

Supporting Information

Synthesis and Reactivity of Taddol-Based Chiral Fe(II) PNP Pincer Complexes - Solution Equilibria between κ^2P,N - and κ^3P,N,P -Bound PNP Pincer Ligands

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[TAD-PCI]. To a solution of 4*R*,5*R*-TADDOL (4.86 g, 10.42 mmol) and NEt₃ (3.6 mL, 26.04 mmol) in toluene (100 mL) PCl₃ (1.0 mL, 11.46 mmol) was added dropwise at 0°C. After stirring the solution for 1 h at 80°C, about half of the solvent was removed under vacuum and the remaining solution was filtered under inert condition over a small pad of pre-dried Celite[®]. After removal of the solvent under reduced pressure, the product was precipitated with 100 mL of pentane. The white powder was washed twice with 15 mL of pentane and dried for 1 h under vacuum. Yield: 3.48 g (63%). ¹H NMR (δ, CDCl₃, 20°C): 7.71-7.48 (m, 6H, ph), 7.48-7.15 (m, 14H, ph), 5.82 (d, ³J_{HH} = 8.1 Hz, 1H, CH), 5.11 (d, ³J_{HH} = 8.1 Hz, 1H, CH), 0.86 (s, 3H, CH₃), 0.49 (s, 3H, CH₃). ¹³C{¹H} NMR (δ, CDCl₃, 20°C): 144.72 (s, Ph¹), 144.12 (s, Ph¹), 140.51 (s, Ph¹), 139.94 (s, Ph¹), 128.87 (Ph), 128.70 (Ph), 128.34 (Ph), 128.06 (Ph), 127.98 (Ph), 127.57 (Ph), 127.35 (Ph), 127.12 (Ph), 126.95 (Ph), 114.22 (s, C(CH₃)₂), 91.00 (d, ²J_{CP} = 14.3 Hz, CPh₂), 88.97 (d, ²J_{CP} = 11.3 Hz, CPh₂), 81.62 (d, ³J_{CP} = 6.6 Hz, CH), 79.20 (d, ³J_{CP} = 6.3 Hz, CH), 26.84 (s, CH₃), 26.23 (s, CH₃). ³¹P{¹H} NMR (δ, CDCl₃, 20°C): 148.0.

Table S1. Details for the crystal structure determinations of **3b**·THF, **4a**·THF and **7b**·2THF.

	3b ·THF	4a ·THF	7b ·2THF
formula	C ₄₆ H ₅₅ Br ₂ FeN ₃ O ₅ P ₂	C ₄₈ H ₅₉ Cl ₂ FeN ₃ O ₅ P ₂	C ₅₁ H ₆₃ Br ₂ FeN ₃ O ₇ P ₂
fw	1007.6	946.7	1107.7
cryst.size, mm	0.54 x 0.22 x 0.02	0.58 x 0.50 x 0.02	0.72 x 0.24 x 0.24
color, shape	yellow plate	yellow plate	dark blue rod
crystal system	triclinic	monoclinic	tetragonal
space group	P1 (no. 1)	P2 ₁ (no. 61)	P4 ₁ (no. 76)
a, Å	9.1105(5)	9.4904(9)	22.454(4)
b, Å	10.3931(6)	10.3270(9)	22.454(4)
c, Å	24.1374(14)	25.295(2)	10.598(4)
α, °	93.0205(19)	90	90
β, °	93.3464(18)	98.334(3)	90
γ, °	91.2982(19)	90	90
V, Å ³	2277.7(2)	10227(3)	5343(2)
T, K	100	100	100
Z, Z'	2, 2	2, 1	4, 1
ρ _{calc} , g cm ⁻³	1.4691	1.2814	1.3770
μ, mm ⁻¹ (MoKα)	2.204	0.528	1.888
F(000)	1036	996	2288
absorption corrections, T _{min} –T _{max}	multi-scan, 0.56–0.96	multi-scan, 0.74–0.94	multi-scan, 0.59–0.78
θ range, deg	0.85–30.2	0.81–0.81	2.57–30.11
no. of rflns measd	55010	52964	138990
R _{int}	0.0406	0.0368	0.0628
no. of rflns unique	25848	14261	15648
no. of rflns I > 3σ(I)	19167	12404	13207
no. of params / restraints	1064 / 0	551 / 0	604 / 2
R (I > 3σ(I)) ^a	0.0327	0.0441	0.0396
R (all data)	0.0553	0.0529	0.0487
wR (I > 3σ(I))	0.0347	0.0471	0.0462
wR (all data)	0.0379	0.0479	0.0475
GooF	0.87	1.86	1.77
Diff.Four.peaks min/max, eÅ ⁻³	-0.33 / 0.34	-0.49 / 0.69	-0.18 / 0.27
Flack Parameter	0.011(3)	0.043(11)	0.031(5)
CCDC no.	1032898	1032899	1032900

^a $R = \Sigma ||F_o| - |F_c|| / \Sigma |F_o|$, $wR = \Sigma w(|F_o| - |F_c|) / \Sigma w|F_o|$, $GooF = \{\Sigma [w(F_o^2 - F_c^2)^2] / (n-p)\}^{1/2}$

Atomic coordinates of all optimized species (B3LYP)

CO				P	6.736202	29.401056	-3.287019
C	0.000000	0.000000	0.001028	P	9.734648	32.374744	0.608202
O	0.000000	0.000000	1.138972	C	10.394334	29.161117	-3.538754
A				H	10.214632	28.386645	-4.274051
Fe	10.738140	26.589023	-1.542368	C	9.409828	29.473283	-2.606476
Br	9.300398	25.754775	-3.283510	C	4.192587	27.589954	-4.054364
Br	10.600808	26.104673	0.774700	H	4.122153	28.342414	-4.852008
O	6.487011	28.106899	-0.779865	C	3.280570	25.672143	-4.974503
N	13.182891	28.524850	-2.136692	C	5.313385	26.601068	-4.376899
O	3.354524	26.774603	-1.945999	H	5.587837	26.056421	-3.462095
P	6.992433	29.572924	-1.390752	C	6.558740	27.246187	-5.011735
P	13.095660	26.799596	-2.238210	C	10.848820	32.228353	2.111828
C	9.859471	30.963068	-1.708583	H	11.369124	31.286067	1.897269
H	8.966251	31.570097	-1.634218	C	10.029676	32.010037	3.396843
C	9.759583	29.562090	-1.774077	H	9.449660	32.895108	3.675158
C	4.356271	27.784393	-1.951665	H	10.709256	31.789958	4.227509
H	3.910419	28.760639	-2.188413	H	9.346145	31.163830	3.289276
C	3.263875	26.221418	-3.275583	C	9.277580	34.179155	0.394425
C	5.268781	27.345487	-3.099151	H	10.199404	34.767918	0.495844
H	5.954540	26.560005	-2.753521	C	8.692334	34.408231	-1.009880
C	6.056603	28.497782	-3.741421	H	9.398730	34.133013	-1.798015
C	13.530677	26.463145	-4.036205	H	8.447671	35.469166	-1.132883
H	12.848868	27.156828	-4.546215	H	7.774181	33.829616	-1.150995
C	13.143498	25.038339	-4.469842	C	4.388873	28.254792	-2.685900
H	13.776446	24.277905	-4.002656	C	2.488556	25.875916	-6.262263
H	13.266186	24.941986	-5.554168	H	2.733808	25.093759	-6.986426
H	12.099997	24.817300	-4.229603	H	2.734854	26.846009	-6.700982
C	14.555083	26.278599	-1.186478	H	1.415134	25.842330	-6.056758
H	15.456913	26.681292	-1.667763	C	10.729900	31.149551	-1.657107
C	14.442322	26.866773	0.230038	C	2.943215	24.367441	-4.258957
H	14.402010	27.959141	0.219910	H	3.106846	23.515266	-4.924397
H	15.317379	26.565893	0.816700	H	1.897189	24.370299	-3.939703
H	13.545194	26.502658	0.738850	H	3.574884	24.252931	-3.374536
C	5.087040	27.833108	-0.601946	C	11.590434	29.885087	-3.508171
C	1.946342	26.627449	-3.926089	H	12.378038	29.666735	-4.223257
H	1.905126	26.265729	-4.957504	C	11.767527	30.891404	-2.574290
H	1.856656	27.716468	-3.933717	H	12.687545	31.464980	-2.529877
H	1.104207	26.205518	-3.370924	C	11.889347	33.346401	2.268705
C	12.081808	29.356056	-1.967649	H	12.501679	33.486948	1.370209
C	3.445060	24.709151	-3.171615	H	12.574604	33.102766	3.087991
H	3.365201	24.248190	-4.160074	H	11.421051	34.306084	2.509817
H	2.679142	24.280371	-2.519085	C	8.278269	34.612771	1.481750
H	4.427024	24.475593	-2.752629	H	7.375394	33.994566	1.449956
C	11.121375	31.535904	-1.760884	H	7.978682	35.652145	1.308694
H	11.223273	32.616001	-1.709322	H	8.701527	34.557266	2.488233
C	12.256140	30.743281	-1.905364	O	6.632791	28.664827	-4.784184
H	13.248108	31.176258	-1.971855	N	9.578802	30.445917	-1.680711
C	14.970623	26.822141	-4.428568	O	4.679806	25.722668	-5.302817
H	15.239580	27.844910	-4.142322	N	8.177382	28.787916	-2.555915
H	15.088587	26.749218	-5.515219	H	3.967050	27.606303	-1.914974
H	15.697184	26.139087	-3.976488	H	3.901953	29.234369	-2.625401
C	14.661562	24.743977	-1.138107	H	6.496413	27.118978	-6.095155
H	13.751814	24.299326	-0.721877	H	7.477033	26.761291	-4.658139
H	15.497230	24.456443	-0.491279	H	8.233942	27.792086	-2.364154
H	14.840675	24.301875	-2.121560	H	11.744454	32.638396	-0.720362
O	6.205711	29.623207	-2.842587	B			
N	10.864389	28.772815	-1.869468	Fe	8.462606	30.143093	0.168683
O	4.329534	26.813414	-4.029630	Br	9.693466	28.570094	1.489806
N	8.550032	28.909770	-1.761135	Br	6.132476	30.680676	0.264090
H	5.037094	26.844609	-0.140973	O	6.234703	27.869038	-2.167484
H	4.634381	28.563082	0.079911	N	10.876698	32.034237	-0.723151
H	5.487310	28.876335	-4.592902	O	3.137965	26.892971	-3.750251
H	7.041453	28.165248	-4.083967	P	7.044035	29.124750	-2.904745
H	8.585781	27.911653	-1.971853	P	9.674413	32.277533	0.507038
H	14.067303	29.006526	-2.233884	C	10.887931	28.772906	-3.271253
TS_{AB}				H	10.834064	27.932103	-3.952812
Fe	8.196380	30.487120	0.023847	C	9.773047	29.122108	-2.502822
Br	9.014835	28.648403	1.331406	C	4.352811	27.628210	-3.683123
Br	6.033780	31.476135	-0.219326	H	4.249831	28.588612	-4.207063
O	5.789022	28.365935	-2.384007	C	3.147672	26.133911	-4.972683
N	10.872242	32.126076	-0.688760	C	5.321852	26.725911	-4.449449
O	3.040880	26.754553	-4.057924	H	5.652562	25.911659	-3.788104
				C	6.540628	27.452791	-5.049552
				C	10.737867	32.481271	2.037774

H	11.401090	31.611233	1.949875	H	1.945096	26.778706	-6.486373
C	9.912081	32.290513	3.322927	H	2.228622	28.133516	-5.375013
H	9.194797	33.101310	3.480875	H	1.071075	26.855690	-4.939164
H	10.584316	32.273459	4.187762	C	11.015443	30.843779	-1.557635
H	9.366351	31.343740	3.303234	C	2.905414	24.774252	-4.734223
C	8.960131	33.949280	0.059963	H	2.760180	24.396197	-5.749938
H	9.793910	34.664185	0.034565	H	2.015771	24.543857	-4.141311
C	8.323911	33.875848	-1.338689	H	3.762386	24.265638	-4.285532
H	9.044609	33.563365	-2.099400	C	12.314570	29.479036	-3.038329
H	7.944221	34.864374	-1.620015	H	13.251835	29.240121	-3.532183
H	7.483315	33.174874	-1.350717	C	12.240083	30.574217	-2.188758
C	4.796914	27.840881	-2.232747	H	13.104016	31.200395	-1.994481
C	2.214680	26.764175	-6.001679	C	11.332170	33.634275	2.136083
H	2.285364	26.231538	-6.954374	H	12.068890	33.707884	1.327365
H	2.491221	27.808639	-6.165599	H	11.893458	33.592310	3.075979
H	1.180048	26.722740	-5.650472	H	10.750042	34.561339	2.144377
C	10.892932	30.945689	-1.580982	C	7.840219	34.411497	0.737164
C	2.783991	24.691841	-4.632105	H	7.015628	33.693553	0.793789
H	2.770482	24.079031	-5.537671	H	7.441322	35.350755	0.338434
H	1.796639	24.651167	-4.163549	H	8.193698	34.611449	1.752112
H	3.515464	24.276732	-3.934130	O	6.648979	29.044655	-4.226491
C	12.034055	29.555605	-3.166741	N	9.918592	30.074667	-1.745105
H	12.915063	29.310328	-3.752478	O	4.375460	26.582555	-5.447789
C	12.044386	30.665881	-2.335076	N	8.840857	28.313362	-2.848218
H	12.923249	31.294636	-2.241167	H	4.983173	26.469408	-1.558459
C	11.589536	33.758440	2.075666	H	4.822107	28.224893	-1.294451
H	12.203201	33.888018	1.176419	H	5.966644	28.322170	-5.996578
H	12.275558	33.722926	2.929091	H	7.319655	27.395546	-5.316226
H	10.971486	34.654635	2.190193	H	8.969522	27.392898	-3.251660
C	7.932110	34.408262	1.109183	H	11.755767	32.480647	-0.616231
H	7.130800	33.671076	1.224117	C			
H	7.475806	35.349900	0.784913	Fe	7.839107	30.766919	-1.051368
H	8.383341	34.584113	2.089305	Br	7.541335	29.176753	0.797059
O	6.739805	28.771341	-4.507196	Br	6.682794	32.477143	-2.336637
N	9.784659	30.171419	-1.644452	O	7.015379	27.293364	-2.445490
O	4.489407	26.210374	-5.485157	N	10.801092	31.955930	-0.621085
N	8.589522	28.392201	-2.579996	O	3.709463	26.022953	-3.123467
H	4.486546	26.980870	-1.635252	P	7.240918	28.910352	-2.728447
H	4.378203	28.749541	-1.787859	P	9.353163	32.341925	0.265039
H	6.364876	27.595078	-6.118229	C	11.158563	29.161989	-3.650294
H	7.451966	26.854509	-4.927374	H	11.214116	28.420070	-4.438735
H	8.706410	27.414140	-2.823307	C	9.937975	29.425397	-3.015282
H	11.722039	32.590625	-0.731244	C	4.681740	27.059619	-3.120008
TS_{BC}				H	4.198584	28.040828	-3.015439
Fe	8.321551	30.125640	-0.073291	C	3.215330	25.895579	-4.466321
Br	9.444568	28.497855	1.285297	C	5.293512	26.928301	-4.517531
Br	6.013171	30.722652	0.303984	H	6.025958	26.107830	-4.514097
O	6.604992	27.544321	-2.148442	C	5.938431	28.221889	-5.048552
N	10.910632	31.930639	-0.702494	C	9.863903	31.878956	2.014409
O	3.328317	26.720178	-3.402217	H	9.956012	30.789373	1.926433
P	7.256220	28.978871	-2.682003	C	8.737690	32.158861	3.023946
P	9.569042	32.212444	0.357253	H	8.616839	33.230144	3.214548
C	11.187265	28.701828	-3.275893	H	8.980439	31.684129	3.980912
H	11.206416	27.868912	-3.969298	H	7.783367	31.747184	2.684588
C	9.998426	29.040239	-2.616625	C	9.318867	34.224622	0.205977
C	4.489722	27.539337	-3.359332	H	10.067367	34.590031	0.921919
H	4.236225	28.579149	-3.607810	C	9.667829	34.760675	-1.192604
C	3.148062	26.279906	-4.758540	H	10.675169	34.478855	-1.511464
C	5.350733	26.936716	-4.471982	H	9.615113	35.855328	-1.182030
H	5.851648	26.035089	-4.090678	H	8.956281	34.395288	-1.938877
C	6.381324	27.908620	-5.074791	C	5.714855	26.834632	-2.010764
C	10.432137	32.396429	2.010764	C	1.866736	26.593558	-4.616311
H	11.059528	31.495897	2.017205	H	1.539996	26.564754	-5.659664
C	9.444745	32.269116	3.184557	H	1.947575	27.638894	-4.307989
H	8.769152	33.126368	3.252824	H	1.113220	26.099581	-3.996841
H	10.004196	32.215130	4.124922	C	10.914694	31.034087	-1.642855
H	8.842306	31.361237	3.099453	C	3.167137	24.410864	-4.808492
C	8.959482	33.898132	-0.185655	H	2.801613	24.268988	-5.829144
H	9.814294	34.586401	-0.135680	H	2.500570	23.885126	-4.119028
C	8.474938	33.814193	-1.643110	H	4.166464	23.976355	-4.726089
H	9.260522	33.460946	-2.316866	C	12.277739	29.879731	-3.245214
H	8.160491	34.807080	-1.983318	H	13.237708	29.698563	-3.719643
H	7.615620	33.141611	-1.731982	C	12.172232	30.825716	-2.237626
C	5.171956	27.454786	-1.989280	H	13.032905	31.393557	-1.901732
C	2.024760	27.061419	-5.432795	C	11.205229	32.456292	2.487141

H	12.033380	32.192554	1.820716
H	11.452442	32.052175	3.475264
H	11.174327	33.547118	2.584491
C	7.926076	34.726029	0.636459
H	7.164610	34.388897	-0.072555
H	7.920964	35.821766	0.649951
H	7.640191	34.382934	1.633824
O	6.239539	29.168940	-4.001926
N	9.812015	30.348619	-2.030121
O	4.165943	26.575450	-5.310869
N	8.811107	28.711395	-3.397158
H	5.823170	25.761562	-1.840284
H	5.443679	27.321699	-1.069251
H	5.219426	28.727832	-5.695338
H	6.843764	28.012415	-5.629586
H	8.994482	27.915908	-3.996677
H	11.671499	32.415624	-0.386962

D

Fe	7.921656	30.755519	-1.019347
Br	7.671355	29.146605	0.824433
Br	6.784067	32.462614	-2.332169
O	7.096058	27.281257	-2.407768
N	10.872899	31.962028	-0.611540
O	3.792573	25.993369	-3.060076
P	7.312462	28.899217	-2.690225
P	9.430282	32.335298	0.289132
C	11.219434	29.177468	-3.651265
H	11.272149	28.438241	-4.442423
C	10.003956	29.429972	-3.002345
C	4.757285	27.037189	-3.062559
H	4.268142	28.014639	-2.951176
C	3.287743	25.865396	-4.398741
C	5.358112	26.912782	-4.465472
H	6.096585	26.097753	-4.469713
C	5.988677	28.212076	-4.999329
C	9.957927	31.871120	2.032894
H	10.048771	30.781519	1.944506
C	8.841322	32.153007	3.052523
H	8.724660	33.224592	3.244240
H	9.091772	31.677559	4.007165
H	7.882435	31.744953	2.721883
C	9.380517	34.217965	0.239320
H	10.122773	34.584717	0.961056
C	9.731693	34.766066	-1.153945
H	10.743743	34.496866	-1.468851
H	9.667430	35.860021	-1.136977
H	9.028390	34.397792	-1.906542
C	5.801062	26.816611	-1.962437
C	1.933320	26.554687	-4.535694
H	1.597939	26.526141	-5.576315
H	2.009789	27.599750	-4.225373
H	1.188449	26.054197	-3.911022
C	10.983556	31.043280	-1.636442
C	3.246638	24.381069	-4.743565
H	2.873353	24.238717	-5.761341
H	2.589598	23.849452	-4.049478
H	4.249598	23.953289	-4.670606
C	12.337404	29.902950	-3.256435
H	13.293422	29.730410	-3.741929
C	12.235977	30.845873	-2.245484
H	13.095937	31.419726	-1.918103
C	11.304120	32.448310	2.491622
H	12.125434	32.181745	1.817940
H	11.560116	32.046351	3.478383
H	11.275470	33.539434	2.586610
C	7.981858	34.704899	0.667578
H	7.226116	34.370193	-0.048447
H	7.969385	35.800392	0.693190
H	7.692473	34.348105	1.658982
O	6.297454	29.156664	-3.952622
N	9.882582	30.349523	-2.013341
O	4.226668	26.553157	-5.250112
N	8.877592	28.709182	-3.373320
H	5.915808	25.744062	-1.793062
H	5.535127	27.302315	-1.018784

H	5.258464	28.716491	-5.634637
H	6.887768	28.010684	-5.592762
H	9.059415	27.916315	-3.976759
H	11.741939	32.427838	-0.384631
C	4.621928	31.430411	0.645190
O	3.942683	30.705234	0.090417

TS_{DE}

Fe	7.899403	30.768803	-0.974950
Br	7.869304	29.053215	0.813794
Br	6.968178	32.473289	-2.480728
O	7.058529	27.284429	-2.389979
N	10.854231	31.954994	-0.587622
O	3.775224	25.960460	-3.066687
P	7.263198	28.910464	-2.643951
P	9.418973	32.340527	0.315576
C	11.162013	29.187243	-3.647722
H	11.203414	28.454264	-4.445373
C	9.954059	29.442962	-2.985754
C	4.721647	27.020859	-3.048218
H	4.215055	27.986757	-2.915644
C	3.275543	25.846011	-4.409039
C	5.322068	26.938795	-4.454079
H	6.075604	26.138067	-4.477792
C	5.926374	28.262516	-4.956967
C	9.947411	31.888635	2.061042
H	10.023422	30.797259	1.985863
C	8.835831	32.199923	3.077228
H	8.721788	33.276554	3.241665
H	9.086596	31.748124	4.043174
H	7.874453	31.786819	2.759507
C	9.367075	34.224197	0.266183
H	10.071186	34.590764	1.025083
C	9.781929	34.781220	-1.105273
H	10.815079	34.532913	-1.363819
H	9.695221	35.873685	-1.092133
H	9.129027	34.397769	-1.894593
C	5.771376	26.795110	-1.954258
C	1.903276	26.501334	-4.533517
H	1.568774	26.483956	-5.574661
H	1.952388	27.541896	-4.203152
H	1.171932	25.969372	-3.918956
C	10.954313	31.039856	-1.618534
C	3.274875	24.368242	-4.783687
H	2.905173	24.236081	-5.804154
H	2.633176	23.804881	-4.100372
H	4.289321	23.966985	-4.719283
C	12.287703	29.902742	-3.256701
H	13.238528	29.728036	-3.751539
C	12.200632	30.839629	-2.238290
H	13.066648	31.406901	-1.915319
C	11.301486	32.455357	2.509152
H	12.117287	32.167088	1.837865
H	11.554211	32.064635	3.501263
H	11.288451	33.548187	2.587856
C	7.947059	34.701164	0.631401
H	7.229744	34.377433	-0.128087
H	7.928920	35.795983	0.676360
H	7.609622	34.325606	1.601104
O	6.225237	29.181759	-3.885918
N	9.848740	30.353772	-1.989567
O	4.195720	26.576086	-5.244667
N	8.817834	28.734155	-3.352120
H	5.899802	25.721143	-1.804448
H	5.497800	27.257259	-1.000756
H	5.183054	28.771106	-5.573587
H	6.824745	28.093981	-5.561501
H	8.989561	27.940006	-3.956824
H	11.727135	32.414113	-0.362749
C	5.173916	31.214743	0.215095
O	4.137535	30.782444	0.027659

E

Fe	7.805300	30.760765	-0.929361
Br	8.110930	28.923509	0.793465
Br	7.124051	32.491144	-2.622098

O	6.998062	27.286943	-2.362997	C	5.315728	27.046589	-4.418574
N	10.810350	31.938729	-0.577515	H	6.033927	26.219234	-4.515744
O	3.750435	25.922018	-3.100526	C	5.926737	28.355650	-4.950052
P	7.212000	28.914178	-2.600111	C	9.717668	31.775847	1.957237
P	9.381588	32.329610	0.324698	H	9.823598	30.686246	1.919107
C	11.096747	29.173889	-3.640437	C	8.516411	32.093273	2.863155
H	11.130287	28.441899	-4.439485	H	8.352394	33.171152	2.968996
C	9.894407	29.437928	-2.972111	H	8.698275	31.691789	3.865946
C	4.667427	27.007101	-3.050216	H	7.596220	31.634348	2.490540
H	4.132459	27.955856	-2.904497	C	9.181099	34.067744	0.149381
C	3.280958	25.806280	-4.454641	H	9.703623	34.421785	1.047461
C	5.284809	26.972359	-4.450416	C	9.831267	34.719727	-1.080857
H	6.063058	26.196086	-4.483115	H	10.908994	34.539139	-1.128585
C	5.850661	28.326188	-4.913902	H	9.679819	35.804278	-1.035079
C	9.911535	31.898734	2.075022	H	9.378092	34.348773	-2.003283
H	9.962024	30.804812	2.024077	C	5.961141	26.847139	-1.968248
C	8.815397	32.263624	3.089819	C	1.884139	26.682925	-4.236681
H	8.716607	33.347155	3.215221	H	1.470640	26.685527	-5.249192
H	9.067459	31.843992	4.069693	H	1.974044	27.717607	-3.896660
H	7.843335	31.854594	2.799376	H	1.194298	26.151732	-3.575244
C	9.327175	34.215917	0.278355	C	11.033179	30.992378	-1.651148
H	9.985124	34.576612	1.080184	C	3.201759	24.535430	-4.620417
C	9.819903	34.787061	-1.060614	H	2.748771	24.422285	-5.609048
H	10.870380	34.552899	-1.254158	H	2.610664	23.969553	-3.894826
H	9.719738	35.878388	-1.046534	H	4.212565	24.120662	-4.644175
H	9.223615	34.399946	-1.891478	C	12.434642	29.923877	-3.276631
C	5.710321	26.786778	-1.947088	H	13.404634	29.773865	-3.743022
C	1.881495	26.397577	-4.592886	C	12.303582	30.823088	-2.228685
H	1.565380	26.381064	-5.639744	H	13.151875	31.386470	-1.856336
H	1.876362	27.433891	-4.246014	C	11.015817	32.386247	2.505587
H	1.166243	25.821963	-3.999110	H	11.892776	32.090582	1.921003
C	10.905588	31.022973	-1.609799	H	11.183213	32.030304	3.528338
C	3.357938	24.336362	-4.852597	H	10.981534	33.480805	2.549150
H	3.008513	24.203194	-5.880093	C	7.696570	34.467246	0.260561
H	2.736069	23.731138	-4.186999	H	7.154862	34.166156	-0.640007
H	4.390119	23.984614	-4.780225	H	7.617753	35.555487	0.364877
C	12.228600	29.881732	-3.252300	H	7.202509	34.019070	1.127854
H	13.176708	29.702065	-3.750545	O	6.334988	29.252838	-3.896056
C	12.149781	30.817653	-2.232154	N	9.950376	30.308383	-2.080196
H	13.019830	31.380086	-1.911220	O	4.115617	26.739206	-5.118822
C	11.280866	32.445130	2.501711	N	8.965240	28.757656	-3.526616
H	12.085403	32.114817	1.836628	H	6.080419	25.767107	-1.860608
H	11.527547	32.077882	3.504241	H	5.779749	27.284534	-0.982170
H	11.296766	33.539965	2.547633	H	5.158759	28.898135	-5.504093
C	7.888850	34.688291	0.568376	H	6.772600	28.165268	-5.619734
H	7.219777	34.384842	-0.241946	H	9.128570	27.969616	-4.140338
H	7.867160	35.781780	0.637831	H	11.697946	32.357023	-0.311078
H	7.493785	34.292113	1.508504	C	6.244407	30.956691	-0.387812
O	6.145012	29.208929	-3.811559	O	5.206657	31.133189	0.059783
N	9.797480	30.345342	-1.976404				
O	4.178278	26.593850	-5.260726				
N	8.748592	28.737707	-3.334114	F			
H	5.845287	25.713267	-1.800120	Fe	8.195752	30.523591	-1.341738
H	5.419975	27.240108	-0.993993	Br	8.610003	28.655592	0.280758
H	5.085813	28.840368	-5.498844	Br	7.795944	32.270678	-3.082249
H	6.743194	28.203255	-5.537410	O	7.417404	27.365816	-2.588370
H	8.910856	27.935390	-3.930357	N	10.868177	31.828496	-0.604946
H	11.684734	32.393400	-0.350742	O	3.970951	26.278253	-2.713310
C	5.895860	31.132685	0.016470	P	7.674964	28.968125	-2.851186
O	4.883809	31.324130	0.503789	P	9.274687	32.033510	0.040004
				C	11.527415	29.290429	-3.799512
CP				H	11.644982	28.624503	-4.646298
Fe	8.005376	30.637623	-1.162911	C	10.273121	29.463993	-3.207555
Br	8.345762	28.784724	0.521023	C	4.999147	27.248312	-2.850213
Br	7.487246	32.372010	-2.906226	H	4.614383	28.252350	-2.622841
O	7.219397	27.325773	-2.491533	C	3.244550	26.233645	-3.954034
N	10.860178	31.872609	-0.603194	C	5.340237	27.145845	-4.338758
O	3.854002	26.095864	-2.923773	H	5.993460	26.275071	-4.498035
P	7.455786	28.939800	-2.747093	C	5.983632	28.411818	-4.933042
P	9.338583	32.186455	0.165354	C	9.517052	31.619097	1.853596
C	11.328744	29.217371	-3.735897	H	9.687932	30.538916	1.819578
H	11.403164	28.517682	-4.560476	C	8.228780	31.861836	2.656803
C	10.098315	29.441210	-3.106482	H	7.994591	32.927529	2.752925
C	4.833644	27.124059	-2.968027	H	8.350647	31.462909	3.669647
H	4.372353	28.103853	-2.781206	H	7.369666	31.355018	2.208710
C	3.251998	26.007775	-4.226990	C	8.979312	33.898434	0.064949
				H	9.364686	34.230857	1.037226

C	9.735576	34.659679	-1.035237	H	2.918114	24.935427	-4.858431
H	10.820268	34.541522	-0.953851	H	2.358677	24.542545	-3.216311
H	9.513949	35.729404	-0.945921	H	4.094793	24.703667	-3.545184
H	9.424254	34.323059	-2.026339	C	10.866238	31.422967	-2.181002
C	6.197259	26.904686	-1.963290	H	10.872614	32.505934	-2.263215
C	1.926515	26.992353	-3.835297	C	12.060566	30.717638	-2.280225
H	1.421589	27.027267	-4.804760	H	13.007424	31.222710	-2.436724
H	2.111882	28.017242	-3.504297	C	15.017503	26.758504	-4.454972
H	1.269695	26.500489	-3.112690	H	15.183104	27.834141	-4.328595
C	11.123265	30.987351	-1.665063	H	15.106901	26.542129	-5.525134
C	3.066641	24.769387	-4.339679	H	15.828396	26.226440	-3.946880
H	2.515225	24.689807	-5.280434	C	15.090438	25.116151	-0.963142
H	2.513462	24.237444	-3.560588	H	14.246768	24.588893	-0.507394
H	4.043121	24.293481	-4.459451	H	15.953022	25.005618	-0.297228
C	12.600572	30.003041	-3.274268	H	15.337028	24.616572	-1.903454
H	13.588670	29.889575	-3.710019	O	6.149079	29.664746	-2.397337
C	12.414192	30.863731	-2.201777	N	10.853982	28.653191	-1.962303
H	13.235265	31.433353	-1.781646	O	4.083357	27.304956	-4.121289
C	10.730874	32.295035	2.508266	N	8.534279	28.619060	-1.754082
H	11.667054	32.050853	1.995988	H	5.069048	26.292705	-0.427368
H	10.831696	31.937597	3.539124	H	4.764487	27.902034	0.265987
H	10.635670	33.385766	2.555572	H	5.281583	29.418761	-4.221127
C	7.470301	34.206970	0.018699	H	6.839400	28.572644	-1.903342
H	7.054498	33.926938	-0.951528	H	8.602016	27.618305	-1.945354
H	7.315963	35.281817	0.166973	H	14.007026	29.112135	-2.499991
H	6.909441	33.684201	0.798848	C	11.550033	23.014313	-0.511943
O	6.500651	29.309790	-3.928339	O	10.695132	22.397131	-0.087463
N	10.073826	30.287446	-2.152144				
O	4.063969	26.914748	-4.924253				
N	9.155746	28.790410	-3.678164				
H	6.294286	25.818933	-1.900519				
H	6.126848	27.316513	-0.952931				
H	5.213310	28.984280	-5.452338				
H	6.777622	28.164267	-5.645633				
H	9.322297	28.018082	-4.309900				
H	11.660563	32.346193	-0.251681				
C	6.548659	30.762696	-0.677854				
O	5.488548	30.910440	-0.254151				
G							
Fe	10.927020	26.534037	-1.369890				
Br	9.548488	25.373988	-2.963283				
Br	10.872539	26.408958	1.003870				
O	6.525201	27.641160	-0.834131				
N	13.171695	28.571850	-2.315597				
O	3.265249	26.736082	-2.046857				
P	7.044083	29.205074	-1.081839				
P	13.239825	26.845576	-2.189070				
C	9.661846	30.752414	-2.015602				
H	8.716791	31.281006	-2.010887				
C	9.688752	29.352195	-1.904435				
C	4.302147	27.693377	-1.868710				
H	3.879281	28.705704	-1.803907				
C	3.032624	26.583562	-3.460762				
C	5.107347	27.554895	-3.162854				
H	5.782011	26.691087	-3.086973				
C	5.893056	28.820490	-3.542226				
C	13.638325	26.314920	-3.947251				
H	12.869262	26.863460	-4.507455				
C	13.385295	24.813472	-4.170549				
H	14.110890	24.188356	-3.641899				
H	13.474697	24.585086	-5.238389				
H	12.380954	24.525938	-3.848716				
C	14.780691	26.611775	-1.152530				
H	15.610614	27.076111	-1.703457				
C	14.628502	27.319754	0.204744				
H	14.454581	28.393373	0.092326				
H	15.547012	27.185925	0.786811				
H	13.793797	26.904665	0.776935				
C	5.131313	27.366051	-0.617396				
C	1.705274	27.224496	-3.851969				
H	1.564954	27.174887	-4.935530				
H	1.694451	28.273770	-3.546800				
H	0.875548	26.704875	-3.365100				
C	12.009384	29.320623	-2.184996				
C	3.105303	25.095789	-3.793069				
				TS_{GH}			
				Fe	10.947472	26.448291	-1.390653
				Br	9.535675	25.494701	-3.129921
				Br	10.849005	26.613176	1.000818
				O	6.533192	27.593343	-0.824033
				N	13.169901	28.528919	-2.337978
				O	3.275312	26.696238	-2.044015
				P	7.052777	29.161777	-1.052259
				P	13.253008	26.808183	-2.202687
				C	9.676383	30.721168	-1.953042
				H	8.734648	31.255073	-1.924517
				C	9.695796	29.317962	-1.878138
				C	4.308288	27.656305	-1.855185
				H	3.880827	28.665838	-1.779207
				C	3.041633	26.561450	-3.459409
				C	5.113237	27.535931	-3.151015
				H	5.790773	26.673518	-3.086290
				C	5.894902	28.808804	-3.513746
				C	13.658989	26.272750	-3.957981
				H	12.883262	26.810848	-4.518798
				C	13.422942	24.768408	-4.178503
				H	14.156404	24.152155	-3.649556
				H	13.515573	24.538387	-5.245647
				H	12.420800	24.470323	-3.859173
				C	14.791882	26.582376	-1.158613
				H	15.635458	26.988398	-1.733596
				C	14.669448	27.362310	0.161904
				H	14.564177	28.437876	-0.002640
				H	15.571427	27.199953	0.762250
				H	13.804190	27.028800	0.742550
				C	5.139598	27.319210	-0.607706
				C	1.711733	27.203170	-3.840955
				H	1.570483	27.167347	-4.924947
				H	1.698011	28.248345	-3.522141
				H	0.884052	26.674730	-3.360080
				C	12.008989	29.279091	-2.178786
				C	3.118316	25.078200	-3.810885
				H	2.930487	24.930909	-4.878036
				H	2.374076	24.515222	-3.240450
				H	4.109416	24.686307	-3.569143
				C	10.882619	31.388731	-2.113459
				H	10.895572	32.473372	-2.168428
				C	12.070784	30.677352	-2.241223
				H	13.020156	31.179367	-2.393040
				C	15.033182	26.728505	-4.467806
				H	15.189400	27.805386	-4.340907
				H	15.122756	26.513803	-5.538282
				H	15.849693	26.203037	-3.961649

C	15.052663	25.089495	-0.890722
H	14.212256	24.632261	-0.359014
H	15.941906	24.981974	-0.260426
H	15.229581	24.519674	-1.806466
O	6.148138	29.637133	-2.357048
N	10.854064	28.612761	-1.964312
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N	8.537565	28.588221	-1.737978
H	5.074935	26.244615	-0.425117
H	4.774313	27.849463	0.279899
H	5.281293	29.414333	-4.184336
H	6.841672	28.569883	-4.008340
H	8.600359	27.595498	-1.968288
H	14.003898	29.073037	-2.516130
C	11.096428	23.735257	-0.715061
O	10.592829	22.812987	-0.280436

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Br	9.560657	25.558491	-3.221816
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O	6.544205	27.542230	-0.851401
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P	7.060856	29.118075	-1.046962
P	13.250127	26.775963	-2.182797
C	9.683539	30.698248	-1.936631
H	8.743367	31.235104	-1.908071
C	9.697270	29.294293	-1.886711
C	4.307287	27.622454	-1.856987
H	3.871922	28.626056	-1.753310
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C	5.868239	28.827831	-3.500479
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H	12.838837	26.771963	-4.490368
C	13.414602	24.737333	-4.168094
H	14.162966	24.128691	-3.651095
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C	14.806533	26.546463	-1.163520
H	15.644818	26.930379	-1.760733
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C	5.153468	27.263306	-0.625426
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H	1.545069	27.184220	-4.912368
H	1.676336	28.231697	-3.484727
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C	12.008743	29.248681	-2.161485
C	3.120349	25.081807	-3.863395
H	2.924196	24.958800	-4.932150
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C	15.053145	25.054436	-0.877639
H	14.224729	24.619026	-0.309169
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H	15.190923	24.464982	-1.787596
O	6.132288	29.623864	-2.324307
N	10.850625	28.584744	-1.974851
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N	8.533574	28.566115	-1.768665
H	5.090578	26.185379	-0.462301
H	4.797250	27.776497	0.275864
H	5.240439	29.447374	-4.144734

H	6.809193	28.609933	-4.015572
H	8.593998	27.582761	-2.036549
H	14.007623	29.035925	-2.478454
C	10.954163	24.246799	-0.683157
O	10.792731	23.194012	-0.282427

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Fe	7.784731	31.059527	-0.067848
Br	8.395976	29.085045	1.281910
Br	6.445583	32.657914	-1.389183
O	5.751063	27.828882	-2.167081
N	10.619546	32.283848	-0.846150
O	3.172481	26.113530	-3.999859
P	6.406830	29.201777	-2.872657
P	9.623980	32.609989	0.533544
C	10.219029	29.004333	-3.328211
H	10.071546	28.140226	-3.965136
C	9.184769	29.430877	-2.488985
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H	10.800228	31.057763	1.862391
C	10.058763	32.439256	3.319691
H	9.984319	33.514151	3.516271
H	10.647645	31.999791	4.131927
H	9.056715	32.003556	3.369176
C	9.498394	34.487714	0.559648
H	10.387288	34.859829	1.085781
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H	10.382264	34.903818	-1.414371
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H	8.621999	34.707608	-1.425541
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H	1.509469	25.475616	-6.078983
C	10.467234	31.203517	-1.706035
C	3.409247	23.877474	-4.826190
H	3.635339	23.264424	-5.702934
H	2.409803	23.620067	-4.464217
H	4.132867	23.651154	-4.039196
C	11.408811	29.726730	-3.345735
H	12.225354	29.421399	-3.993320
C	11.543104	30.843071	-2.537528
H	12.462521	31.418787	-2.517135
C	12.157925	32.734780	1.917410
H	12.682743	32.472111	0.993022
H	12.755201	32.337421	2.745594
H	12.157354	33.826134	2.015508
C	8.242329	34.899355	1.352643
H	7.340454	34.574712	0.825690
H	8.209633	35.990219	1.448622
H	8.221770	34.479549	2.362500
O	6.248022	28.814660	-4.488083
N	9.305468	30.515453	-1.688268
O	4.816041	25.724777	-5.564460
N	7.997777	28.685594	-2.428278
H	4.145651	26.646130	-1.788621
H	3.724128	28.346121	-2.097352
H	6.234128	27.616581	-6.128602
H	7.432319	27.146993	-4.905258
H	8.146729	27.681958	-2.464681
H	11.515853	32.745683	-0.930560
C	6.239884	31.359348	1.488366
O	5.388326	31.437781	2.240208

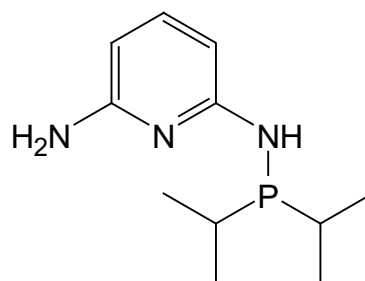
[Fe(κ^2 (P,N)-PNP-iPr/TAD)Br₂]

Fe	8.855669	11.599061	28.360055
O	11.161326	6.547713	30.168059
C	11.351155	7.944752	32.161347

N	10.970513	11.020617	28.292883	C	12.318644	10.377261	33.188228
P	9.898494	13.817764	28.159226	H	12.691360	11.318027	33.583572
N	10.403802	8.873333	28.982447	Br	7.907722	11.098404	26.237702
C	12.617870	9.273378	28.056372	C	12.601346	8.442459	31.764476
H	12.899925	8.238249	28.200647	H	13.195053	7.877229	31.053712
C	13.159526	11.540384	27.426460	N	11.484840	13.249749	27.768687
H	13.852510	12.280446	27.041420	Br	8.045950	11.185497	30.580978
C	11.873403	11.915812	27.833637	C	11.340205	9.719524	28.436380
O	7.915255	4.513423	31.662112	C	13.510261	10.198475	27.532779
C	11.083715	9.881971	33.601652	H	14.501900	9.876321	27.228461
H	10.485516	10.434944	34.319873	P	10.399737	7.142669	28.823500
O	9.051227	5.900747	33.089823	O	8.785853	7.097024	29.233343
C	10.879421	6.599276	31.598796	C	13.078682	9.649968	32.267230
C	8.185054	3.522130	28.586858	H	14.046886	10.022411	31.944002
H	8.267399	3.111203	29.588217	H	9.640622	9.319025	29.492687
C	9.485322	14.888429	26.677175	H	12.204563	13.884743	27.450191
H	9.677290	14.173604	25.866052	C	11.393892	15.715761	29.783245
C	9.339229	6.374520	31.785042	H	11.516838	16.104867	30.800291
H	8.830094	7.327668	31.611071	H	12.303989	15.160400	28.537411
C	7.983652	15.226062	26.637322	H	11.319454	16.574992	29.111596
H	7.745035	15.704092	25.680997	H	10.274478	14.017161	30.461259
H	7.695008	15.920487	27.431822	[Fe(κ^3(P,N)-PNP-<i>i</i>Pr/TAD)Br₂]			
H	7.371671	14.323987	26.720093	Fe	8.819697	12.308493	29.172056
C	7.988650	4.942809	33.031898	O	7.644858	8.985184	28.194979
C	11.693412	5.446962	32.213893	C	8.901696	7.124318	27.242229
C	11.902682	5.396204	33.600475	N	10.799531	11.351838	28.784239
H	11.500214	6.179427	34.232114	P	10.156523	14.331553	28.408352
C	8.780927	5.287395	30.850278	N	9.961025	9.280635	29.520698
H	9.595695	4.644706	30.502056	C	12.297093	9.464903	28.991510
C	6.668195	5.590550	33.444138	H	12.431922	8.415746	29.226999
H	6.717961	5.904945	34.490873	C	13.149073	11.599961	28.278937
H	5.847186	4.878127	33.328299	H	13.964075	12.243467	27.966269
H	6.455951	6.461180	32.820606	C	11.848953	12.118159	28.400477
C	8.065123	5.885179	29.581476	O	5.106066	6.479541	30.236674
C	8.081838	4.906799	28.400225	C	10.682713	5.488861	27.003849
C	7.935359	5.405133	27.097005	H	11.098100	4.516918	27.255204
H	7.837154	6.474924	26.943438	O	6.544110	5.529040	28.724532
C	7.915864	4.539956	26.005046	C	7.549381	7.583034	27.800602
H	7.808976	4.944178	25.002498	C	4.290059	9.413516	31.218950
C	8.028263	3.160667	26.197699	H	3.855058	8.556689	30.714080
H	8.011473	2.486388	25.346167	C	9.812865	15.094445	26.725681
C	8.156509	2.655476	27.490723	H	9.393000	14.226966	26.201278
H	8.236515	1.584266	27.653177	C	7.116124	6.776374	29.071298
C	12.232556	4.428809	31.417907	H	8.001929	6.615771	29.696786
H	12.100674	4.465819	30.343652	C	8.696903	16.148663	26.811328
C	12.955926	3.380824	31.994547	H	8.359555	16.405354	25.801307
H	13.368894	2.603204	31.357845	H	9.044161	17.072211	27.285327
C	13.152482	3.335408	33.373340	H	7.828667	15.774286	27.361158
H	13.717257	2.522471	33.821060	C	5.443596	5.239286	29.596937
C	12.622587	4.350289	34.174162	C	6.478455	7.548170	26.697340
H	12.773030	4.330686	35.249978	C	6.295652	6.382018	25.937535
C	6.323404	7.674321	30.150977	H	6.914752	5.513012	26.126858
H	7.095648	8.431358	30.111873	C	6.022557	7.498366	29.871707
C	6.627807	6.332895	29.889089	H	5.508064	8.218656	29.228649
C	5.591796	5.387734	29.928750	C	5.865238	4.213700	30.647517
H	5.804381	4.345311	29.721151	H	6.130908	3.270577	30.160942
C	4.287290	5.774460	30.229612	H	5.045410	4.029073	31.346777
H	3.499516	5.026468	30.253043	H	6.724669	4.577300	31.214694
C	10.360406	16.130366	26.453648	C	6.582916	8.282469	31.118527
H	11.432741	15.909440	26.488837	C	5.665207	9.451035	31.494551
H	10.150697	16.910808	27.191096	C	6.190715	10.558911	32.171278
H	10.151838	16.552621	25.464218	H	7.251307	10.613663	32.386898
C	10.601189	8.672294	33.092536	C	5.364392	11.619907	32.540523
H	9.646790	8.293830	33.441864	H	5.800933	12.481158	33.036656
C	5.013501	8.060420	30.450427	C	3.997226	11.578193	32.262499
H	4.804776	9.108838	30.642741	H	3.354220	12.404676	32.551460
C	3.991235	7.114139	30.492694	C	3.462469	10.469442	31.606114
H	2.972706	7.415411	30.721270	H	2.399863	10.424896	31.384559
C	8.365696	3.750337	33.902702	C	5.682877	8.667398	26.420267
H	9.308671	3.322590	33.556547	H	5.840493	9.591610	26.963072
H	7.583628	2.987883	33.850540	C	4.712143	8.611431	25.415592
H	8.479636	4.063632	34.944182	H	4.109849	9.492046	25.211385
C	8.865173	15.587433	30.103623	C	4.524624	7.445379	24.676368
H	8.697028	16.443895	29.443305	H	3.770995	7.405874	23.894777
H	8.955639	15.973776	31.124320	C	5.324443	6.330351	24.939793
H	7.980073	14.944881	30.072204				
C	10.145642	14.823396	29.726435				

H	5.197044	5.418356	24.363126
C	8.088261	6.879470	32.650133
H	8.943595	7.205263	32.071894
C	6.811451	7.353049	32.322846
C	5.726016	6.949860	33.114947
H	4.731090	7.314242	32.888880
C	5.912420	6.089247	34.194679
H	5.057309	5.792535	34.795521
C	11.022377	15.599957	25.925967
H	11.791646	14.829672	25.814267
H	11.481162	16.486660	26.372969
H	10.698300	15.875885	24.915803
C	9.458300	5.878706	27.558143
H	8.928956	5.193476	28.211904
C	8.274555	6.016986	33.734295
H	9.275442	5.669021	33.974445
C	7.188179	5.615771	34.509376
H	7.332872	4.949224	35.354825
C	4.264671	4.777280	28.749286
H	4.021972	5.540362	28.007447
H	3.393323	4.601334	29.385934
H	4.512459	3.846939	28.230550
C	9.503218	16.369551	30.251364
H	9.034897	17.045362	29.530301
H	9.836096	16.975628	31.101484
H	8.749966	15.668133	30.618773
C	10.710623	15.623959	29.653775
C	11.361735	6.336921	26.131330
H	12.312177	6.033397	25.701674
Br	7.229695	12.458560	27.323515
C	9.584638	7.965893	26.350129
H	9.151389	8.927571	26.093665
N	11.628062	13.453551	28.114033
Br	9.123192	12.733393	31.568808
C	11.026435	10.050303	29.089726
C	13.356695	10.261079	28.578498
H	14.352211	9.835420	28.492822
P	8.301624	9.745946	29.488777
O	7.912169	8.762330	30.762904
C	10.805761	7.578137	25.804727
H	11.323273	8.243639	25.119673
H	10.183803	8.309772	29.703800
H	12.460432	13.951403	27.826299
C	11.823620	16.588800	29.221909
H	12.175019	17.157092	30.090972
H	12.695761	16.072921	28.804922
H	11.470379	17.313339	28.481750
H	11.099748	14.969245	30.444403

¹H-NMR (400 MHz, CDCl₃)



1a

7.2711
7.2514
7.2318

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6.4551

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5.8886

4.4098
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4.1839

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0.82

0.92

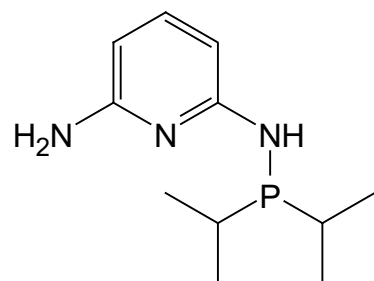
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1.89

12.00

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$^{31}\text{P}\{^1\text{H}\}$ -NMR (162 MHz, CDCl_3)



1a

—47.4360

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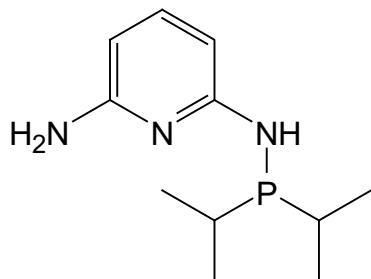
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157.2784

139.4274
139.4071

98.0777
97.9882
97.8955

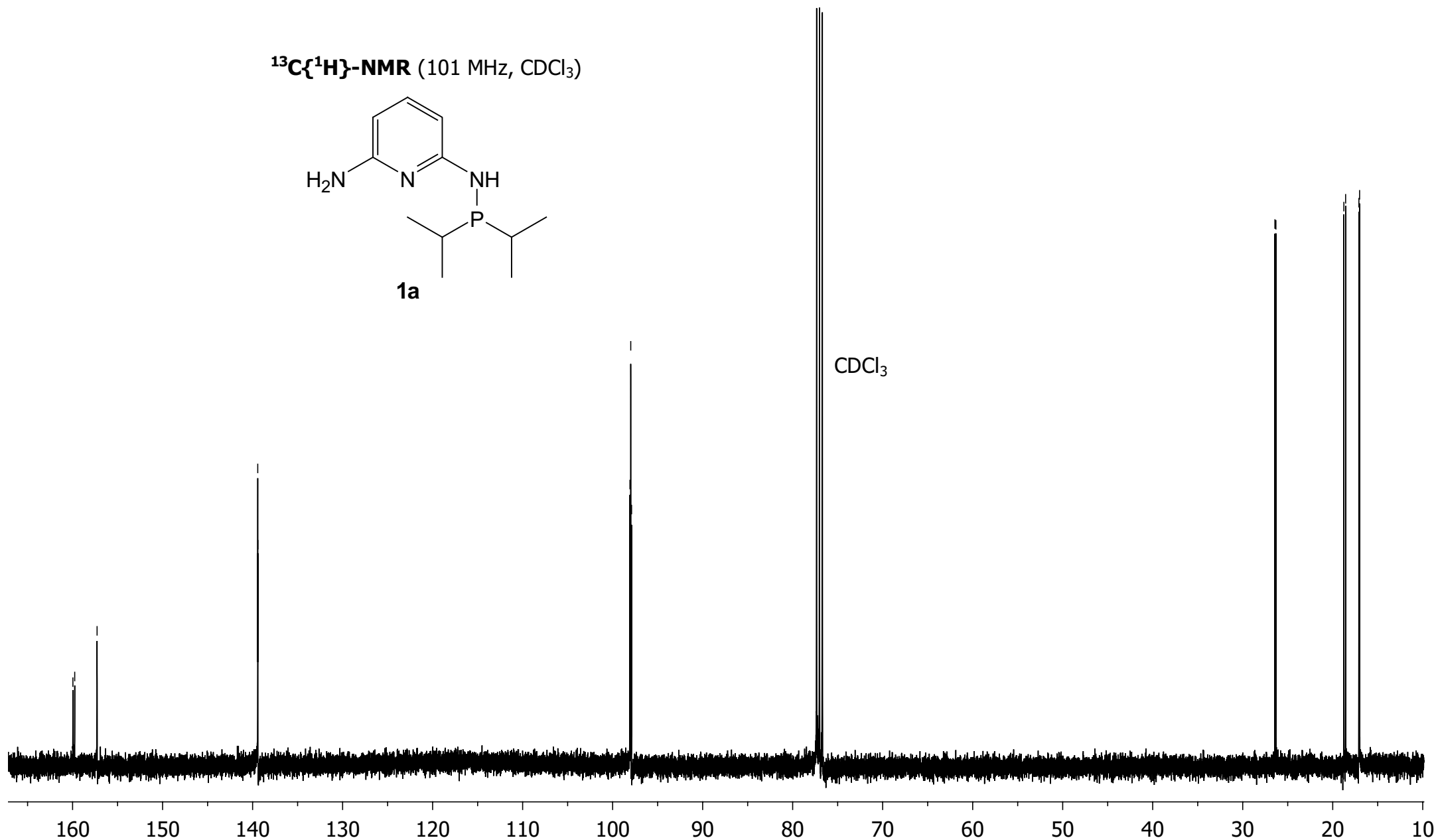
26.4224
26.3116
18.7617
18.5659
17.0909
17.0132

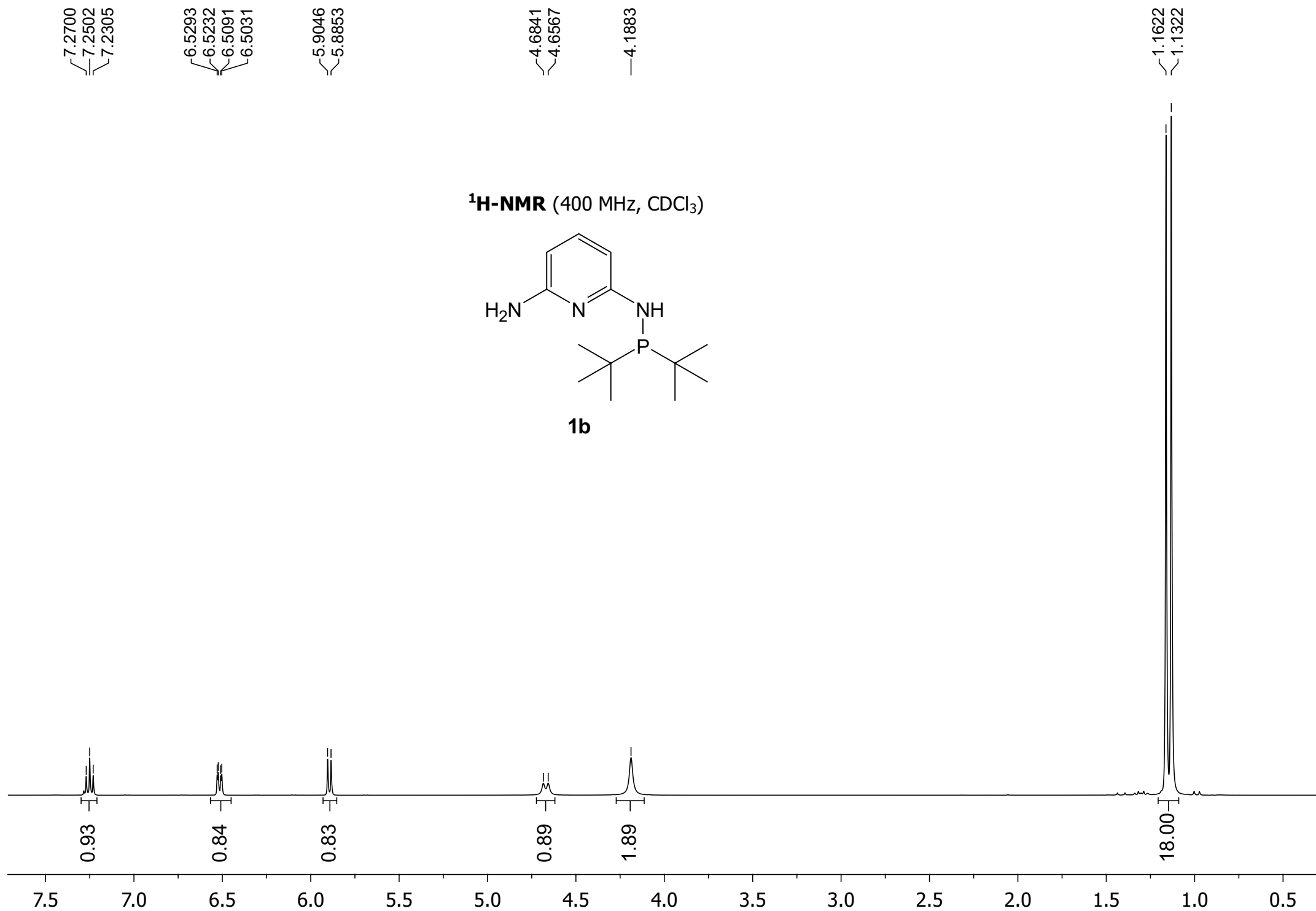
$^{13}\text{C}\{^1\text{H}\}$ -NMR (101 MHz, CDCl_3)



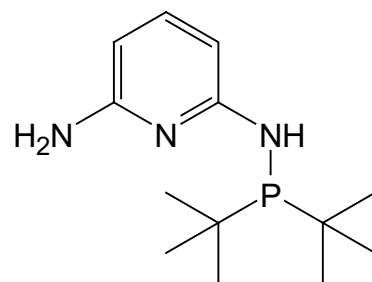
1a

CDCl_3



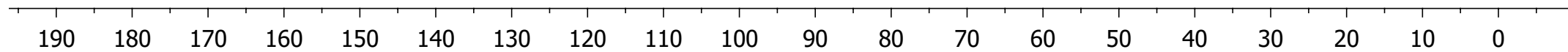


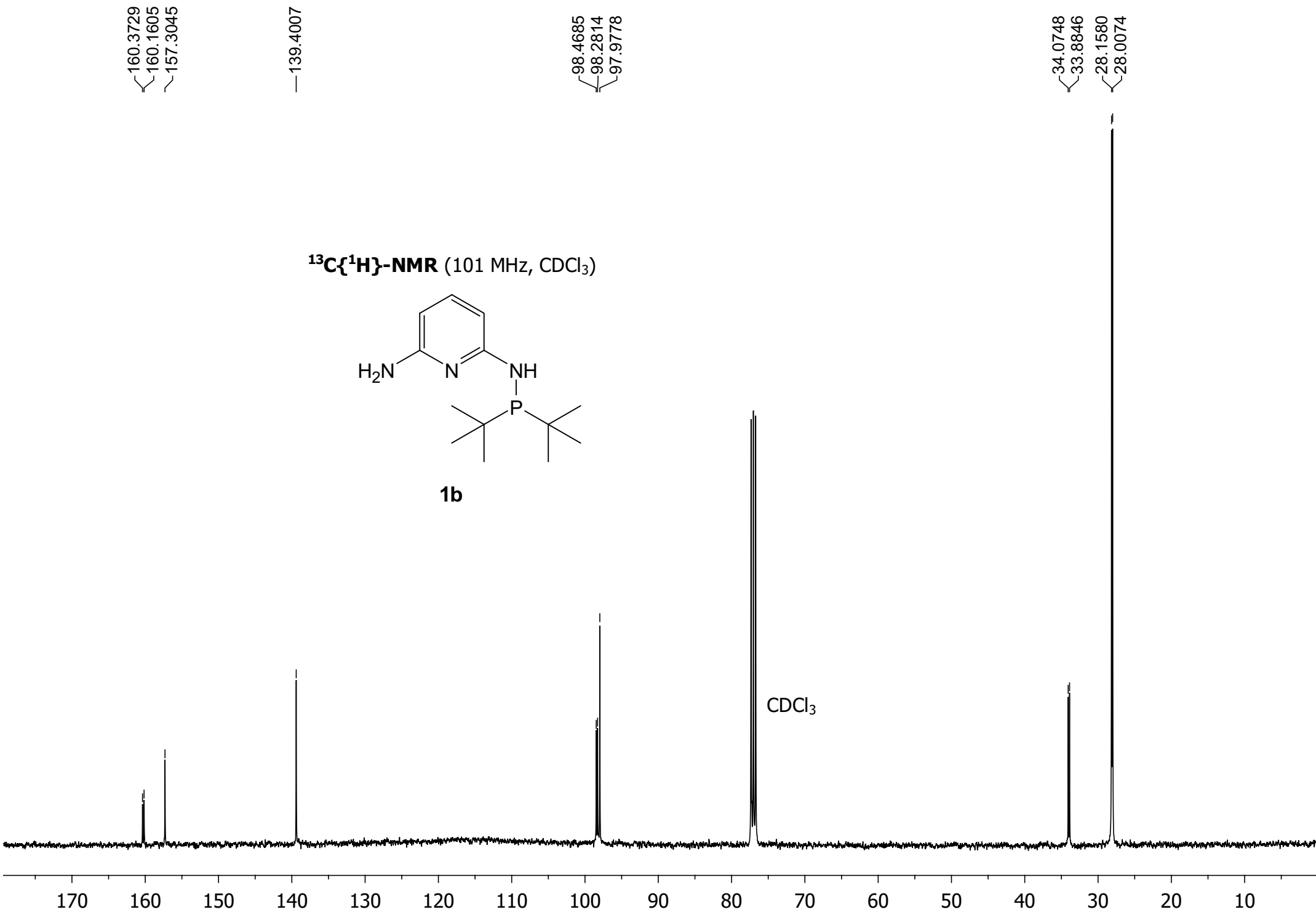
$^{31}\text{P}\{^1\text{H}\}$ -NMR (162 MHz, CDCl_3)

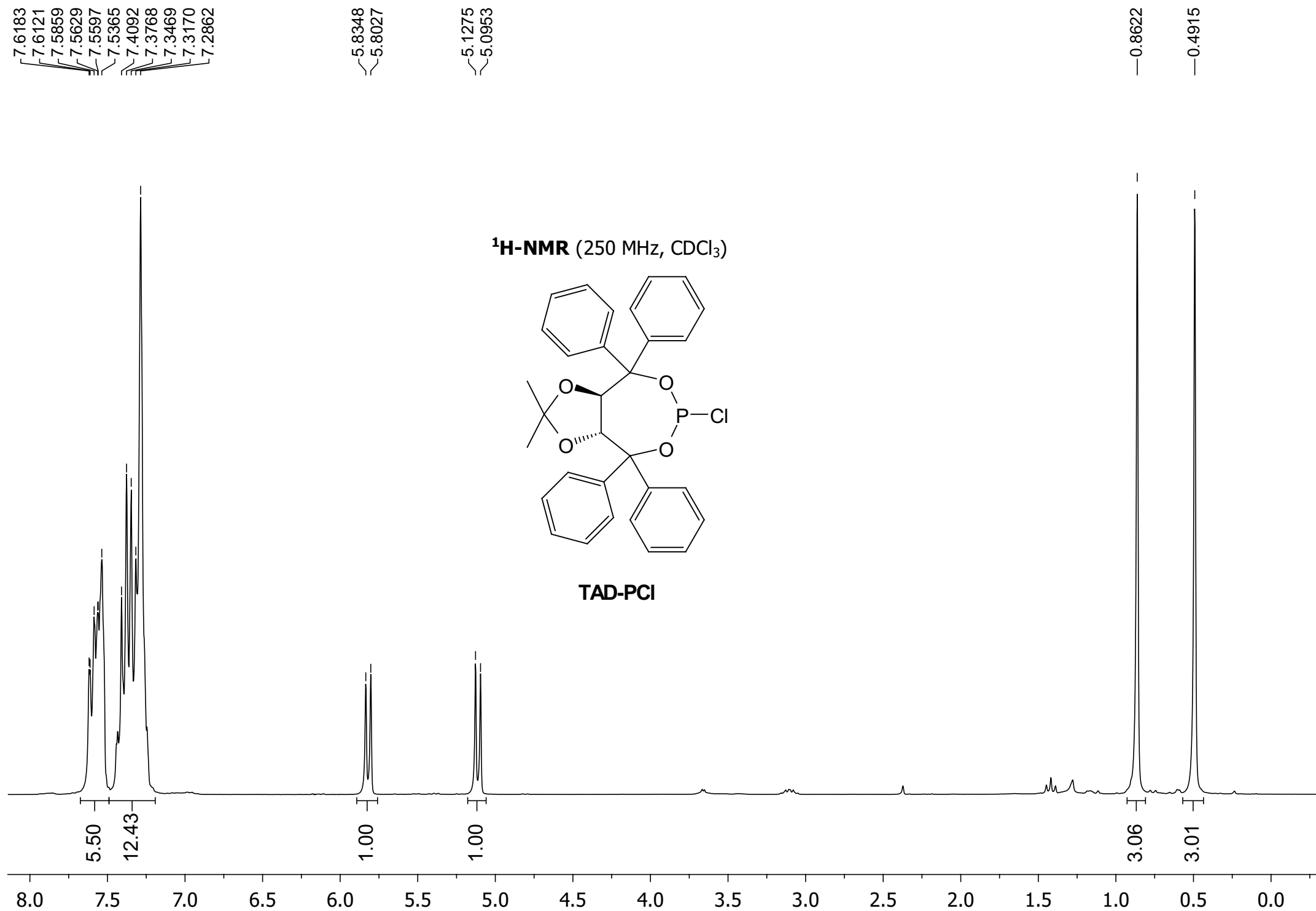


1b

—58.1892



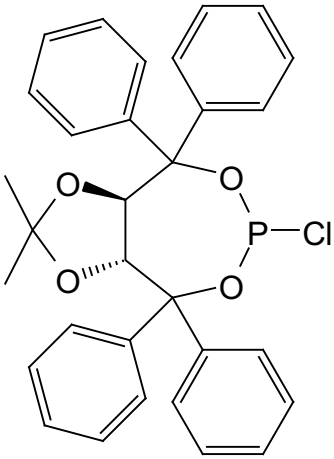




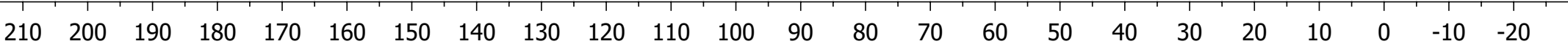
CHS0052
(TADDOL)PCl in CDCl₃

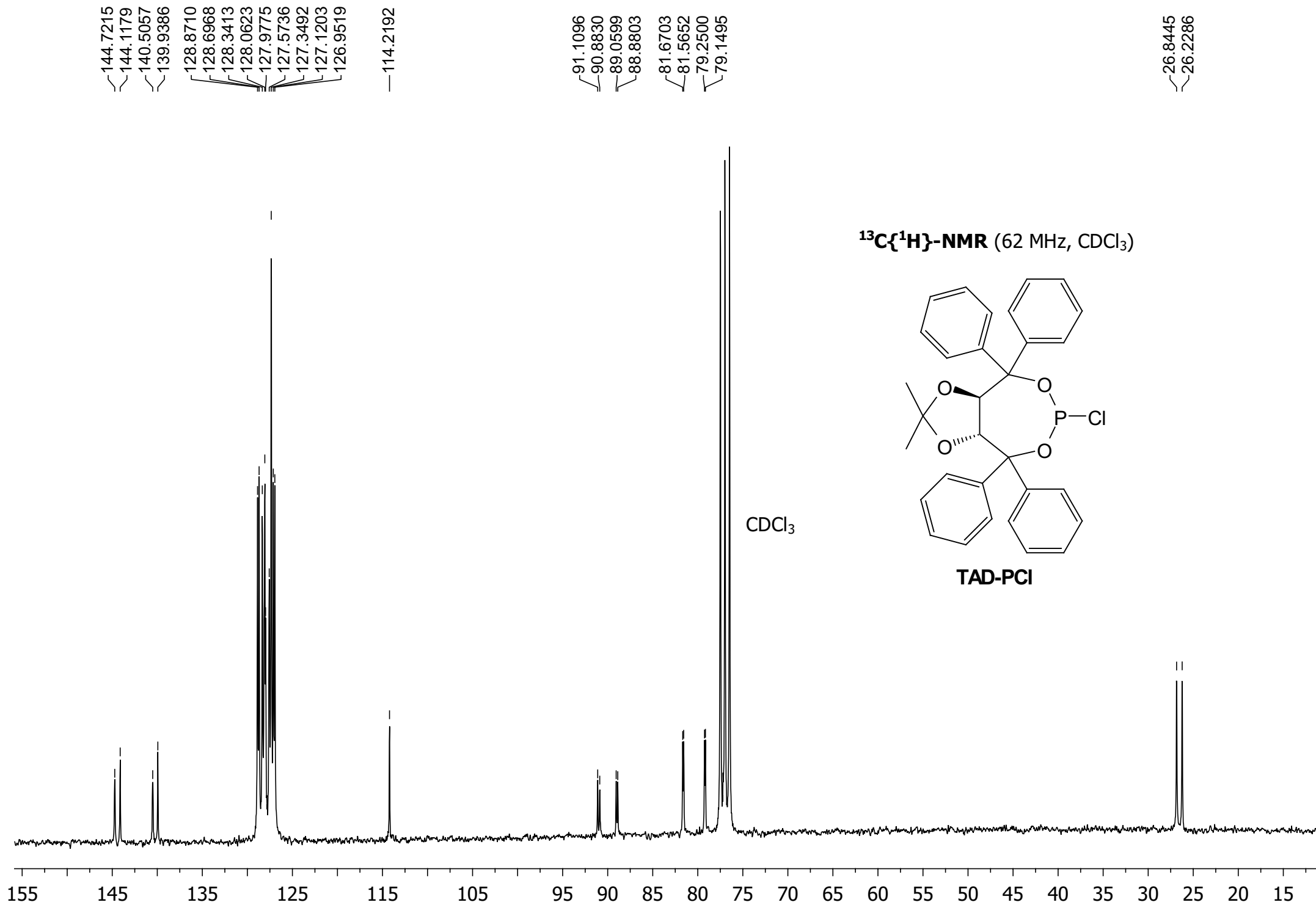
—148.0122

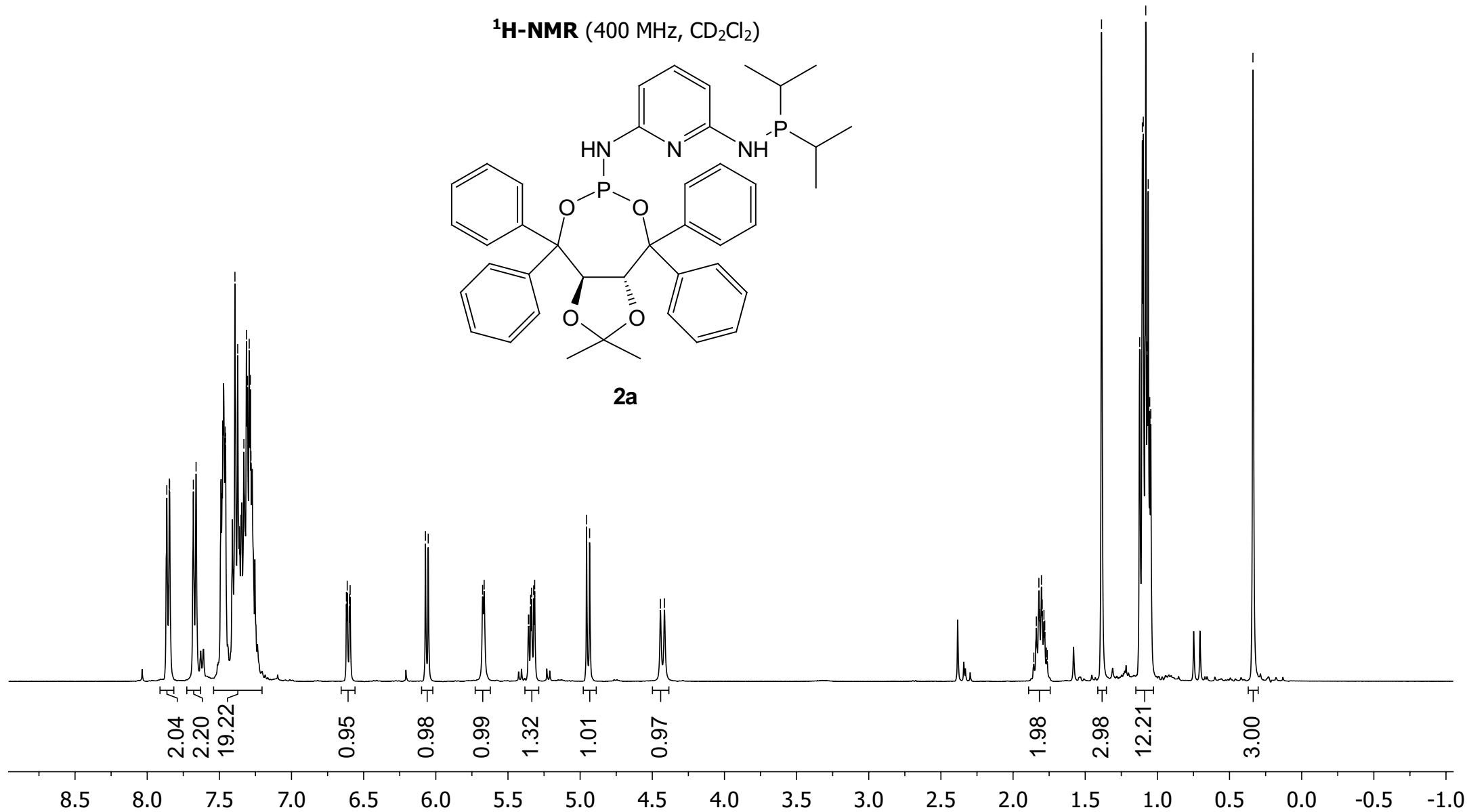
³¹P{¹H}-NMR (101 MHz, CDCl₃)

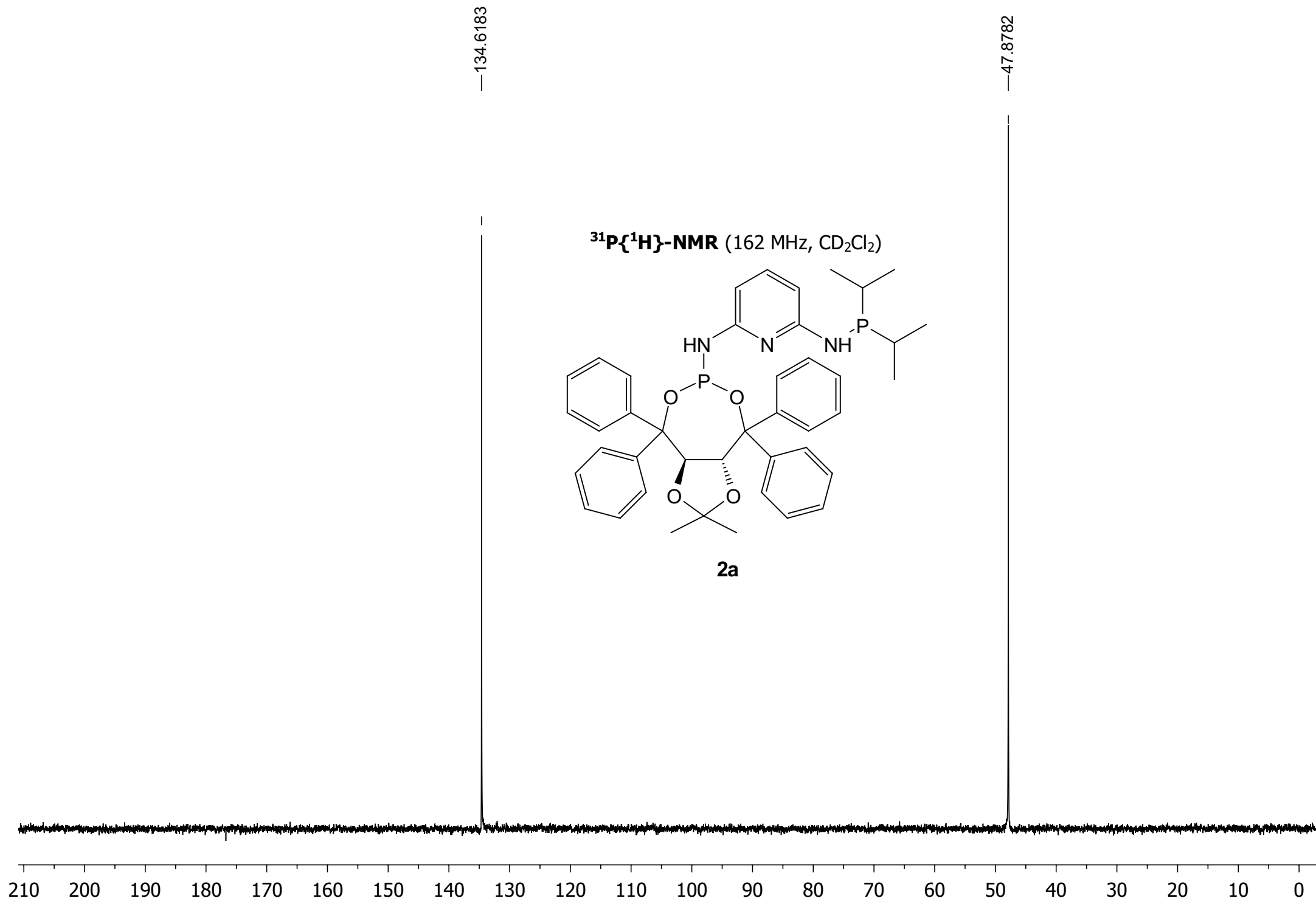


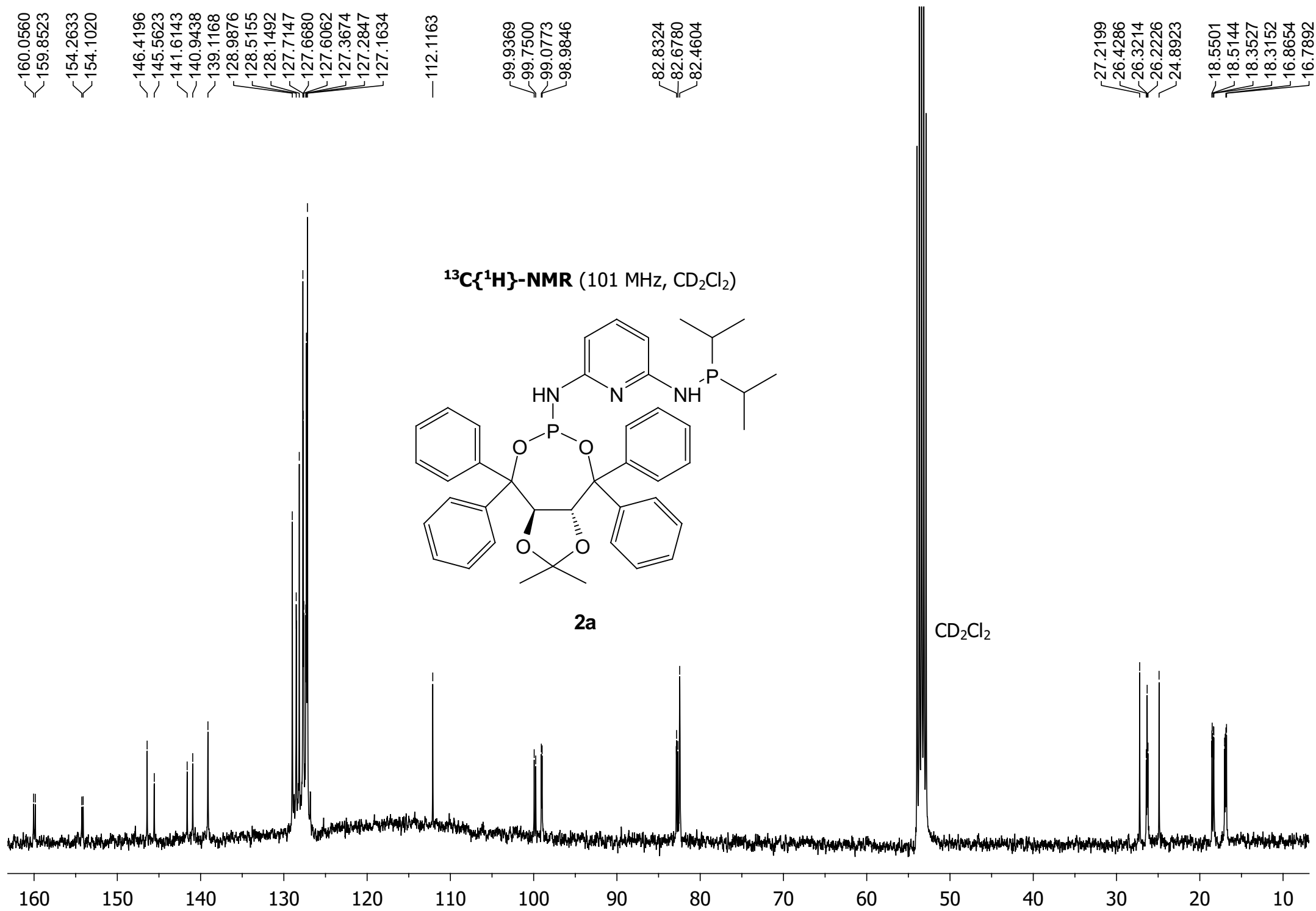
TAD-PCl

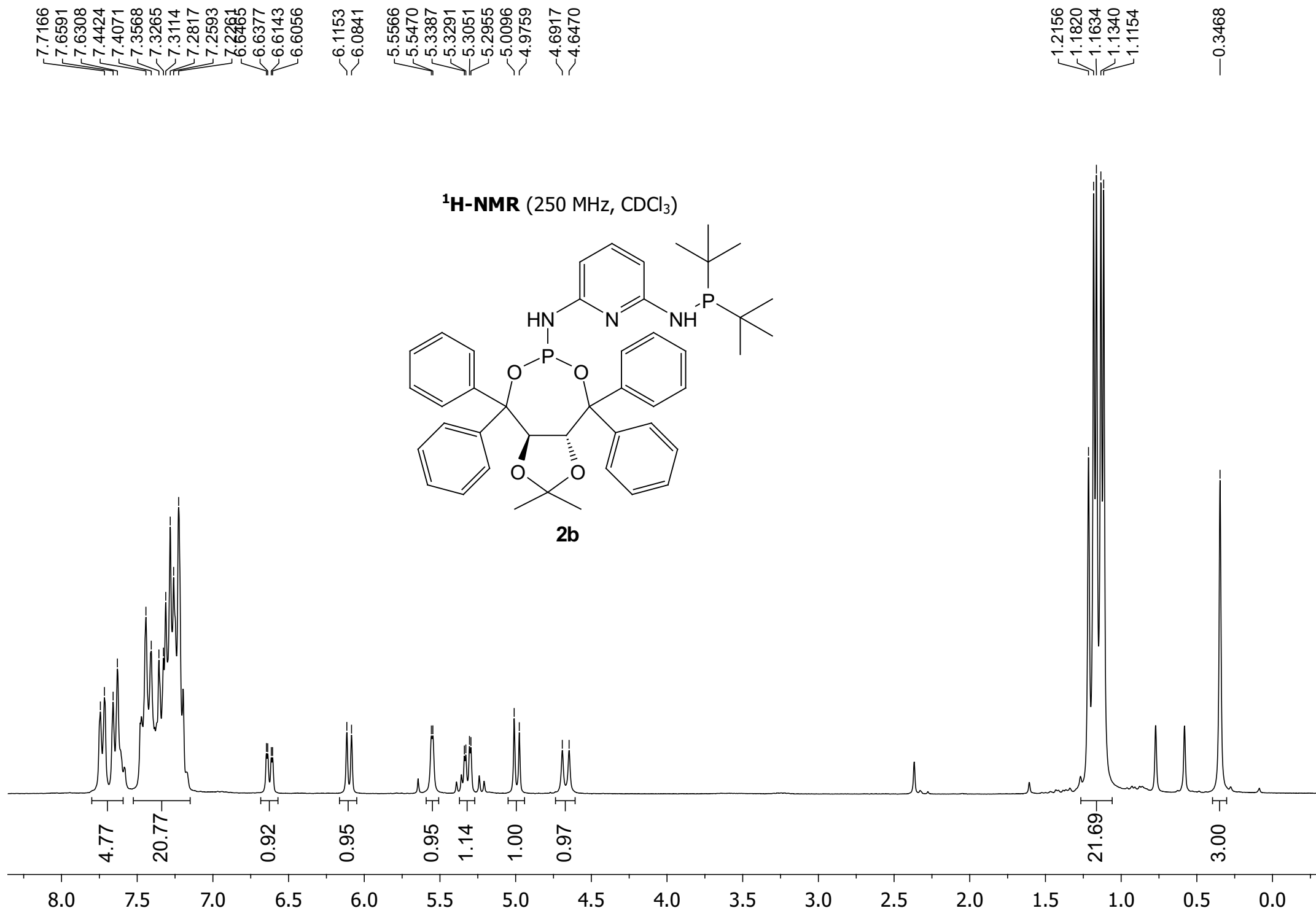


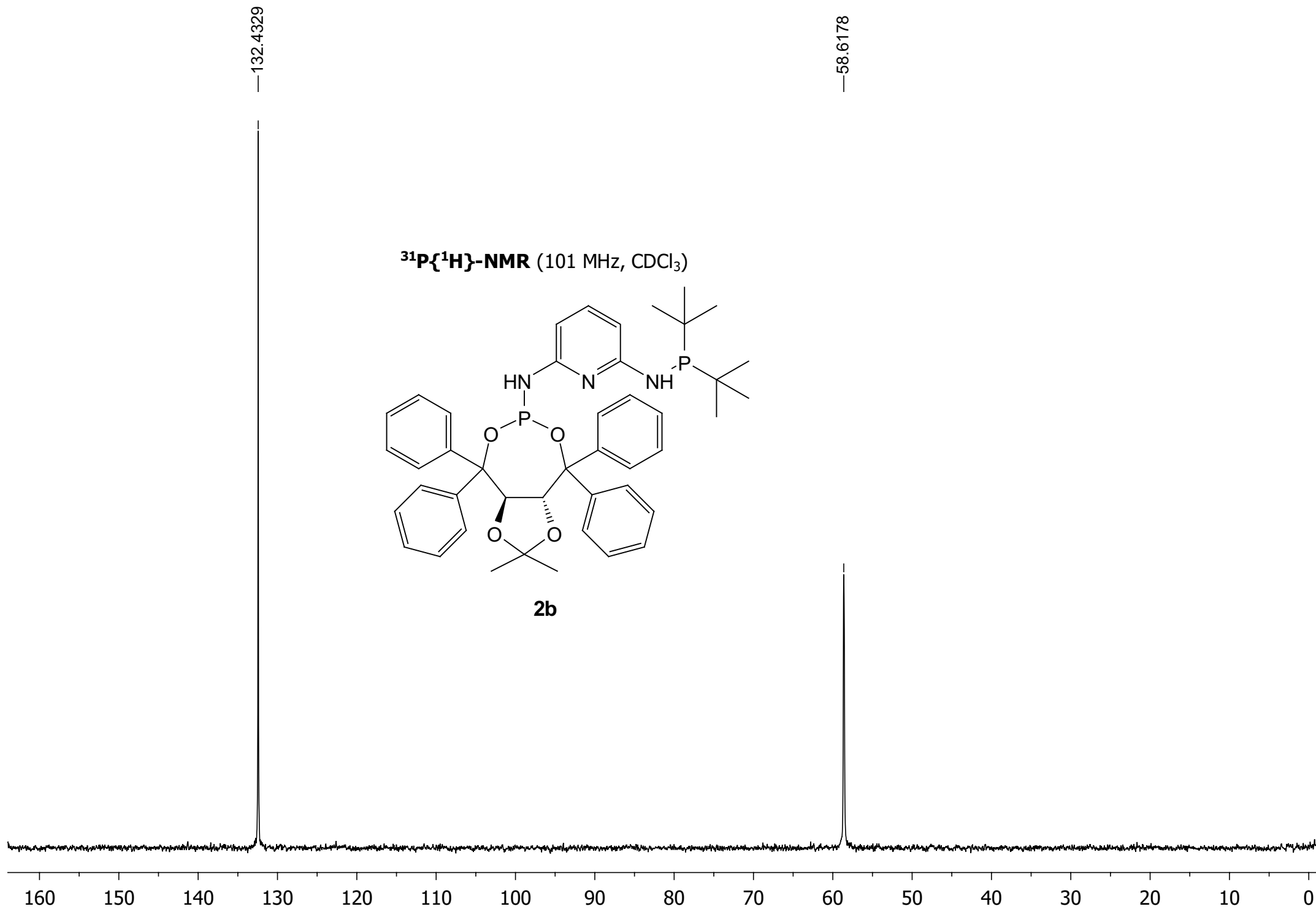


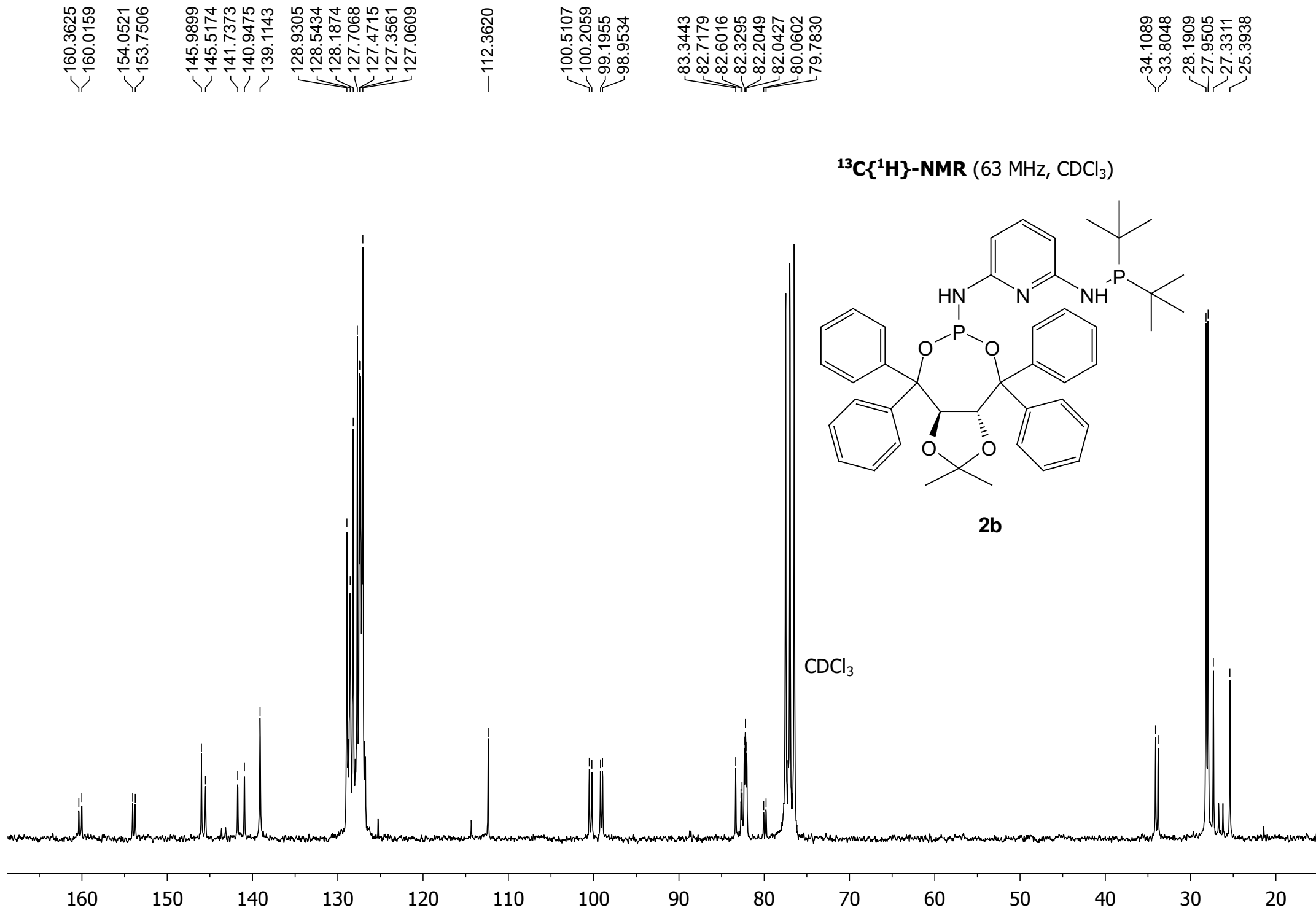


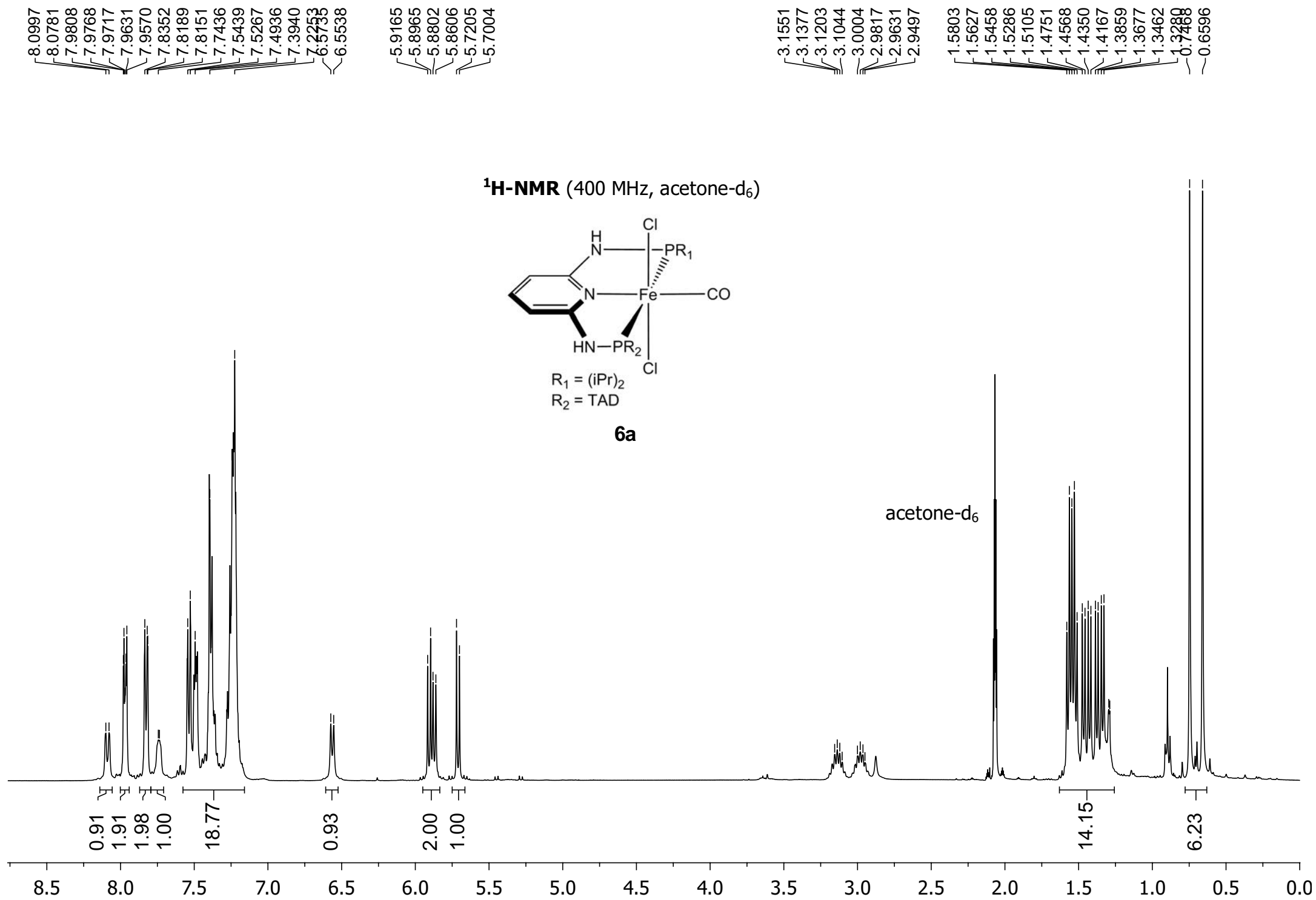


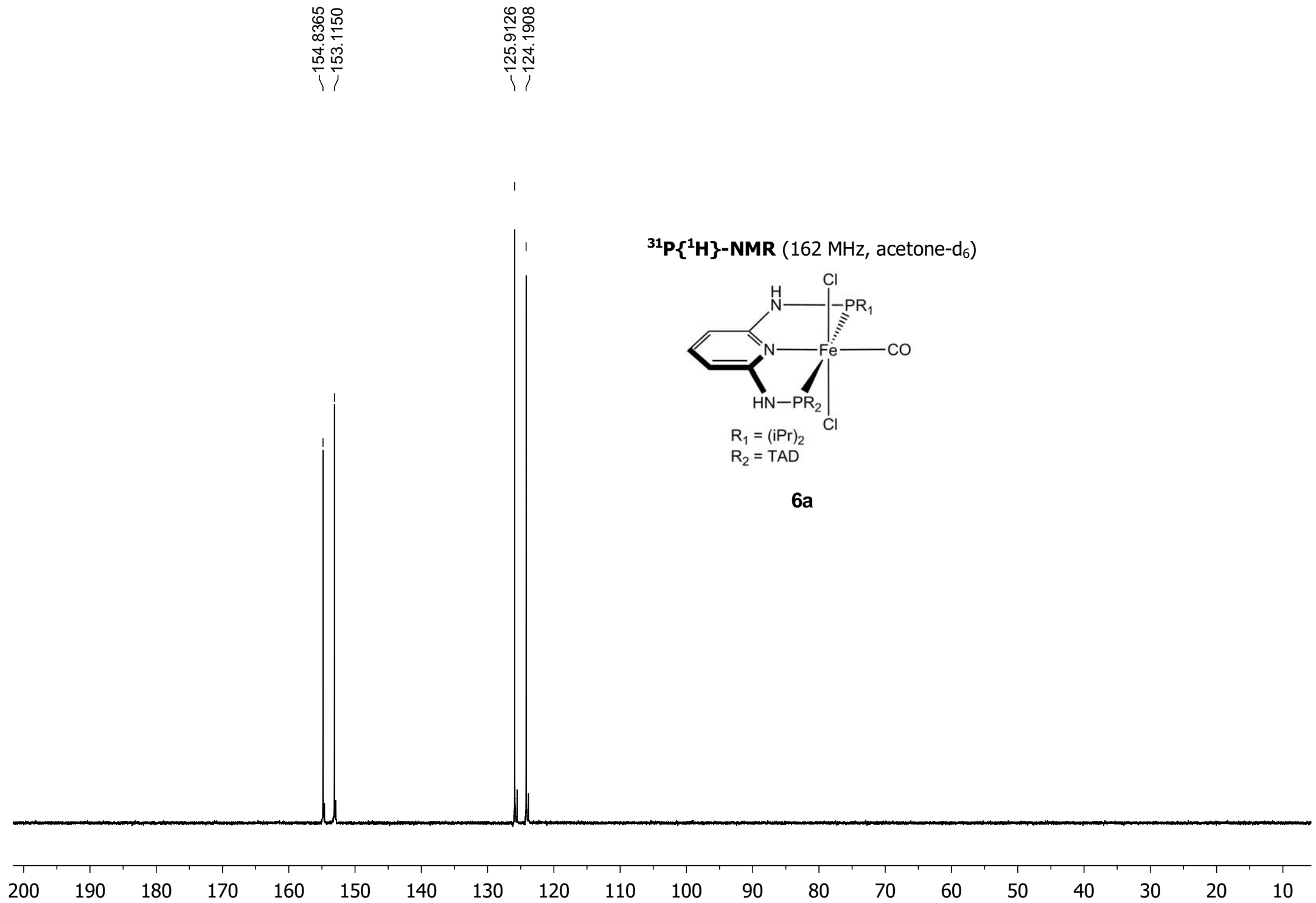


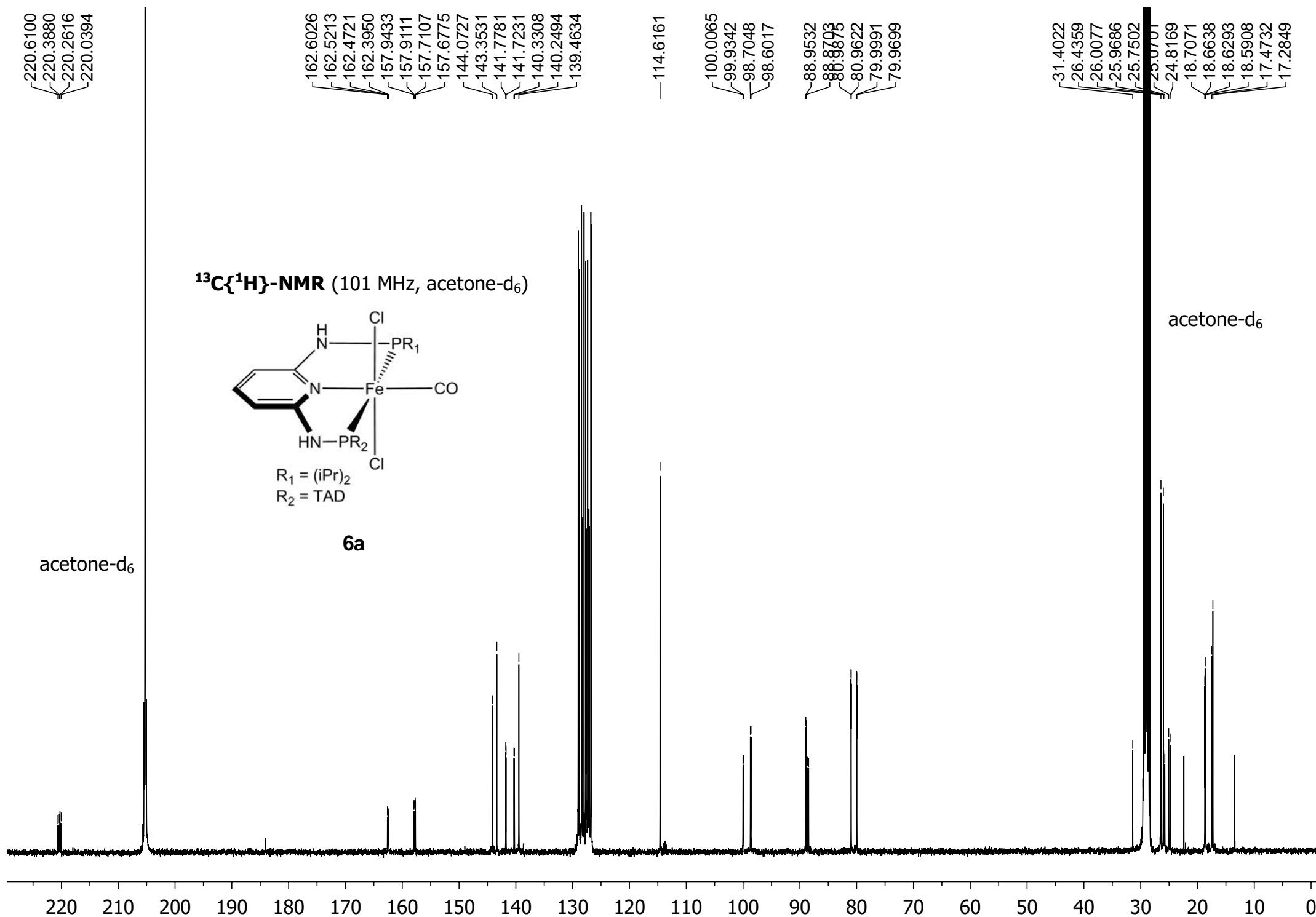


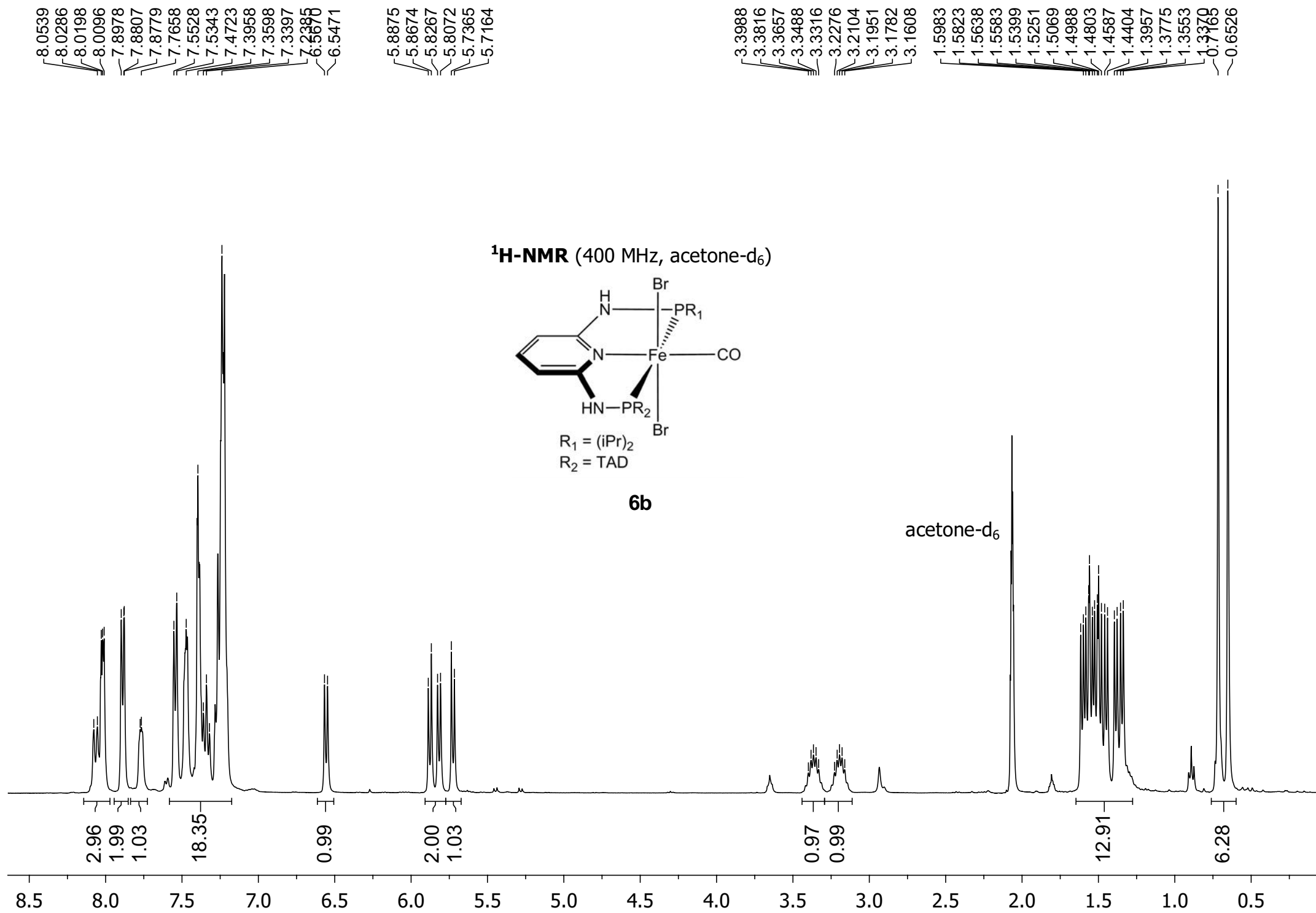


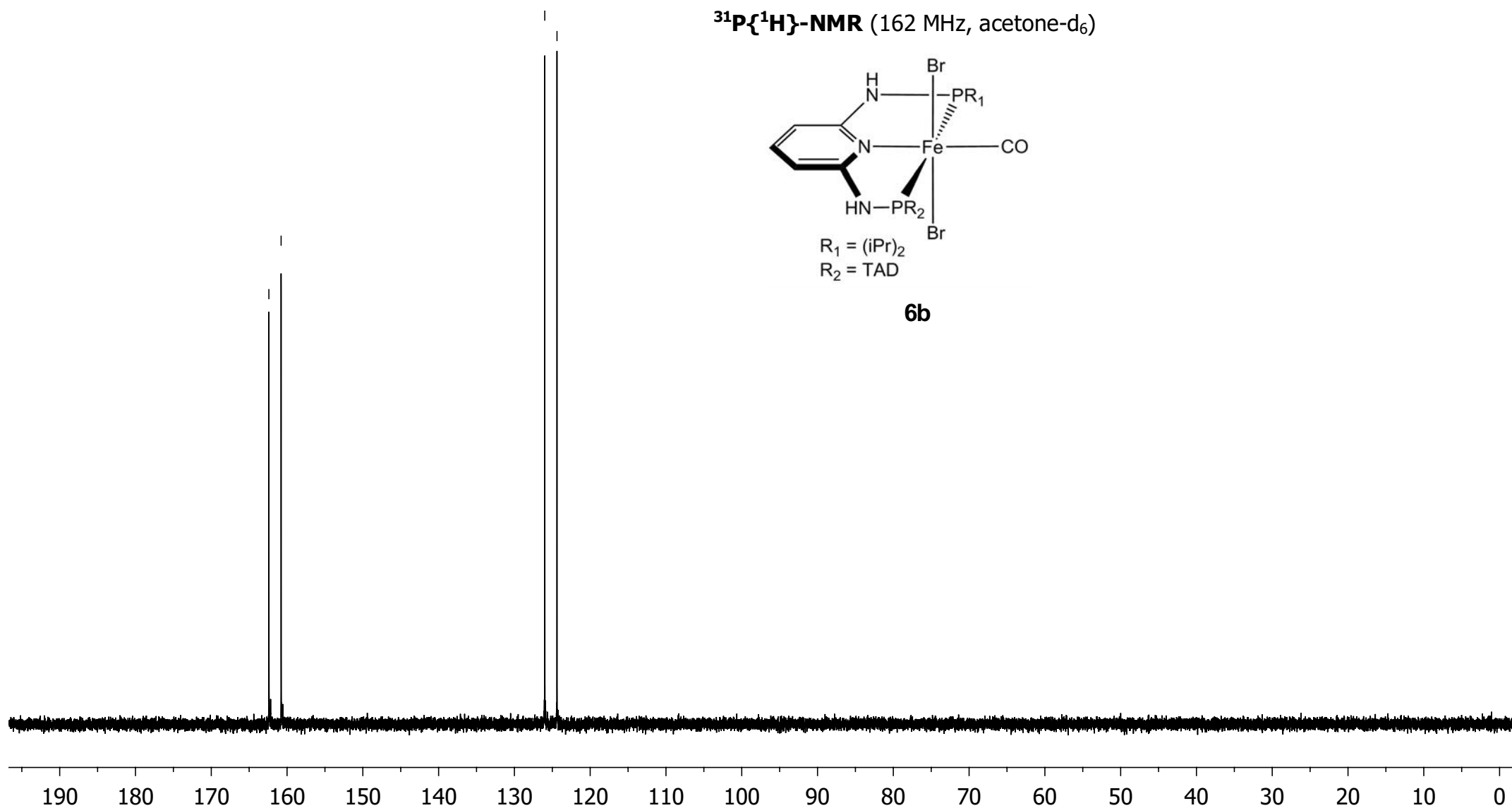


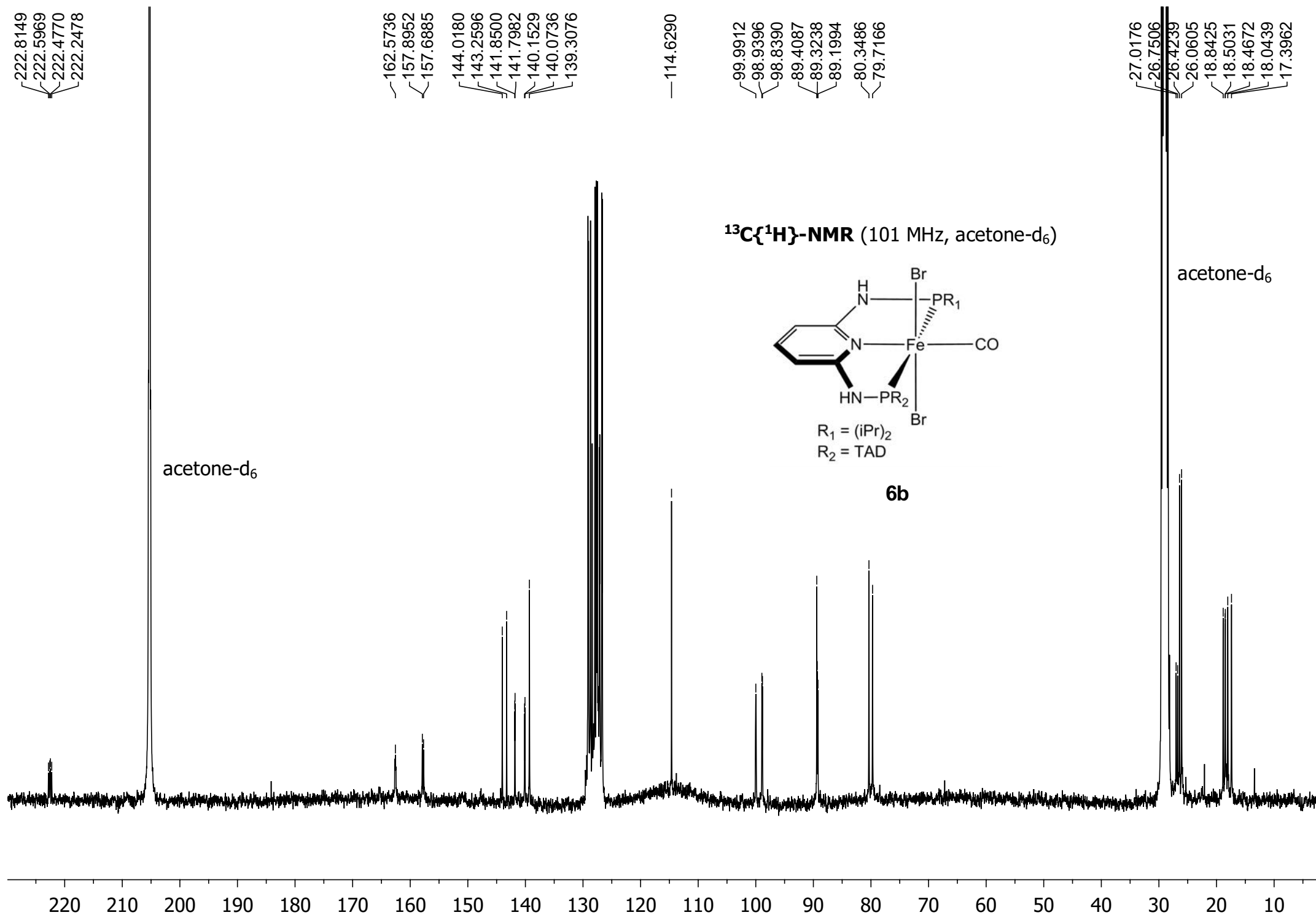


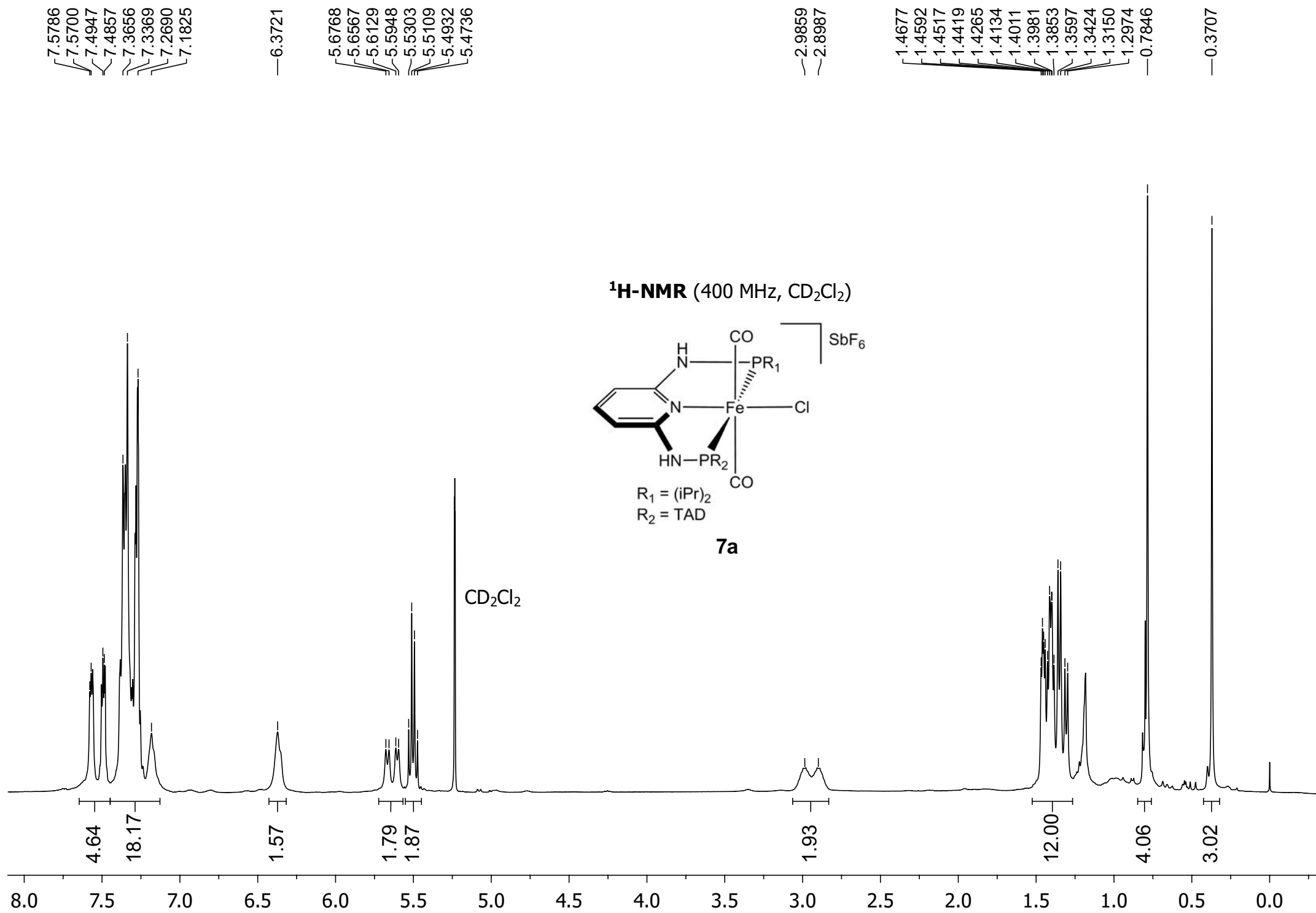


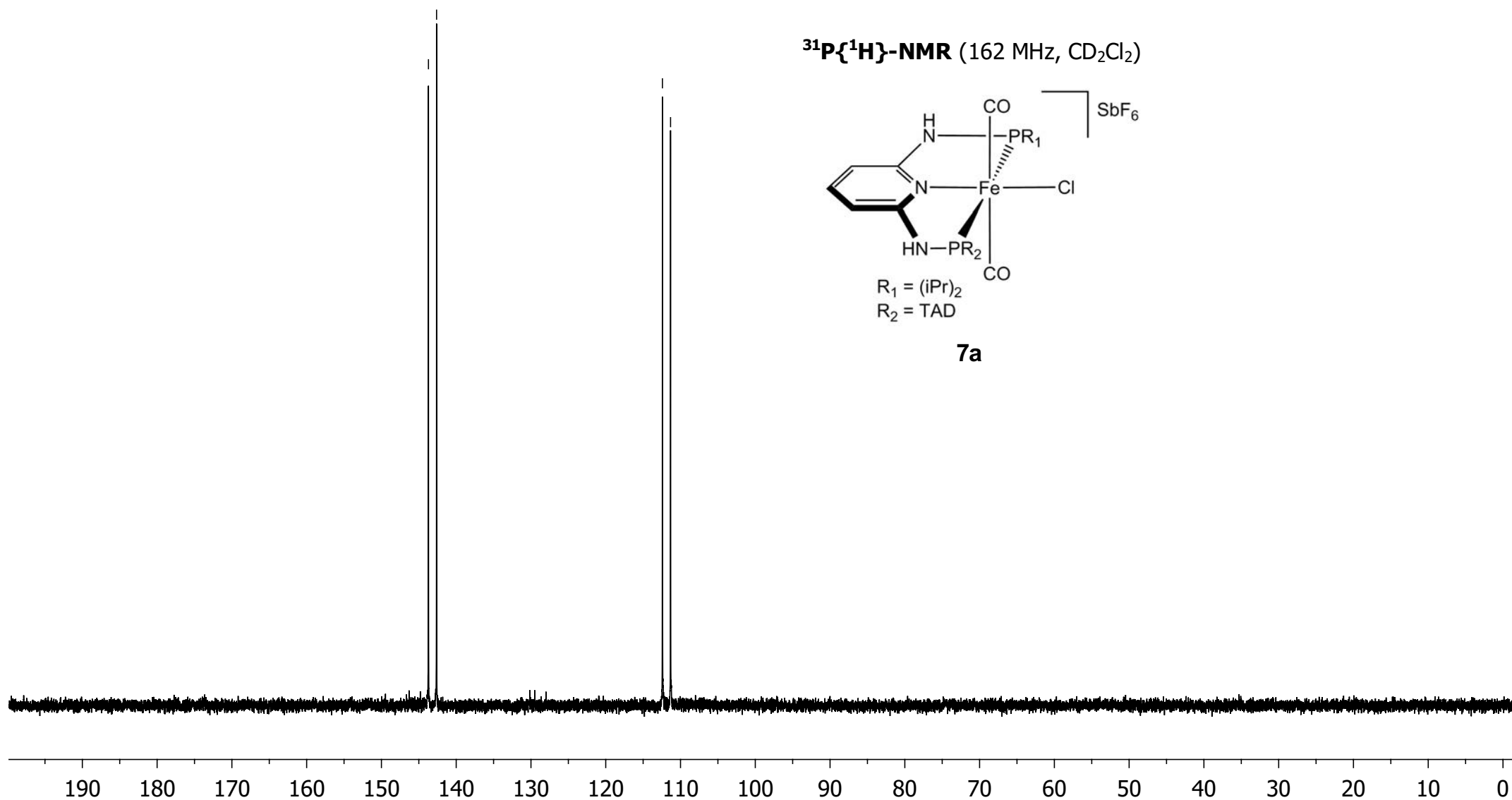


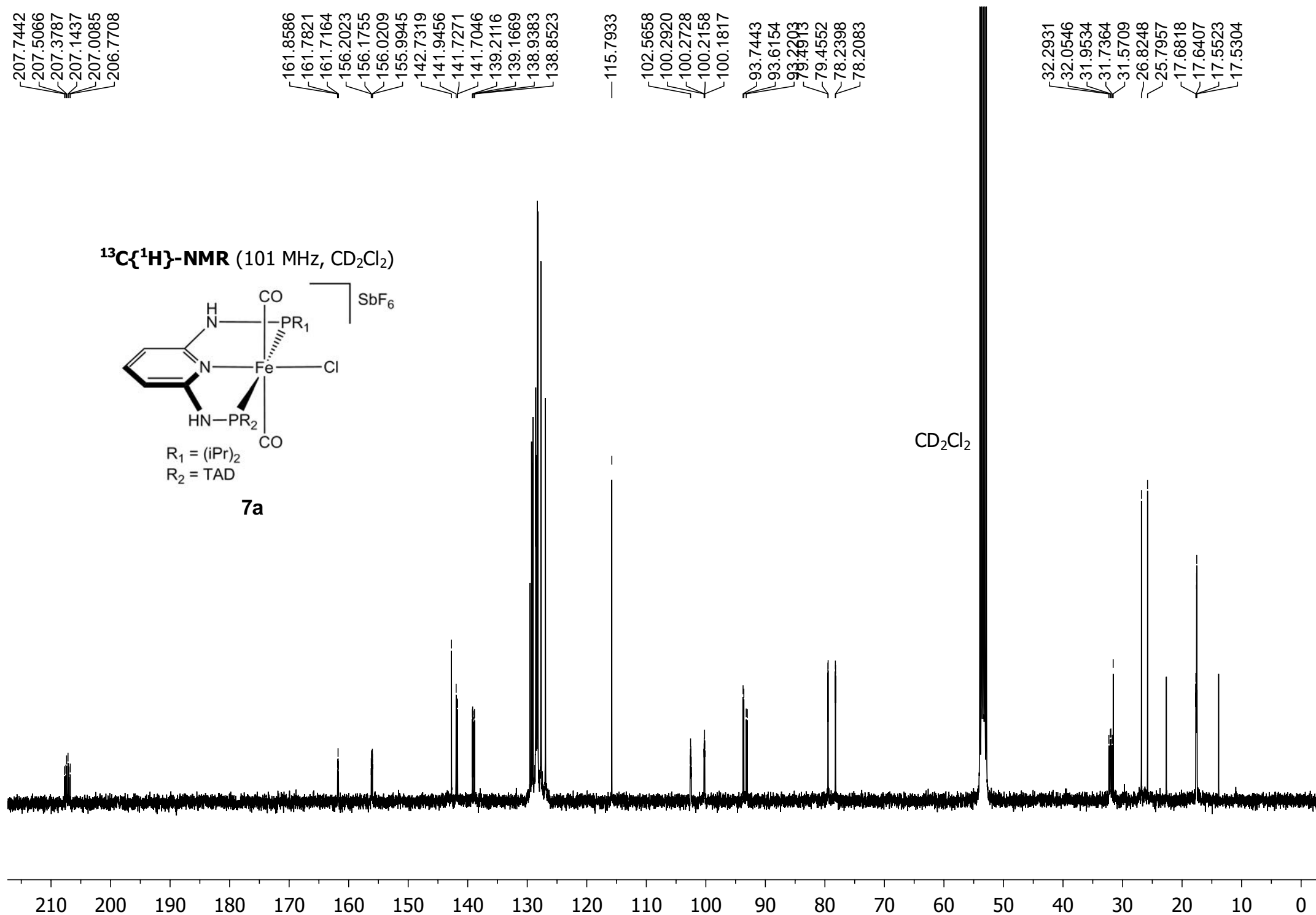


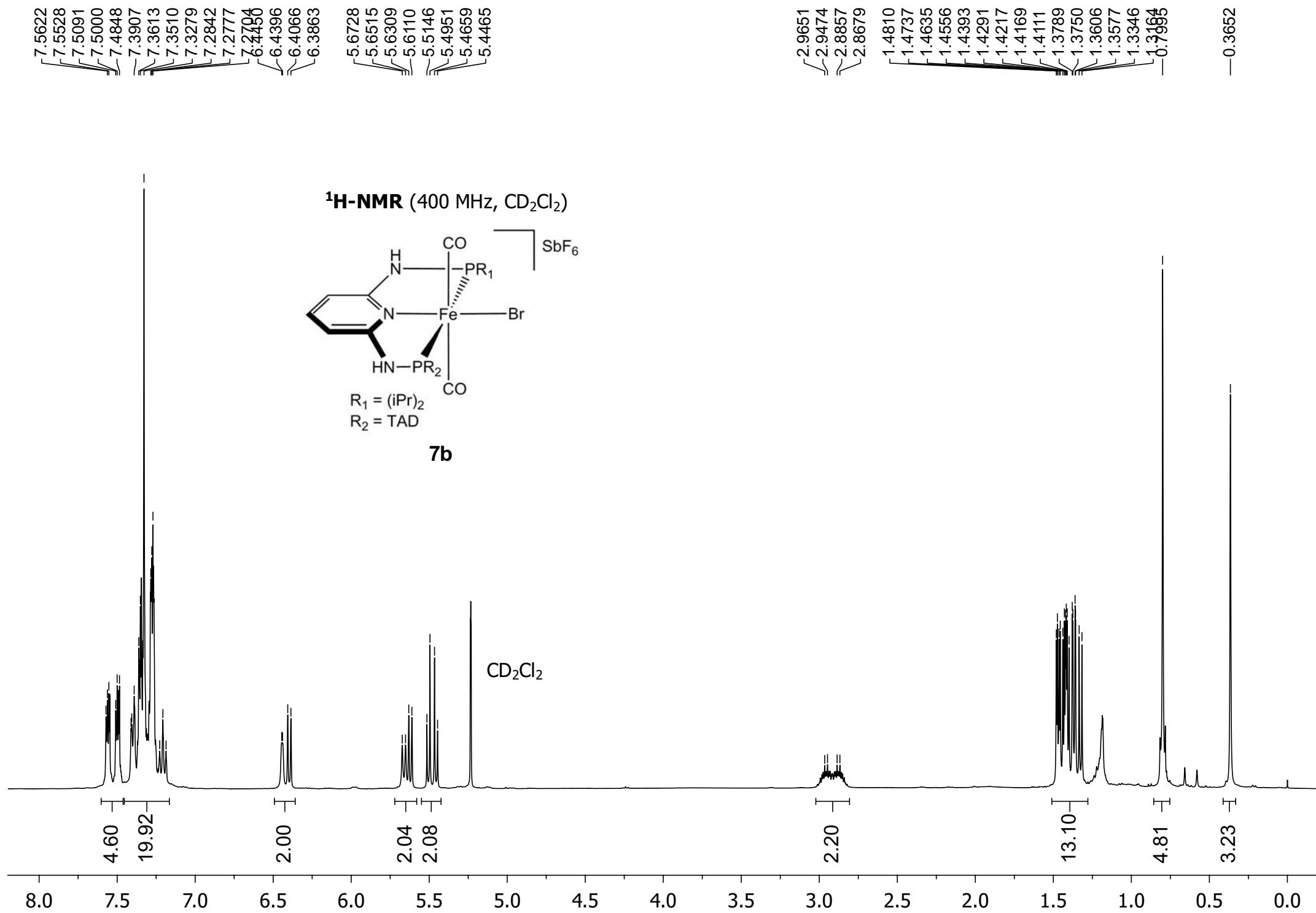


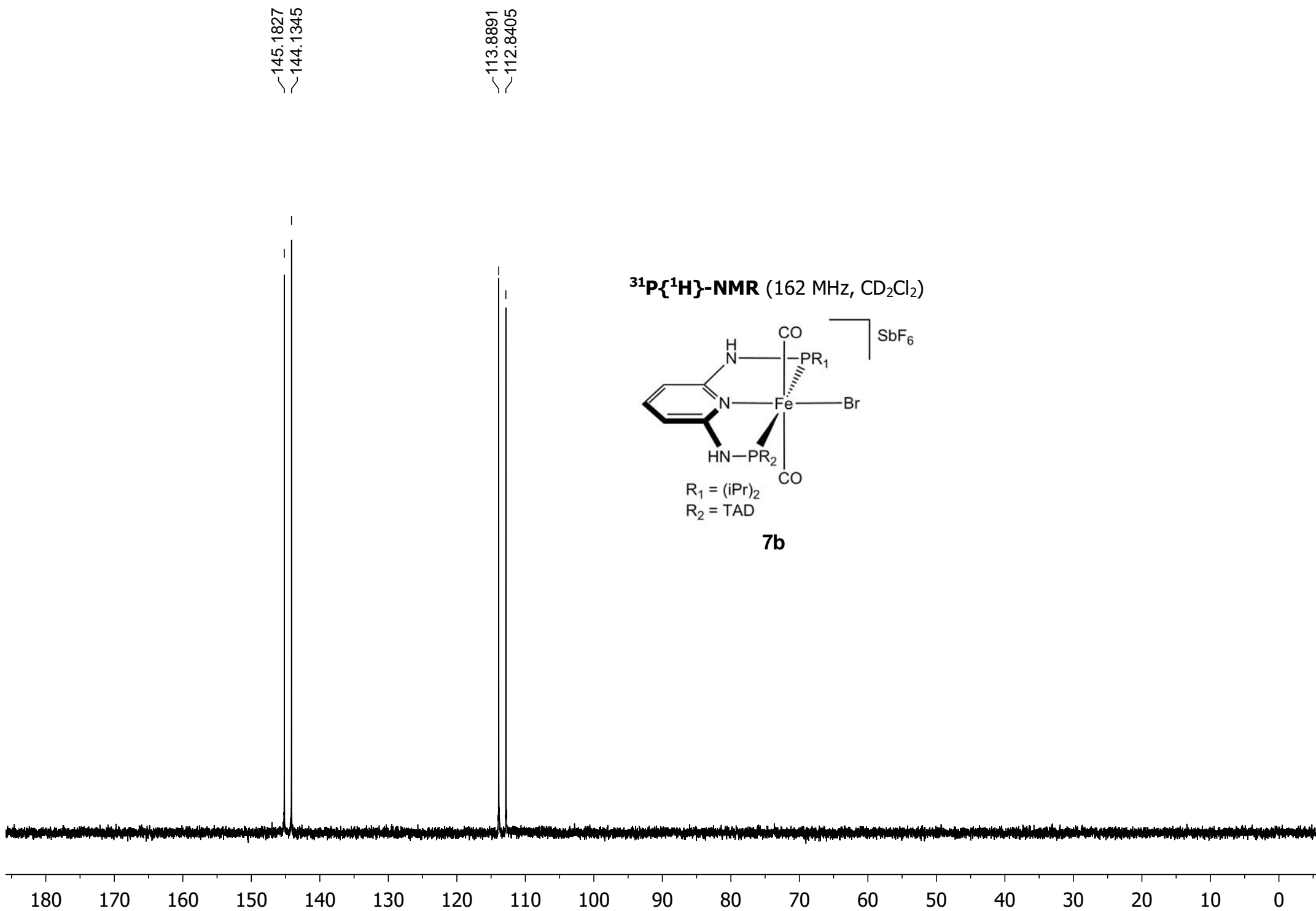












208.0618
207.8261
207.7117
207.6598
207.4743
207.4249
207.2907
207.0543

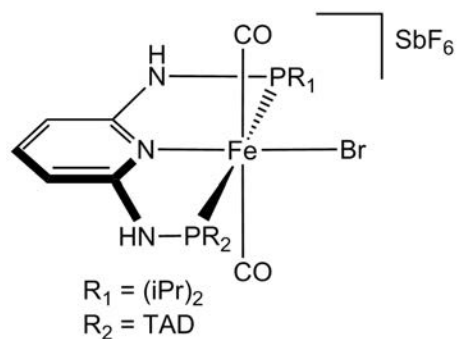
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161.7551
161.7362
161.6746
156.2504
156.2221
156.0669
156.0384
142.7725
141.8979
141.8732
139.2555
139.2126
138.9583
138.8711

—115.7710

102.5295
102.4666
100.2225
100.1313
94.0776
93.9402
93.1173
92.9229
79.5372
79.5005
78.2695
78.2370

32.5764
32.5450
32.3415
32.3098
32.2519
32.2199
32.0284
31.9972
31.5694
26.8515
25.7735
18.0075
17.9163
17.8424

$^{13}\text{C}\{^1\text{H}\}$ -NMR (101 MHz, CD_2Cl_2)



7b

CD_2Cl_2

