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Electropolymerizable N-heterocyclic carbene complexes of Rh and Ir with enantiotropic polymorphic phases.

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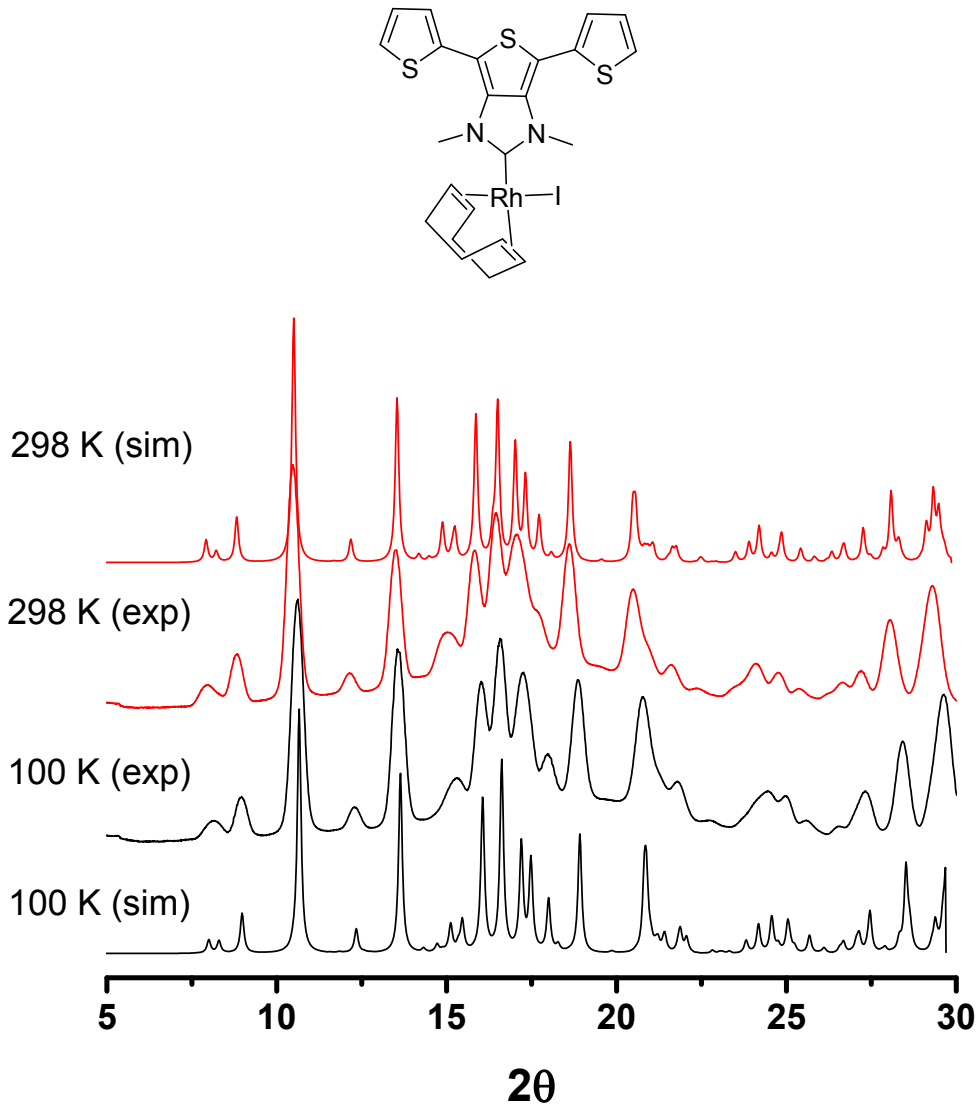
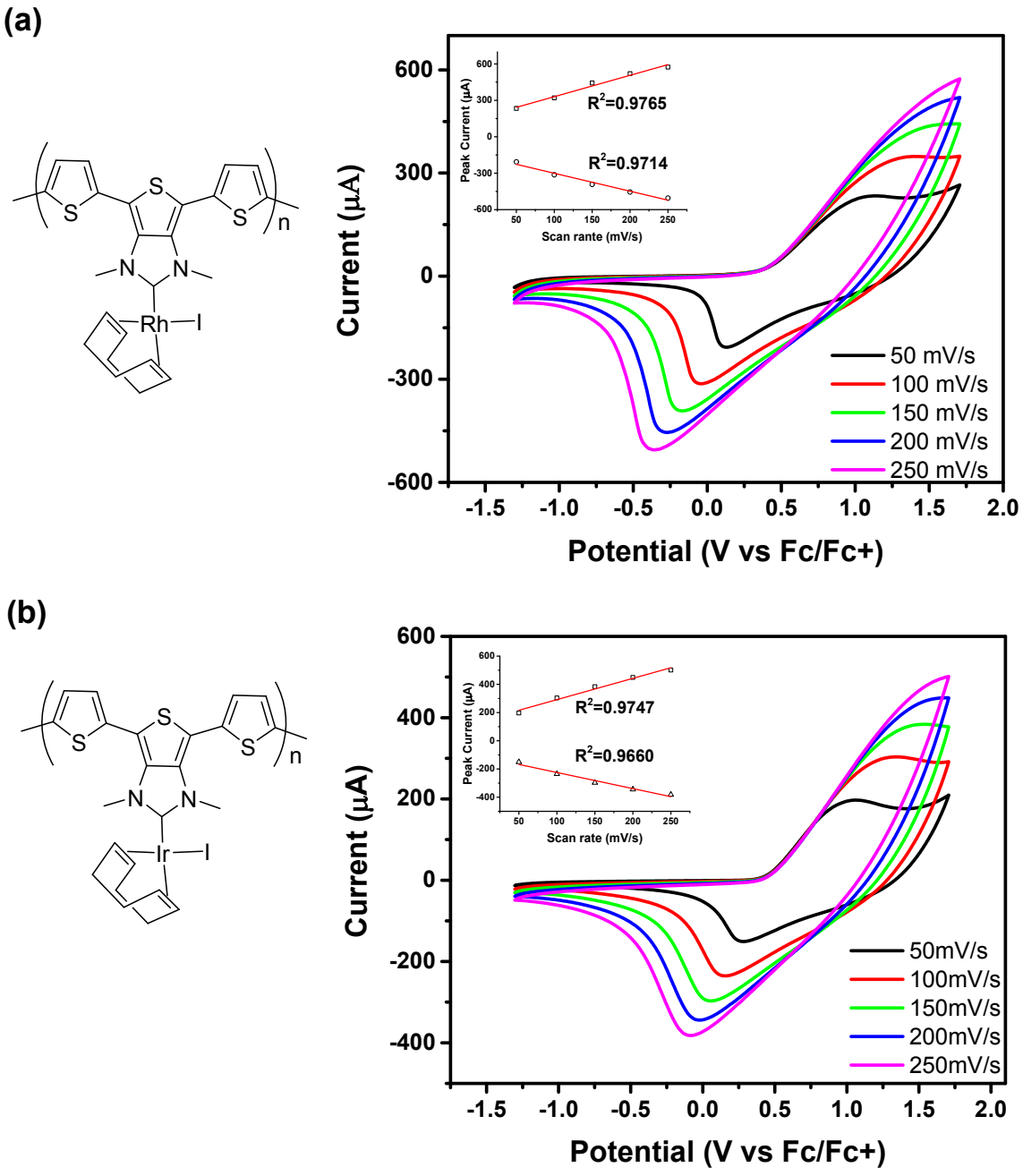


Fig. S1. Simulated and experimental PXRD traces of polycrystalline **1** at 100 K and 298 K.



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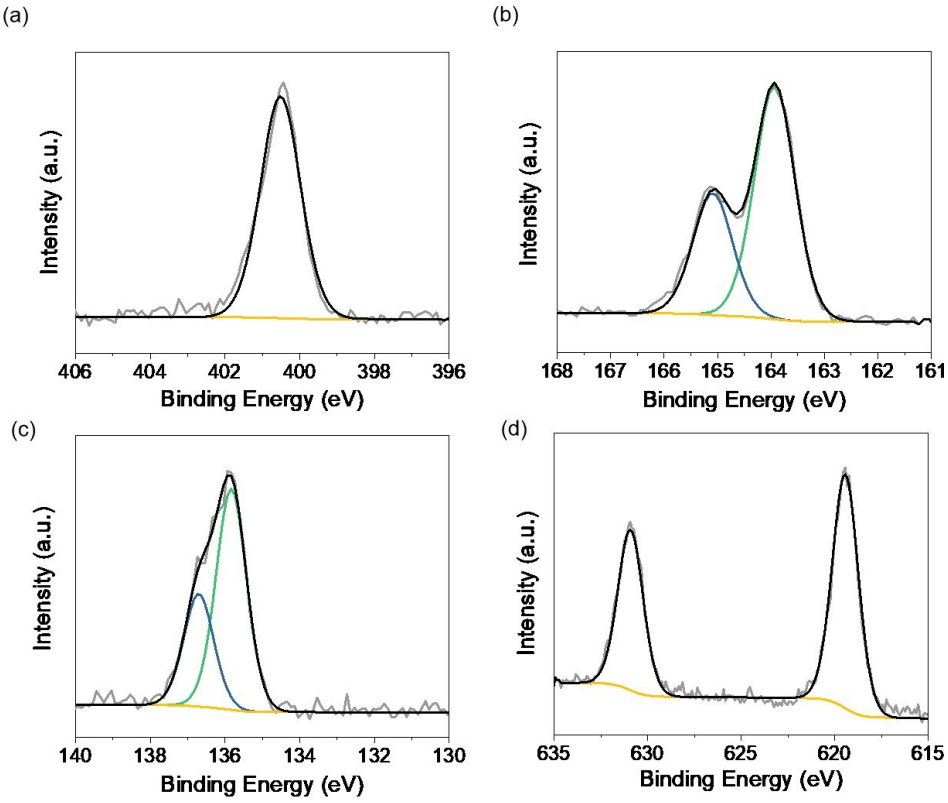


Fig. S3. Deconvoluted (a) N 1s, (b) S 2p, (c) P 2p and (d) I 3d XPS spectra of **poly-1** on ITO coated glasses.

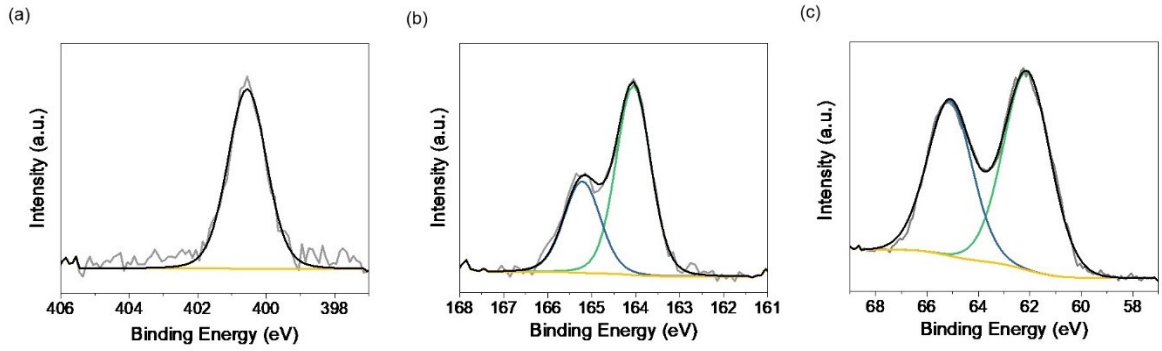
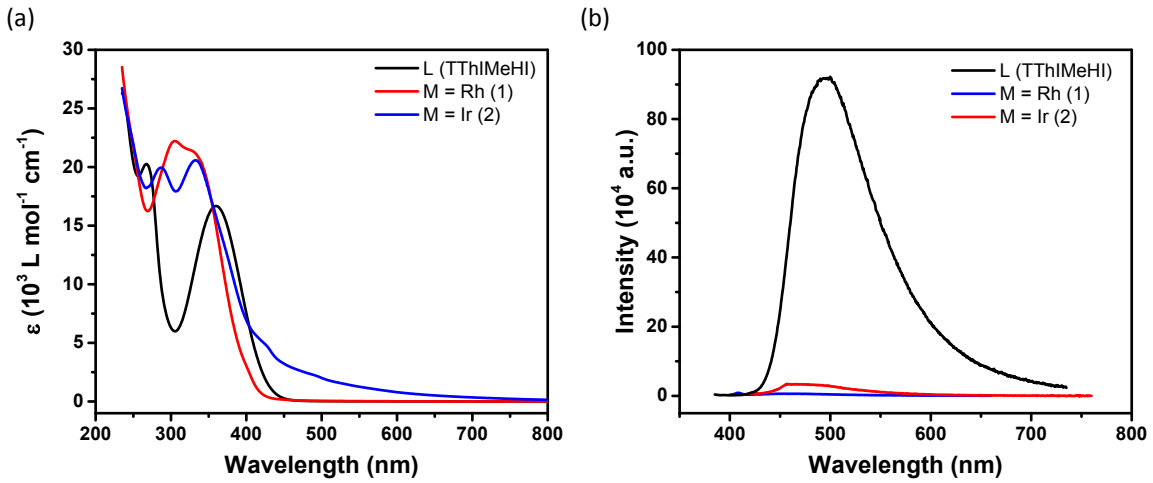


Fig. S4. Deconvoluted (a) N 1s, (b) S 2p and (c) Ir 4f XPS spectra of **poly-2** on ITO coated glasses.



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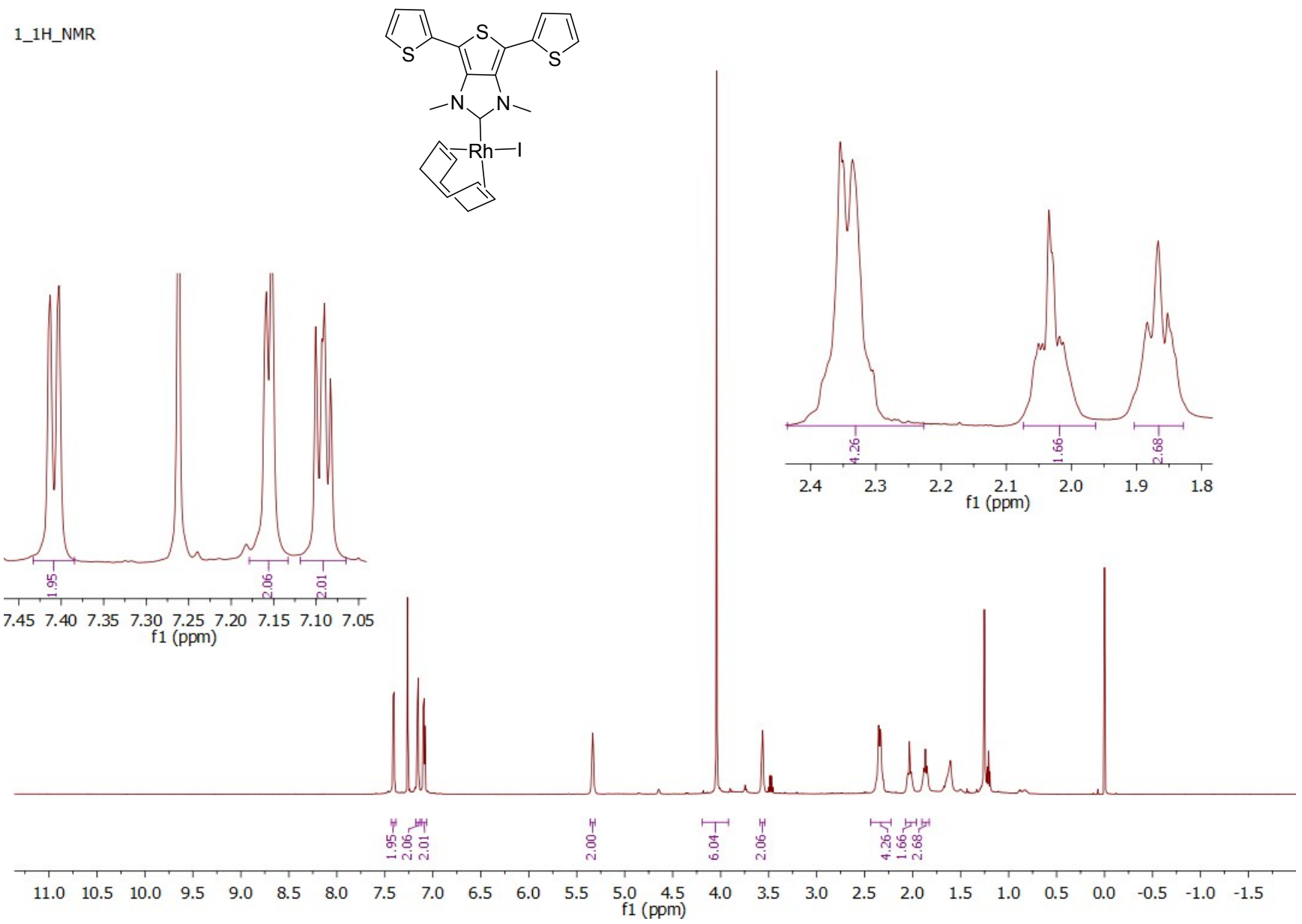
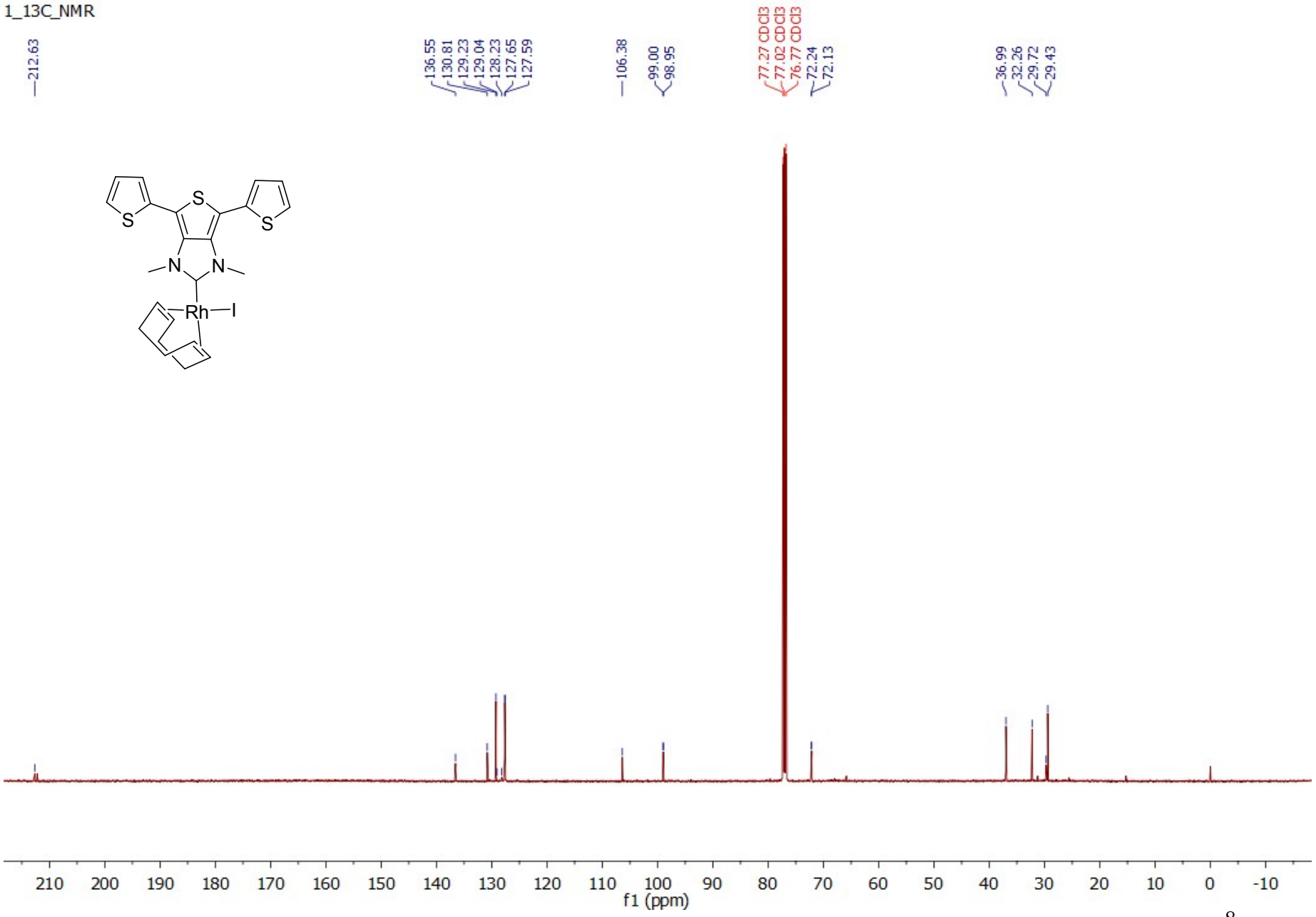
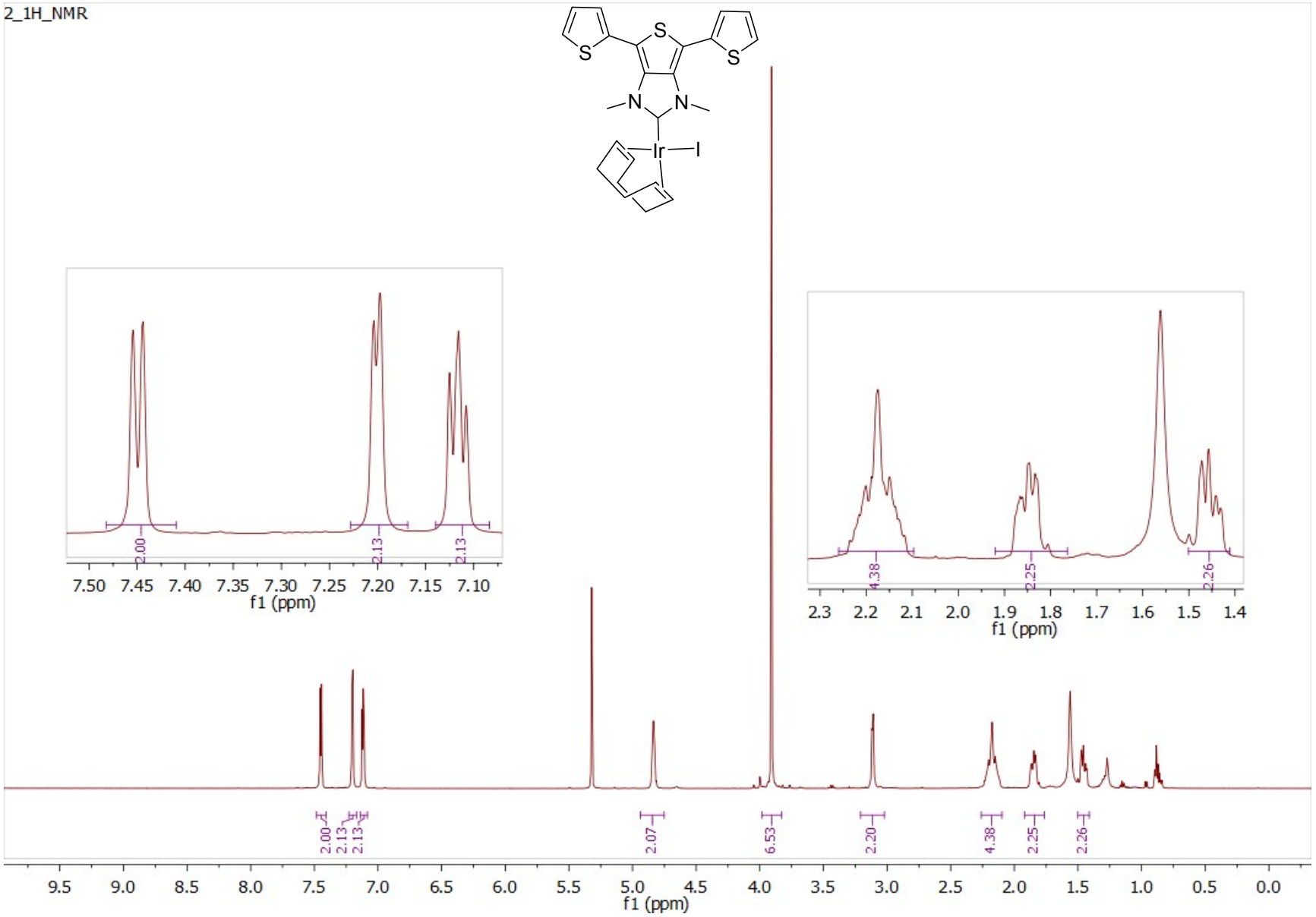
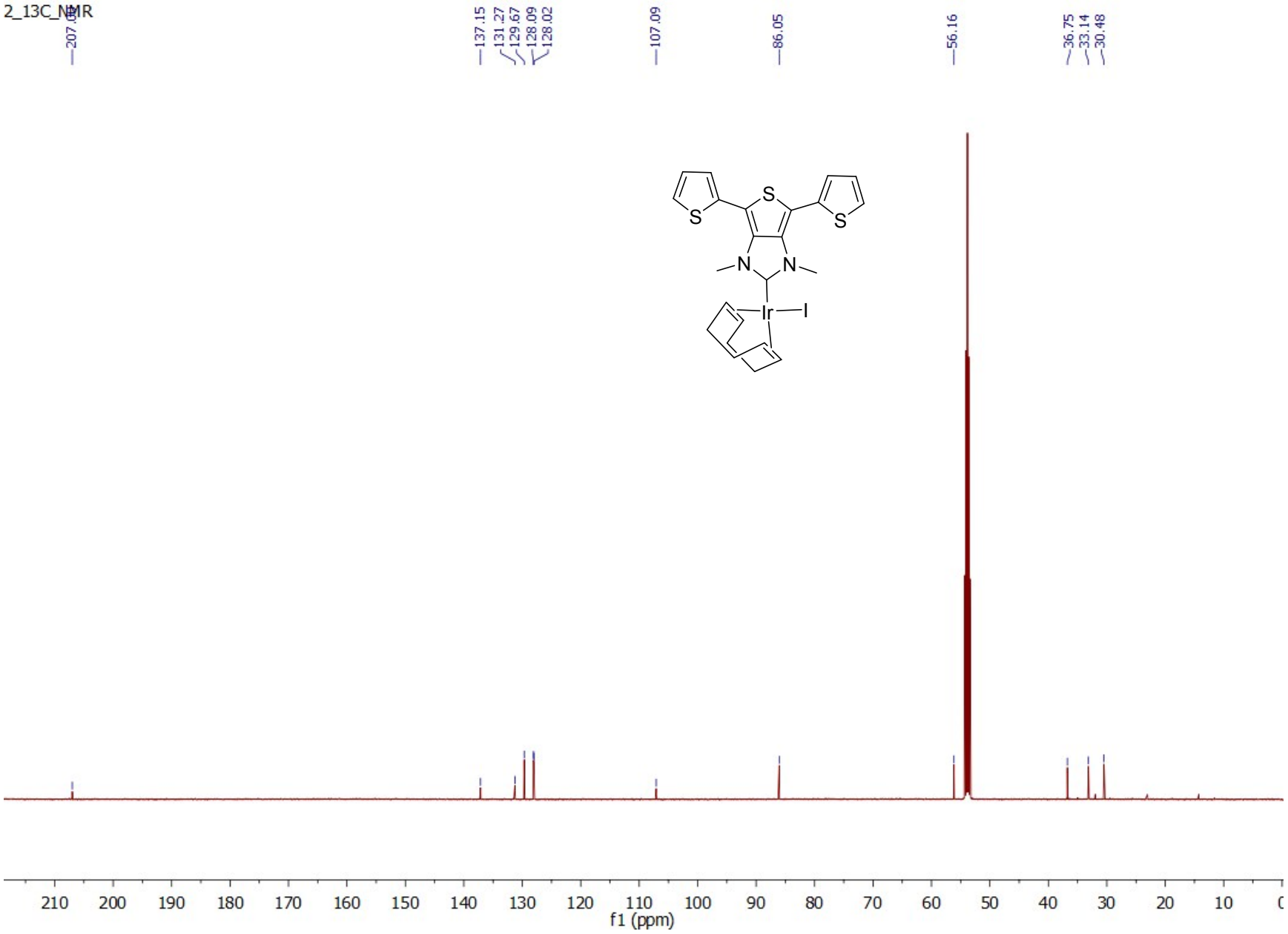

1_1H_NMR
S
S
S
N
N
Rh
I
1.95
2.06
2.01
7.45 7.40 7.35 7.30 7.25 7.20 7.15 7.10 7.05
f1 (ppm)
4.26
1.66
2.68
2.4 2.3 2.2 2.1 2.0 1.9 1.8
f1 (ppm)
1.95
2.06
2.01
2.00
6.04
2.06
4.26
1.66
2.68
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0 -1.5
f1 (ppm)


1_13C_NMR
212.63
136.55
130.81
129.23
129.04
128.23
127.65
127.59
106.38
99.00
98.95
77.27 CDCl3
77.02 CDCl3
76.77 CDCl3
72.24
72.13
36.99
32.26
29.72
29.43
S
S
S
N
N
Rh
I
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


2_1H_NMR
S
S
S
N
N
Ir
I
7.50 7.45 7.40 7.35 7.30 7.25 7.20 7.15 7.10
f1 (ppm)
2.00
2.13
2.13
2.3 2.2 2.1 2.0 1.9 1.8 1.7 1.6 1.5 1.4
f1 (ppm)
4.38
2.25
2.26
2.00
2.13
2.13
2.07
6.53
2.20
4.38
2.25
2.26
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


2_13C_NMR
207.08
137.15
131.27
129.67
128.09
128.02
107.09
86.05
56.16
36.75
33.14
30.48
S
S
S
N
N
Ir
I
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)