Electronic Supplementary Material (ESI) for RSC Advances.

Electronic Supplementary Information

Structural exploration of rhodium catalysts and their kinetic studies for efficient parahydrogen-induced polarization by side arm hydrogenation

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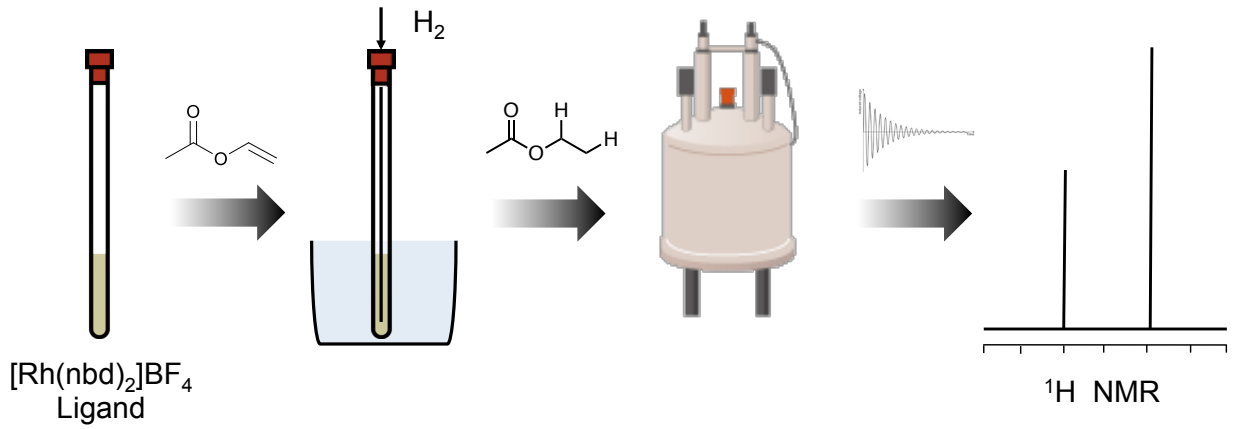
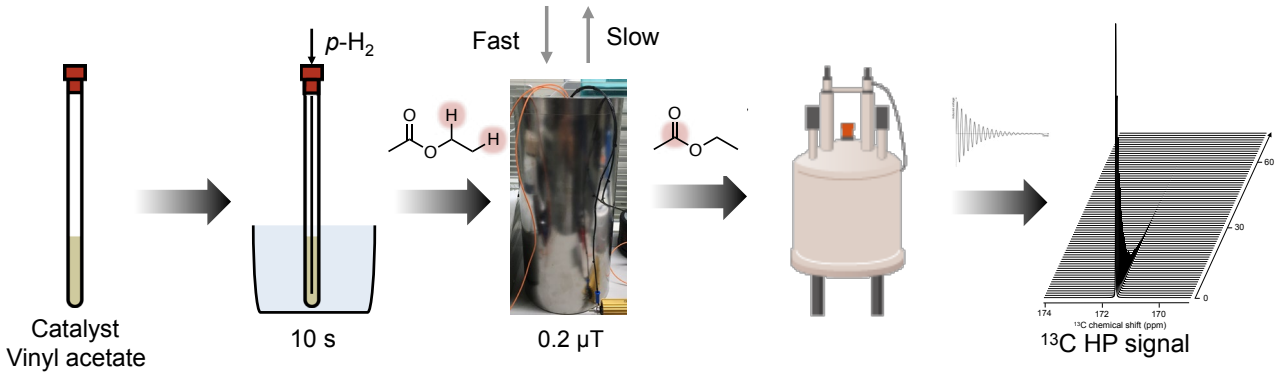
1. Supporting schemes



Scheme S1. Schematic illustration of ligand screening for hydrogenation of vinyl acetate.



Scheme S2. Schematic illustration of PHIP experiments in this study.

2. Supporting figure

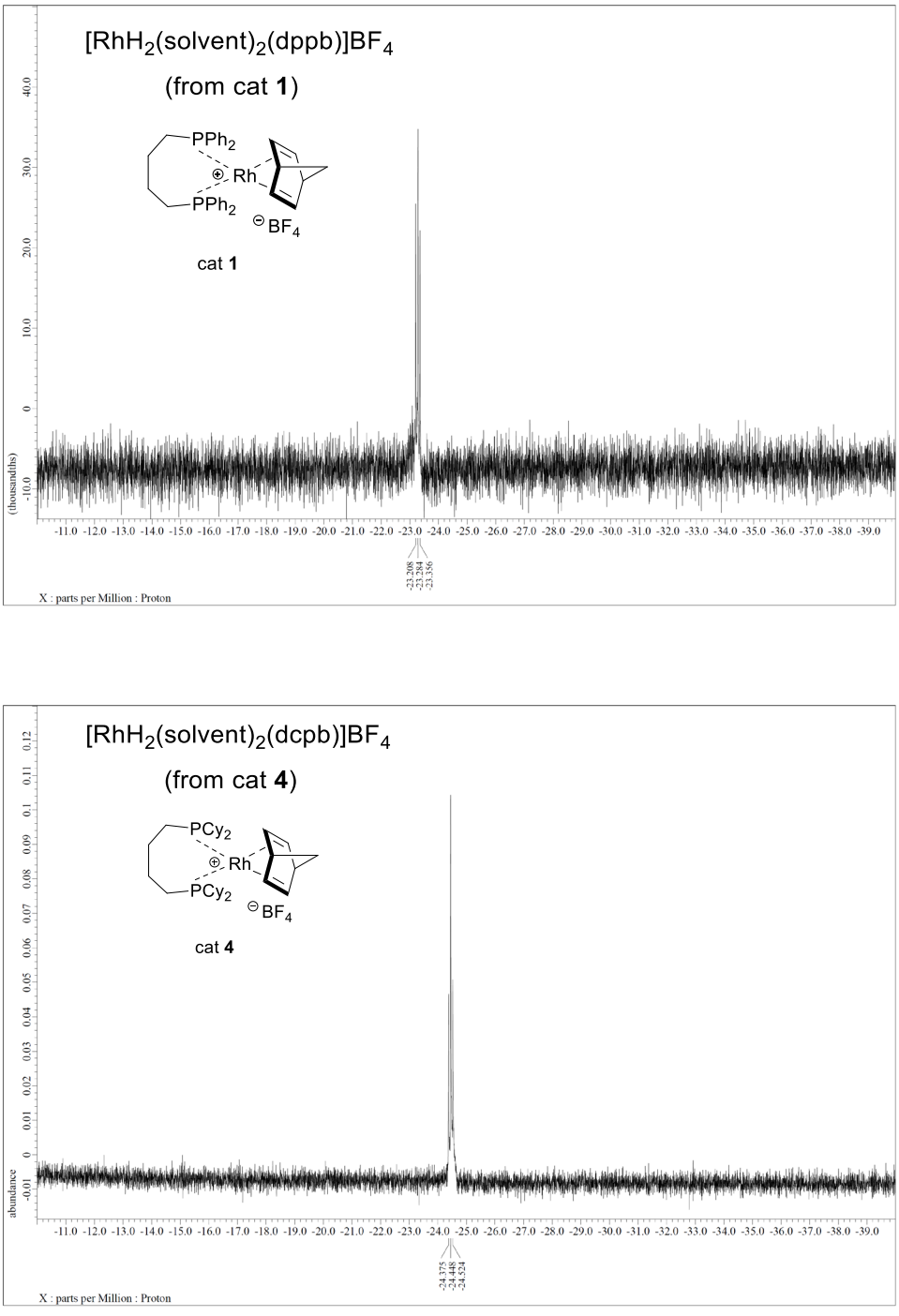
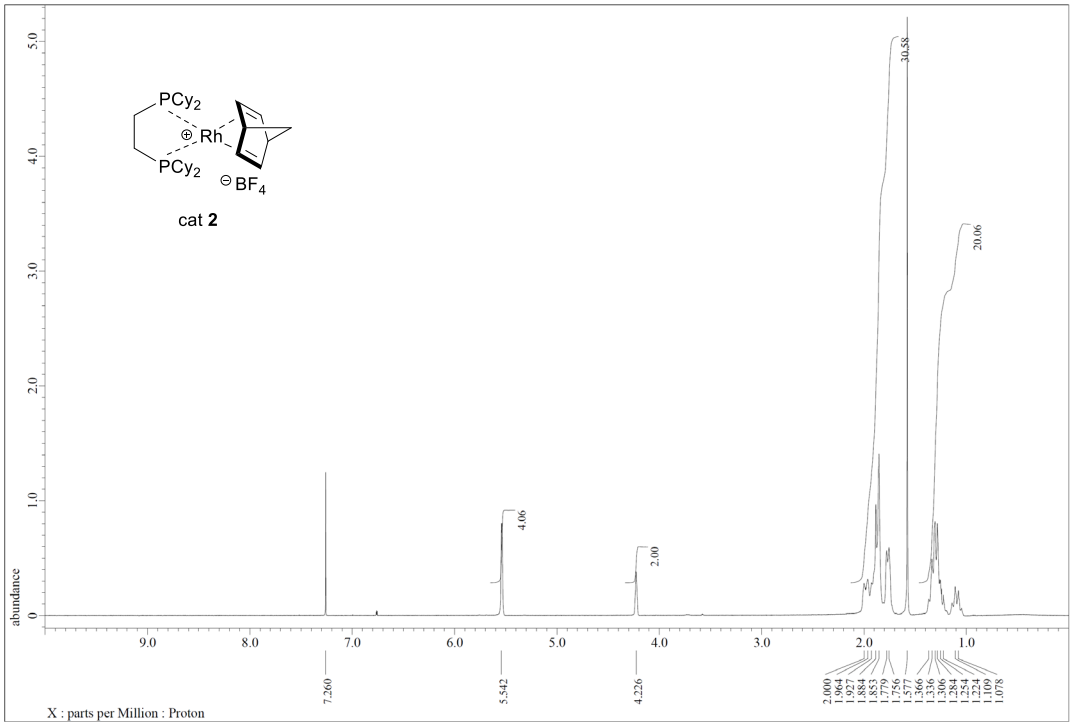
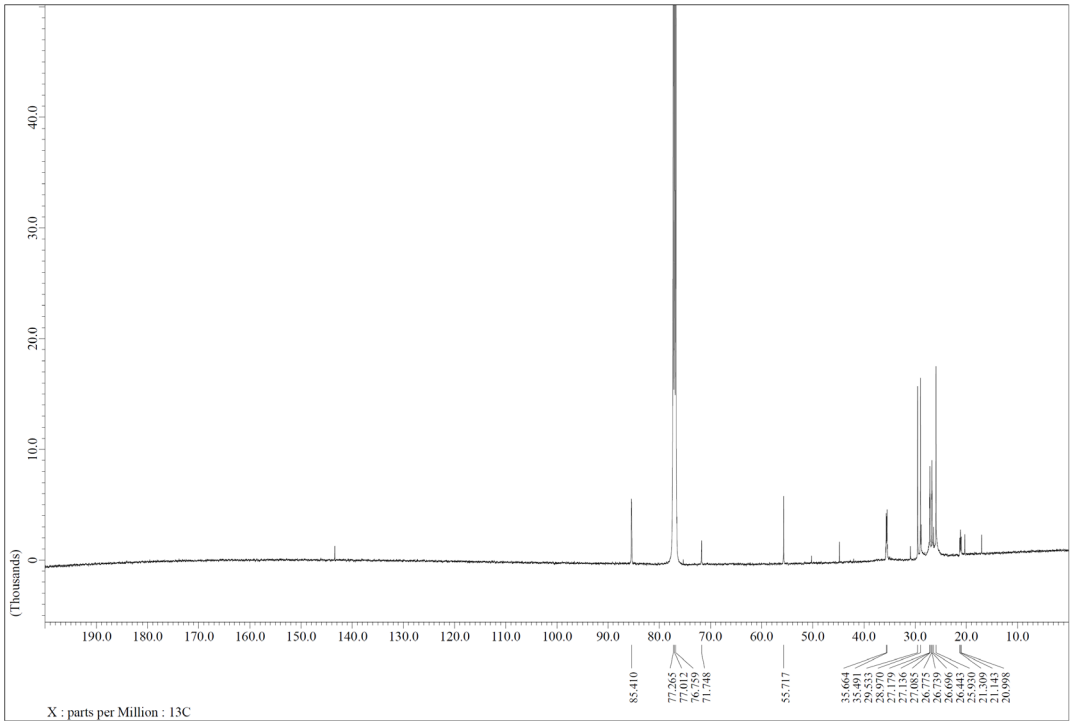
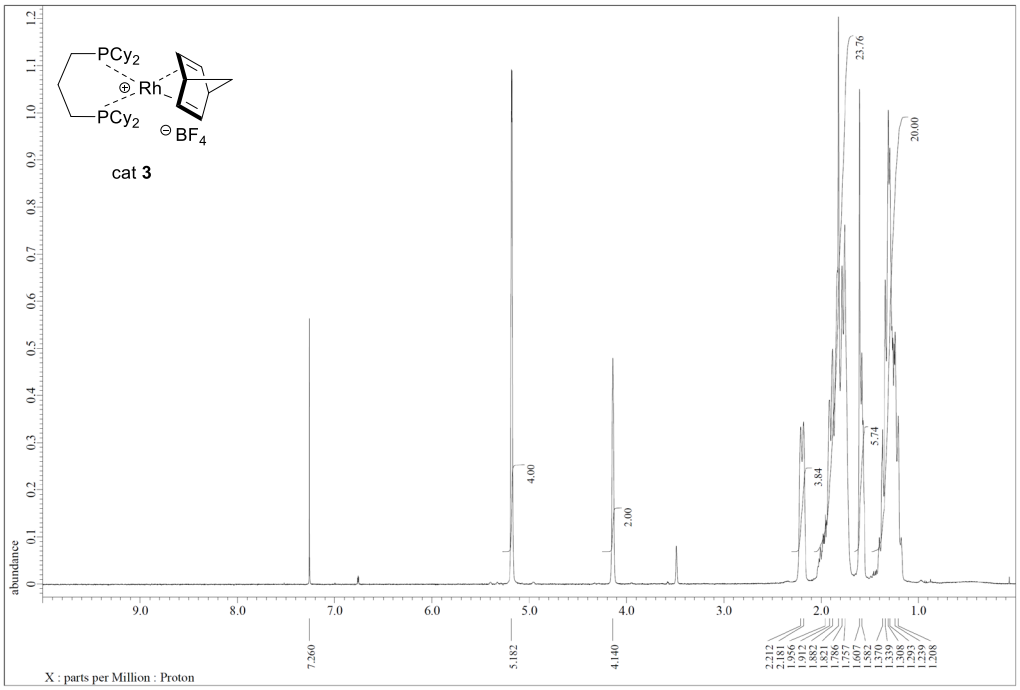


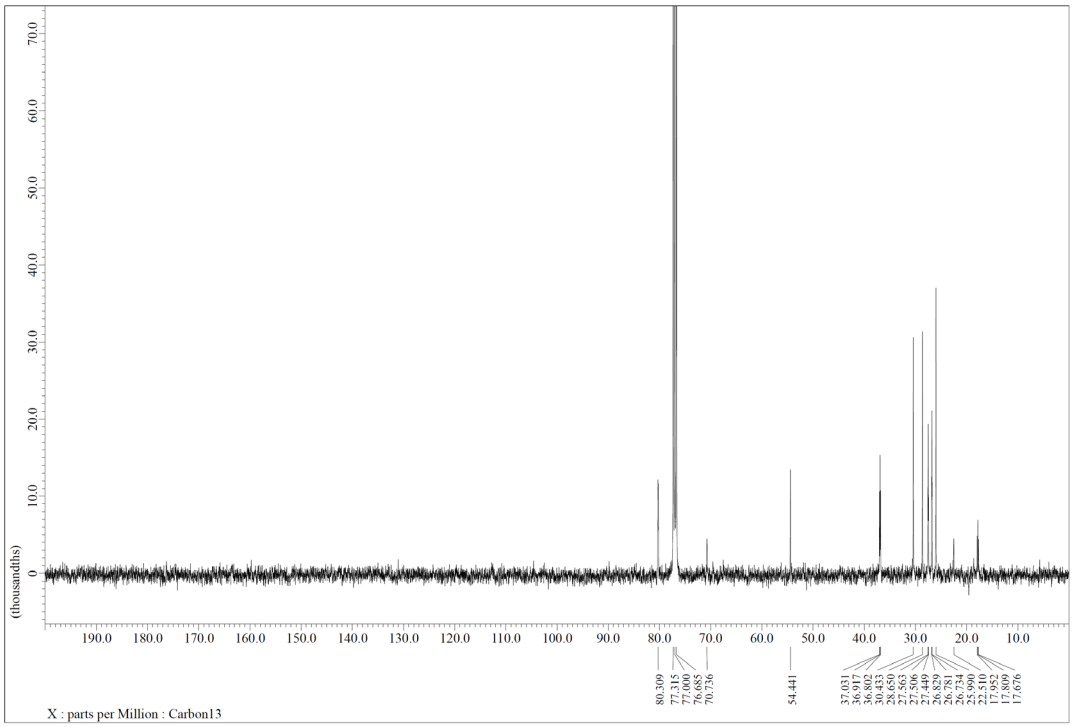
Fig. S1 Observation of rhodium hydride species in the hydrogenation of cat **1** and **4**. 5 mM of cat **1** or **4** in 700 μL of methanol-d_4 was set into an NMR tube with a cap. After normal hydrogen bubbling at 24 ºC under 1 atm for 120 s, ^{1}H NMR spectrum was measured immediately.

3. NMR spectrum (^{1}H and ^{13}C NMR in $CDCl_3$)






PCy2
Rh
PCy2
BF4
cat 3
abundance
23.76
20.00
5.74
4.00
3.84
2.00
7.260
5.182
4.140
X : parts per Million : Proton


(thousandths)
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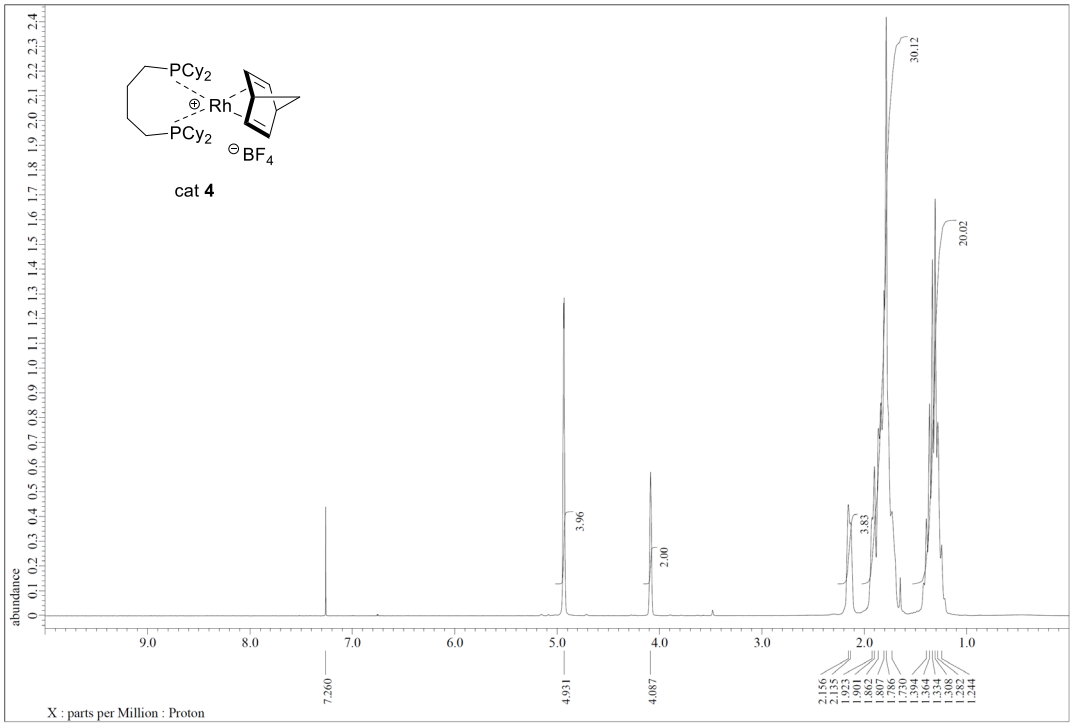
77.000
76.685
70.736
54.441
37.031
36.917
36.802
30.433
28.650
27.566
27.506
27.449
26.829
26.781
26.734
25.990
22.510
17.952
17.809
17.676
X : parts per Million : Carbon13


PCy2
Rh
PCy2
BF4
cat 4
abundance
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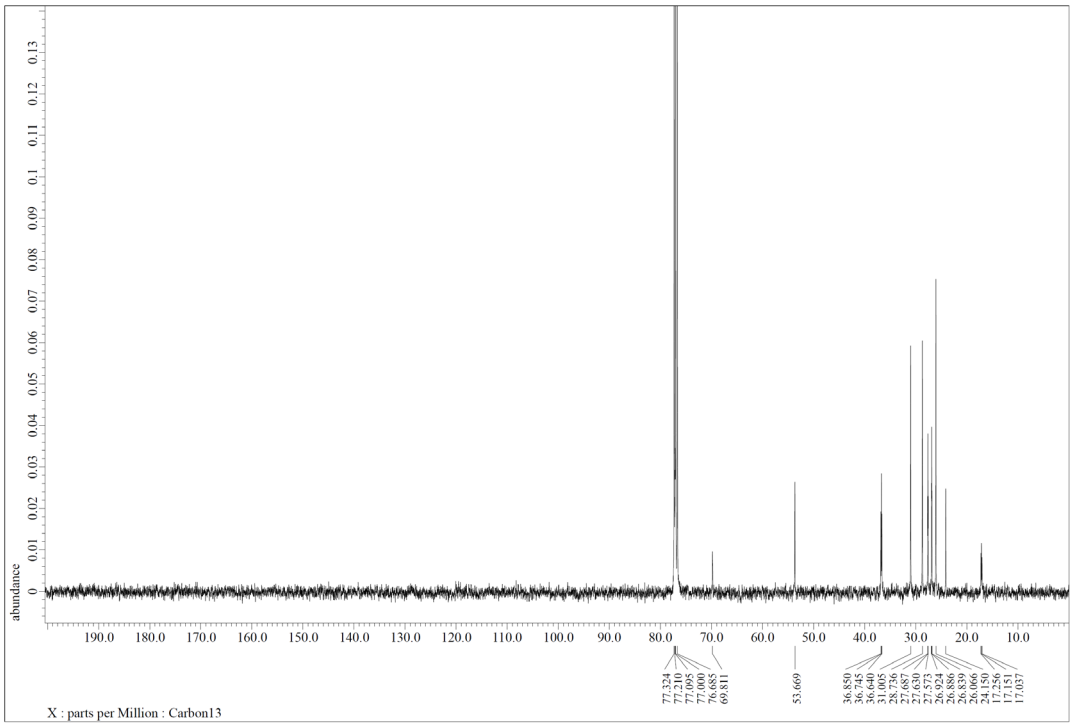
20.02
3.96
3.83
2.00
7.260
4.931
4.087
X : parts per Million : Proton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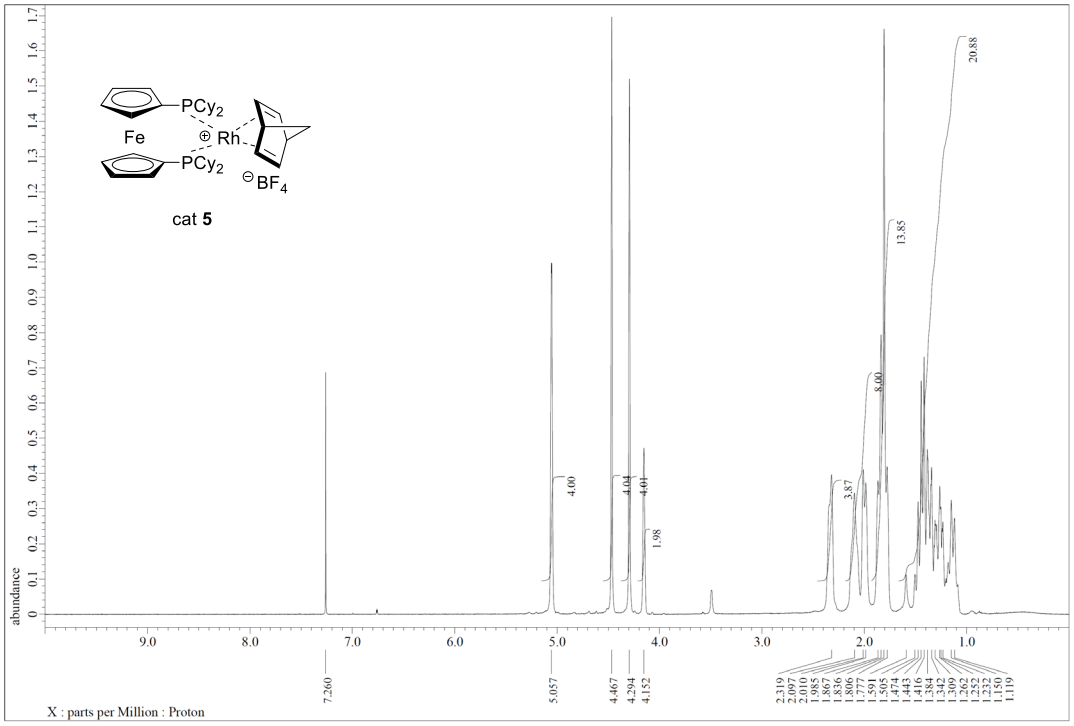
77.095
77.000
76.685
69.811
53.669
36.850
36.745
36.640
31.005
28.736
27.687
27.630
27.573
26.924
26.886
26.839
26.066
24.150
17.256
17.151
17.037
X : parts per Million : Carbon13


PCy2
Fe
Rh
PCy2
BF4
cat 5
abundance
X : parts per Million : Proton
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5.057
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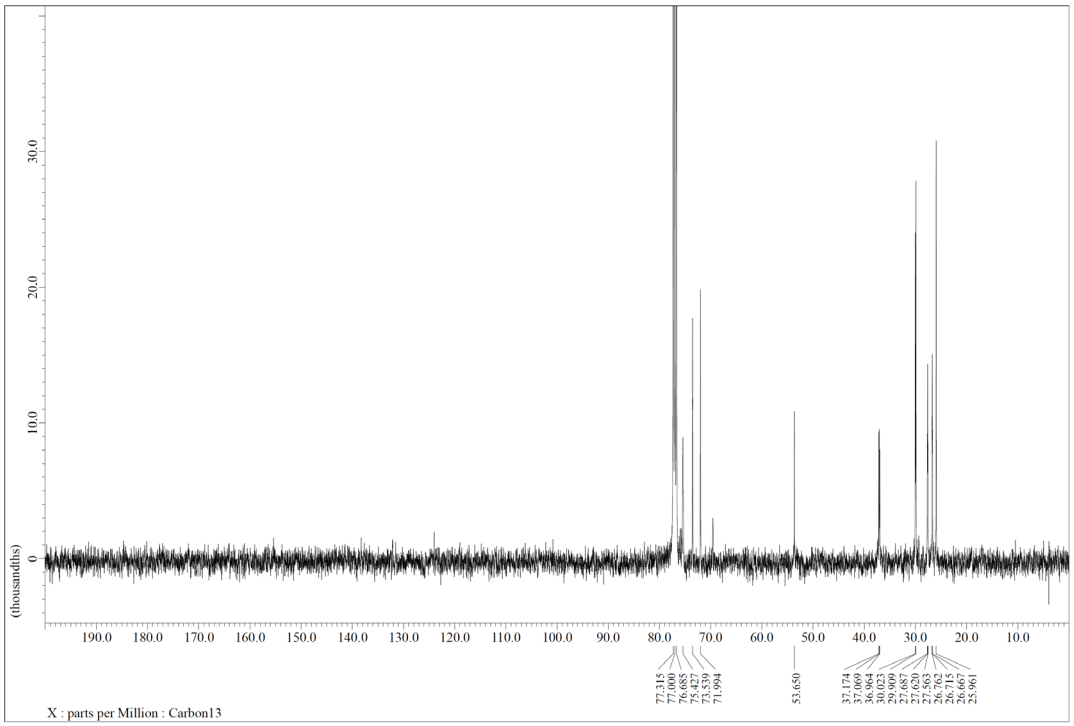
4.152
4.00
4.04
4.01
1.98
3.87
8.00
13.85
20.88


(thousandths)
X : parts per Million : Carbon13
77.315
77.000
76.685
75.427
73.539
71.994
53.650
37.174
37.069
36.964
30.023
29.909
27.687
27.620
27.563
26.762
26.715
26.667
25.961