Supporting Information

for

Rhenium complexes of peripherally π-extended N-confused porphyrin

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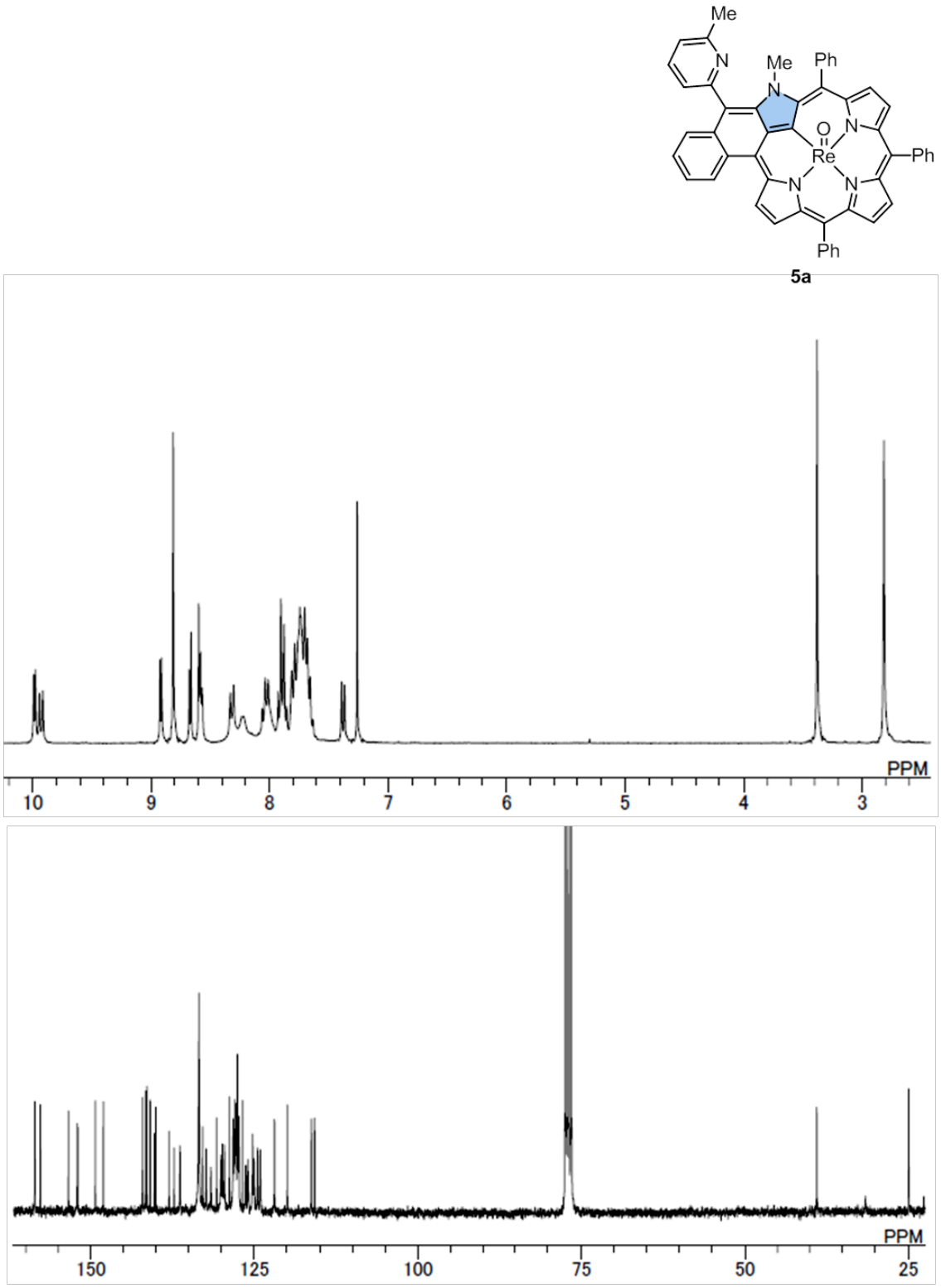


Fig. S1. ^{1}H and ^{13}C NMR spectra of **5a** in $CDCl_3$.

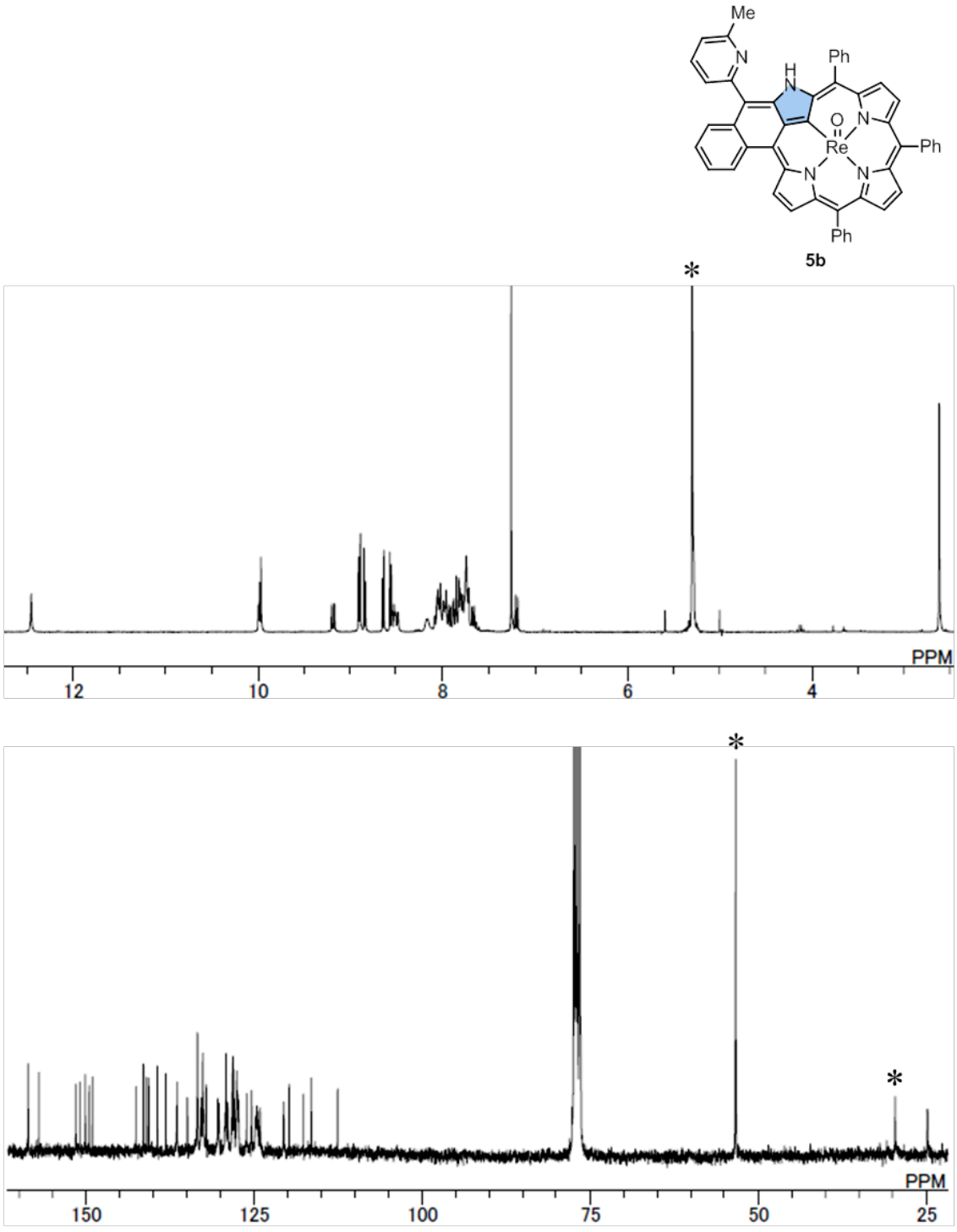


Fig. S2. ^{1}H and ^{13}C NMR spectra of **5b** in $CDCl_3$.

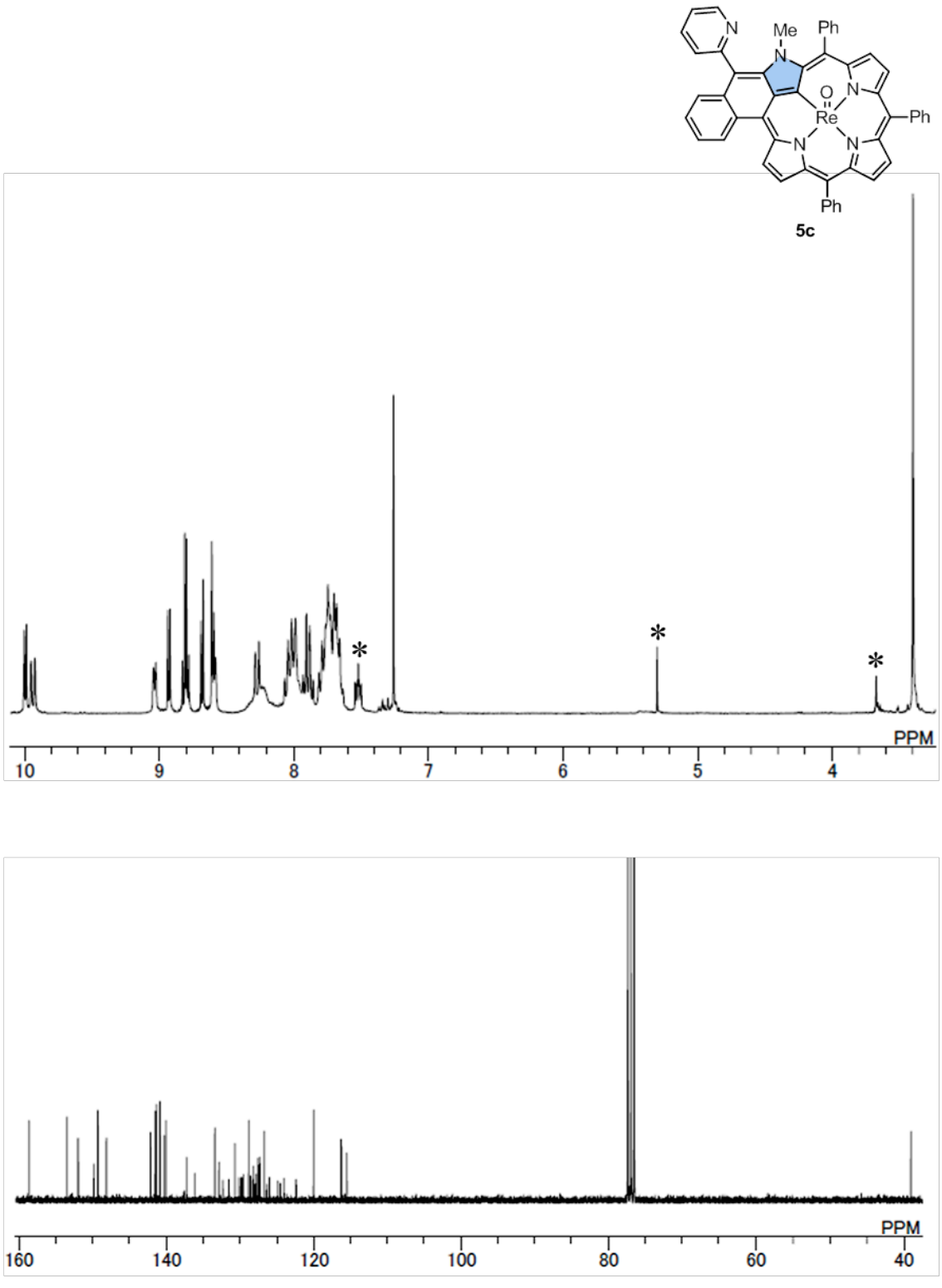


Fig. S3. ^{1}H and ^{13}C NMR spectra of **5c** in $CDCl_3$.

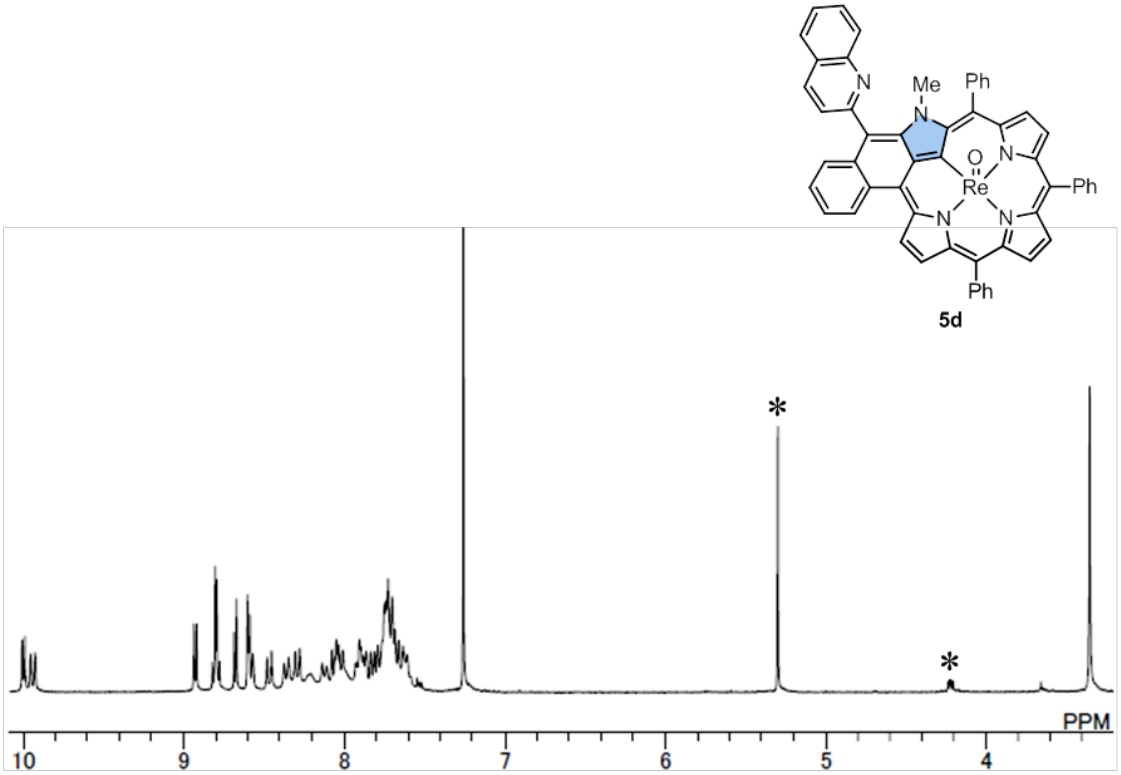


Fig. S4. ^{1}H NMR spectrum of **5d** in $CDCl_3$.

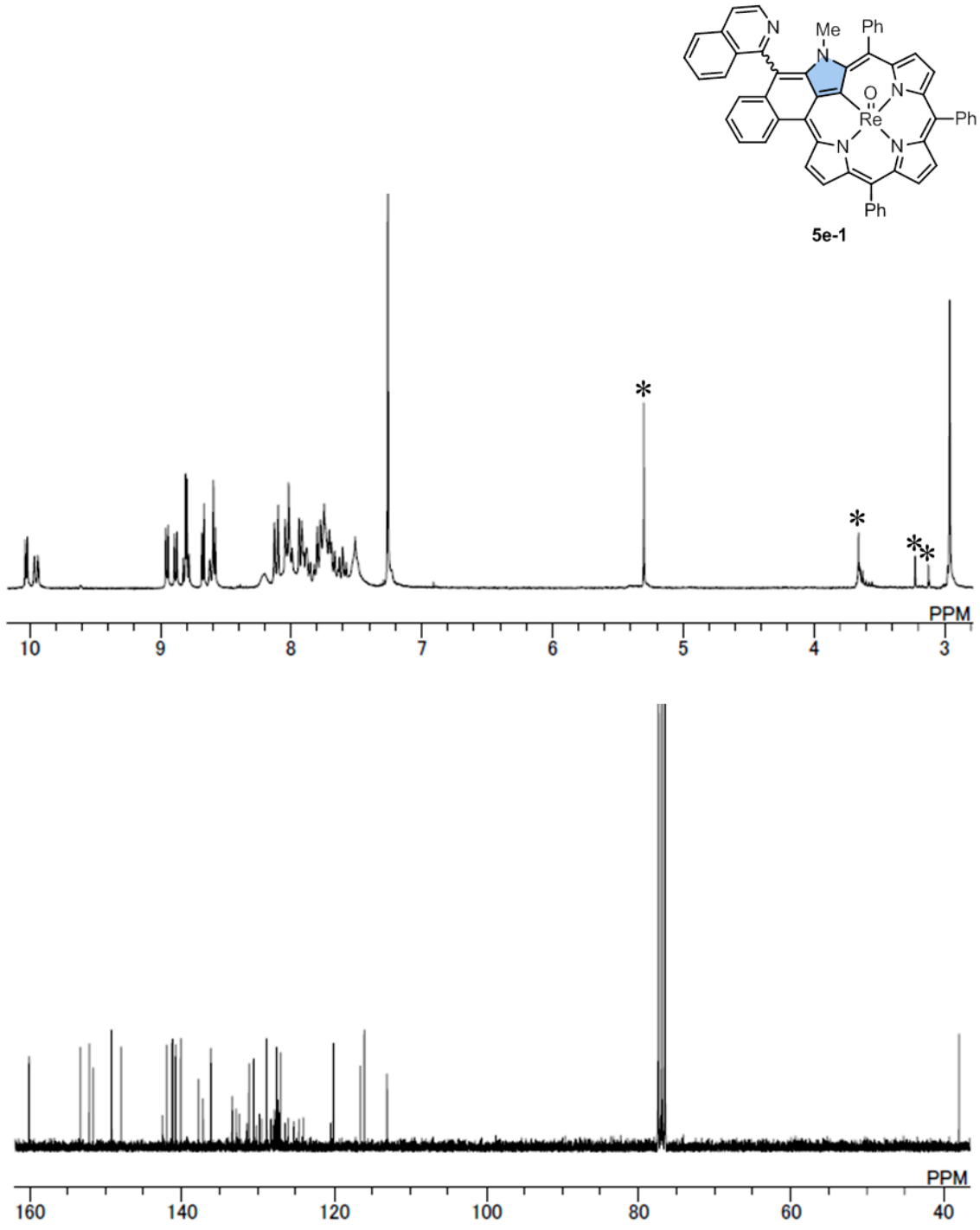


Fig. S5. ^{1}H and ^{13}C NMR spectra of **5e-1** in $CDCl_3$.

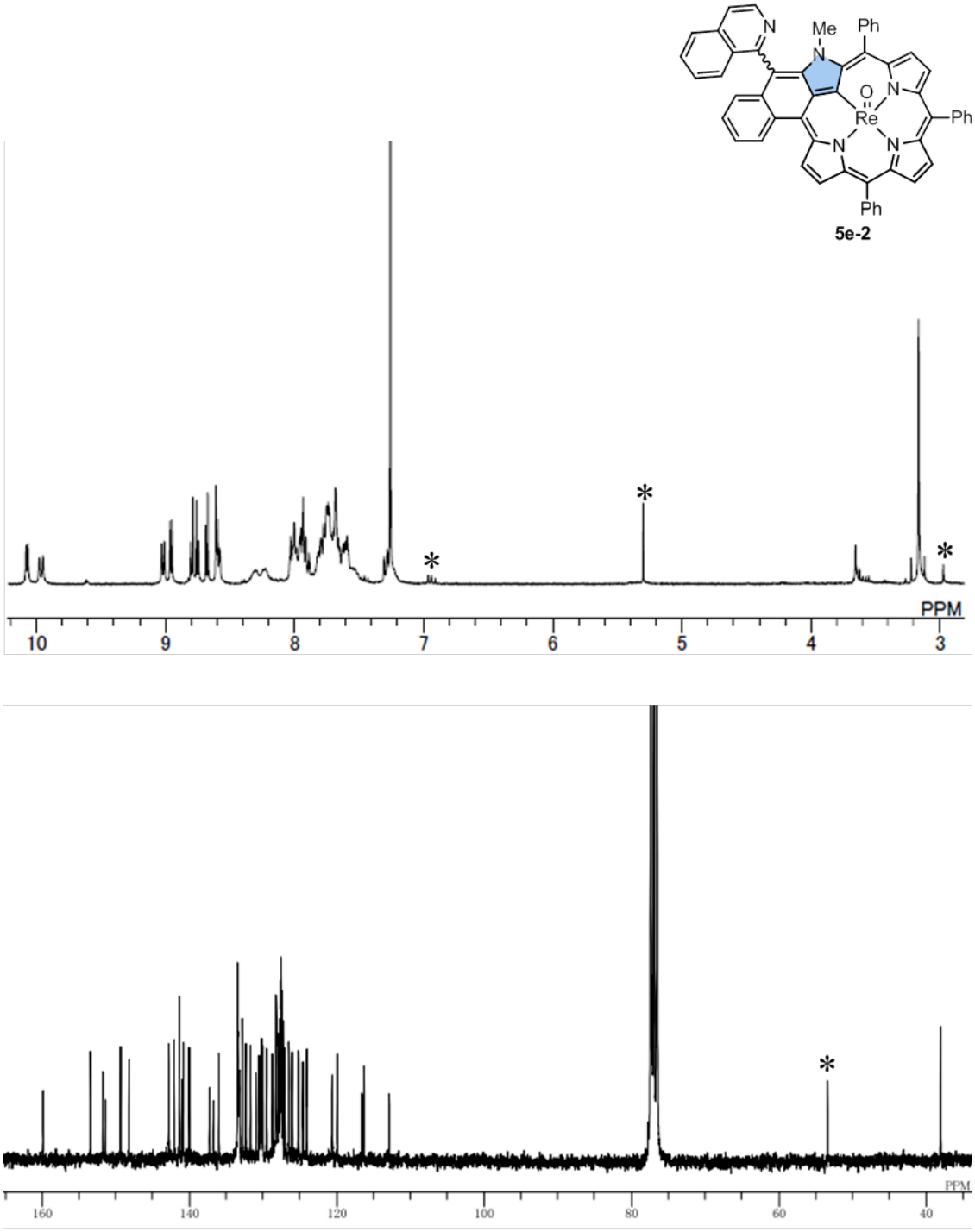


Fig. S6. ^{1}H and ^{13}C NMR spectra of **5e-2** in $CDCl_3$.

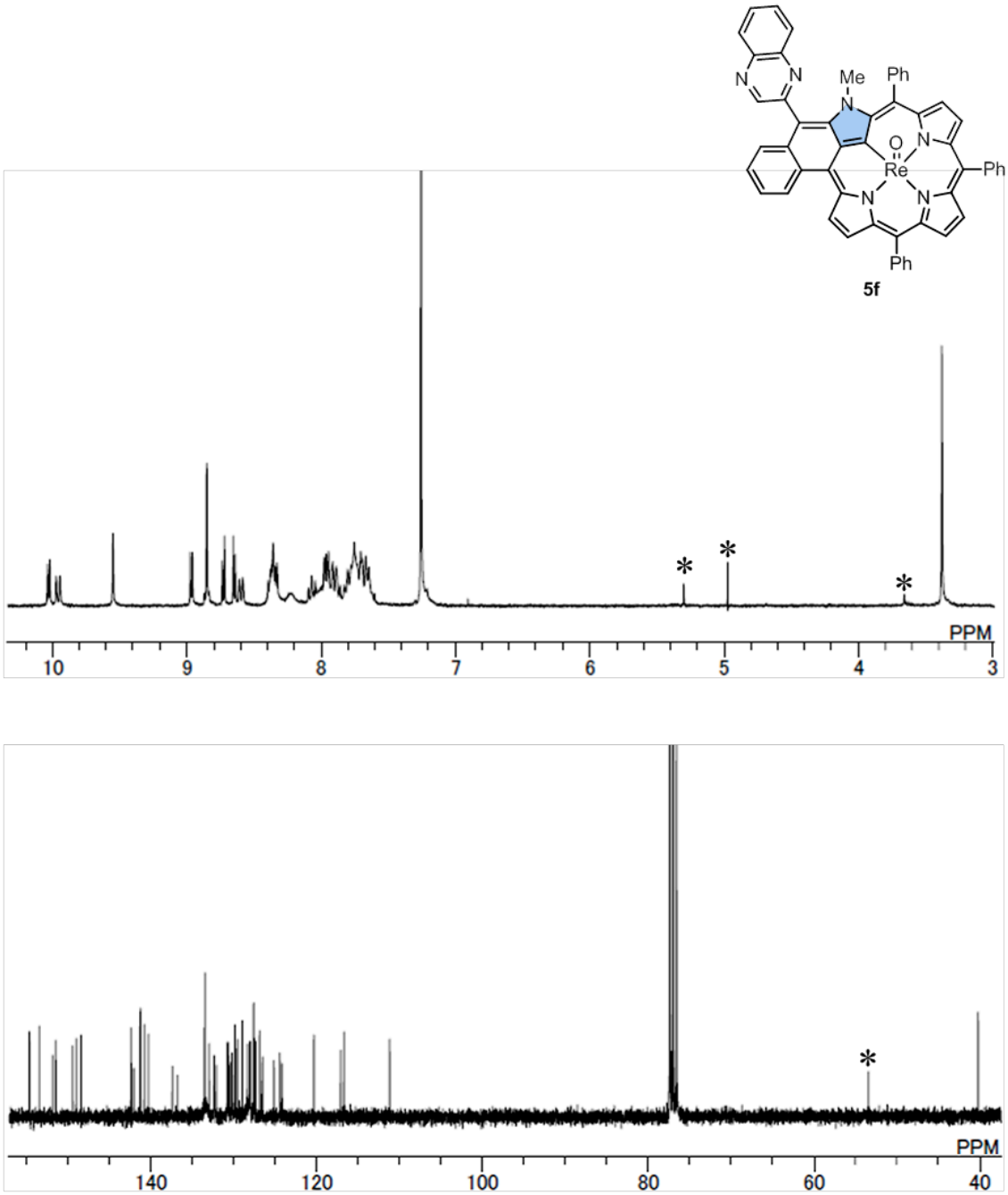


Fig. S7. ^{1}H and ^{13}C NMR spectra of **5f** in $CDCl_3$.

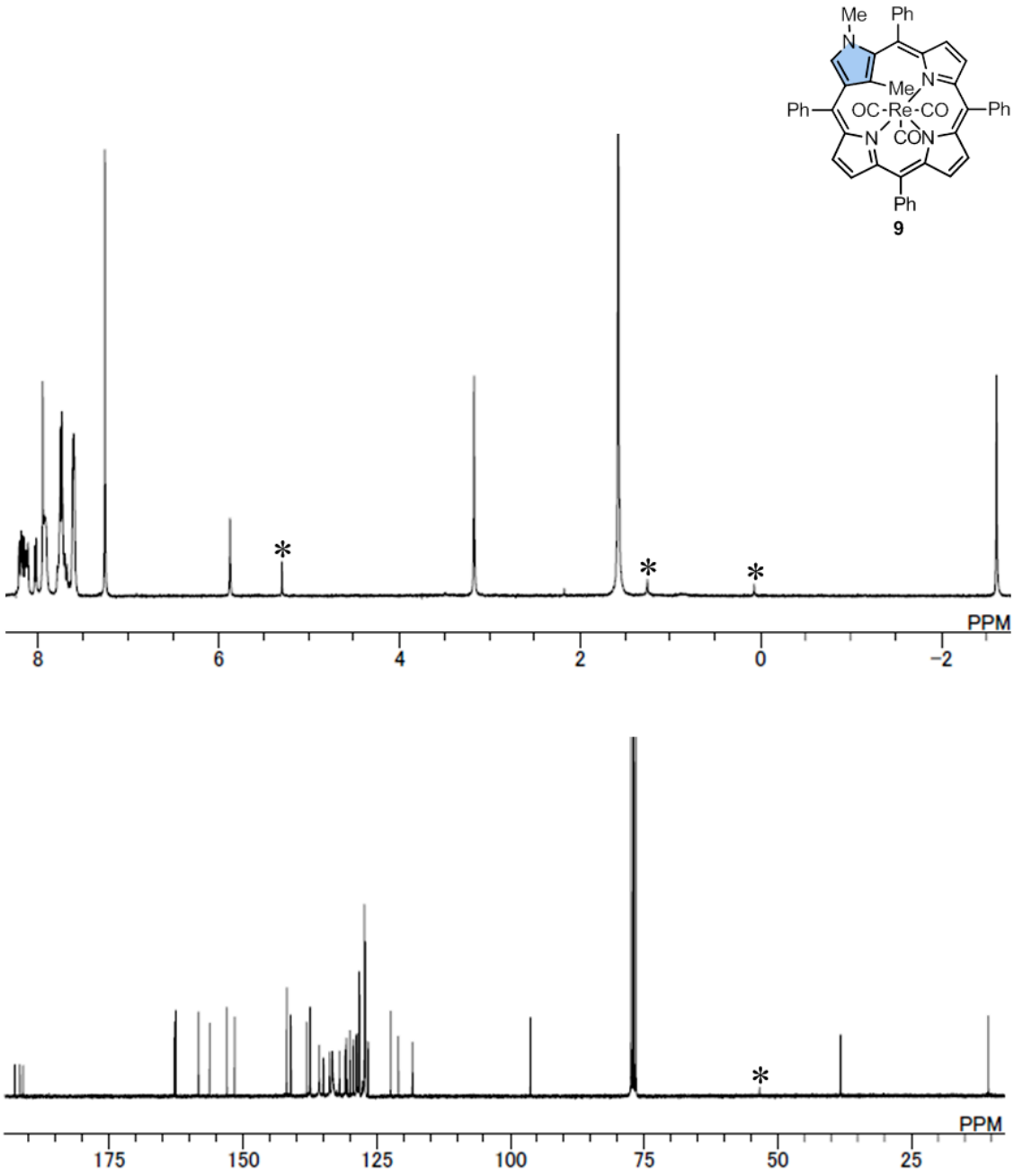
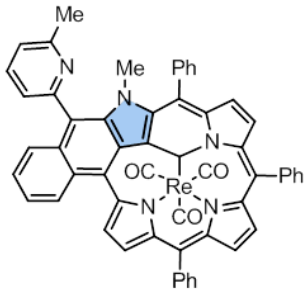


Fig. S8. ^{1}H and ^{13}C NMR spectra of **9** in $CDCl_3$.



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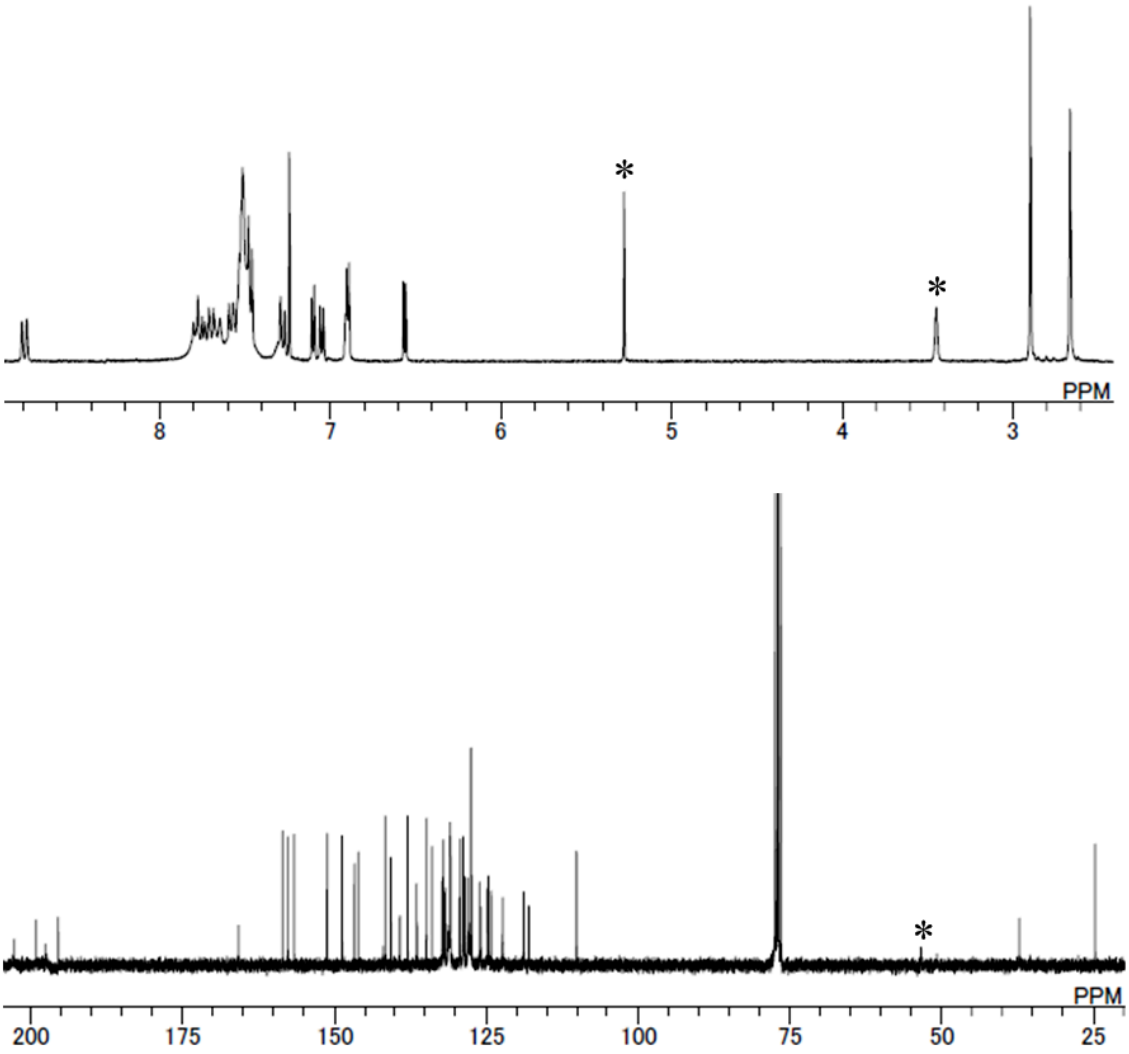


Fig. S9. ^{1}H and ^{13}C NMR spectra of **10** in $CDCl_3$.

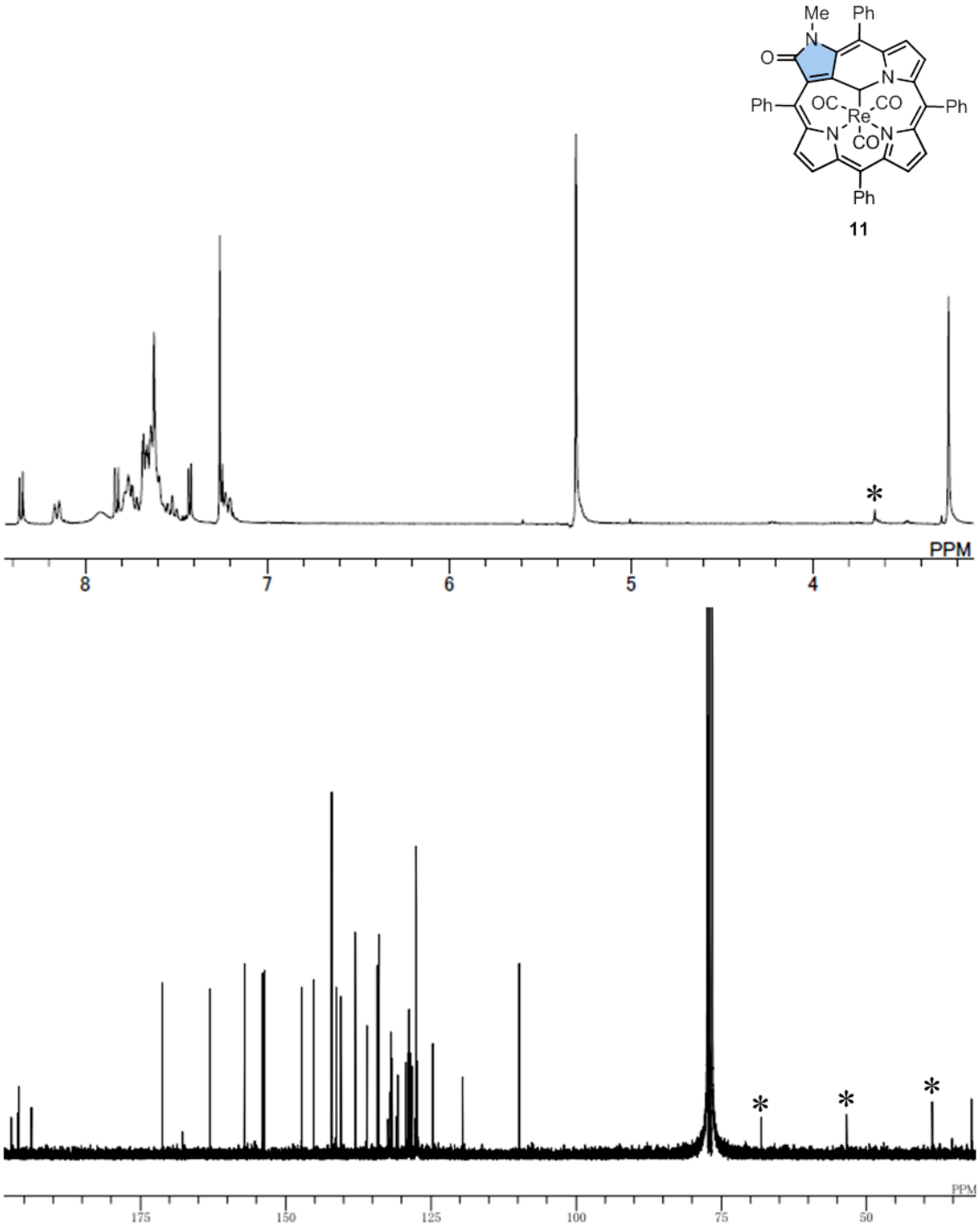


Fig. S10. ^{1}H and ^{13}C NMR spectra of **11** in $CDCl_3$.

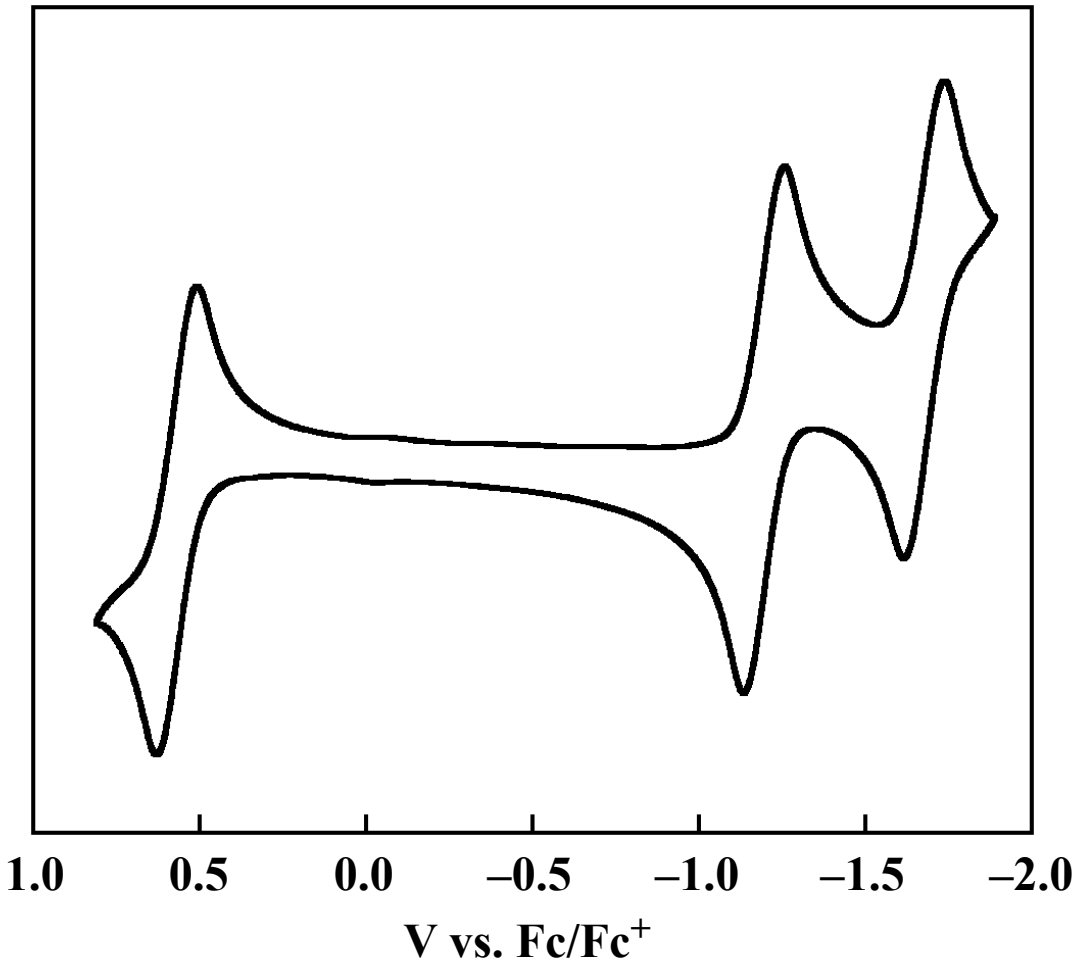
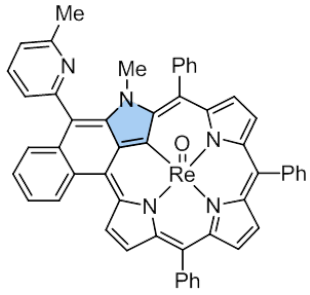


Fig. S11 Cyclic voltammogram of **11** in CH_2Cl_2 with 0.1 M Bu_4NPF_6 (Pt electrode, scan rate 100 mV/s).

Cartesian coordinates and vibrational frequencies for the optimized structures

5a



5a

E(RB3LYP) = -2430.23103213

Stoichiometry	C52H34N5ORe		
Framework group	C1[X(C52H34N5ORe)]		
Deg. of freedom	273		
Full point group	C1	NOp	1
Largest Abelian subgroup	C1	NOp	1
Largest concise Abelian subgroup	C1	NOp	1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	75	0	–1.041287	–0.064480	–0.615856
2	8	0	–1.009556	–0.117848	–2.298209
3	6	0	–0.182808	2.882054	0.101495
4	6	0	–0.768017	4.186160	0.249651
5	6	0	–2.113195	4.065172	0.090544
6	6	0	–2.400239	2.677479	–0.110759
7	6	0	–3.686156	2.157980	–0.186446
8	6	0	–3.967249	0.783676	–0.090137
9	6	0	–5.275674	0.217321	–0.090951
10	6	0	–5.138120	–1.128148	0.120463
11	6	0	–3.744143	–1.404182	0.230174
12	6	0	–3.193186	–2.669642	0.451042
13	6	0	–1.824871	–2.944255	0.412808
14	6	0	–1.257515	–4.202429	0.755657
15	6	0	0.090758	–4.118003	0.534910
16	6	0	0.372437	–2.805014	0.062254
17	6	0	1.675390	–2.293024	–0.204193
18	6	0	1.870871	–0.910741	–0.098594
19	6	0	3.196223	–0.368150	–0.032168
20	6	0	0.921445	0.139282	–0.024700
21	6	0	1.698244	1.330226	0.077283
22	6	0	1.192863	2.639725	0.197031
23	6	0	–4.830403	3.115377	–0.305205
24	6	0	–4.993362	3.880519	–1.470868
25	6	0	–6.053655	4.779966	–1.591271
26	6	0	–6.967588	4.930956	–0.546864
27	6	0	–6.814438	4.177813	0.619097
28	6	0	–5.755042	3.277728	0.738989
29	6	0	–4.131005	–3.799578	0.737830
30	6	0	–4.241152	–4.883067	–0.148514
31	6	0	–5.120337	–5.933323	0.117136
32	6	0	–5.899253	–5.920830	1.275884
33	6	0	–5.796619	–4.849926	2.165985
34	6	0	–4.922123	–3.796334	1.897761
35	6	0	2.834227	–3.117357	–0.475334
36	6	0	4.154098	–2.557579	–0.333759
37	6	0	5.269883	–3.420169	–0.502380
38	6	0	5.117686	–4.739315	–0.875325
39	6	0	3.832654	–5.256154	–1.125191
40	6	0	2.724140	–4.457904	–0.930360
41	6	0	2.071712	3.799787	0.553094
42	6	0	2.259023	4.885634	-0.318230
43	6	0	3.066179	5.964072	0.046021
44	6	0	3.700173	5.978344	1.290246
45	6	0	3.518929	4.907340	2.167495
46	6	0	2.711900	3.828932	1.802385
47	6	0	4.333215	–1.155769	–0.031701
48	6	0	5.671052	–0.603096	0.339926
49	6	0	5.847306	–0.033259	1.612246
50	6	0	7.095667	0.479783	1.950241
51	6	0	8.131406	0.407633	1.020581
52	6	0	7.881402	–0.184989	–0.223244
53	6	0	8.958776	–0.309407	–1.272575
54	6	0	4.126606	1.913974	–0.425104
55	1	0	–0.215195	5.086622	0.466059
56	1	0	–2.858791	4.843226	0.152784
57	1	0	–6.189856	0.772603	–0.234344
58	1	0	–5.920738	–1.869603	0.176398
59	1	0	–1.809308	–5.044958	1.143735
60	1	0	0.832039	–4.871722	0.747241
61	1	0	–4.285834	3.759735	–2.285908
62	1	0	–6.166959	5.359461	–2.503140
63	1	0	–7.792995	5.630901	–0.640118

64	1	0	–7.517100	4.294427	1.439439
65	1	0	–5.633715	2.698730	1.649734
66	1	0	–3.638794	–4.891757	–1.051818
67	1	0	–5.198405	–6.759852	–0.583442
68	1	0	–6.581723	–6.739915	1.483808
69	1	0	–6.395048	–4.835179	3.072517
70	1	0	–4.839855	–2.966112	2.592754
71	1	0	6.264211	–3.011086	–0.381725
72	1	0	5.994416	–5.365727	–1.013698
73	1	0	3.711507	–6.272437	–1.488915
74	1	0	1.743785	–4.847962	–1.173671
75	1	0	1.773994	4.874486	–1.290179
76	1	0	3.202379	6.791654	–0.644528
77	1	0	4.328575	6.817583	1.573959
78	1	0	4.000691	4.913683	3.141335
79	1	0	2.567986	2.999933	2.489262
80	1	0	5.017419	–0.002645	2.310179
81	1	0	7.261758	0.925627	2.927183
82	1	0	9.117335	0.799213	1.251059
83	1	0	9.197512	–1.363560	–1.451749
84	1	0	9.875735	0.206287	–0.975772
85	1	0	8.612080	0.103865	–2.224504
86	1	0	4.822884	1.335326	–1.031980
87	1	0	4.674738	2.384076	0.394743
88	1	0	3.694711	2.694255	–1.049214
89	7	0	–1.200835	1.948102	–0.117095
90	7	0	–3.019385	–0.220922	0.075769
91	7	0	–0.803117	–2.060353	0.024462
92	7	0	3.067731	1.018159	0.049285
93	7	0	6.674873	–0.676715	–0.552242

Harmonic frequencies (cm**-1), IR intensities (KM/Mole), Raman scattering activities (A**4/AMU), depolarization ratios for plane and unpolarized incident light, reduced masses (AMU), force constants (mDyne/A), and normal coordinates:

	1	2	3
	A	A	A
Frequencies --	10.9989	15.0243	26.8254
Red. masses --	5.6742	5.6764	3.7498
Frc consts --	0.0004	0.0008	0.0016
IR Inten --	0.0509	0.1789	0.5465

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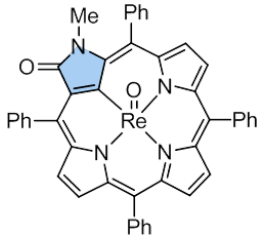

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E(RB3LYP) = -2180.93508253

Stoichiometry	C45H29N4O2Re			
Framework group	C1[X(C45H29N4O2Re)]			
Deg. of freedom	237			
Full point group		C1	NOp	1
Largest Abelian subgroup		C1	NOp	1
Largest concise Abelian subgroup		C1	NOp	1

Standard orientation:

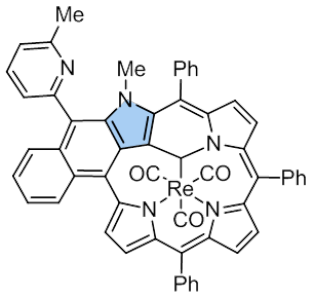
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.005887	–0.035180	0.001015
2	6	0	0.002883	–0.011976	1.492282
3	6	0	1.339743	–0.005574	1.956349
4	6	0	2.158165	0.077625	0.777492
5	6	0	3.541951	0.257046	0.748643
6	6	0	4.314603	0.122747	1.918347
7	6	0	5.742739	0.214151	1.942230
8	6	0	6.158662	–0.095171	3.205679
9	6	0	4.994182	–0.367872	3.984019
10	6	0	5.007619	–0.789425	5.309035
11	6	0	3.847474	–1.045785	6.052063
12	6	0	3.844915	–1.524620	7.396754
13	6	0	2.543421	–1.583067	7.808394
14	6	0	1.730264	–1.156053	6.715386
15	6	0	0.337203	–1.032771	6.772542
16	6	0	–0.451863	–0.652145	5.690495
17	6	0	–1.880481	–0.593715	5.716589
18	6	0	–2.299393	–0.288810	4.454992
19	6	0	–1.137744	–0.176011	3.627435
20	6	0	–1.174750	–0.008189	2.235962
21	6	0	1.709121	–0.175052	–1.763601
22	6	0	4.279522	0.636321	–0.501065
23	6	0	5.094014	–0.281392	–1.181806
24	6	0	5.789289	0.098319	–2.330780
25	6	0	5.685864	1.404655	–2.813479
26	6	0	4.887109	2.329447	–2.138043
27	6	0	4.191010	1.948555	-0.989452
28	6	0	6.333068	–0.990448	5.978586
29	6	0	7.157664	–2.068790	5.623279
30	6	0	8.391372	–2.256855	6.248275
31	6	0	8.819573	–1.368691	7.236592
32	6	0	8.007258	–0.291789	7.597446
33	6	0	6.772623	–0.104659	6.974343
34	6	0	–0.347288	–1.350237	8.068280
35	6	0	–0.838254	–0.320341	8.884408
36	6	0	–1.477395	–0.613598	10.090172
37	6	0	–1.634182	–1.939955	10.496822
38	6	0	–1.149493	–2.972304	9.691370
39	6	0	–0.510765	–2.679685	8.485291
40	6	0	–2.516090	0.150245	1.585955
41	6	0	–2.945113	1.413542	1.156893
42	6	0	–4.204641	1.576756	0.581626
43	6	0	–5.053040	0.478885	0.425772
44	6	0	–4.634590	–0.782837	0.850835
45	6	0	–3.375595	–0.945603	1.429842
46	1	0	6.358248	0.466611	1.092883
47	1	0	7.171785	–0.140388	3.575376
48	1	0	4.729044	–1.778162	7.961652
49	1	0	2.167907	–1.883001	8.774785
50	1	0	–2.487290	–0.781496	6.589381
51	1	0	–3.313192	–0.178843	4.101679
52	1	0	2.135438	0.720491	–2.219224
53	1	0	2.422916	–0.995279	–1.864332
54	1	0	0.779655	–0.429871	–2.275366
55	1	0	5.174160	–1.298456	–0.808463
56	1	0	6.410313	–0.626726	–2.849270
57	1	0	6.226542	1.700481	–3.707831
58	1	0	4.807574	3.349755	–2.502294
59	1	0	3.573085	2.670089	–0.462585
60	1	0	6.823376	–2.763049	4.857871
61	1	0	9.015700	–3.099420	5.964734
62	1	0	9.779987	–1.514564	7.722521
63	1	0	8.335083	0.406114	8.362609
64	1	0	6.143330	0.735489	7.253248
65	1	0	–0.713943	0.711862	8.569945
66	1	0	–1.850290	0.195123	10.712209

67	1	0	–2.131770	–2.167761	11.435063
68	1	0	–1.271443	–4.007018	9.998870
69	1	0	–0.138168	–3.483467	7.856883
70	1	0	–2.285365	2.268383	1.275004
71	1	0	–4.523426	2.562559	0.254666
72	1	0	–6.033473	0.606037	–0.024481
73	1	0	–5.286933	–1.643252	0.730102
74	1	0	–3.049512	–1.929423	1.754886
75	7	0	1.349649	0.035258	–0.367405
76	7	0	3.850306	–0.180060	3.192923
77	7	0	2.537807	–0.843218	5.622340
78	7	0	0.008101	–0.353447	4.402759
79	8	0	–0.919933	–0.141002	–0.789774
80	8	0	1.948367	1.910947	4.206398
81	75	0	1.948419	0.252258	3.921677

Harmonic frequencies (cm**-1), IR intensities (KM/Mole), Raman scattering activities (A**4/AMU), depolarization ratios for plane and unpolarized incident light, reduced masses (AMU), force constants (mDyne/A), and normal coordinates:

	1	2	3
	A	A	A
Frequencies --	11.0304	19.2731	25.3269
Red. masses --	6.0879	4.4441	4.8052
Frc consts --	0.0004	0.0010	0.0018
IR Inten --	0.0366	0.1604	0.1713

10



10

E(RB3LYP) = -2733.11344912

Stoichiometry	C56H34N5O3Re		
Framework group	C1[X(C56H34N5O3Re)]		
Deg. of freedom	291		
Full point group	C1	NOp	1
Largest Abelian subgroup	C1	NOp	1
Largest concise Abelian subgroup	C1	NOp	1

Standard orientation:

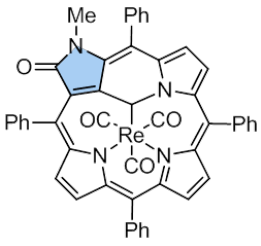
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.679918	3.319138	0.615307
2	6	0	0.081774	4.604045	0.440564
3	6	0	–1.238569	4.424657	0.174018
4	6	0	–1.565981	3.024182	0.232354
5	6	0	–2.879879	2.600645	0.375504
6	6	0	–3.399427	1.325451	0.770754
7	6	0	–4.644189	1.130687	1.462228
8	6	0	–4.693225	–0.195359	1.818510
9	6	0	–3.492192	–0.800199	1.323079
10	6	0	–3.024989	–2.109734	1.615151
11	6	0	–1.715254	–2.540316	1.387571
12	6	0	–1.085133	–3.703430	1.952606
13	6	0	0.239015	–3.636215	1.619470
14	6	0	0.410239	–2.454560	0.804348
15	6	0	1.704119	–1.964836	0.343012
16	6	0	2.070292	–0.608173	0.407504
17	6	0	3.471654	–0.290556	0.535844
18	6	0	1.345261	0.656176	0.508768
19	6	0	2.335617	1.647219	0.789783
20	6	0	2.022817	3.014768	0.814359
21	6	0	4.736213	1.668816	1.532695
22	6	0	0.008945	0.994581	0.175985
23	6	0	–3.939189	3.660859	0.206995
24	6	0	–4.585337	3.795849	–1.029650
25	6	0	–5.586915	4.753777	–1.197596
26	6	0	–5.960426	5.576976	–0.133469
27	6	0	–5.323296	5.444213	1.101834
28	6	0	–4.315344	4.492996	1.270836
29	6	0	–3.979413	–3.028961	2.308232
30	6	0	–5.077026	–3.540924	1.598827
31	6	0	–5.983691	–4.398683	2.222111
32	6	0	–5.813332	–4.746811	3.563619
33	6	0	–4.730353	–4.233612	4.279541
34	6	0	–3.817993	–3.380511	3.656720
35	6	0	2.727866	–2.926882	0.014873
36	6	0	2.384481	–4.243855	–0.401616
37	6	0	3.343293	–5.164107	–0.763284
38	6	0	4.706069	–4.802199	–0.737822
39	6	0	5.076075	–3.528353	–0.369300
40	6	0	4.113566	–2.551876	0.015733
41	6	0	3.011079	4.131661	0.881934
42	6	0	3.932020	4.328771	–0.159794
43	6	0	4.836832	5.389741	–0.115263
44	6	0	4.832972	6.273073	0.966741
45	6	0	3.916674	6.091077	2.004008
46	6	0	3.011840	5.028832	1.961625
47	6	0	4.494828	–1.213307	0.366196
48	6	0	5.944477	–0.851795	0.419512
49	6	0	6.806157	–1.470662	1.341306
50	6	0	8.154674	–1.129252	1.330914
51	6	0	8.607512	–0.188883	0.406224
52	6	0	7.686510	0.388090	–0.475895
53	6	0	8.103567	1.419957	–1.494704
54	6	0	–1.906223	0.961300	–2.148986
55	6	0	–2.526180	–1.669637	–1.709071
56	6	0	0.078289	–0.871228	–2.151621
57	1	0	0.621426	5.536857	0.502568
58	1	0	–1.972096	5.198457	0.013721
59	1	0	–5.358217	1.904023	1.702048
60	1	0	–5.453447	–0.694337	2.401373
61	1	0	–1.571793	–4.441408	2.572437
62	1	0	1.031612	–4.300723	1.929452
63	1	0	5.235032	0.911373	2.138979
64	1	0	4.395485	2.468571	2.187483
65	1	0	5.450329	2.069453	0.811399
66	1	0	–4.288419	3.158672	–1.857058

67	1	0	–6.075701	4.854773	–2.162342
68	1	0	–6.742961	6.318593	–0.265941
69	1	0	–5.608154	6.081217	1.934489
70	1	0	–3.817008	4.390655	2.230808
71	1	0	–5.205126	–3.273207	0.554247
72	1	0	–6.822948	–4.795019	1.657866
73	1	0	–6.521734	–5.412035	4.048863
74	1	0	–4.596246	–4.492930	5.325910
75	1	0	–2.982024	–2.972884	4.217092
76	1	0	1.336874	–4.508849	–0.479407
77	1	0	3.046594	–6.153669	–1.097630
78	1	0	5.464991	–5.518621	–1.039284
79	1	0	6.123074	–3.252214	–0.398774
80	1	0	3.930756	3.648610	–1.006672
81	1	0	5.539571	5.531511	–0.931447
82	1	0	5.537095	7.099361	0.999270
83	1	0	3.906543	6.773912	2.848795
84	1	0	2.302930	4.885498	2.772244
85	1	0	6.415460	–2.200405	2.042530
86	1	0	8.844354	–1.588154	2.033958
87	1	0	9.654388	0.095739	0.366977
88	1	0	7.759039	1.128896	–2.491419
89	1	0	9.188426	1.551197	–1.519062
90	1	0	7.644291	2.389138	–1.268902
91	7	0	–0.300186	2.332254	0.408724
92	7	0	–2.744922	0.143985	0.664051
93	7	0	–0.759894	–1.818414	0.667932
94	7	0	3.578960	1.063692	0.880451
95	7	0	6.382114	0.062173	–0.463652
96	8	0	–2.299465	1.750773	–2.914953
97	8	0	–3.262917	–2.437301	–2.175295
98	8	0	0.899178	–1.168555	–2.921230
99	75	0	–1.300291	–0.364415	–0.895417

Harmonic frequencies (cm**-1), IR intensities (KM/Mole), Raman scattering activities (A**4/AMU), depolarization ratios for plane and unpolarized incident light, reduced masses (AMU), force constants (mDyne/A), and normal coordinates:

	1	2	3
	A	A	A
Frequencies --	15.1303	16.7465	26.1867
Red. masses --	5.6749	5.8838	4.1885
Frc consts --	0.0008	0.0010	0.0017
IR Inten --	0.0632	0.2095	0.1798

11



11

E(RB3LYP) = -2483.80822144

Stoichiometry	C49H29N4O4Re		
Framework group	C1[X(C49H29N4O4Re)]		
Deg. of freedom	255		
Full point group	C1	NOp	1
Largest Abelian subgroup	C1	NOp	1
Largest concise Abelian subgroup	C1	NOp	1

Standard orientation:

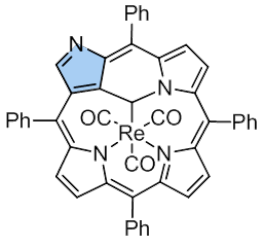
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	–2.776543	1.875760	–0.494847
2	6	0	–2.985961	3.282978	–0.465626
3	6	0	–1.798038	3.879092	–0.170229
4	6	0	–0.762107	2.886824	–0.082053
5	6	0	0.578080	3.254808	–0.164547
6	6	0	1.737962	2.468562	–0.445407
7	6	0	2.934001	2.972600	–1.073066
8	6	0	3.739658	1.889647	–1.311631
9	6	0	3.043761	0.737466	–0.809397
10	6	0	3.430370	–0.617343	–0.969551
11	6	0	2.559679	–1.700702	–0.770931
12	6	0	2.791644	–3.072102	–1.143817
13	6	0	1.626226	–3.746443	–0.912596
14	6	0	0.679885	–2.785606	–0.389971
15	6	0	–0.709985	–3.078371	–0.135784
16	6	0	–1.756081	–2.169693	–0.111658
17	6	0	–1.872612	–0.711932	–0.234131
18	6	0	–3.248992	–0.436538	–0.534425
19	6	0	–3.723544	0.867233	–0.676408
20	6	0	–5.416475	–1.788185	–0.669002
21	6	0	–0.962135	0.322841	0.082546
22	6	0	0.861474	4.732477	–0.052474
23	6	0	1.206855	5.268320	1.195821
24	6	0	1.498515	6.628063	1.319557
25	6	0	1.457224	7.461944	0.200555
26	6	0	1.116590	6.932842	–1.046014
27	6	0	0.817194	5.575038	–1.172159
28	6	0	4.809956	–0.876918	–1.477843
29	6	0	5.912699	–0.546024	–0.673488
30	6	0	7.211769	–0.780957	–1.123785
31	6	0	7.428161	–1.335703	–2.386768
32	6	0	6.338208	–1.657397	–3.197823
33	6	0	5.037146	–1.432182	–2.746861
34	6	0	–0.982923	–4.553076	0.018028
35	6	0	–0.955631	–5.118421	1.298828
36	6	0	–1.132669	–6.492696	1.464286
37	6	0	–1.331650	–7.315672	0.355110
38	6	0	–1.354456	–6.757034	–0.924567
39	6	0	–5.132625	1.260501	–0.987290
40	6	0	–5.988612	1.722444	0.024077
41	6	0	–7.295131	2.112299	–0.275666
42	6	0	–7.761291	2.051209	–1.590425
43	6	0	–6.913833	1.603664	–2.605769
44	6	0	–5.606935	1.215025	–2.306849
45	6	0	0.497270	1.419319	2.460559
46	6	0	2.508176	–0.413708	2.199449
47	6	0	–0.107532	–1.224828	2.472639
48	1	0	–3.940083	3.758784	–0.635937
49	1	0	–1.614261	4.938085	–0.089274
50	1	0	3.113051	4.000324	–1.350150
51	1	0	4.692430	1.874530	–1.819997
52	1	0	3.708262	–3.464629	–1.557493
53	1	0	1.417778	–4.786828	–1.106751
54	1	0	–5.597855	–2.853718	–0.525024
55	1	0	–5.765074	–1.483124	–1.657519
56	1	0	–5.959602	–1.217864	0.088174
57	1	0	1.232423	4.618479	2.065429
58	1	0	1.758928	7.034103	2.292702
59	1	0	1.688042	8.518716	0.298947
60	1	0	1.081253	7.575750	–1.920927
61	1	0	0.548261	5.163260	–2.140931
62	1	0	5.742992	–0.124025	0.312453
63	1	0	8.054544	–0.531500	–0.485711
64	1	0	8.440333	–1.514521	–2.737770
65	1	0	6.499210	–2.080528	–4.185197

66	1	0	4.190941	–1.671906	–3.383498
67	1	0	–0.804684	–4.477307	2.162167
68	1	0	–1.113261	–6.919151	2.463274
69	1	0	–1.467912	–8.385454	0.485790
70	1	0	–1.511167	–7.390206	–1.793517
71	1	0	–5.627612	1.768394	1.047594
72	1	0	–7.948210	2.462277	0.518534
73	1	0	–8.778132	2.353807	–1.822744
74	1	0	–7.267624	1.560509	–3.631811
75	1	0	–4.945276	0.875310	–3.098750
76	7	0	–1.433666	1.606225	–0.206641
77	7	0	1.846055	1.131235	–0.266653
78	7	0	1.271670	–1.579495	–0.268609
79	7	0	–3.977897	–1.605212	–0.538983
80	8	0	0.324690	2.316862	3.187683
81	8	0	3.511645	–0.612472	2.749301
82	8	0	–0.657436	–1.943052	3.207408
83	75	0	0.818294	–0.045368	1.259040
84	6	0	–1.179160	–5.383977	–1.092712
85	1	0	–1.204739	–4.950195	–2.088538
86	6	0	–3.161057	–2.696690	–0.195261
87	8	0	–3.601057	–3.822665	–0.043030

Harmonic frequencies (cm**-1), IR intensities (KM/Mole), Raman scattering activities (A**4/AMU), depolarization ratios for plane and unpolarized incident light, reduced masses (AMU), force constants (mDyne/A), and normal coordinates:

	1	2	3
	A	A	A
Frequencies --	13.4947	18.8734	22.6270
Red. masses --	5.9651	4.4698	4.3465
Frc consts --	0.0006	0.0009	0.0013
IR Inten --	0.1481	0.0698	0.1696

13



13

E(RB3LYP) = -2369.25339738

Stoichiometry	C48H27N4O3Re		
Framework group	C1[X(C48H27N4O3Re)]		
Deg. of freedom	243		
Full point group	C1	NOp	1
Largest Abelian subgroup	C1	NOp	1
Largest concise Abelian subgroup	C1	NOp	1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.134637	–1.432460	–0.546885
2	6	0	3.501865	–2.808378	–0.553340
3	6	0	2.390989	–3.550611	–0.290265
4	6	0	1.246801	–2.685939	–0.177700
5	6	0	–0.049337	–3.199640	–0.259030
6	6	0	–1.294770	–2.543887	–0.505456
7	6	0	–2.433294	–3.173058	–1.141386
8	6	0	–3.373785	–2.198420	–1.323439
9	6	0	–2.821797	–0.980558	–0.783383
10	6	0	–3.384187	0.310903	–0.881615
11	6	0	–2.647203	1.497823	–0.667898
12	6	0	–3.074909	2.843181	–0.961844
13	6	0	–1.997658	3.655722	–0.743200
14	6	0	–0.908586	2.803905	–0.321524
15	6	0	0.445684	3.232642	–0.180773
16	6	0	1.588018	2.431241	–0.239808
17	6	0	1.859130	0.993766	–0.329545
18	6	0	3.250671	0.921798	–0.650770
19	6	0	3.930350	–0.298389	–0.728976
20	6	0	1.108726	–0.140144	0.030030
21	6	0	–0.161189	–4.702932	–0.190560
22	6	0	–0.441564	–5.310426	1.041175
23	6	0	–0.573402	–6.697771	1.126694
24	6	0	–0.435861	–7.489568	–0.014874
25	6	0	–0.158948	–6.889928	–1.245292
26	6	0	–0.018957	–5.503634	–1.332825
27	6	0	–4.800972	0.409461	–1.340298
28	6	0	–5.825198	–0.109081	–0.530847
29	6	0	–7.157353	–0.027711	–0.936417
30	6	0	–7.484670	0.560236	–2.159706
31	6	0	–6.472657	1.069258	–2.976133
32	6	0	–5.140081	0.997251	–2.569629
33	6	0	0.643266	4.720481	–0.062777
34	6	0	0.782093	5.288745	1.211758
35	6	0	0.956878	6.666622	1.352385
36	6	0	0.995541	7.489845	0.225594
37	6	0	0.860600	6.929830	–1.046297
38	6	0	5.392945	–0.392705	–0.962475
39	6	0	6.213890	–1.160037	–0.118958
40	6	0	7.587593	–1.244693	–0.346858
41	6	0	8.163412	–0.562861	–1.419610
42	6	0	7.358310	0.213183	–2.256580
43	6	0	5.986731	0.302424	–2.029115
44	6	0	–0.143926	–1.419743	2.425908
45	6	0	–2.351909	0.181404	2.254390
46	6	0	0.168287	1.285845	2.446433
47	1	0	4.501019	–3.168982	–0.745628
48	1	0	2.331851	–4.625989	–0.250421
49	1	0	–2.482243	–4.203326	–1.459511
50	1	0	–4.328643	–2.285708	–1.820535
51	1	0	–4.054321	3.129011	–1.314569
52	1	0	–1.934837	4.722332	–0.896993
53	1	0	–0.541479	–4.692630	1.928706
54	1	0	–0.784525	–7.158284	2.087447
55	1	0	–0.542340	–8.568322	0.053425
56	1	0	–0.049077	–7.499831	–2.137469
57	1	0	0.201283	–5.036861	–2.288910
58	1	0	–5.571028	–0.555507	0.425734
59	1	0	–7.939151	–0.422566	–0.294169
60	1	0	–8.521954	0.619797	–2.476111
61	1	0	–6.718939	1.518884	–3.933750
62	1	0	–4.353923	1.381596	–3.212381
63	1	0	0.755702	4.645705	2.086606
64	1	0	1.064473	7.094951	2.344711
65	1	0	1.132891	8.561474	0.337191
66	1	0	0.895198	7.563399	–1.928033
67	1	0	5.776925	–1.667723	0.735501

68	1	0	8.207604	–1.835976	0.320928
69	1	0	9.232940	–0.628555	–1.597499
70	1	0	7.800165	0.753398	–3.088924
71	1	0	5.366665	0.915912	–2.672840
72	7	0	1.757437	–1.342483	–0.264376
73	7	0	–1.573217	–1.241963	–0.270593
74	7	0	–1.341707	1.520225	–0.229009
75	7	0	3.848971	2.170183	–0.734346
76	8	0	0.147975	–2.301114	3.133782
77	8	0	–3.352560	0.257996	2.839166
78	8	0	0.662944	2.071876	3.150658
79	75	0	–0.661199	0.014117	1.256850
80	6	0	0.685433	5.552294	–1.190726
81	1	0	0.585378	5.116709	–2.181001
82	6	0	2.894538	3.031274	–0.478838
83	1	0	3.088007	4.097178	–0.498137

Harmonic frequencies (cm**-1), IR intensities (KM/Mole), Raman scattering activities (A**4/AMU), depolarization ratios for plane and unpolarized incident light, reduced masses (AMU), force constants (mDyne/A), and normal coordinates:

	1	2	3
	A	A	A
Frequencies --	15.6115	24.9111	26.3272
Red. masses --	6.1015	4.2428	4.2993
Frc consts --	0.0009	0.0016	0.0018
IR Inten --	0.0231	0.1379	0.2325