Ruthenium PNN(O) Complexes: Cooperative Reactivity and Application as Catalysts for Acceptorless Dehydrogenative Coupling Reactions

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SUPPORTING INFORMATION FOR

Ruthenium PNN(O) Complexes: Cooperative Reactivity and Application as Catalysts for Acceptorless Dehydrogenative Coupling Reactions

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Spectra of relevant compounds
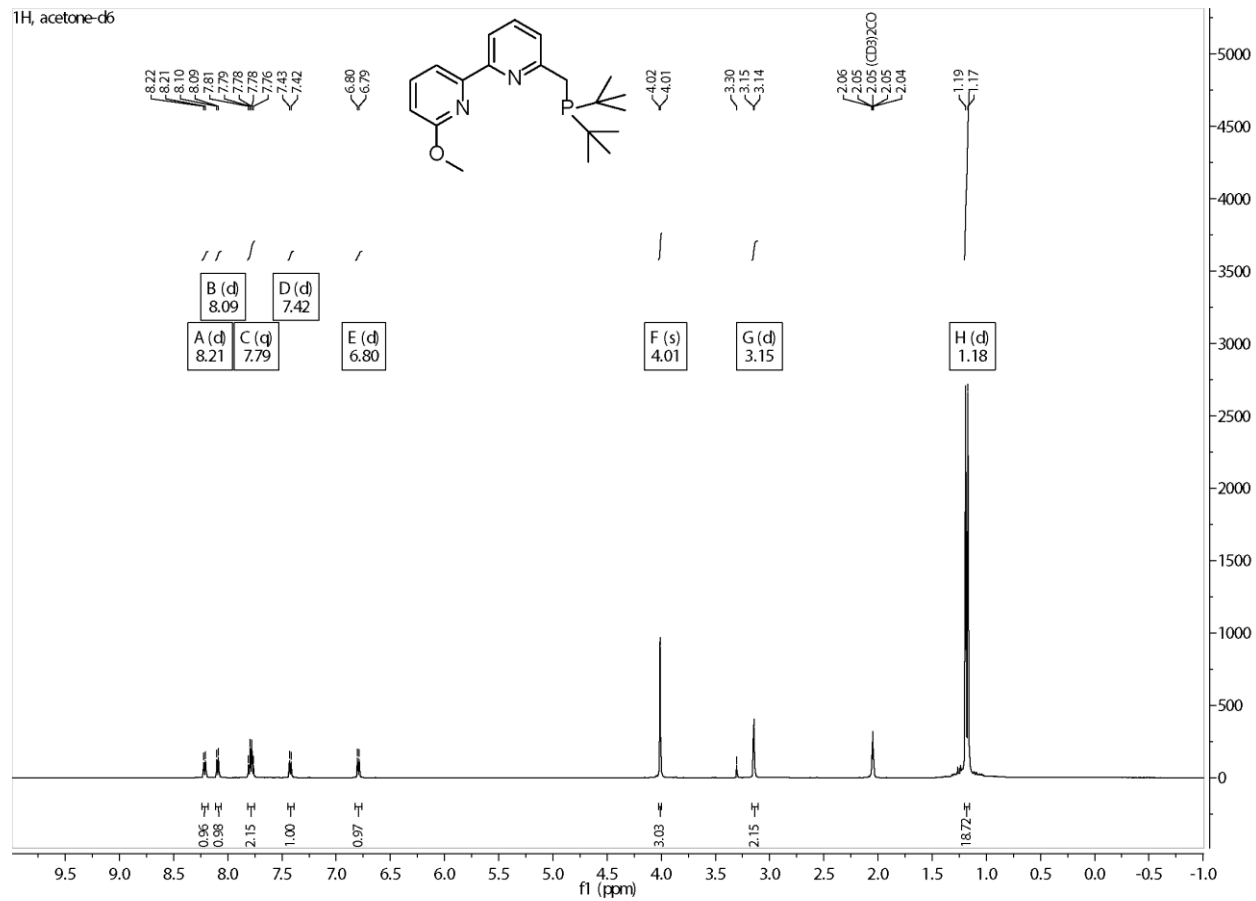
Figure S1. ^{1}H NMR spectrum (acetone-d_6) of L^{Me}.
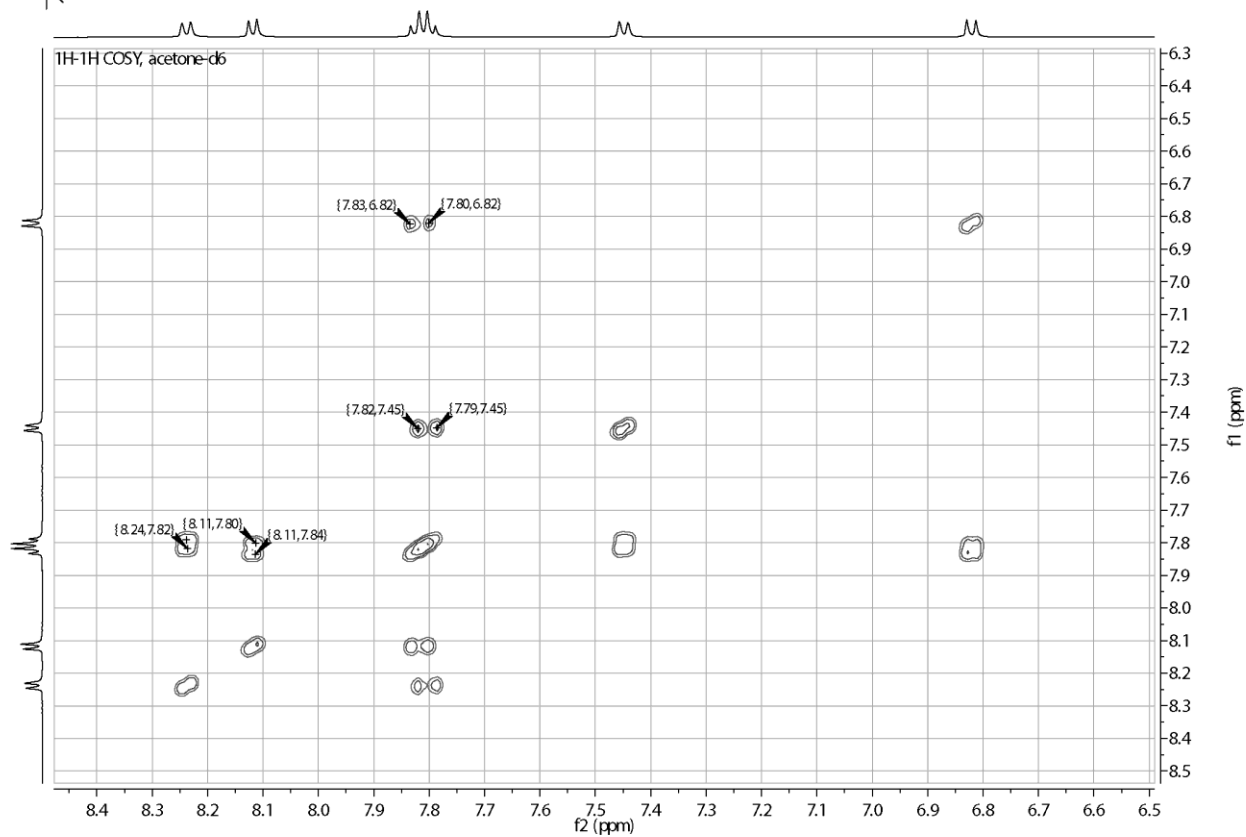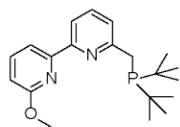
Figure S2. 2D [^{1}H-^{1}H]-COSY NMR spectrum (acetone-d_6) of L^{Me}.
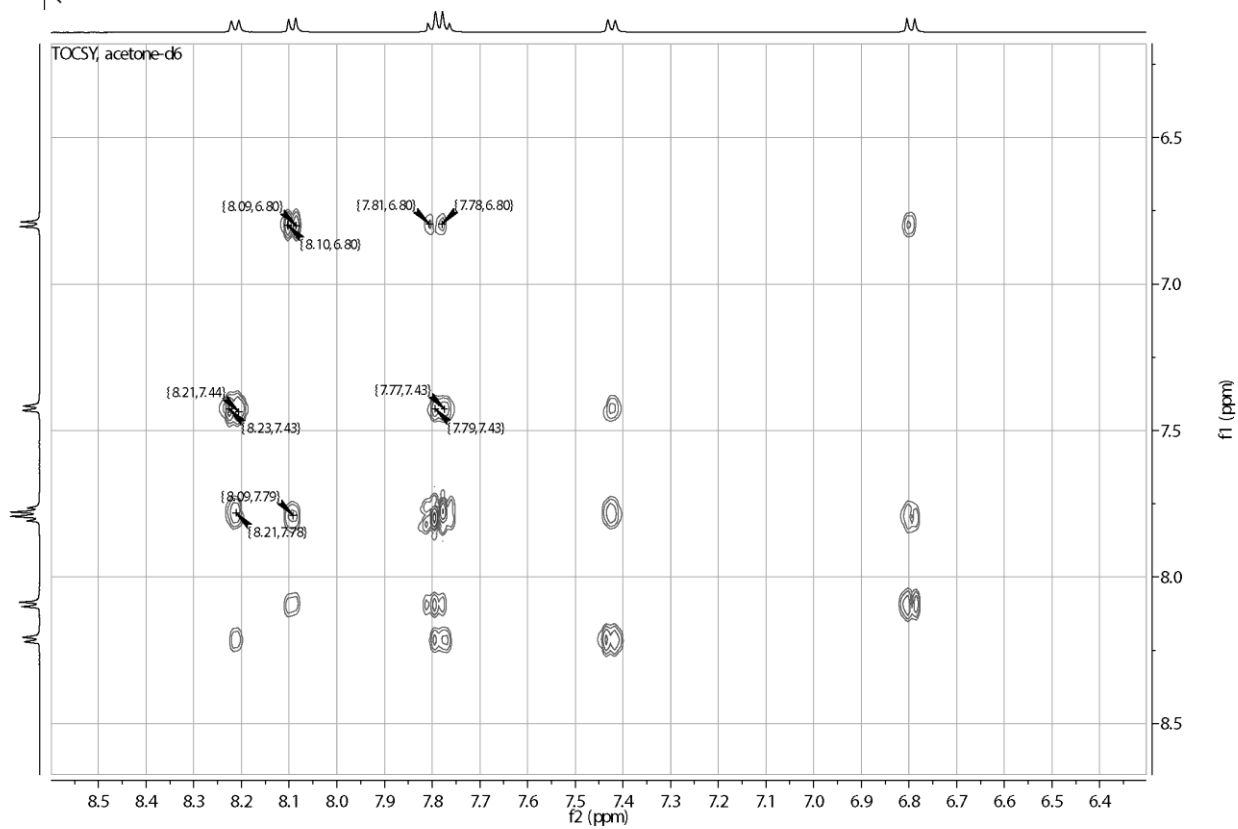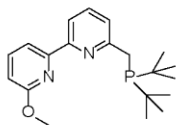
Figure S3. 2D [^{1}H-^{1}H]-TOCSY NMR spectrum (acetone-d_6) of L^{Me}.
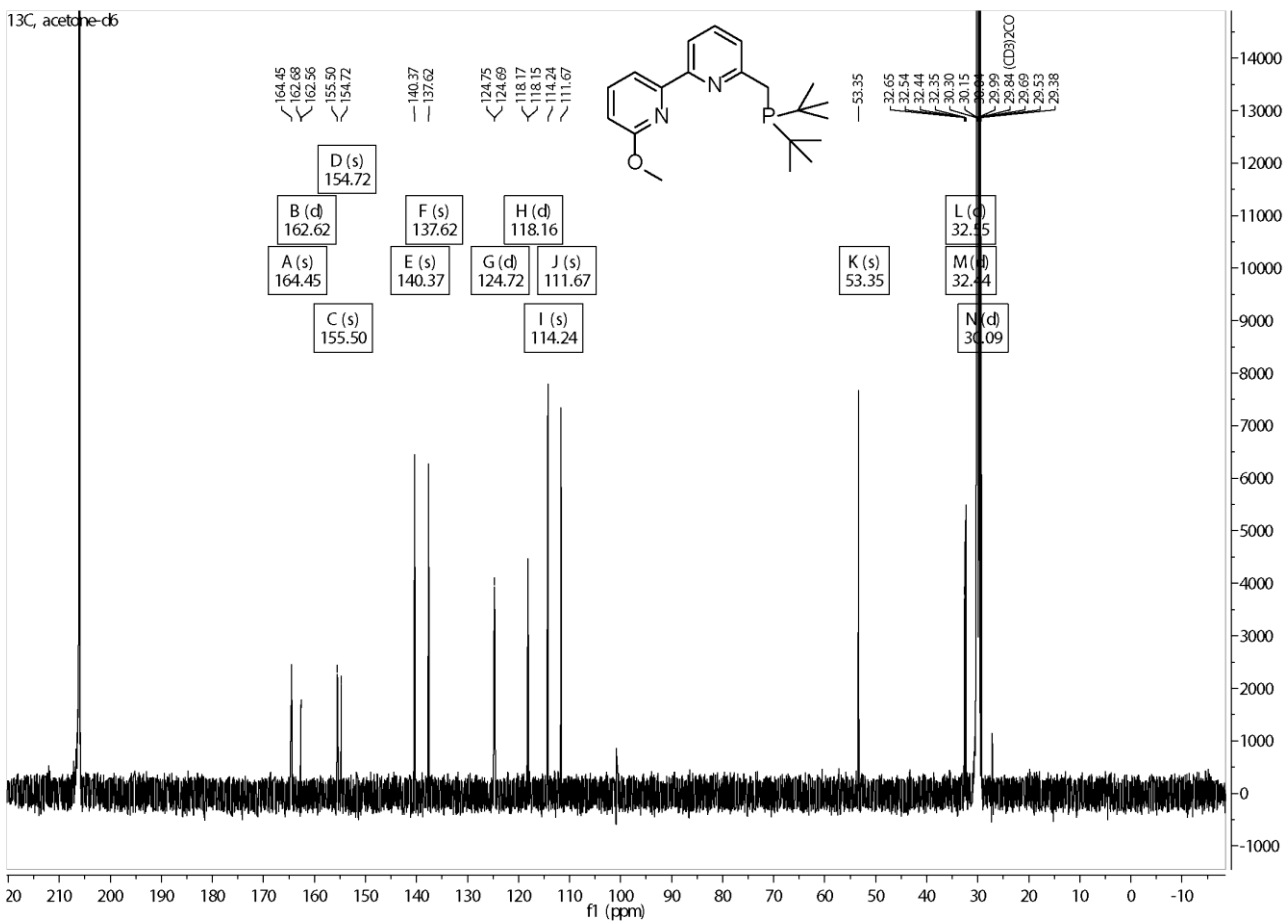
Figure S4. ^{13}C NMR spectrum (acetone-d_6) of L^{Me}.
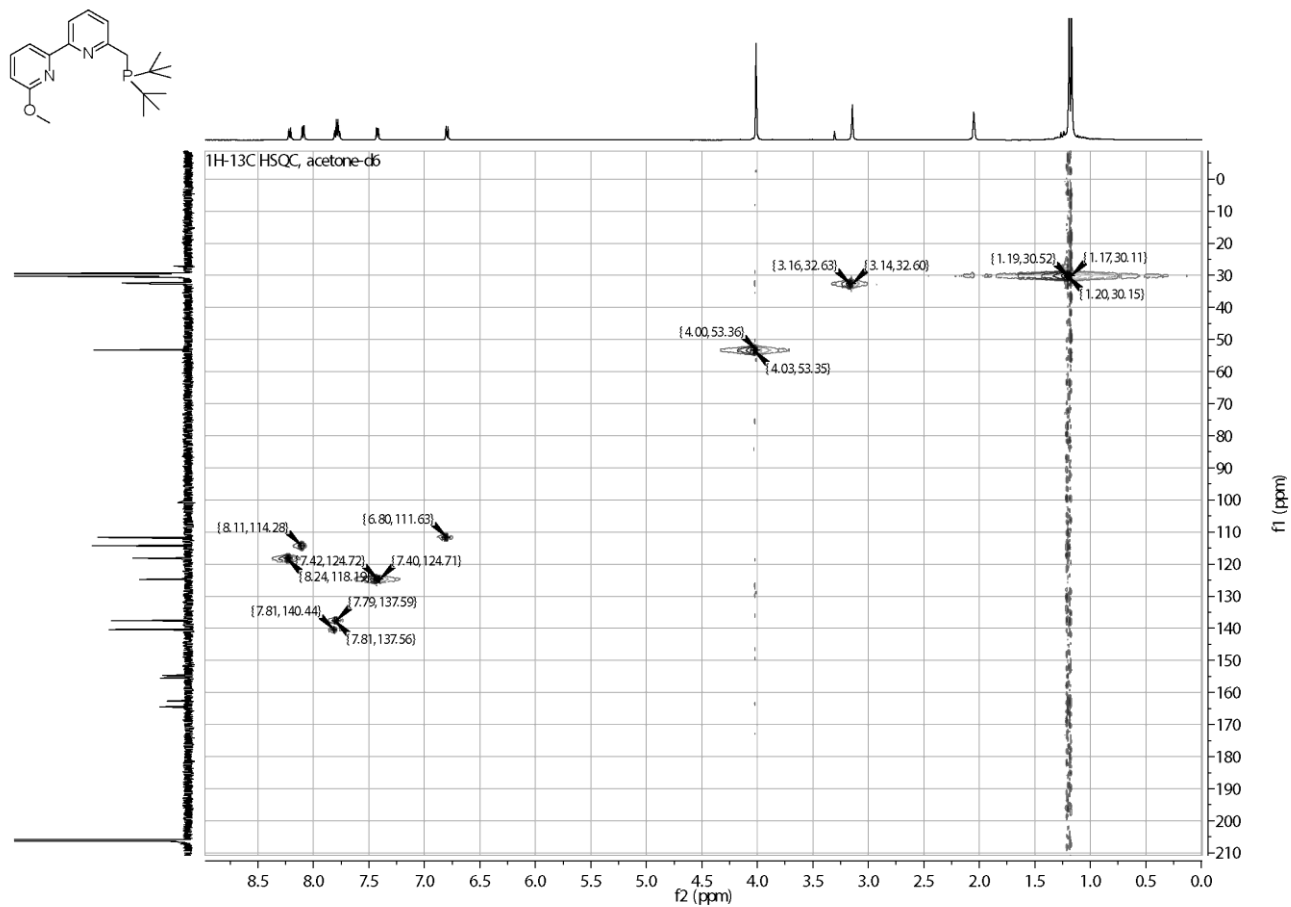
Figure S5. 2D [^{1}H-^{13}C]-HSQC NMR spectrum (acetone-d_6) of L^{Me}.
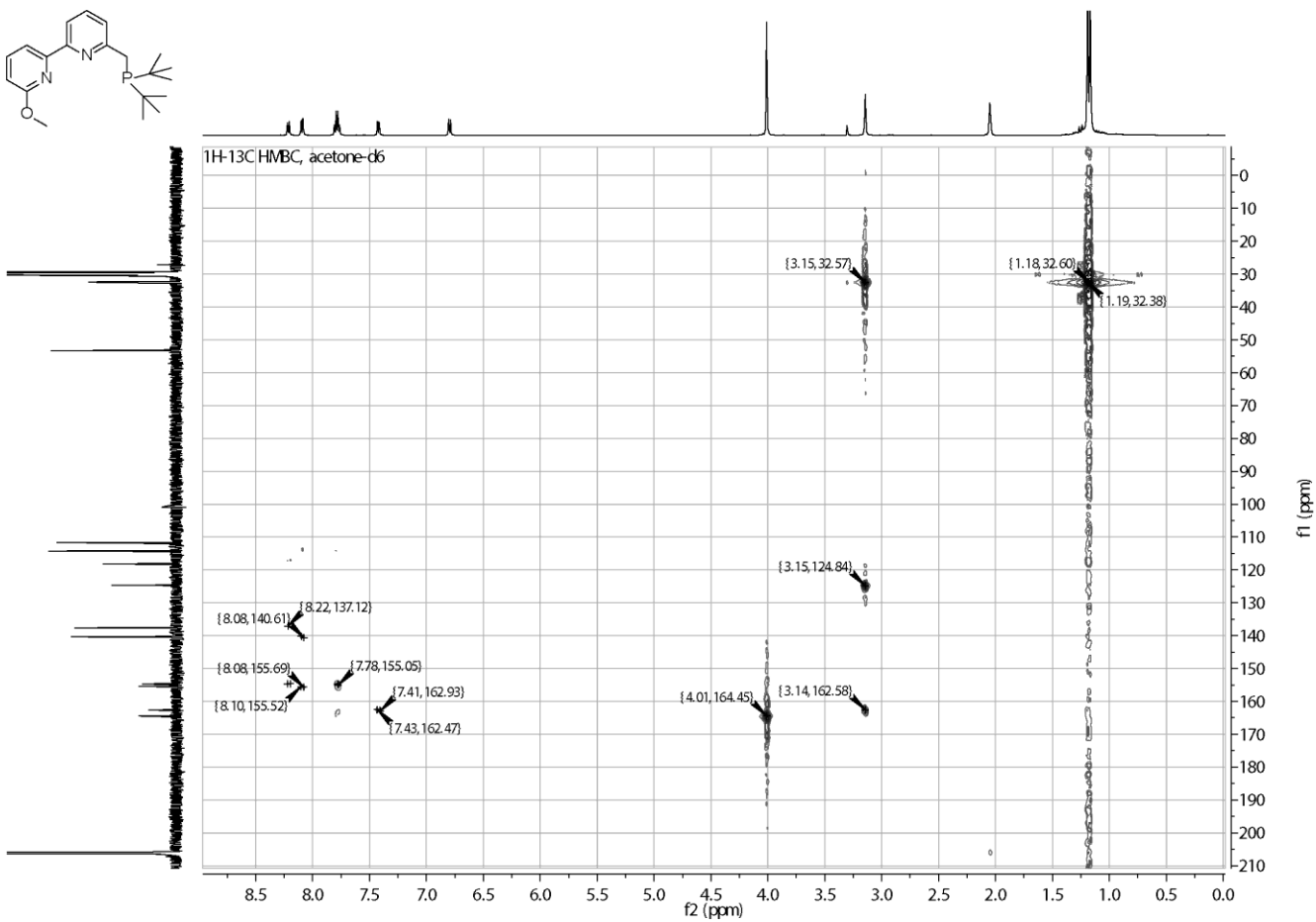
Figure S6. 2D [^{1}H-^{13}C]-HMBC NMR spectrum (acetone-d_6) of L^{Me}.
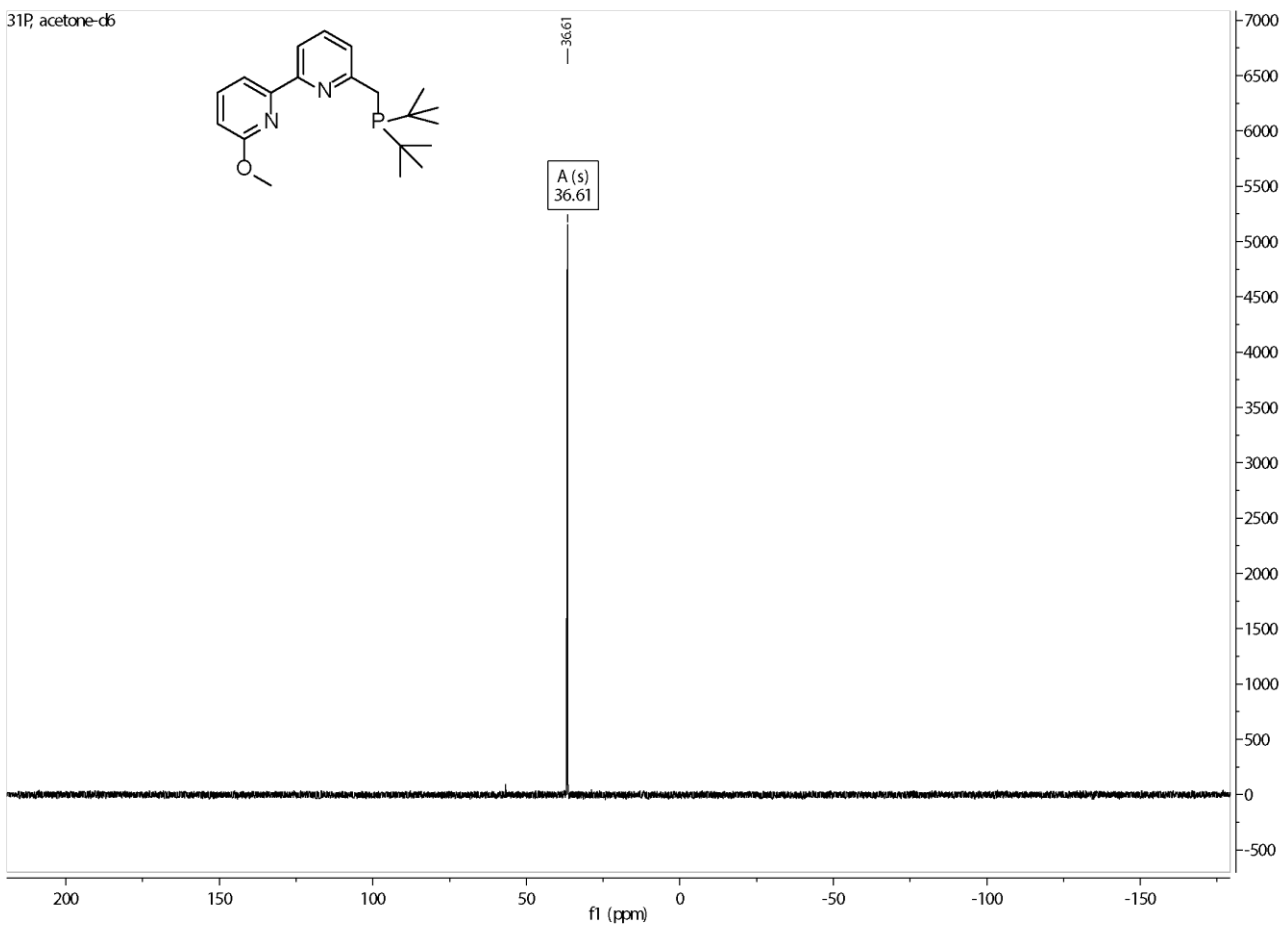
Figure S7. ^{31}P NMR spectrum (acetone-d_6) of L^{Me}.
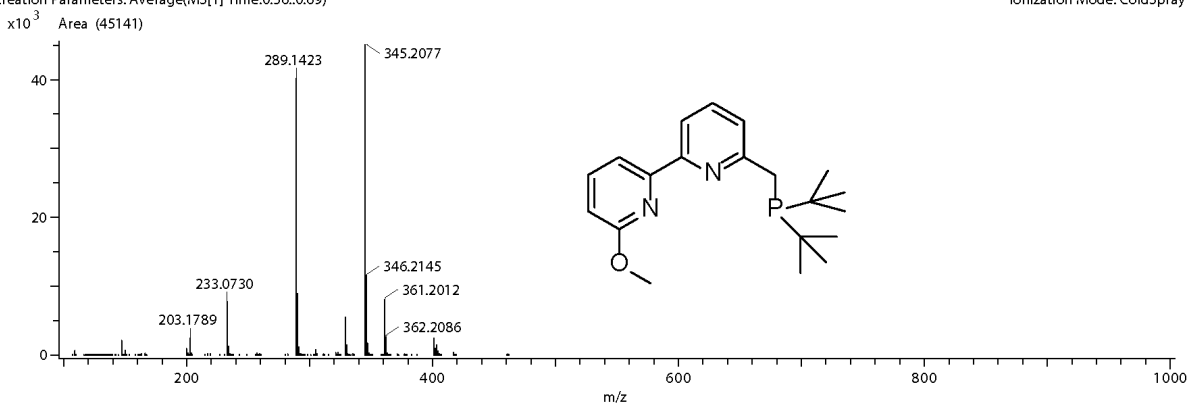
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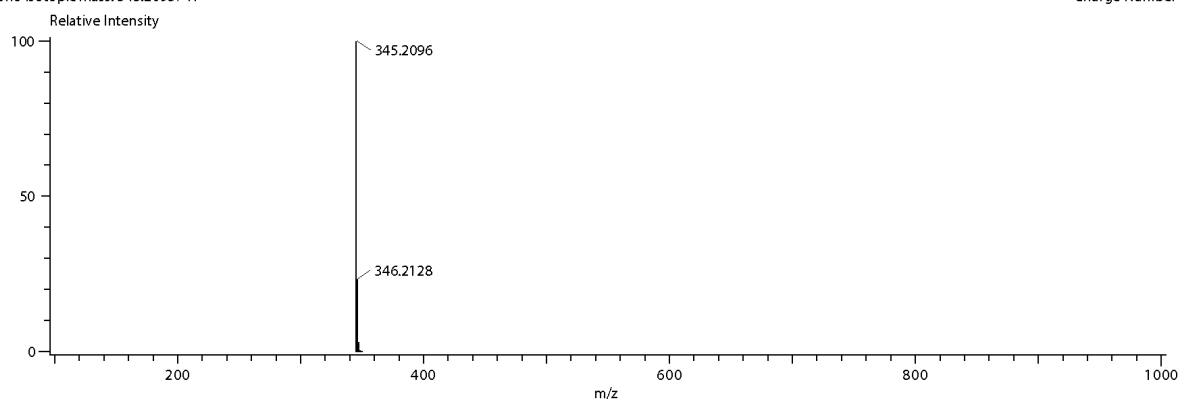
Figure S8. CSI-MS of L^{Me}.

$x10^3$ Area (45141)
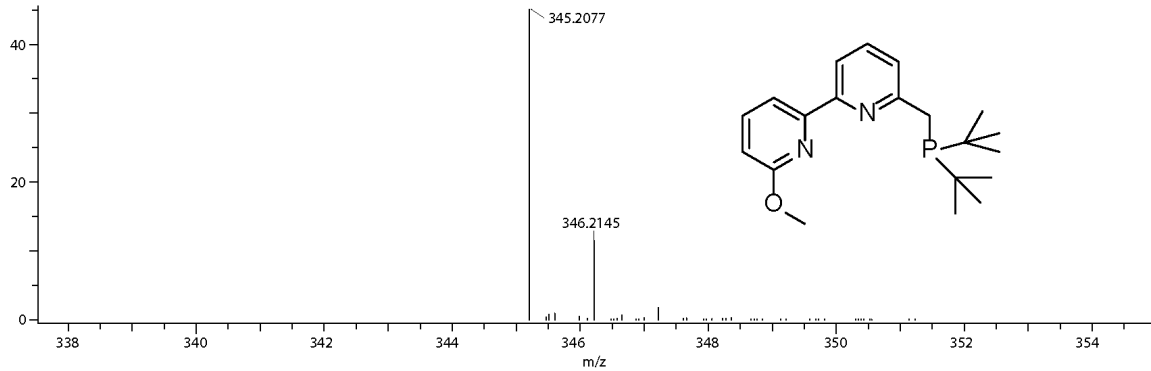
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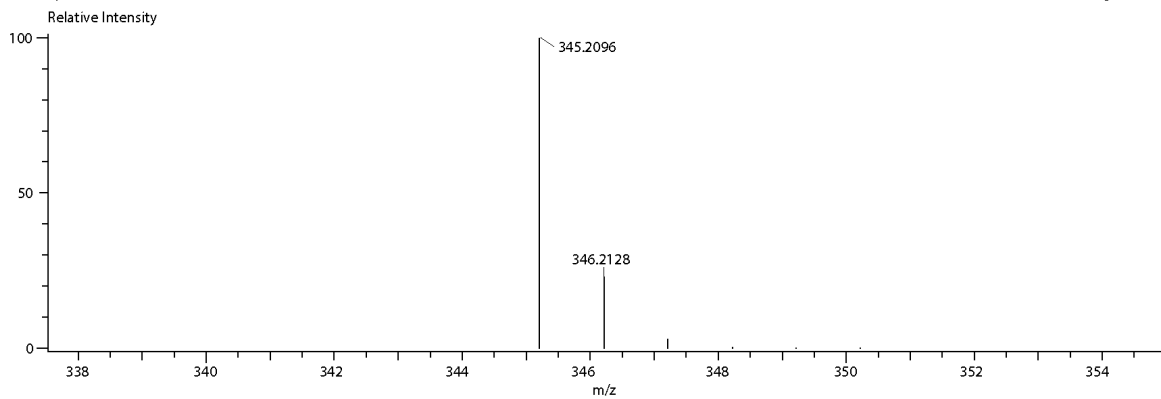
Figure S9. CSI-MS of L^{Me}.
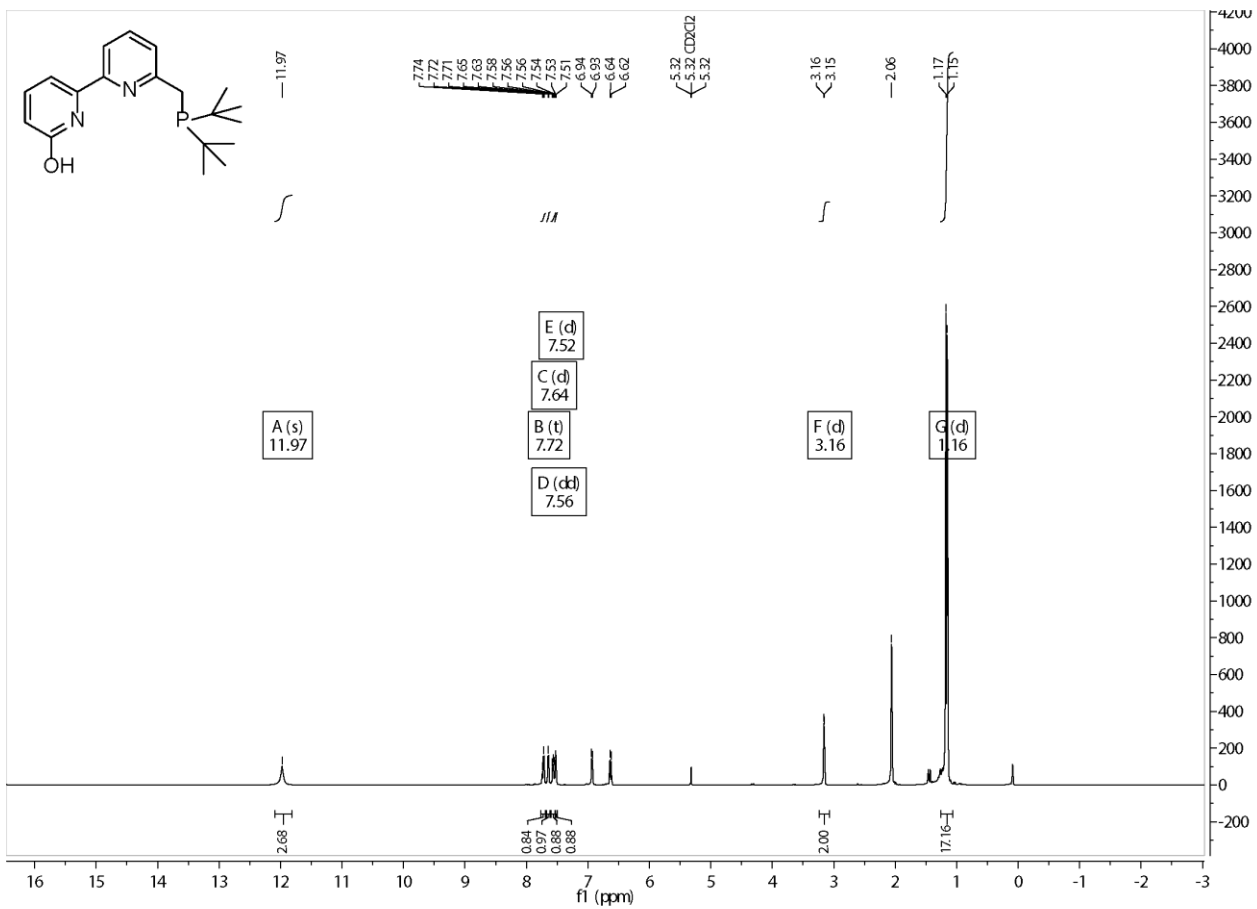
Figure S10. ¹H NMR spectrum (CD₂Cl₂) of L^{H2}.
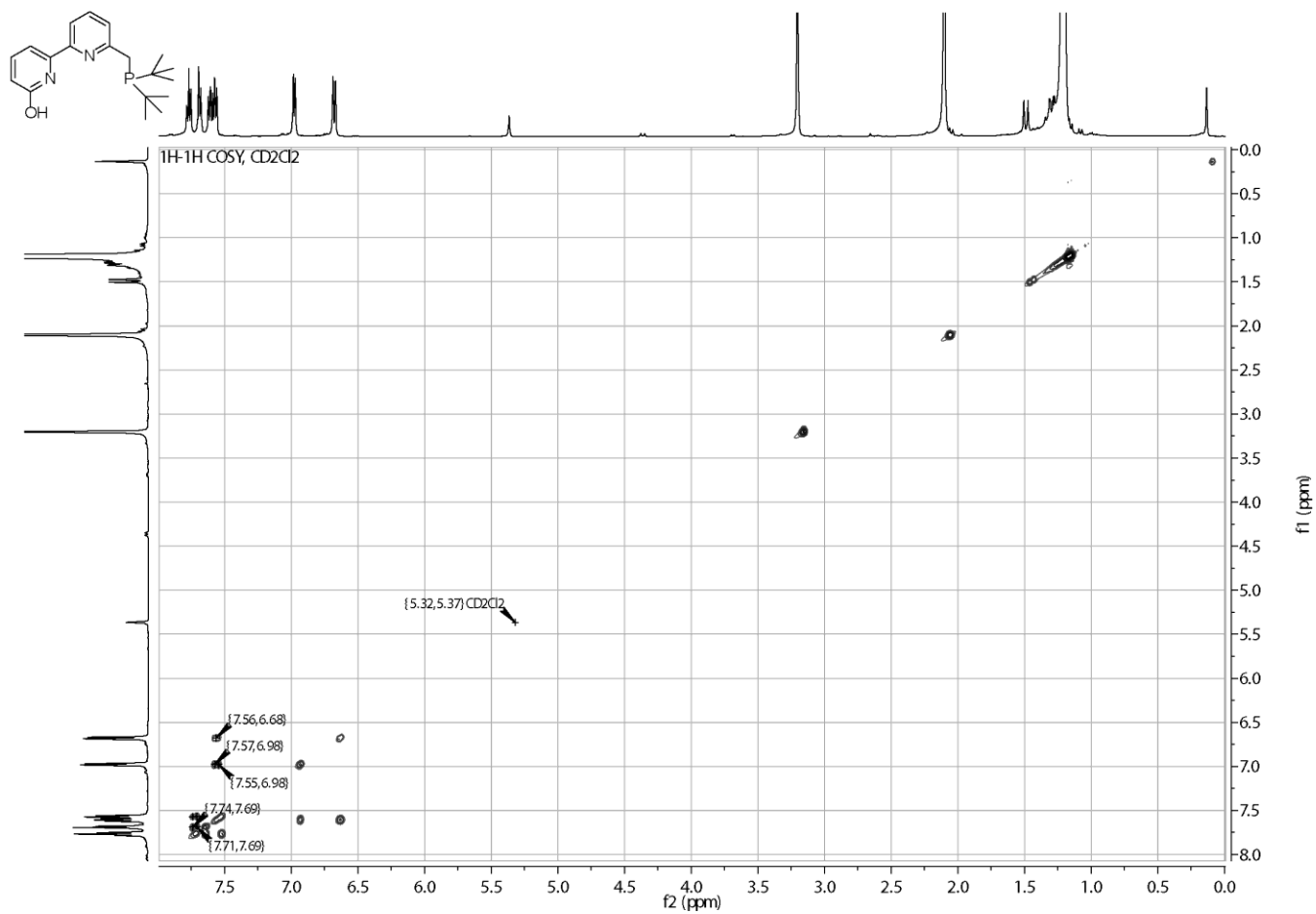
Figure S11. 2D [¹H-¹H]-COSY NMR spectrum (CD₂Cl₂) of L^{H2}.
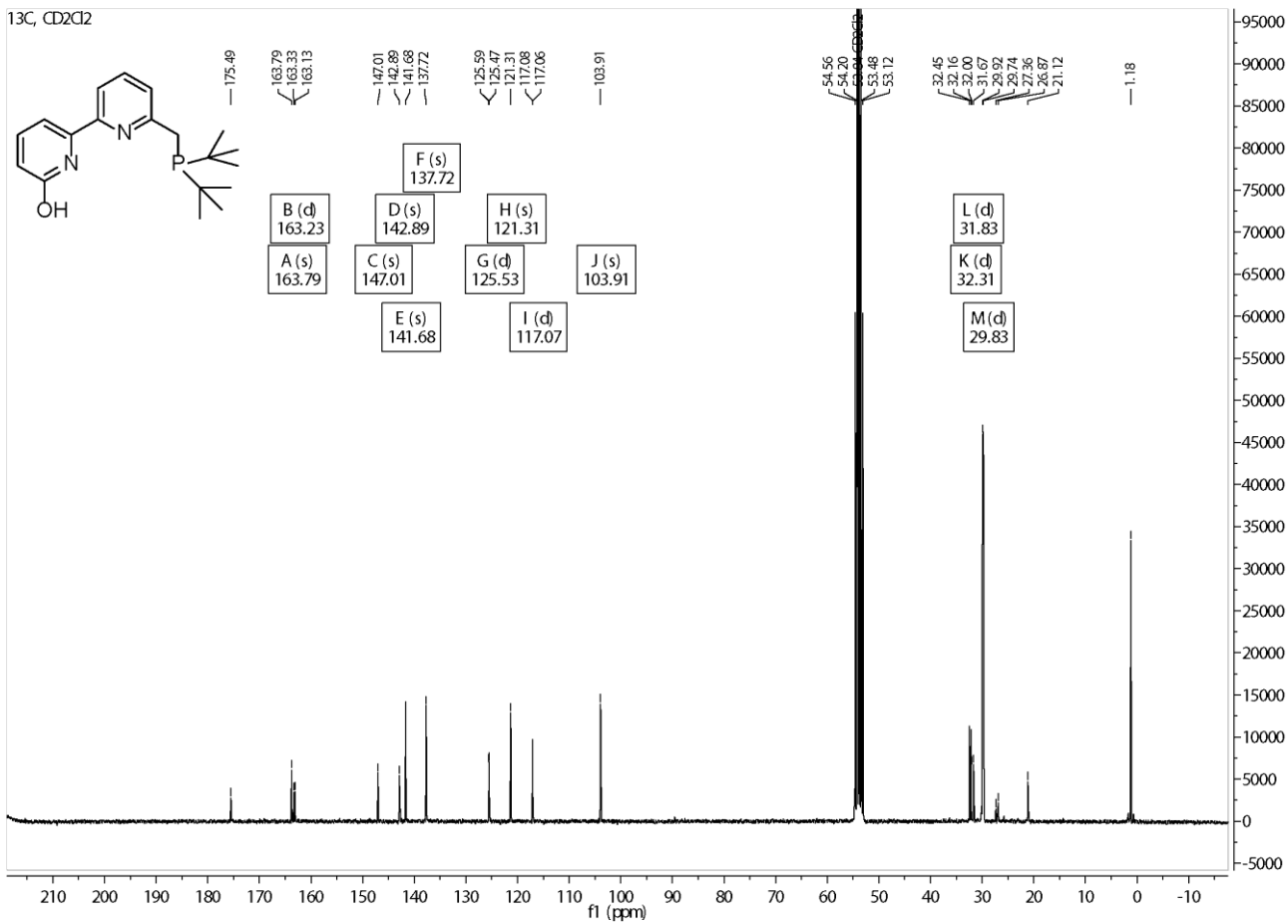
Figure S12. ^{13}C NMR spectrum (CD$_2$Cl$_2$) of L^{H2}.
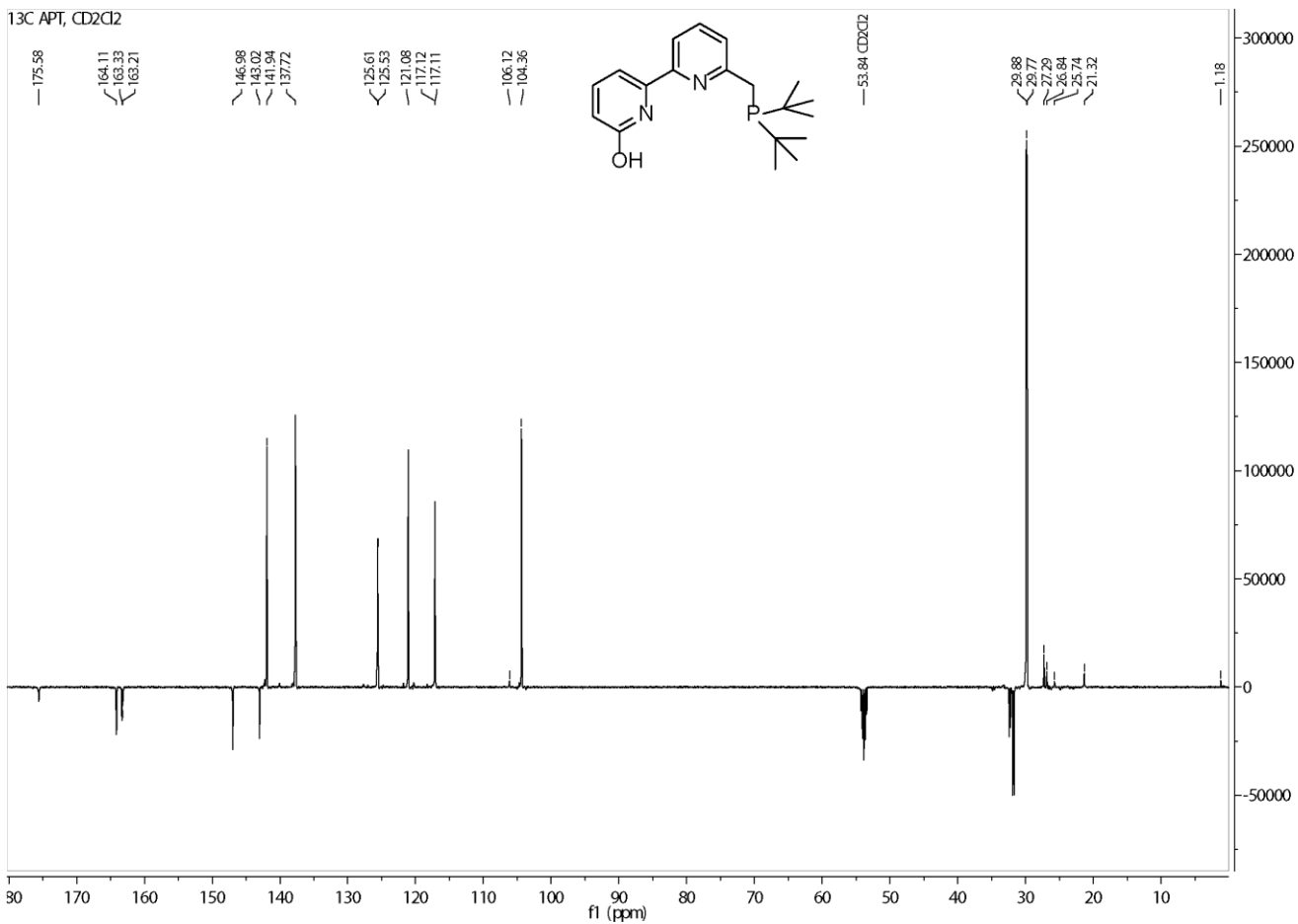
Figure S13. ^{13}C APT NMR spectrum (CD$_2$Cl$_2$) of L^{H2}.
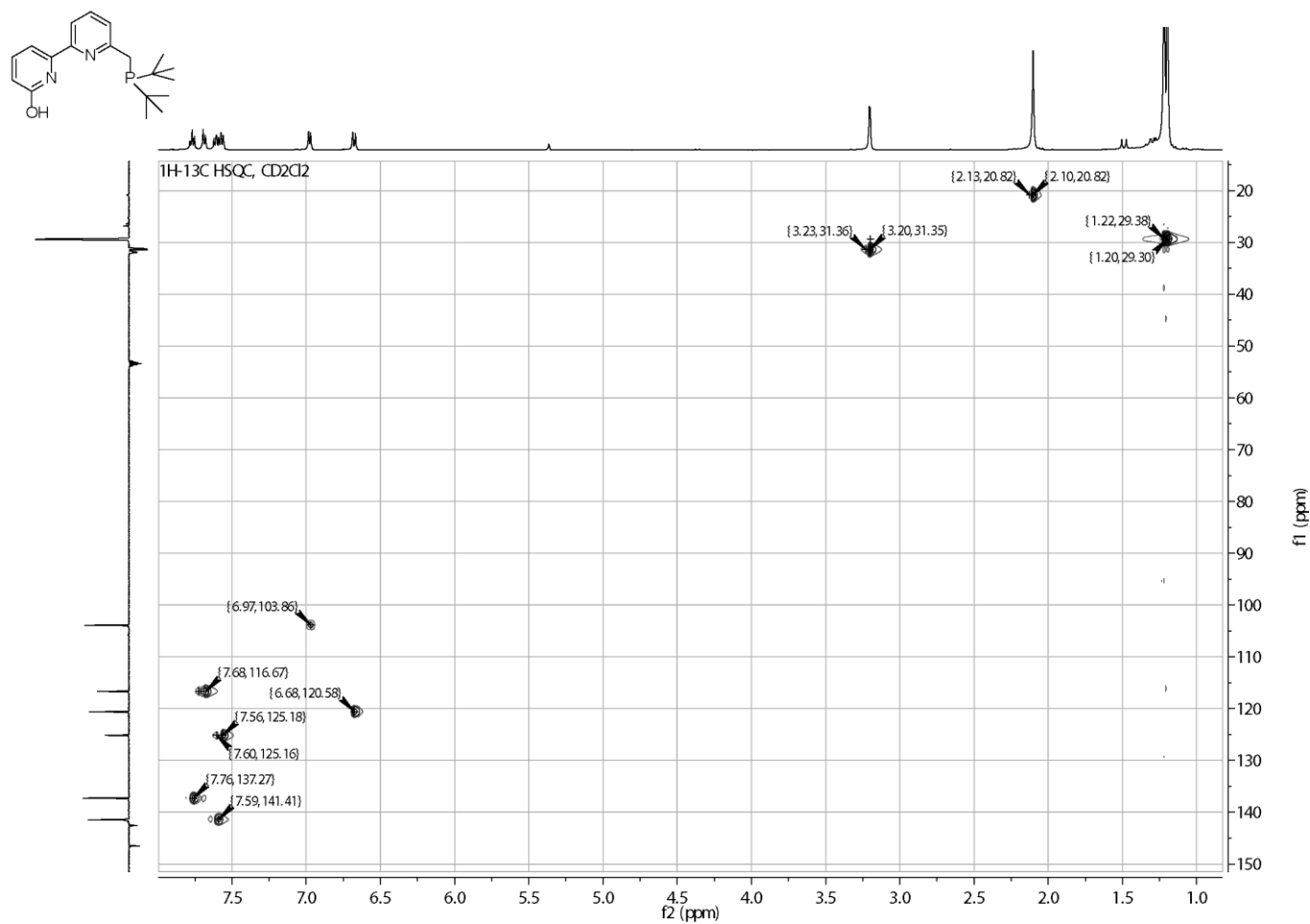
Figure S14. 2D [^{1}H-^{13}C]-HSQC NMR spectrum (CD$_2$Cl$_2$) of L^{H2}.
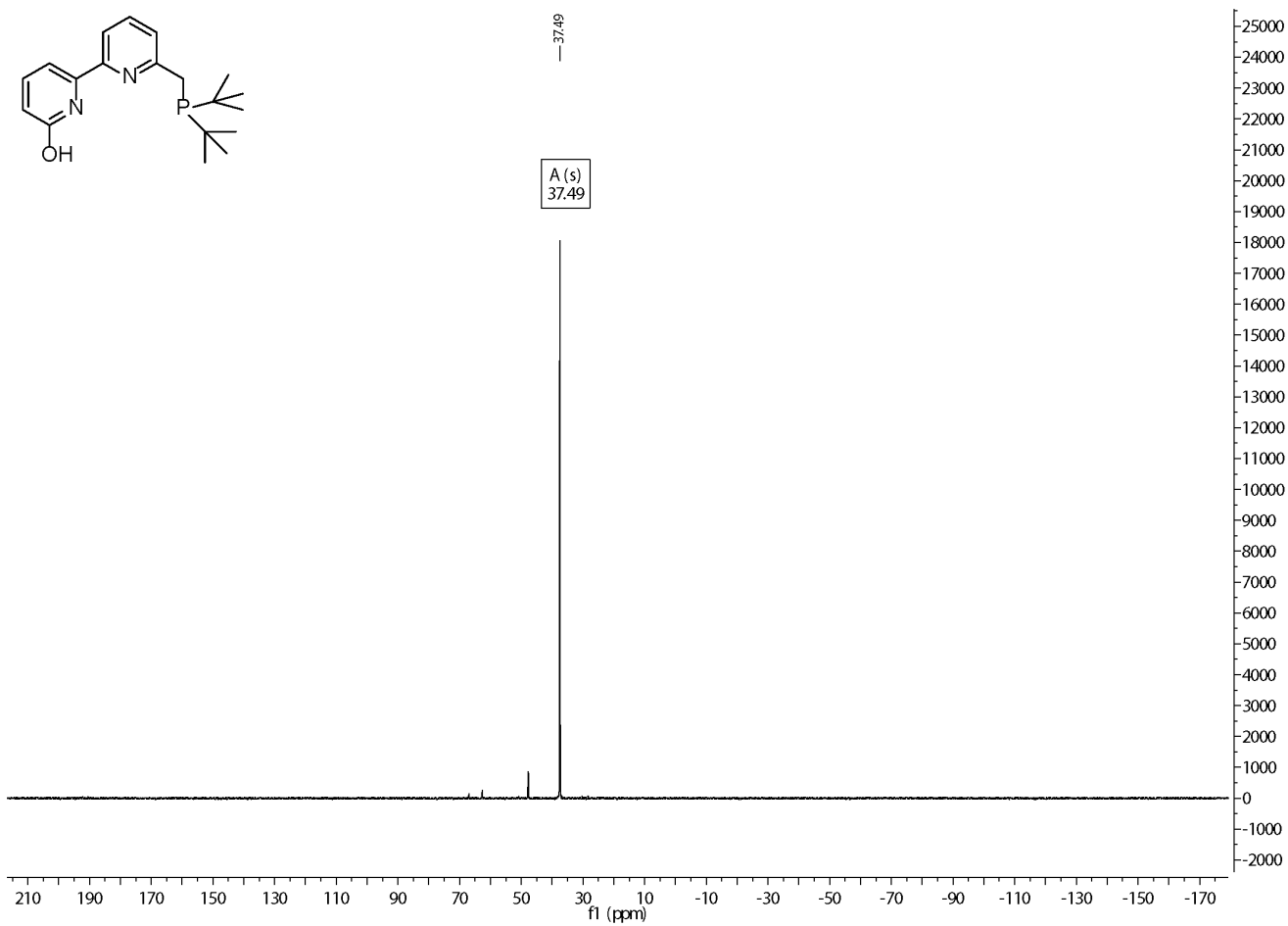
Figure S15. ^{31}P NMR spectrum (CD$_2$Cl$_2$) of L^{H2}.

Figure S16. CSI-MS of L^{H2}.

x10^3 Area (1682286)
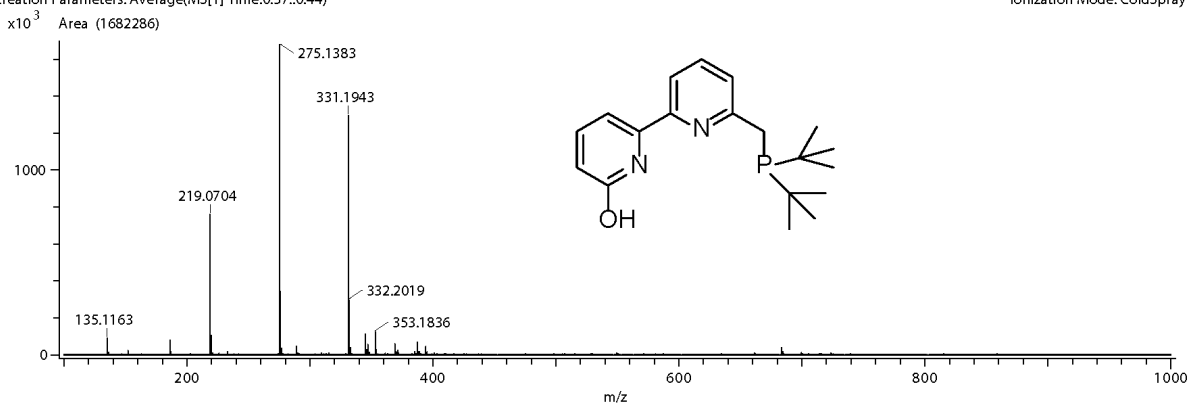
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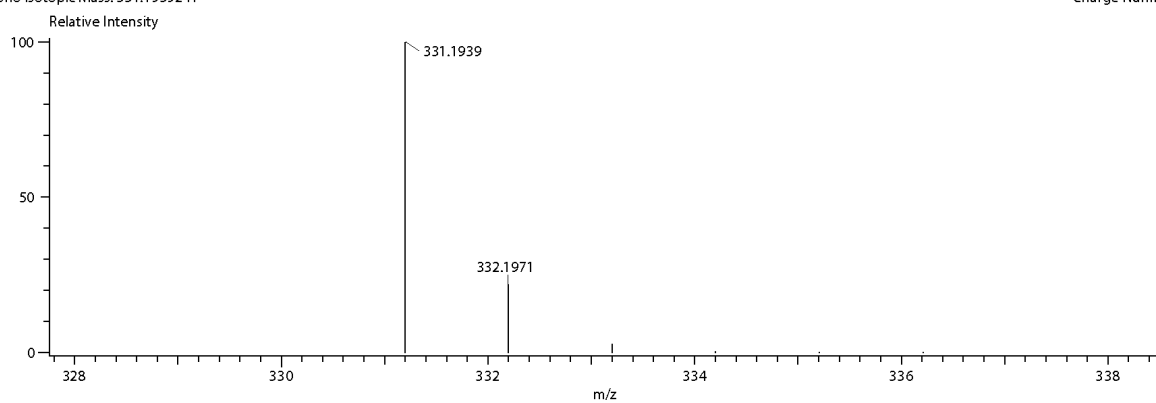
Figure S17. CSI-MS of L^{H2}.
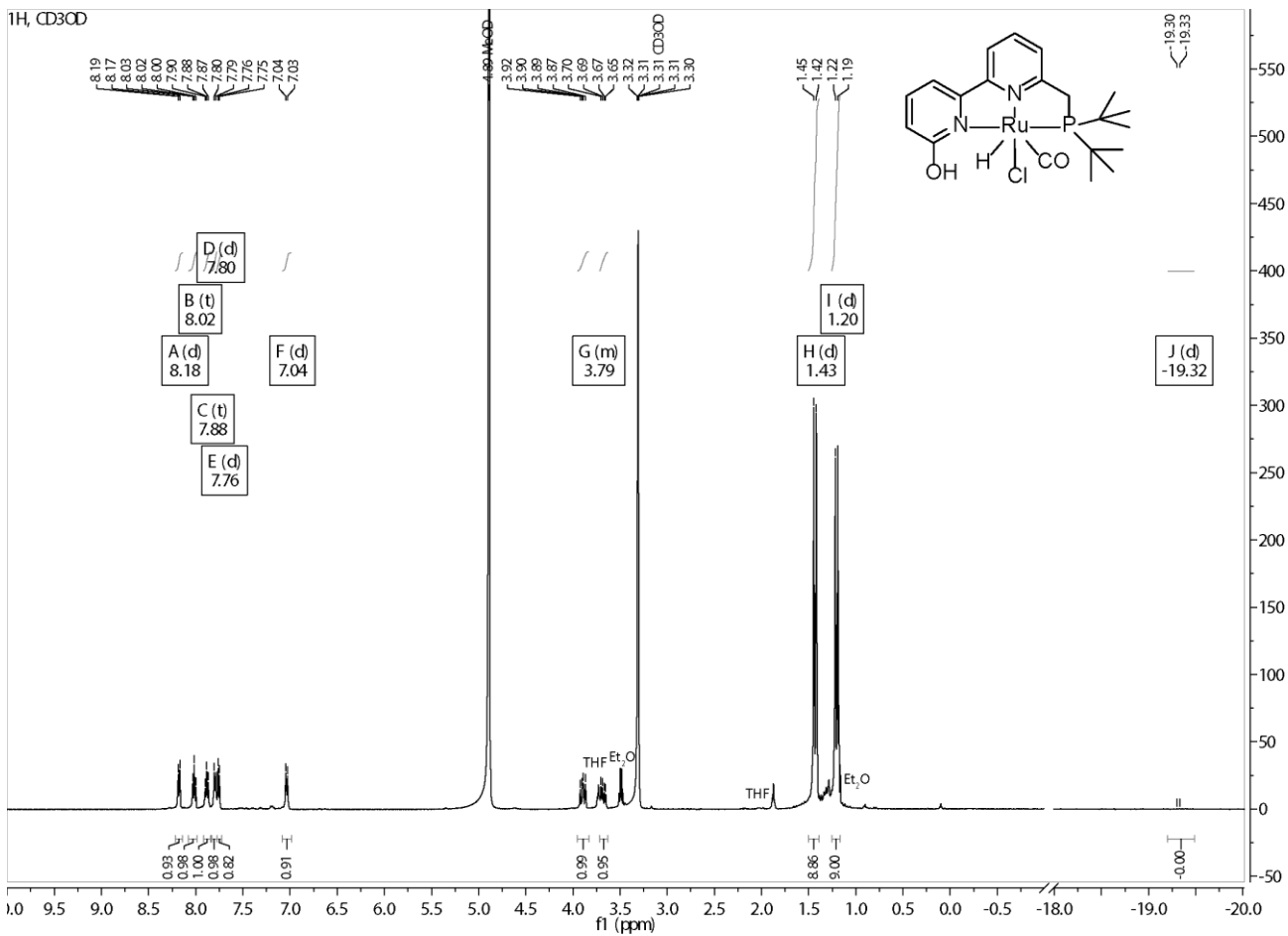
Figure S18. ^{1}H NMR spectrum (CD$_3$OD) of **1**.
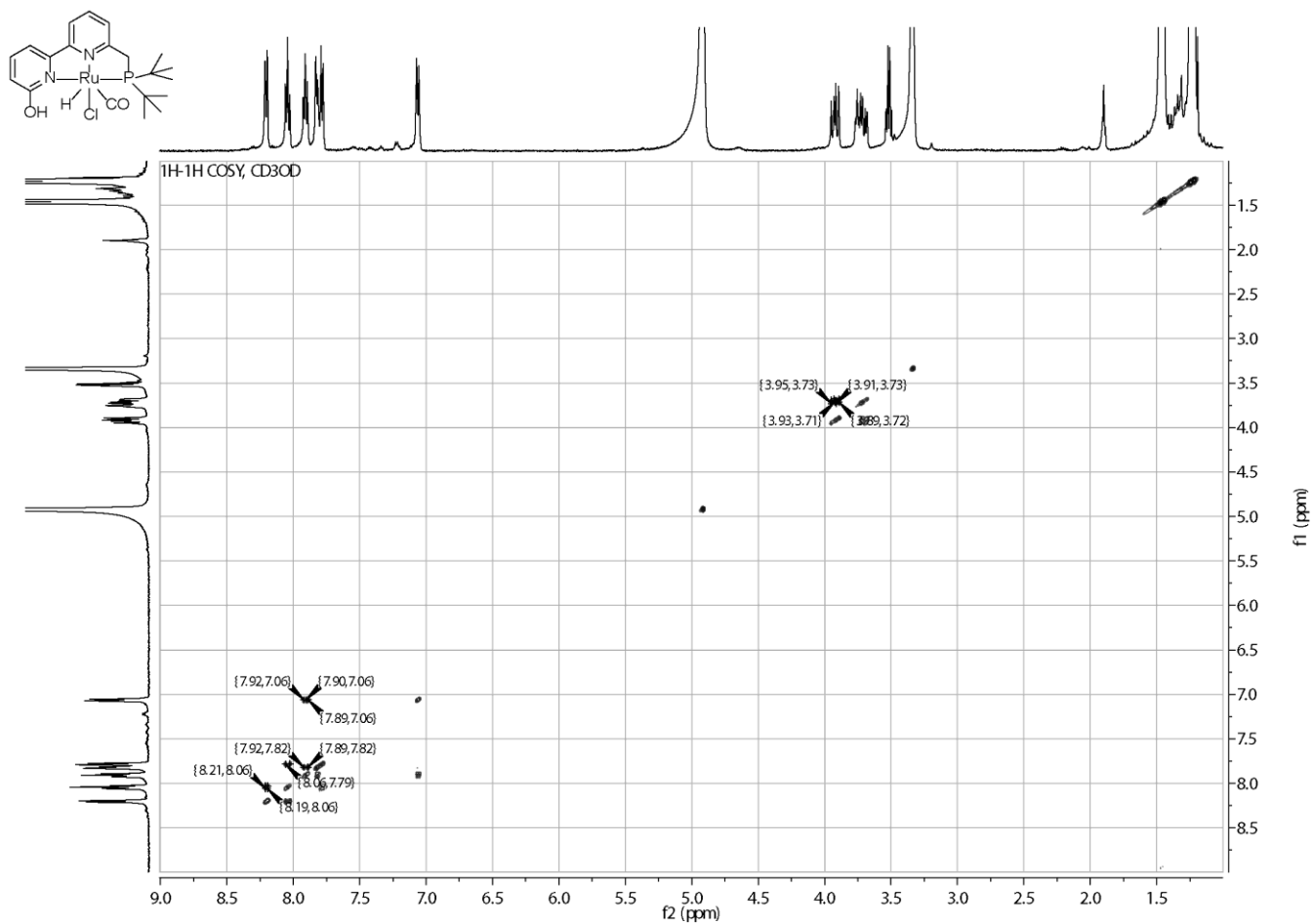
Figure S19. 2D [¹H-¹H]-COSY NMR spectrum (CD₃OD) of 1.
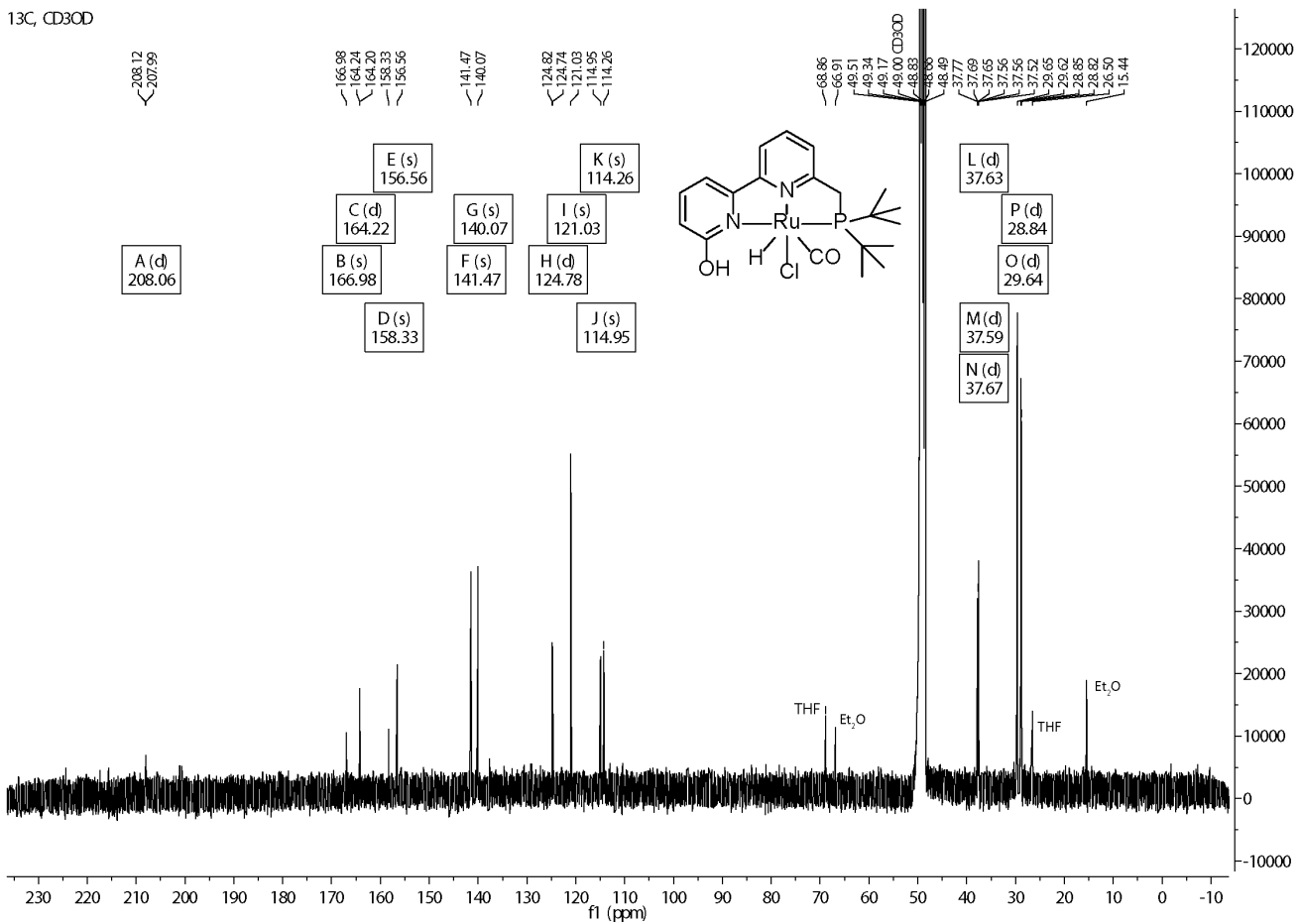
Figure S20. ^{13}C NMR spectrum (CD$_3$OD) of 1.
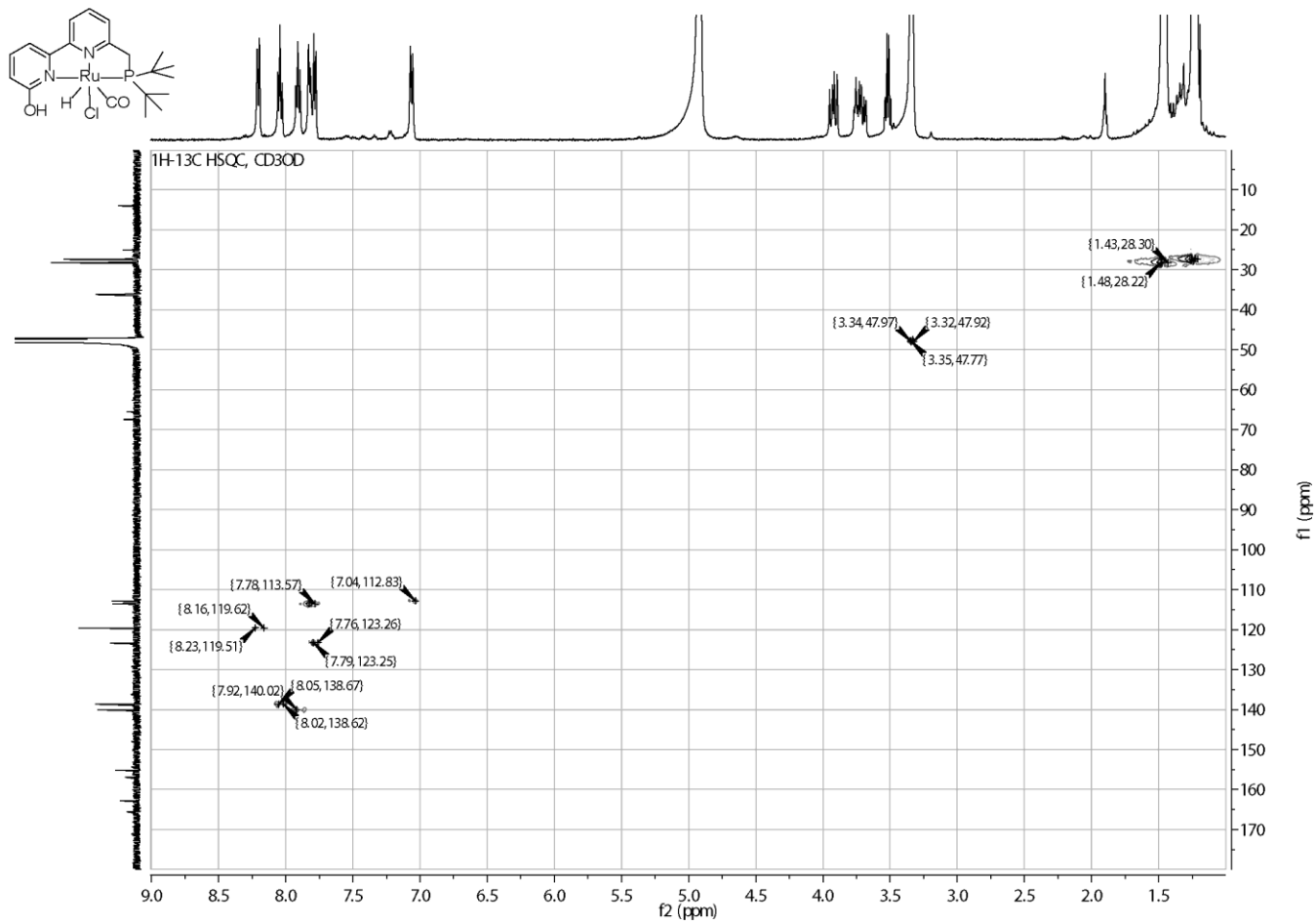
Figure S21. 2D [^{1}H-^{13}C]-HSQC NMR spectrum (CD$_3$OD) of 1.
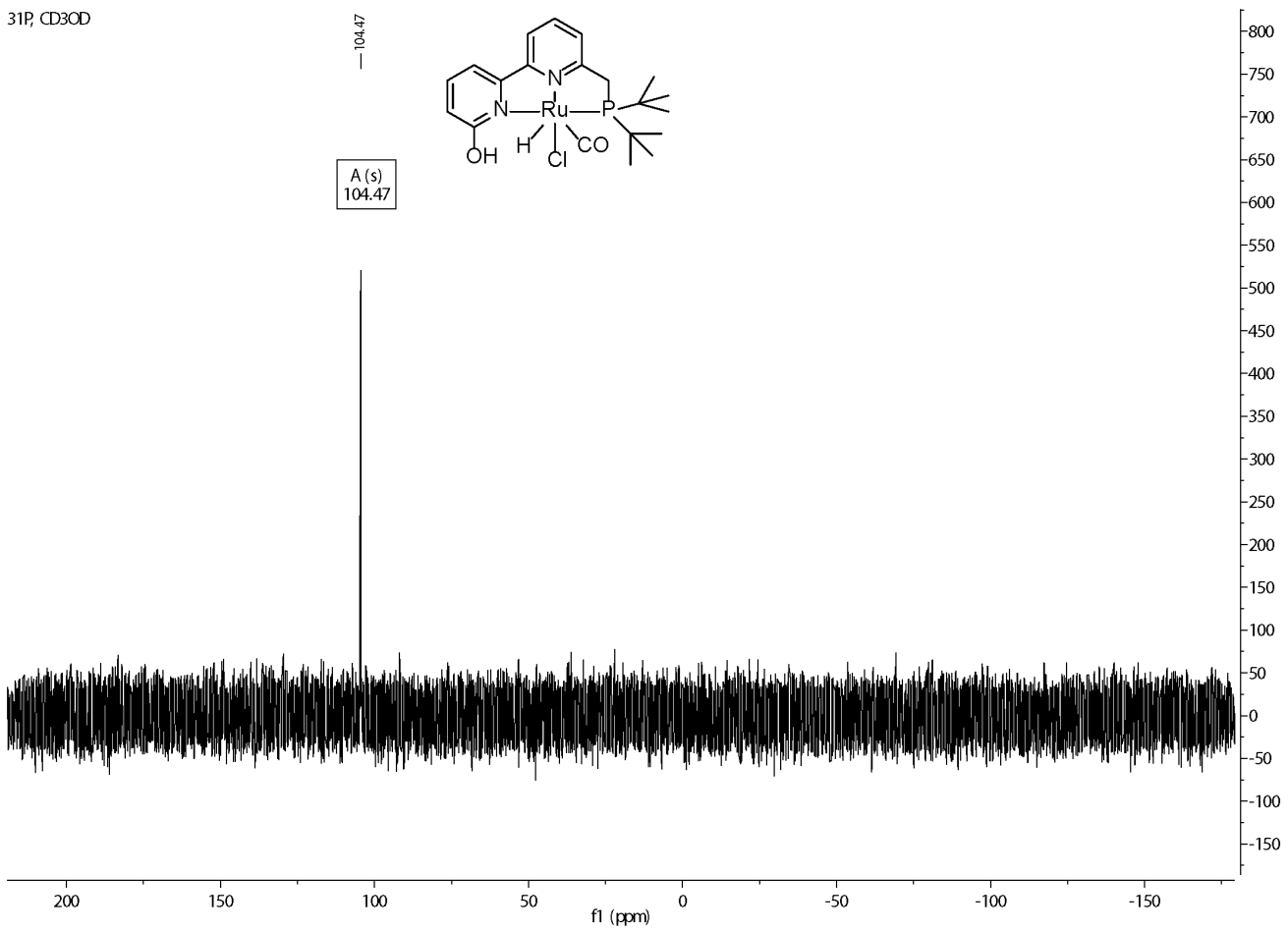
Figure S22. ^{31}P NMR spectrum (CD$_3$OD) of **1**.
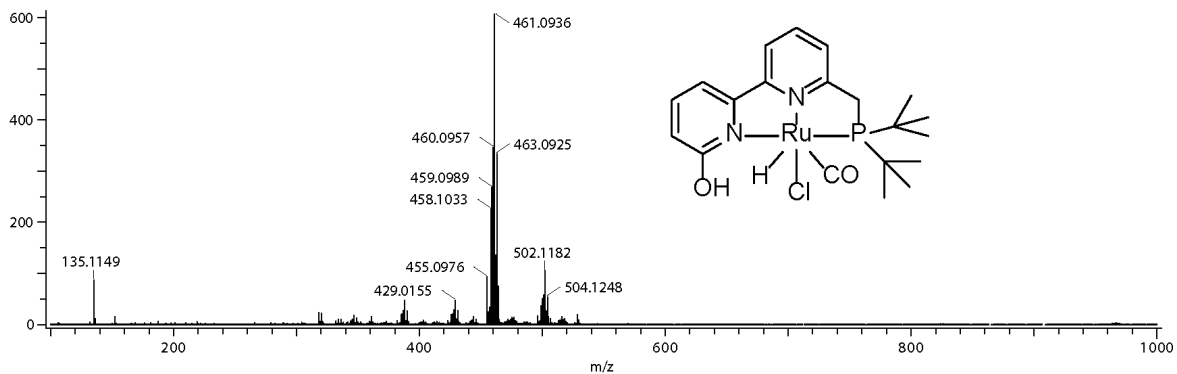
Formula: C20H28N2O2P1Ru1   Addition/Desorption Ion: None
Mono Isotopic Mass: 461.0931875   Charge Number : -

Figure S23. CSI-MS of 1.
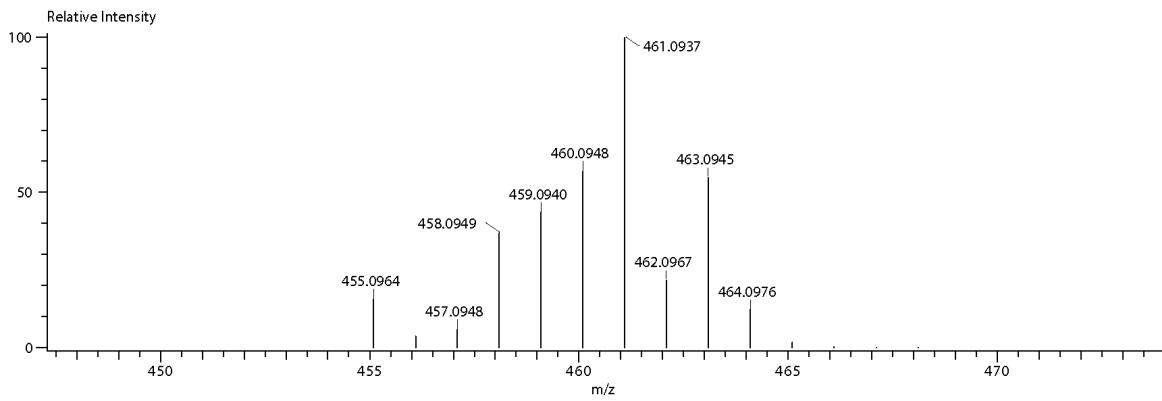
Figure S24. CSI-MS of 1.
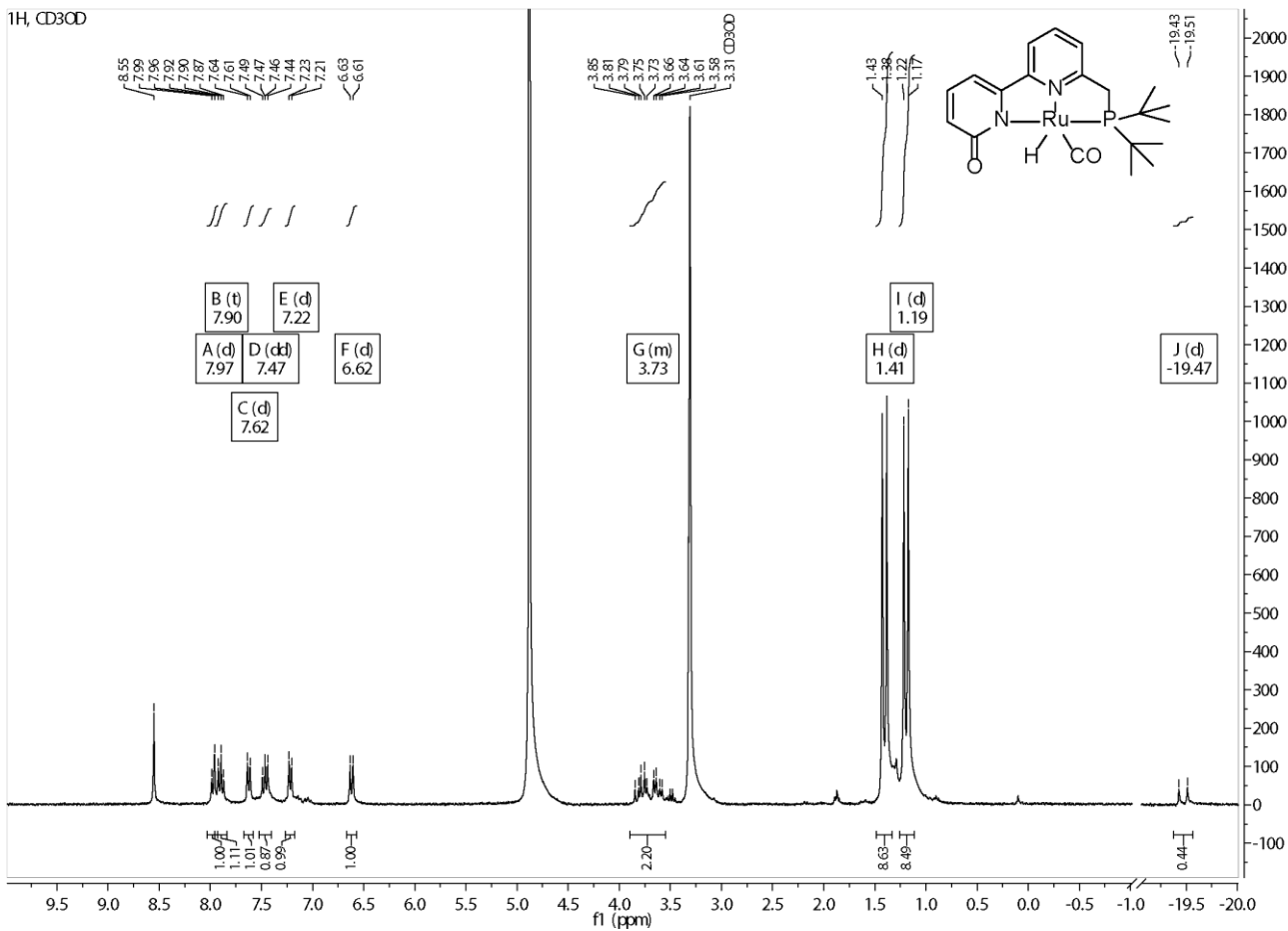
Figure S25. ^{1}H NMR spectrum (CD$_3$OD) of 1'.
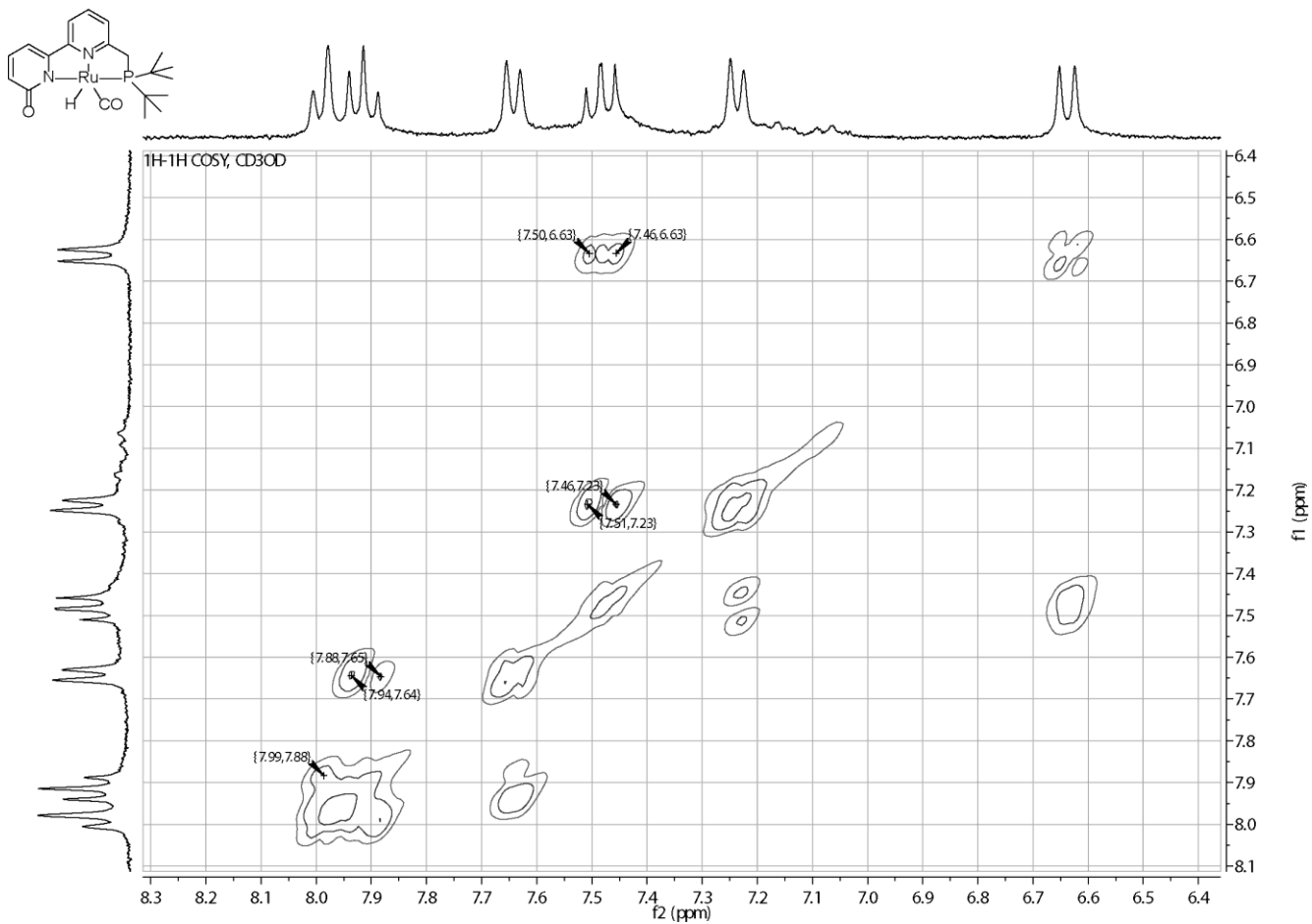
Figure S26. 2D [^{1}H-^{1}H]-COSY NMR spectrum (CD$_3$OD) of 1'.
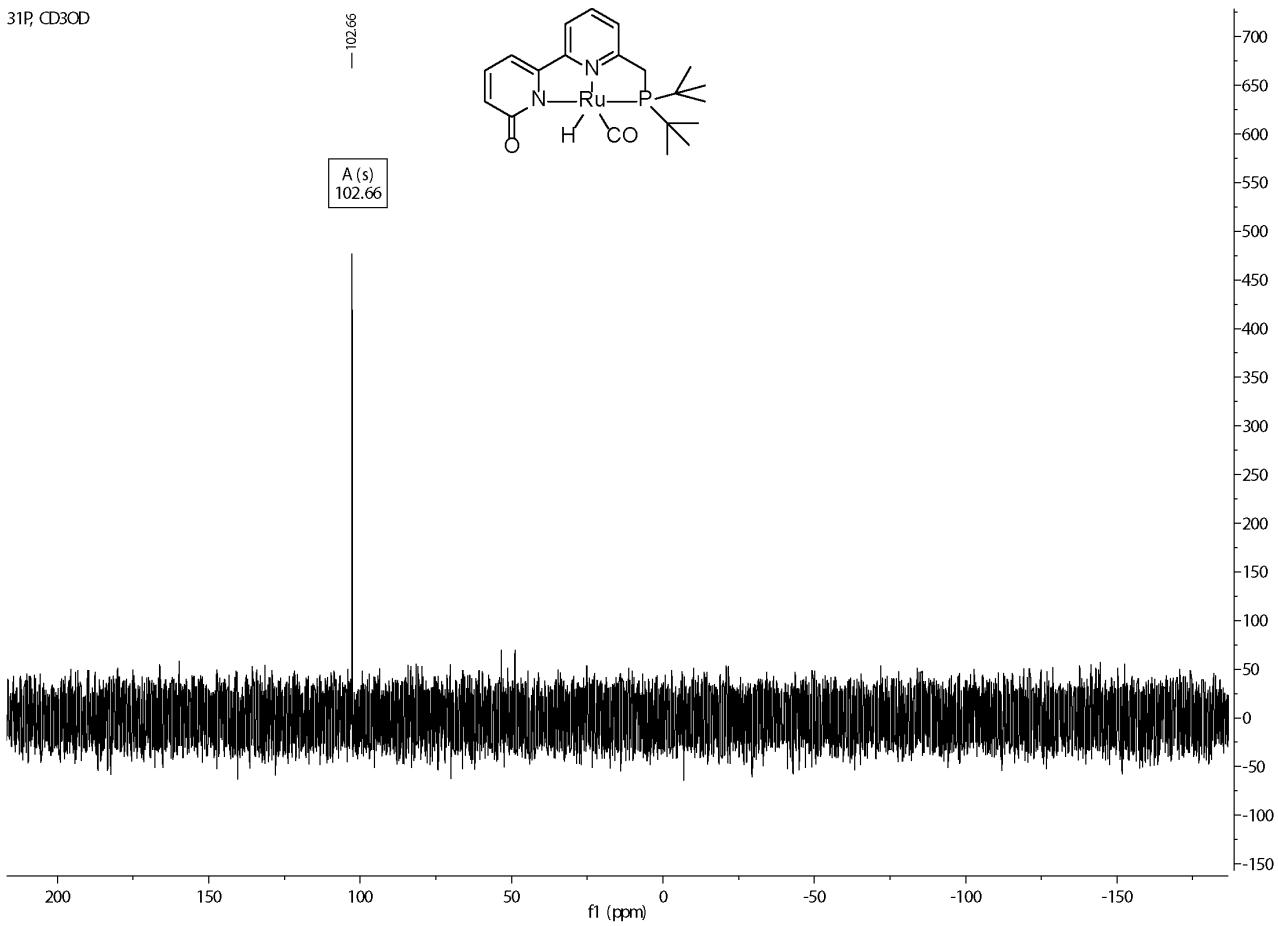
Figure S27. ^{31}P NMR spectrum (CD$_3$OD) of 1'.

Crystallographic details of complex 1^Me
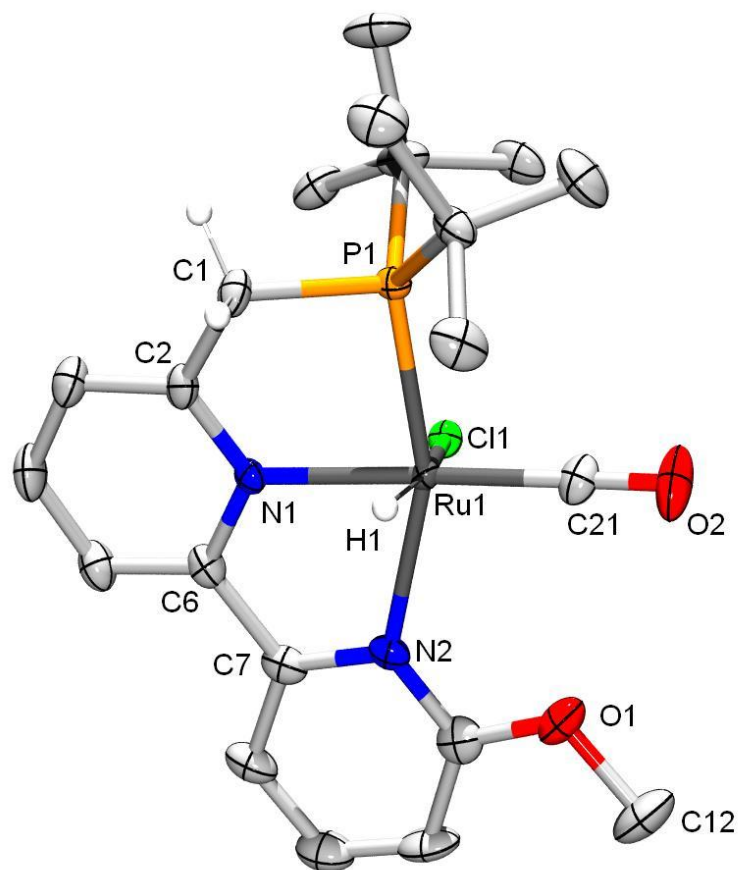
Figure S28. ORTEP plot of 1^Me.

		Complex 1_MeCN	**Complex 1^Me**
Ru1-P1	(Å)	2.2711(6)	2.2779(12)
Ru1-N1	(Å)	2.0964(19)	2.0943(39)
Ru1-N2	(Å)	2.1598(18)	2.1740(40)
Ru1-C20^a	(Å)	1.8524(25)	1.8404(53)
Ru1-H1	(Å)	1.7125(309)	1.9415(447)
Ru1-Cl1^b	(Å)	2.1855(21)	2.5634(12)
C20-O2^a	(Å)	1.1512(30)	1.1481(65)
P1-Ru1-N1	(°)	82.72(5)	83.21(11)
P1-Ru1-N2	(°)	157.27(7)	159.24(12)
N1-Ru1-N2	(°)	76.24(7)	76.31(16)

Table S1. Selected bond lengths (Å), angles and torsion angles (°) for complexes 1 and 2

N1-Ru1-C20[a]	(°)	171.49(9)	173.16(19)
H1-Ru1-Cl1[b]	(°)	171.90(1.04)	172.13(1.30)
N2-C7-C6-N1	(°)	-1.00	-0.58
N1-C2-C1-P1	(°)	29.04	27.14

[a] In complex **2**, the corresponding bond lengths are between Ru1-C21 and C21-O2, and bond angle between N1-Ru1-C21. [b] In complex **1$_{MeCN}$**, the chloride ligand is replaced by an NCMe ligand, thus the bond length represents the Ru1-N3 bond and H1-Ru1-N3 bond angle.

Details for complex 1^{Me}, [RuCl(CO)(H)(L^{Me})]: $C_{21}H_{30}ClN_2O_2PRu$, Fw = 509.96, orange-red rectangular block, 0.255×0.168×0.145 mm, triclinic $P\bar{1}$ (No: 2)), a = 8.053(6), b = 8.281(5), c = 17.447(11) Å, α = 103.250(17), β = 94.156(14), γ = 90.651(13)°, V = 1129.0(2) Å^3, Z = 2, D_x = 1.459 g/cm^3, μ = 0.905 mm^{-1}. 42825 Reflections were measured up to a resolution of (sin θ/λ)$_{max}$ = 0.75 Å^{-1}. 5605 Reflections were unique (R_{int} = 0.0664), of which 5035 were observed [I>2σ(I)]. 264 Parameters were refined with 0 restraints. R1/wR2 [I > 2σ(I)]: 0.0540/0.1349. R1/wR2 [all refl.]: 0.0629/ 0.1387. S = 1.187. Residual electron density between -1.49 and 1.64 e/Å^3.

Computational details, energies and BP86-calculated structures

Table S2. Relative **f**ree energies of the calculated complexes using different functionals (BP86 was used in combination with disp3 dispersion corrections, TPSS and b3-lyp without).

	Free energy (kcal mol⁻¹)		
Complex	**BP86 / disp3**	**TPSS**	**b3-lyp**
1ᴴᴴ	0	0	0
TS''	22.5	24.4	28.1
TS'PS'	22.3	25.0	28.3
TS'	5.0	6.2	7.7
Int''	4.7	4.6	4.7
Int'	0.0	-2.0	-2.1
1''	0.9	-2.0	-4.9
1'	-4.1	-6.6	-9.8

1ᴴᴴ
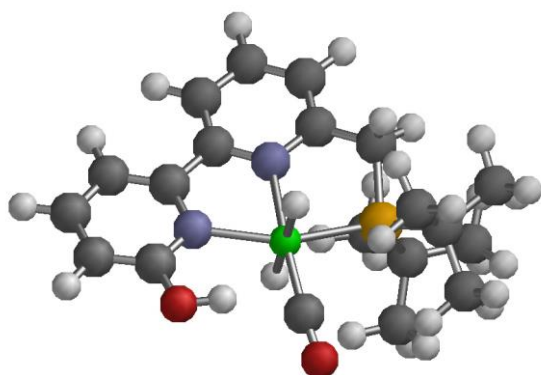
55

Energy = -1476.645732639

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N	0.723217	-1.363071	-0.9690875
C	0.4683446	-3.5007987	0.0800503
C	0.9963542	-3.3724807	-2.2615696
C	1.0117247	-1.9760763	-2.1546206
C	0.4949954	-2.1106657	0.1447718
H	0.2689409	-4.0747679	0.9844525
H	1.2058847	-3.8489765	-3.2176271
C	0.3353654	-1.3481377	1.4266346
H	1.3430059	-1.1886669	1.8457849
H	-0.2472089	-1.9090638	2.1699962
P	-0.3196921	0.3733144	1.106949
C	-2.2198565	0.1551461	1.2360094

C	-2.7457238	-0.1129528	2.6543968
H	-2.2646972	-0.9844713	3.1217455
H	-3.8241509	-0.331003	2.5953412
H	-2.6266589	0.7505427	3.3201975
C	-2.59019	-1.0544151	0.3526044
H	-2.1799045	-0.9467206	-0.6607621
H	-3.6873627	-1.1083441	0.2720349
H	-2.2473454	-2.0063499	0.7821854
C	-2.8997512	1.4062337	0.6493198
H	-2.5718841	1.5781695	-0.3840426
H	-2.6942163	2.3123555	1.2319608
H	-3.9906328	1.2518955	0.6450436
C	0.3244297	1.3571015	2.6150733
C	0.2460773	0.5739592	3.94088
H	0.8618356	-0.3360012	3.9208214
H	-0.7732669	0.2926903	4.221714
H	0.6433541	1.2115486	4.7471962
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H	-0.4618742	3.2374713	1.7904641
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C	1.8038464	1.7017641	2.3583661
H	1.9274236	2.3368619	1.4749481
H	2.4229421	0.8077467	2.2006945
H	2.1936744	2.2336249	3.2415527
C	1.3475754	-1.0559142	-3.2385806
C	2.1074021	0.8471326	-5.0885181
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C	1.7408905	-1.4592653	-4.51688
C	2.1083025	-0.4941489	-5.4544534
C	1.7091907	1.1909326	-3.7905644
H	1.7697732	-2.516111	-4.7723183
H	2.4116004	-0.7887277	-6.4589698
H	2.4147636	1.640396	-5.7671705
Ru	0.5084527	0.7117581	-0.9736245
O	1.7473414	2.4690023	-3.4093132
H	1.4816134	2.4729123	-2.4466967
H	2.0594188	0.8946026	-0.3277167
C	0.1304718	2.5179273	-0.8904206
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H	-1.0318688	0.5070267	-1.6258448

1^{HH} + tBuOH
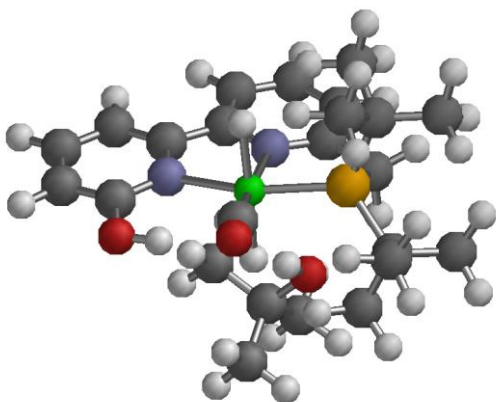
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C	1.2367287	-3.108944	-0.5632311
C	2.4952096	-2.4217511	-2.4923879
C	1.7847885	-1.216125	-2.4913528
C	0.5520163	-1.8962809	-0.5979135
H	0.9801544	-3.8453494	0.1973571
H	3.245996	-2.6147176	-3.2562408
C	-0.5833758	-1.5797085	0.3281233
H	-0.4821488	-2.0957158	1.2923761
P	-0.8146841	0.2629988	0.5053284
C	-2.664862	0.4320891	0.9507544
C	-3.1585727	-0.6573454	1.9232175
H	-3.0573755	-1.6647398	1.4970701
H	-4.2324691	-0.495809	2.1099205
H	-2.6524905	-0.6385915	2.892873
C	-3.4831568	0.3058324	-0.3490287
H	-3.2208129	1.0853649	-1.0723772
H	-4.5503244	0.4056213	-0.0915534
H	-3.347966	-0.6652251	-0.8447564
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H	-2.5448153	2.6282558	0.8924411
H	-2.4736088	1.9520855	2.5405893
H	-4.0069896	1.9744558	1.6554697
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C	-0.2817861	0.1987998	3.3691032
H	-0.464402	-0.8857097	3.3681379

H	-1.207345	0.7083119	3.6647136
H	0.4643187	0.4015923	4.1539037
C	0.4671967	2.2266964	2.0739383
H	0.9205119	2.5904136	1.143478
H	1.144613	2.4723045	2.9075127
H	-0.470655	2.7713042	2.2355372
C	1.6462502	0.0418358	1.7994332
H	2.0622258	0.3124672	0.8193872
H	1.6050755	-1.0533773	1.8824992
H	2.3398187	0.4033835	2.5751183
C	1.9175354	-0.1696541	-3.5053913
C	1.8605377	1.8253161	-5.4136076
N	1.096208	0.9112383	-3.3144427
C	2.7527005	-0.2615719	-4.6195339
C	2.7318707	0.755533	-5.5745472
C	1.044192	1.8618917	-4.2753001
H	3.4013834	-1.125099	-4.7480395
H	3.3798142	0.702931	-6.4494298
H	1.7790698	2.6308649	-6.1405202
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O	0.1711433	2.859734	-4.1258712
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C	-3.2723948	-1.4161106	-4.4149448
H	-4.2138434	-1.558545	-3.8663395
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H	-2.9755869	-0.3614262	-4.3193723
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H	-0.0628839	-2.7216717	-4.1001725
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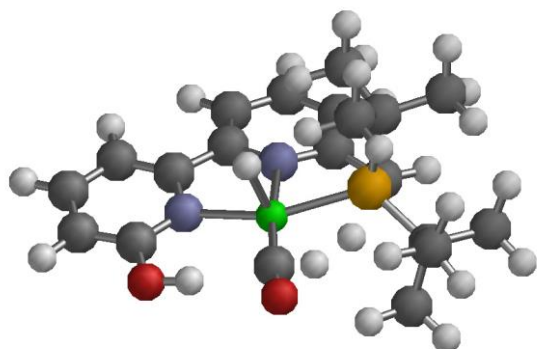
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C	2.1547579	-3.7351918	-0.4344063
N	0.9139997	-1.2965242	-0.8390966
C	1.1509143	-3.3195929	0.4282095
C	2.4919326	-2.9518976	-1.5477411
C	1.8366742	-1.7369319	-1.735441
C	0.5081564	-2.0830199	0.2100765
H	0.8484677	-3.932896	1.2766153
H	3.2290615	-3.3009606	-2.2677854
C	-0.6516209	-1.5956088	0.9136981
H	-1.0047292	-2.2067534	1.7495515
P	-0.7304196	0.2318422	1.0071583
C	-2.5220679	0.5780709	1.5657515
C	-2.9516318	-0.3171025	2.7448291
H	-2.9554243	-1.3789454	2.4652565
H	-3.9836449	-0.0507769	3.0241956
H	-2.3292538	-0.1956867	3.6366147
C	-3.4857261	0.2904326	0.396401
H	-3.281979	0.9149385	-0.4791491
H	-4.5100932	0.5064381	0.7411833
H	-3.4537562	-0.7604671	0.0834305
C	-2.6630386	2.062109	1.9505409
H	-2.3189607	2.7285152	1.1483136
H	-2.1207278	2.3080087	2.8726968
H	-3.7272648	2.2815613	2.1307196
C	0.5190081	0.8711614	2.3019155
C	0.1291516	0.5591307	3.7548087
H	-0.0537057	-0.5142022	3.9085357
H	-0.7561781	1.1177812	4.0838038

H	0.9609464	0.8508593	4.4161278
C	0.7129728	2.3884818	2.1141116
H	1.0072098	2.6220034	1.0827946
H	1.5151297	2.7294948	2.78857
H	-0.1868059	2.9667242	2.3534036
C	1.8649305	0.1780977	2.0064554
H	2.1816965	0.334218	0.9676558
H	1.8258991	-0.9007376	2.2056965
H	2.6330025	0.6136049	2.6653364
C	1.9650386	-0.8744748	-2.9123415
C	1.9396933	0.7794451	-5.1230044
N	1.0503157	0.1502593	-2.965357
C	2.8939015	-1.0783648	-3.9331376
C	2.8794444	-0.2410951	-5.0488759
C	1.0450638	0.949162	-4.0582106
H	3.6187743	-1.8853518	-3.8529225
H	3.5971128	-0.3858209	-5.8564316
H	1.8753054	1.4581714	-5.9711691
Ru	-0.0879909	0.4963258	-1.1876031
O	0.1496624	1.9384609	-4.1144592
H	-0.3564084	1.8999904	-3.2569025
H	1.1337894	1.4751888	-0.8175515
C	-1.1095646	2.0199366	-1.3804046
O	-1.7778532	2.9868567	-1.4113346
H	-1.4775398	-0.8328635	-1.2754955
H	-1.3987059	-1.3660924	-0.3496814

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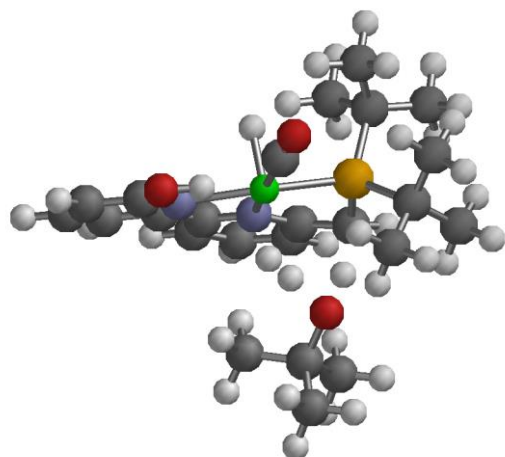
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N	0.8654135	-0.8227624	-1.761752
C	1.1226705	-3.0639149	-0.9587418
C	2.5385889	-2.2398664	-2.7320933
C	1.856504	-1.0248204	-2.6682206
C	0.45482	-1.8195987	-0.916038
H	0.8052837	-3.8561345	-0.2816256
H	3.3338588	-2.3960697	-3.4572313
C	-0.7327371	-1.5518405	-0.1322838
H	-0.941577	-2.2809633	0.6572369
P	-0.8787086	0.217809	0.2977374
C	-2.7100254	0.527263	0.7569948
C	-3.3188277	-0.7133317	1.4371869
H	-3.3170198	-1.5764779	0.758151
H	-4.3678411	-0.4959069	1.6945998
H	-2.8042122	-0.9955986	2.3638248
C	-3.5203696	0.8166832	-0.522102
H	-3.1492921	1.7043778	-1.048539
H	-4.5634013	1.0125269	-0.2231715
H	-3.5172236	-0.0284444	-1.2189461
C	-2.845082	1.7649295	1.6645548
H	-2.4117957	2.6592247	1.1965401
H	-2.3938856	1.6317177	2.6546644
H	-3.9175922	1.9616411	1.8198733
C	0.2267937	0.4562373	1.8504314
C	-0.3461046	-0.2353381	3.0994636

H	-0.5337895	-1.3043727	2.9216433
H	-1.2740601	0.2241371	3.4589577
H	0.3910883	-0.1641106	3.9154678
C	0.4673296	1.9536382	2.1149877
H	0.9132267	2.4377986	1.2367066
H	1.1710437	2.0594487	2.9565246
H	-0.44547	2.4974897	2.378992
C	1.5916932	-0.1951497	1.5471002
H	2.0360814	0.2013502	0.6250741
H	1.5186723	-1.2871967	1.46279
H	2.2778637	0.0309257	2.3786271
C	2.0801974	0.1068829	-3.5798672
C	2.2568464	2.2923578	-5.2667153
N	1.2661154	1.1869274	-3.3654213
C	3.0095184	0.0995222	-4.6192056
C	3.0992052	1.2081664	-5.464812
C	1.3433144	2.2423858	-4.2028706
H	3.6515609	-0.7646743	-4.7726475
H	3.8215198	1.2185983	-6.2812324
H	2.2739835	3.1752479	-5.9023258
Ru	0.0021641	1.0879633	-1.6411856
O	0.5119505	3.2681564	-4.0056205
H	-0.0323516	3.0301061	-3.20271
H	1.2955538	1.5590562	-0.8067013
C	-0.6869135	2.7536524	-1.2402189
O	-1.1168446	3.7807579	-0.8723614
H	-1.3641159	0.6748013	-2.7721188
H	-1.6493662	-0.1916716	-2.5324894
O	-2.296775	-1.4378473	-2.2457011
H	-1.6287104	-1.6392102	-1.1806147
C	-2.305551	-2.4634327	-3.2475255
C	-3.573973	-2.2544866	-4.0861536
H	-4.4608124	-2.2983241	-3.4388932
H	-3.670646	-3.0200862	-4.8711425
H	-3.5473341	-1.2648329	-4.5639866
C	-2.3426253	-3.8278834	-2.5438044
H	-3.2144973	-3.8862799	-1.8770411
H	-1.4326379	-3.9727567	-1.9427666
H	-2.4042974	-4.6480744	-3.2745824
C	-1.0557237	-2.3617998	-4.1381374
H	-0.1497847	-2.5831858	-3.5600998
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H	-1.108046	-3.0740305	-4.9752098

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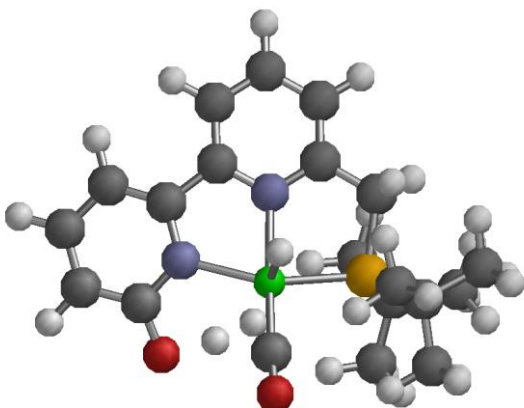
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N	0.8172319	0.8994929	-1.3950262
C	0.8668816	-0.2435743	-3.5000114
C	1.7084478	2.0011236	-3.3436203
C	1.3855806	2.000935	-1.981572
C	0.6086551	-0.2251893	-2.1305302
H	0.6644468	-1.1505692	-4.0692959
H	2.1740218	2.8788733	-3.7885603
C	0.2158481	-1.4721099	-1.3865759
H	1.1192416	-2.1000712	-1.324827
H	-0.5323233	-2.0584406	-1.9384043
P	-0.2715354	-1.1397092	0.3901962
C	-2.1854616	-1.159756	0.328775
C	-2.8066327	-2.5287884	0.0139649
H	-2.4004392	-2.9773953	-0.9040692
H	-3.8906668	-2.4017337	-0.1378142
H	-2.6772211	-3.2426834	0.8371435
C	-2.5848838	-0.1703849	-0.7872503
H	-2.1388367	0.8202281	-0.626949
H	-3.6801424	-0.0547914	-0.7820583
H	-2.2976861	-0.5267924	-1.7865398
C	-2.7420896	-0.6342013	1.6646124
H	-2.3135491	0.3449027	1.9146806
H	-2.5468408	-1.3193328	2.4982775
H	-3.8340391	-0.5182964	1.5771408
C	0.3876635	-2.6937512	1.2834342
C	0.1321572	-4.0151071	0.532602

H	0.6068999	-4.0310757	-0.4582757
H	-0.9304601	-4.242692	0.4065473
H	0.5769628	-4.8395574	1.1128782
C	-0.2362388	-2.7634586	2.6884338
H	-0.1342324	-1.8132419	3.229258
H	0.2842977	-3.5372452	3.2746206
H	-1.2986534	-3.0369414	2.6546434
C	1.91241	-2.5199154	1.4347639
H	2.1681526	-1.6659311	2.0700358
H	2.4188103	-2.3777094	0.4696274
H	2.3225283	-3.4323788	1.8964669
C	1.5470894	3.1429949	-1.0816102
C	1.2448611	5.2216375	0.7127705
N	1.1846516	2.8723405	0.2061391
C	1.8936072	4.4341298	-1.4767381
C	1.7993509	5.4681776	-0.5328756
C	0.833833	3.9037687	1.0466104
H	2.1926565	4.6421016	-2.5019446
H	2.0991558	6.4810981	-0.8051027
H	1.0586851	6.0161347	1.4334975
O	0.0994143	3.6110739	2.0661236
C	0.9937767	0.7072447	2.5096067
O	1.2934106	0.4959117	3.6174526
Ru	0.6477531	0.903773	0.6996386
H	2.1071493	0.2216444	0.5016997
H	-0.4674011	2.5103434	1.6325127
H	-0.9280984	1.7519736	1.1021958

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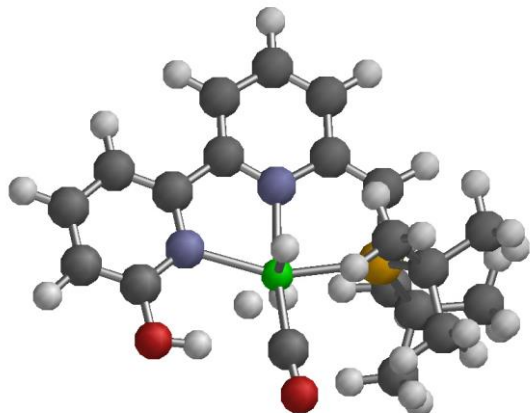
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H	1.7498748	-5.1742343	-0.8319498
C	1.4740359	-4.1187046	-0.8491362
N	0.7364141	-1.4410274	-0.92569
C	0.8610828	-3.5512934	0.2405053
C	1.7642872	-3.3387358	-1.9910361
C	1.3798212	-2.0023136	-1.9827384
C	0.4970694	-2.1599721	0.2433449
H	0.6496437	-4.1403761	1.1328463
H	2.2762608	-3.7730514	-2.8455504
C	-0.0613333	-1.5085497	1.3367203
H	-0.2653314	-2.065589	2.2497261
P	-0.4769982	0.1962111	1.1729033
C	-2.3775135	0.342198	1.4508671
C	-2.7826945	0.1769267	2.9260665
H	-2.4065317	-0.7646918	3.3494737
H	-3.8827381	0.1506211	2.9923249
H	-2.4407481	1.00758	3.5545551
C	-3.0441629	-0.8059676	0.670957
H	-2.8084388	-0.7888966	-0.4012333
H	-4.1377579	-0.7095462	0.763889
H	-2.7416804	-1.7869311	1.058652
C	-2.9011421	1.6853856	0.9132837
H	-2.731035	1.780642	-0.1669622
H	-2.4335502	2.5497773	1.3990036
H	-3.9873991	1.7492817	1.0892542
C	0.4396233	1.1226865	2.5808645
C	0.3863988	0.3202864	3.8977522

H	0.8342715	-0.6747083	3.7733426
H	-0.6251009	0.200057	4.2973714
H	0.9768413	0.8576916	4.6569836
C	-0.1025544	2.5442081	2.799957
H	-0.0958281	3.1349515	1.87554
H	0.5411378	3.0626641	3.5290317
H	-1.1211546	2.5490148	3.2087912
C	1.9226514	1.2166739	2.1743666
H	2.0749059	1.90647	1.3363527
H	2.3239827	0.2340717	1.8889807
H	2.5007229	1.5884028	3.0359973
C	1.6475728	-1.0767955	-3.0936941
C	2.0901446	0.8248171	-5.0650091
N	1.217447	0.2098816	-2.9016876
C	2.3022328	-1.4391635	-4.2721963
C	2.5245117	-0.4787992	-5.2599634
C	1.4314152	1.1304004	-3.8658631
H	2.6370317	-2.463571	-4.4130158
H	3.0377262	-0.7511607	-6.1825332
H	2.2356854	1.6130006	-5.800534
Ru	0.2141032	0.5914796	-1.0286026
O	0.987898	2.3761615	-3.6677873
H	0.5671521	2.3788535	-2.7644147
H	1.6593721	0.8605205	-0.4265976
C	-0.1029719	2.4042662	-0.8307598
O	-0.2755658	3.5411429	-0.600242
H	-1.2353195	0.3198496	-2.12829
H	-1.5021631	0.0498386	-1.3922403

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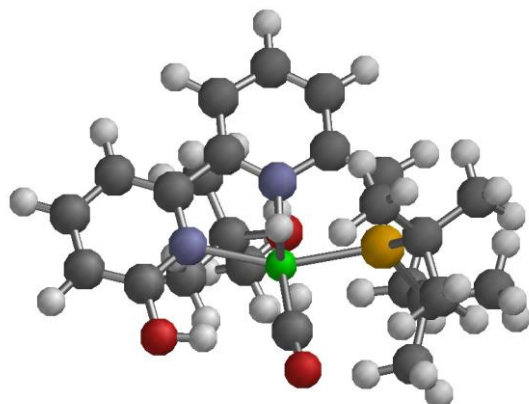
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N	0.6261708	-1.1849254	-1.460415
C	0.6920891	-3.4239917	-0.5514304
C	1.8525687	-2.9099268	-2.6102748
C	1.413732	-1.5980411	-2.495295
C	0.3216943	-2.0412672	-0.3966012
H	0.386635	-4.1276046	0.2226455
H	2.4765002	-3.2243882	-3.4425031
C	-0.307053	-1.5262632	0.724455
H	-0.5920613	-2.1937704	1.5361121
P	-0.6490816	0.207479	0.7805196
C	-2.5474921	0.4050261	0.9994687
C	-3.027972	0.0680745	2.421942
H	-2.7202732	-0.9414739	2.7278165
H	-4.1297897	0.0923867	2.436374
H	-2.6787097	0.787486	3.1723713
C	-3.2264207	-0.5927681	0.043663
H	-2.9409576	-0.4722297	-1.0086014
H	-4.3173628	-0.4482166	0.103133
H	-2.9983664	-1.6322786	0.3126255
C	-2.9790628	1.8354682	0.6295704
H	-2.7510403	2.0656594	-0.4189298
H	-2.4981966	2.6001352	1.2511693
H	-4.0688866	1.9303218	0.7643281
C	0.2480192	0.8754728	2.33959
C	0.0961348	-0.0988149	3.5257745
H	0.5107513	-1.0863662	3.2825676

H	-0.9383683	-0.227618	3.8575937
H	0.6672263	0.3001302	4.3792216
C	-0.2383287	2.2789316	2.7360314
H	-0.1632762	2.9914814	1.9047475
H	0.3958498	2.6582853	3.553658
H	-1.2727159	2.2794485	3.1023485
C	1.7505825	0.9484495	2.0096339
H	1.9735335	1.7396408	1.2846599
H	2.1201379	-0.0037637	1.6039692
H	2.3038322	1.1652748	2.9377897
C	1.7143687	-0.5514011	-3.4807646
C	2.1186587	1.5398254	-5.2557238
N	1.2425961	0.6976717	-3.1718782
C	2.3976762	-0.7801183	-4.6758153
C	2.6026079	0.2762877	-5.5640832
C	1.4336785	1.709972	-4.0443759
H	2.7529168	-1.7792851	-4.9138868
H	3.133513	0.1085196	-6.5014584
H	2.2408733	2.3964724	-5.9150499
Ru	0.1710736	0.8664538	-1.3086221
O	0.9367177	2.9134033	-3.7420658
H	0.5013298	2.8166408	-2.8501552
H	1.6044174	0.9673554	-0.6249977
C	-0.0376925	2.6504222	-0.8656884
O	-0.1305593	3.7540143	-0.4818865
H	-1.2527504	0.8548887	-2.4643383
H	-1.5522377	0.4724906	-1.7949477
O	-2.1436925	-1.9657938	-2.7758148
H	-1.2185824	-1.8468652	-2.4815541
C	-2.156163	-2.1359278	-4.2107739
C	-3.6166289	-2.4301576	-4.5545737
H	-3.950803	-3.3391502	-4.035989
H	-3.7413712	-2.5743097	-5.6366516
H	-4.2569295	-1.5960163	-4.2348099
C	-1.2537045	-3.3130546	-4.6008147
H	-1.5724649	-4.2218563	-4.0723199
H	-0.2090188	-3.1057999	-4.3237468
H	-1.2917786	-3.5019083	-5.6838177
C	-1.6880863	-0.8429493	-4.8946883
H	-0.648529	-0.6138268	-4.6220642
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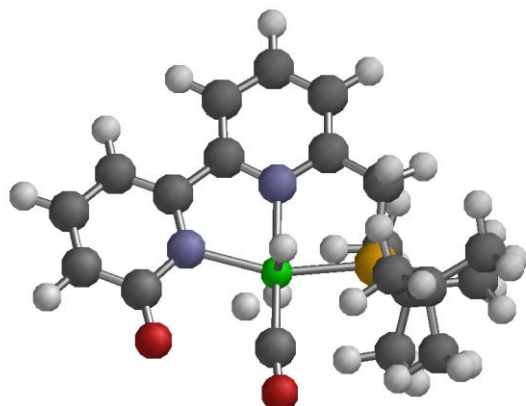
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N	0.7080339	0.9632258	-1.3727234
C	0.5637045	-0.116083	-3.5003718
C	1.2029862	2.2029565	-3.3587883
C	1.1168552	2.1242904	-1.9606044
C	0.4984795	-0.1576078	-2.1091831
H	0.3734819	-1.0199791	-4.0778823
H	1.5064681	3.1342016	-3.8323089
C	0.2997603	-1.4376777	-1.3439484
H	1.2960497	-1.8914465	-1.212905
H	-0.3085155	-2.1623168	-1.9023095
P	-0.3180356	-1.1250296	0.3958235
C	-2.2158844	-1.3253049	0.2123331
C	-2.6939701	-2.7639203	-0.0388915
H	-2.2047757	-3.2220382	-0.9100996
H	-3.7766023	-2.7492078	-0.2434894
H	-2.537876	-3.413329	0.8307413
C	-2.6437582	-0.4699987	-0.9989762
H	-2.2836755	0.5653381	-0.9369471
H	-3.743516	-0.4345335	-1.0379404
H	-2.2950327	-0.8917936	-1.9515931
C	-2.8982008	-0.7713234	1.4775141
H	-2.5945791	0.2620997	1.6870173
H	-2.6734407	-1.3702769	2.3679514
H	-3.9902804	-0.7821127	1.3344829
C	0.4107282	-2.5913492	1.3750574
C	0.3434786	-3.9404121	0.6329293

H	0.8974877	-3.9207874	-0.3157295
H	-0.6781844	-4.2724452	0.4265804
H	0.8162341	-4.7101646	1.2634374
C	-0.3124483	-2.6942719	2.7304669
H	-0.3280919	-1.7308223	3.2572482
H	0.225016	-3.413048	3.3687509
H	-1.3430151	-3.0579146	2.6270164
C	1.89528	-2.272989	1.6455056
H	2.0168954	-1.3867937	2.2771903
H	2.4659068	-2.1043871	0.7211369
H	2.3460278	-3.1345971	2.1630841
C	1.4669435	3.2012333	-1.0245785
C	2.153969	5.0935921	0.8535151
N	1.3212684	2.8881706	0.2964955
C	1.942795	4.4369304	-1.455458
C	2.3004699	5.3884723	-0.4799793
C	1.6099542	3.8257457	1.3082744
H	2.0481153	4.6593411	-2.5145429
H	2.692974	6.35945	-0.7895125
H	2.4174127	5.8073159	1.6335739
O	1.3947817	3.5654951	2.5034309
C	0.501817	0.9440956	2.5733188
O	0.5546821	0.7831398	3.7232176
Ru	0.4616399	0.9960228	0.7083412
H	1.9267074	0.3673909	0.7548379
H	-0.9467189	2.180961	0.8565257
H	-1.3034893	1.5479988	0.4777957

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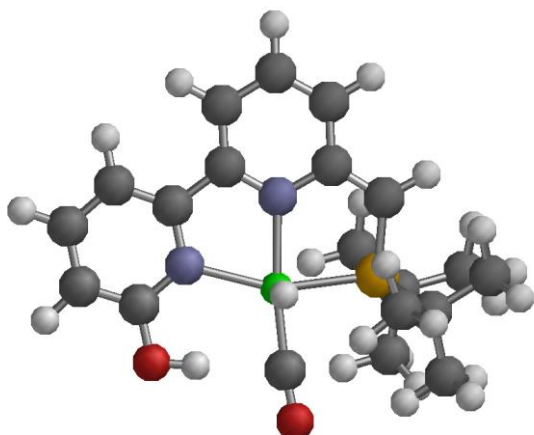
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H	1.5041022	-5.1944942	-0.8767945
C	1.2869727	-4.1253091	-0.8790426
N	0.7291003	-1.3964981	-0.9154289
C	0.8151263	-3.5177242	0.2554282
C	1.4990738	-3.3709531	-2.0597208
C	1.2118501	-2.0149592	-2.0318433
C	0.523811	-2.1078225	0.2734195
H	0.6528406	-4.0878335	1.1701323
H	1.8824446	-3.8467957	-2.958598
C	0.0534529	-1.4274006	1.3854133
H	-0.1353764	-1.9660304	2.3116601
P	-0.3787124	0.2766922	1.1569204
C	-2.2972314	0.338879	1.1746303
C	-2.8805188	-0.133987	2.5140662
H	-2.4734906	-1.1093238	2.8157996
H	-3.9733032	-0.243487	2.417445
H	-2.6957899	0.5887001	3.3196826
C	-2.7269658	-0.6427998	0.0640726
H	-2.3763674	-0.3120679	-0.9274497
H	-3.8271738	-0.6855285	0.0221821
H	-2.3439058	-1.6562449	0.2424145
C	-2.8504858	1.7298019	0.822078
H	-2.4842014	2.0767844	-0.1523288
H	-2.6003699	2.4936564	1.5659426
H	-3.9499706	1.6702992	0.7658973
C	0.3605502	1.2129331	2.6365183
C	0.2293406	0.3998932	3.9388169

H	0.7730451	-0.5514595	3.8734644
H	-0.8120867	0.1875818	4.207936
H	0.672363	0.9813437	4.7633518
C	-0.2719666	2.6002695	2.8227216
H	-0.2728704	3.1850986	1.8942171
H	0.312461	3.1602138	3.5703888
H	-1.3013917	2.5348995	3.1993486
C	1.8615038	1.3791559	2.3262239
H	2.0270899	2.080332	1.4989453
H	2.3239847	0.4169285	2.0636075
H	2.370628	1.7744925	3.220076
C	1.4088697	-1.1183681	-3.1818056
C	1.7517659	0.7383952	-5.2129831
N	1.1021087	0.2001441	-2.9485886
C	1.8763966	-1.5348448	-4.4275569
C	2.0448712	-0.5973517	-5.4488968
C	1.2838434	1.1011207	-3.9423966
H	2.1083004	-2.5832073	-4.5977146
H	2.4093953	-0.9124653	-6.4268418
H	1.8711575	1.5115679	-5.9689907
Ru	0.3722431	0.6492516	-0.9860684
O	1.0052565	2.3841582	-3.6965988
H	0.7071621	2.4248418	-2.7453873
H	1.7805082	0.9880353	-0.4382291
C	0.0251887	2.4553512	-0.8346784
O	-0.1846296	3.5961349	-0.6348579

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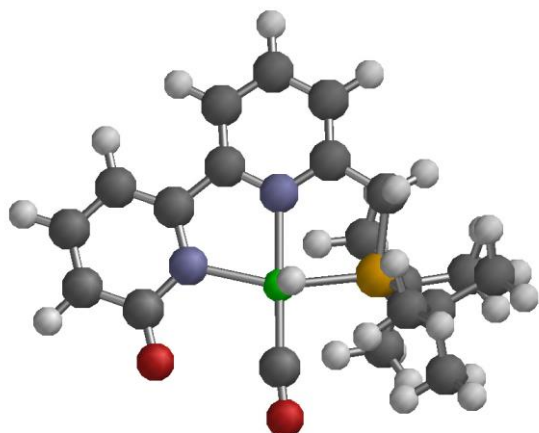
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Energy = -1475.45404301

H	0.9120119	1.1957997	-5.1861796
C	0.8817535	1.1319791	-4.0981356
N	0.777971	0.9753302	-1.3363503
C	0.6014572	-0.0872836	-3.4717763
C	1.1291979	2.2611449	-3.3260465
C	1.0778498	2.1690481	-1.9283278
C	0.56555	-0.142848	-2.0807096
H	0.4195857	-0.9901936	-4.0535379
H	1.3540224	3.2136709	-3.8013557
C	0.3361536	-1.4206868	-1.3213596
H	1.3119204	-1.9168736	-1.1919288
H	-0.3035139	-2.1166779	-1.8817796
P	-0.2655496	-1.0721054	0.4216515
C	-2.1718386	-1.0903946	0.252746
C	-2.7922538	-2.4590881	-0.0578142
H	-2.357739	-2.9212592	-0.9557746
H	-3.8713738	-2.3334601	-0.2444387
H	-2.687794	-3.1611071	0.7789132
C	-2.510041	-0.1225301	-0.9013018
H	-2.0810014	0.877397	-0.7409019
H	-3.6037066	-0.0080185	-0.9625522
H	-2.1618234	-0.4882275	-1.8771896
C	-2.779822	-0.5161937	1.547229
H	-2.3636551	0.4738948	1.7799986
H	-2.6101559	-1.1614014	2.4166607
H	-3.8685344	-0.4077677	1.4183423
C	0.3419803	-2.5999315	1.3826735

C	0.1794518	-3.9277495	0.6195094
H	0.7557313	-3.9423842	-0.3156953
H	-0.8634469	-4.1630431	0.3827272
H	0.5653488	-4.7466685	1.2475951
C	-0.3904506	-2.6723145	2.7343826
H	-0.3467644	-1.7161124	3.2729813
H	0.0959316	-3.4333266	3.3651693
H	-1.4419085	-2.9665099	2.6212295
C	1.8426826	-2.3779303	1.6606097
H	2.0102577	-1.5069406	2.304928
H	2.4254627	-2.2327049	0.7393286
H	2.243273	-3.2691077	2.1694703
C	1.3164025	3.2764178	-0.9898586
C	1.7631923	5.2595022	0.872896
N	1.1700065	2.9558687	0.3365917
C	1.6691905	4.546576	-1.4249652
C	1.894875	5.5520615	-0.4590842
C	1.3973656	3.9303327	1.3424862
H	1.7735875	4.7659394	-2.4849624
H	2.1750923	6.5574586	-0.7800141
H	1.9338576	6.0061127	1.6480386
Ru	0.5647669	0.9925625	0.7387346
O	1.2872751	3.6532679	2.5435845
H	1.948045	0.3190589	0.9345046
C	0.4196054	0.9896641	2.5918223
O	0.3305174	0.867753	3.7472356

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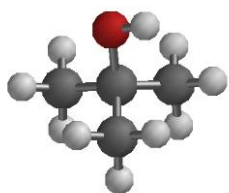
15

Energy =   -233.786168453

C	0.0058838	-0.009202	1.1341675
C	-0.7262433	-1.2685983	1.6159565
H	-0.2128871	-2.1761135	1.2609055
H	-1.7539638	-1.2792841	1.2287458
H	-0.7631432	-1.3132873	2.7142969
C	1.4620839	-0.0049546	1.616962
H	1.9853429	0.8800066	1.2301917
H	1.9914605	-0.9031148	1.2615535
H	1.5192859	0.0040821	2.7154246
C	-0.7241079	1.2541075	1.5891552
H	-0.2115429	2.1468471	1.205552
H	-0.7560219	1.3102177	2.6858795
H	-1.7532505	1.2556733	1.2056529
O	-0.0261879	0.0483643	-0.3136908
H	0.4259649	-0.7461275	-0.6486993

H₂

 2

Energy =   -10.177530179

H	0	0	0.3754185
H	0	0	-0.3754185