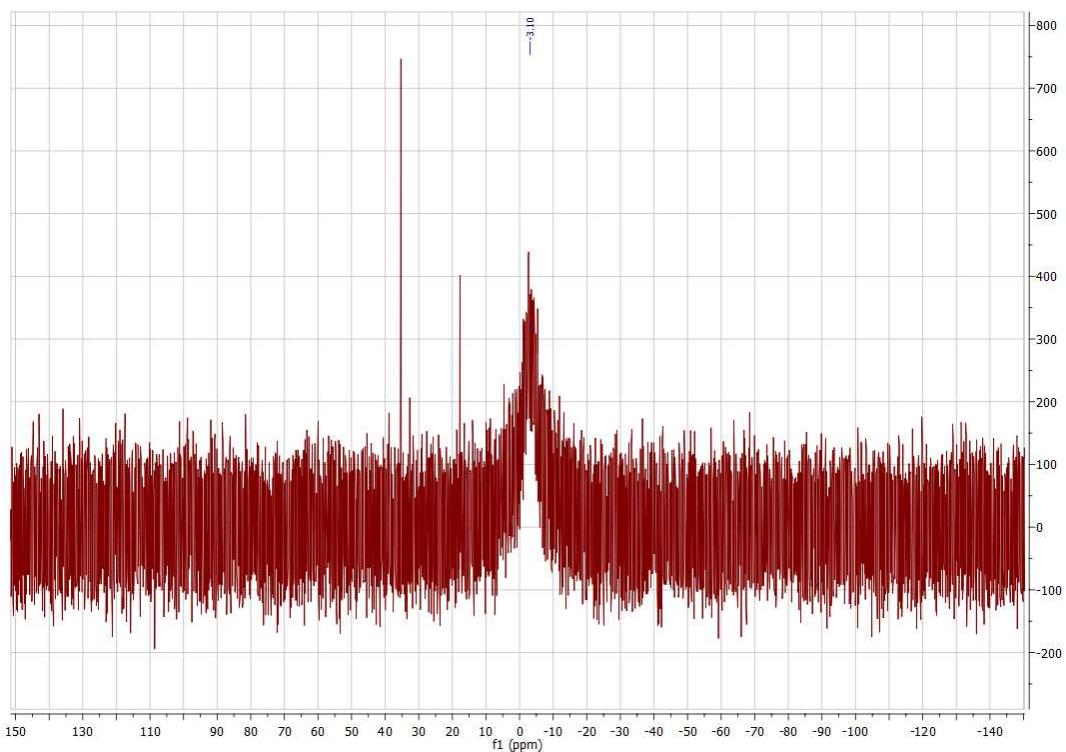


Figure 12. $^{31}\text{P}\{\text{H}\}$ NMR spectrum of **2** (121 MHz, 20 °C) in CD_2Cl_2

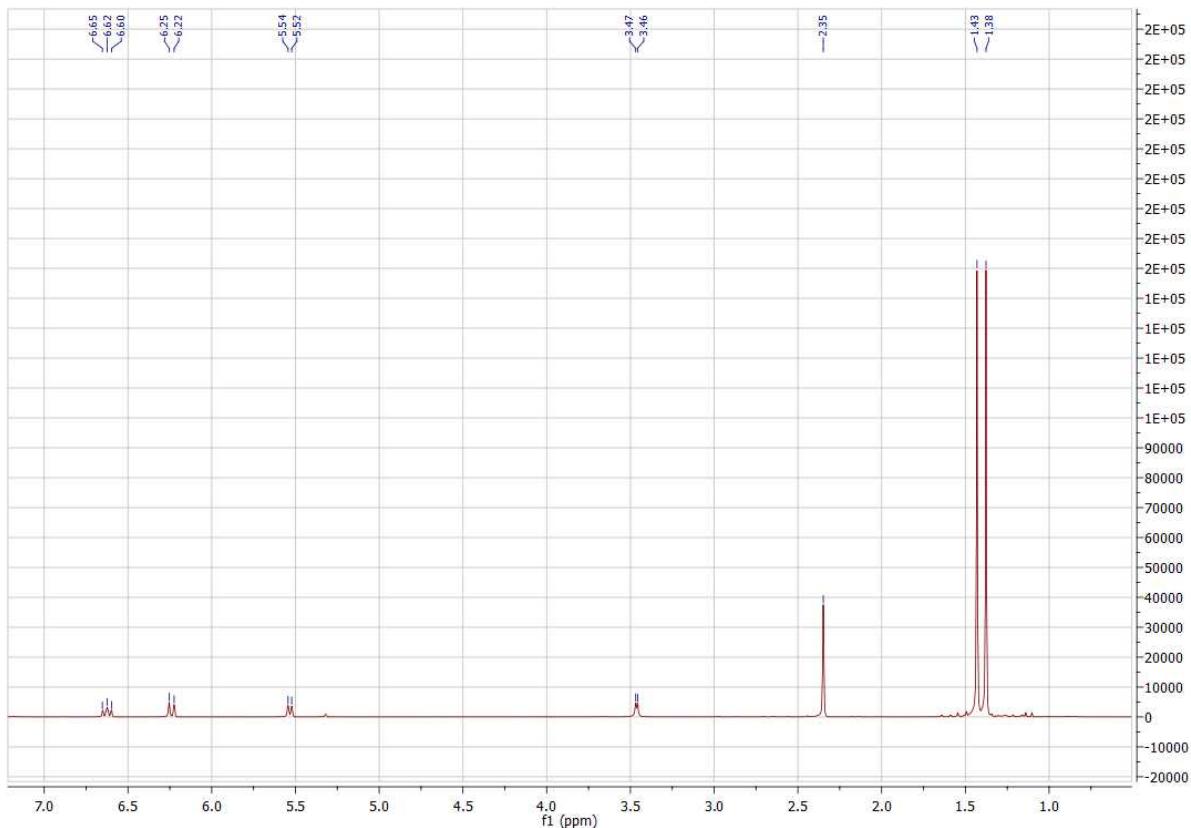


Figure 13. ^1H NMR spectrum of **2** (300 MHz, 20 °C) in CD_2Cl_2

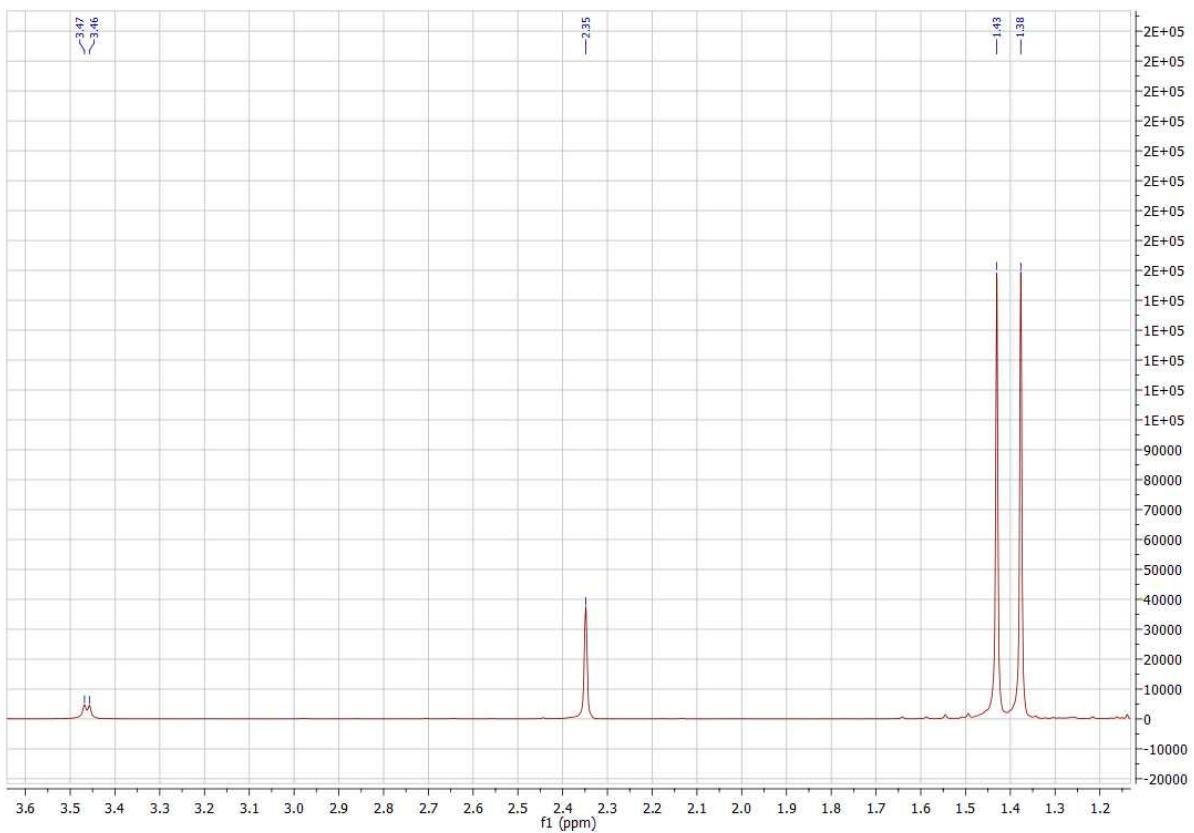


Figure 14. ¹H NMR spectrum of **2** (300 MHz, 20 °C) in CD₂Cl₂: zoom 1

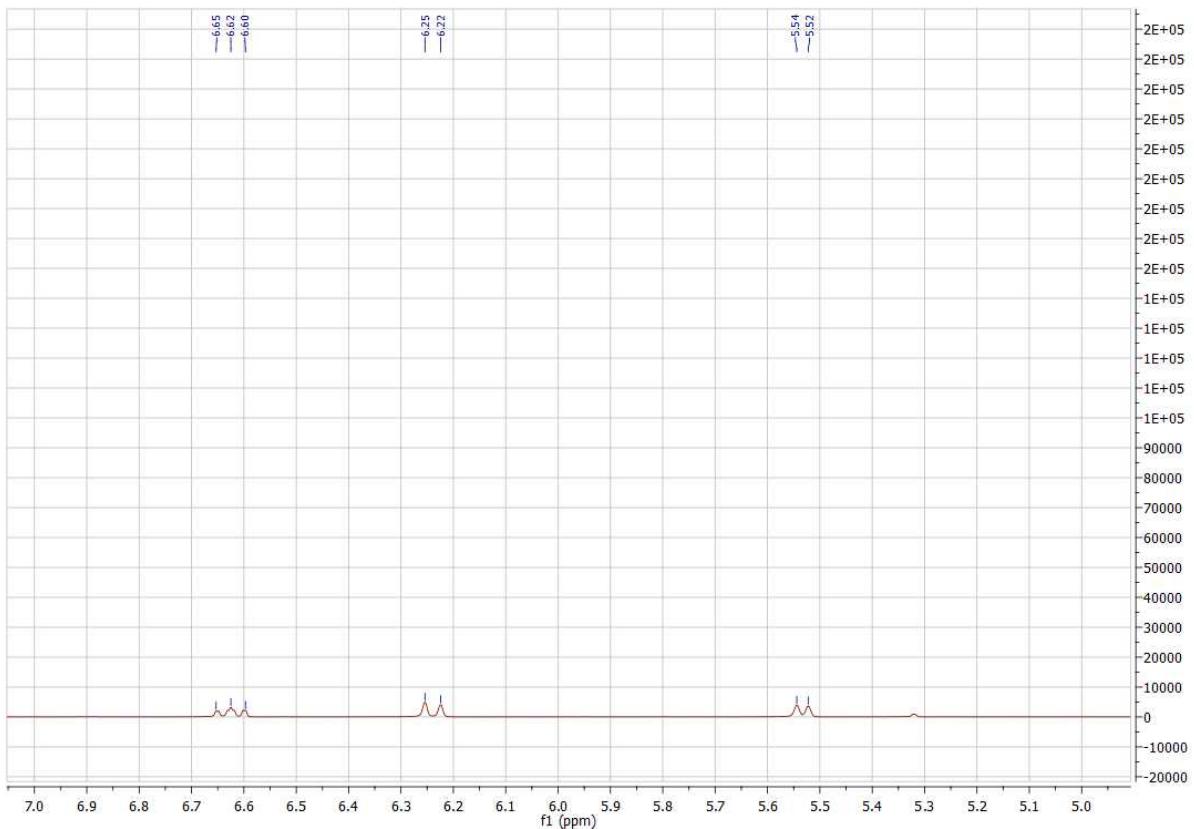


Figure 15. ¹H NMR spectrum of **2** (300 MHz, 20 °C) in CD₂Cl₂: zoom 2

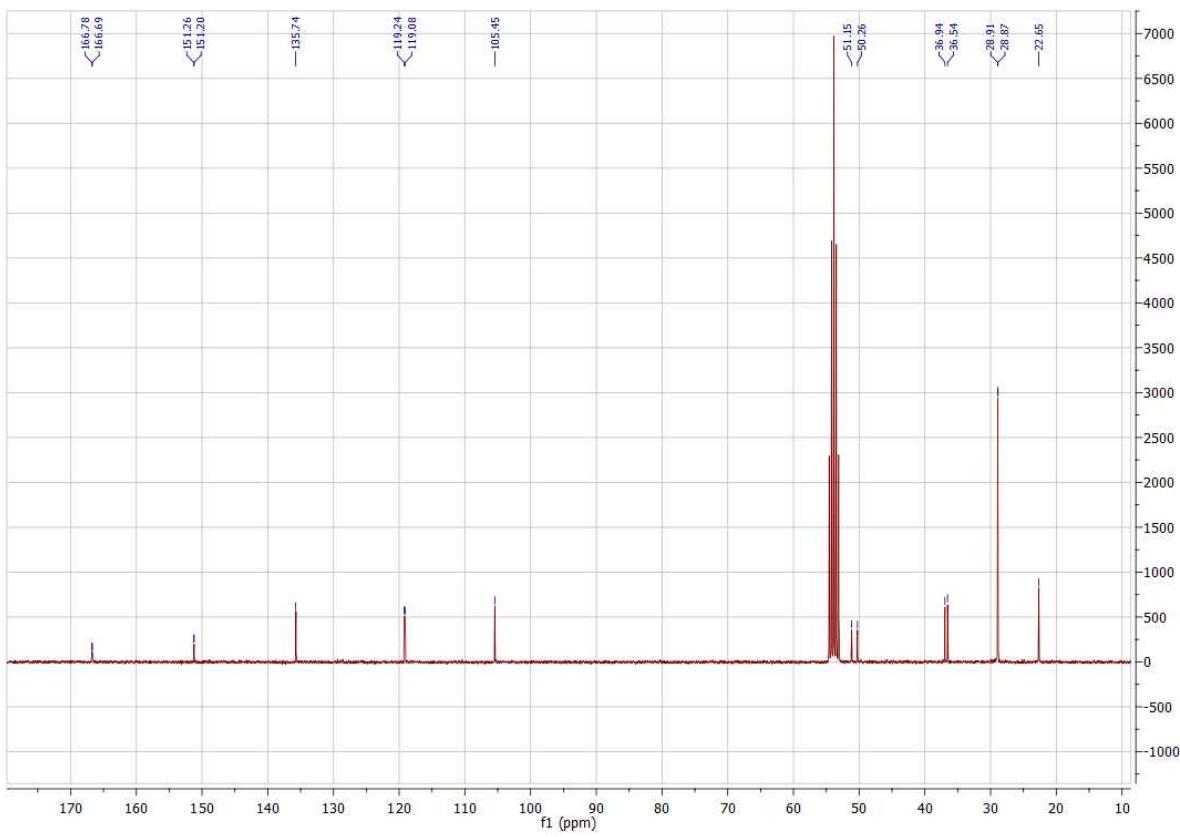


Figure 16. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **2** (75 MHz, 20 °C) in CD_2Cl_2

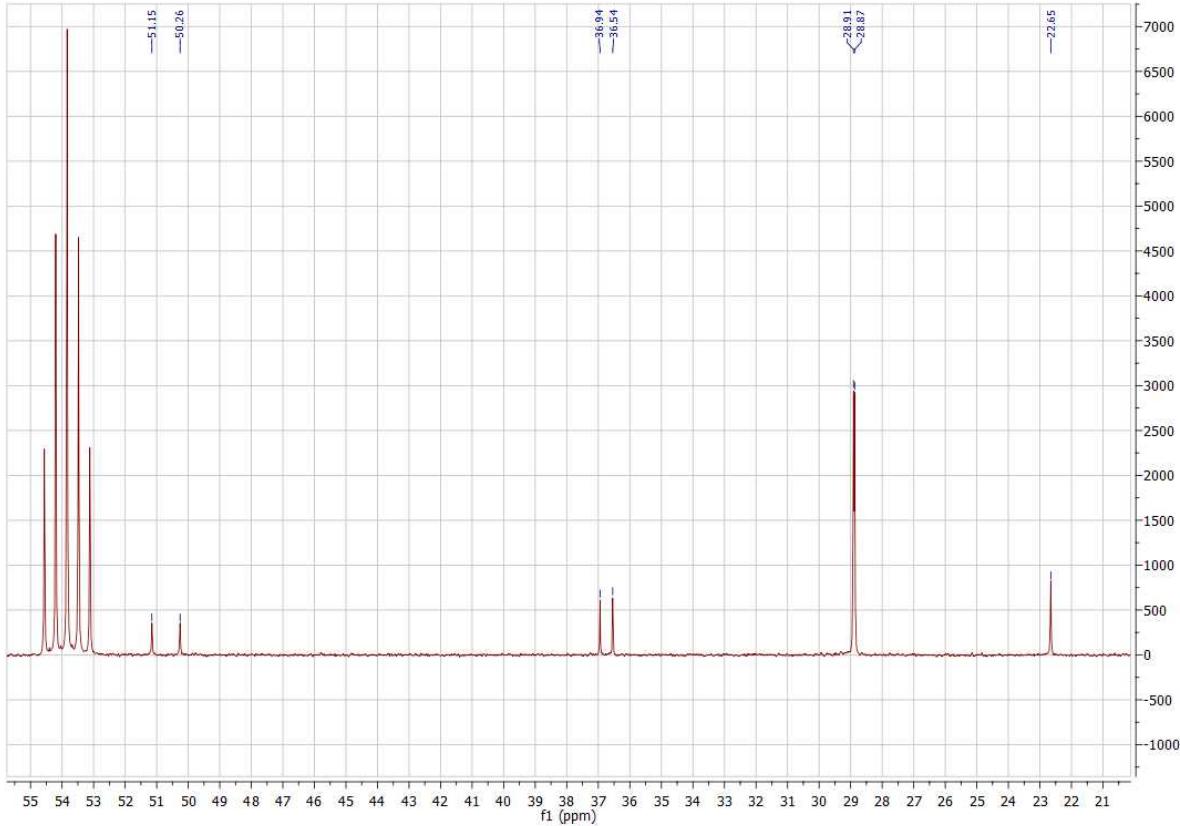


Figure 17. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **2** (75 MHz, 20 °C) in CD_2Cl_2 : zoom 1

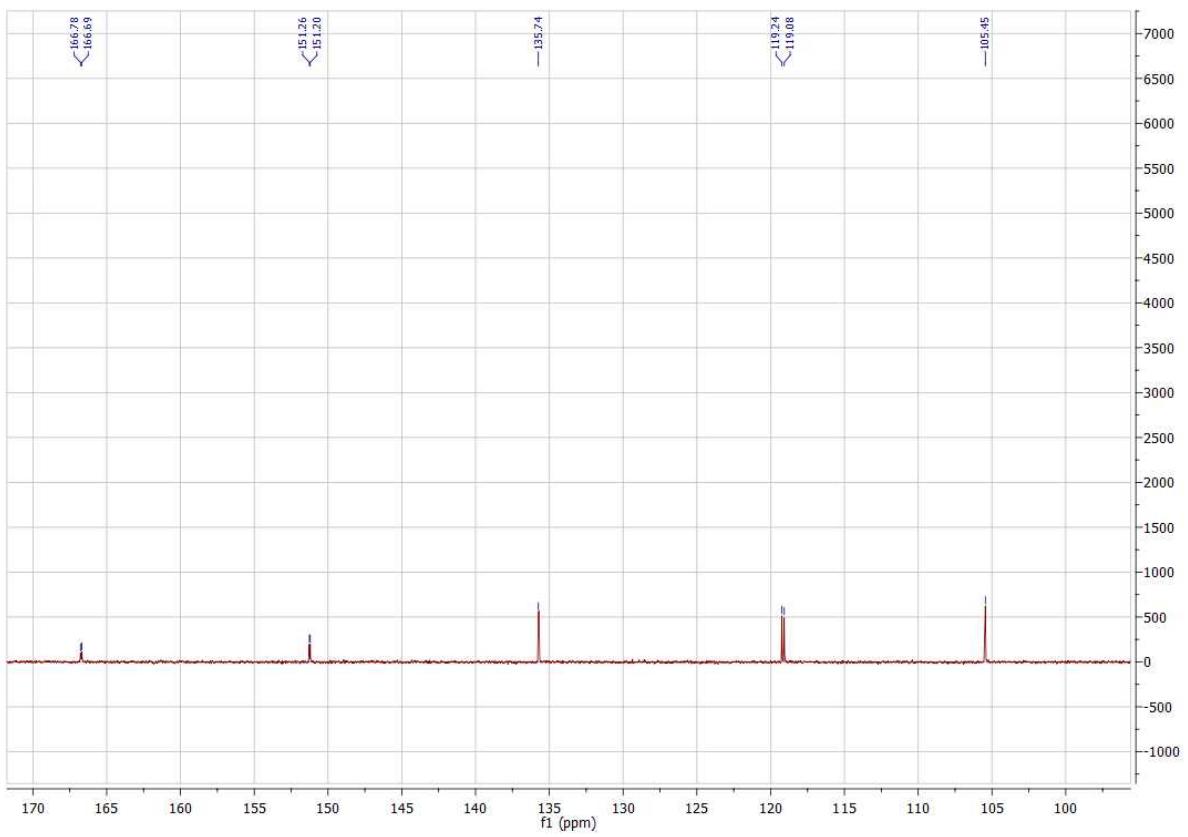


Figure 18. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **2** (75 MHz, 20 °C) in CD_2Cl_2 : zoom 2

NMR spectra of 3

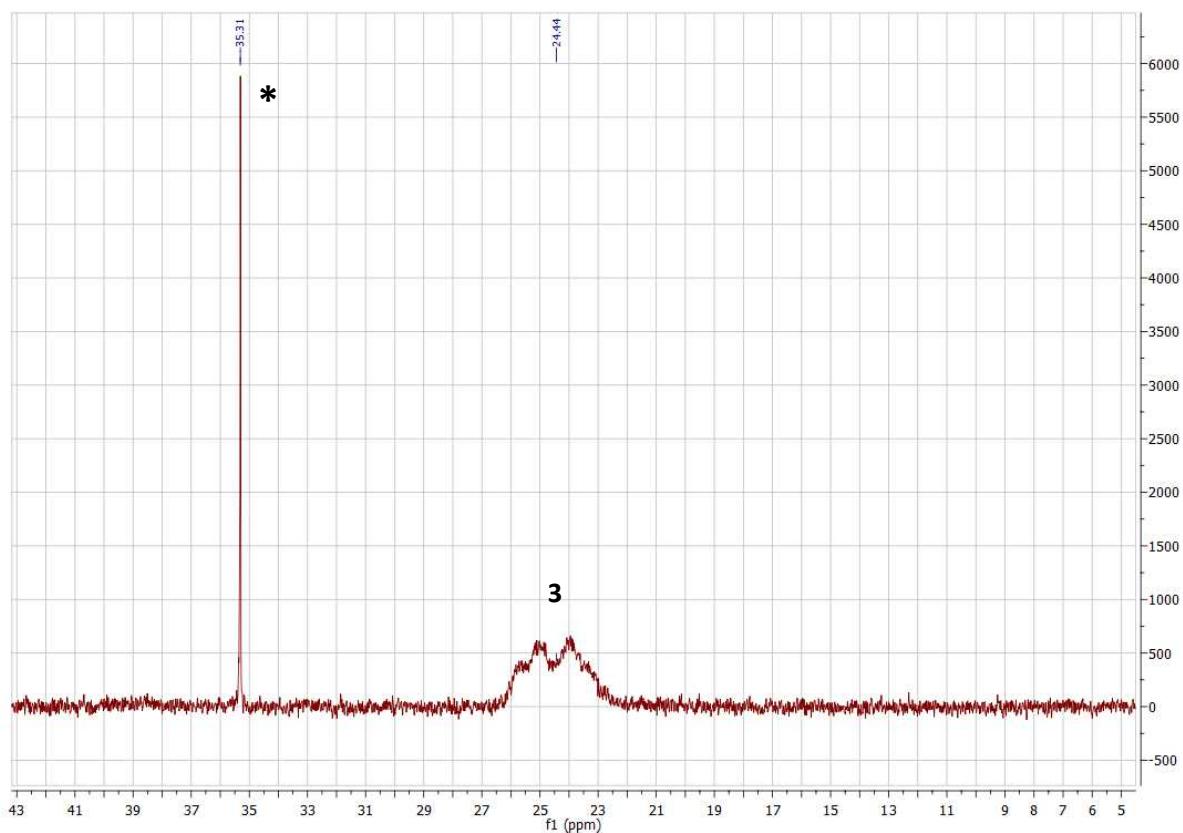


Figure 19. $^{31}\text{P}\{\text{H}\}$ NMR spectrum of **3** (121 MHz, 20 °C) in CD_2Cl_2 . *Signal attributed to L^{H}

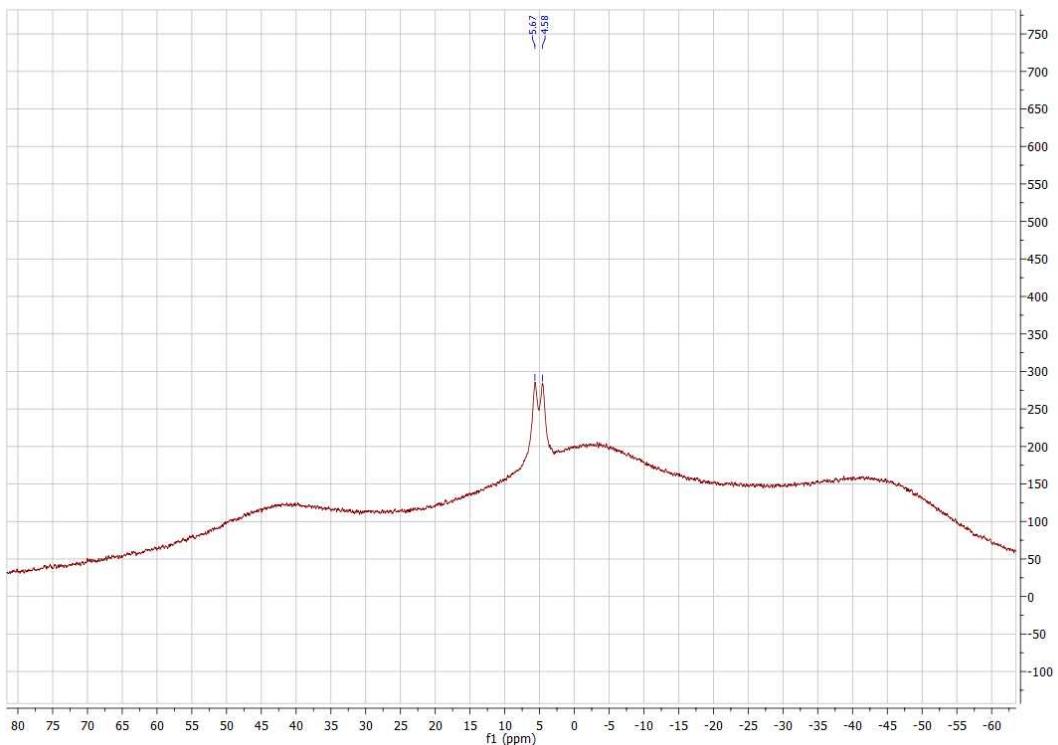


Figure 20. $^{11}\text{B}\{\text{H}\}$ NMR spectrum of **3** (96 MHz, 20 °C) in CD_2Cl_2

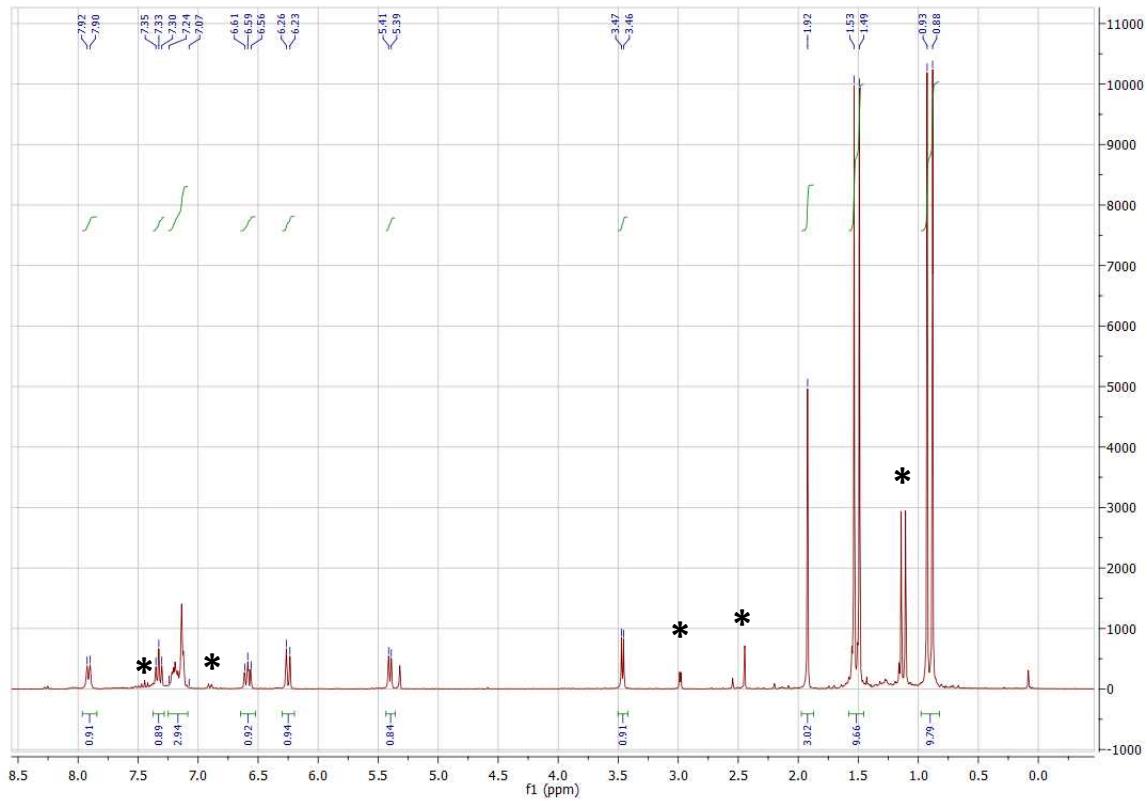


Figure 21. ^1H NMR spectrum of **3** (300 MHz, 20 °C) in CD_2Cl_2 . *Signal attributed to L^{H}

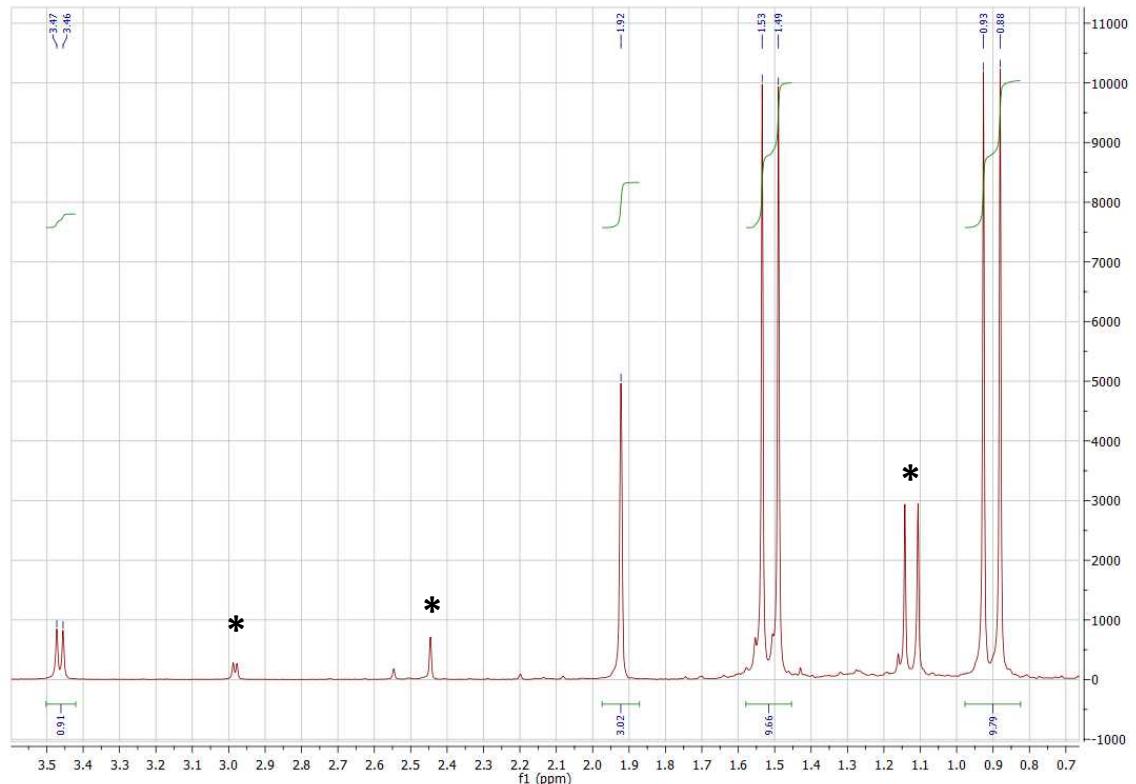


Figure 22. ^1H NMR spectrum of **3** (300 MHz, 20 °C) in CD_2Cl_2 : zoom 1. *Signal attributed to L^{H}

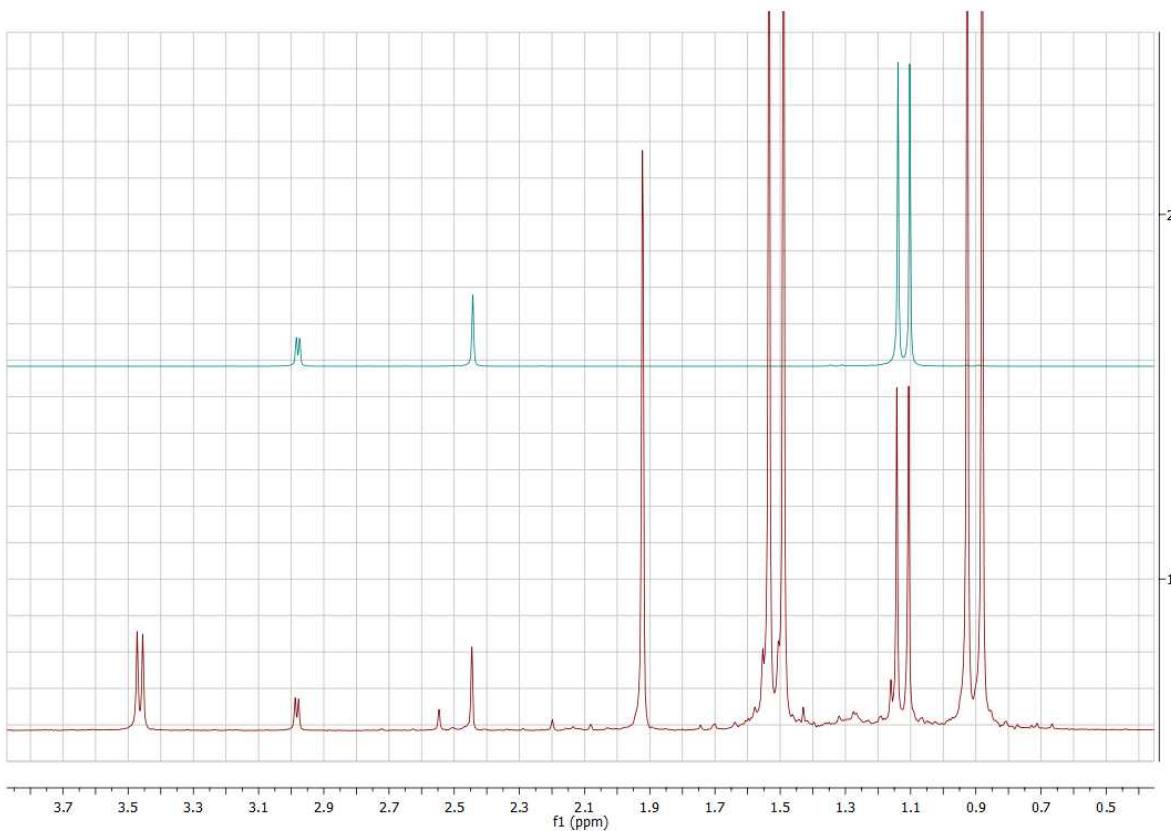


Figure 23. Stacked ^1H NMR spectra of **3** (bottom) and L^H (top) (300 MHz, 20 °C) in CD_2Cl_2 : zoom 1

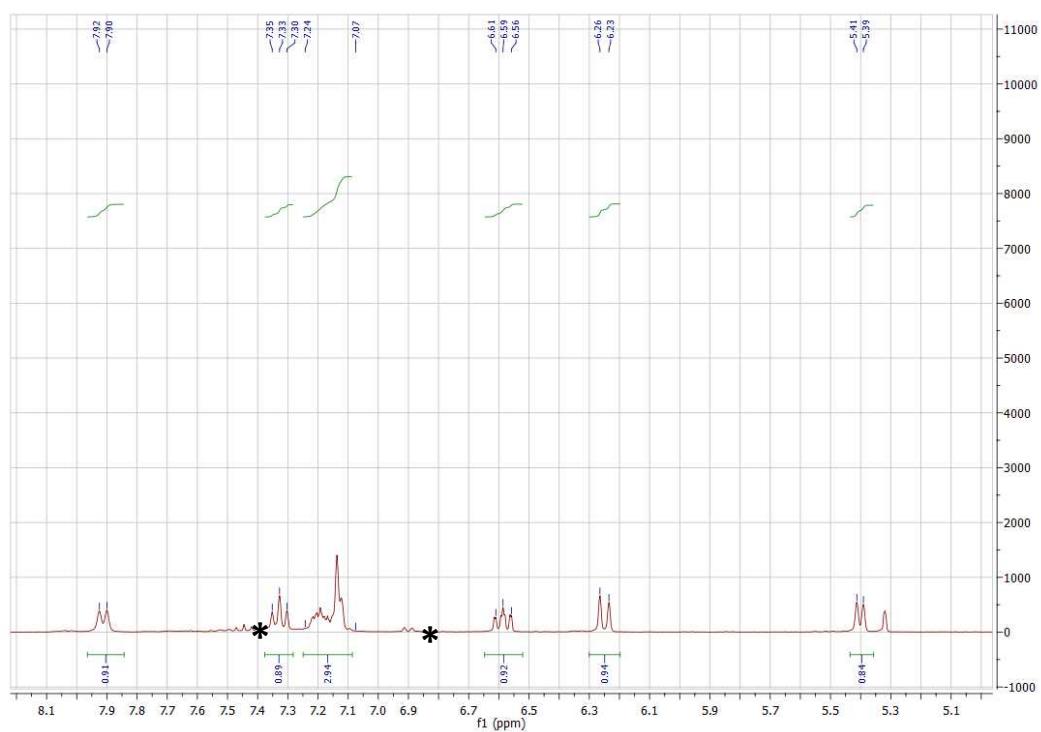


Figure 24. ^1H NMR spectrum of **3** (300 MHz, 20 °C) in CD_2Cl_2 : zoom 2. *Signal attributed to L^H

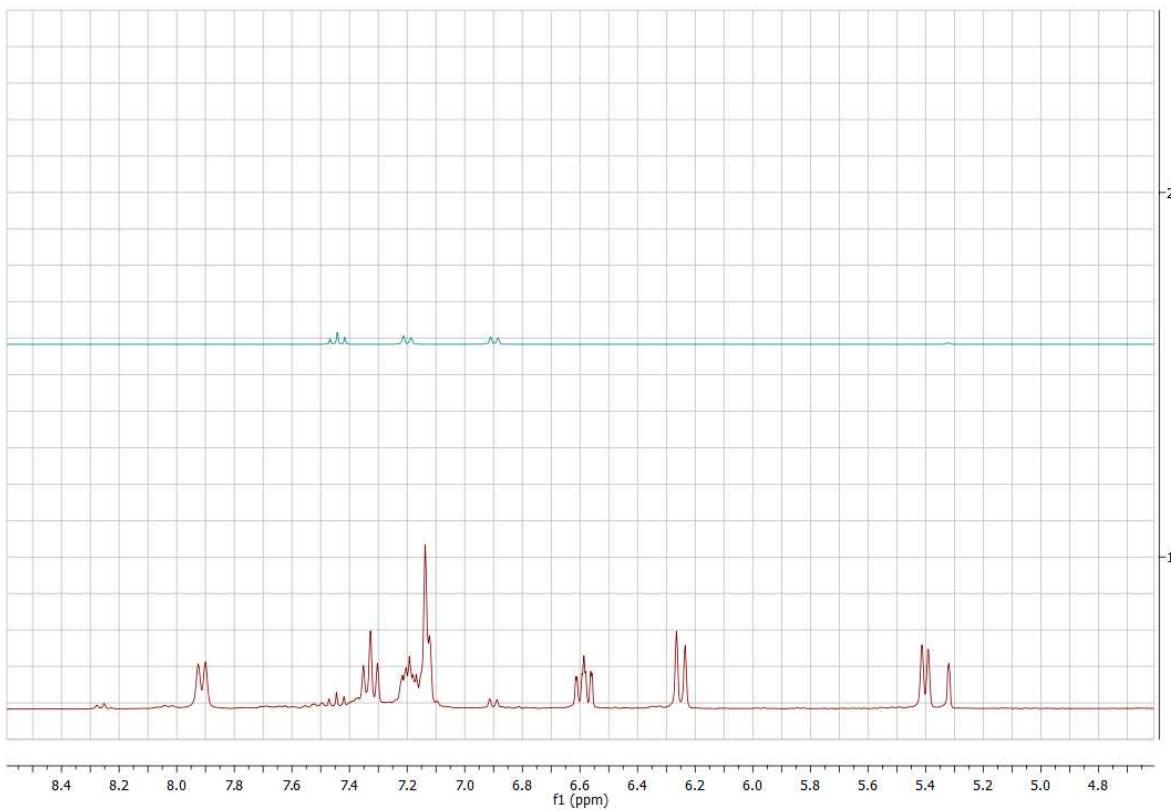


Figure 25. Stacked ^1H NMR spectra of **3** (bottom) and L^{H} (top) (300 MHz, 20 °C) in CD_2Cl_2 : zoom 1

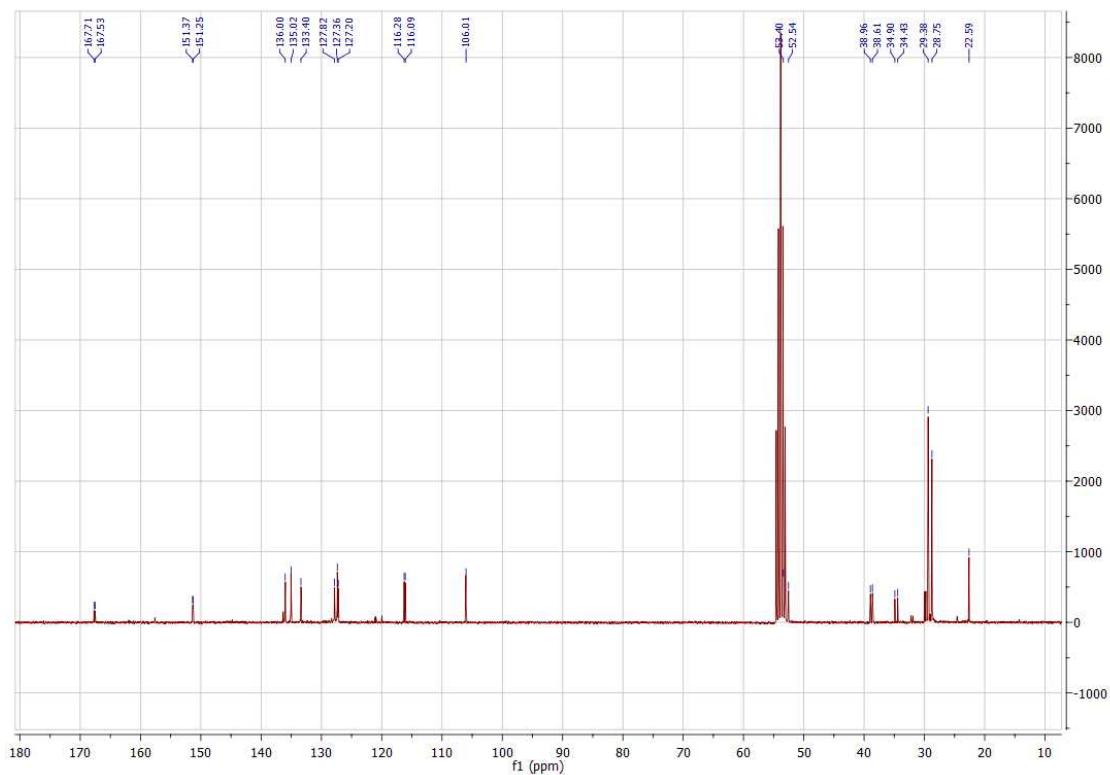


Figure 26. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **3** (75 MHz, 20 °C) in CD_2Cl_2 . *Signal attributed to L^{H}

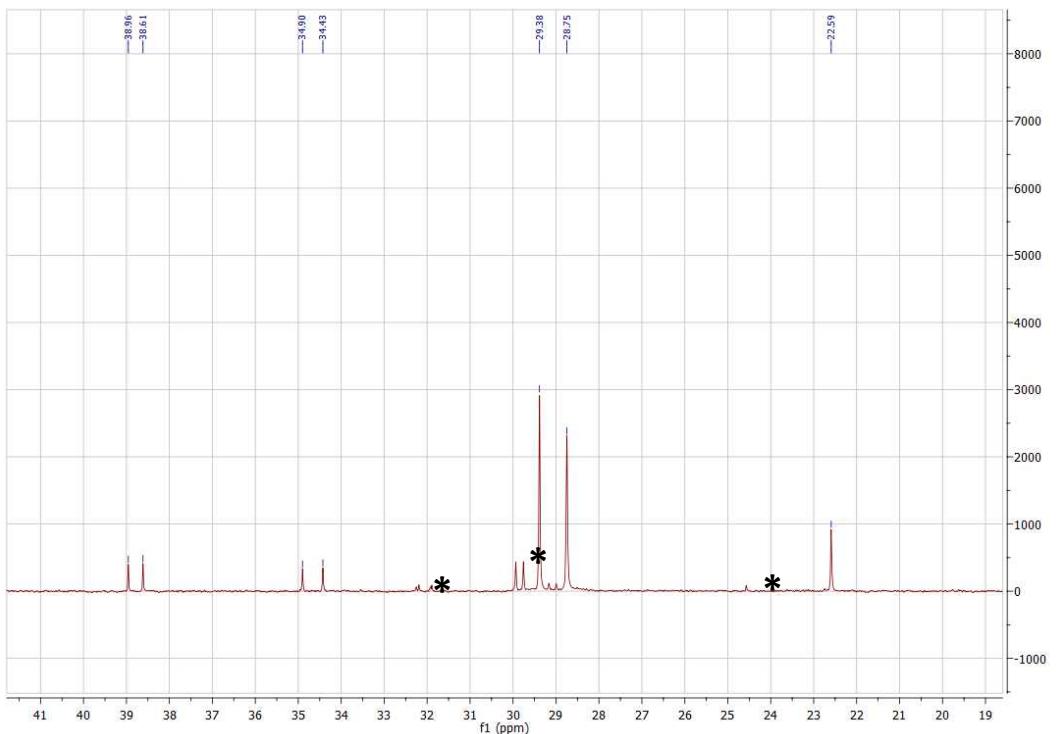


Figure 27. $^{13}\text{C}\{\text{H}\}$ NMR spectrum of **3** (75 MHz, 20 °C) in CD_2Cl_2 : zoom 1. *Signal attributed to L^{H}

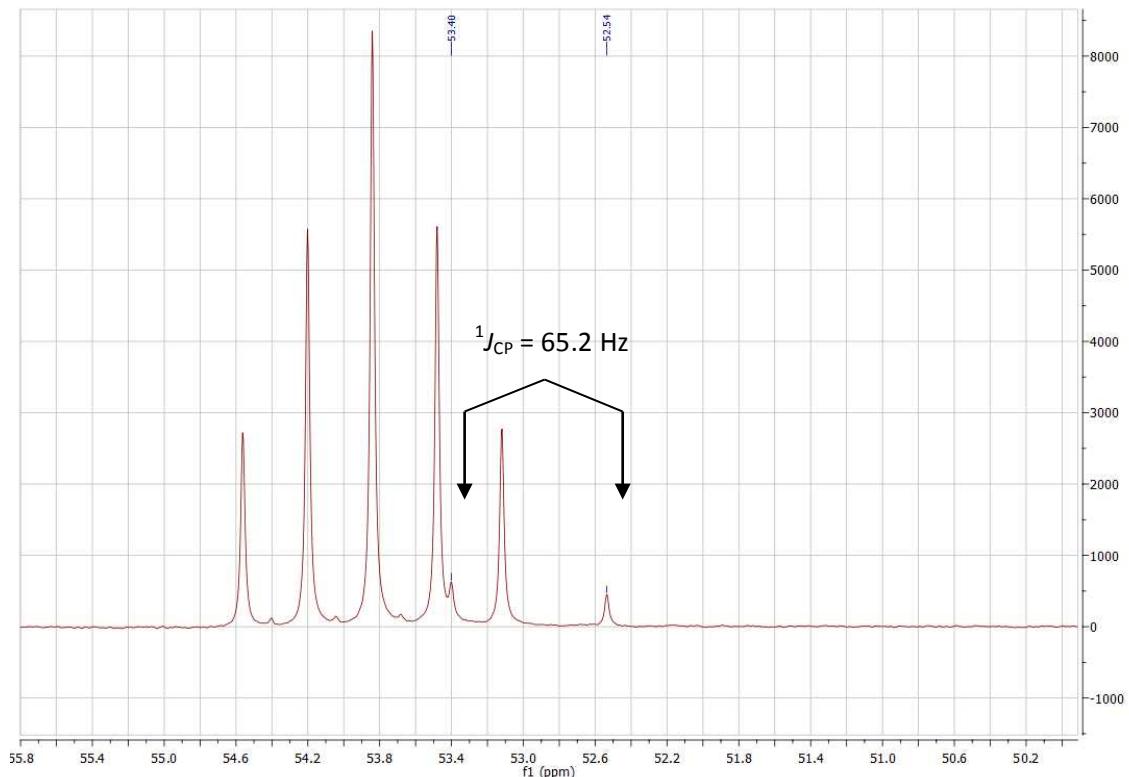


Figure 28. $^{13}\text{C}\{\text{H}\}$ NMR spectrum of **3** (75 MHz, 20 °C) in CD_2Cl_2 : zoom 2 (=CH-PPh₂ signal)

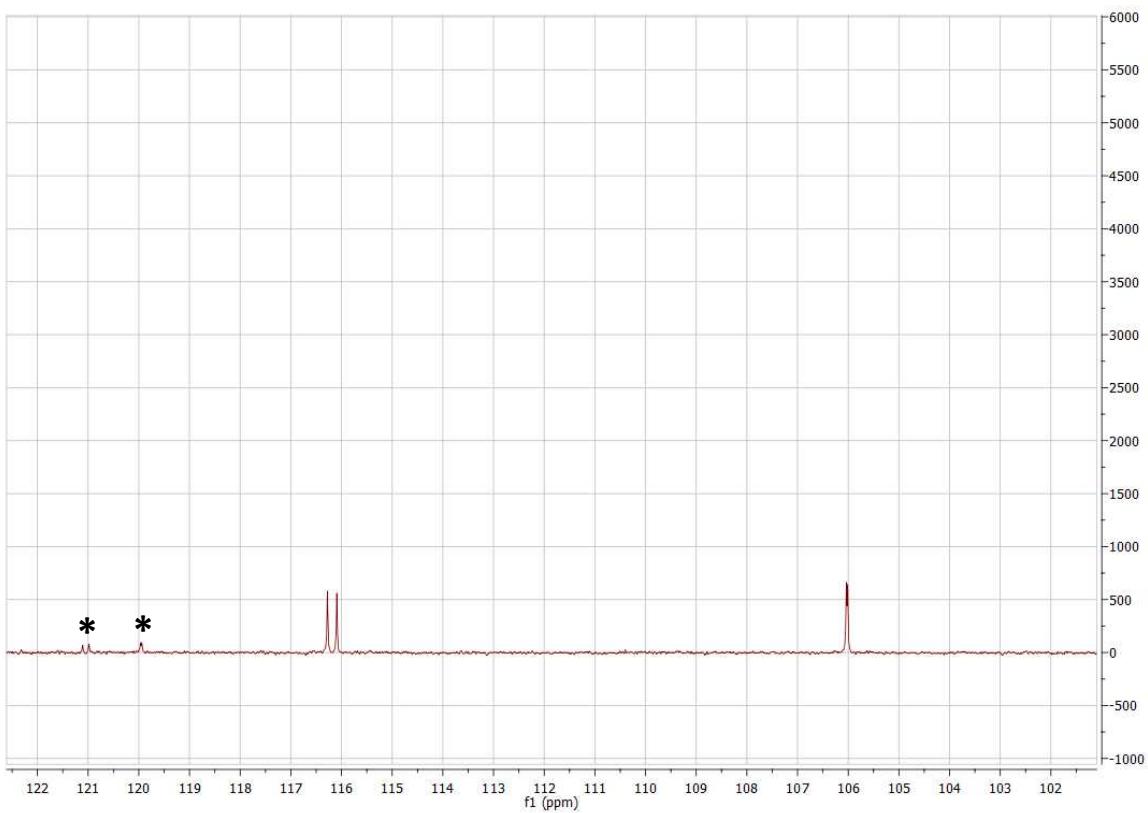


Figure 29. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **3** (75 MHz, 20 °C) in CD_2Cl_2 : zoom 3. *Signal attributed to L^H

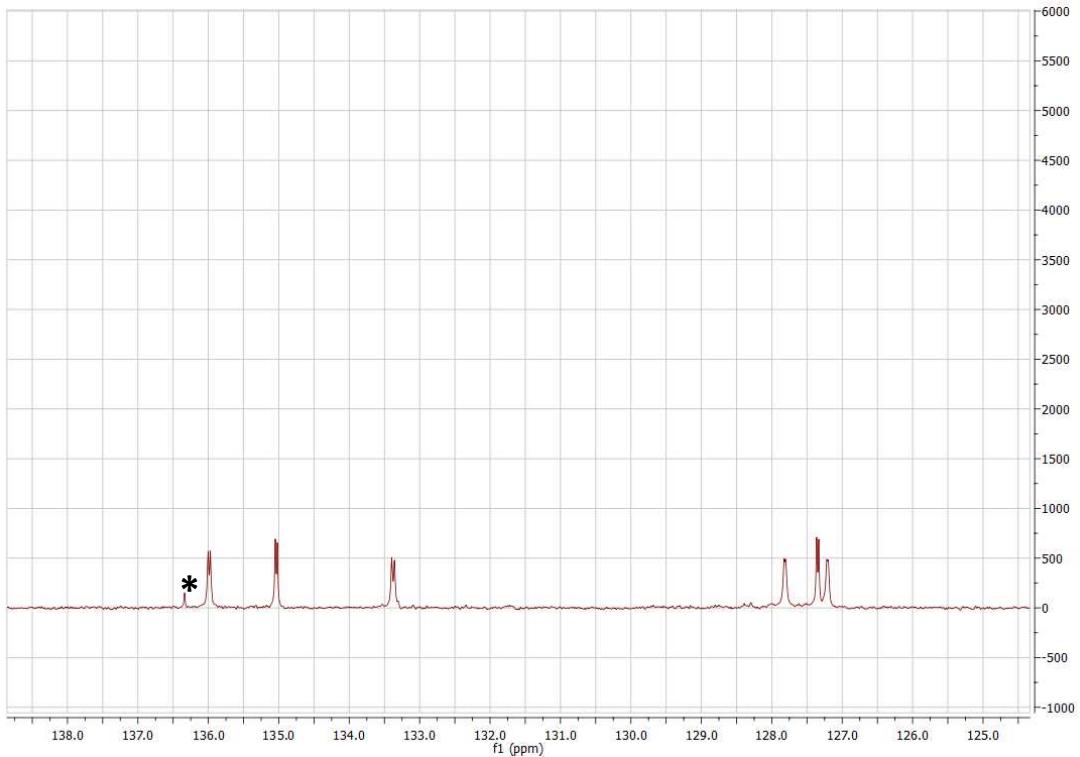


Figure 30. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **3** (75 MHz, 20 °C) in CD_2Cl_2 : zoom 4. *Signal attributed to L^H

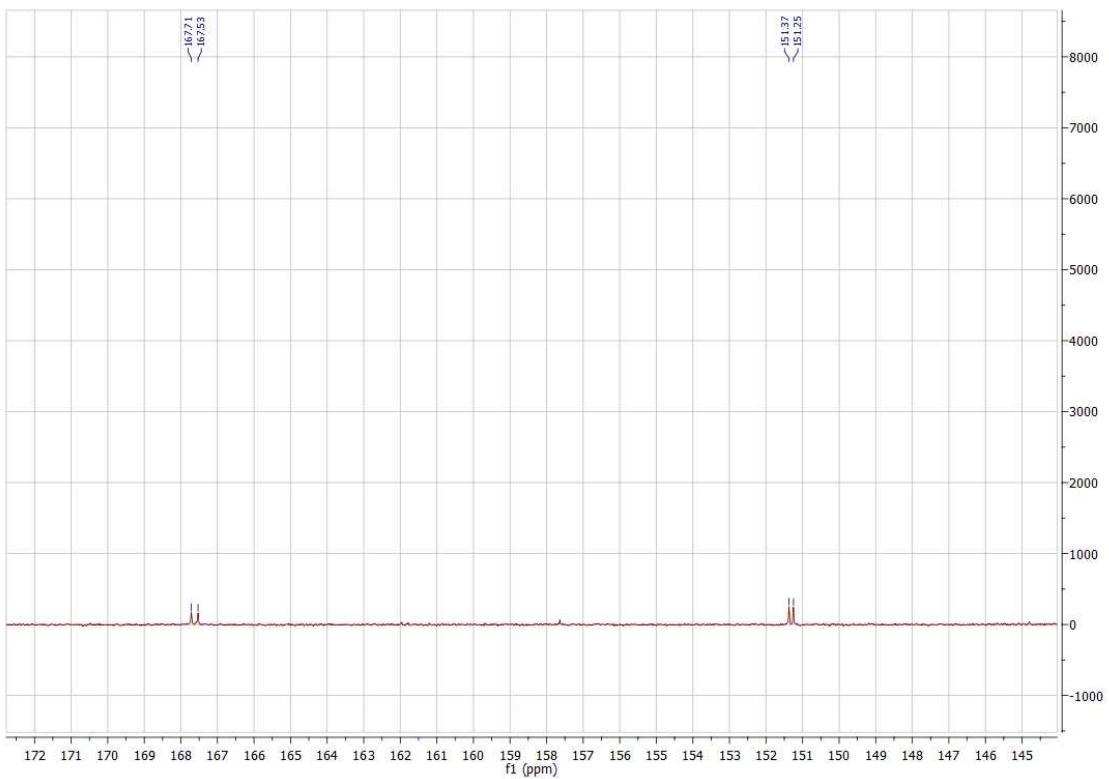


Figure 31. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **3** (75 MHz, 20 °C) in CD_2Cl_2 : zoom 5

NMR spectra of *anti*-3.GaCl₃

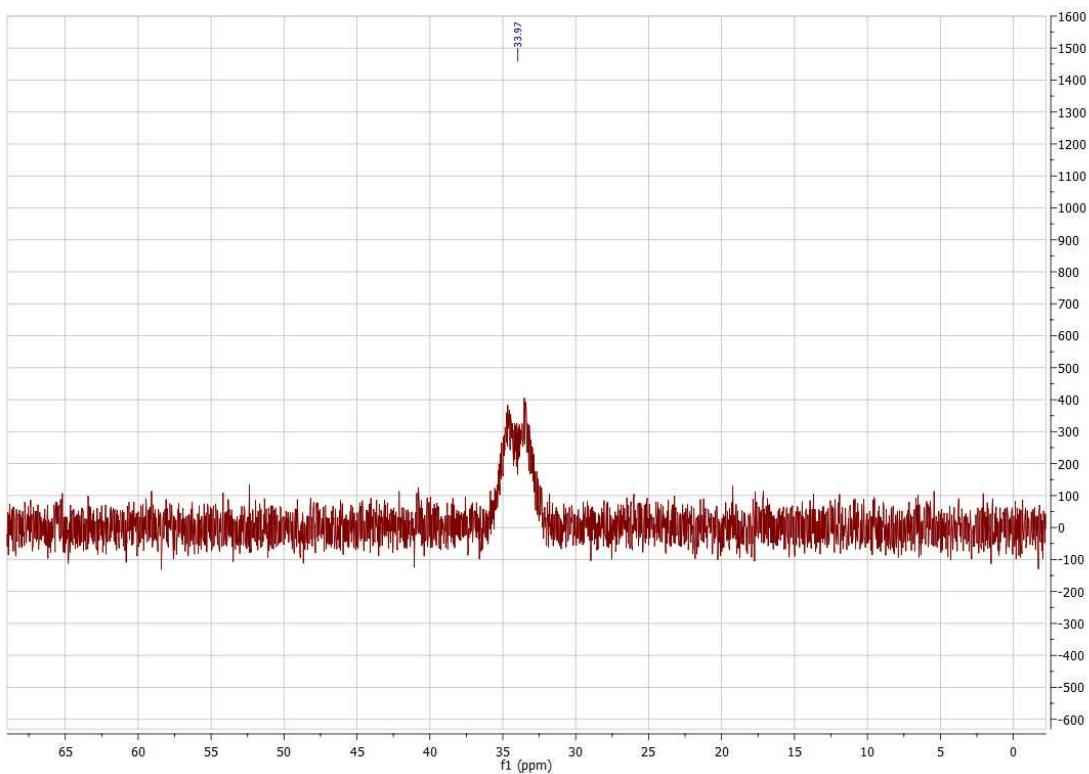


Figure 32. ³¹P{¹H} NMR spectrum of *anti*-3.GaCl₃ (121 MHz, 20 °C) in CD₂Cl₂

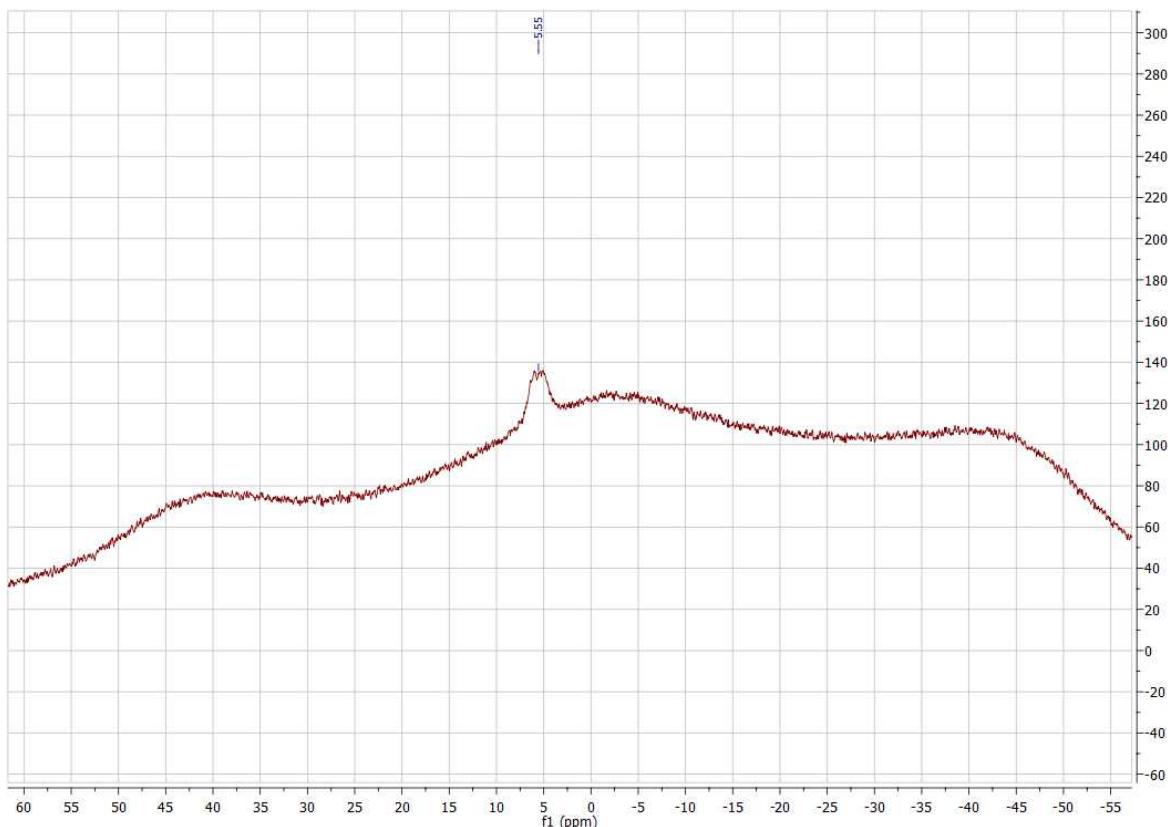


Figure 33. ¹¹B{¹H} NMR spectrum of *anti*-3.GaCl₃ (96 MHz, 20 °C) in CD₂Cl₂

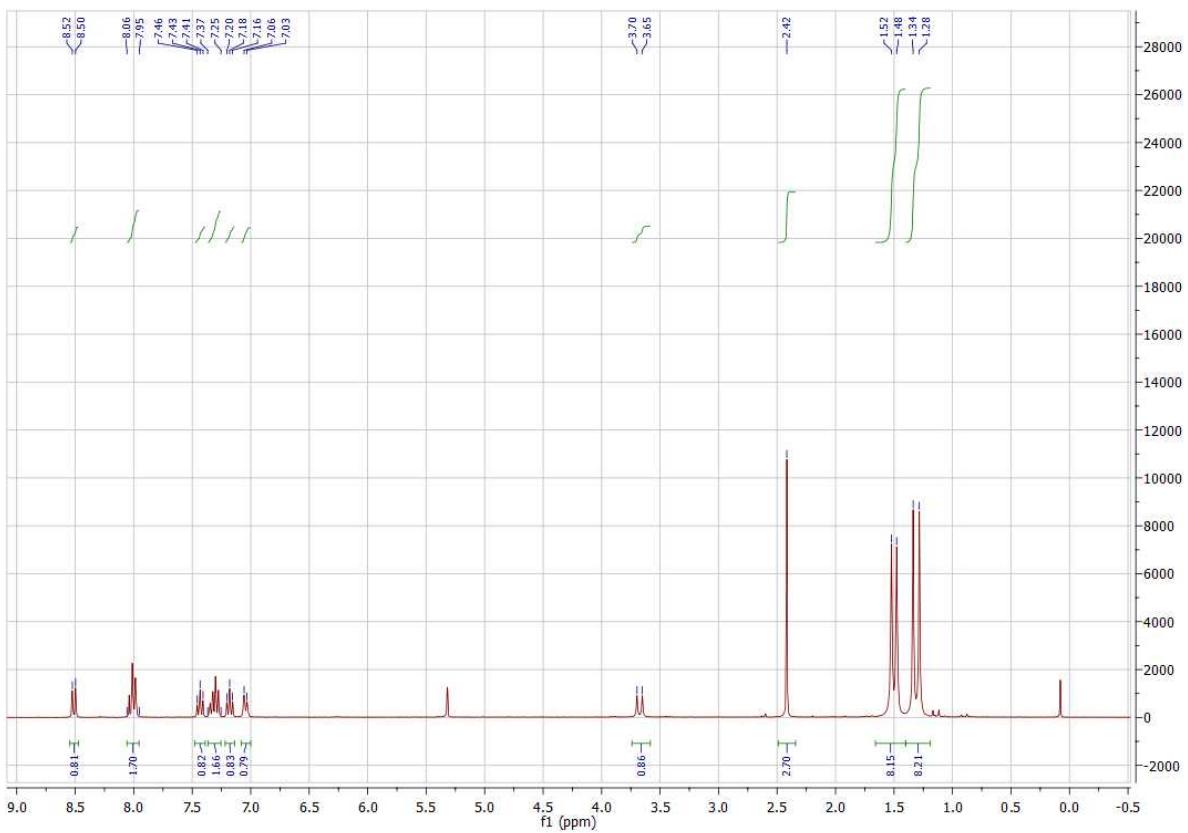


Figure 34. ¹H NMR spectrum of *anti*-3.GaCl₃ (300 MHz, 20 °C) in CD₂Cl₂

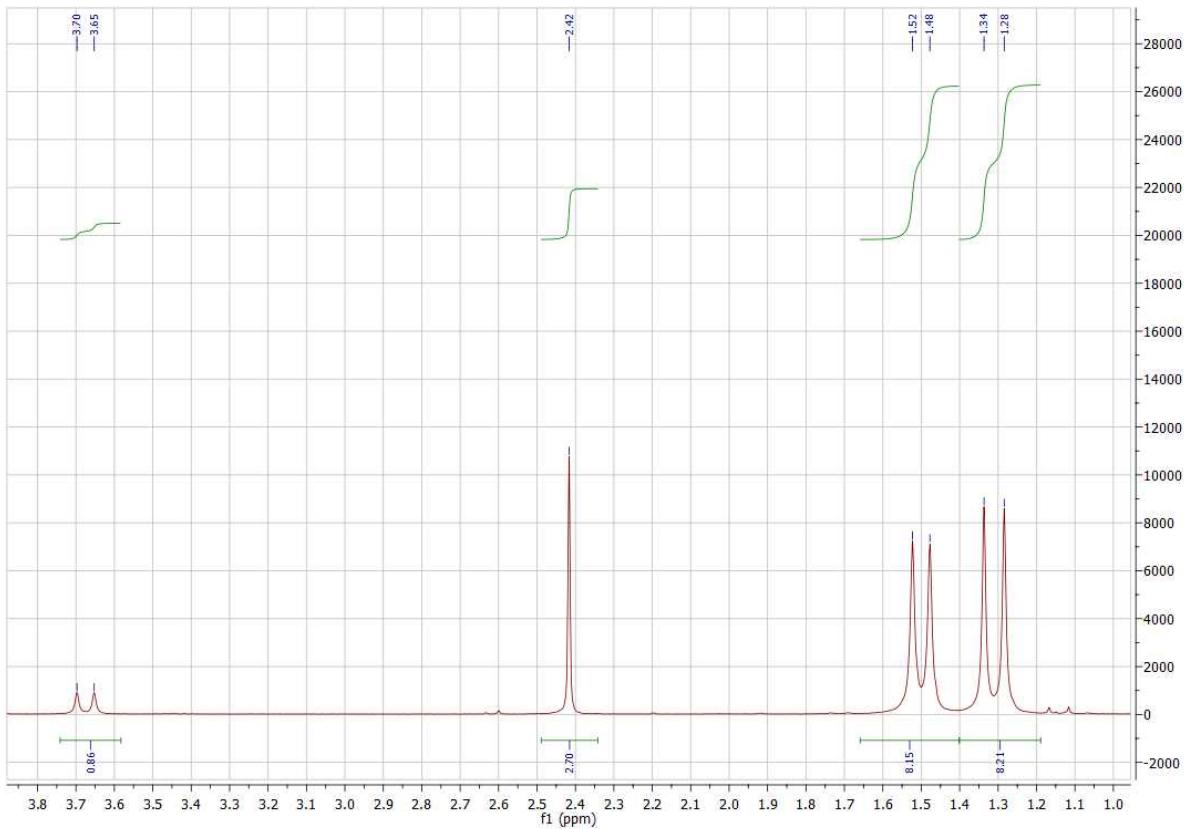


Figure 35. ¹H NMR spectrum of *anti*-3.GaCl₃ (300 MHz, 20 °C) in CD₂Cl₂; zoom 1

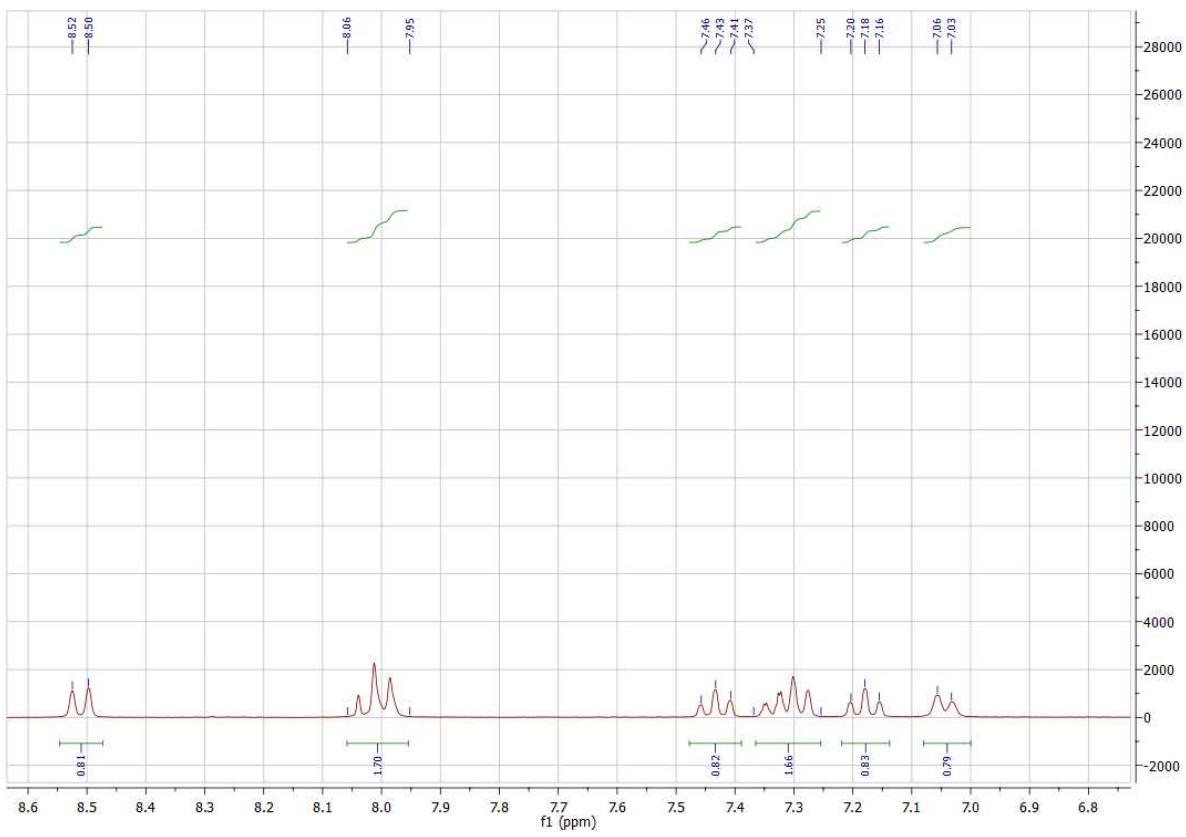


Figure 36. ^1H NMR spectrum of *anti*-3.GaCl₃ (300 MHz, 20 °C) in CD₂Cl₂: zoom 2

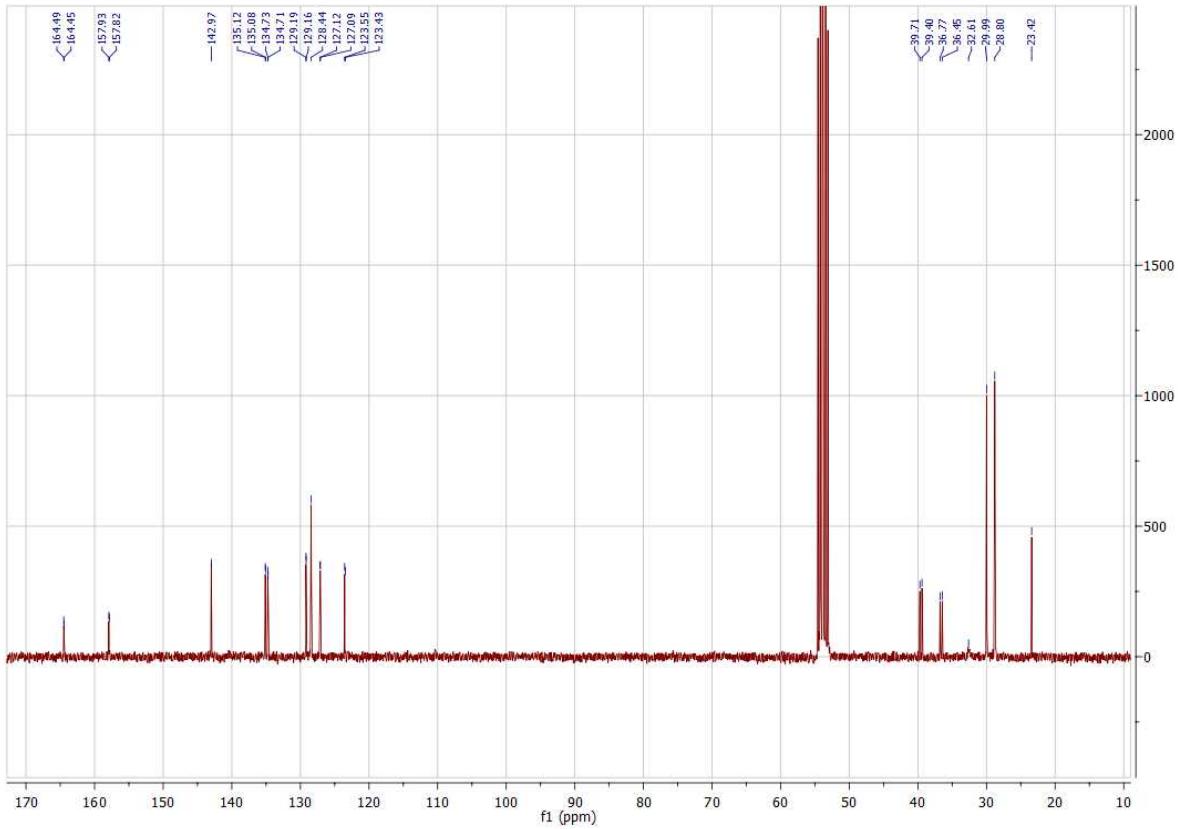


Figure 37. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of *anti*-3.GaCl₃ (75 MHz, 20 °C) in CD₂Cl₂

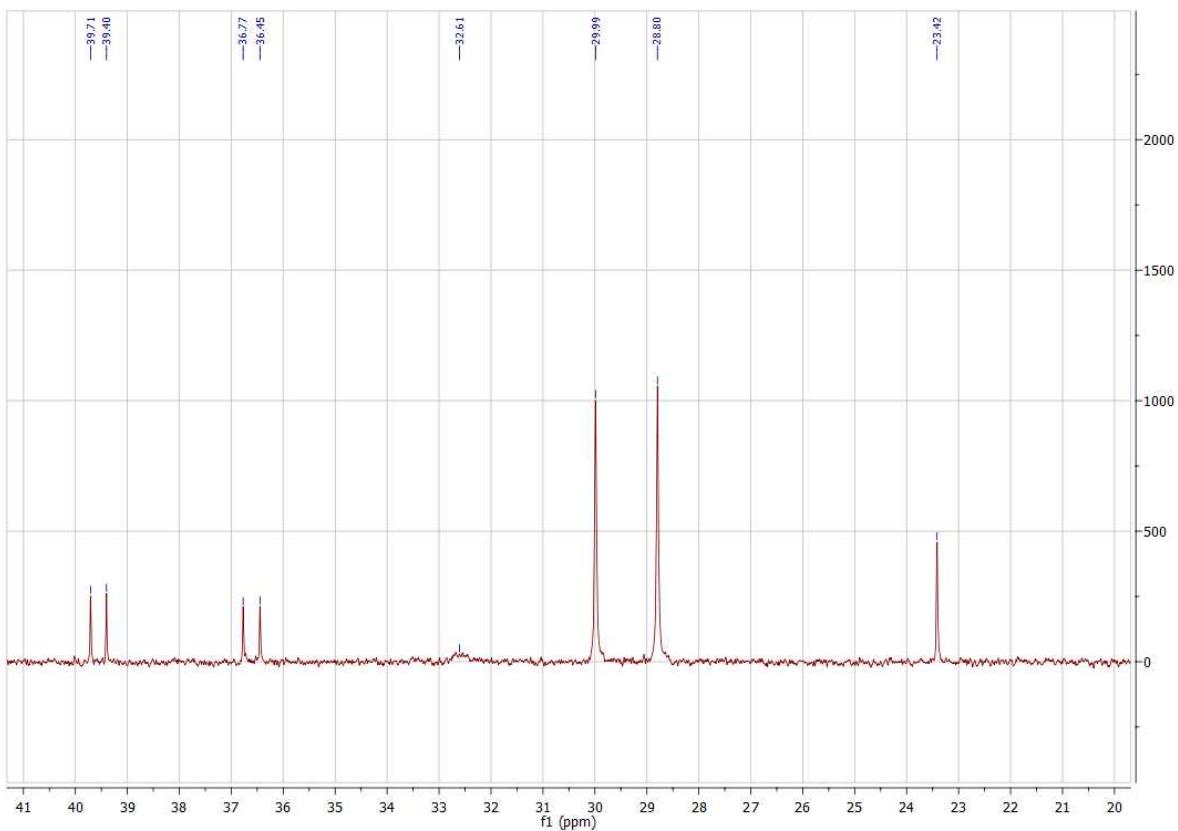


Figure 38. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of *anti*-3.GaCl₃ (75 MHz, 20 °C) in CD₂Cl₂: zoom 1

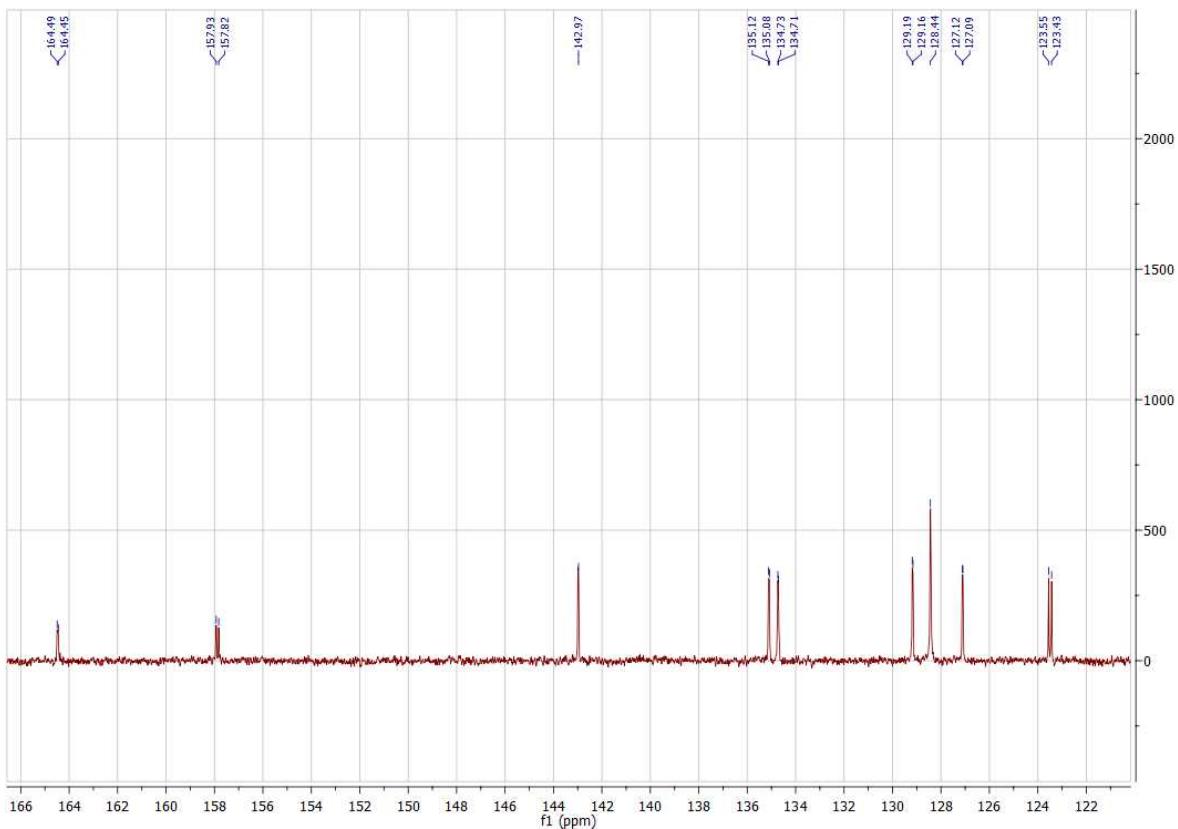


Figure 39. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of *anti*-3.GaCl₃ (75 MHz, 20 °C) in CD₂Cl₂: zoom 2

Isomerization of *anti*-3.GaCl₃

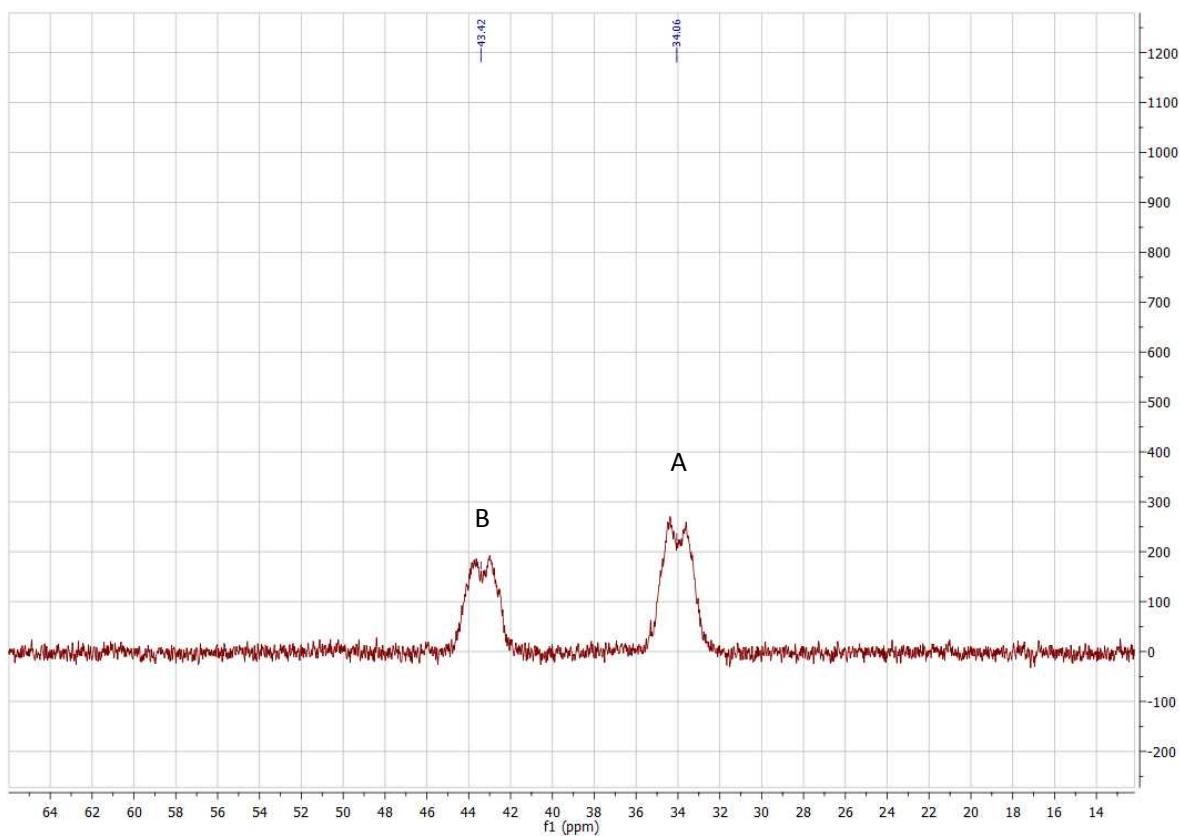


Figure 40. ³¹P{¹H} NMR spectrum of the mixture of diastereoisomers (162 MHz, 20 °C) in CD₂Cl₂. ^ASignal attributed to *anti*-3.GaCl₃. ^BSignal attributed to *syn*-3.GaCl₃

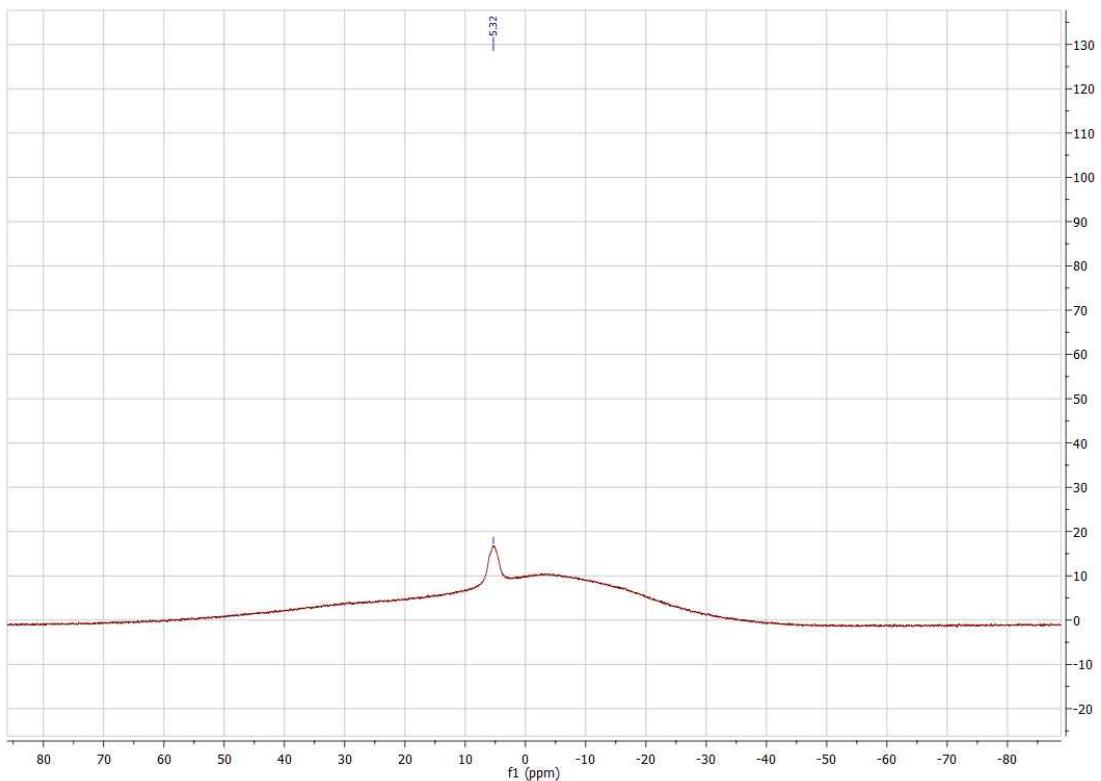


Figure 41. $^{11}\text{B}\{\text{H}\}$ NMR spectrum of the mixture of diastereoisomers (128 MHz, 20 °C) in CD_2Cl_2

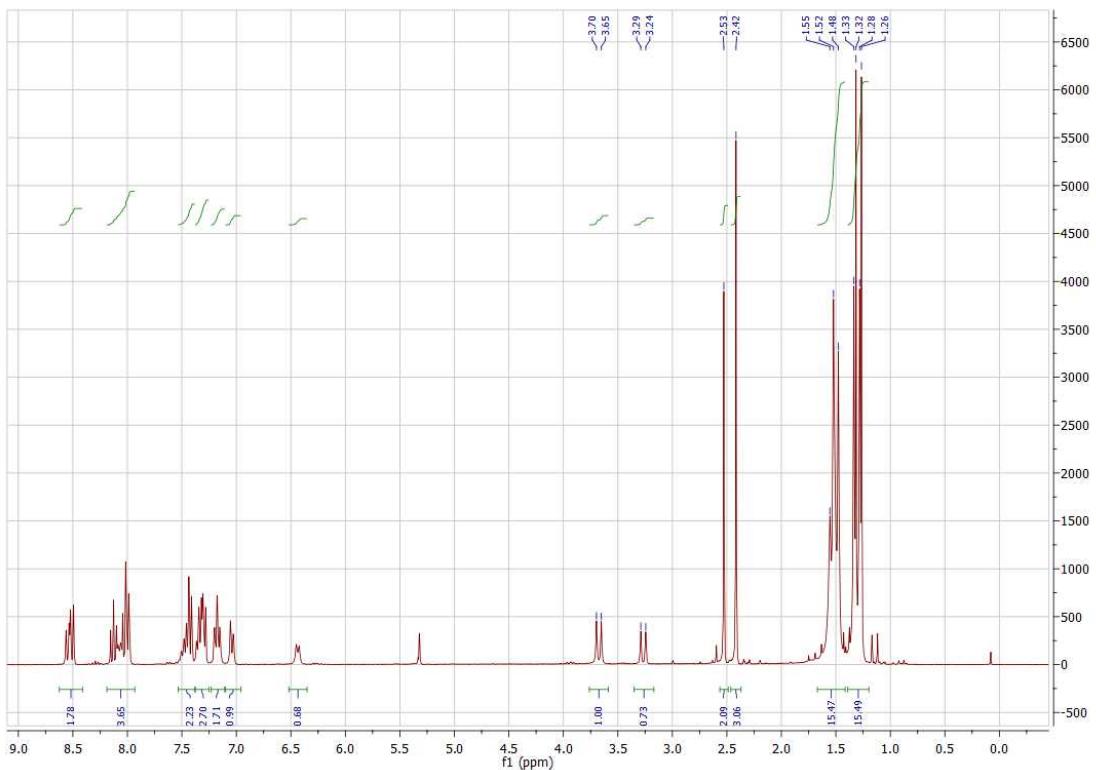


Figure 42. ^1H NMR spectrum (300 MHz, 20 °C) in CD_2Cl_2

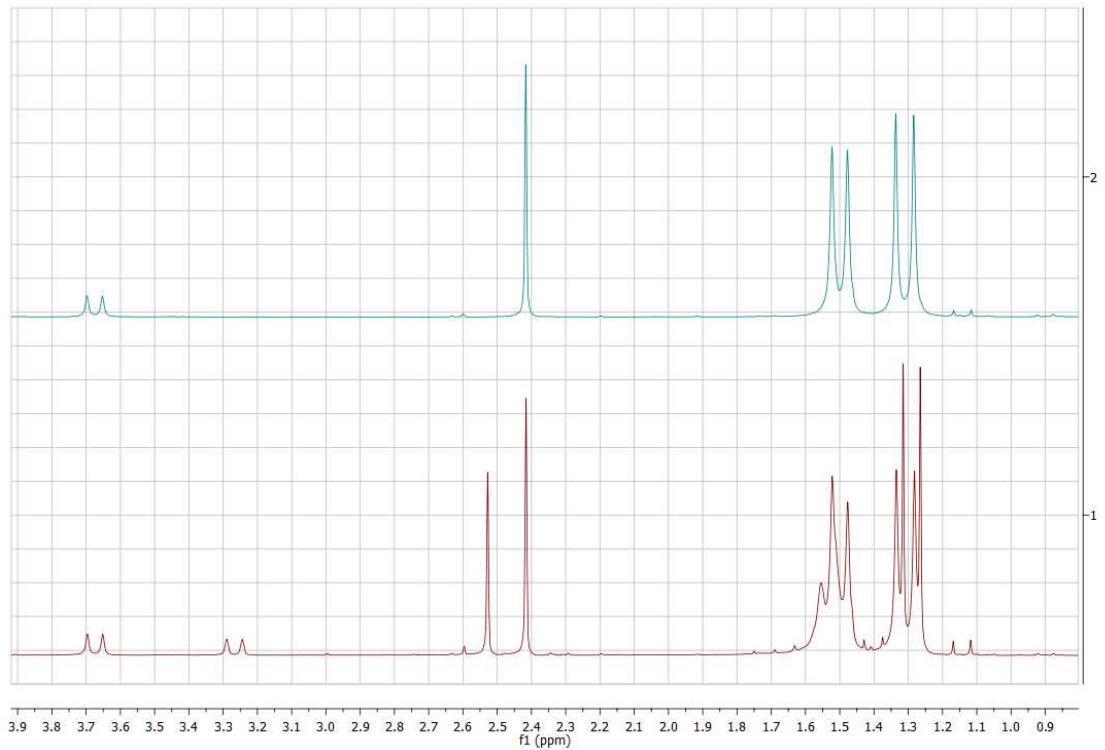


Figure 43. Stacked ^1H NMR spectrum of the mixture of diastereoisomers and ^1H NMR spectrum of pure *anti*-3.GaCl₃ (top) (300 MHz, 20 °C) in CD₂Cl₂: aliphatic region

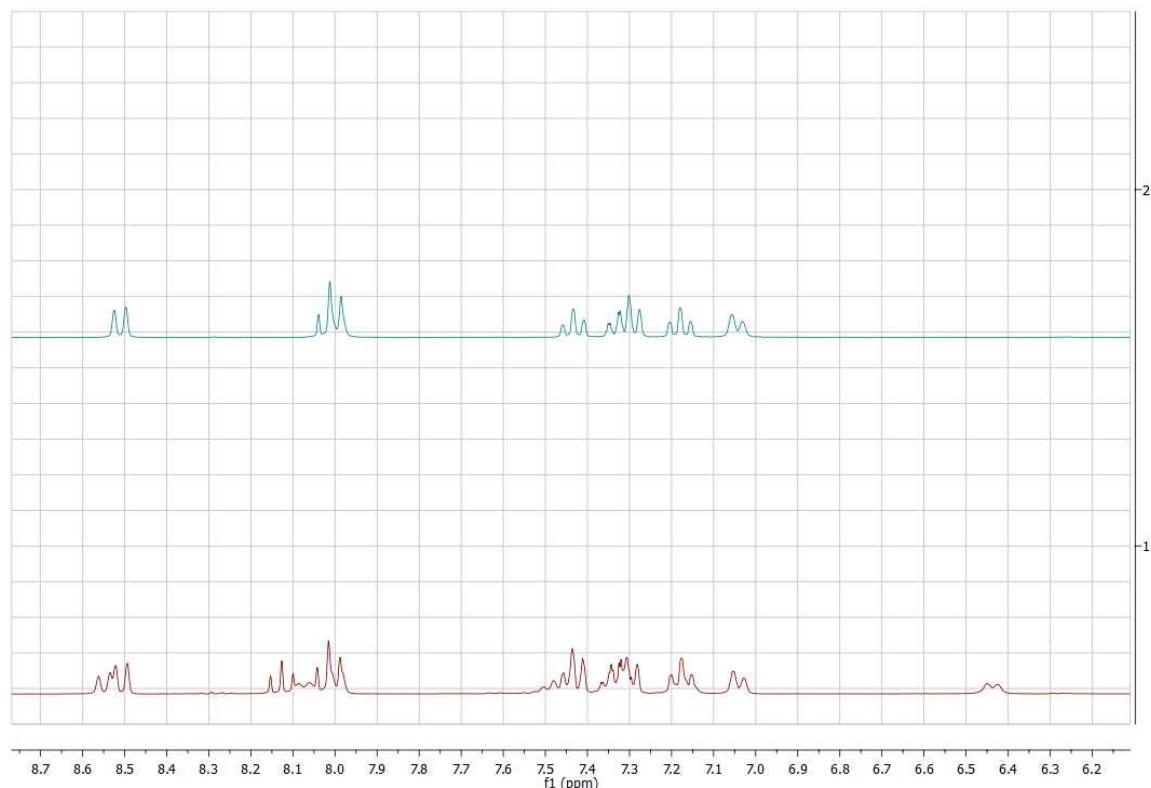


Figure 44. Stacked ^1H NMR spectrum of the mixture of diastereoisomers (bottom) and ^1H NMR spectrum of *anti*-3.GaCl₃ (top) (300 MHz, 20 °C) in CD₂Cl₂: aromatic region

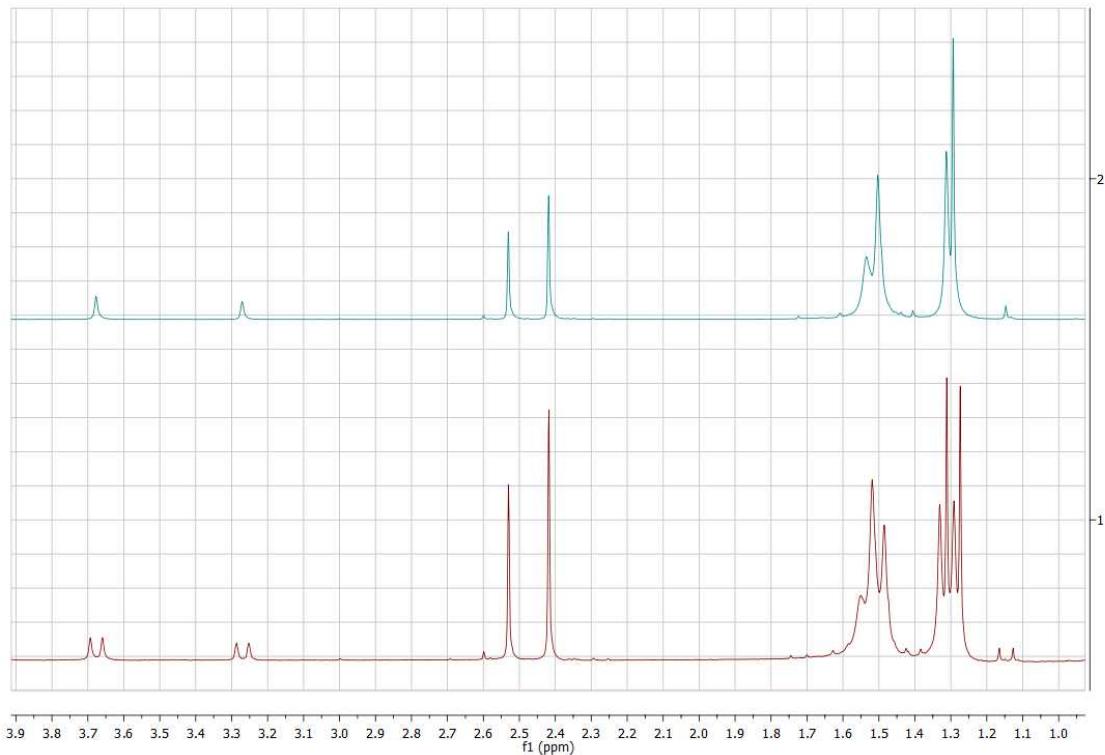


Figure 45. Stacked ^1H (bottom) and $^1\text{H}\{^{31}\text{P}\}$ (top) NMR spectra of the mixture of diastereoisomers (400 MHz, 20 °C) in CD_2Cl_2 : aliphatic region

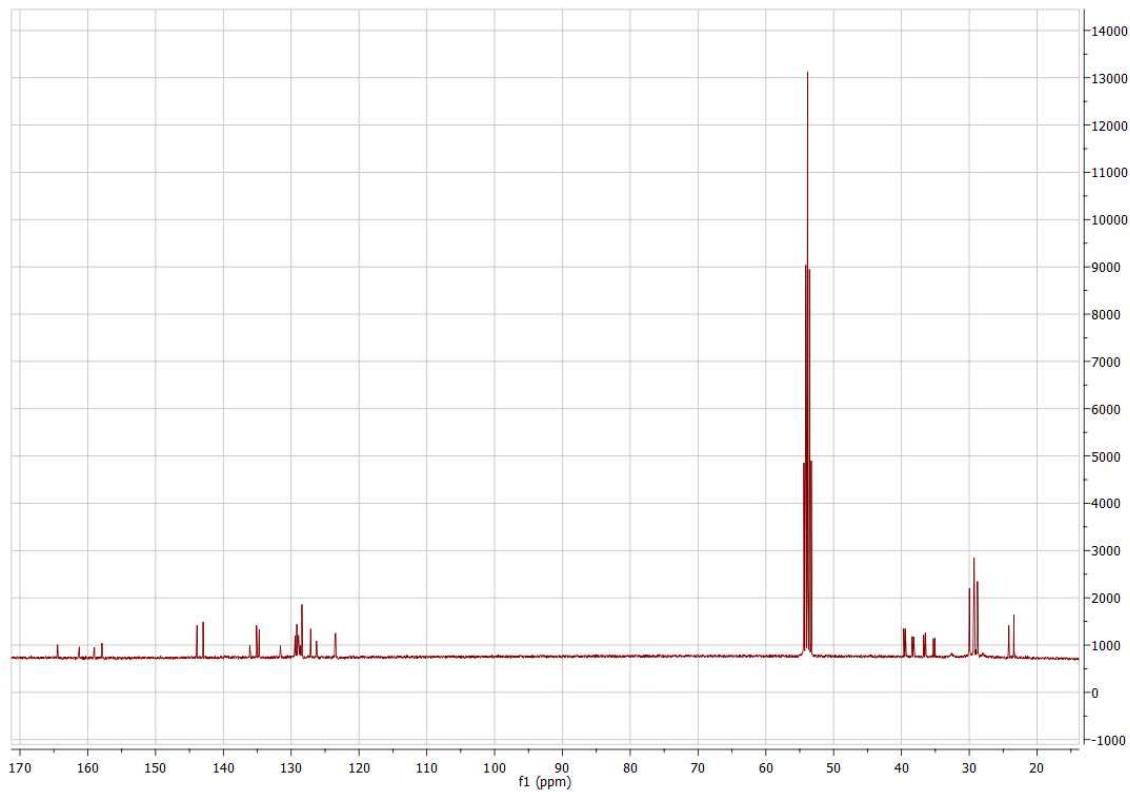


Figure 46. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of the mixture of diastereoisomers (101 MHz, 20 °C) in CD_2Cl_2

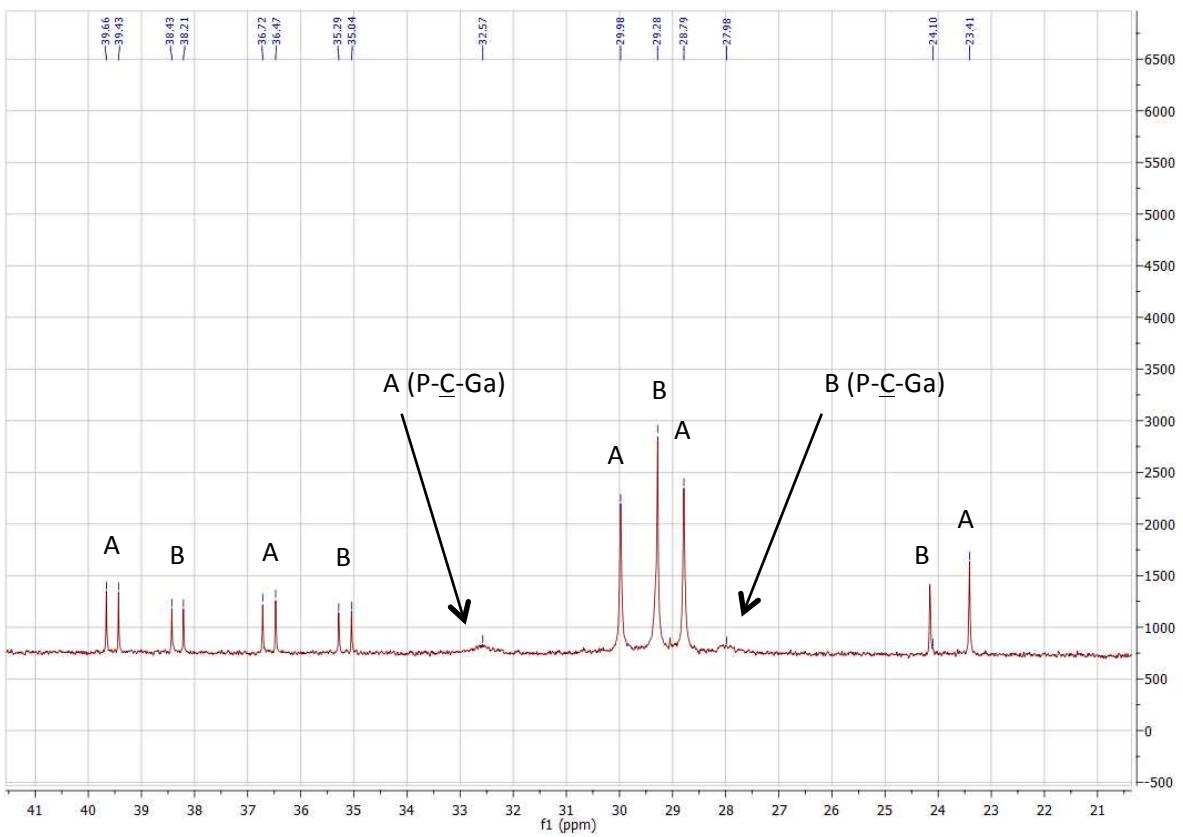


Figure 47. $^{13}\text{C}\{\text{H}\}$ NMR spectrum of the mixture of diastereoisomers (101 MHz, 20 °C) in CD_2Cl_2 : zoom 1. ^ASignal attributed to *anti*-3.GaCl₃. Figure 70. $^{13}\text{C}\{\text{H}\}$ NMR spectrum of the mixture of diastereoisomers (101 MHz, 20 °C) in CD_2Cl_2 : zoom 1. ^BSignal attributed to *syn*-3.GaCl₃

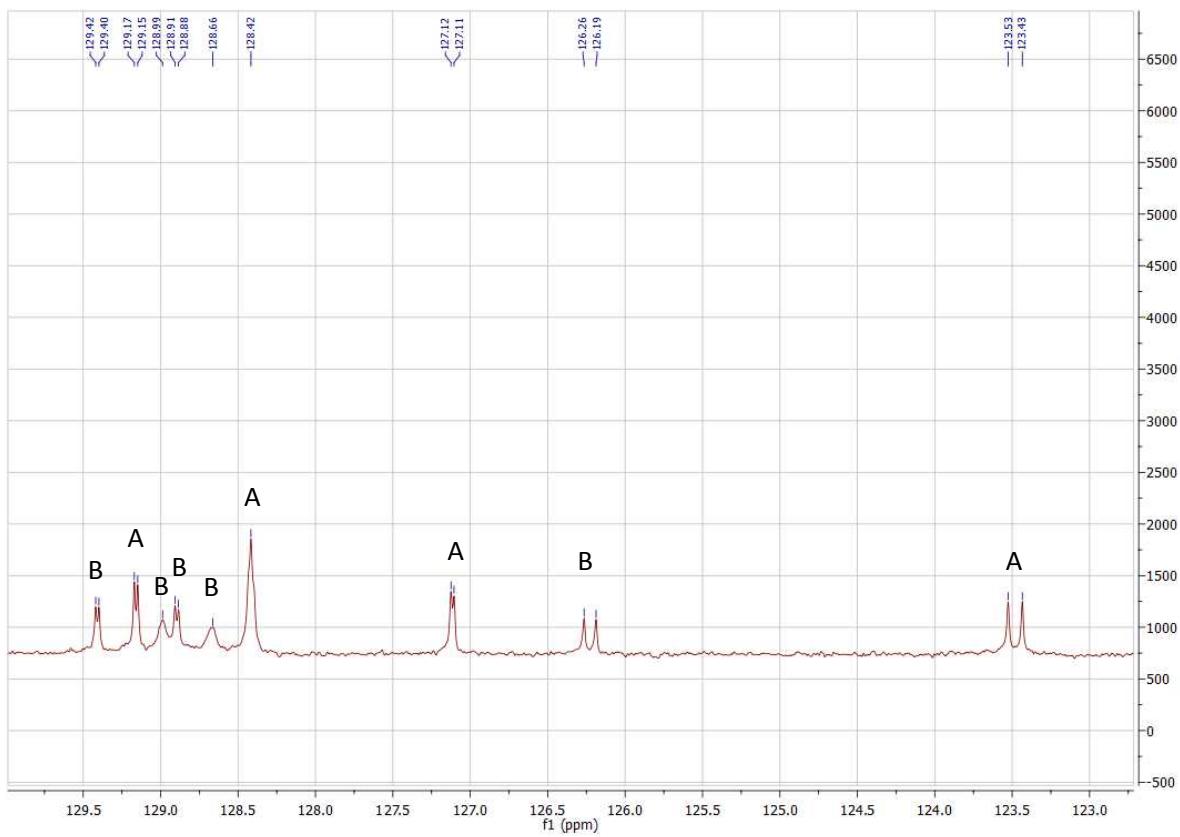


Figure 48. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of the mixture of diastereoisomers (101 MHz, 20 °C) in CD_2Cl_2 : zoom 2. ^ASignal attributed to *anti*-3.GaCl₃. ^BSignal attributed to *syn*-3.GaCl₃

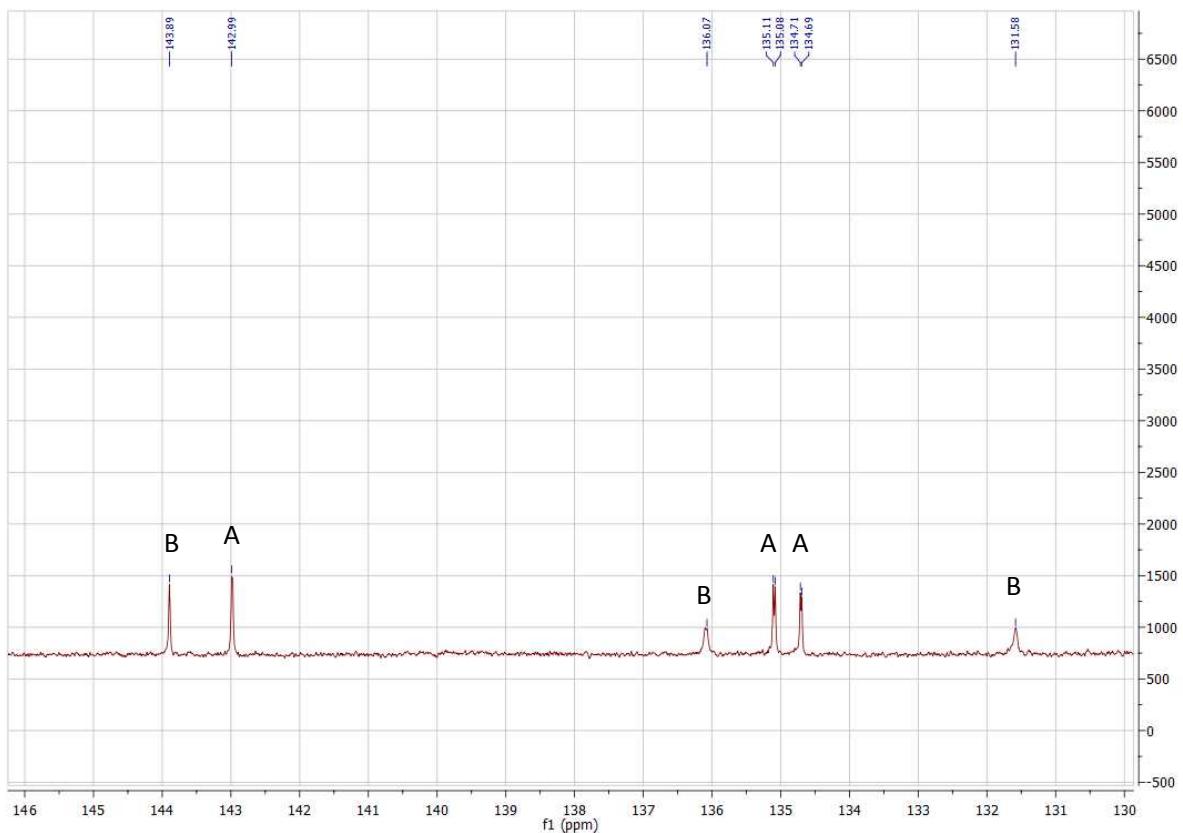


Figure 49. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of the mixture of diastereoisomers (101 MHz, 20 °C) in CD_2Cl_2 : zoom 3. ^ASignal attributed to *anti*-3.GaCl₃. ^BSignal attributed to *syn*-3.GaCl₃

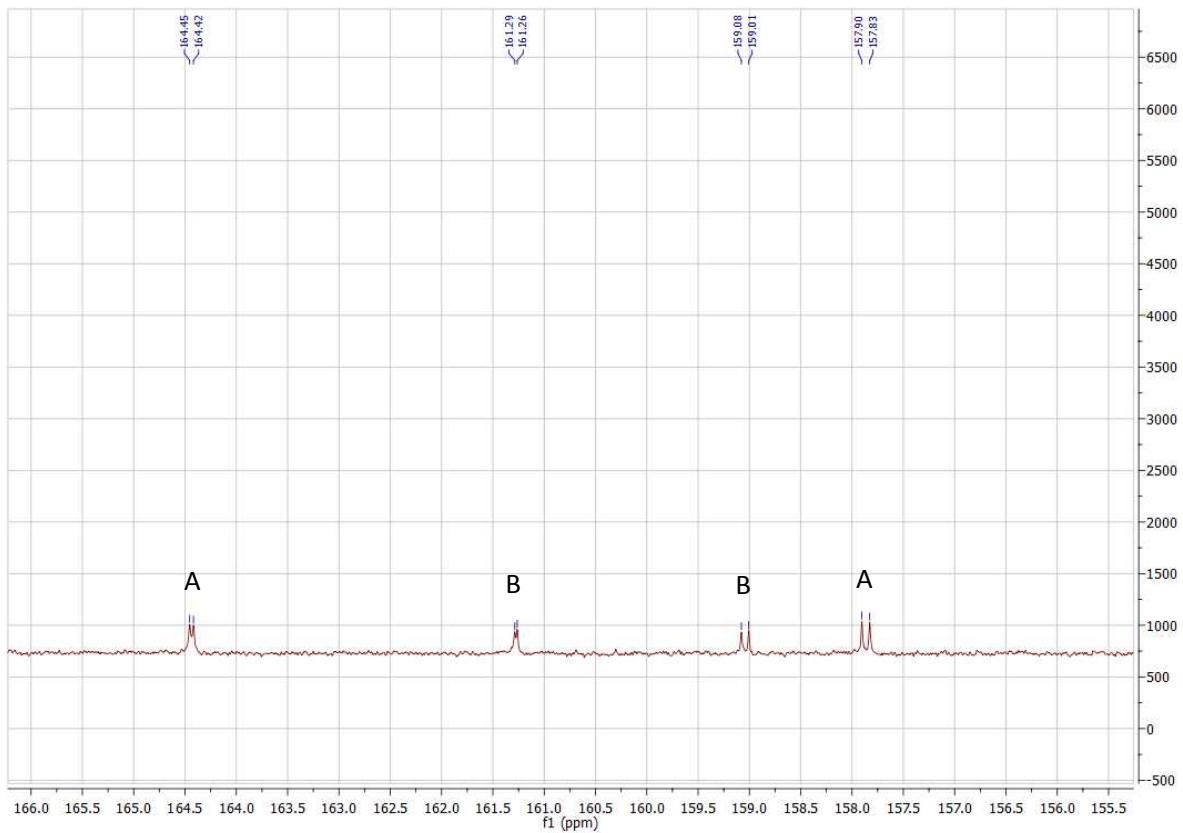


Figure 50. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of the mixture of diastereoisomers (101 MHz, 20 °C) in CD_2Cl_2 : zoom 4. ^ASignal attributed to *anti*-3.GaCl₃. ^BSignal attributed to *syn*-3.GaCl₃

NMR spectra of 4

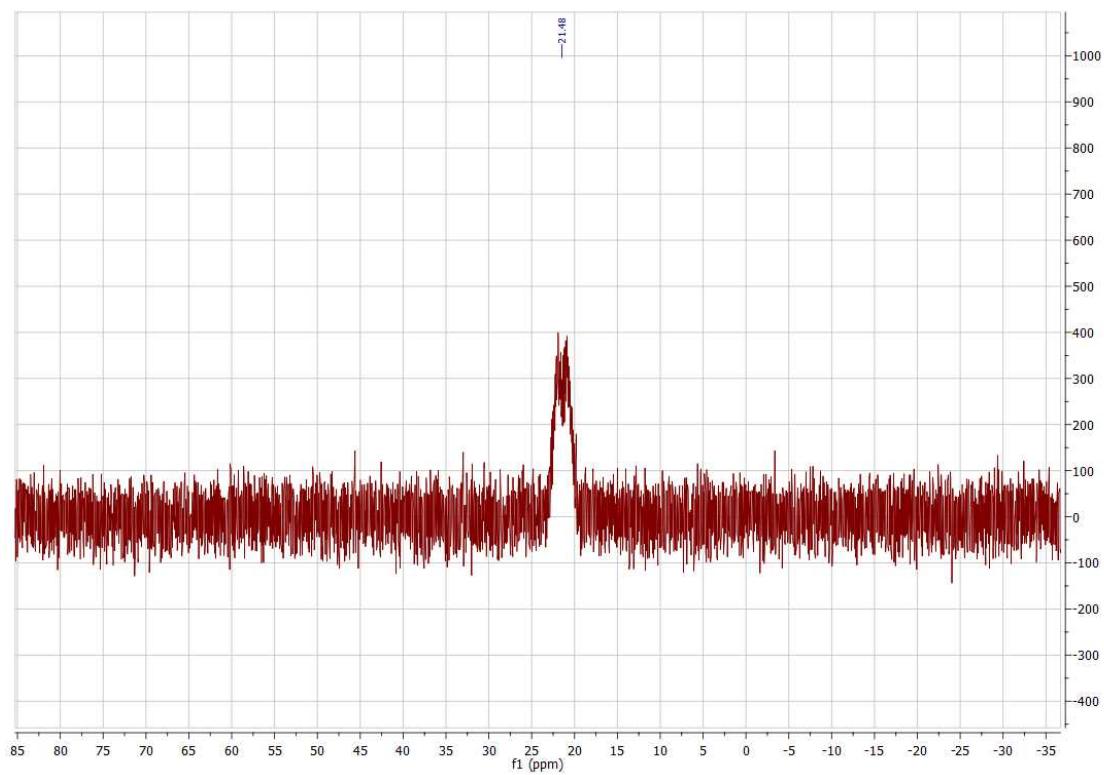


Figure 51. $^{31}\text{P}\{\text{H}\}$ NMR spectrum of 4 (121 MHz, 20 °C) in CD_2Cl_2

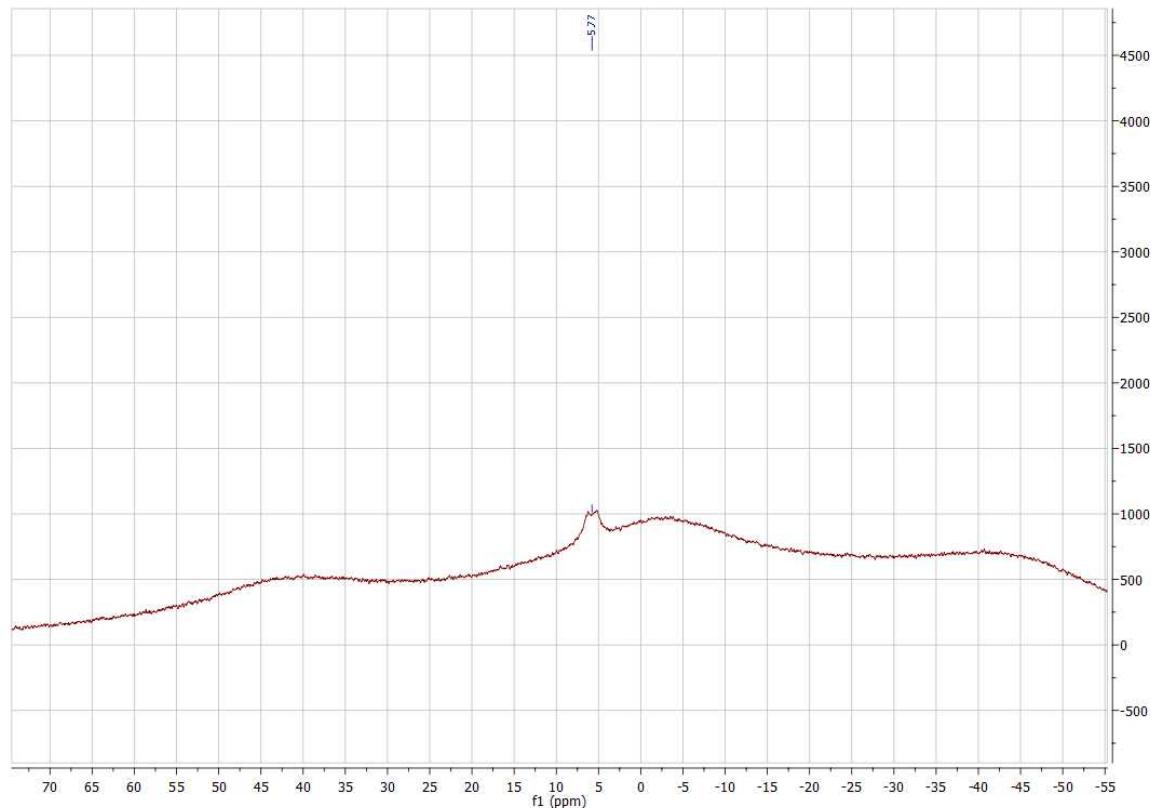


Figure 52. $^{11}\text{B}\{\text{H}\}$ NMR spectrum of 4 (96 MHz, 20 °C) in CD_2Cl_2

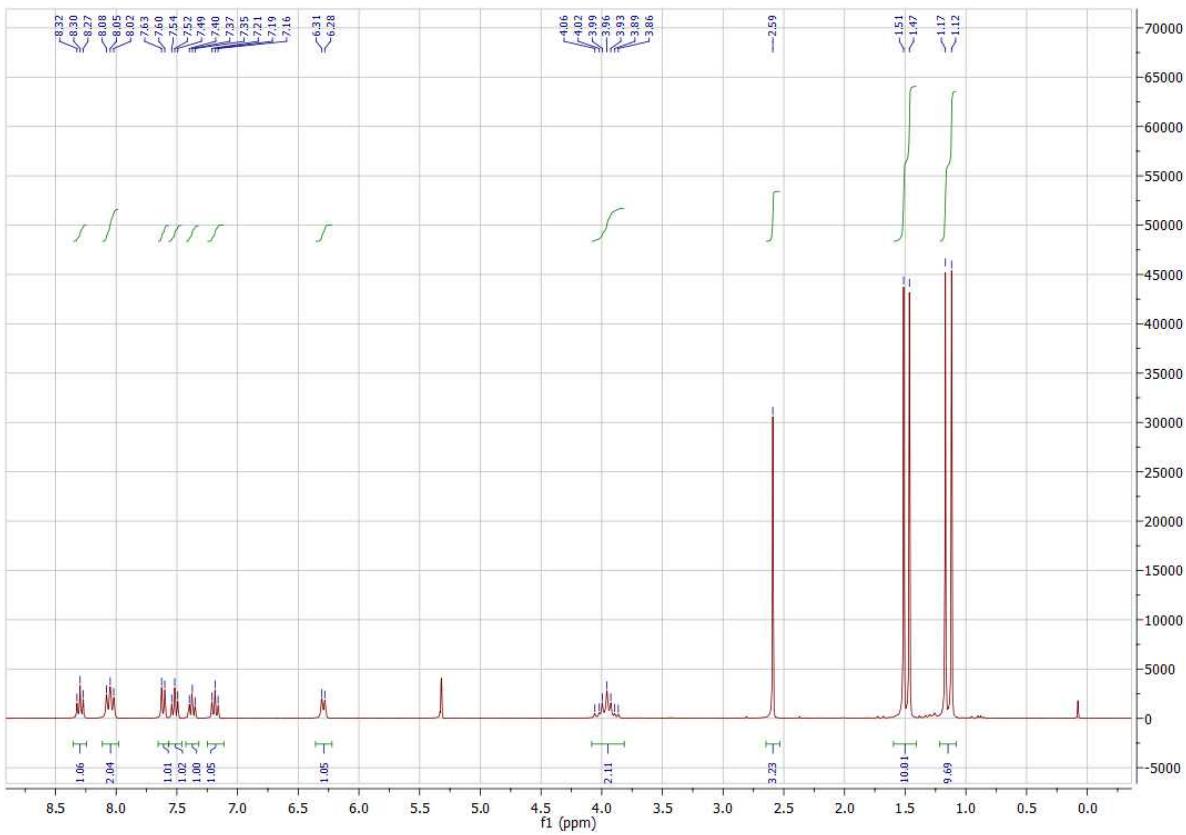


Figure 53. ^1H NMR spectrum of **4** (300 MHz, 20 °C) in CD_2Cl_2

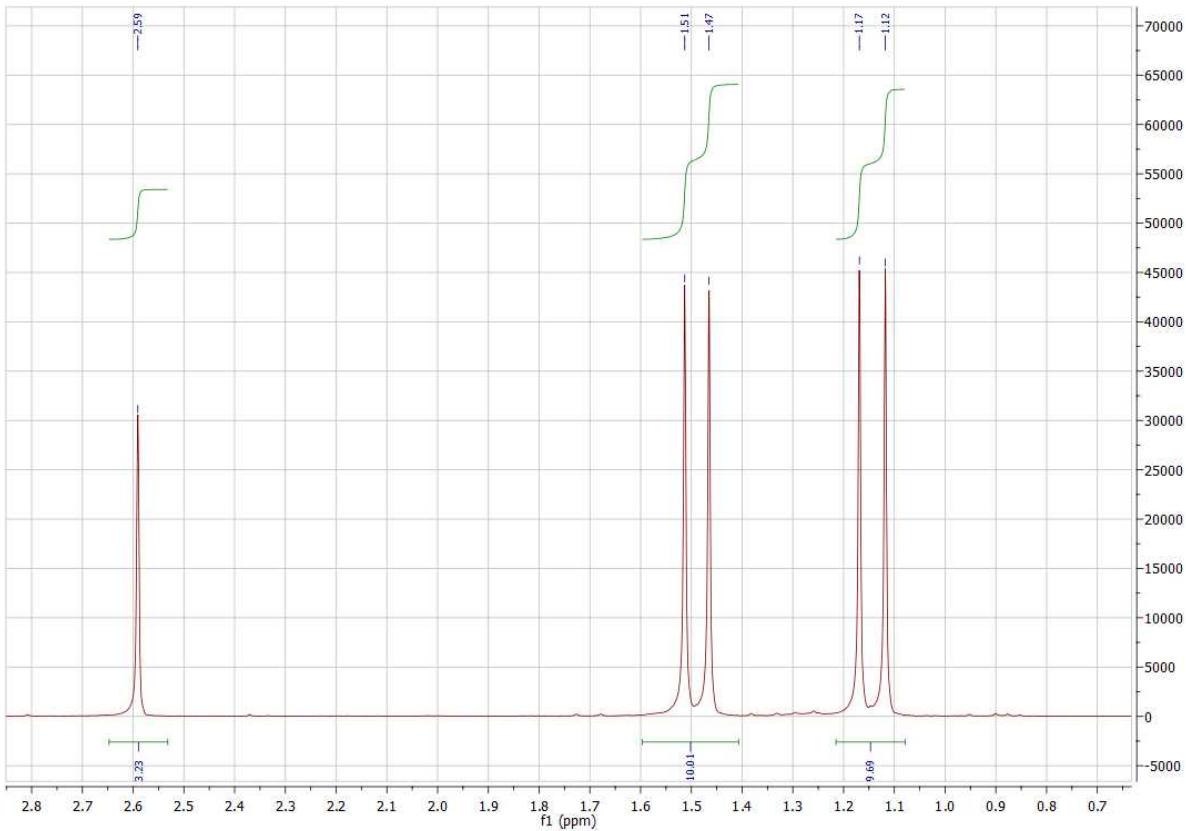


Figure 54. ^1H NMR spectrum of **4** (300 MHz, 20 °C) in CD_2Cl_2 , aliphatic region

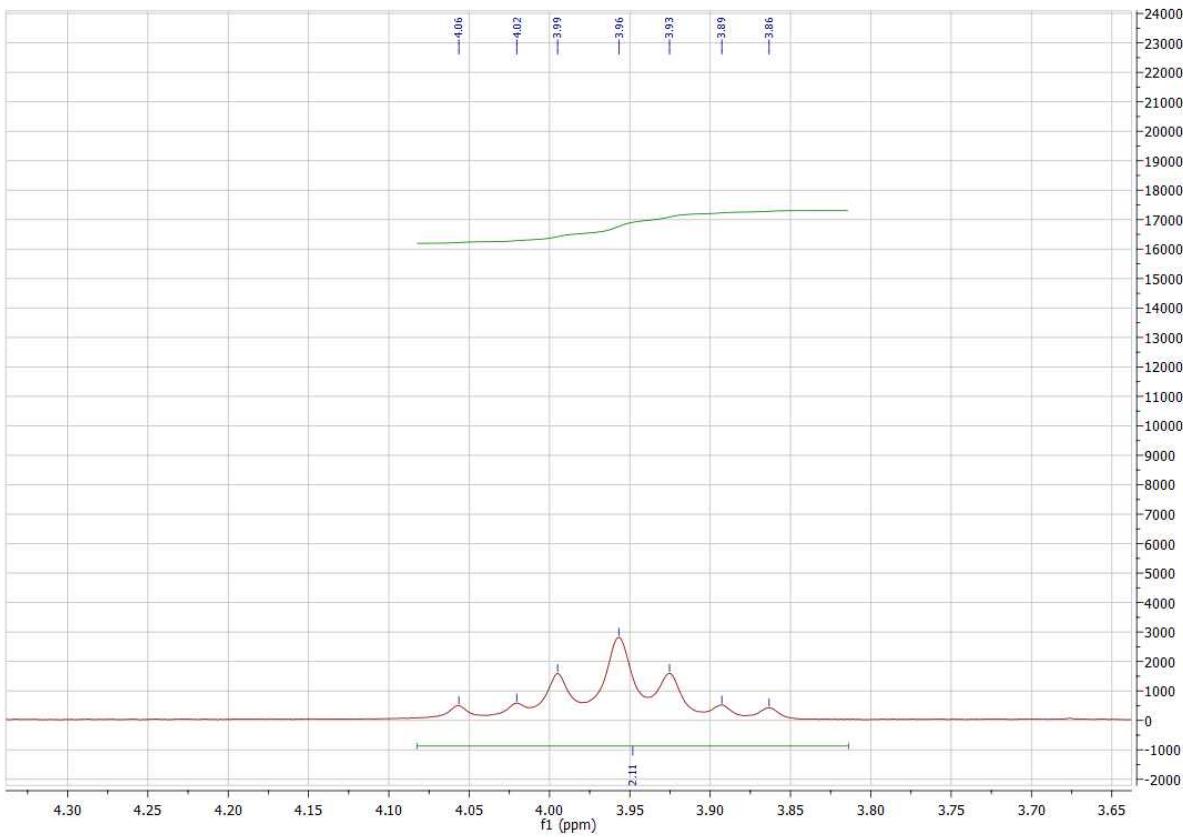


Figure 55. ^1H NMR spectrum of **4** (300 MHz, 20 °C) in CD_2Cl_2 , methylene arm

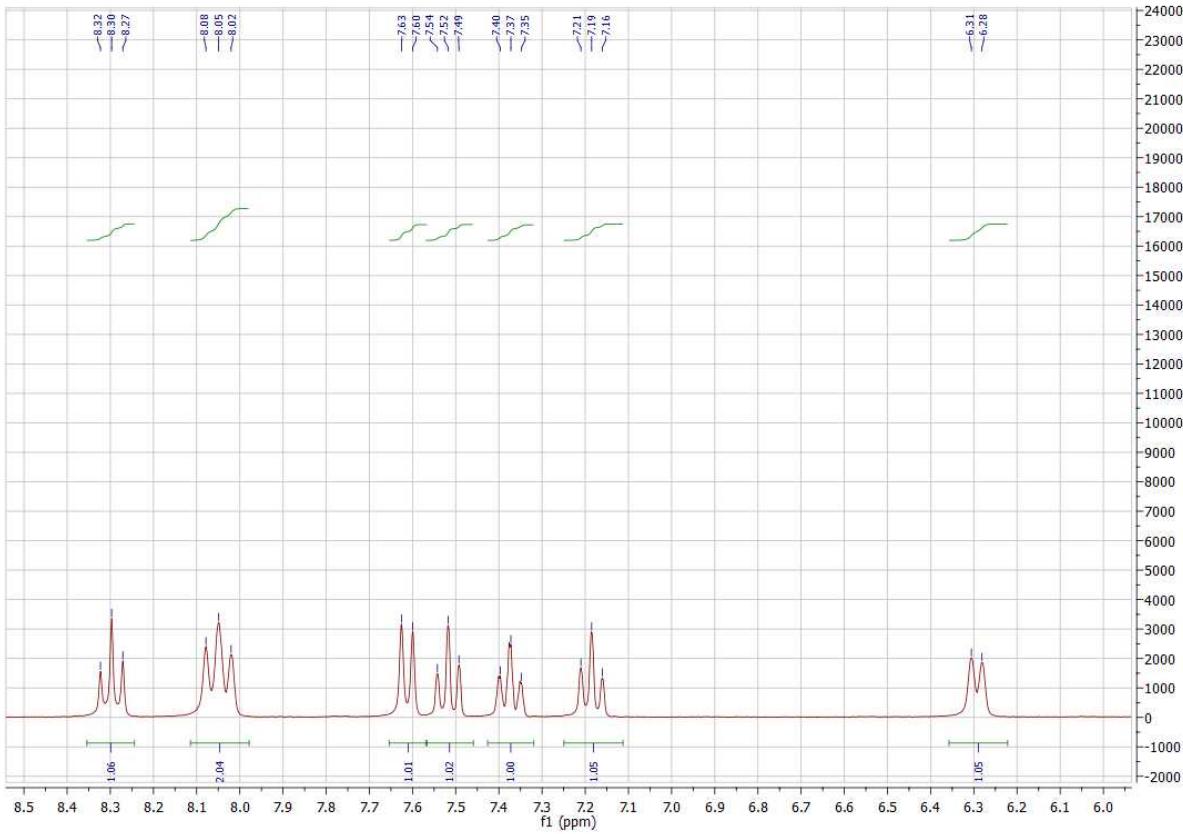


Figure 56. ^1H NMR spectrum of **4** (300 MHz, 20 °C) in CD_2Cl_2 , aromatic region

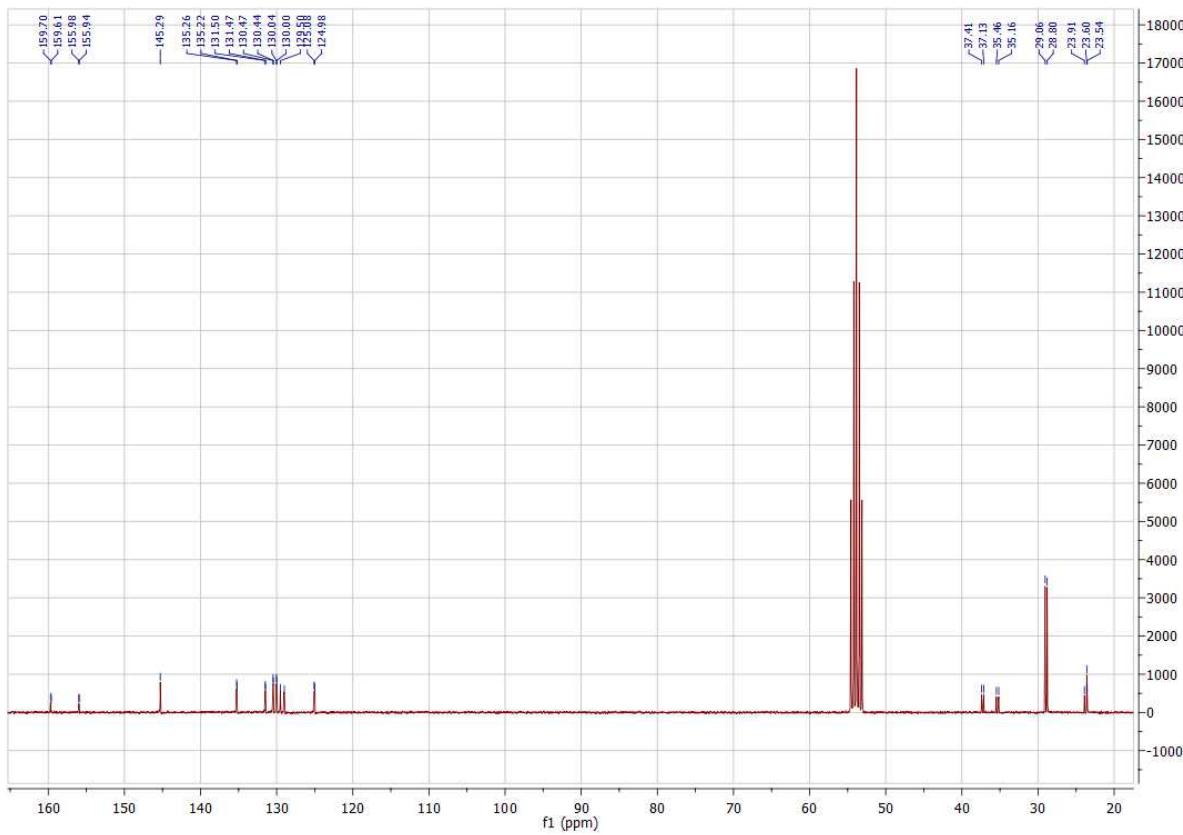


Figure 57. $^{13}\text{C}\{\text{H}\}$ NMR spectrum of **4** (75 MHz, 20 °C) in CD_2Cl_2

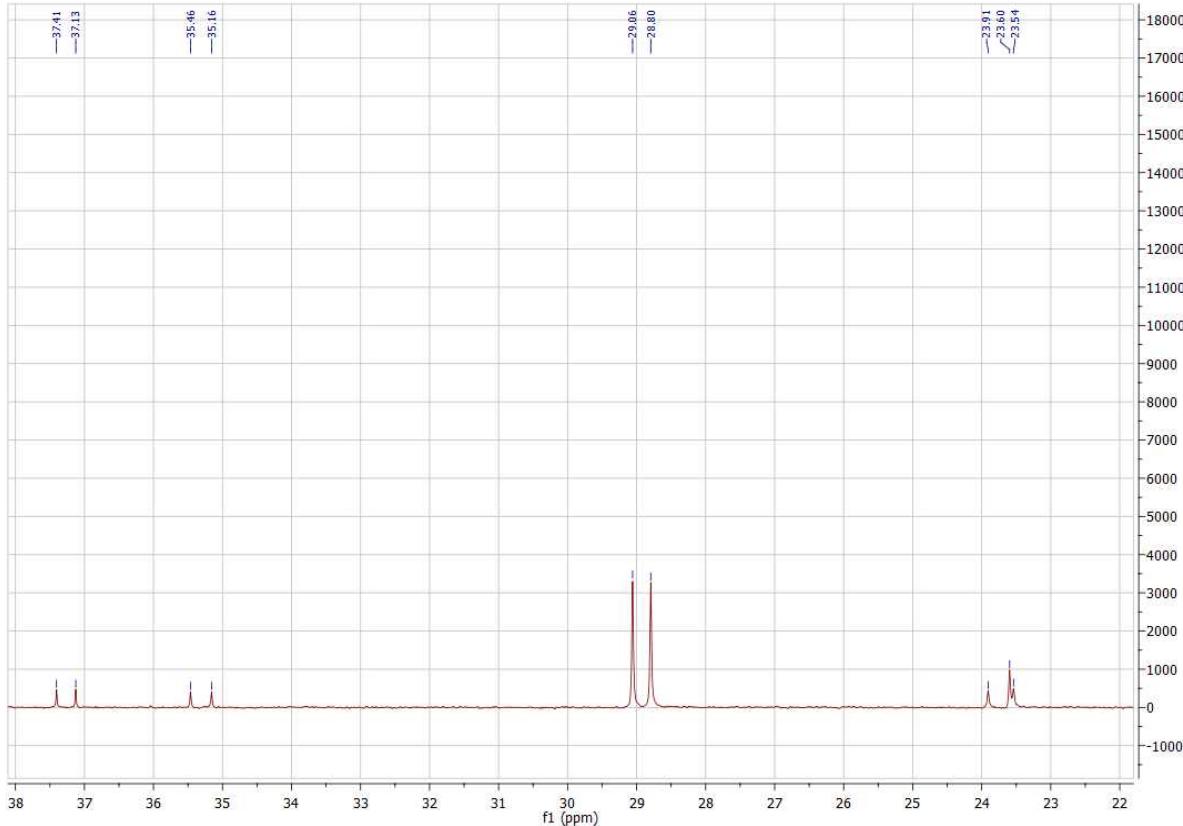


Figure 58. $^{13}\text{C}\{\text{H}\}$ NMR spectrum of **4** (75 MHz, 20 °C) in CD_2Cl_2 , aliphatic region

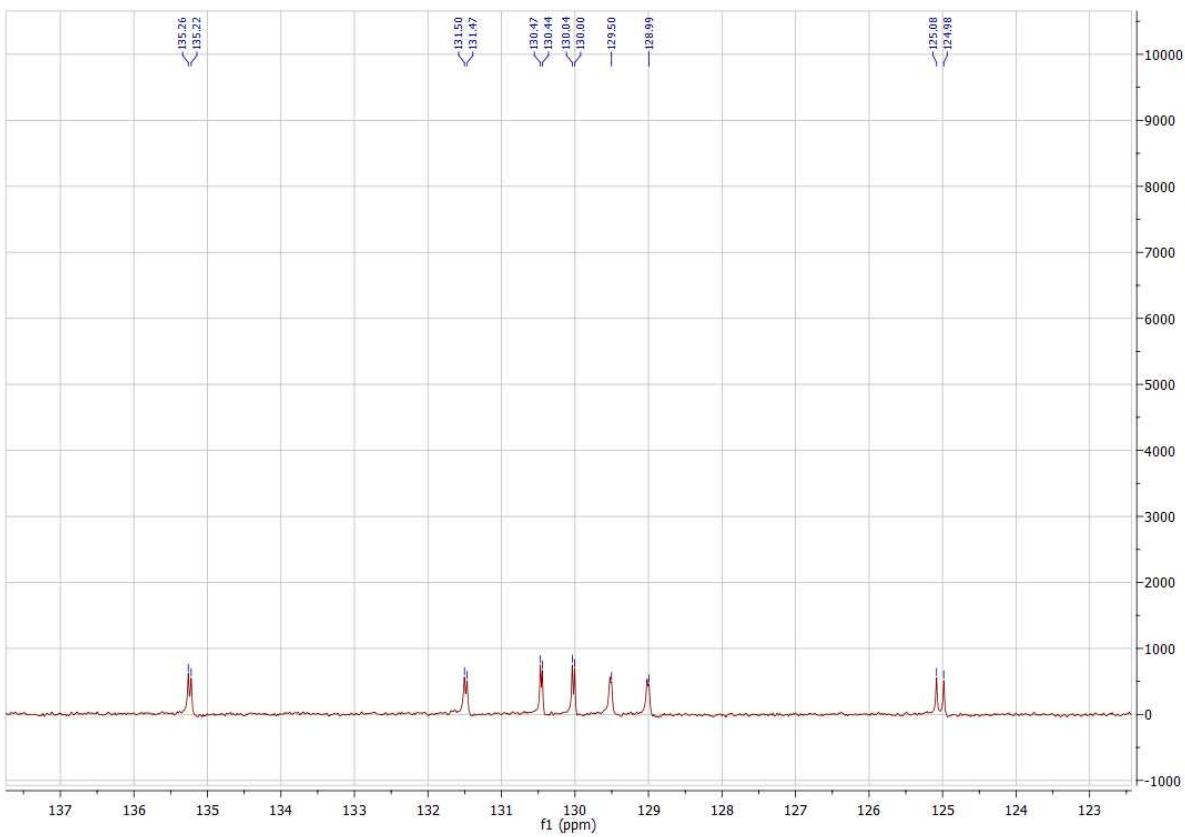


Figure 59. $^{13}\text{C}\{\text{H}\}$ NMR spectrum of **4** (75 MHz, 20 °C) in CD_2Cl_2 , aromatic region 1

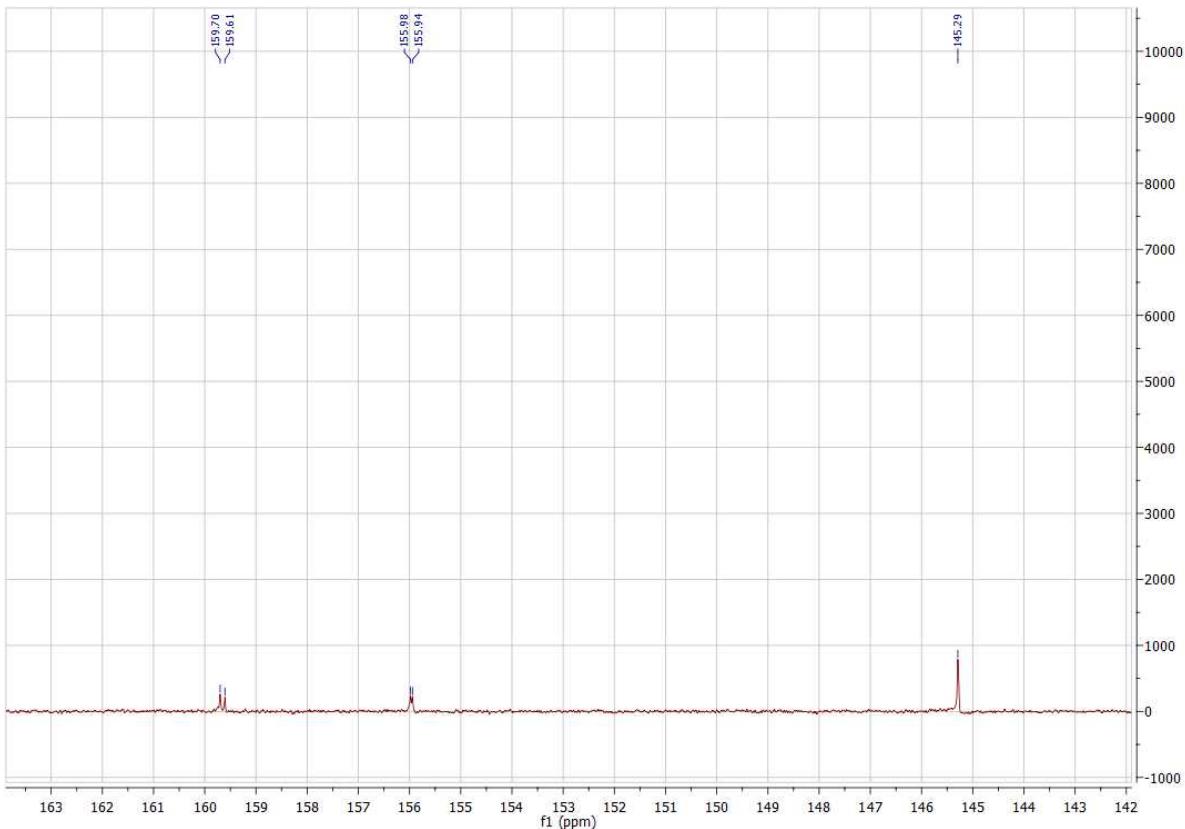


Figure 60. $^{13}\text{C}\{\text{H}\}$ NMR spectrum of **4** (75 MHz, 20 °C) in CD_2Cl_2 , aromatic region 2

NMR spectra of **5.BCl₂**

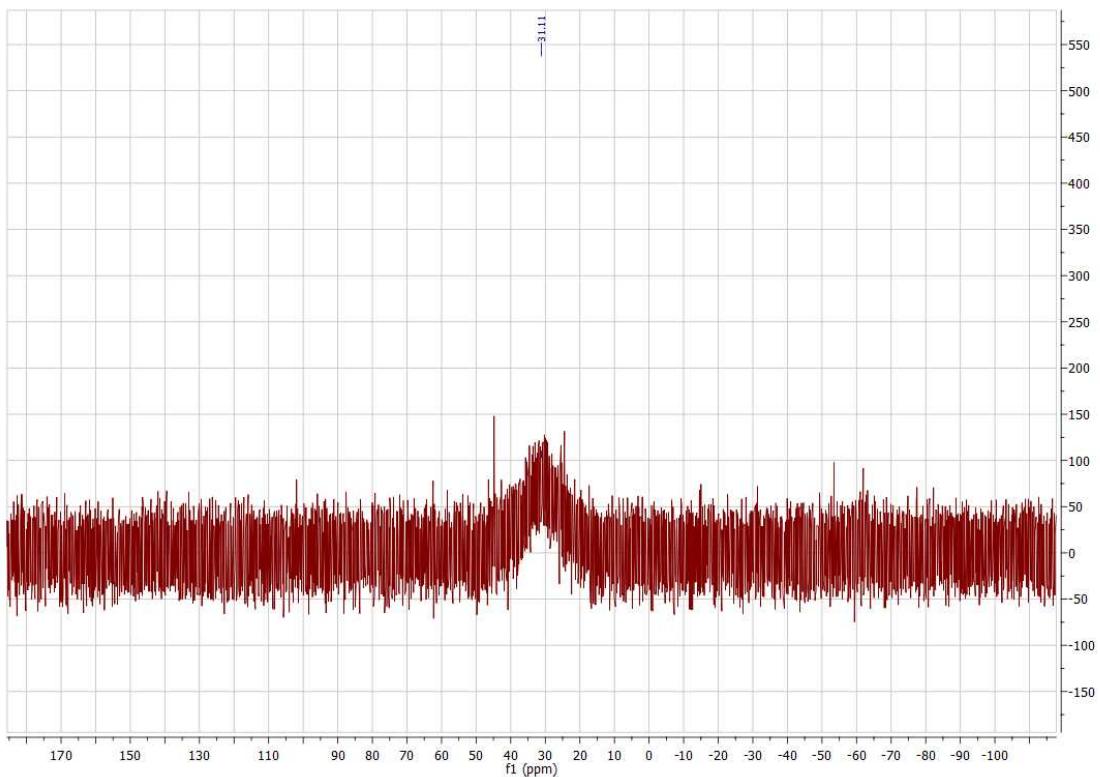


Figure 61. ³¹P{¹H} NMR spectrum of **5.BCl₂** (121 MHz, 20 °C) in CD₂Cl₂

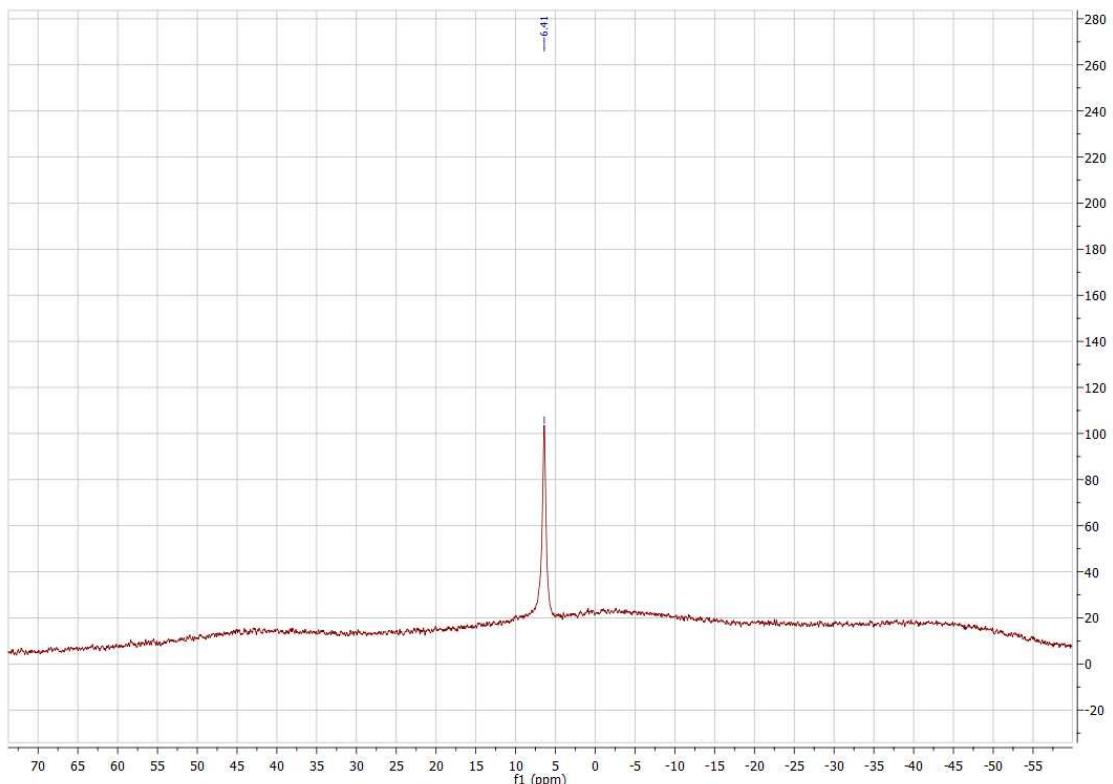


Figure 62. ¹¹B{¹H} NMR spectrum of **5.BCl₂** (96 MHz, 20 °C) in CD₂Cl₂

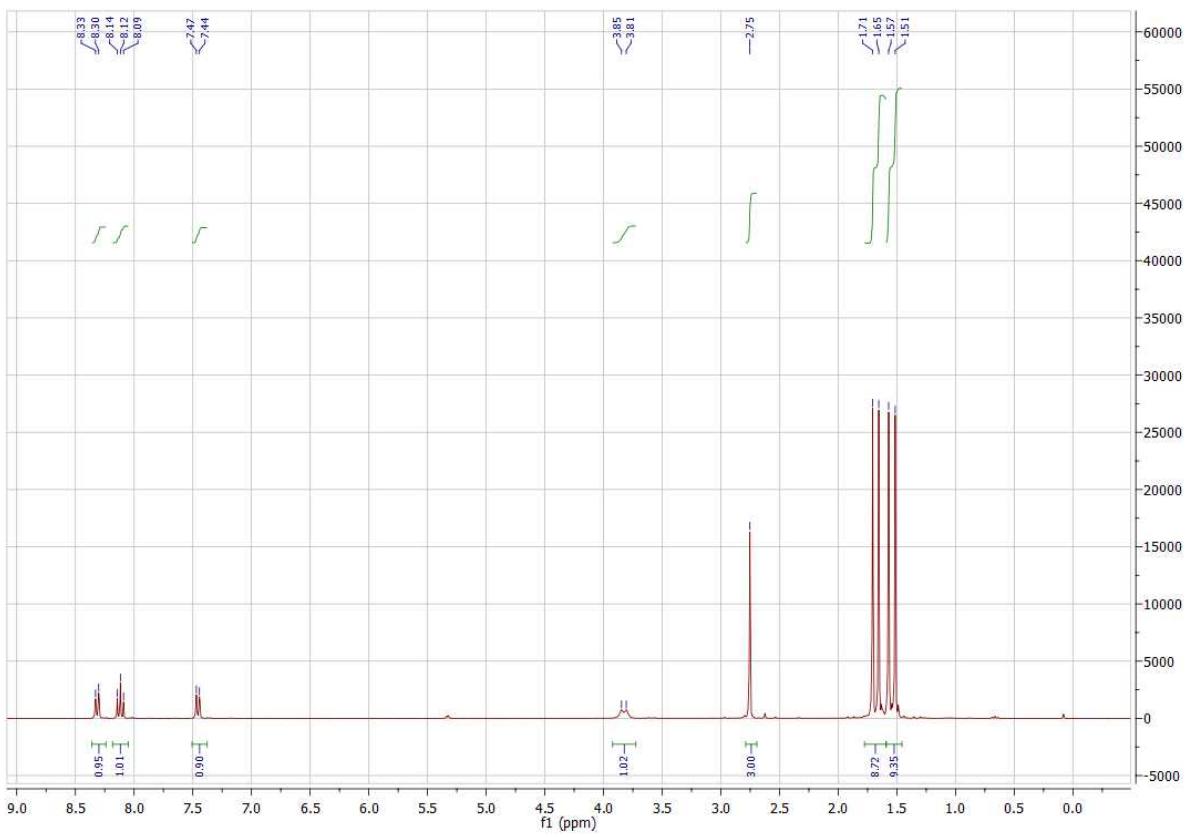


Figure 63. ^1H NMR spectrum of **5.BCl₂** (300 MHz, 20 °C) in CD₂Cl₂

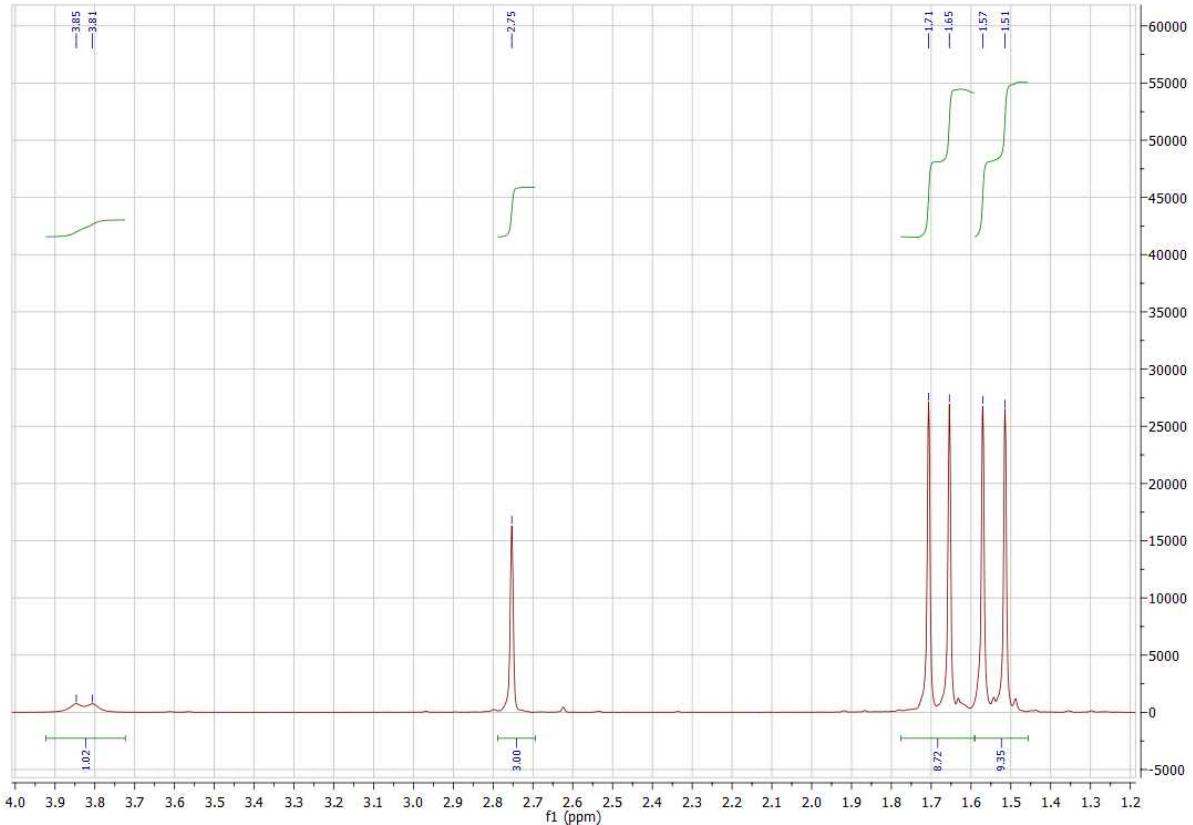


Figure 64. ^1H NMR spectrum of **5.BCl₂** (300 MHz, 20 °C) in CD₂Cl₂: zoom 1

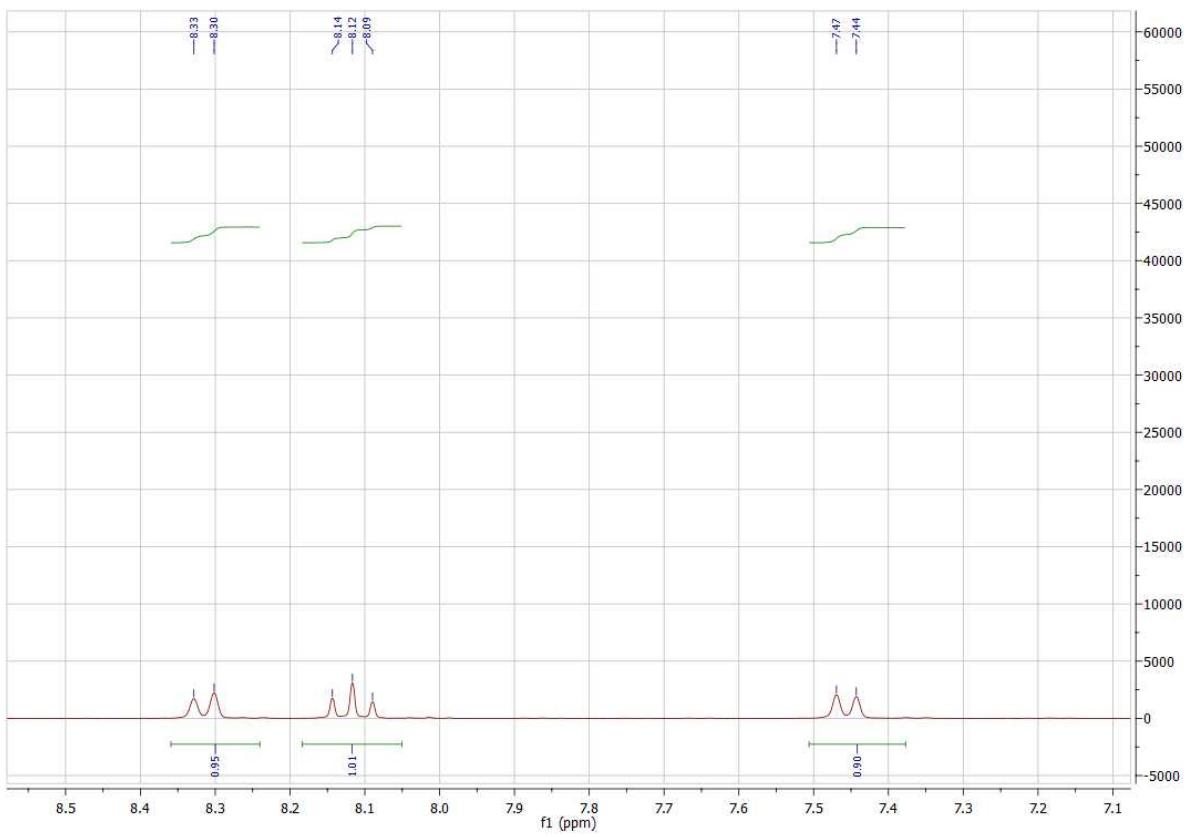


Figure 65. ^1H NMR spectrum of **5.BCl₂** (300 MHz, 20 °C) in CD₂Cl₂: zoom 2

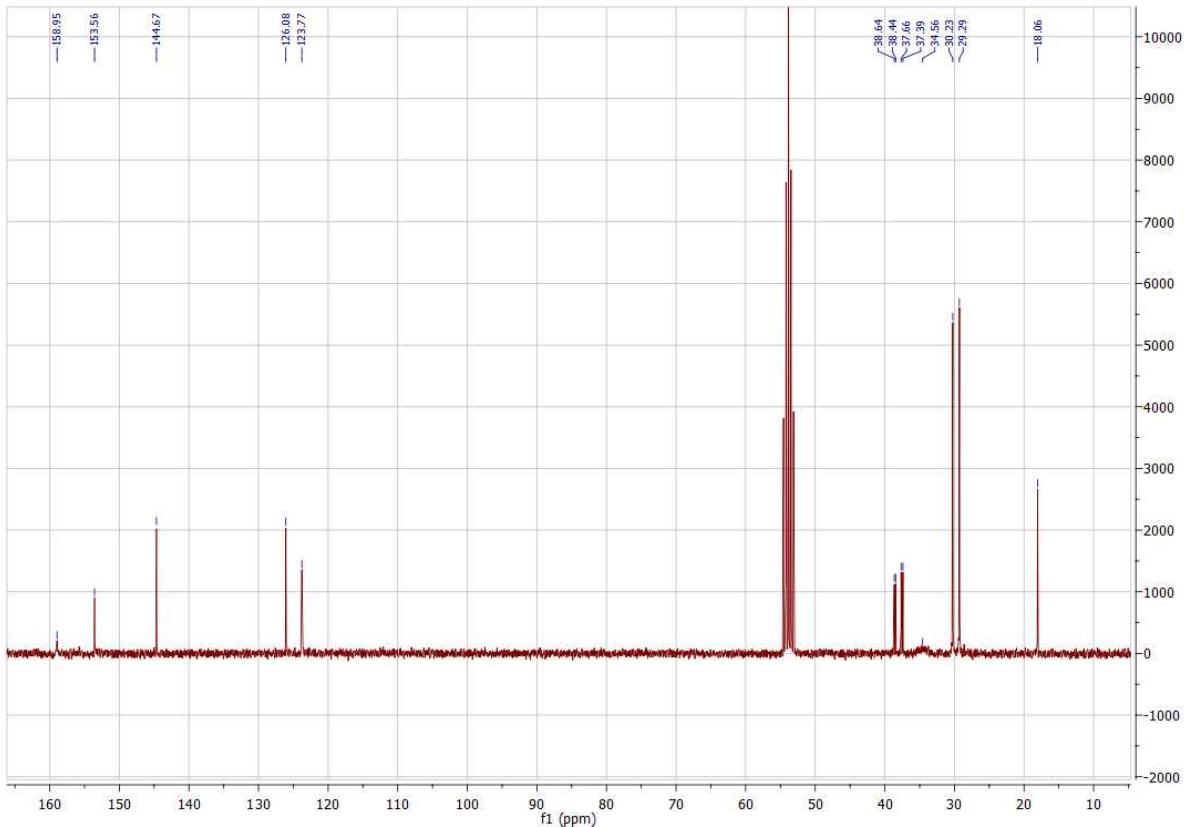


Figure 66. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **5.BCl₂** (75 MHz, 20 °C) in CD₂Cl₂

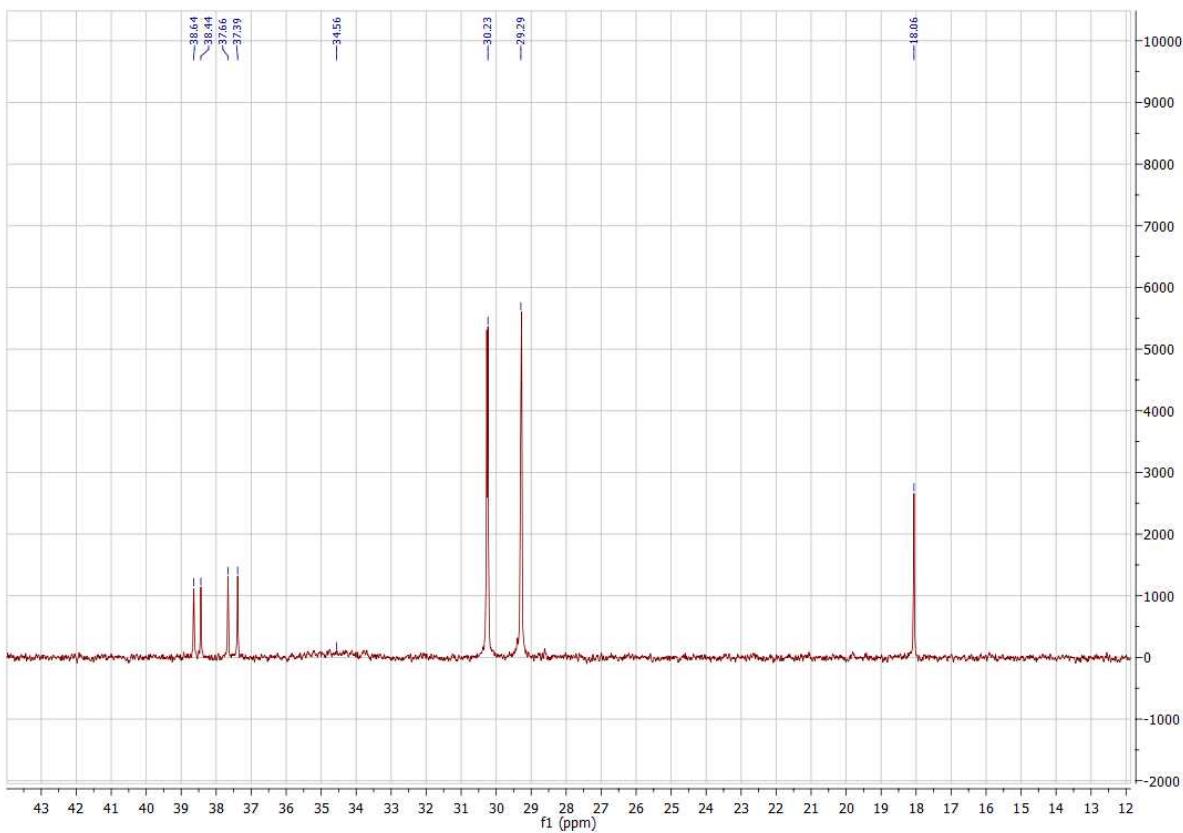


Figure 67. $^{13}\text{C}\{\text{H}\}$ NMR spectrum of **5.BCl₂** (75 MHz, 20 °C) in CD₂Cl₂: zoom 1

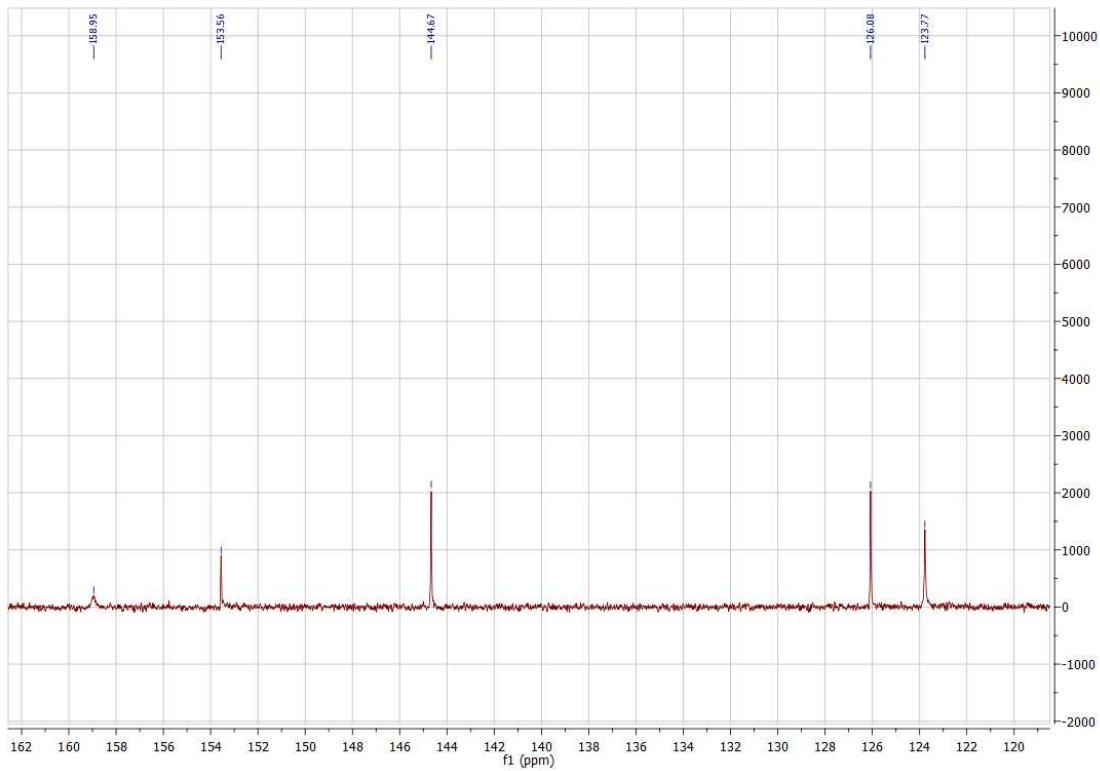


Figure 68. $^{13}\text{C}\{\text{H}\}$ NMR spectrum of **5.BCl₂** (75 MHz, 20 °C) in CD₂Cl₂: zoom 2

NMR spectra of **5.B(Cl)(Ph)**

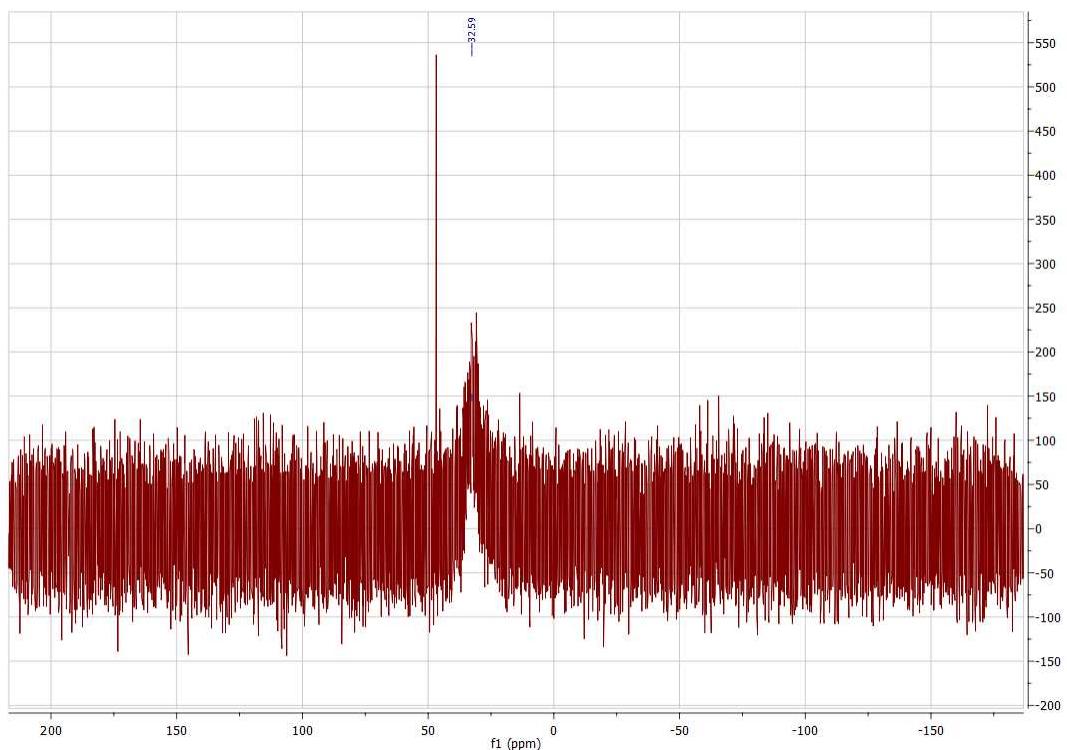


Figure 69. $^{31}\text{P}\{\text{H}\}$ NMR spectrum of **5.B(Cl)(Ph)** (121 MHz, 20 °C) in CD_2Cl_2

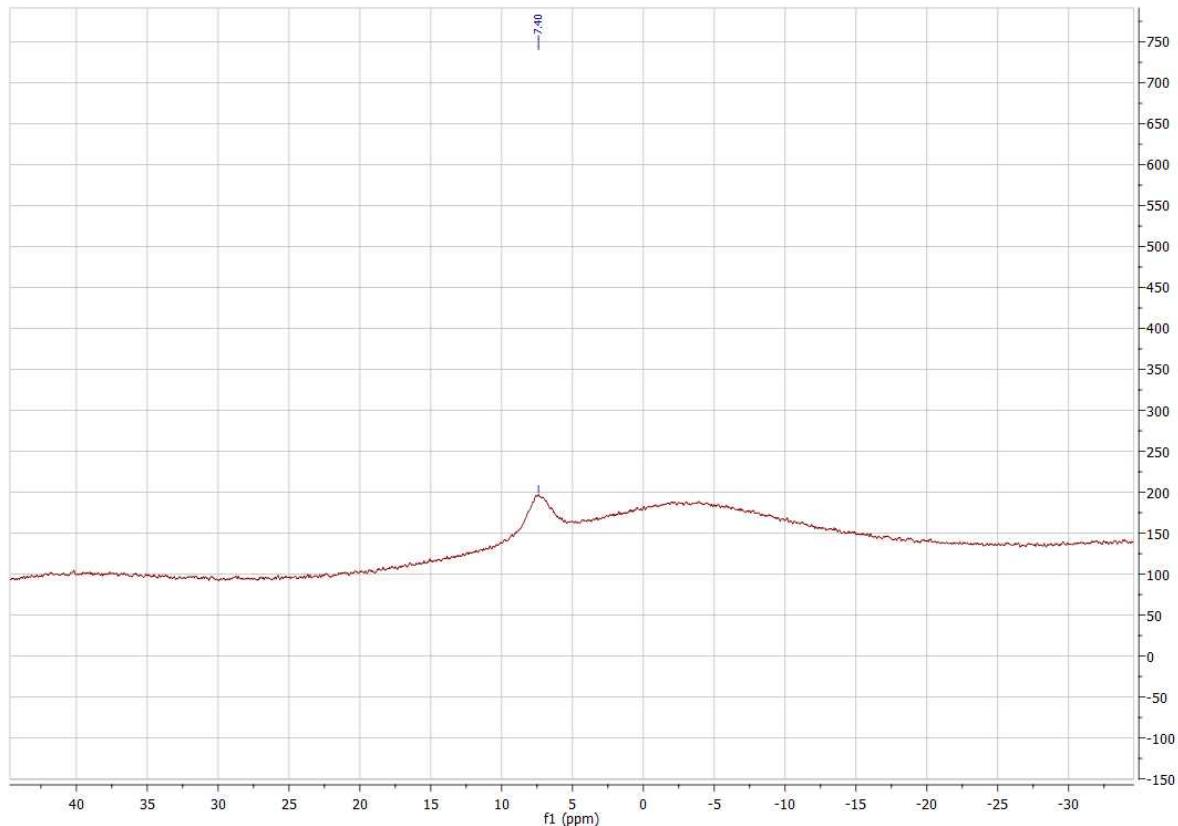


Figure 70. $^{11}\text{B}\{\text{H}\}$ NMR spectrum of **5.B(Cl)(Ph)** (96 MHz, 20 °C) in CD_2Cl_2

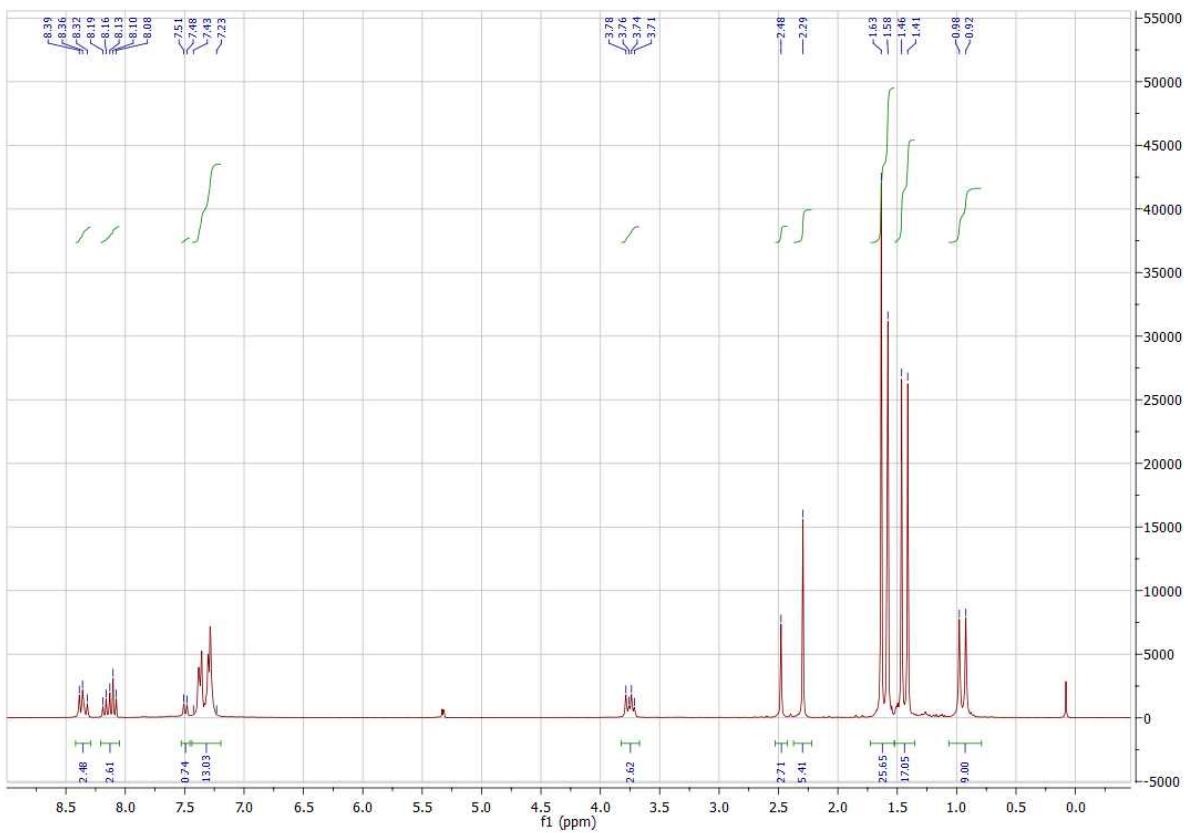


Figure 71. ^1H NMR spectrum of **5.B(Cl)(Ph)** (400 MHz, 20 °C) in CD_2Cl_2

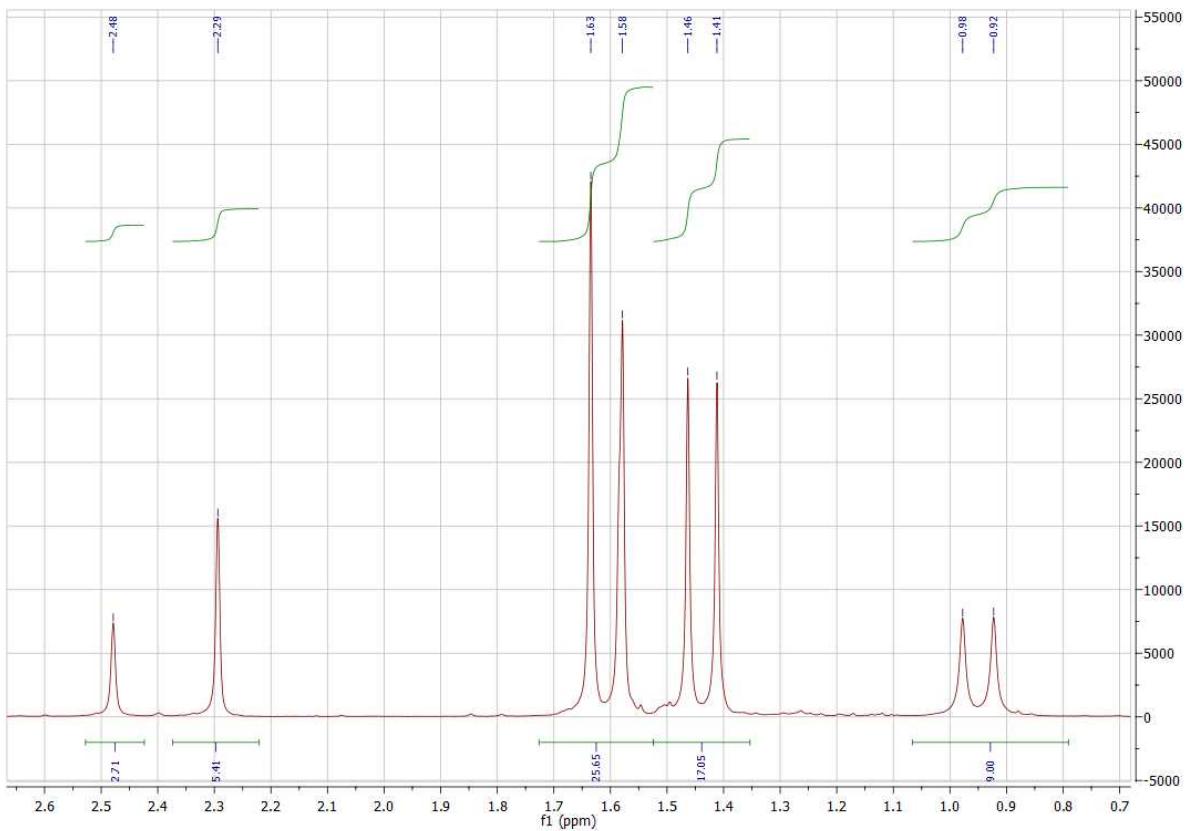


Figure 72. ^1H NMR spectrum of **5.B(Cl)(Ph)** (400 MHz, 20 °C) in CD_2Cl_2 : zoom 1

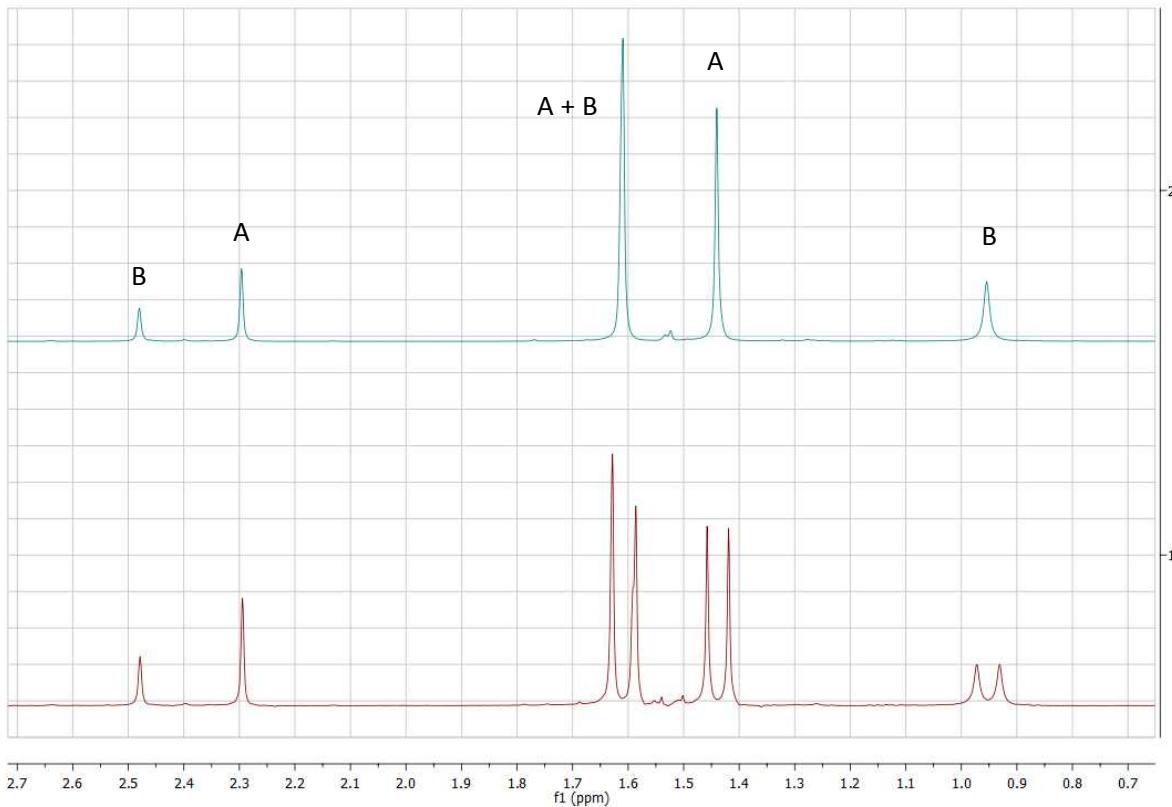


Figure 73. Stacked $^1\text{H}\{^{31}\text{P}\}$ NMR (top) and ^1H NMR (bottom) spectra of **5.B(Cl)(Ph)** (400 MHz, 20 °C) in CD_2Cl_2 : zoom 1. ^A Signal attributed to the *syn*-**5.B(Cl)(Ph)**; **A**. ^B Signal attributed to the *anti*-**5.B(Cl)(Ph)**; **B**. ^{A+B} Here, one signal of the *t*Bu group of **A** overlap with one signal of the *t*Bu group of **B** as evidenced by integration

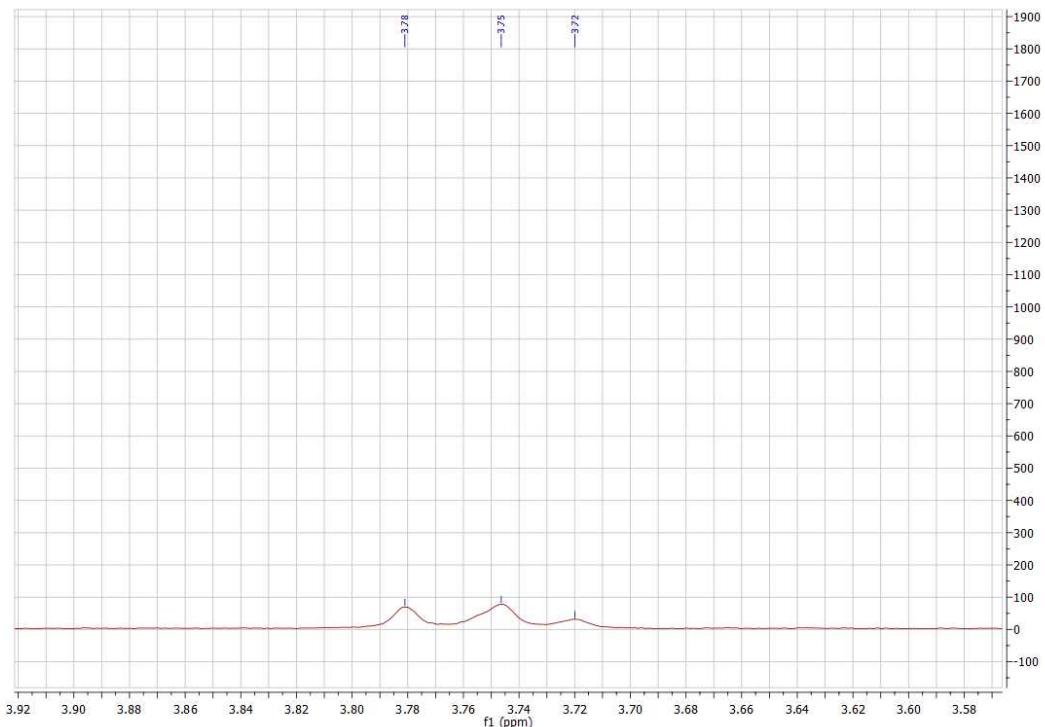


Figure 74. ^1H NMR spectrum of **5.B(Cl)(Ph)** (400 MHz, 20 °C) in CD_2Cl_2 : zoom 2 ($=\text{CH-PPh}_2$)

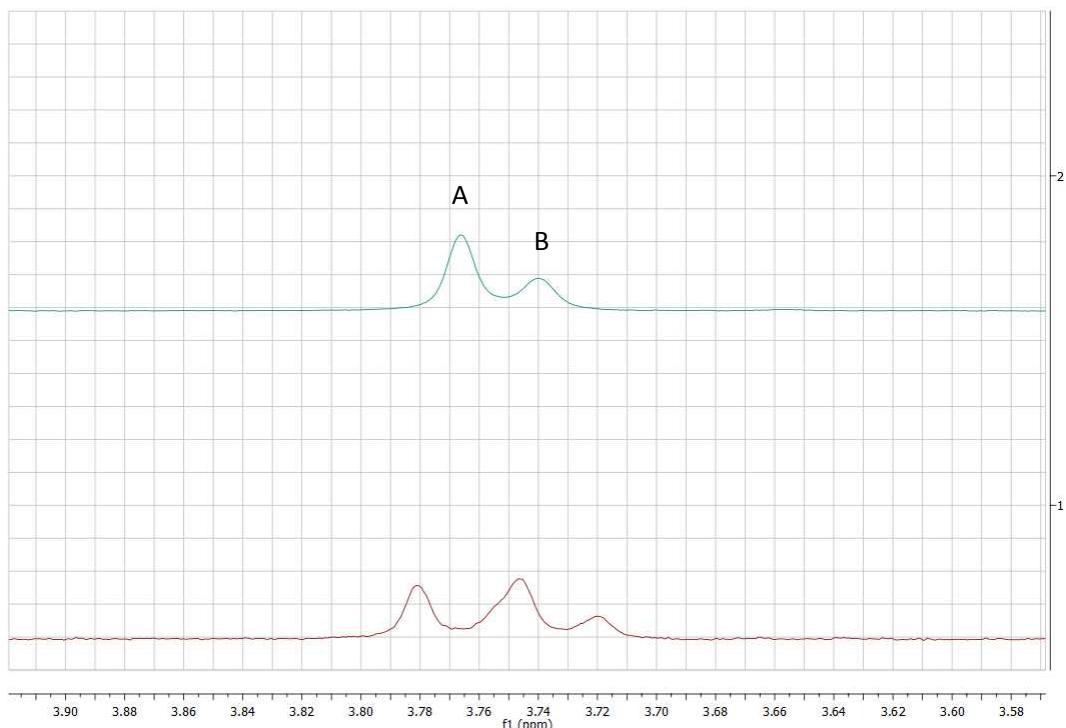


Figure 75. Stacked ^1H NMR (bottom) and $^1\text{H}\{\text{P}^{31}\}$ NMR (top) spectra of **5.B(Cl)(Ph)** (400 MHz, 20 °C) in CD_2Cl_2 : zoom 2, B-C(H)-P signals. ^A Signal attributed to the *syn*-**5.B(Cl)(Ph)**; **A**. ^B Signal attributed to the *anti*-**5.B(Cl)(Ph)**; **B**

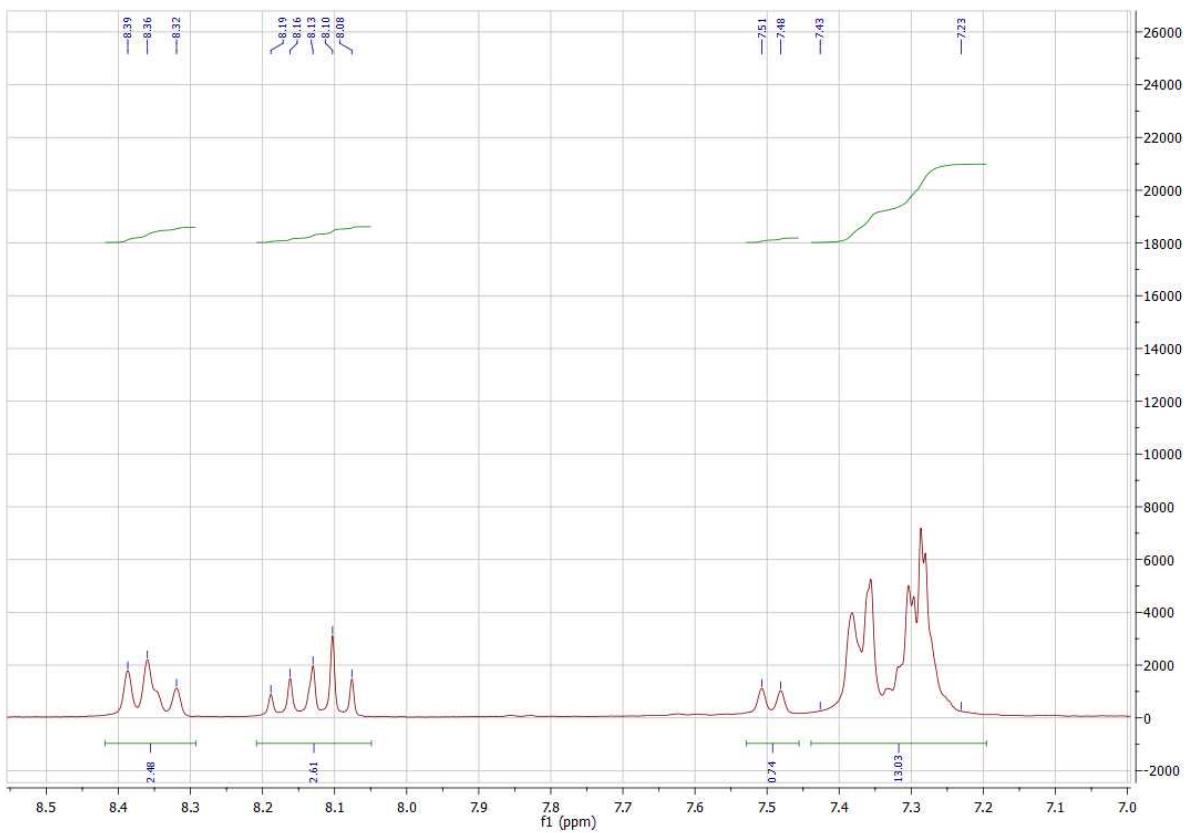


Figure 76. ^1H NMR spectrum of **5.B(Cl)(Ph)** (400 MHz, 20 °C) in CD_2Cl_2 : zoom 3

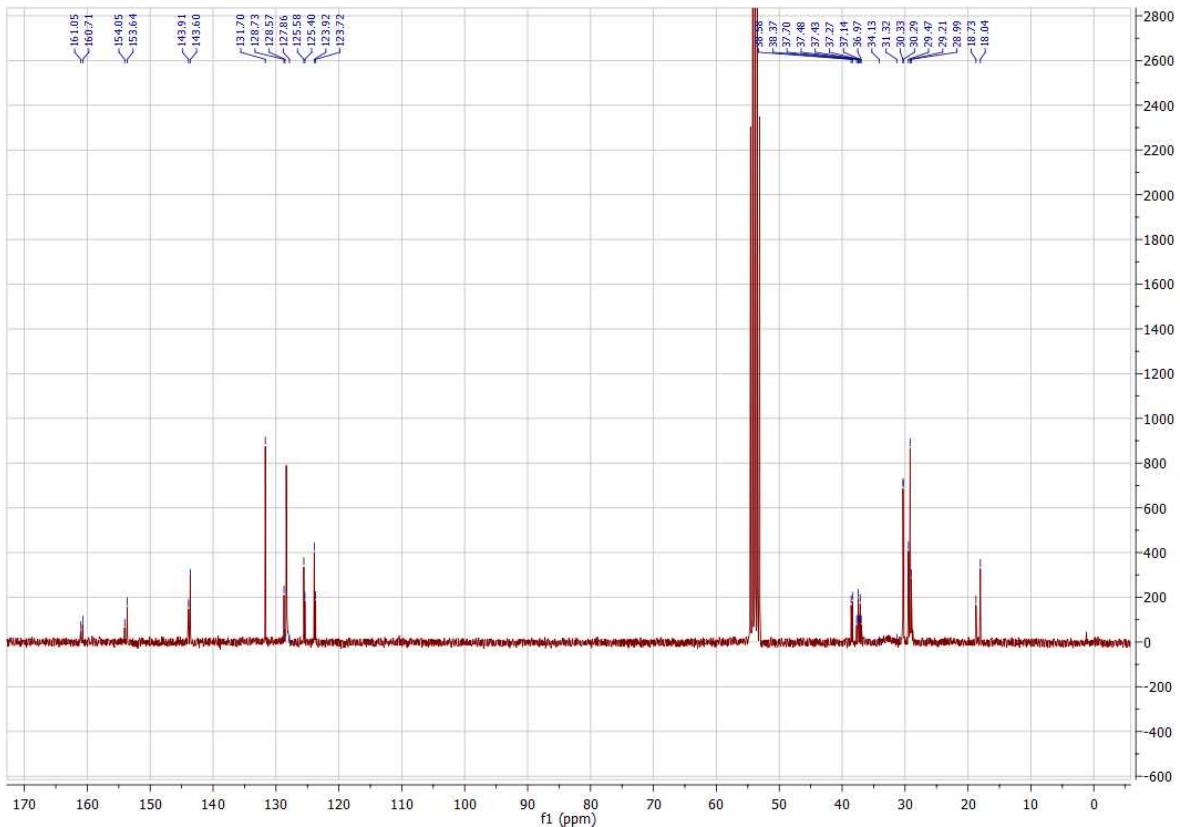


Figure 77. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **5.B(Cl)(Ph)** (75 MHz, 20 °C) in CD_2Cl_2

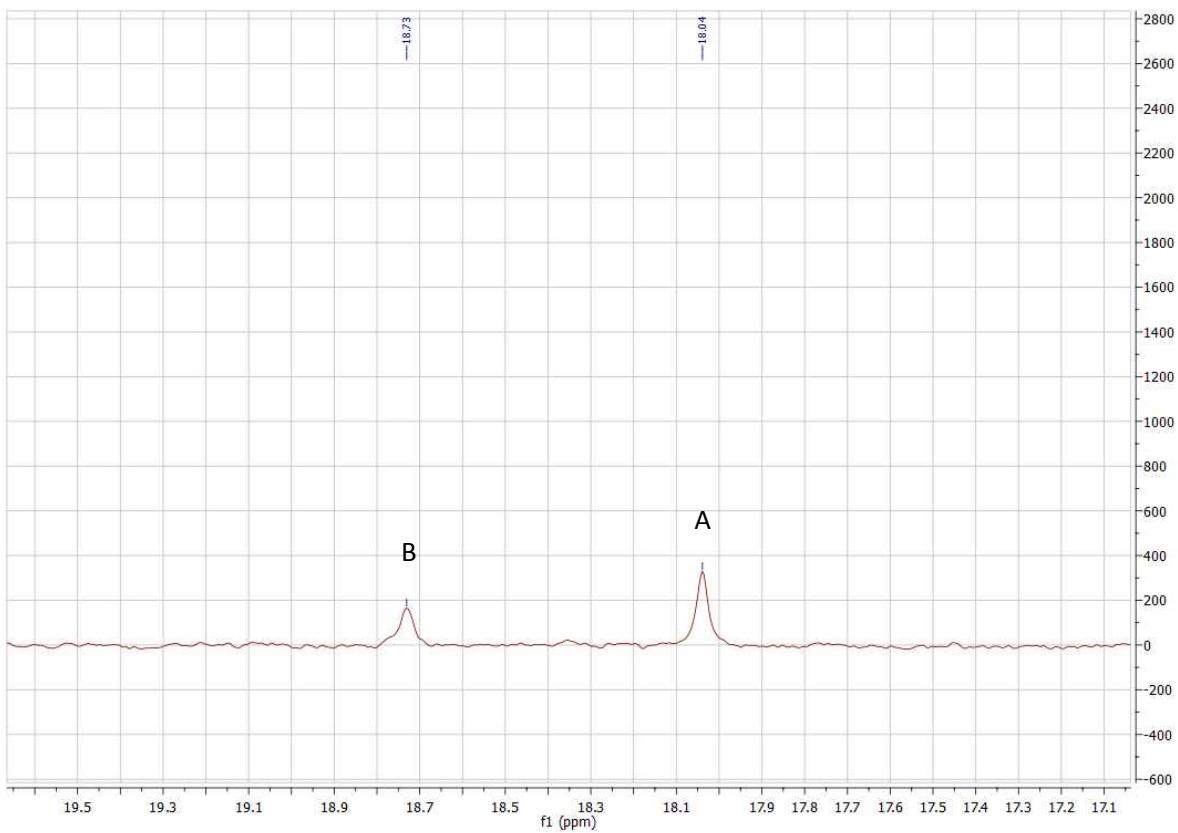


Figure 78. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **5.B(Cl)(Ph)** (75 MHz, 20 °C) in CD_2Cl_2 : zoom 1.
^A Signal attributed to the *syn*-**5.B(Cl)(Ph)**; ^B Signal attributed to the *anti*-**5.B(Cl)(Ph)**; **B**

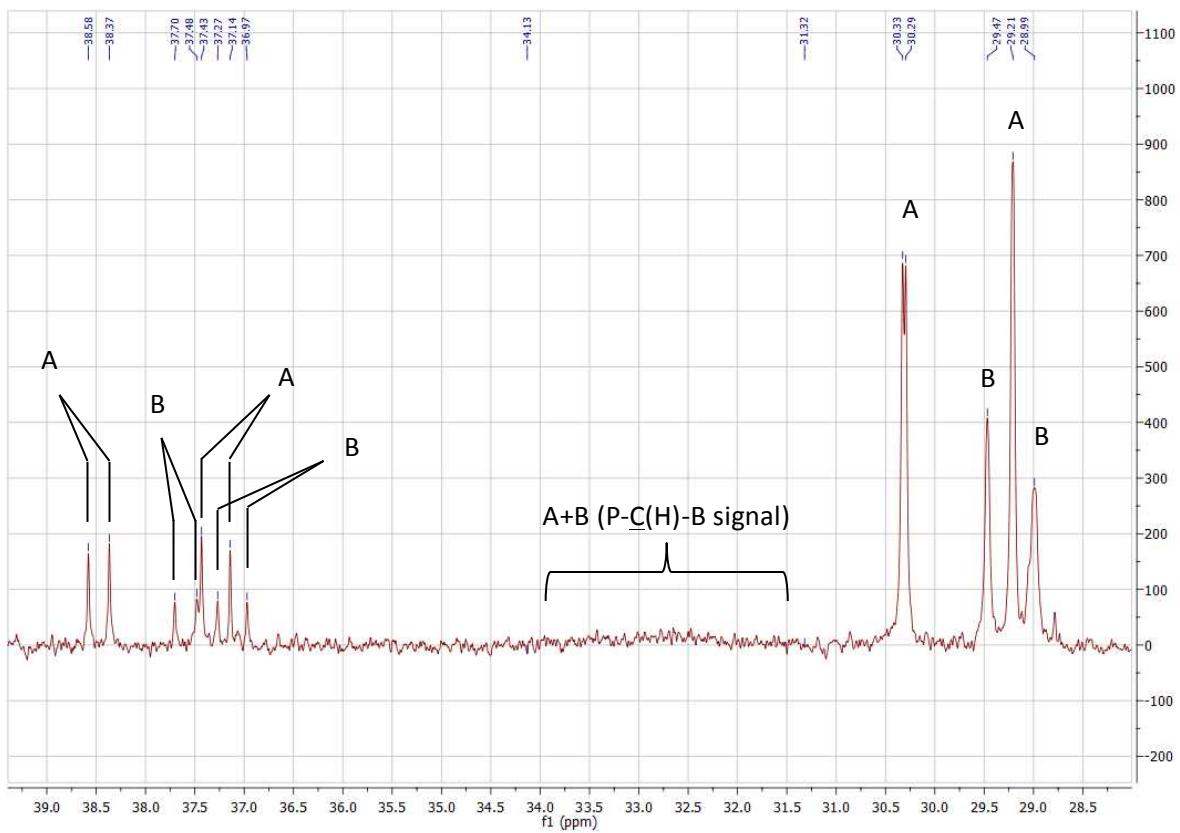


Figure 79. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **5.B(Cl)(Ph)** (75 MHz, 20 °C) in CD_2Cl_2 : zoom 2.
^A Signal attributed to the *syn*-**5.B(Cl)(Ph)**; **A**. ^B Signal attributed to the *anti*-**5.B(Cl)(Ph)**; **B**

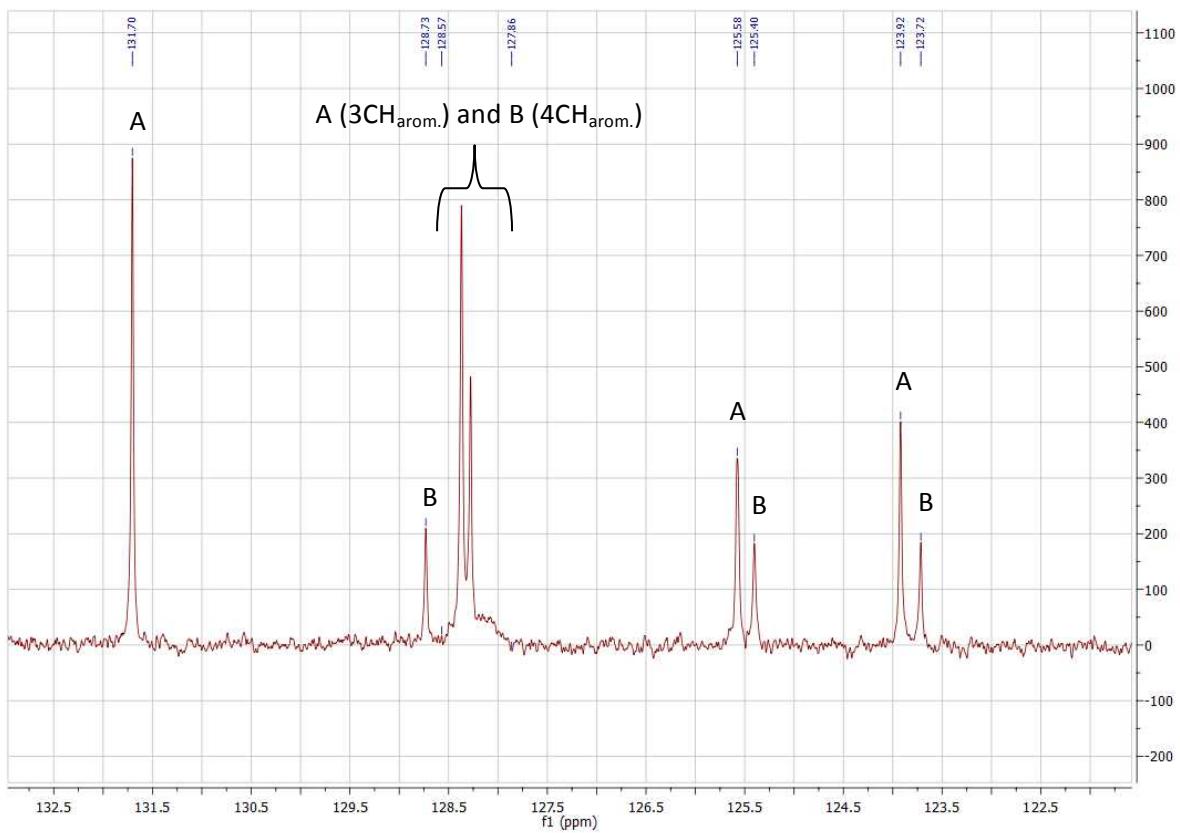


Figure 80. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **5.B(Cl)(Ph)** (75 MHz, 20 °C) in CD₂Cl₂: zoom 3.
^A Signal attributed to the *syn*-5.B(Cl)(Ph); A. ^B Signal attributed to the *anti*-5.B(Cl)(Ph); B

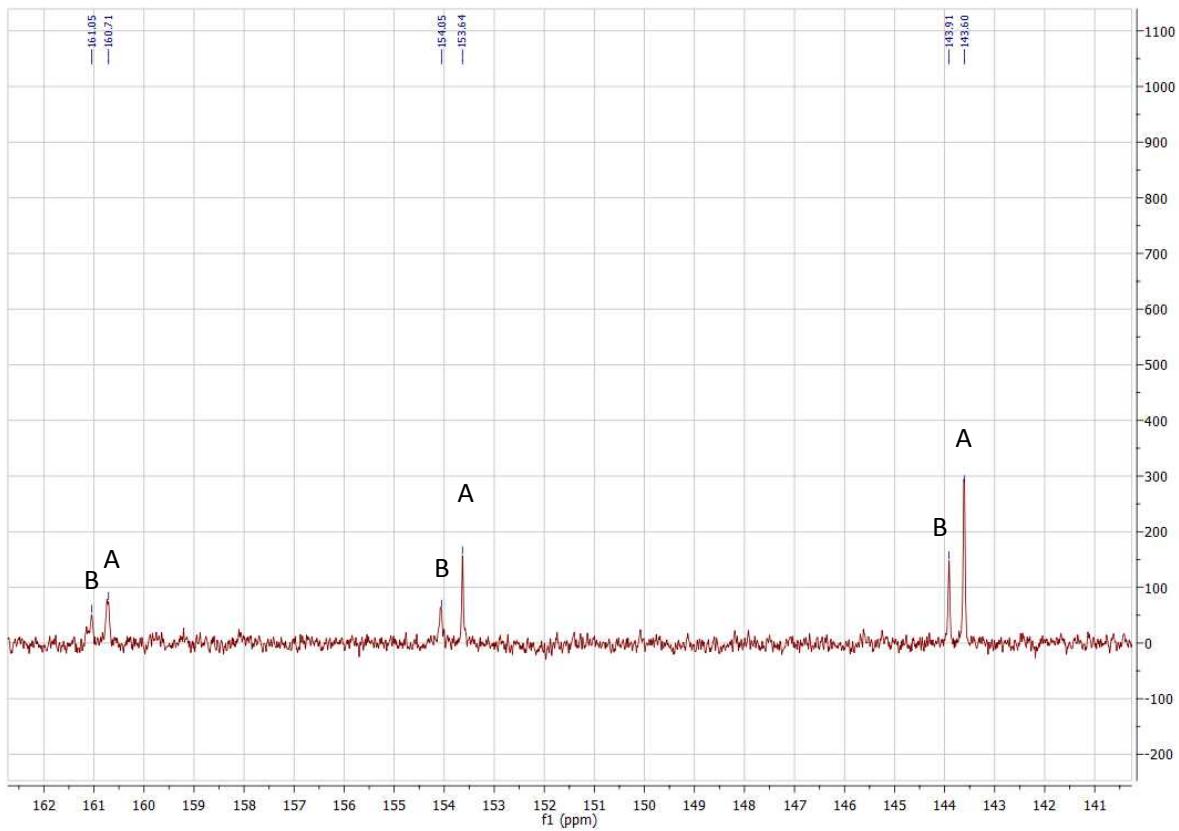


Figure 81. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **5.B(Cl)(Ph)** (75 MHz, 20 °C) in CD_2Cl_2 : zoom 4.
^A Signal attributed to the *syn*-**5.B(Cl)(Ph)**; **A**. ^B Signal attributed to the *anti*-**5.B(Cl)(Ph)**; **B**

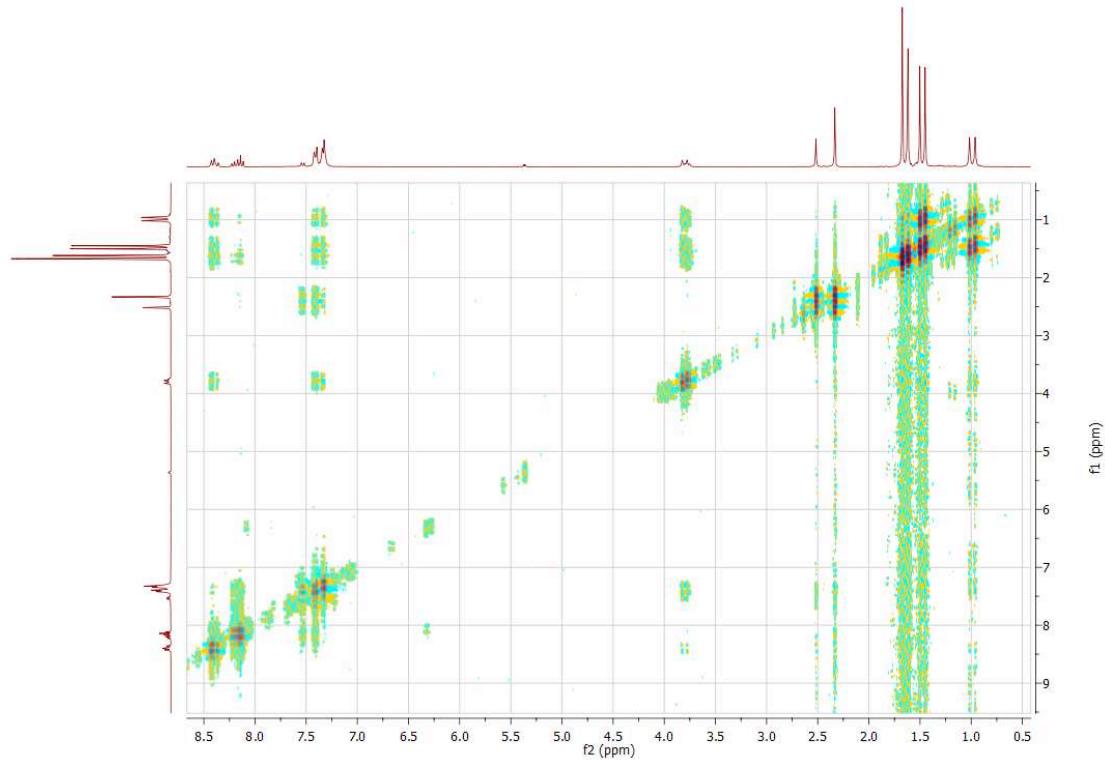


Figure 82. 2D [1H,1H] NOESY NMR spectrum of **5.B(Cl)(Ph)** (300 MHz, 20 °C) in CD_2Cl_2

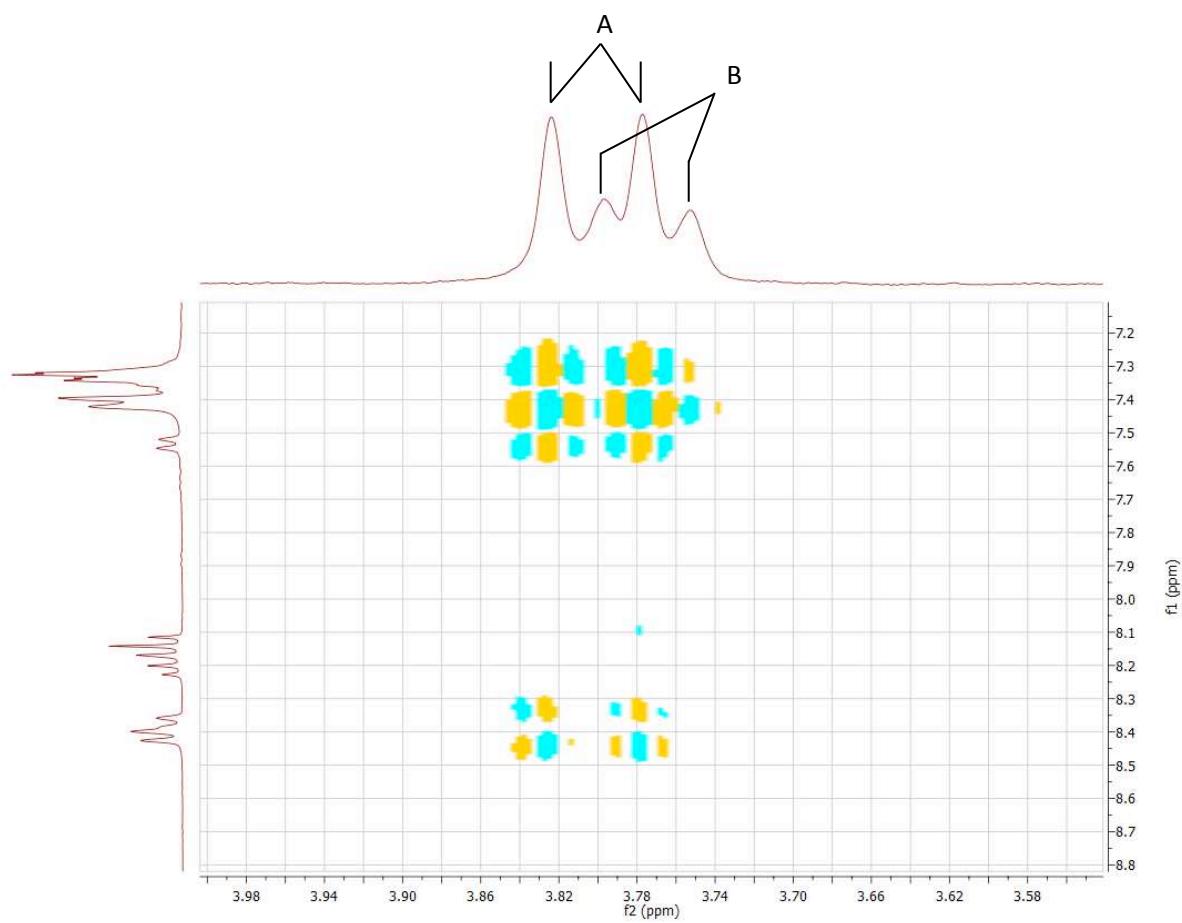


Figure 83. 2D $[1\text{H}, 1\text{H}]$ NOESY NMR spectrum of **5.B(Cl)(Ph)** (300 MHz, 20 °C) in CD_2Cl_2 ; zoom on the B-C(H)-P signals. ^A Signal attributed to the *syn*-**5.B(Cl)(Ph)**; **A**. ^B Signal attributed to the *anti*-**5.B(Cl)(Ph)**; **B**

Isomerization of 5.B(Cl)(Ph) to 3.GaCl₃

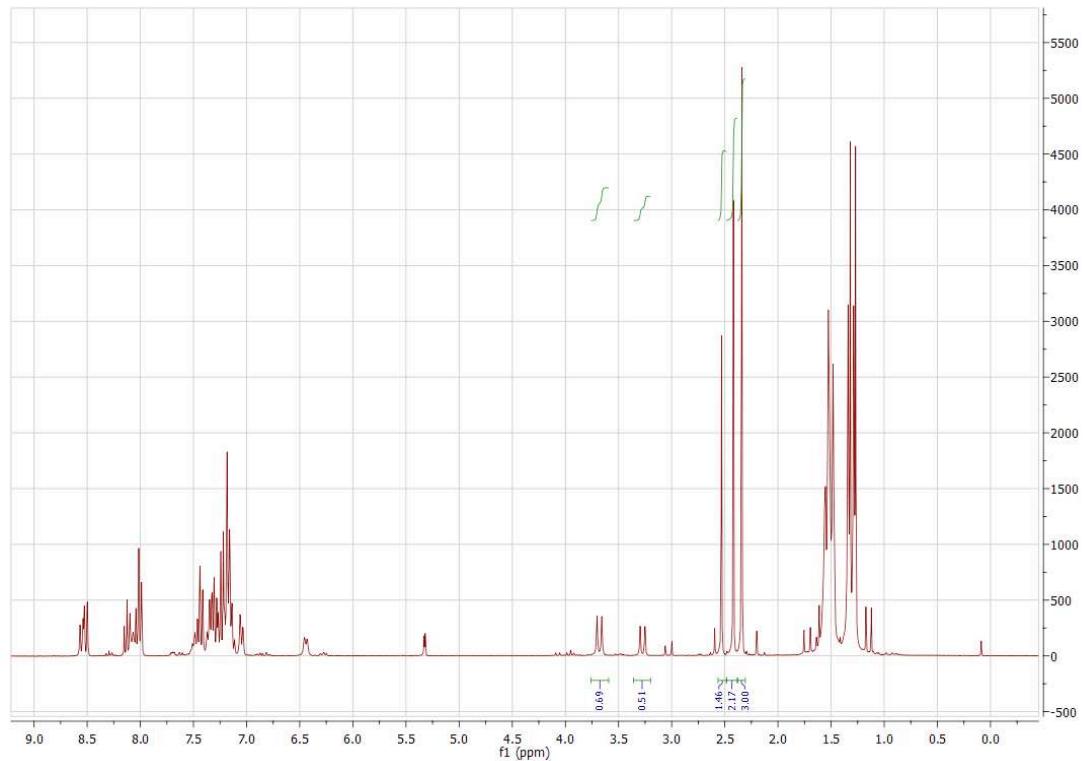


Figure 84. ¹H NMR spectrum of the crude mixture (300 MHz, 20 °C) in CD₂Cl₂

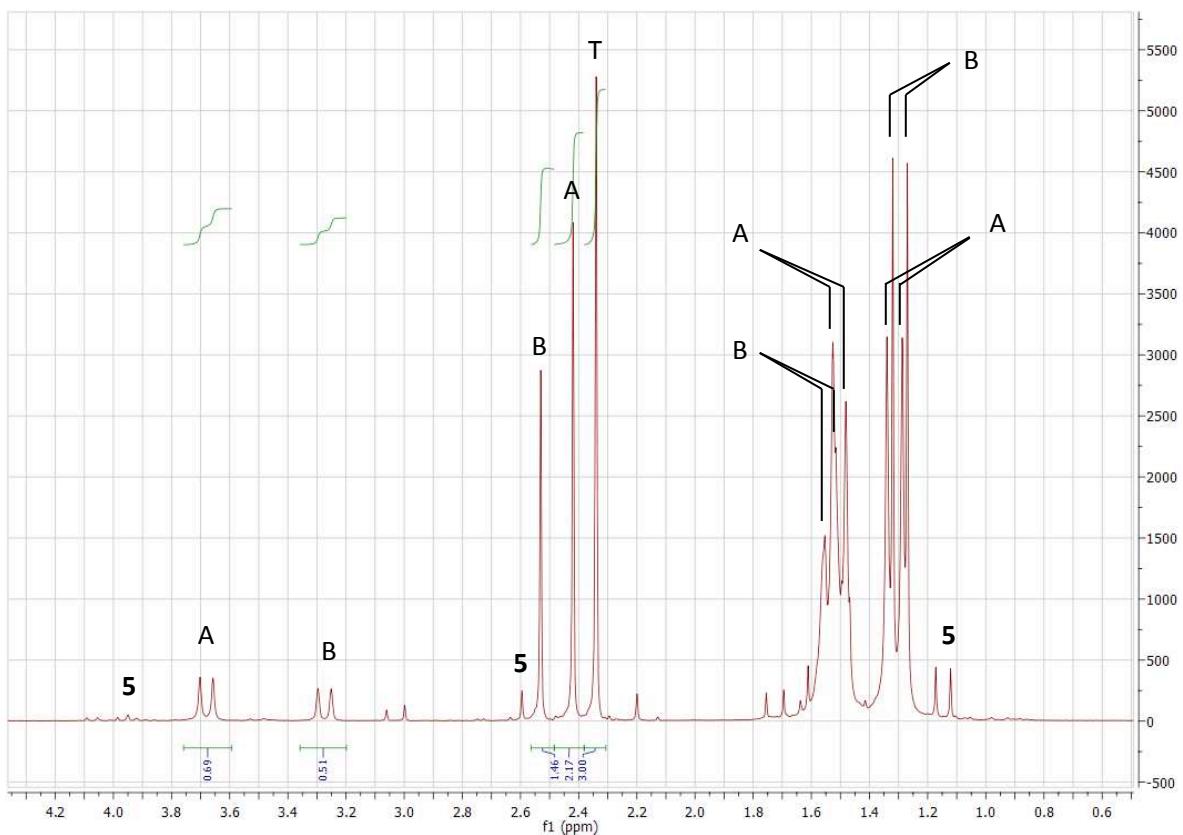


Figure 85. ^1H NMR spectrum of the crude mixture (300 MHz, 20 °C) in CD_2Cl_2 , aliphatic region

^ASignal attributed to *anti*-**3.GaCl₃**

^BSignal attributed to *syn*-**3.GaCl₃**

^TSignal attributed to the CH₃ group of toluene (internal standard)

⁵Signal attributed to compound **4**

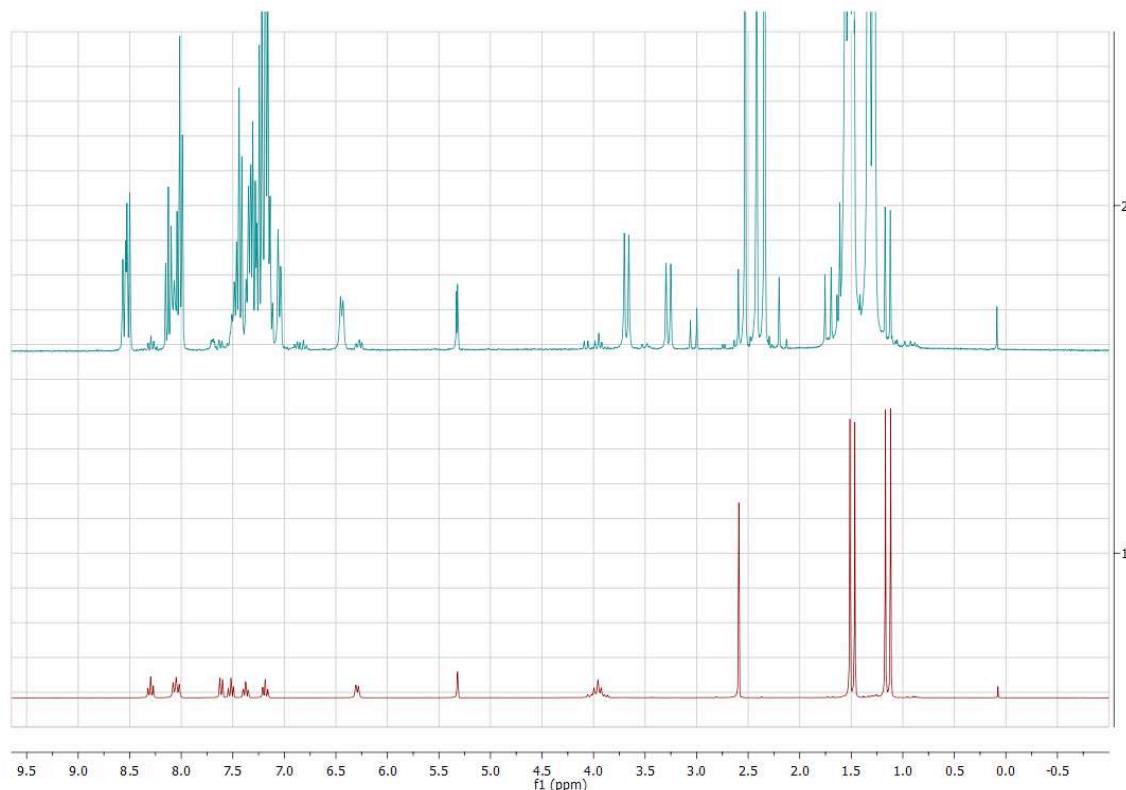


Figure 86. Stacked ^1H NMR spectrum of the crude mixture (top) and ^1H NMR spectrum of **4** (bottom) (300 MHz, 20 °C) in CD_2Cl_2

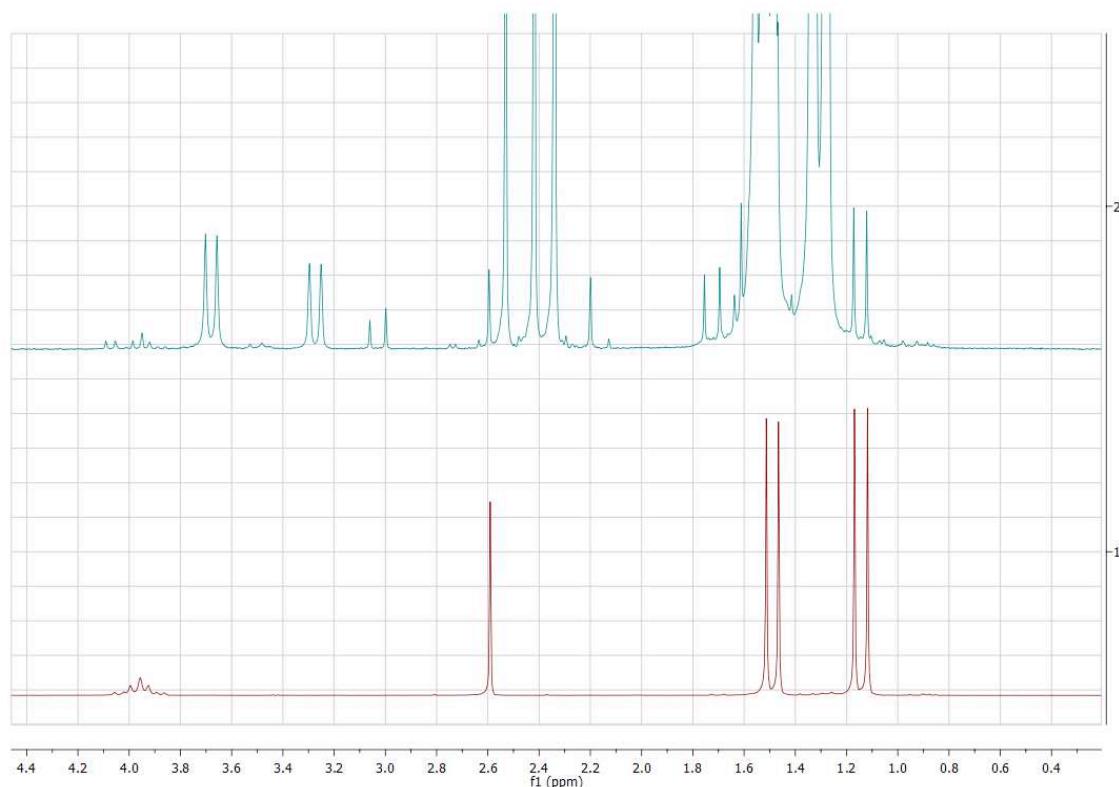


Figure 87. Stacked ^1H NMR spectrum of the crude mixture (top) and ^1H NMR spectrum of **4** (bottom) (300 MHz, 20 °C) in CD_2Cl_2 : aliphatic region

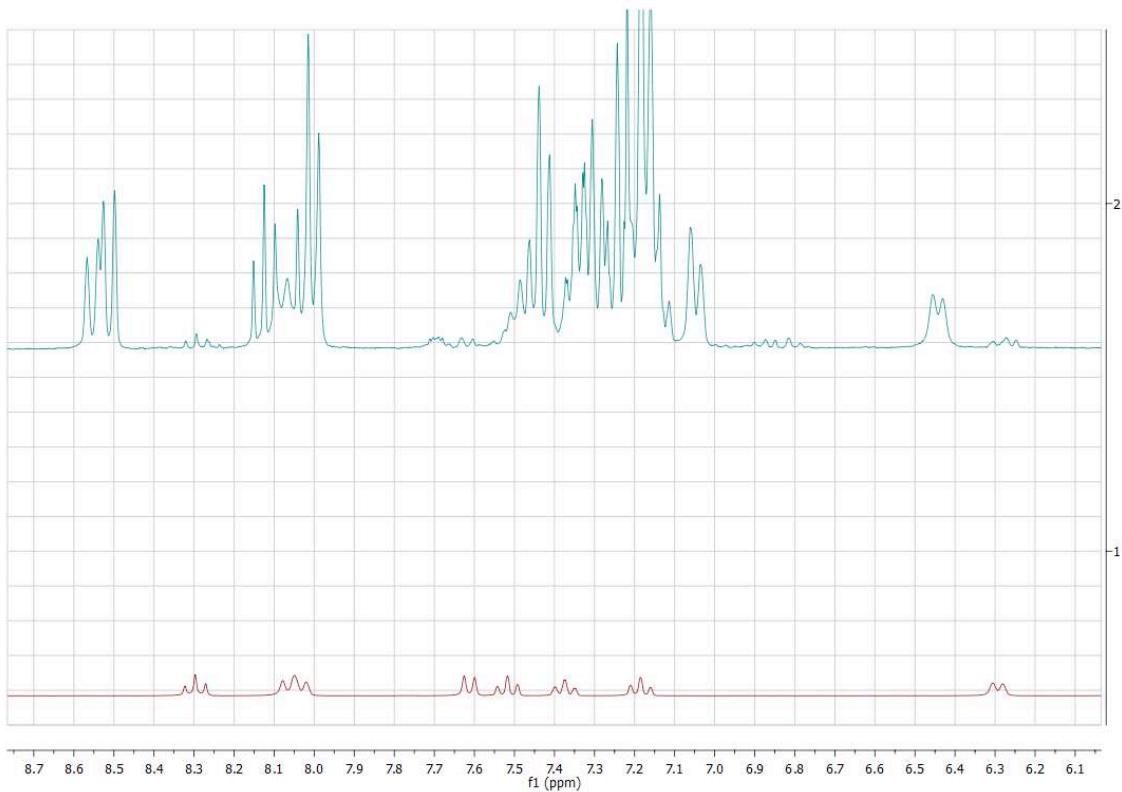


Figure 88. Stacked ^1H NMR spectrum of the crude mixture (top) and ^1H NMR spectrum of **4** (bottom) (300 MHz, 20 °C) in CD_2Cl_2 : aromatic region

NMR spectra of 6

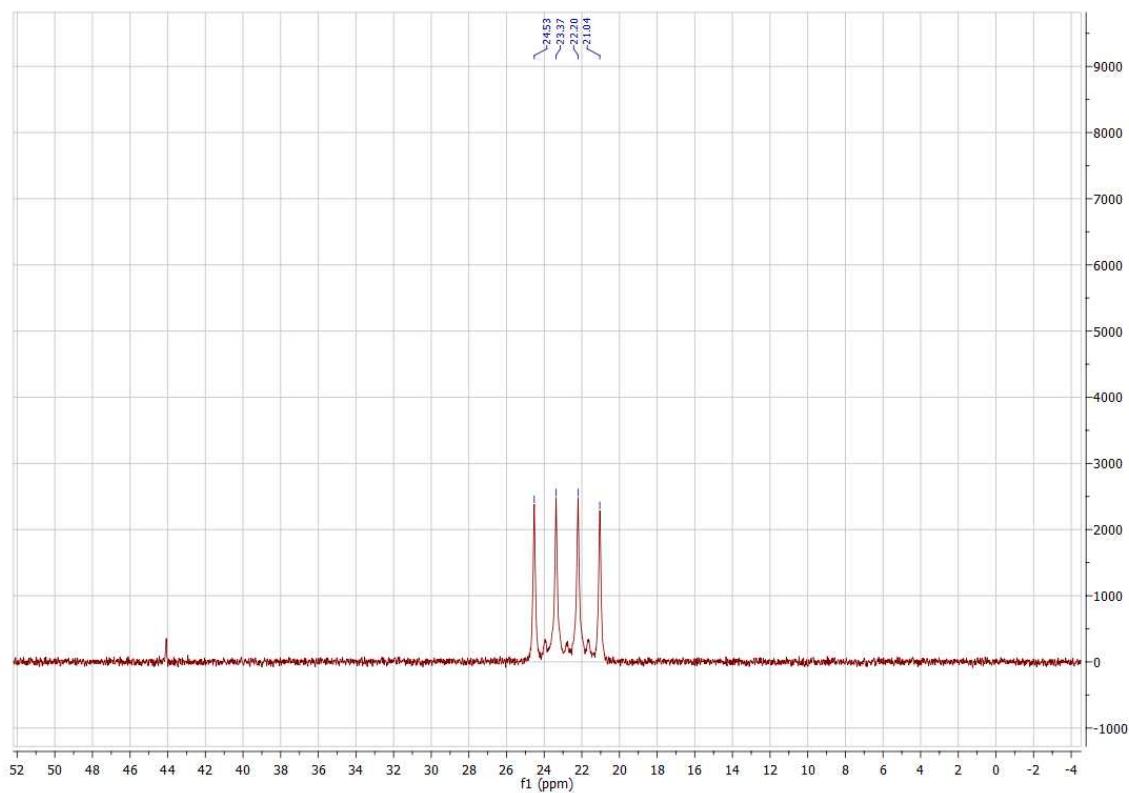


Figure 89. $^{31}\text{P}\{\text{H}\}$ NMR spectrum of **6** (121 MHz, 20 °C) in CD_2Cl_2

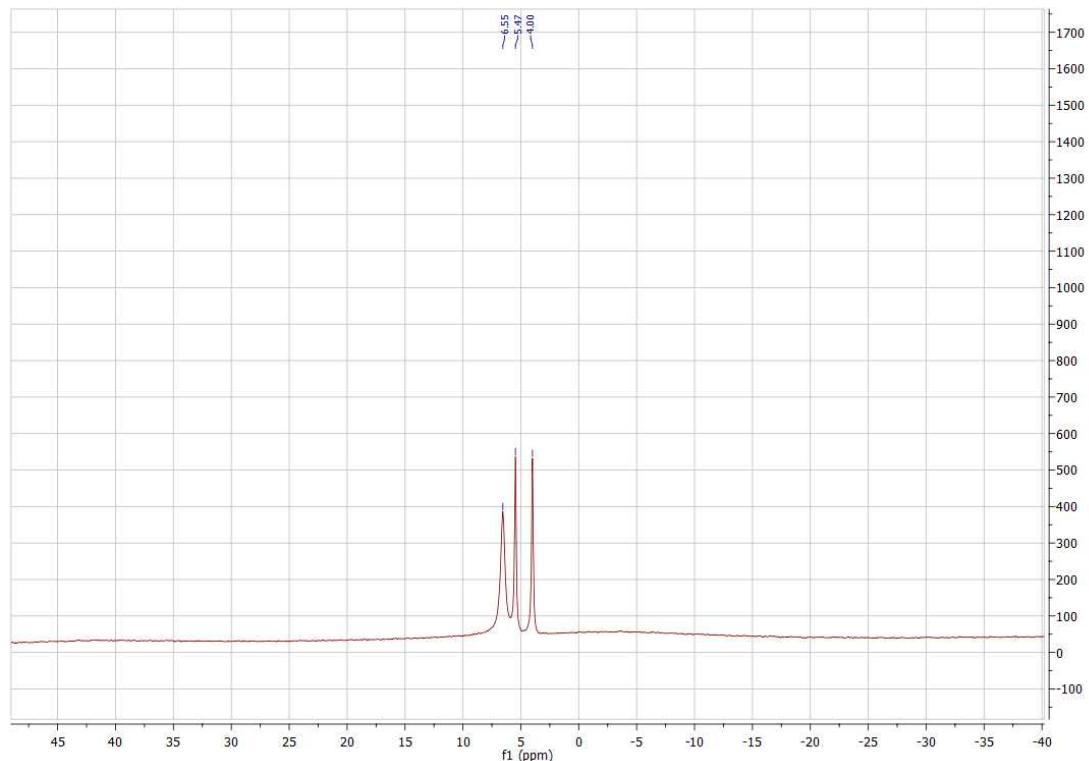


Figure 90. $^{11}\text{B}\{\text{H}\}$ NMR spectrum of **6** (96 MHz, 20 °C) in CD_2Cl_2

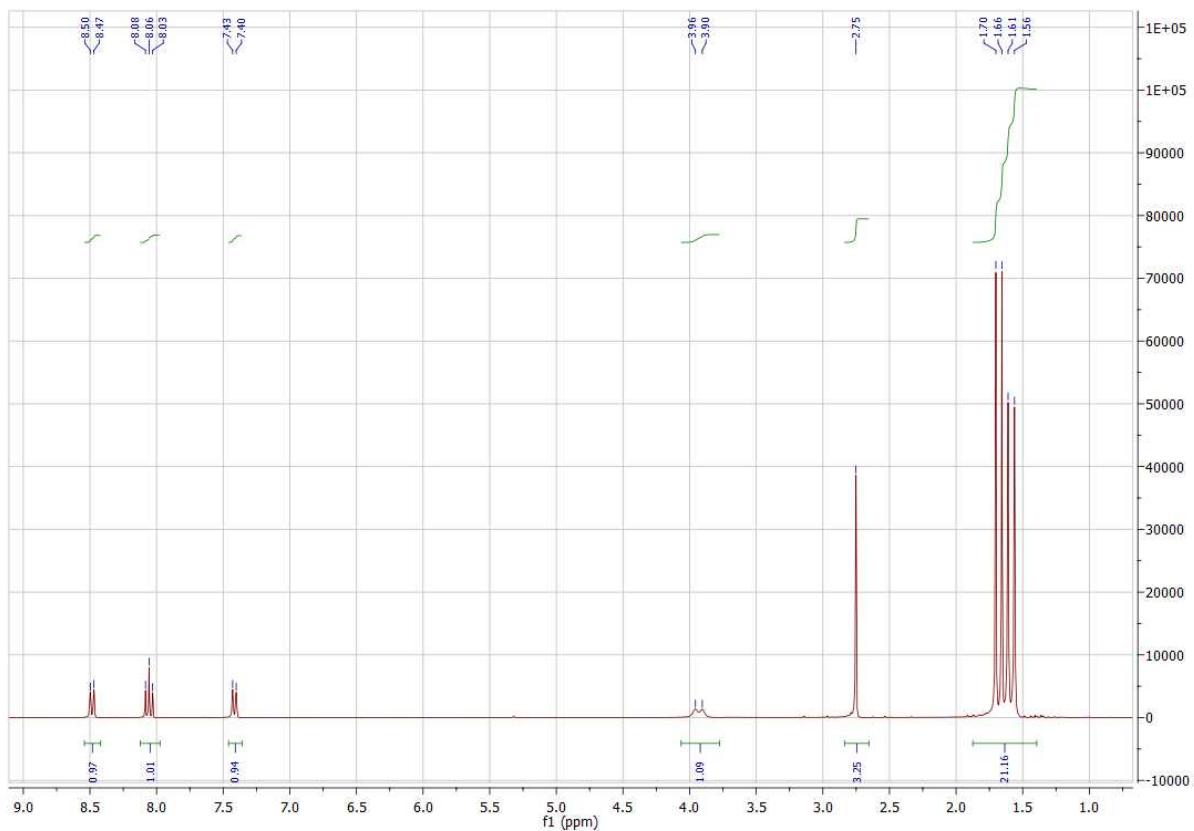


Figure 91. ^1H NMR spectrum of **6** (300 MHz, 20 °C) in CD_2Cl_2

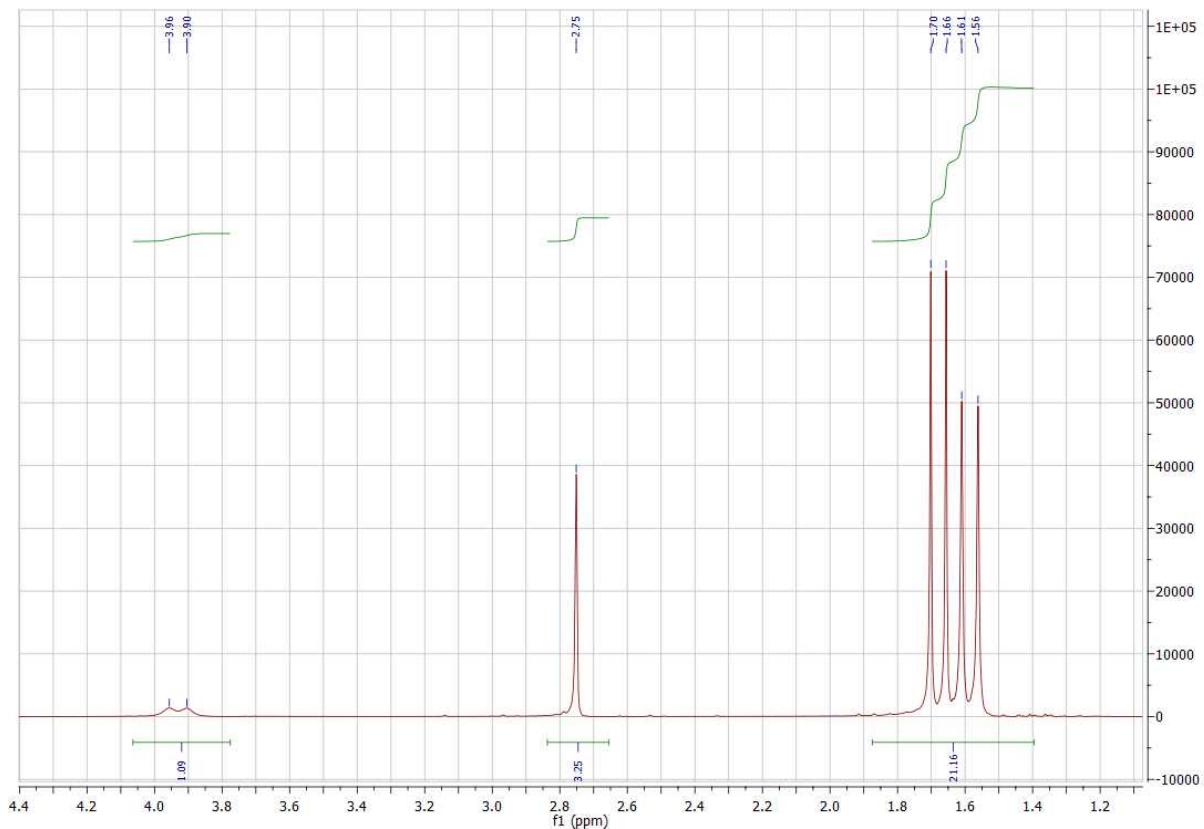


Figure 92. ^1H NMR spectrum of **6** (300 MHz, 20 °C) in CD_2Cl_2 , aliphatic region

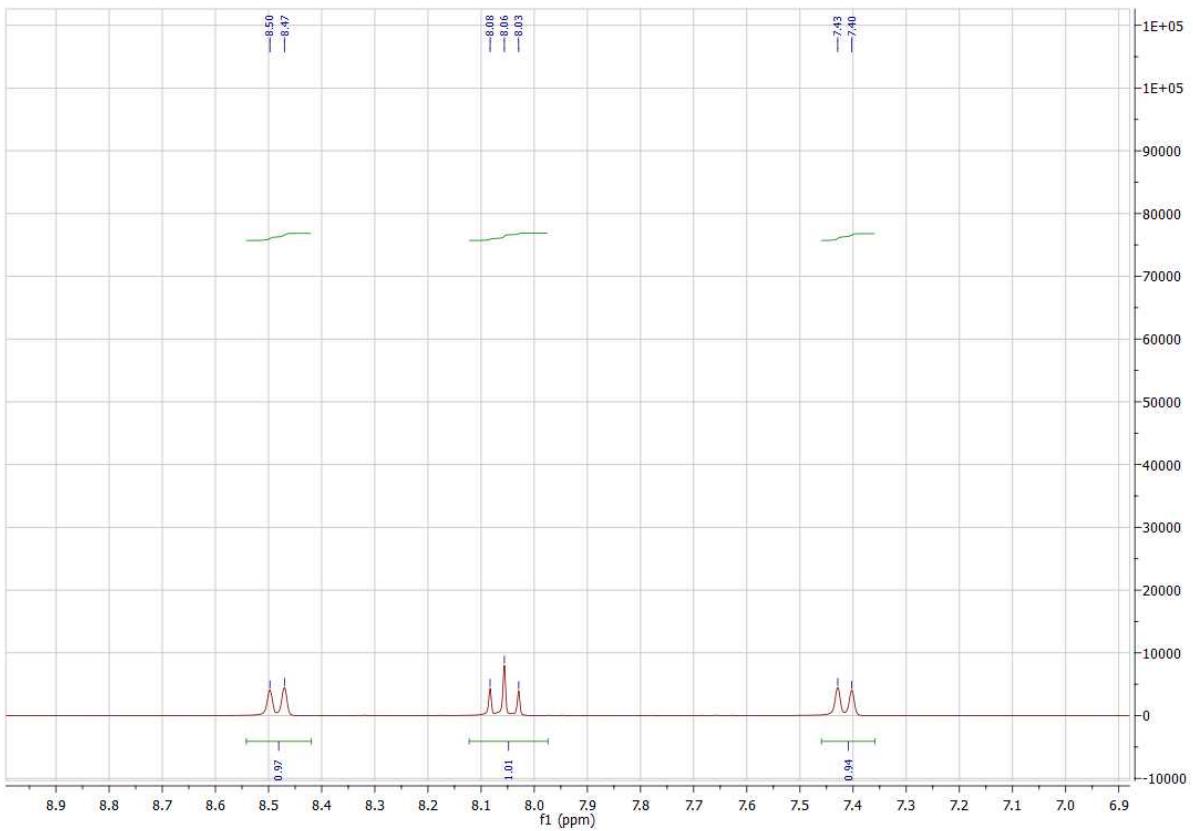


Figure 93. ^1H NMR spectrum of **6** (300 MHz, 20 °C) in CD_2Cl_2 , aromatic region

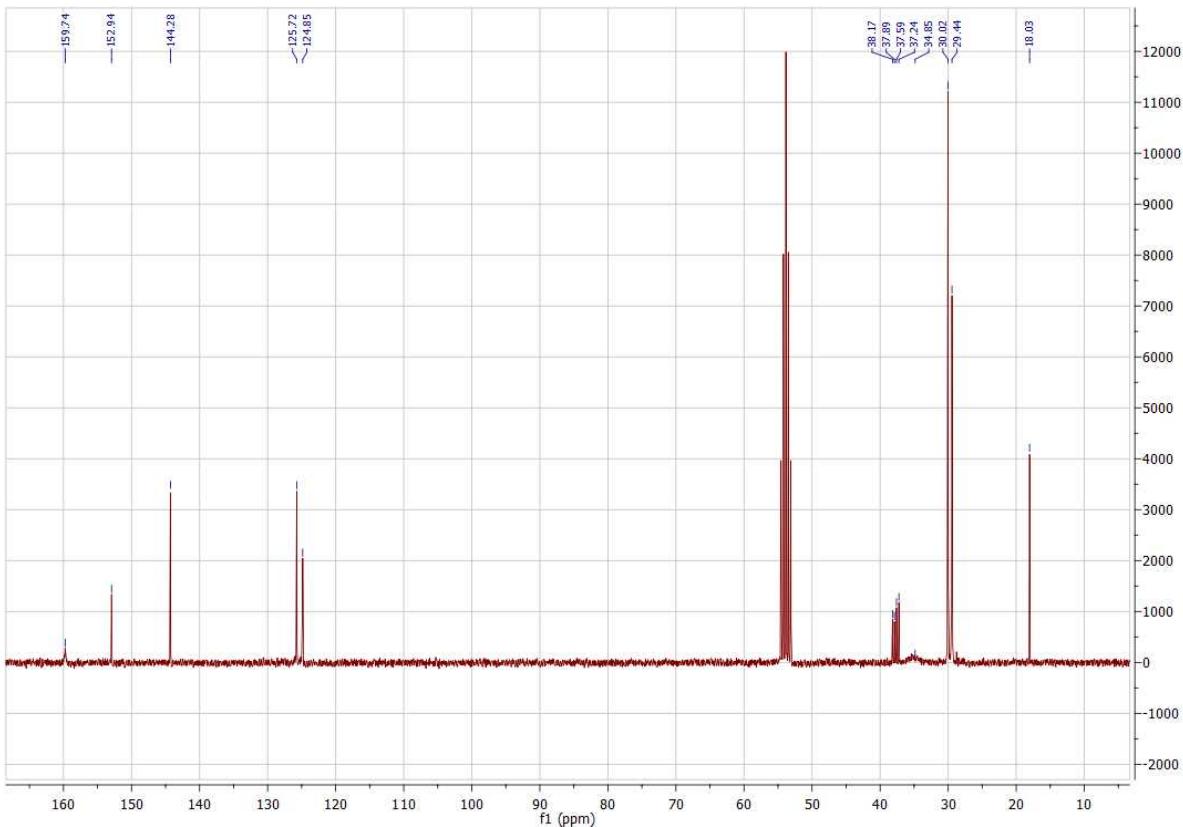


Figure 94. $^{13}\text{C}\{\text{H}\}$ NMR spectrum of **6** (75 MHz, 20 °C) in CD_2Cl_2

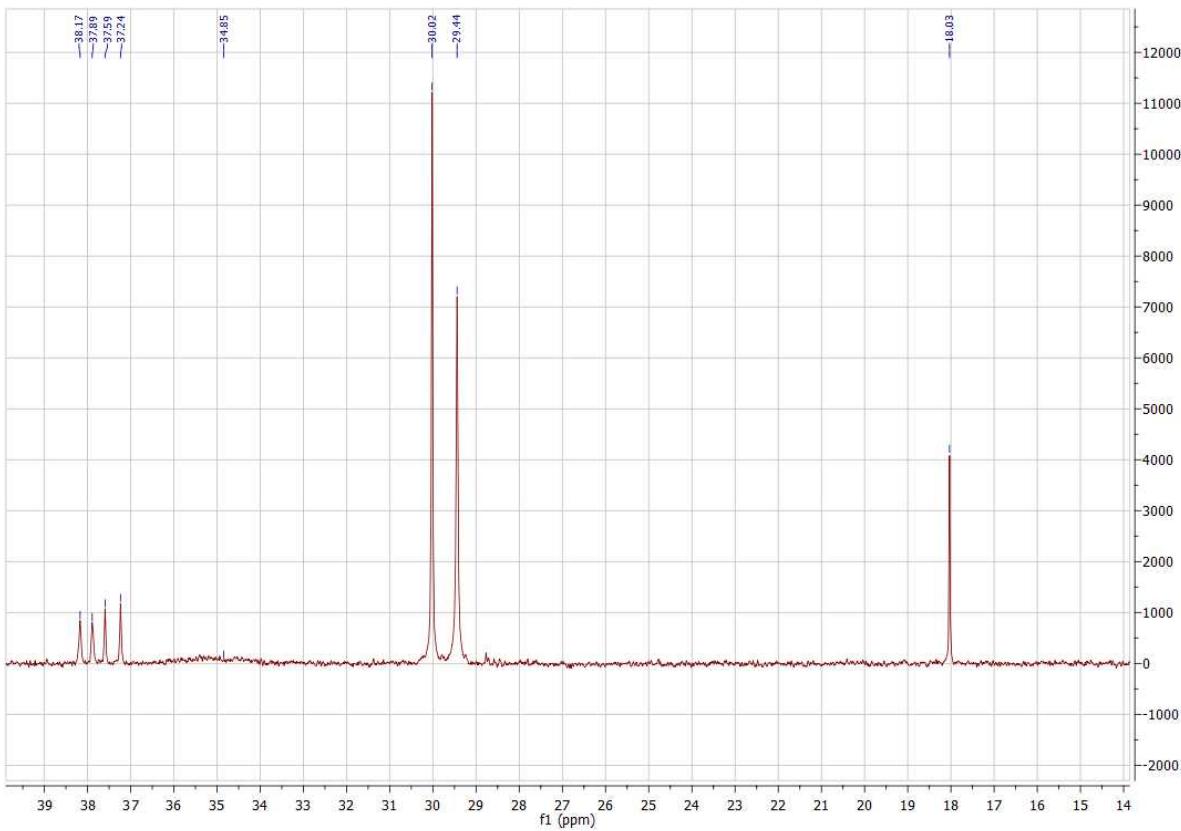


Figure 95. $^{13}\text{C}\{\text{H}\}$ NMR spectrum of **6** (75 MHz, 20 °C) in CD_2Cl_2 , aliphatic region

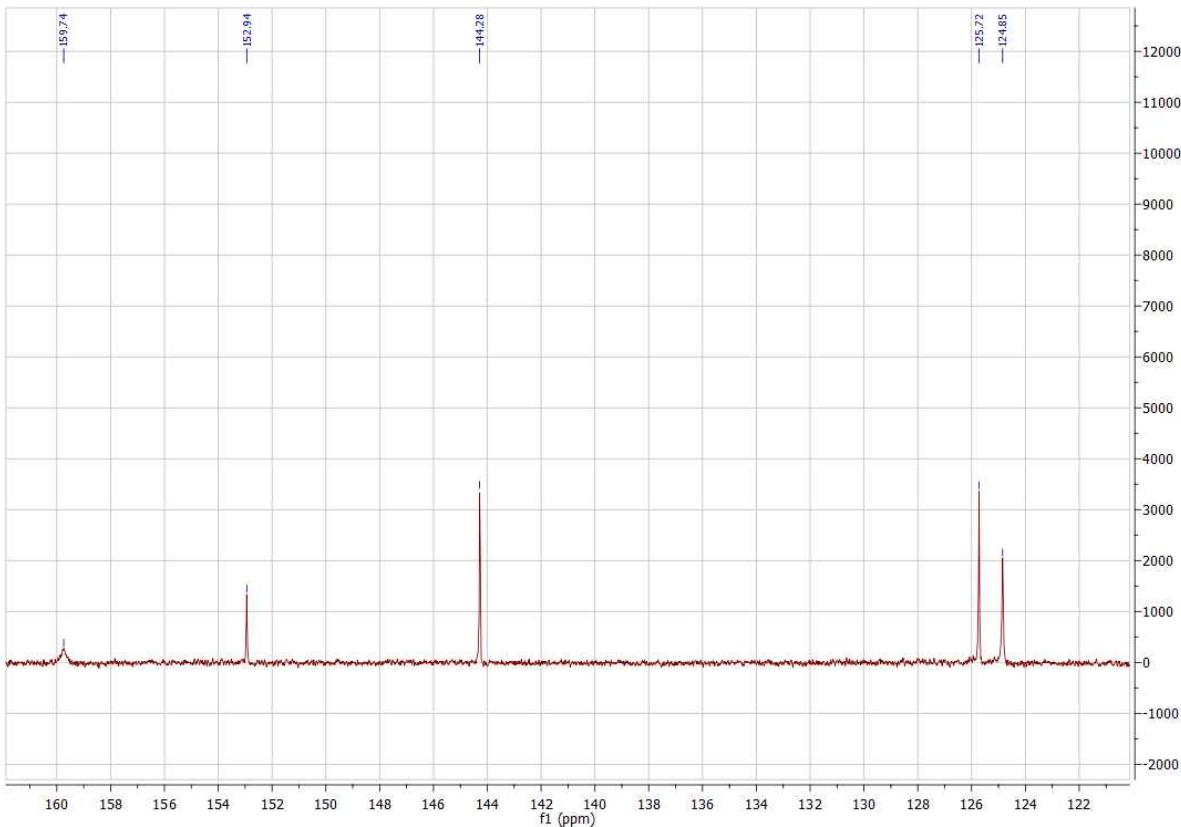


Figure 96. $^{13}\text{C}\{\text{H}\}$ NMR spectrum of **6** (75 MHz, 20 °C) in CD_2Cl_2 , aromatic region

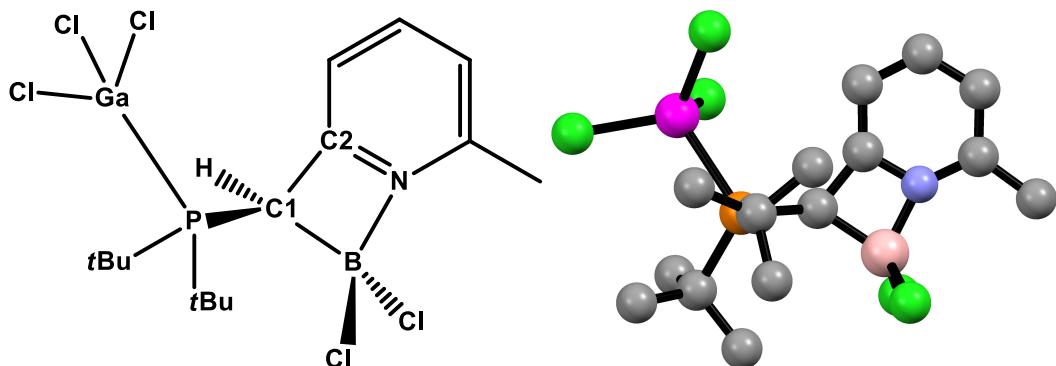
Computational Details

1) Relative energies of the 4 structural isomers **5.B(Cl)(Ph)** and **3.GaCl₃**

	DH (Hartree)	Relative DH (kcal.mol ⁻¹)
<i>anti</i> -5.B(Cl)(Ph)	-966.09945	1.5
<i>syn</i> -5.B(Cl)(Ph)	-966.10176	0
<i>anti</i> -3.GaCl ₃	-966.0978	2.5
<i>syn</i> -3.GaCl ₃	-966.09193	6.2

2) MO analysis and NBO calculations on **5.BCl₂**

Both Molecular Orbital analysis and Natural Bond Orbital (NBO) calculations were carried out to study the bonding of the atoms involved in the 4-membered ring of the structure.



	Distance (Å) from XRD analysis	Distance (Å) from DFT calculations	Occupancy of the natural bonding orbital	Wiberg bond index
B-N	1.586(3)	1.61	1.96	0.58
B-C1	1.682(3)	1.69	1.95	0.77
C2-N	1.352(3)	1.35	1.97	1.25
C1-C2	1.516(4)	1.5	1.97	1.03

Atomic charge from the natural population analysis

B	+0.4
N	-0.5
C2	+0.3
C1	-0.9

3) Z-matrices

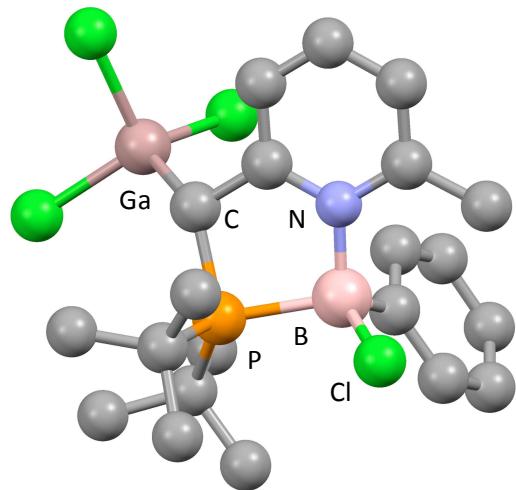
Compound 1

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15	2.523320000	3.457604000	14.067084000
7	1.762598000	1.688156000	11.665640000
6	1.775670000	3.976165000	12.510486000
1	1.540977000	5.019724000	12.333681000
6	1.499036000	3.051910000	11.513010000
6	0.923223000	3.485938000	10.267105000
1	0.713980000	4.544439000	10.150690000
6	0.652794000	2.599081000	9.270226000
1	0.218319000	2.944739000	8.335421000
6	0.936911000	1.223047000	9.452614000
1	0.731397000	0.496395000	8.675441000
6	1.480981000	0.815674000	10.645606000
6	1.796355000	-0.632935000	10.881731000
1	1.483024000	-1.237148000	10.027938000
1	1.278157000	-1.016494000	11.768424000
1	2.870536000	-0.788867000	11.029356000
6	4.243921000	4.394820000	14.166445000
6	5.130773000	3.709535000	13.121407000
1	6.085947000	4.245608000	13.051511000
1	4.661713000	3.728970000	12.132214000
1	5.347837000	2.671398000	13.382262000
6	4.095555000	5.868072000	13.775836000
1	3.505137000	6.445034000	14.490528000
1	3.641226000	5.967885000	12.785833000

1	5.092933000	6.324296000	13.729524000
6	4.869984000	4.262043000	15.554632000
1	4.927409000	3.219332000	15.882386000
1	4.324830000	4.831667000	16.312709000
1	5.893959000	4.656107000	15.528858000
6	1.328209000	3.978134000	15.529157000
6	-0.075887000	3.543454000	15.097765000
1	-0.788593000	3.799686000	15.892090000
1	-0.141478000	2.465656000	14.927361000
1	-0.383120000	4.048718000	14.178000000
6	1.328334000	5.488500000	15.768560000
1	0.563554000	5.733644000	16.517173000
1	1.085260000	6.044942000	14.857905000
1	2.285376000	5.850000000	16.153702000
6	1.738267000	3.233071000	16.803132000
1	2.725505000	3.532339000	17.163999000
1	1.746100000	2.149819000	16.651894000
1	1.016850000	3.451895000	17.600906000
6	4.228528000	0.160344000	13.311838000
1	4.866125000	0.603890000	12.535110000
1	4.051795000	-0.873172000	12.976166000
6	4.994196000	0.094387000	14.642574000
1	5.931714000	-0.470335000	14.558601000
1	4.401763000	-0.388295000	15.428714000
1	5.258546000	1.090195000	15.017463000
6	1.047849000	0.046341000	14.402895000
1	0.860678000	0.537086000	15.367556000

1	0.093368000	0.128322000	13.861497000
6	1.354733000	-1.434927000	14.679571000
1	2.259217000	-1.553317000	15.286549000
1	1.522830000	-2.008181000	13.759850000
1	0.539039000	-1.934274000	15.218400000

anti-3.GaCl₃



Ga 8.452836 6.111389 6.357727

Cl 6.662118 4.845230 6.716983

Cl 10.190398 4.973915 5.539710

Cl 9.186864 6.977356 8.302570

Cl 5.757029 9.840473 2.087173

P 7.952535 7.852872 3.280358

N 5.857852 8.902360 4.805750

C 7.645509 5.029114 2.910186

C 7.647838 6.474205 0.862285

C 9.797387 5.964017 2.051037

C 8.302129 6.231593 2.229937

C 8.774572 10.562827 3.599568

C 9.268863 9.564542 1.354698

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C 9.233933 9.297868 2.862298

C 4.560720 6.325203 4.034760

C 3.626601 5.311138 3.828535

C 2.997582 5.180770 2.591611

C 3.308855 6.074712 1.568229
C 4.244565 7.086108 1.781088
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C 4.747124 9.567663 5.264713
C 4.704526 10.011887 6.577145
C 5.775889 9.781998 7.434541
C 6.867581 9.074431 6.972757
C 6.893662 8.611430 5.653089
C 8.049740 7.810395 5.160601
B 5.958760 8.406054 3.289245
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H 9.917095 10.430460 1.173165
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H 10.662373 8.689940 4.433008

H 11.074578 8.084609 2.826853

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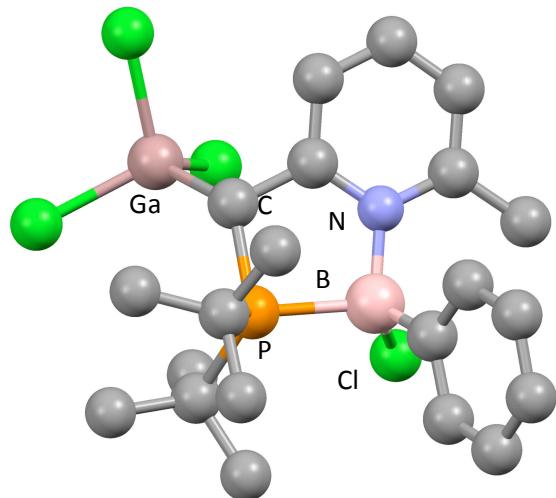
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syn-3.GaCl₃



Ga 8.375845 6.215926 6.351854

Cl 4.876221 7.121359 2.718764

Cl 6.513708 5.046310 6.638340

Cl 10.120936 5.017614 5.637940

Cl 9.071757 7.108158 8.300946

P 7.984485 7.898226 3.226866

N 5.793612 8.857500 4.722031

C 5.551335 12.228246 1.839378

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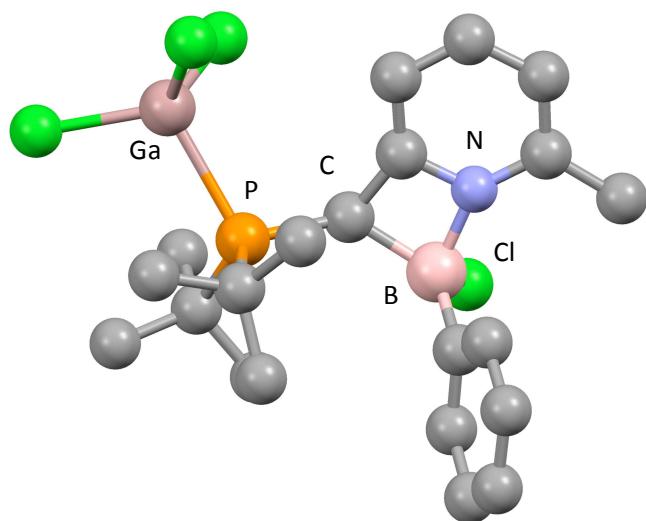
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anti-5.BClPh



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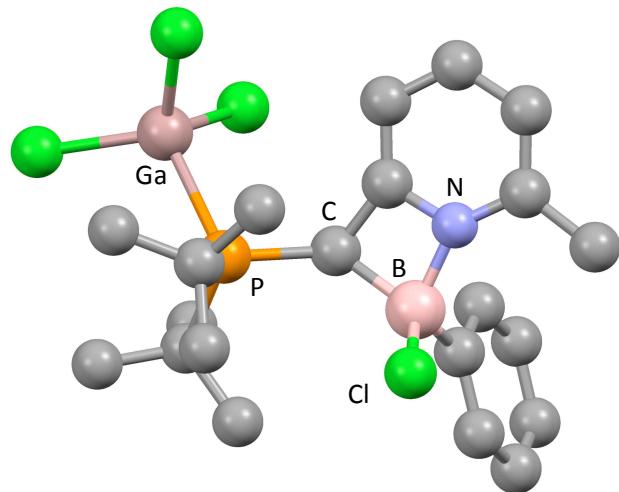
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syn-**5.BClPh**



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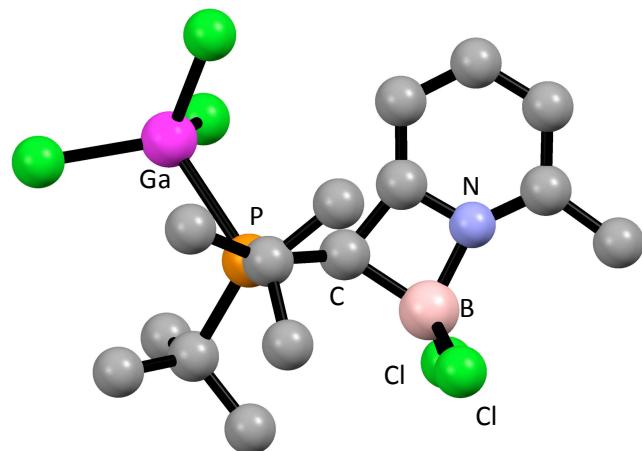
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5.BCl₂



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