

Supporting Information

Insight into the Steric and Electronic Effects of Ancillary Ligands: Synthesis and Structure–Reactivity Relationship of Well-defined, Air- and Moisture-stable (NHC)Pd(sal)Cl complexes (sal = Salicylaldimine)

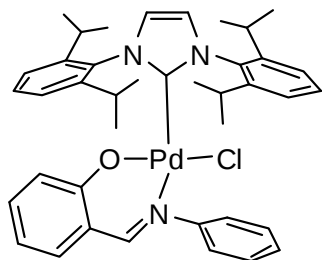
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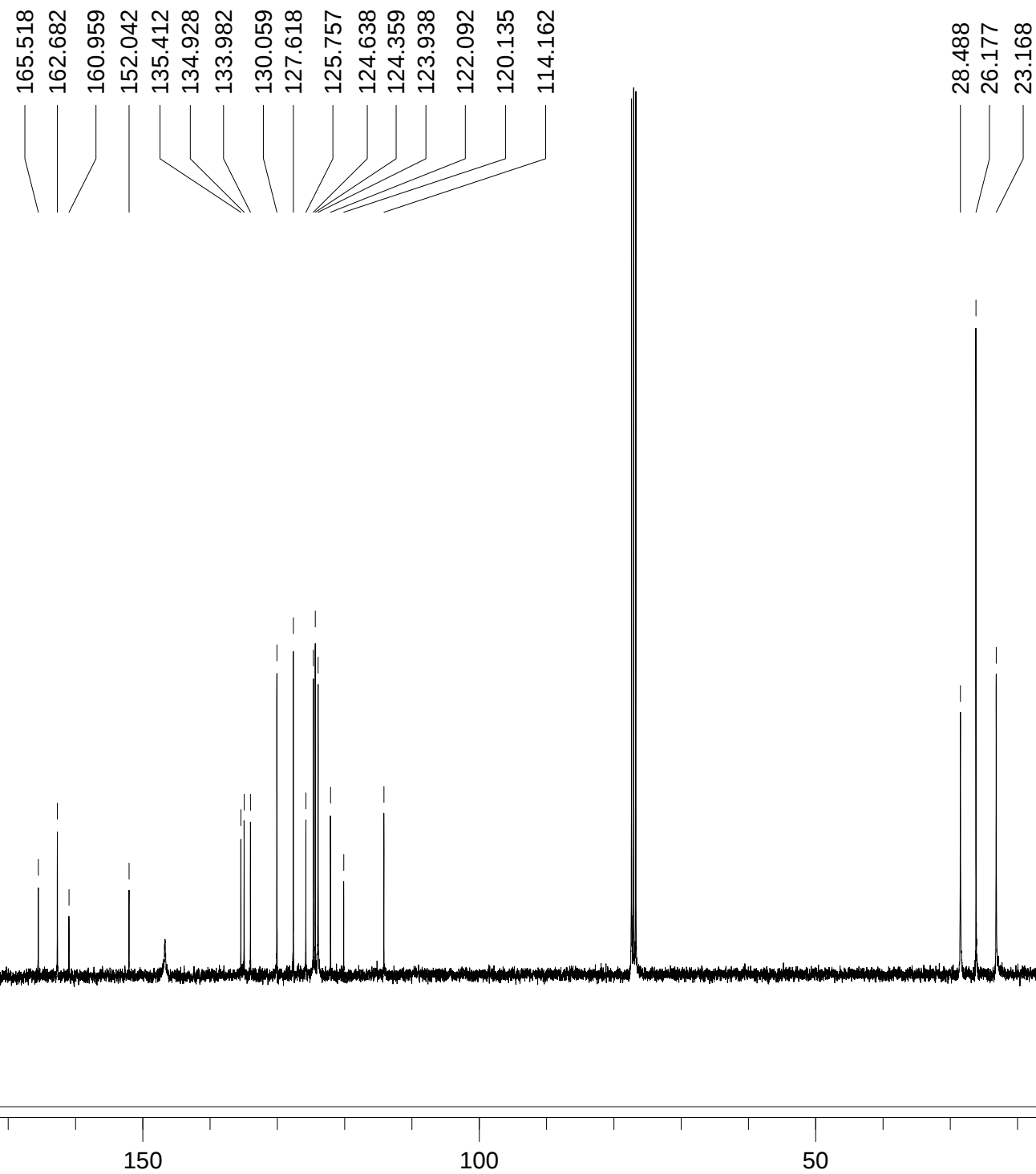
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Table 1. Crystal Data and Summary of X-ray Data Collection for complex **1a–c**, **2a–c**, and **5b**

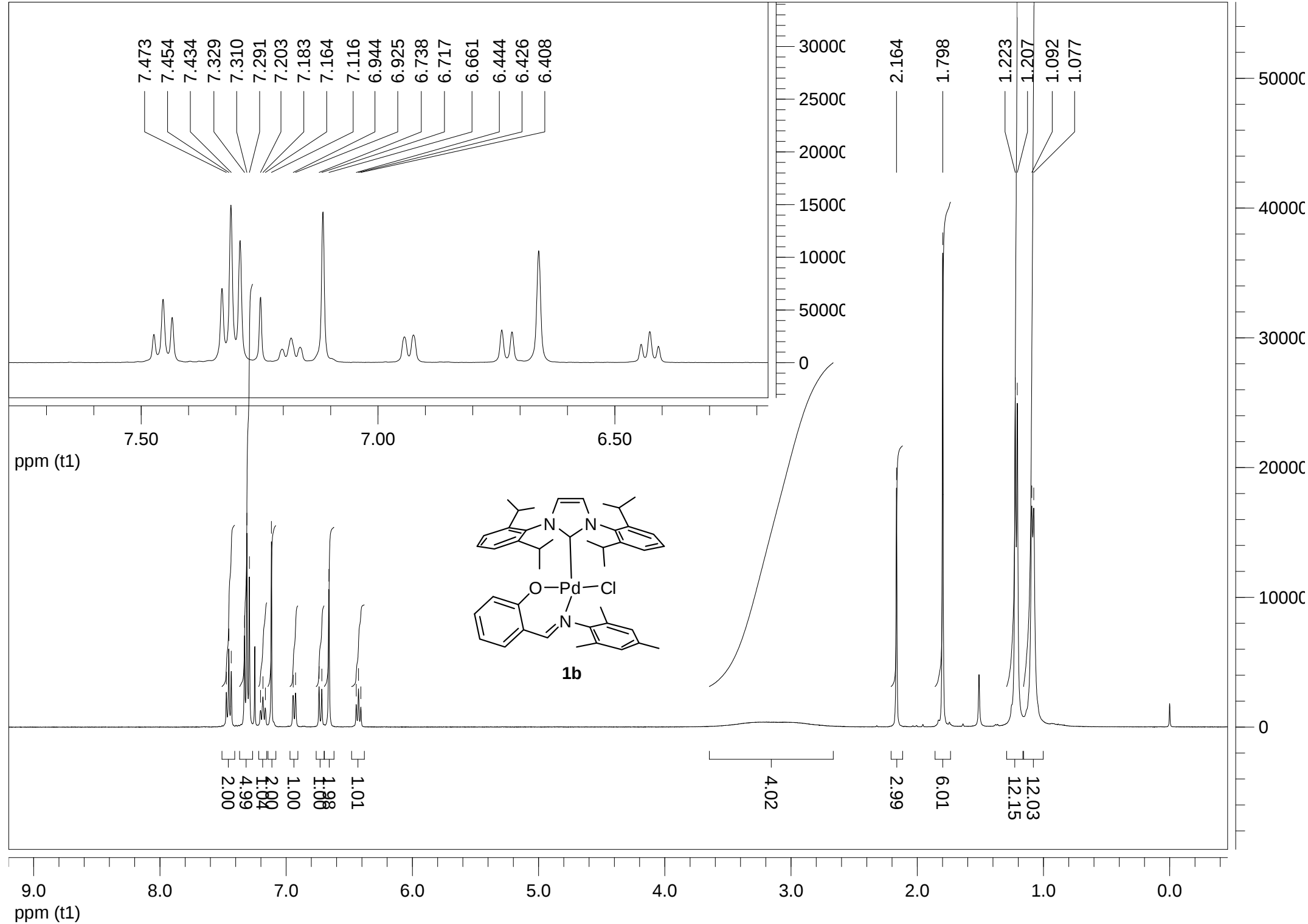
	1a	1b	1c	2a	2b	2c	5b
formula	C ₄₀ H ₄₆ ClN ₃ OPd	C ₄₃ H ₅₂ ClN ₃ OPd	C ₄₆ H ₅₈ ClN ₃ OPd	C ₄₀ H ₄₈ ClN ₃ OPd	C ₄₃ H ₅₄ ClN ₃ OPd	C ₄₆ H ₆₀ ClN ₃ OPd	C ₄₂ H ₅₀ ClF ₆ N ₃ OPd
fw	726.65	768.73	810.80	728.66	770.74	812.82	838.48
cryst syst	Monoclinic	Monoclinic	Triclinic	Monoclinic	Monoclinic	Triclinic	Triclinic
space group	<i>P</i> 2 ₁ / <i>n</i>	<i>P</i> 12 ₁ / <i>m</i> 1	<i>P</i> [−] 1	<i>P</i> 2 ₁ / <i>n</i>	<i>P</i> 2 ₁ / <i>c</i>	<i>P</i> [−] 1	<i>P</i> [−] 1
<i>a</i> (Å)	12.0410 (10)	10.455 (4)	11.3608 (8)	12.112 (2)	24.795 (2)	11.2600 (10)	11.010 (4)
<i>b</i> (Å)	14.123 (3)	17.283 (6)	12.4600 (10)	14.188 (2)	14.9470 (10)	12.4340 (12)	11.797 (5)
<i>c</i> (Å)	21.275 (4)	11.175 (4)	15.9450 (14)	21.125 (3)	21.1820 (16)	15.9760 (14)	17.681 (7)
<i>α</i> (deg)	90	90	84.306 (8)	90	90	84.330 (9)	100.061 (4)
<i>β</i> (deg)	101.433 (7)	98.818 (5)	69.835 (6)	101.620 (6)	91.080 (3)	70.865 (8)	105.612 (3)
<i>γ</i> (deg)	90	90	81.668 (8)	90	90	82.210 (10)	107.596 (4)
<i>V</i> (Å ³)	3546.1 (10)	1995.4 (13)	2093.4 (3)	3555.8 (9)	7848.9 (10)	2090.1 (3)	2024.6 (14)
<i>Z</i>	4	2	2	4	8	2	2
<i>D</i> _{calcd} (g cm ^{−3})	1.361	1.279	1.286	1.361	1.304	1.292	1.375
<i>μ</i> (mm ^{−1})	0.63	0.57	0.54	0.63	0.58	0.55	0.59
<i>F</i> (000)	1512	804	852	1520	3232	856	836
cryst size (mm)	0.20 × 0.14 × 0.06	0.22 × 0.18 × 0.16	0.20 × 0.18 × 0.16	0.24 × 0.22 × 0.16	0.18 × 0.16 × 0.14	0.22 × 0.18 × 0.16	0.20 × 0.20 × 0.20
<i>θ</i> range (deg)	1.74 to 25.00	1.84 to 27.88	1.36 to 27.88	1.74 to 27.88	1.64 to 27.91	1.66 to 27.86	1.89 to 27.89
no. of reflns collected	26164	18636	19419	31830	62267	16473	26201
no. of indep reflns/ <i>R</i> _{int}	6243/0.068	4917/0.036	9814/0.027	8427/0.063	18652/0.046	9678/0.036	9617/0.054
no. of params	423	250	481	423	905	481	482
goodness-of-fit on <i>F</i> ²	1.204	1.025	1.032	0.981	1.111	1.112	1.616
<i>R</i> ₁ , <i>wR</i> ₂ (<i>I</i> > 2 σ (<i>I</i>))	0.0587, 0.1009	0.0301, 0.0660	0.0321, 0.0740	0.0447, 0.1033	0.0398, 0.0838	0.0532, 0.0990	0.0354, 0.0753
<i>R</i> ₁ , <i>wR</i> ₂ (all data)	0.0656, 0.1035	0.0373, 0.0686	0.0387, 0.0768	0.0614, 0.1095	0.0455, 0.0864	0.0616, 0.1033	0.0402, 0.0773

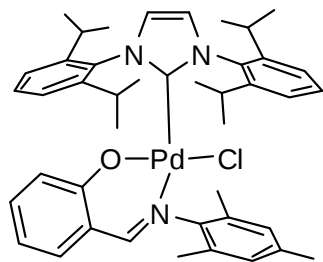


1a



ppm (t1)





1b

165.142
163.077
162.819
147.916
135.394
134.849
134.296
133.831
130.585
129.818
127.886
124.493
123.884
123.788
122.093
119.501
113.653

28.479
26.265
23.270
21.013
18.388

20000

15000

10000

50000

0

200

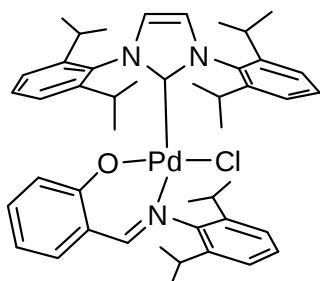
150

100

50

0

ppm (t1)



1c

165.234
163.091
162.563
147.581
140.971
135.356
135.065
133.886
129.830
126.063
124.557
122.358
122.282
118.554
113.665

28.136
26.365
24.052
22.595

30000

25000

20000

15000

10000

50000

0

200

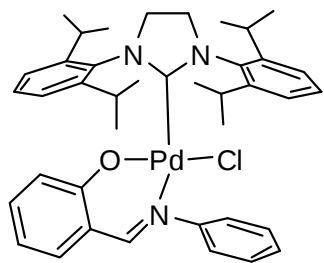
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100

50

0

ppm (t1)

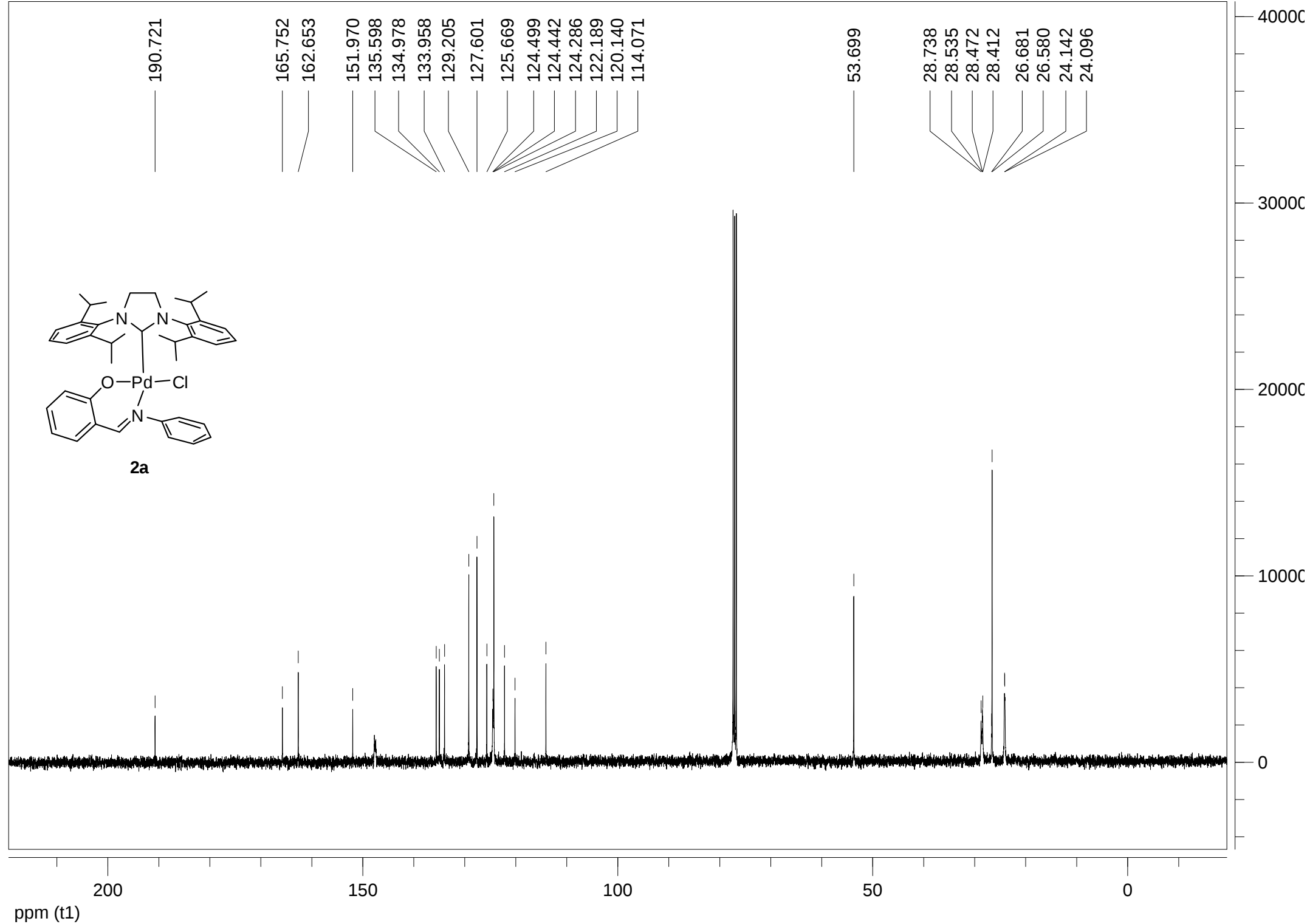


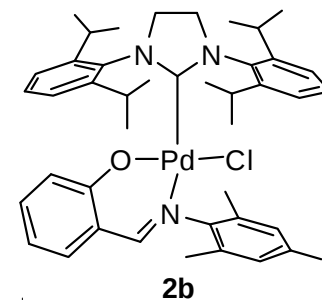
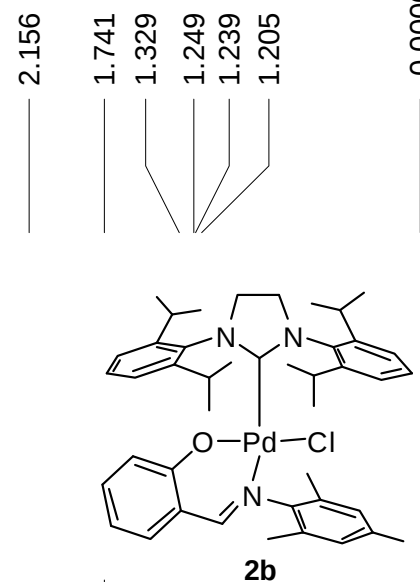
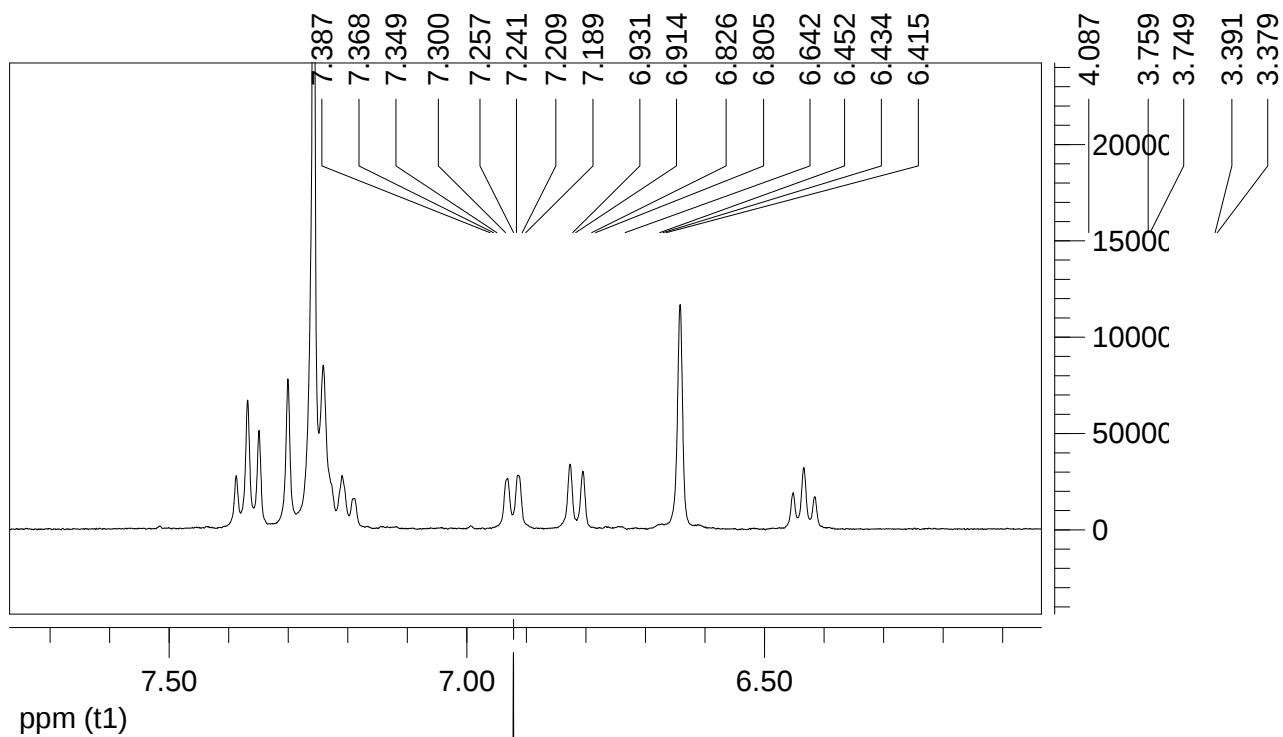
2a

190.721
165.752
162.653
151.970
135.598
134.978
133.958
129.205
127.601
125.669
124.499
124.442
124.286
122.189
120.140
114.071

53.699

28.738
28.535
28.472
28.412
26.681
26.580
24.142
24.096

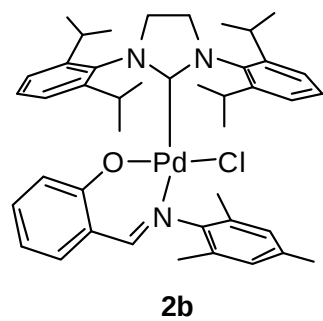




10.0
ppm (t1)

5.0

0.0



192.415
165.335
163.070
147.815
135.580
134.847
134.221
133.829
130.523
129.001
127.847
124.476
124.444
122.100
119.622
113.604

53.588
28.674
28.453
28.404
26.592
24.206
24.111
24.074
20.960
18.297
0.0000

50000

0

ppm (t1)

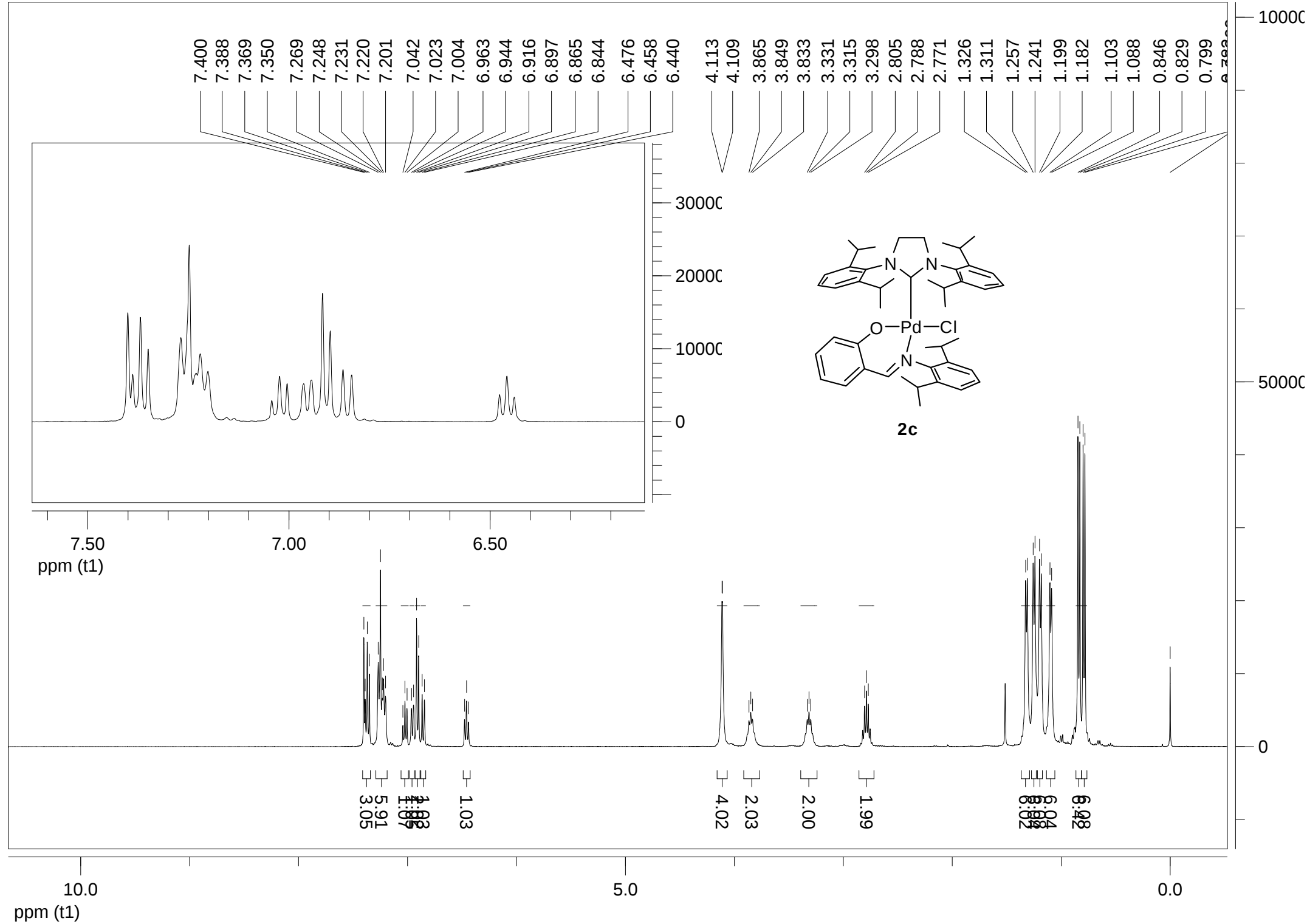
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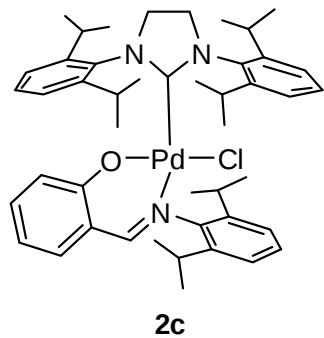
150

100

50

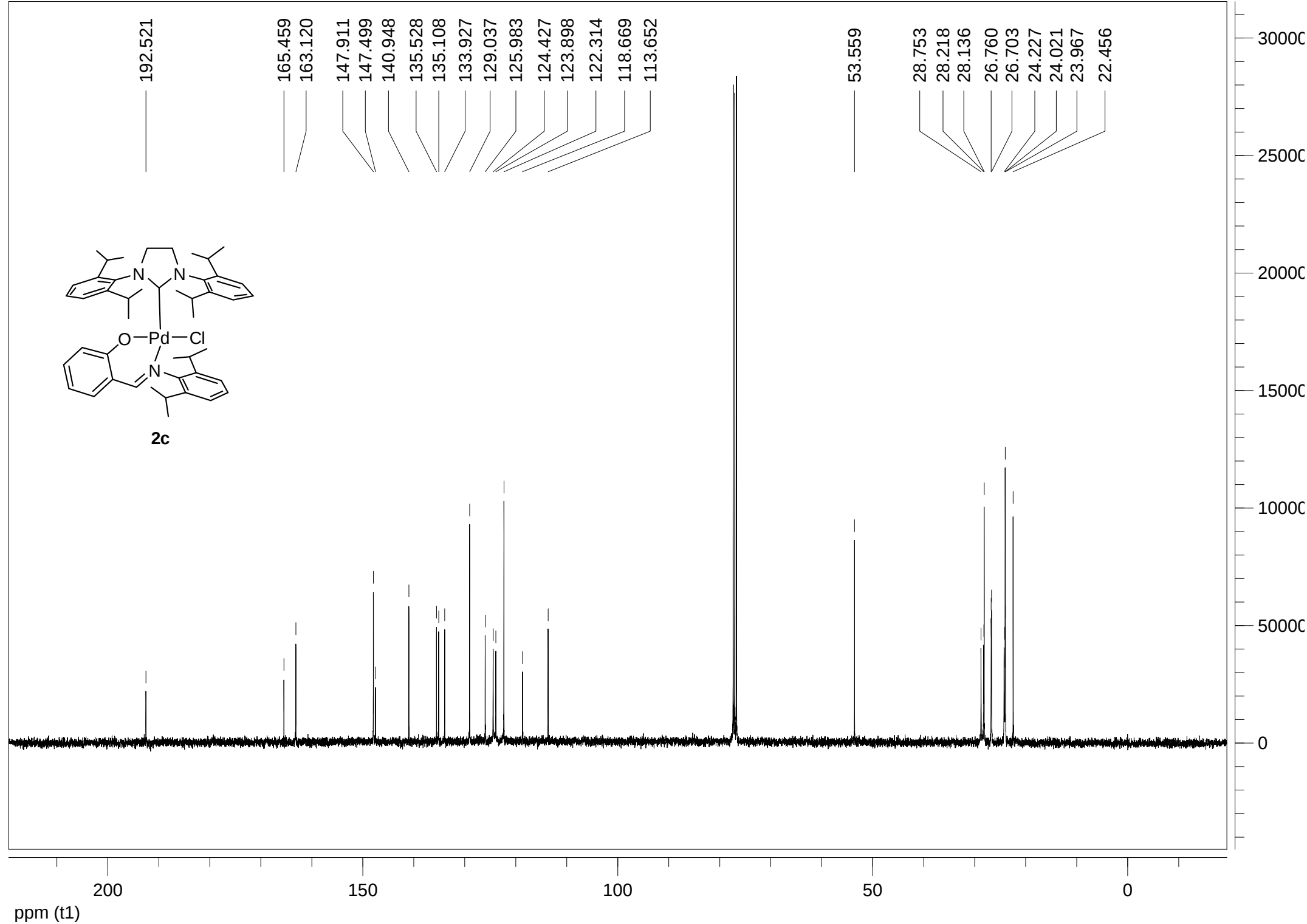
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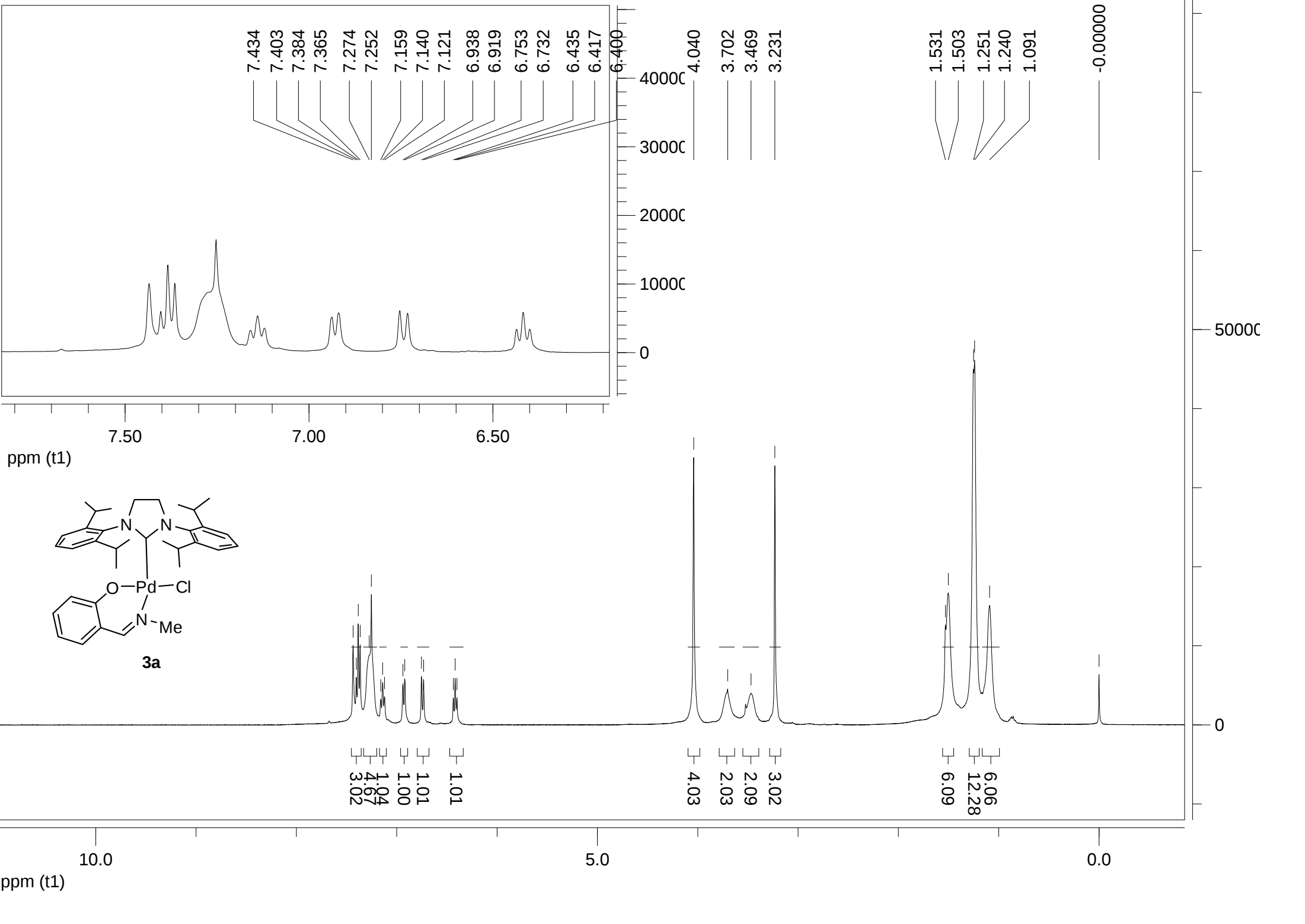


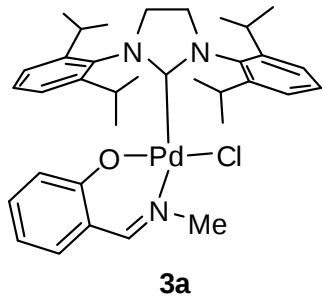


192.521
165.459
163.120
147.911
147.499
140.948
135.528
135.108
133.927
129.037
125.983
124.427
123.898
122.314
118.669
113.652

53.559
28.753
28.218
28.136
26.760
26.703
24.227
24.021
23.967
22.456

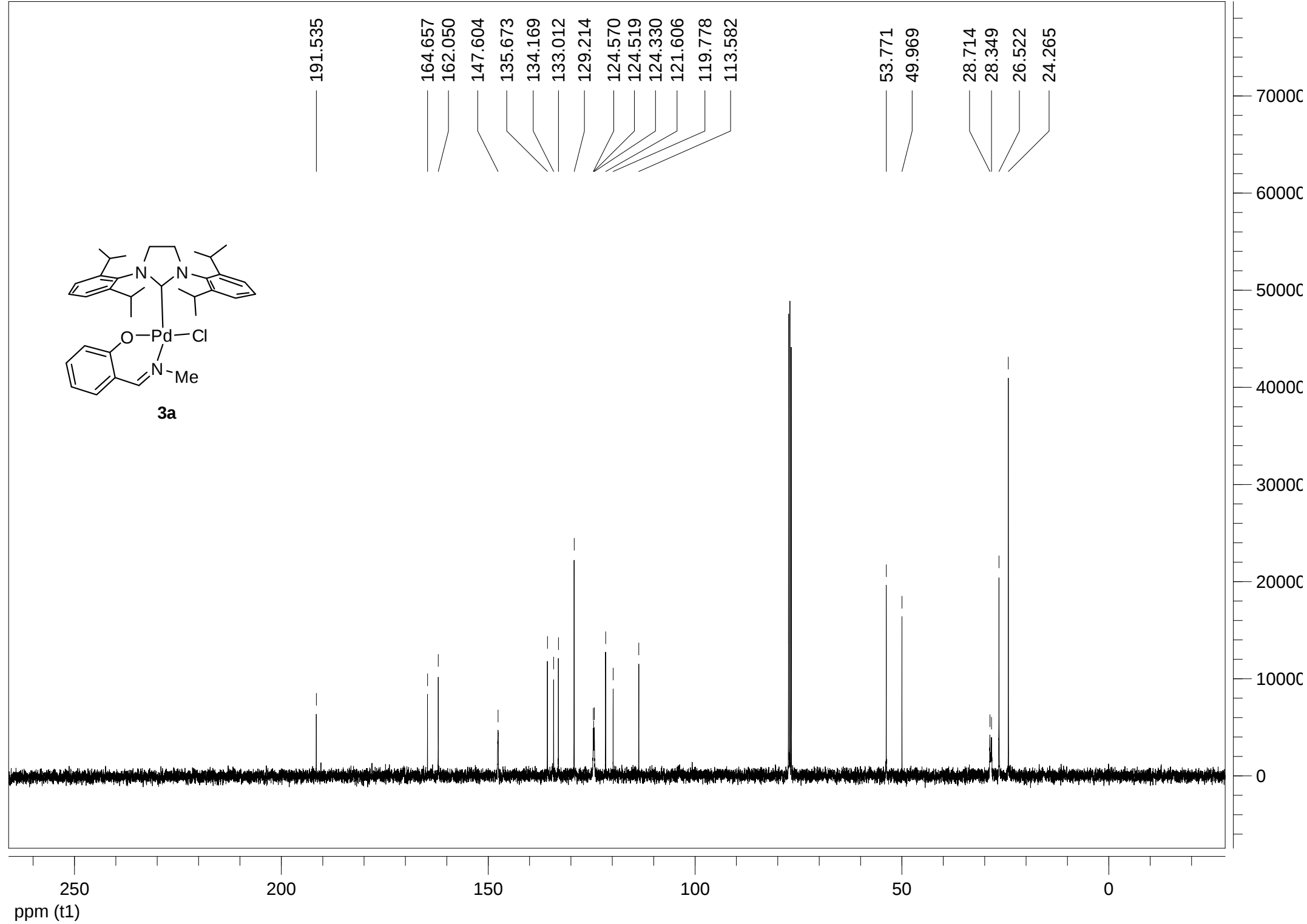


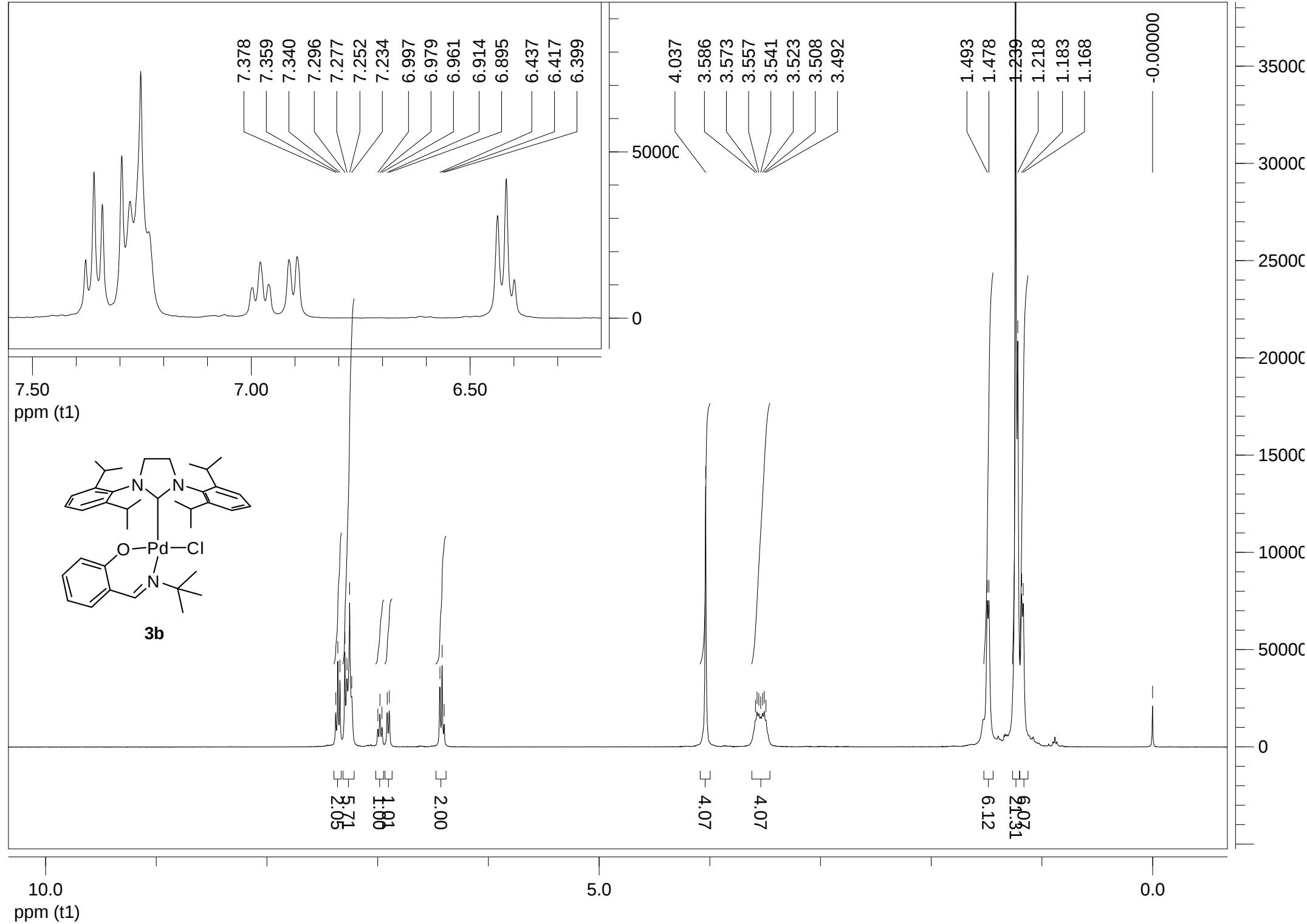


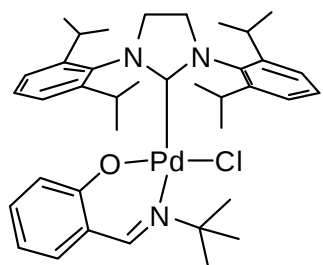


191.535
164.657
162.050
147.604
135.673
134.169
133.012
129.214
124.570
124.519
124.330
121.606
119.778
113.582

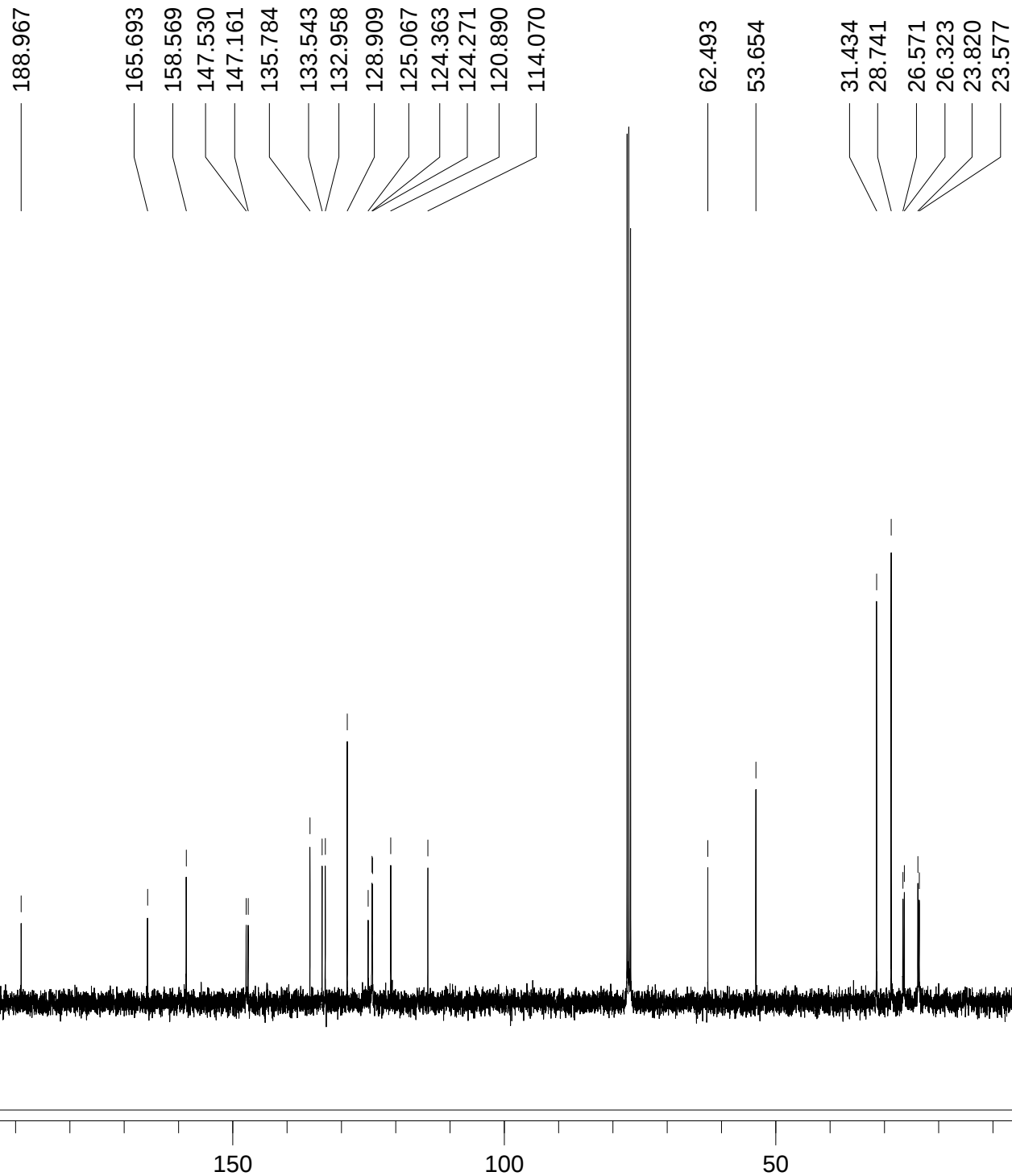
53.771
49.969
28.714
28.349
26.522
24.265

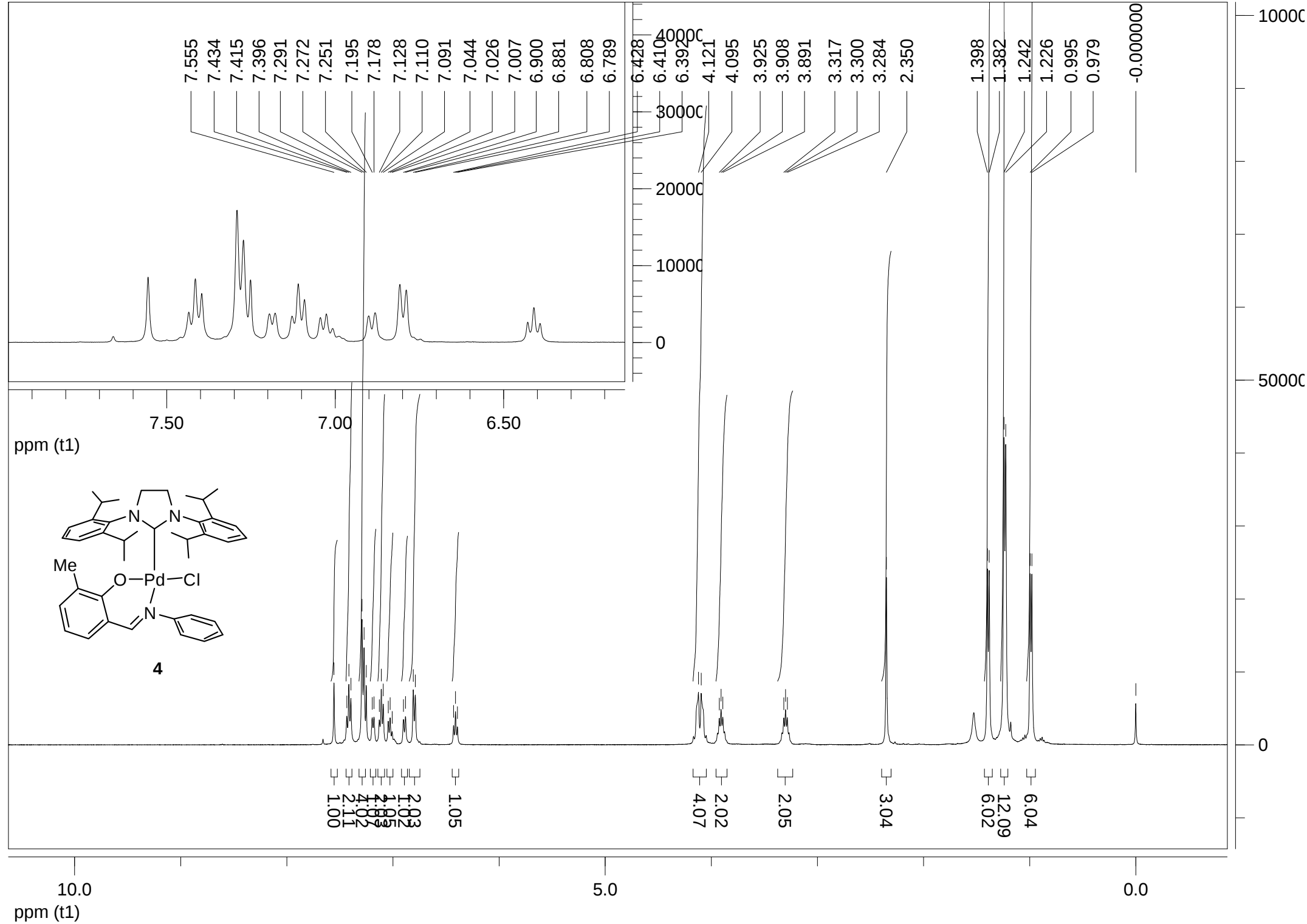


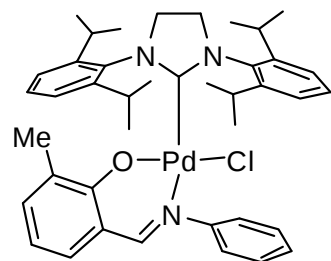




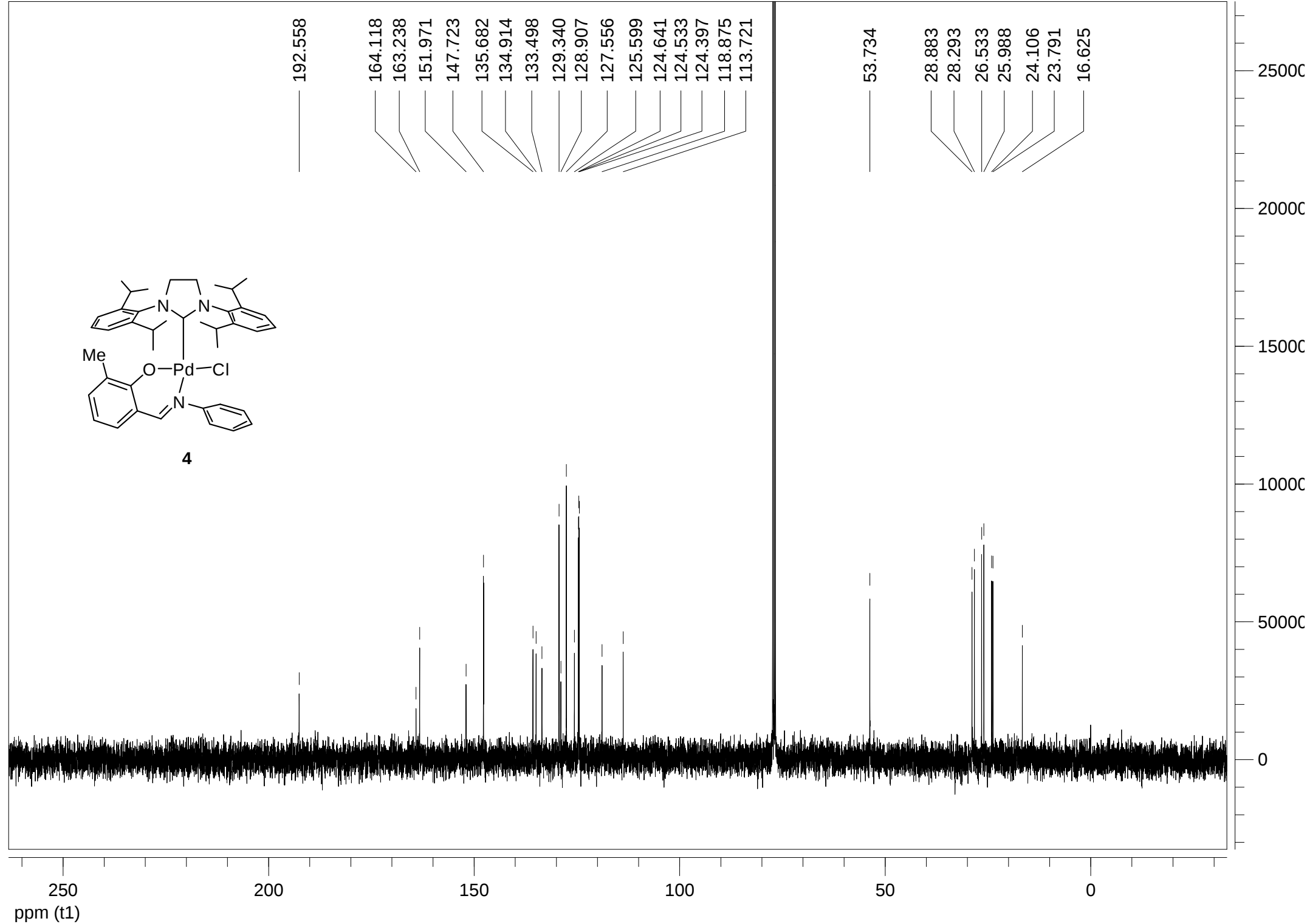
3b

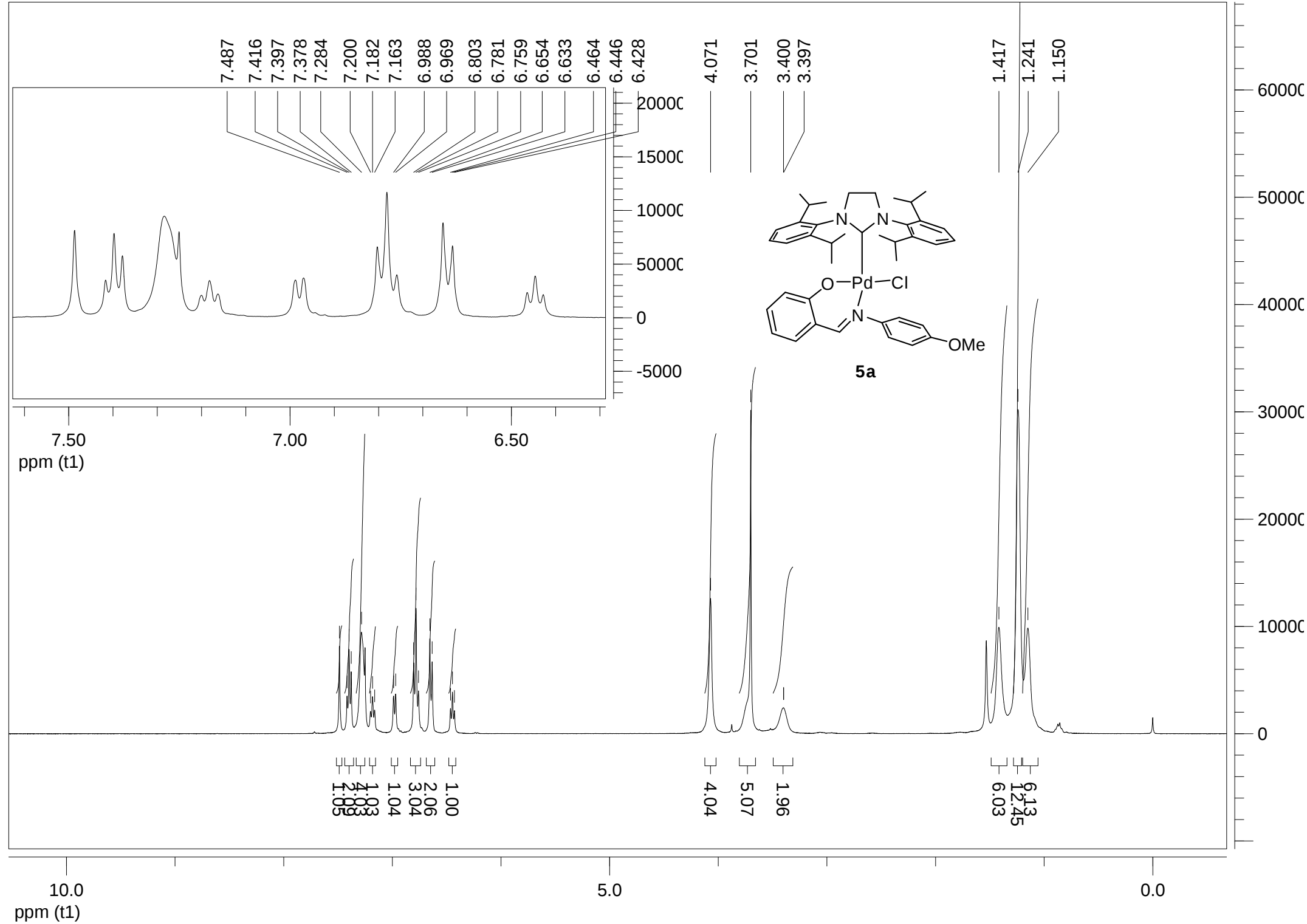


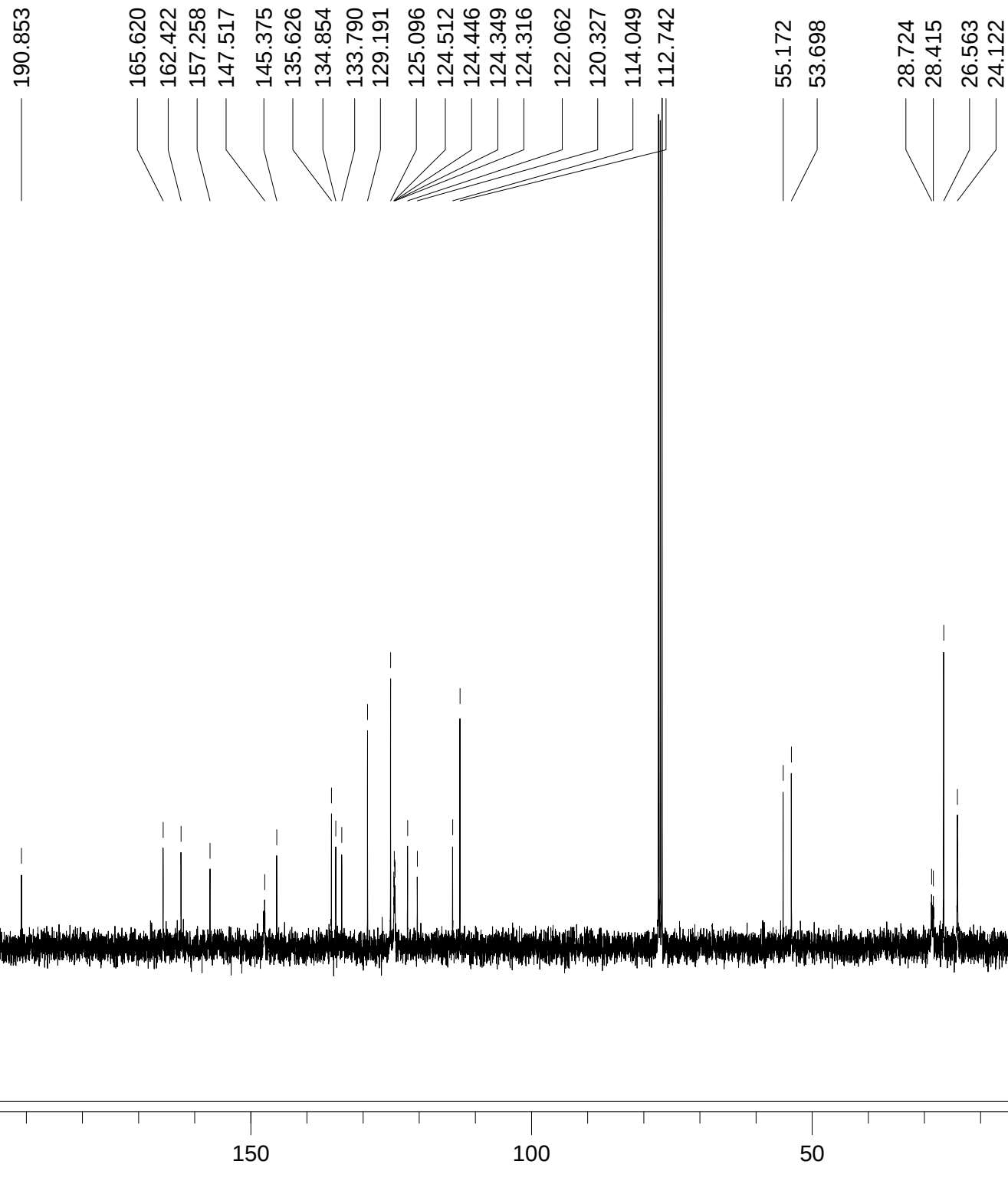
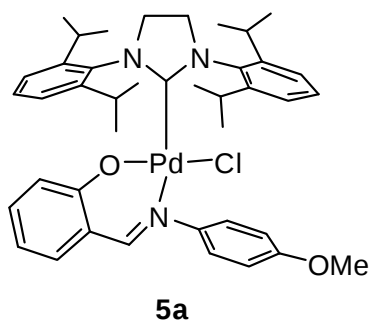


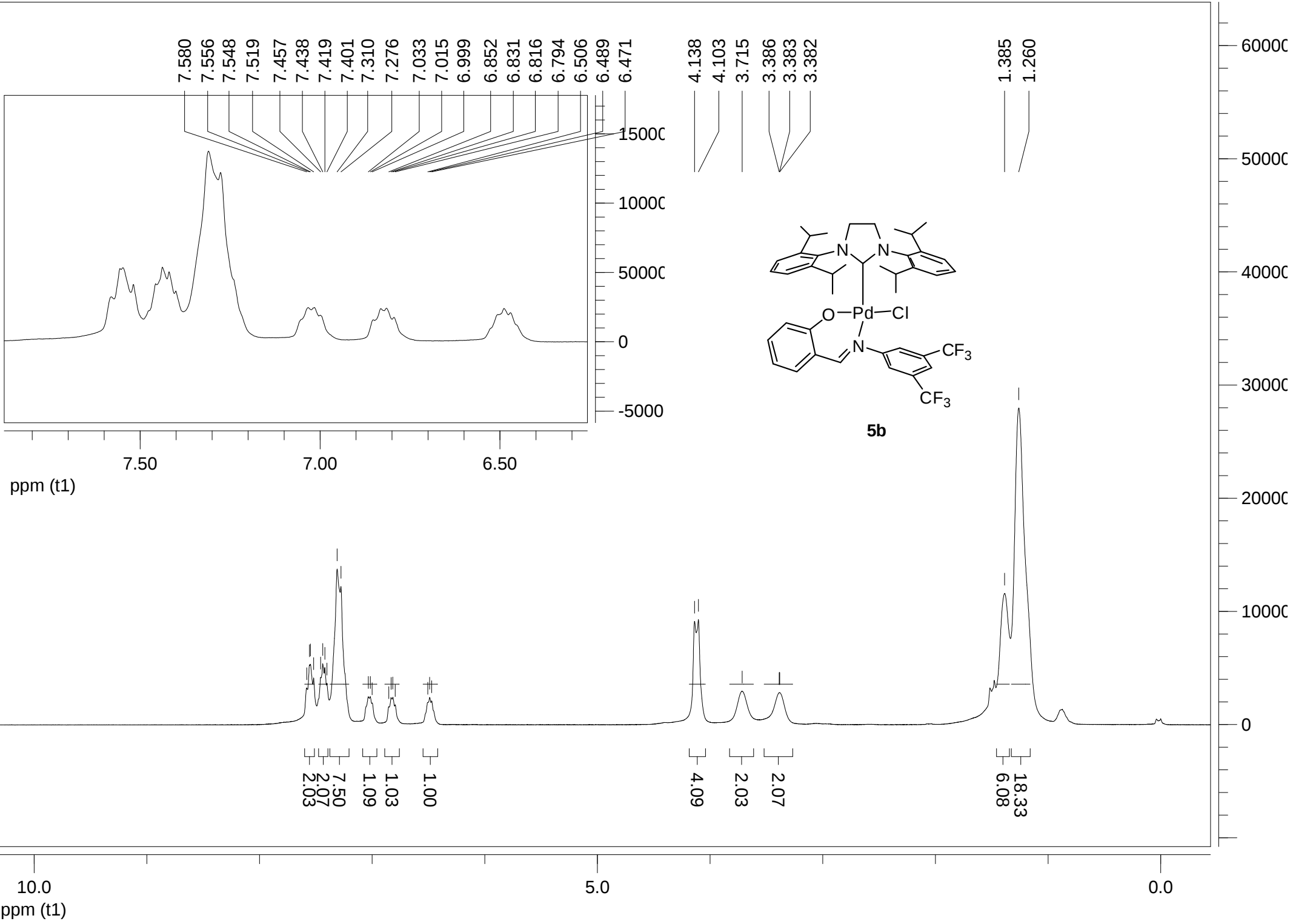


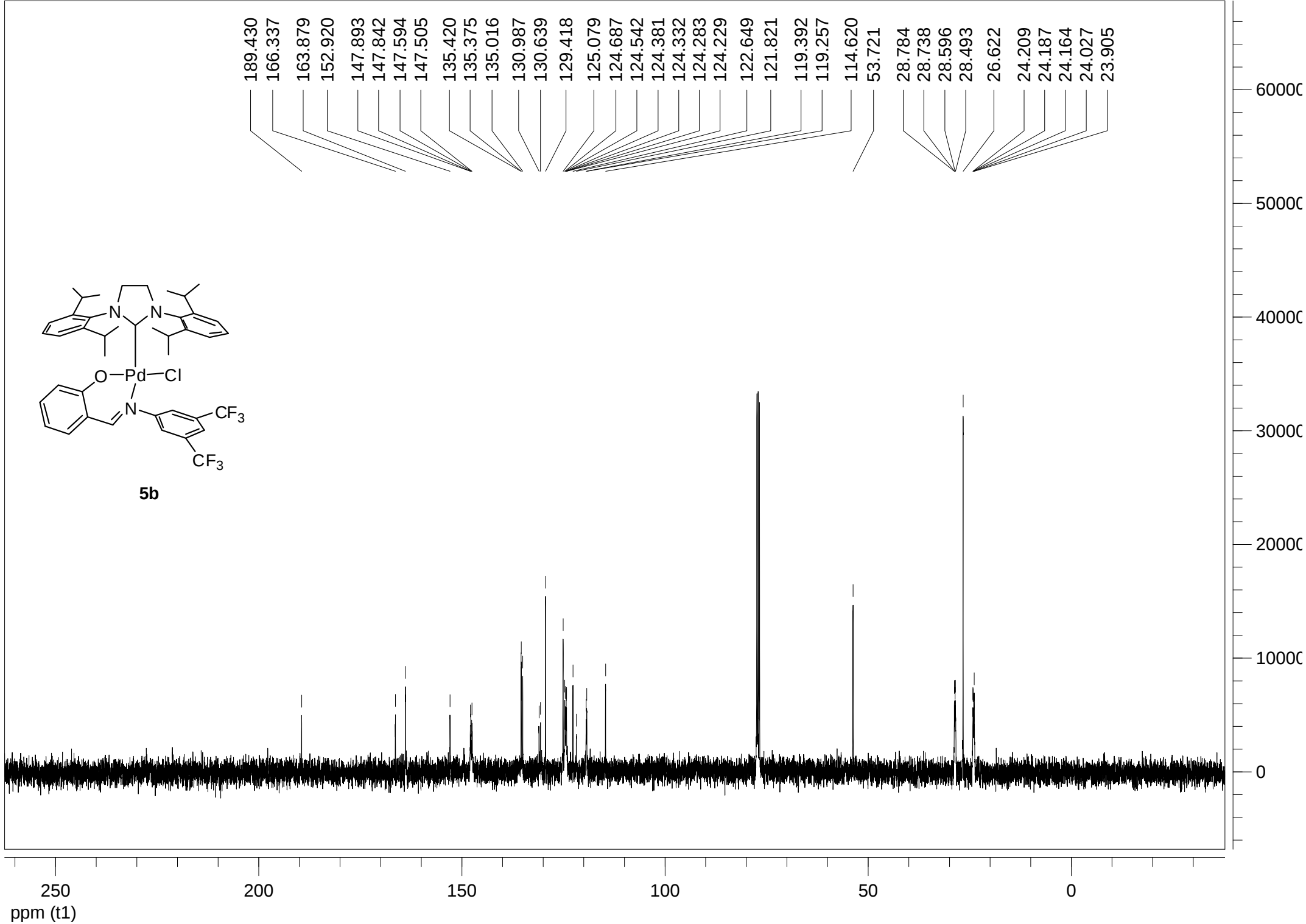
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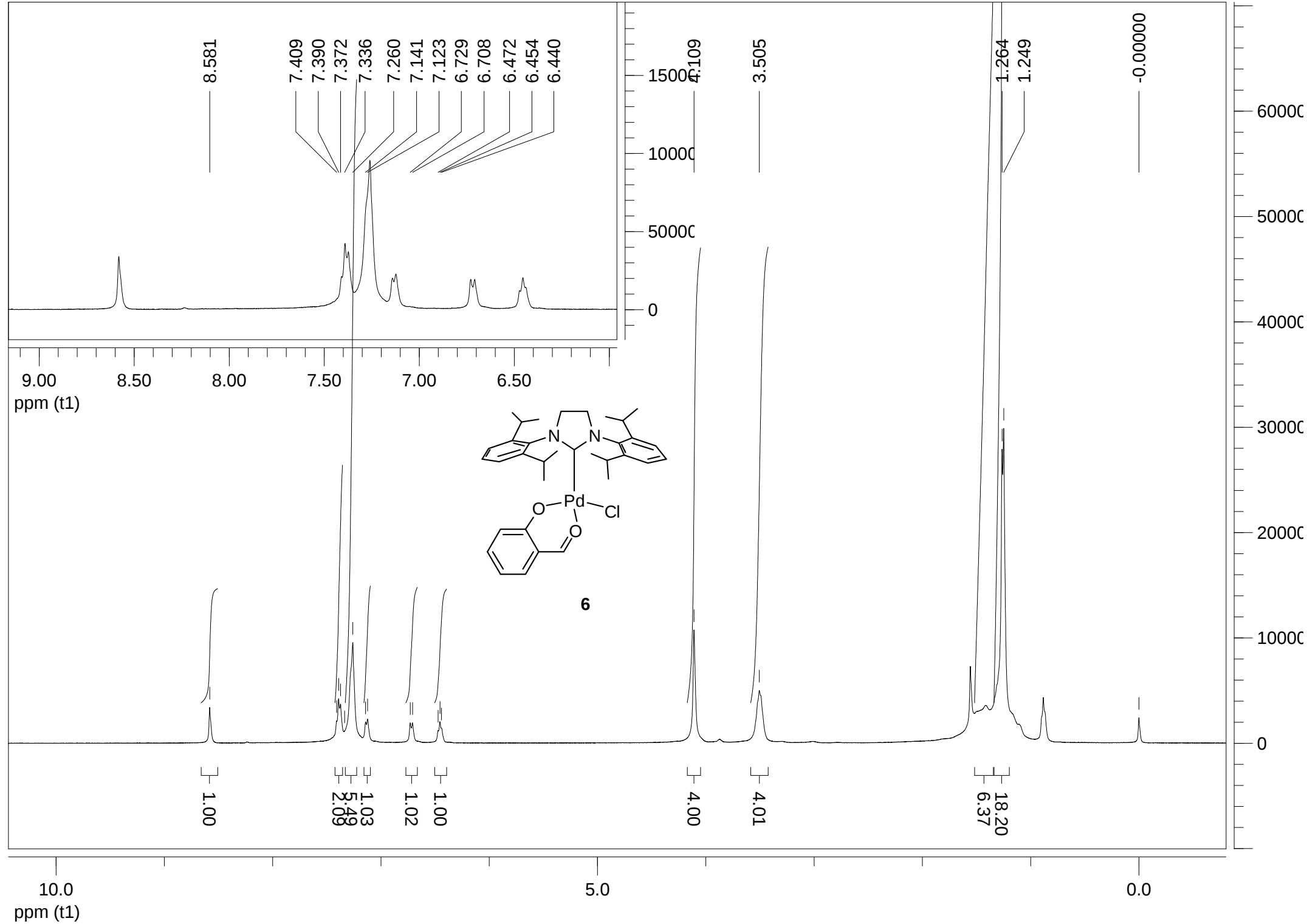


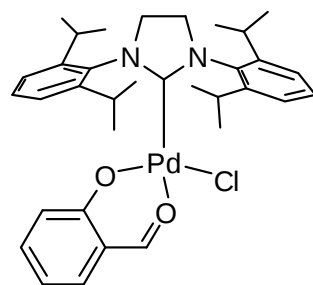












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