

Supporting information for:

Activation of aldehydes by exocyclic iridium (I)- $\eta^4:\pi^2$ -diene complexes derived from 1,3-oxazolidin-2-ones

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A. NMR characterization of 4e-k and 5a-b.

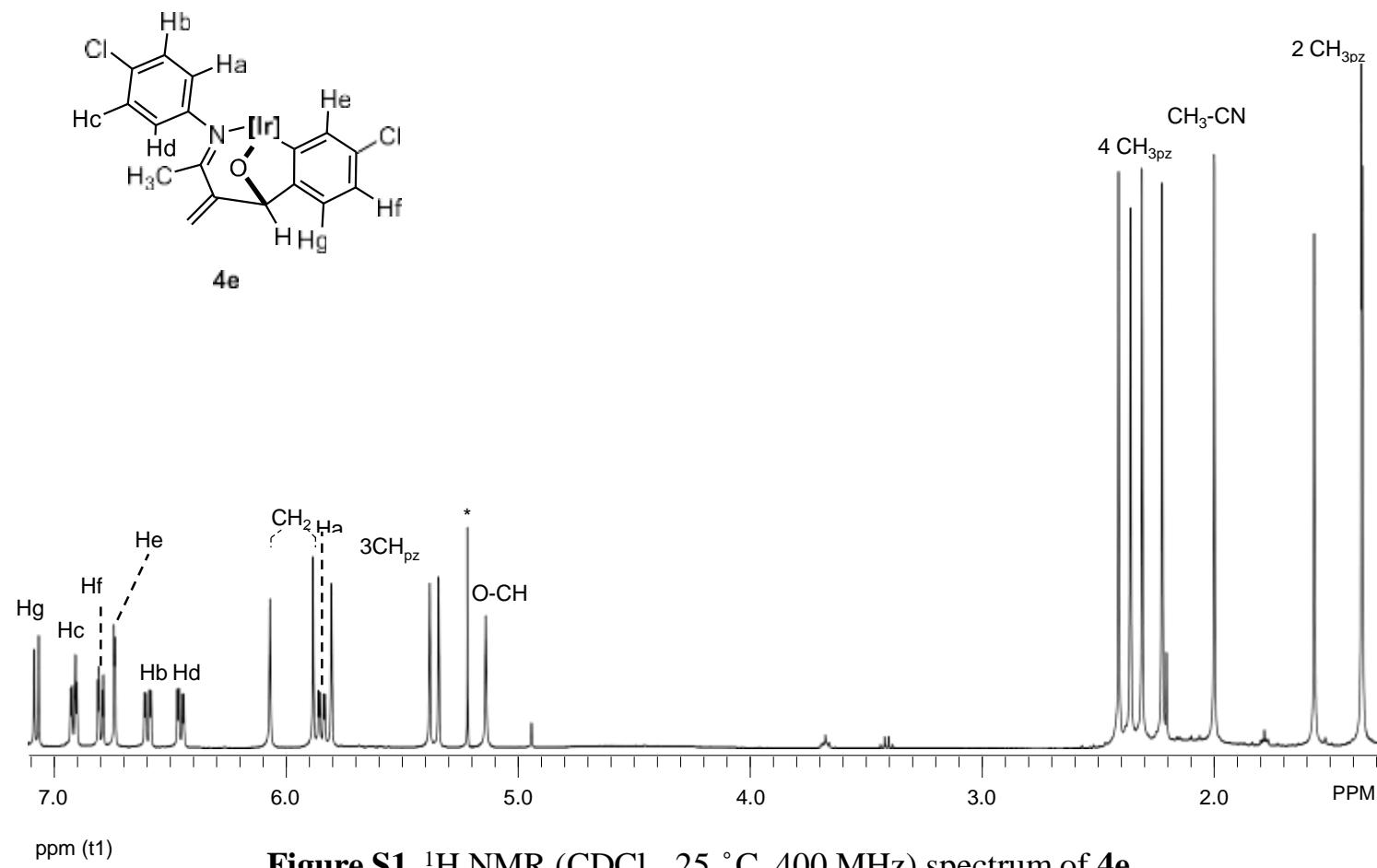


Figure S1. ¹H NMR (CDCl₃, 25 °C, 400 MHz) spectrum of **4e**.

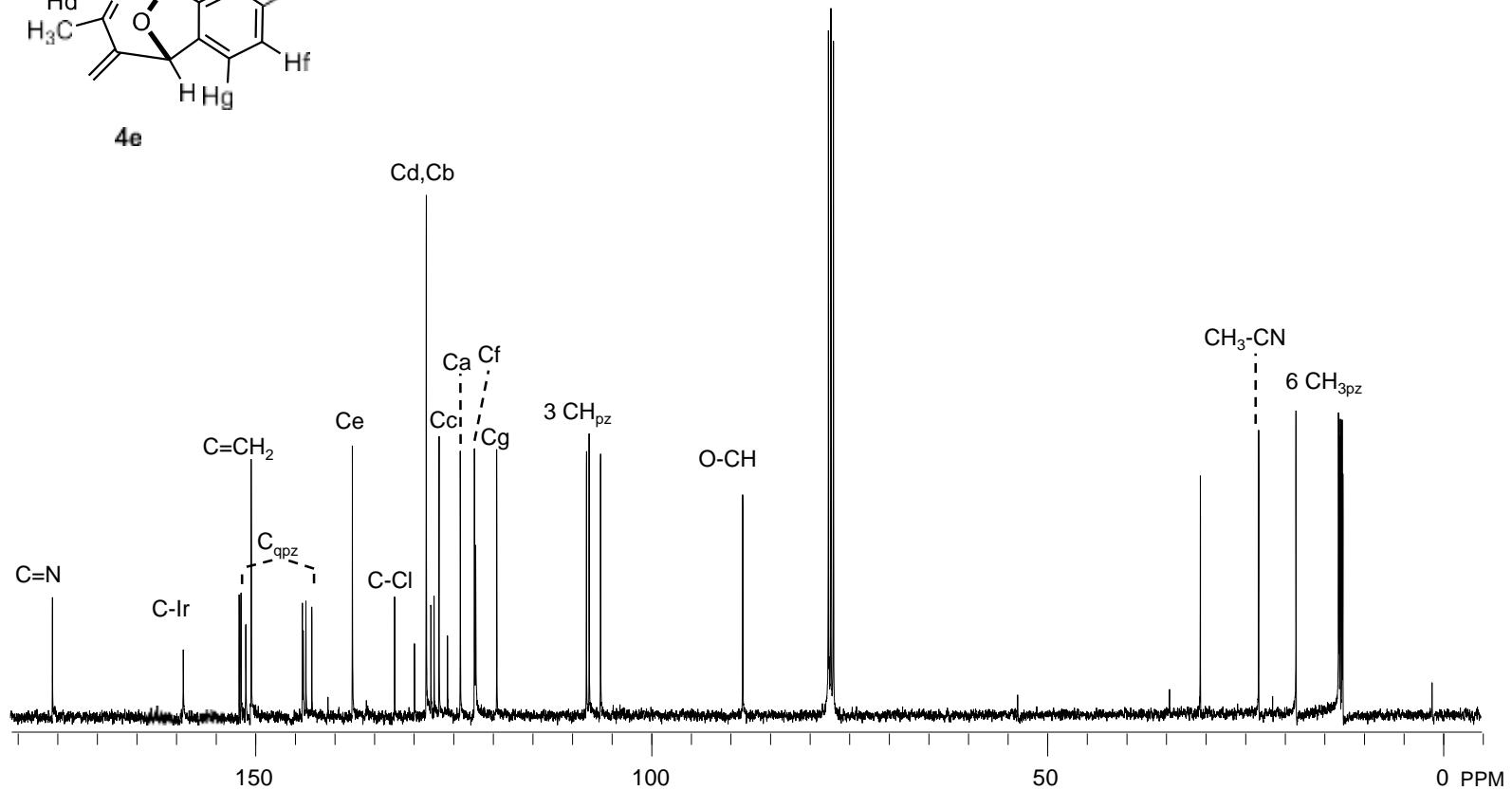
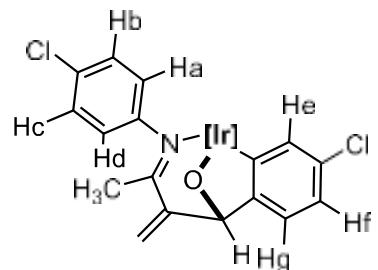


Figure S2. ^{13}C { ^1H } NMR (CDCl_3 , 25 °C, 100.6 MHz) spectrum of **4e**.

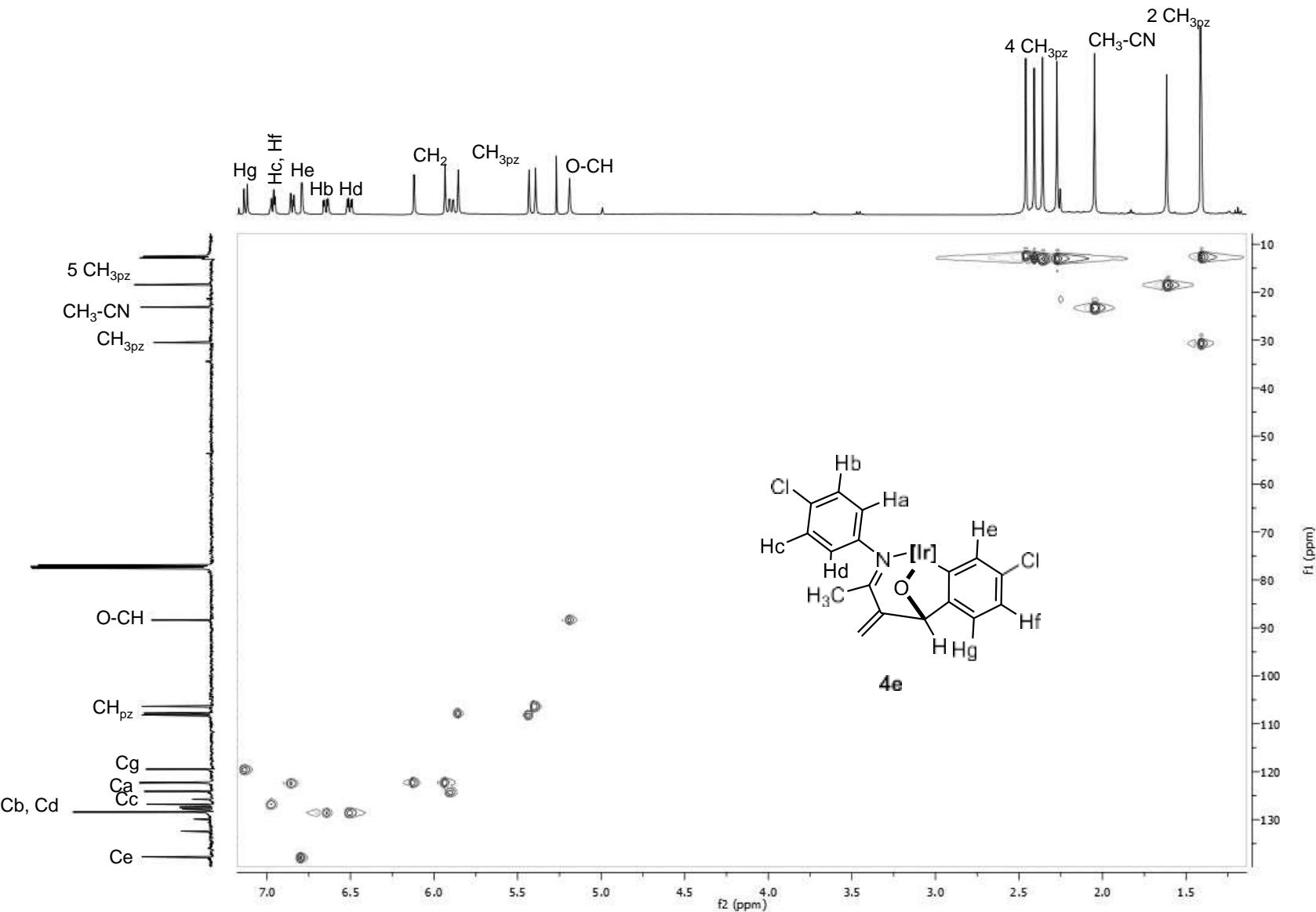


Figure S3. HMQC diagram of **4e**.

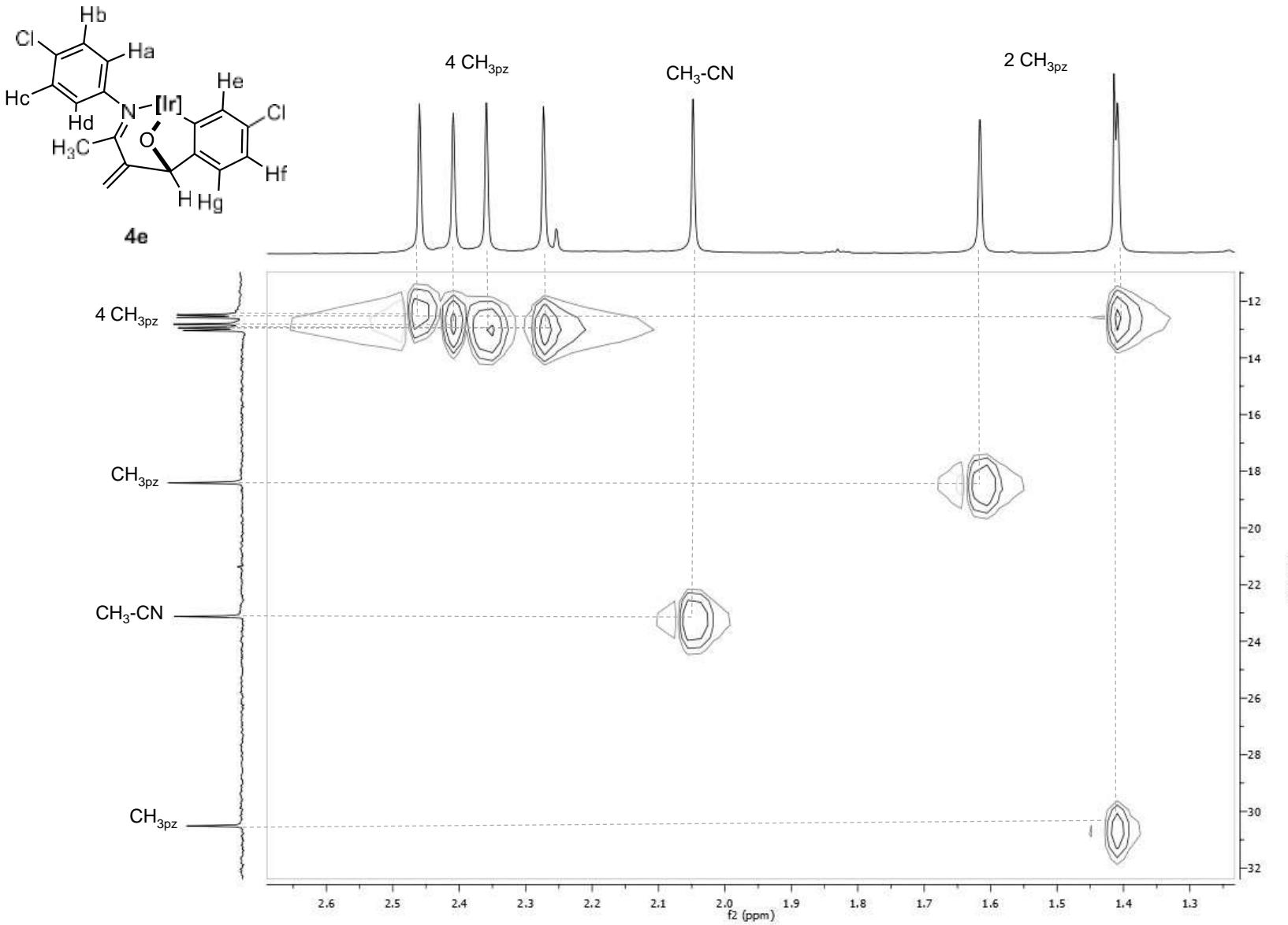


Figure S4. HMQC diagram of **4e**.

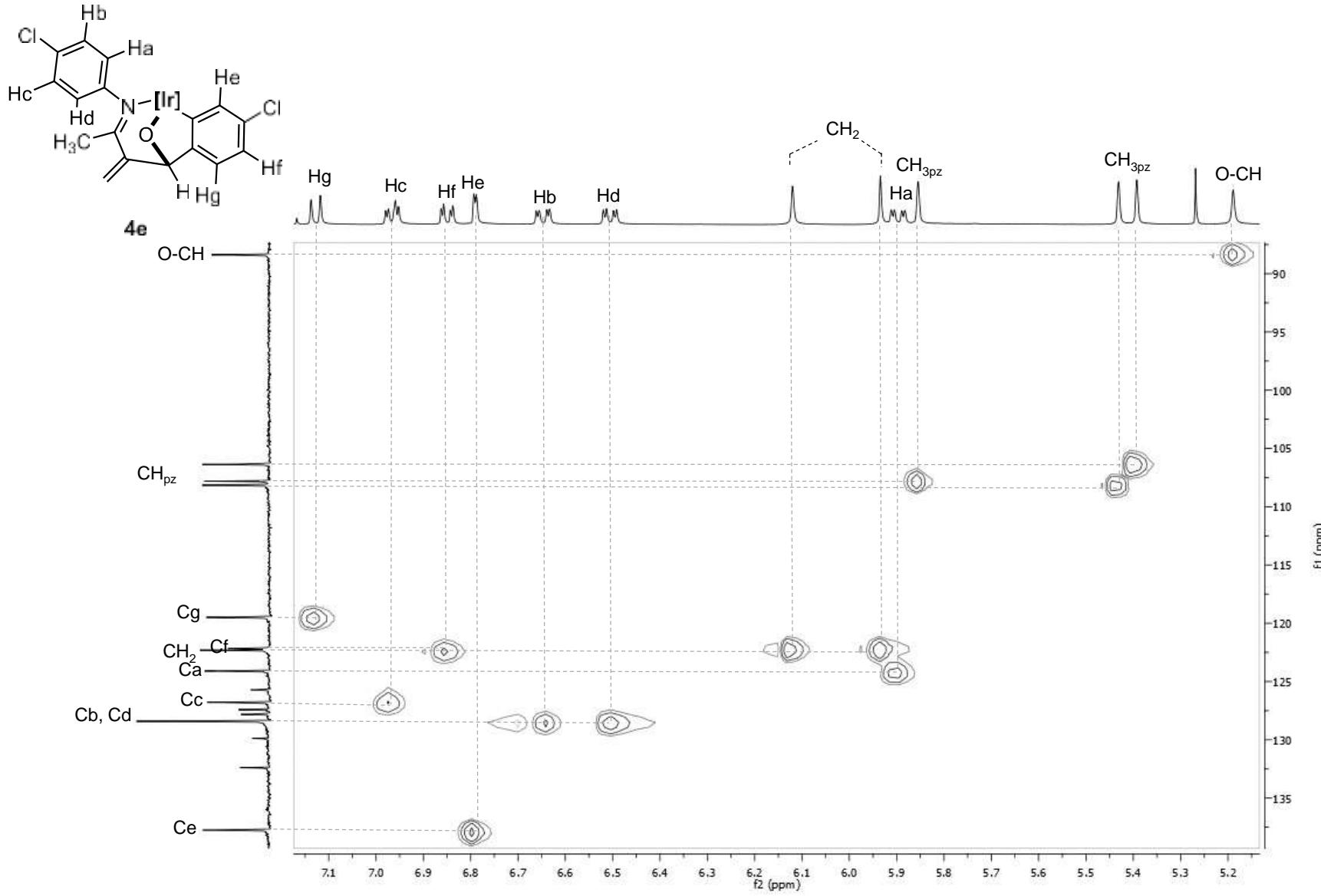


Figure S5. HMQC diagram of **4e**.

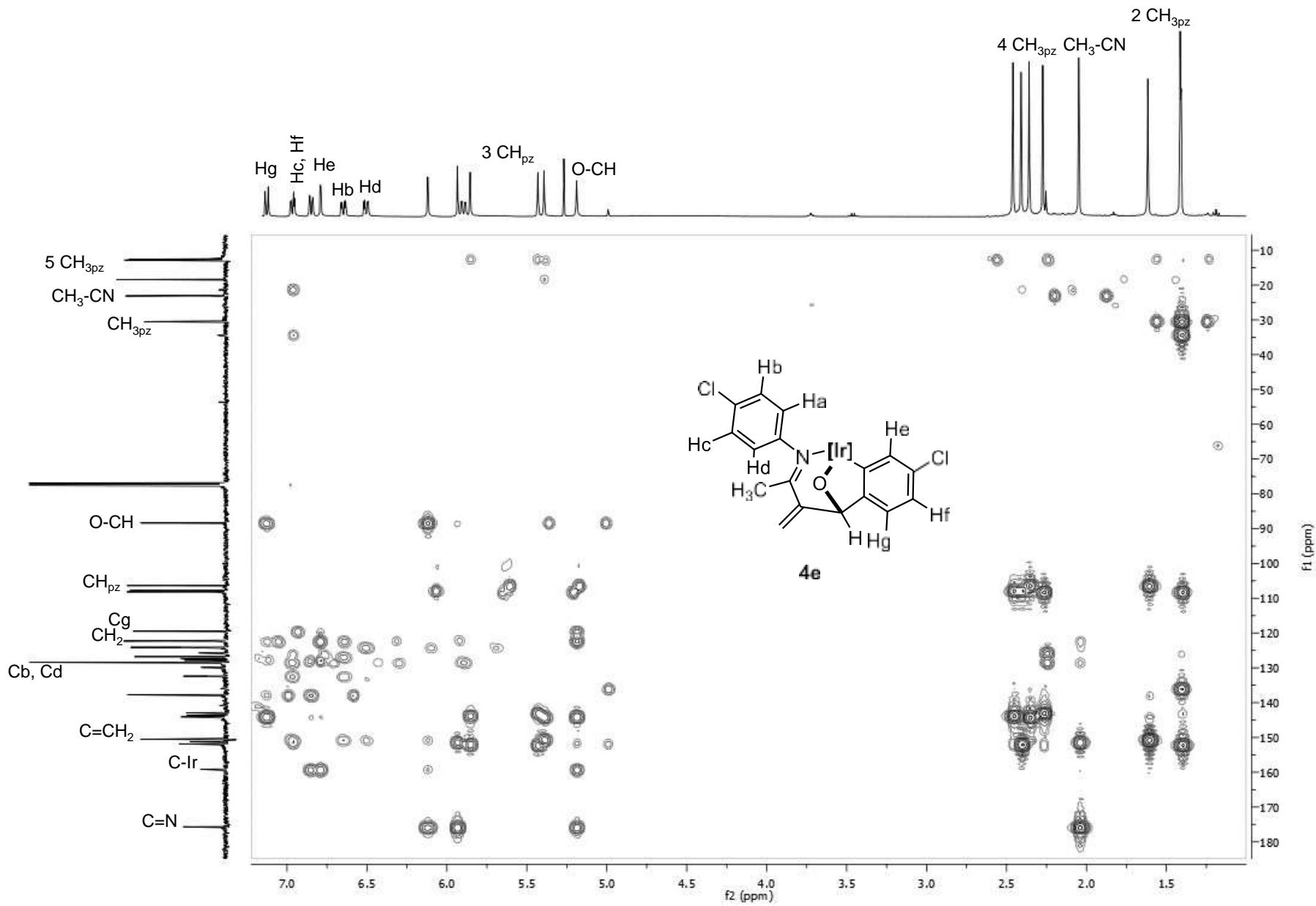


Figure S6. HMBC diagram of **4e**.

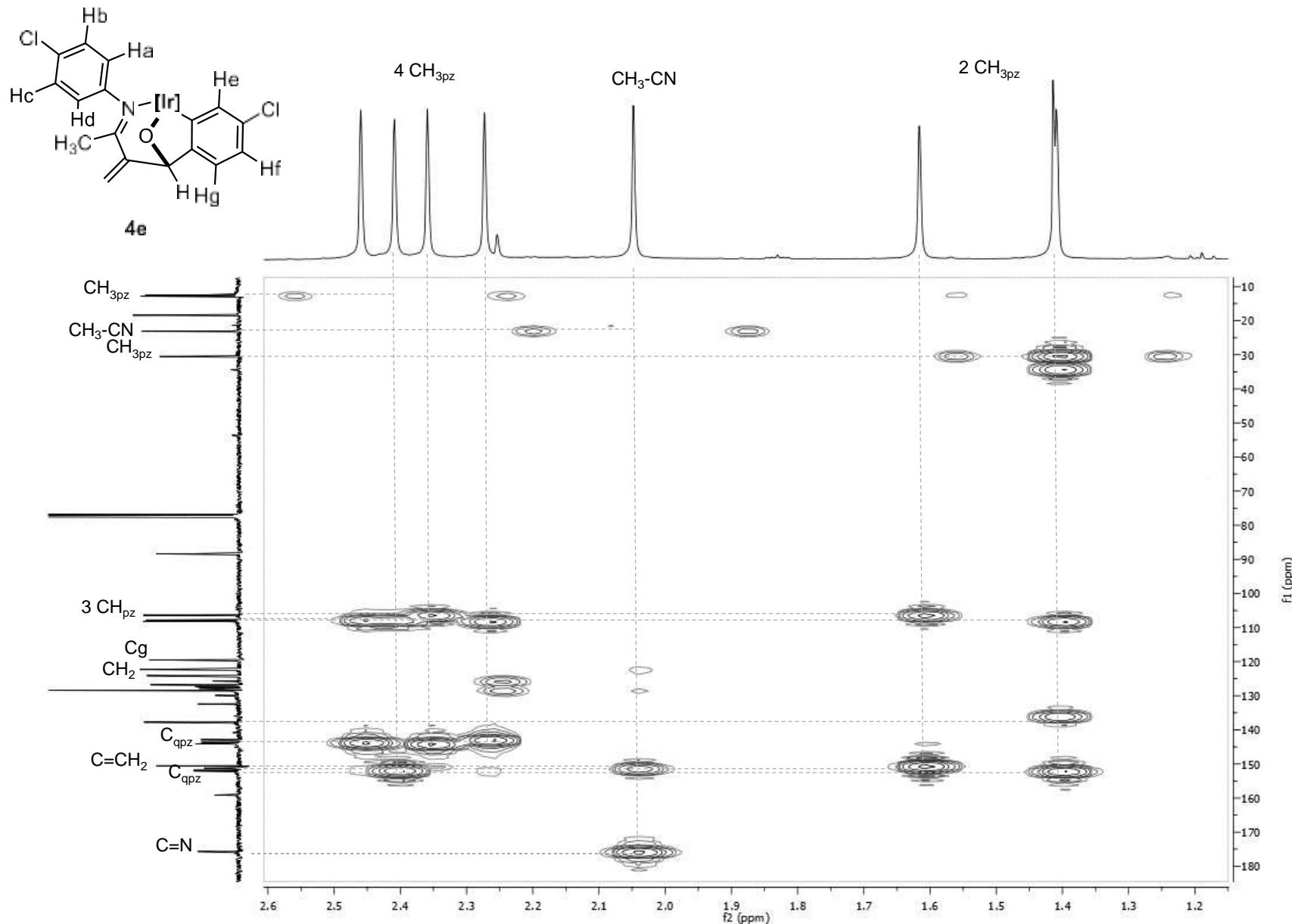


Figure S7. HMBC diagram of **4e**.

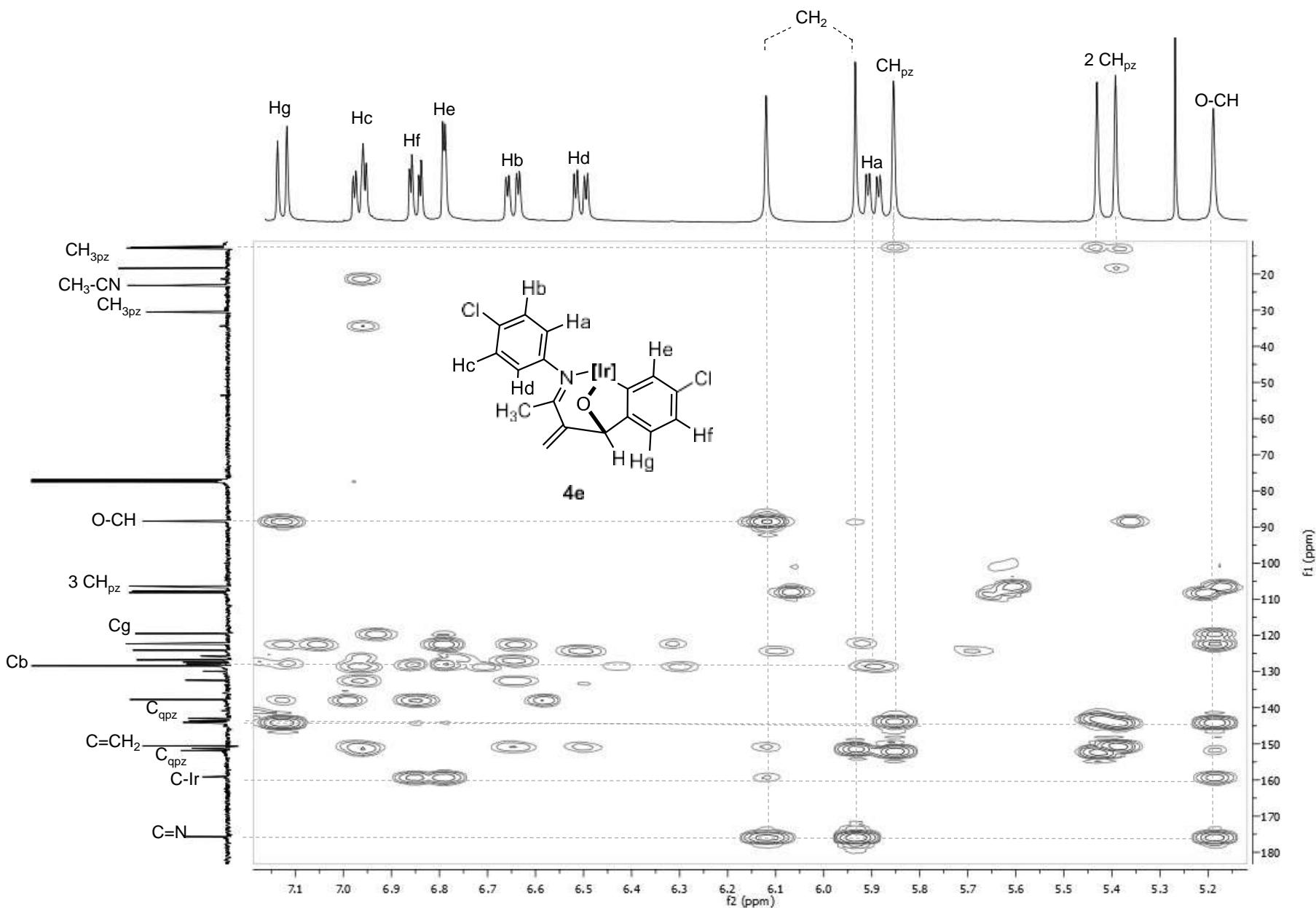


Figure S8. HMBC diagram of **4e**.

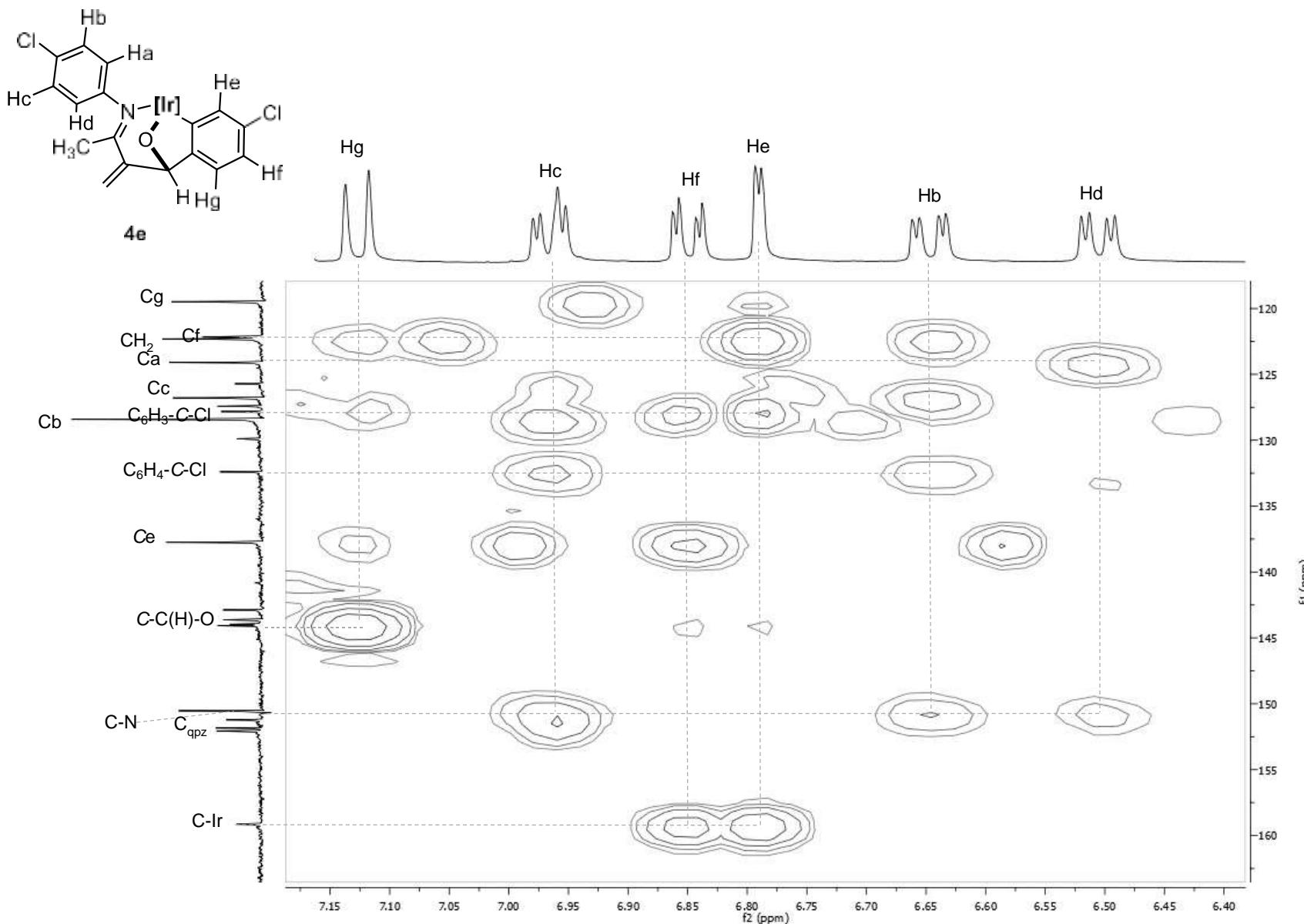


Figure S9. HMBC diagram of **4e**.

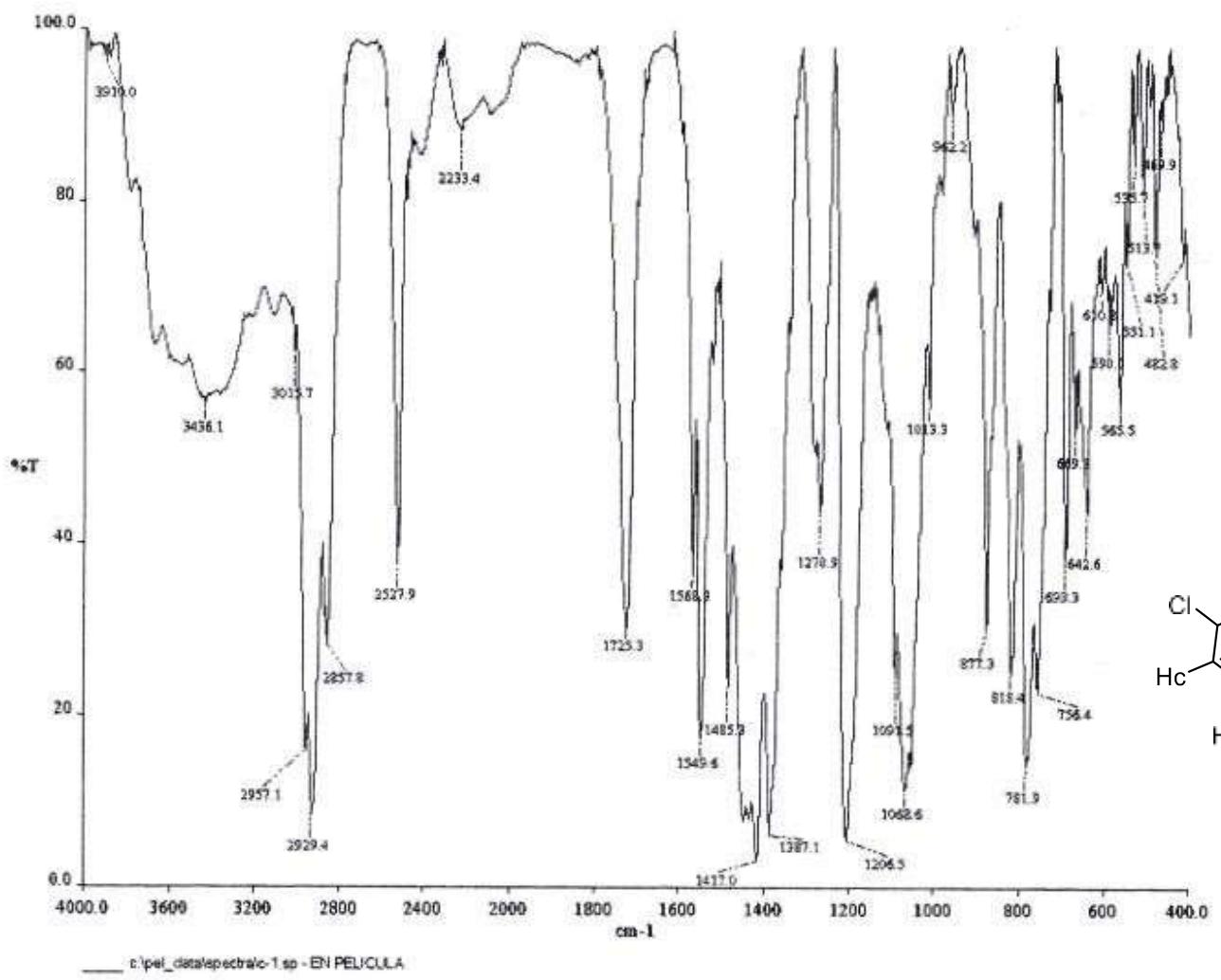


Figure S10. IR spectrum of **4e**.

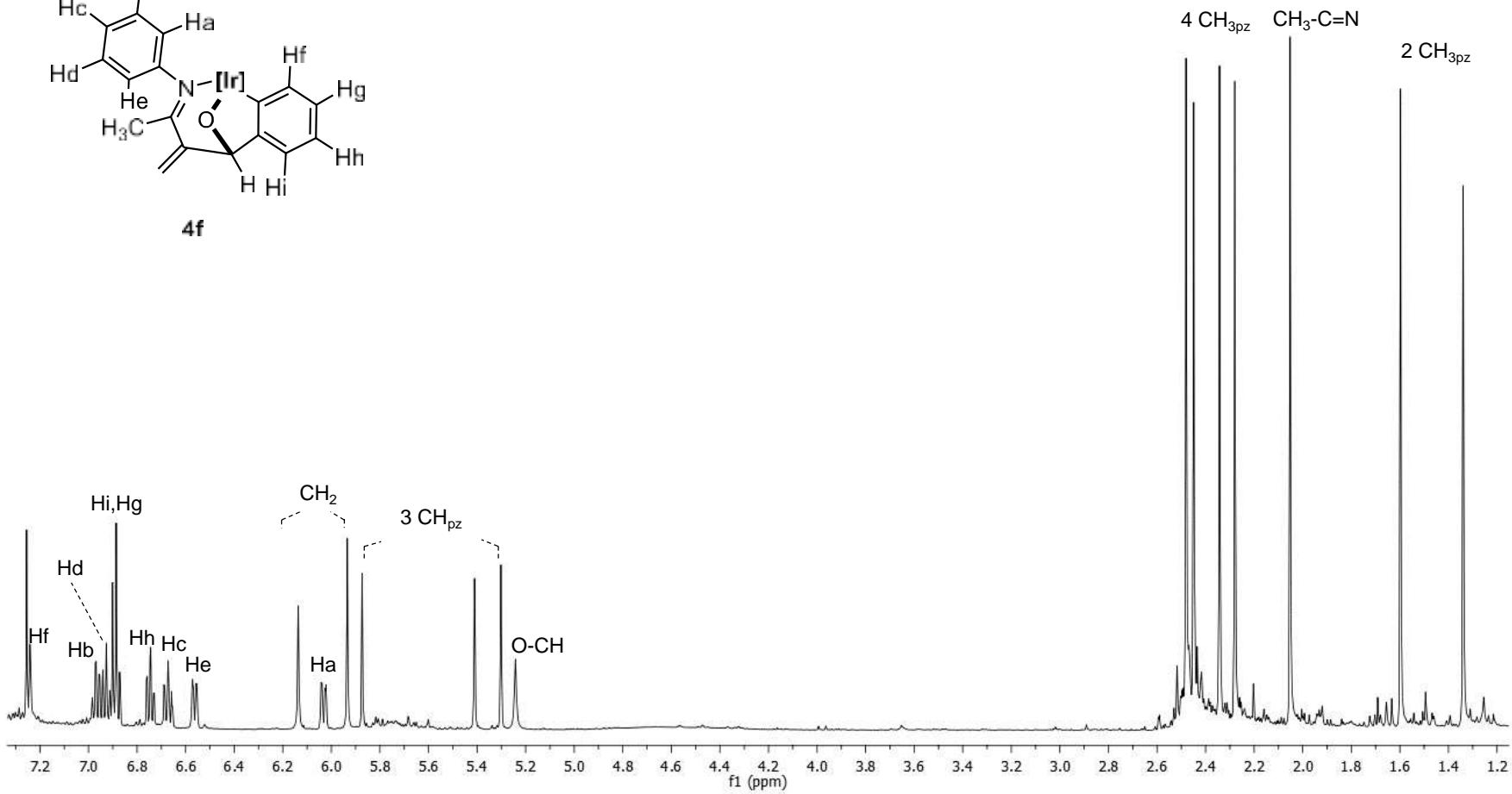
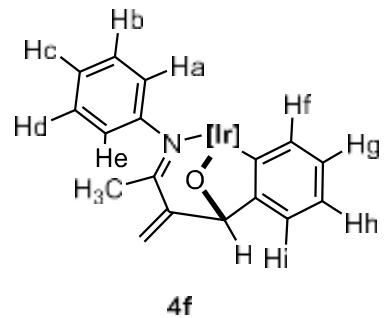
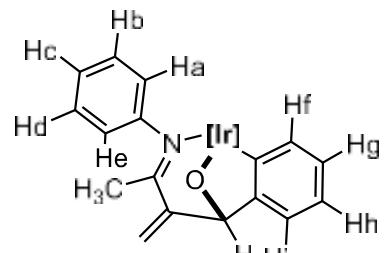


Figure S11. ^1H NMR (CDCl_3 , 25 °C, 400 MHz) spectrum of **4f**.



4f

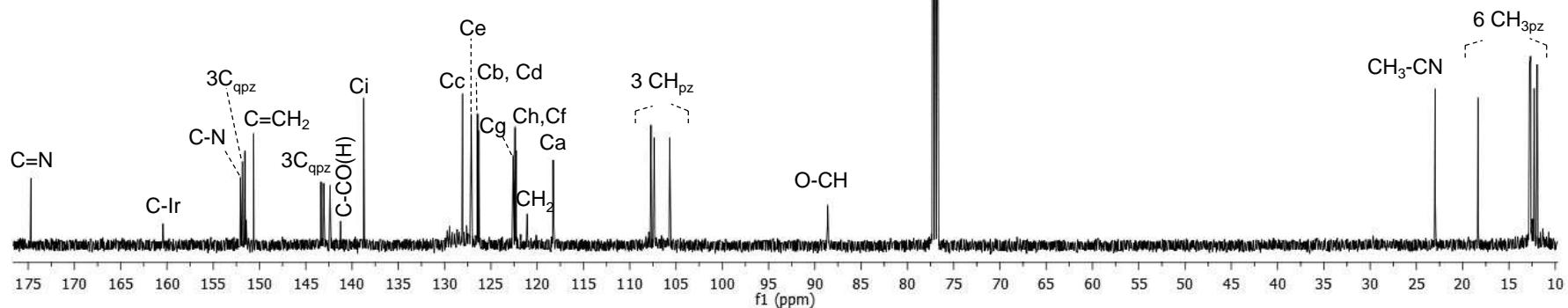


Figure S12. ¹³C {¹H} NMR (CDCl₃, 25 °C, 100.6 MHz) spectrum of **4f**.

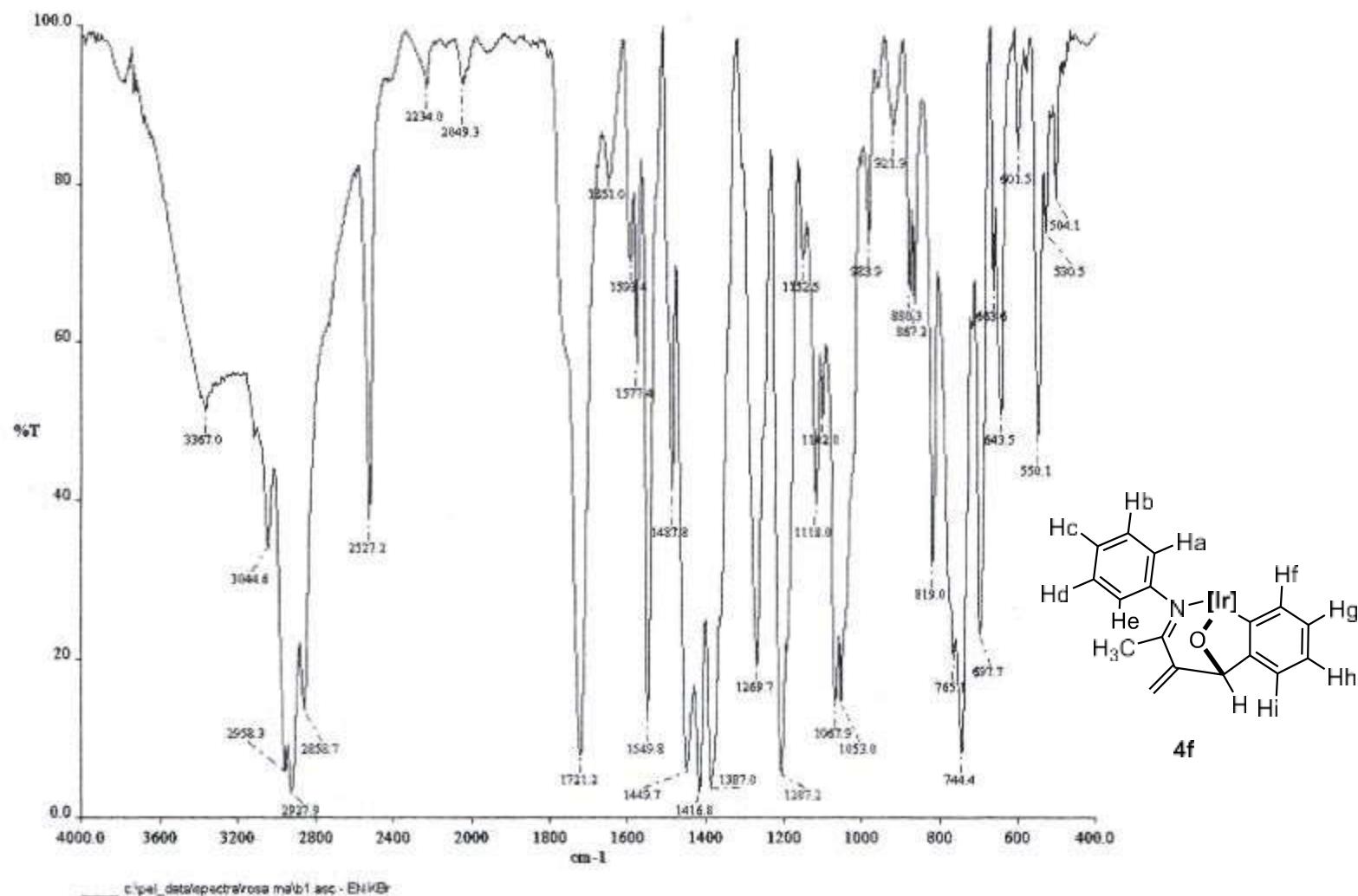


Figure S13. IR spectrum of **4f**.

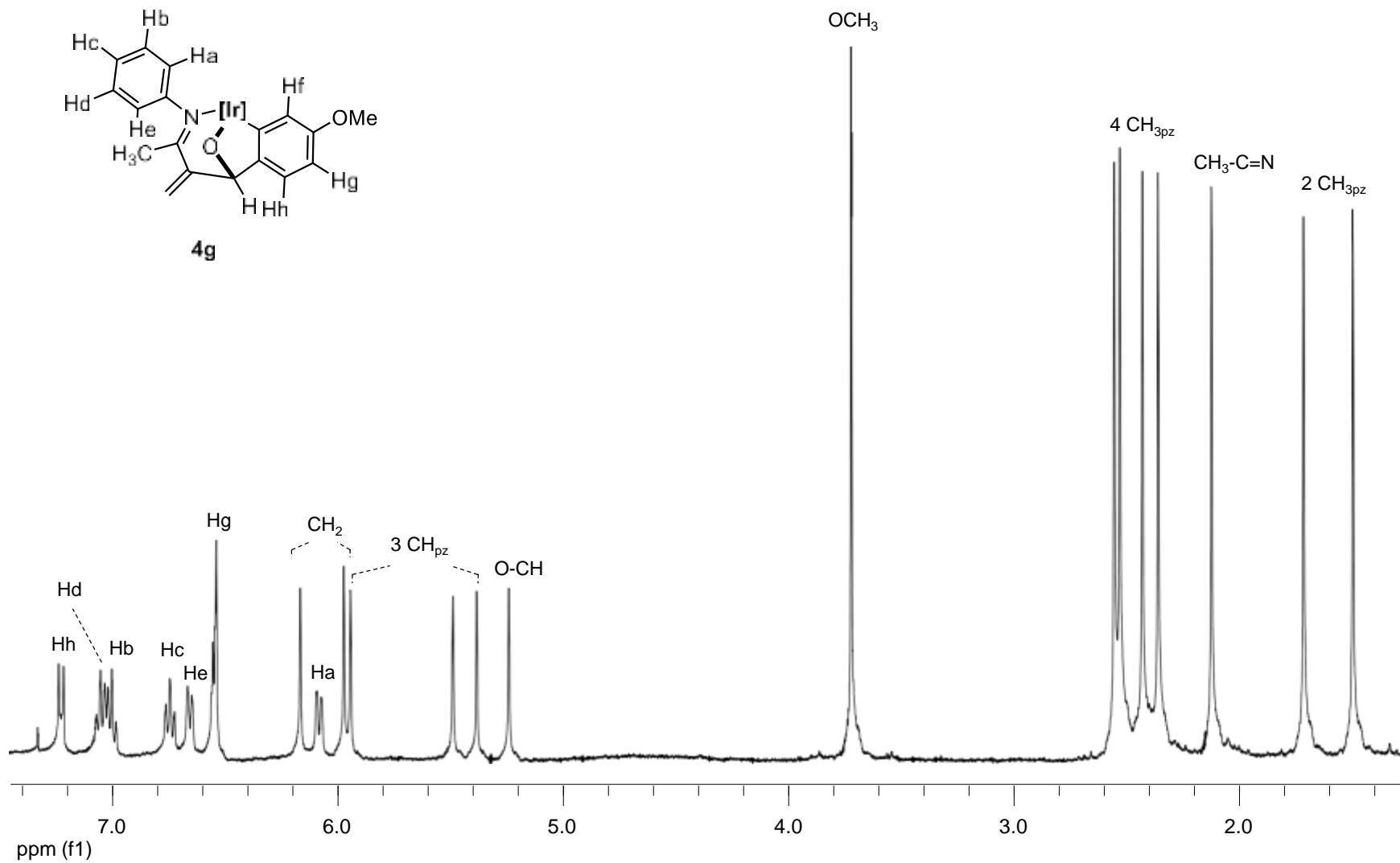
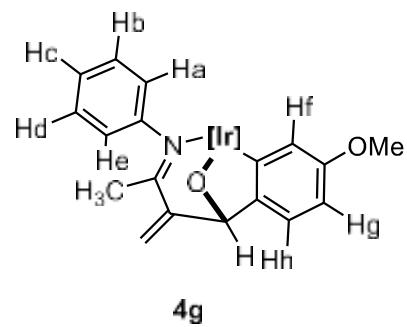


Figure S14. ^1H NMR (CDCl_3 , 25 °C, 400 MHz) spectrum of **4g**.

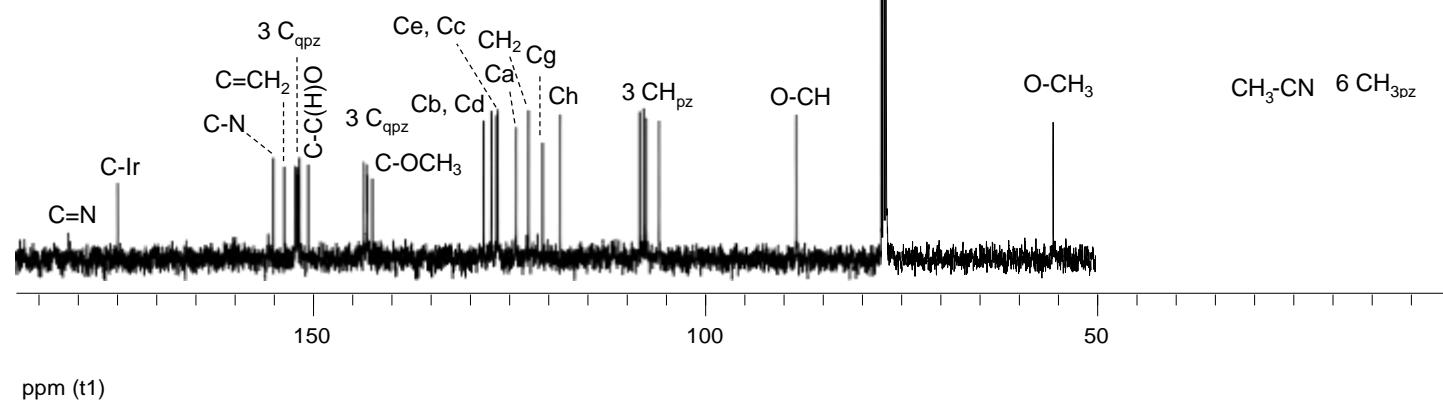
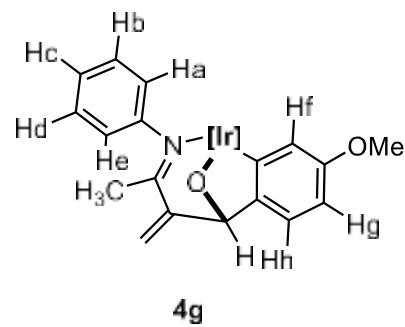


Figure S15. ^{13}C $\{\text{H}\}$ NMR (CDCl_3 , 25°C , 100.6 MHz) spectrum of **4g**.

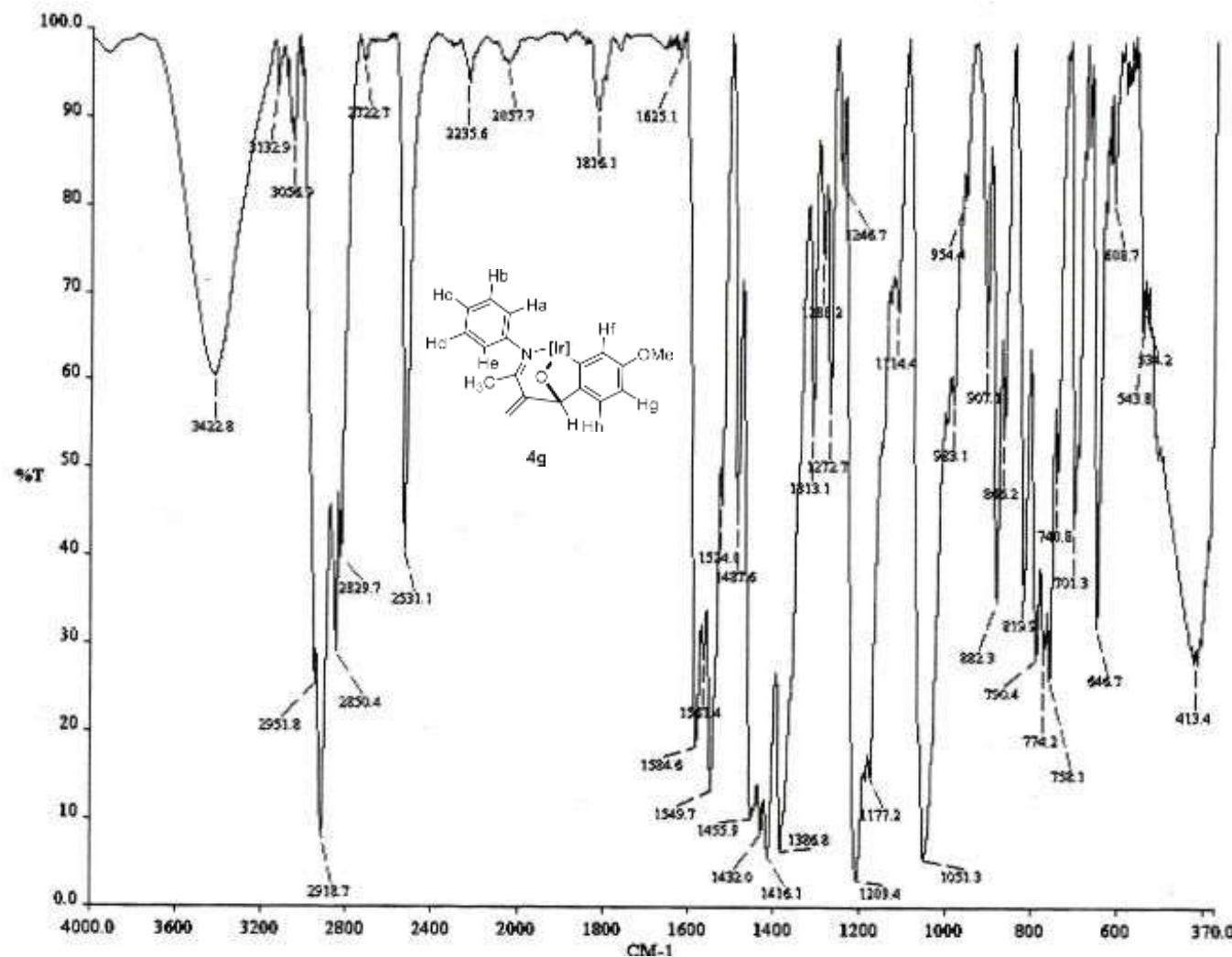
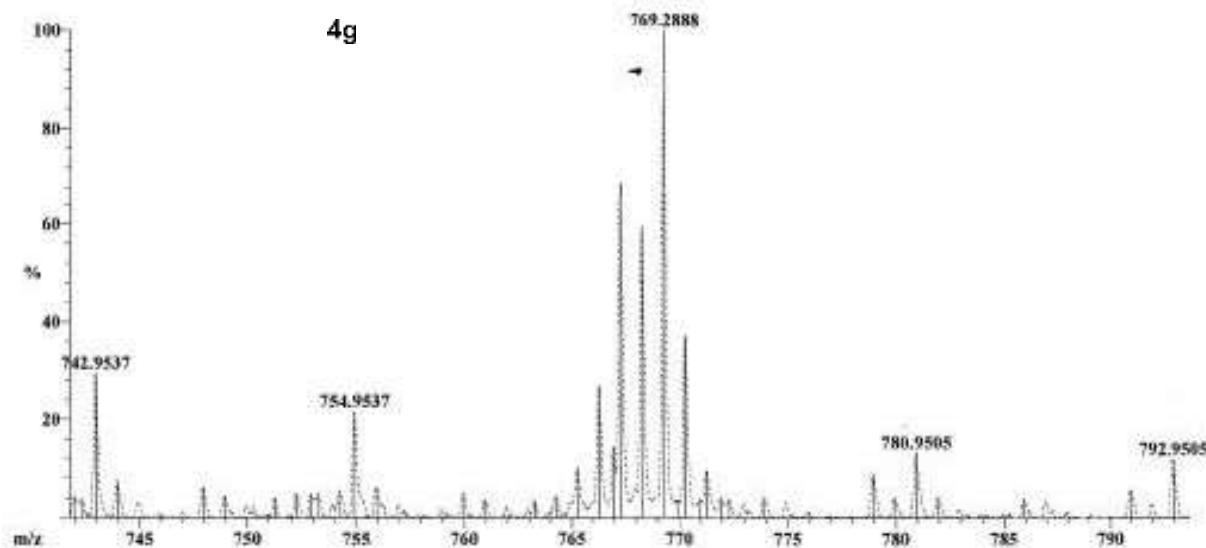
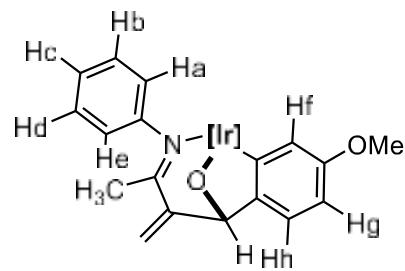
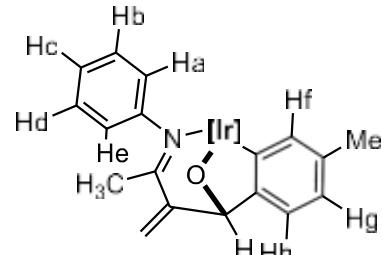


Figure S16. IR spectrum of **4g**.



MS Calcd: 769.2888 for $C_{33}H_{39}N_7BO_2Ir$, observed: 769.2888

Figure S17. MS Spectra of complex **4g**.



4h

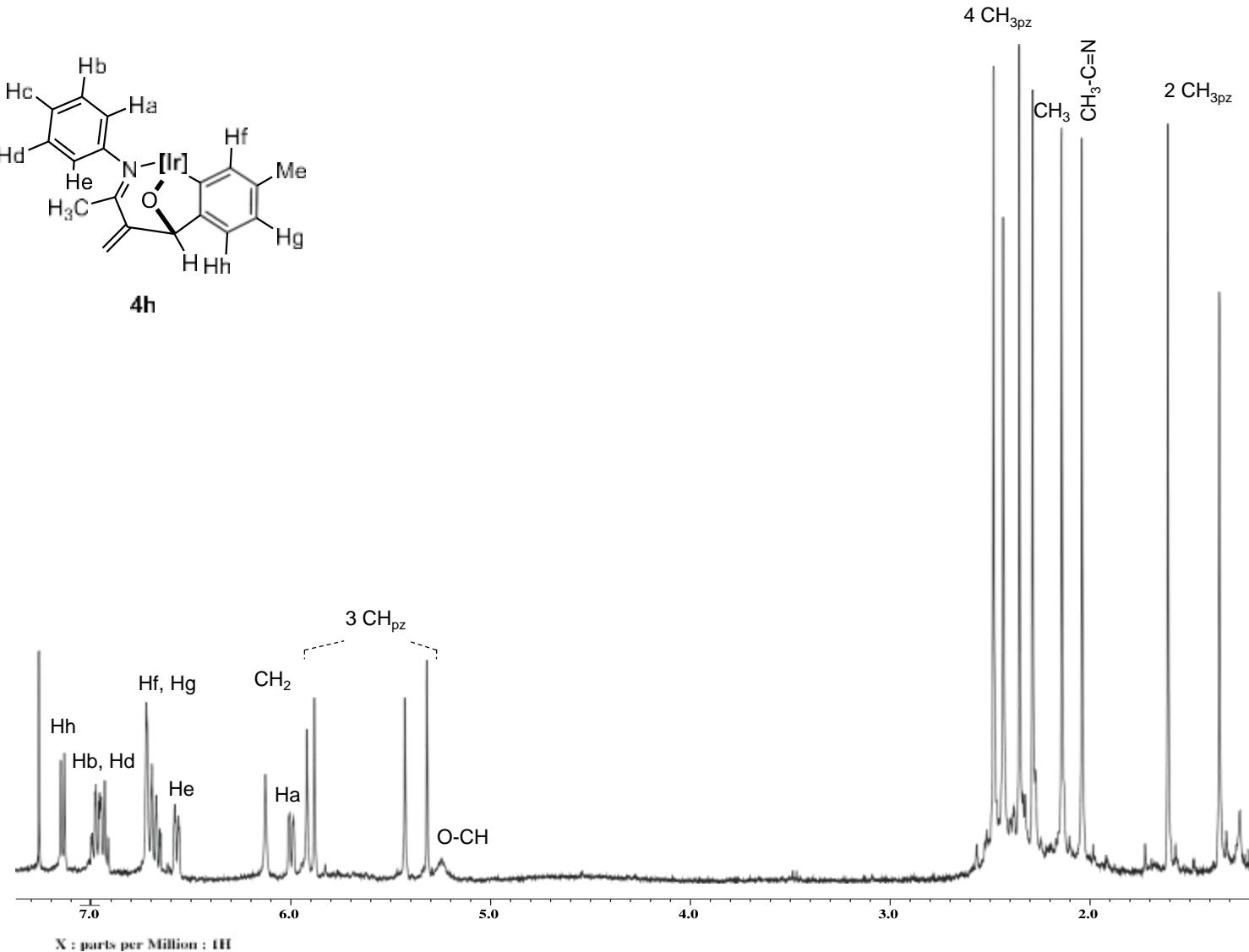


Figure S18. ^1H NMR (CDCl_3 , 25 °C, 400 MHz) spectrum of **4h**.

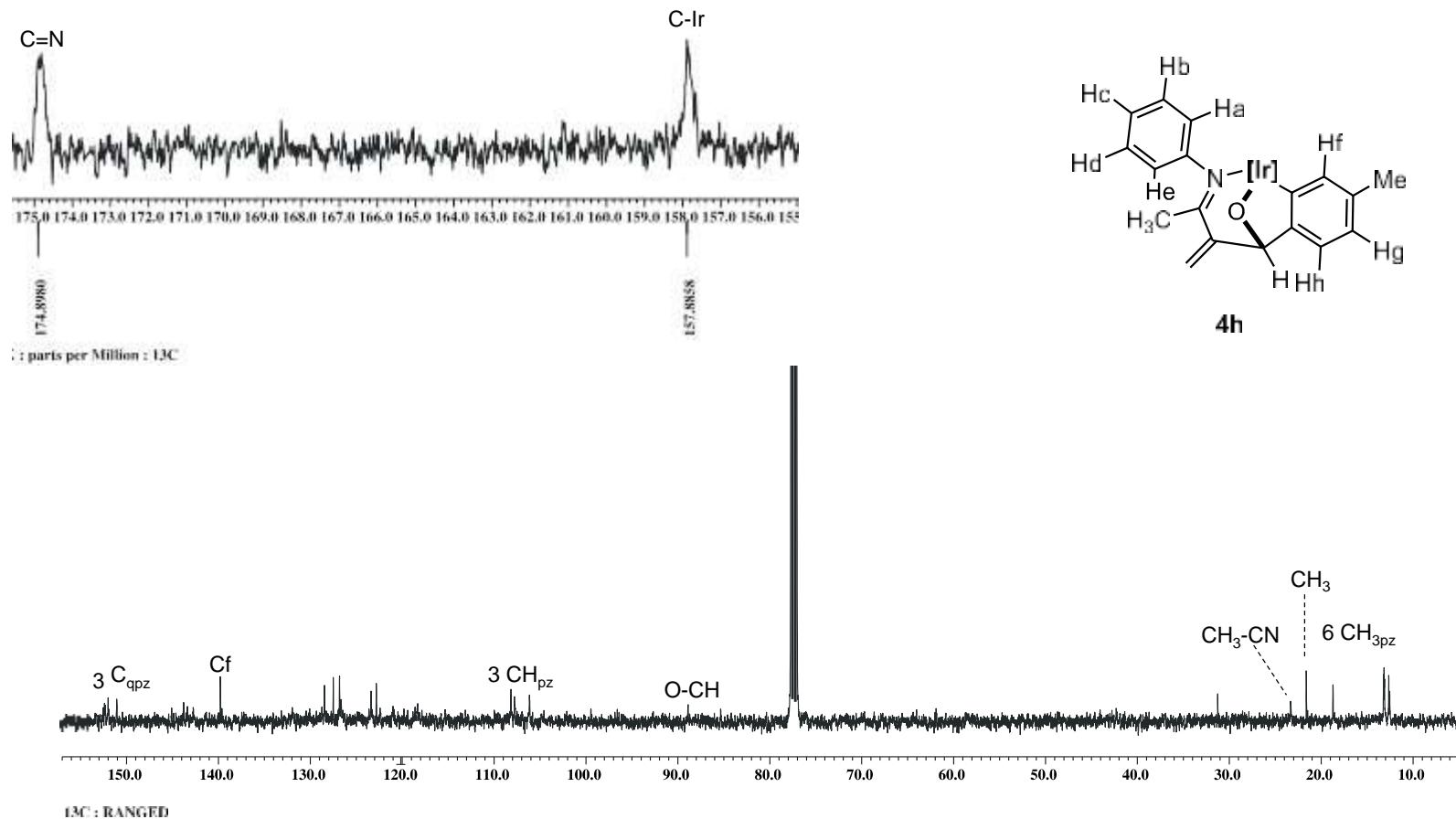


Figure S19. ^{13}C { ^1H } NMR (CDCl_3 , 25 °C, 100.6 MHz) spectrum of **4h**.

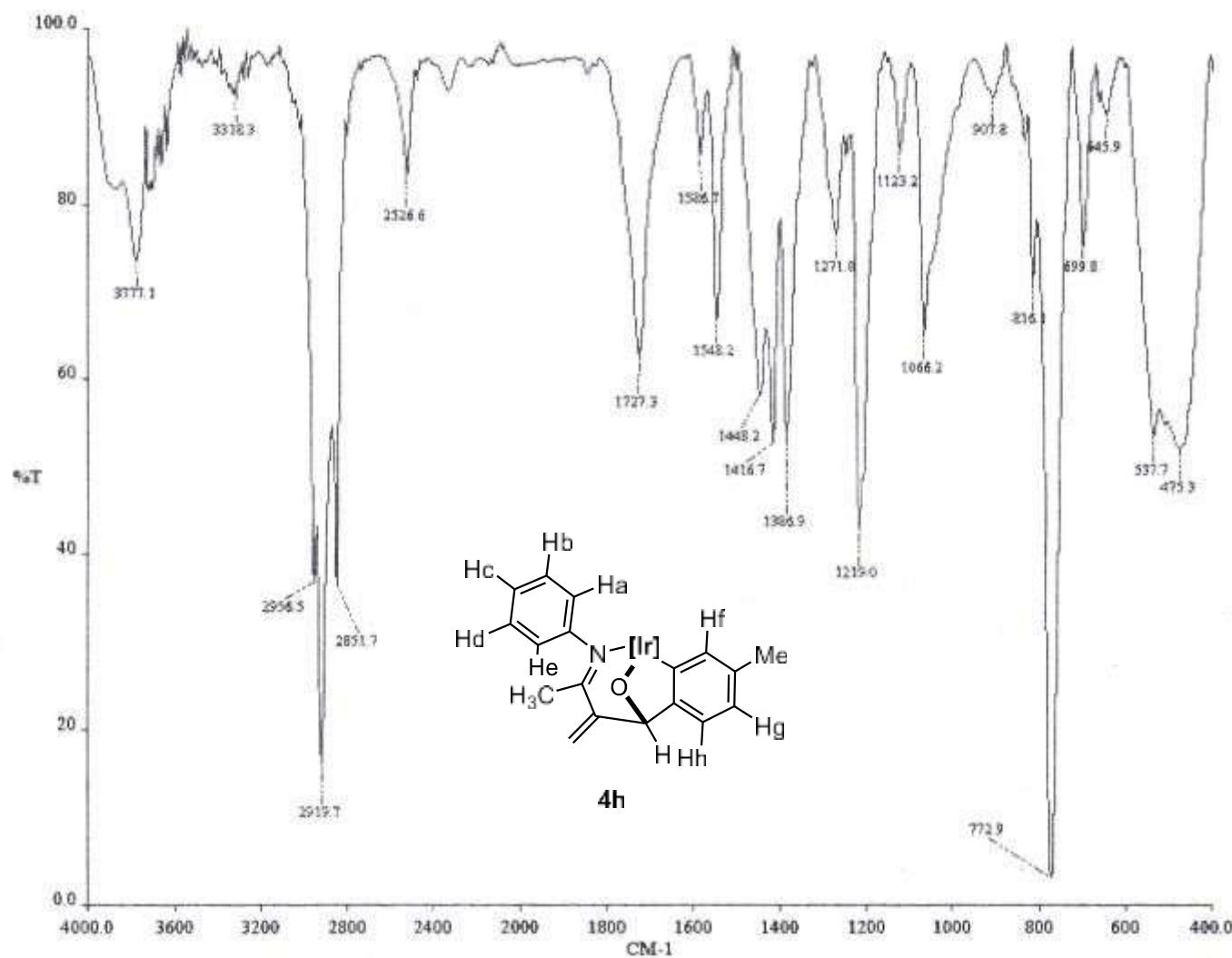


Figure S20. IR spectrum of **4h**.

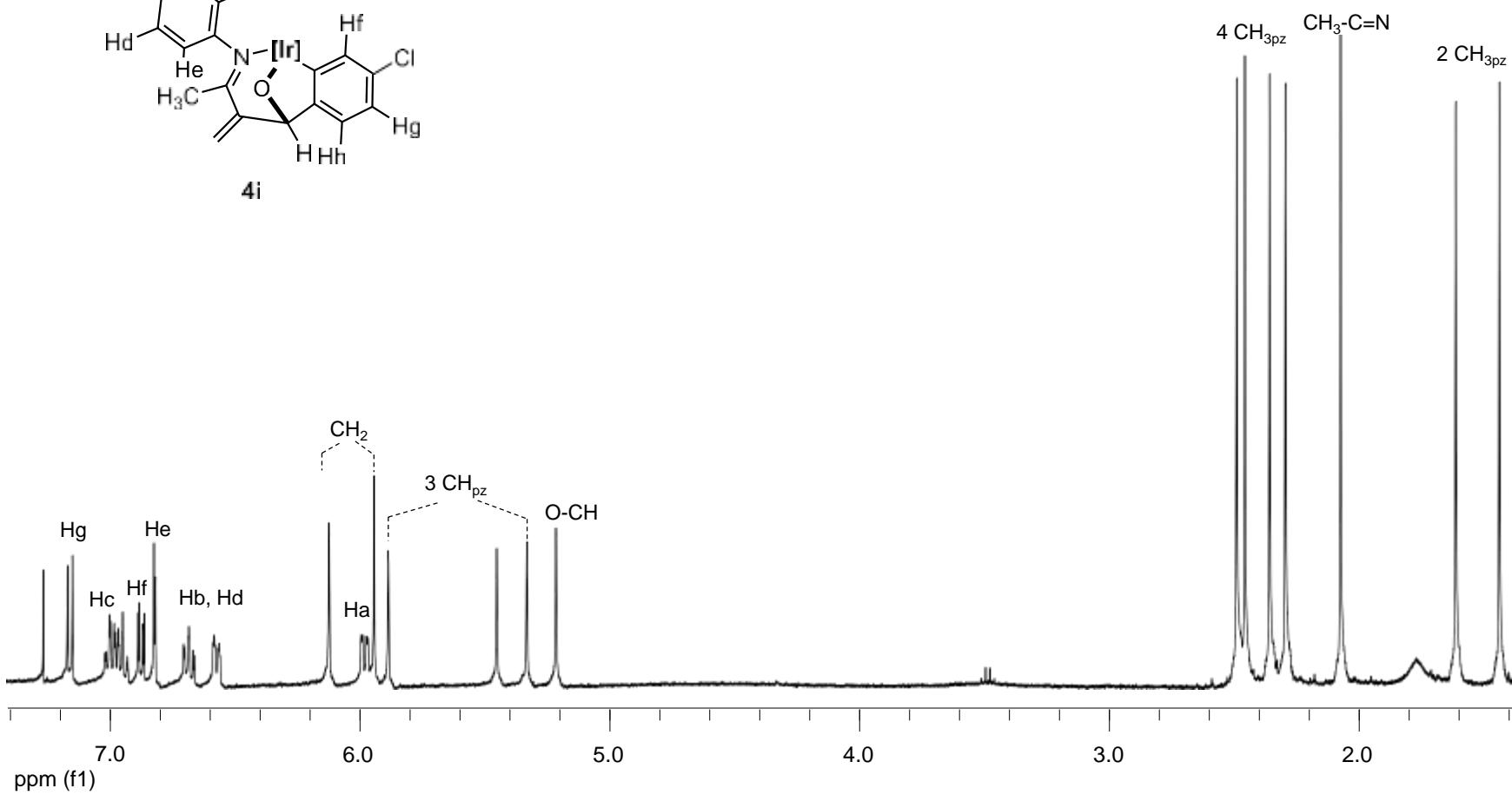
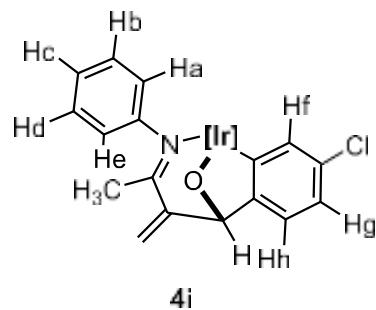


Figure S21. ^1H NMR (CDCl_3 , 25 °C, 400 MHz) spectrum of **4i**.

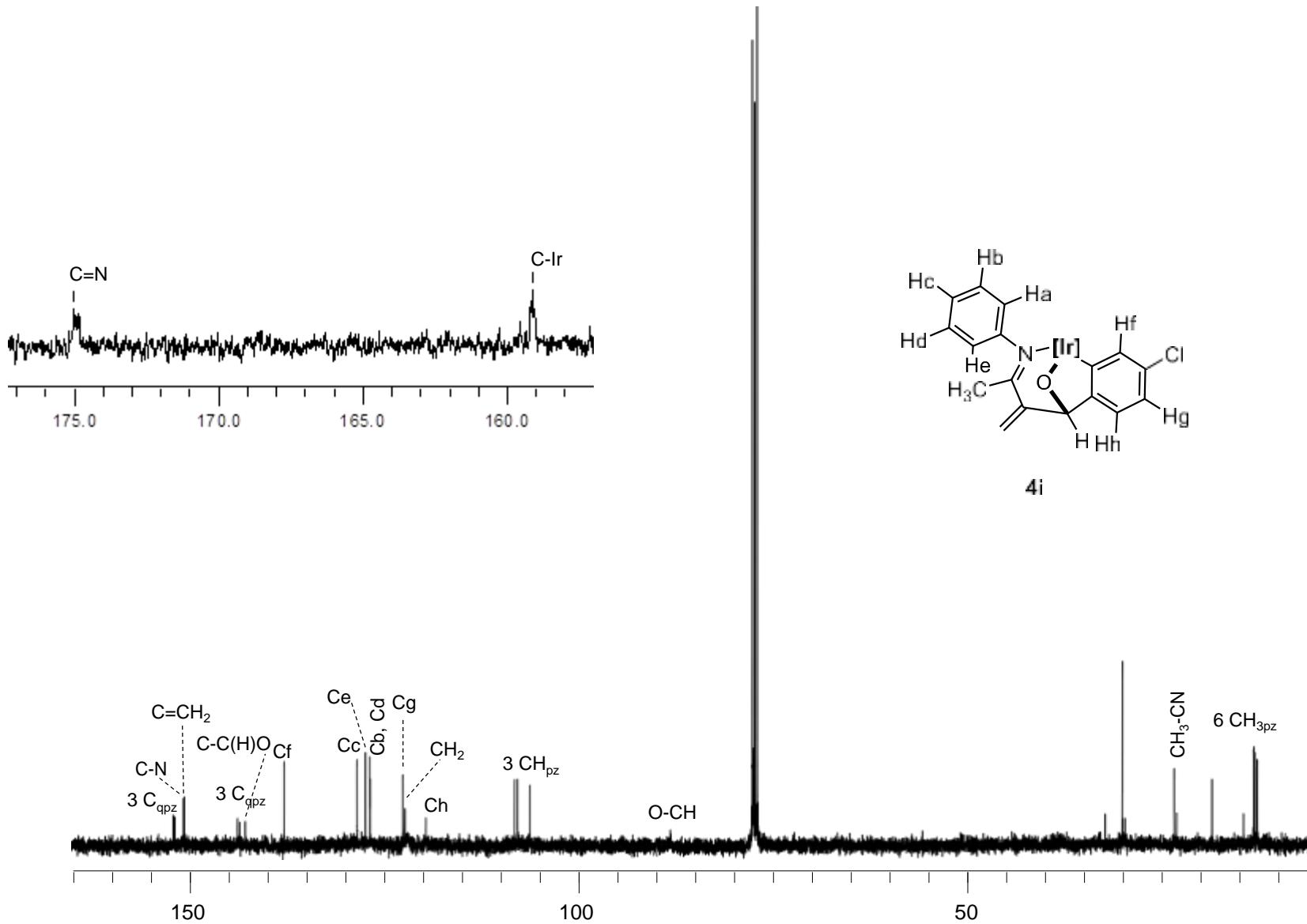


Figure S22. ^{13}C { ^1H } NMR (CDCl_3 , 25 °C, 100.6 MHz) spectrum of **4i**.

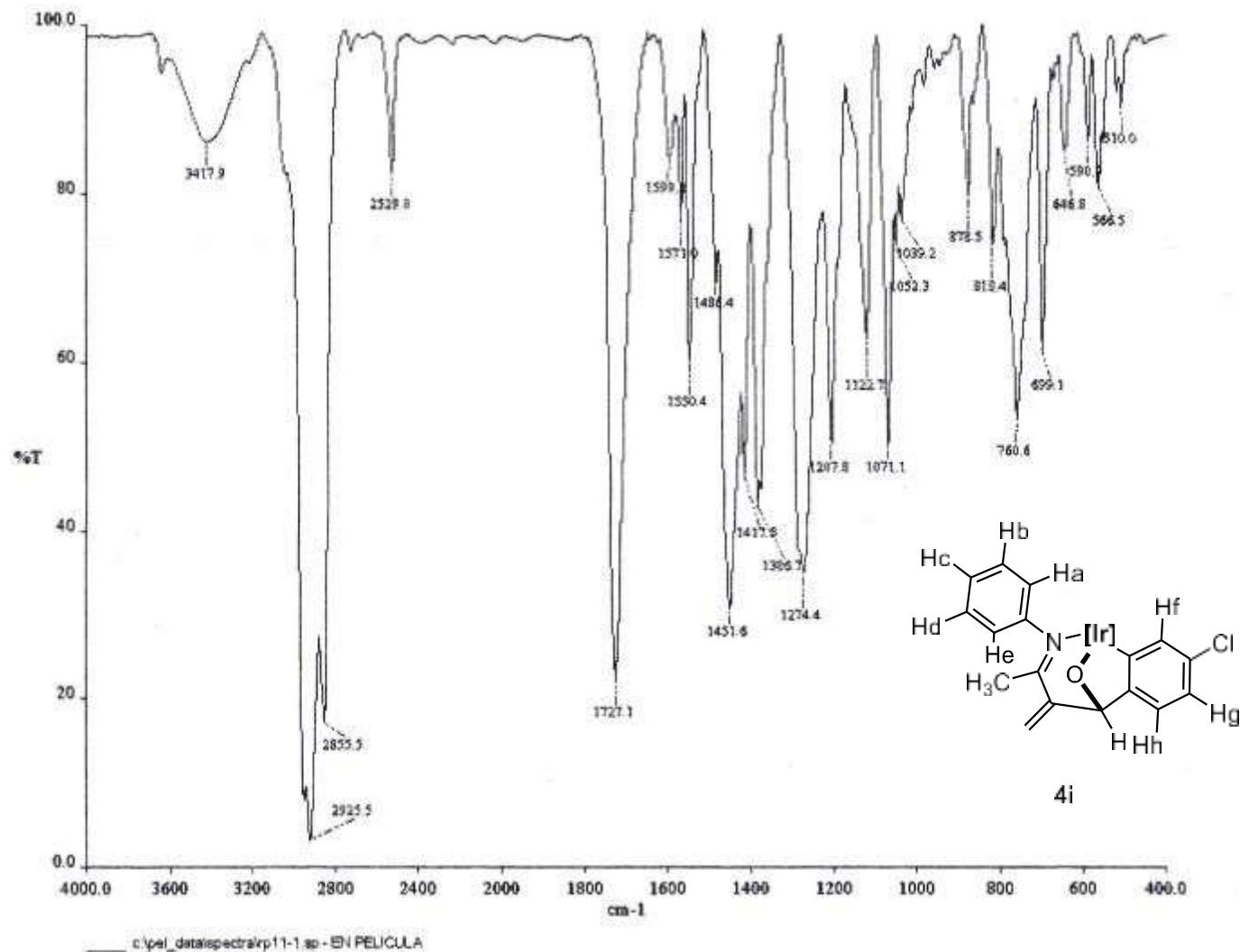
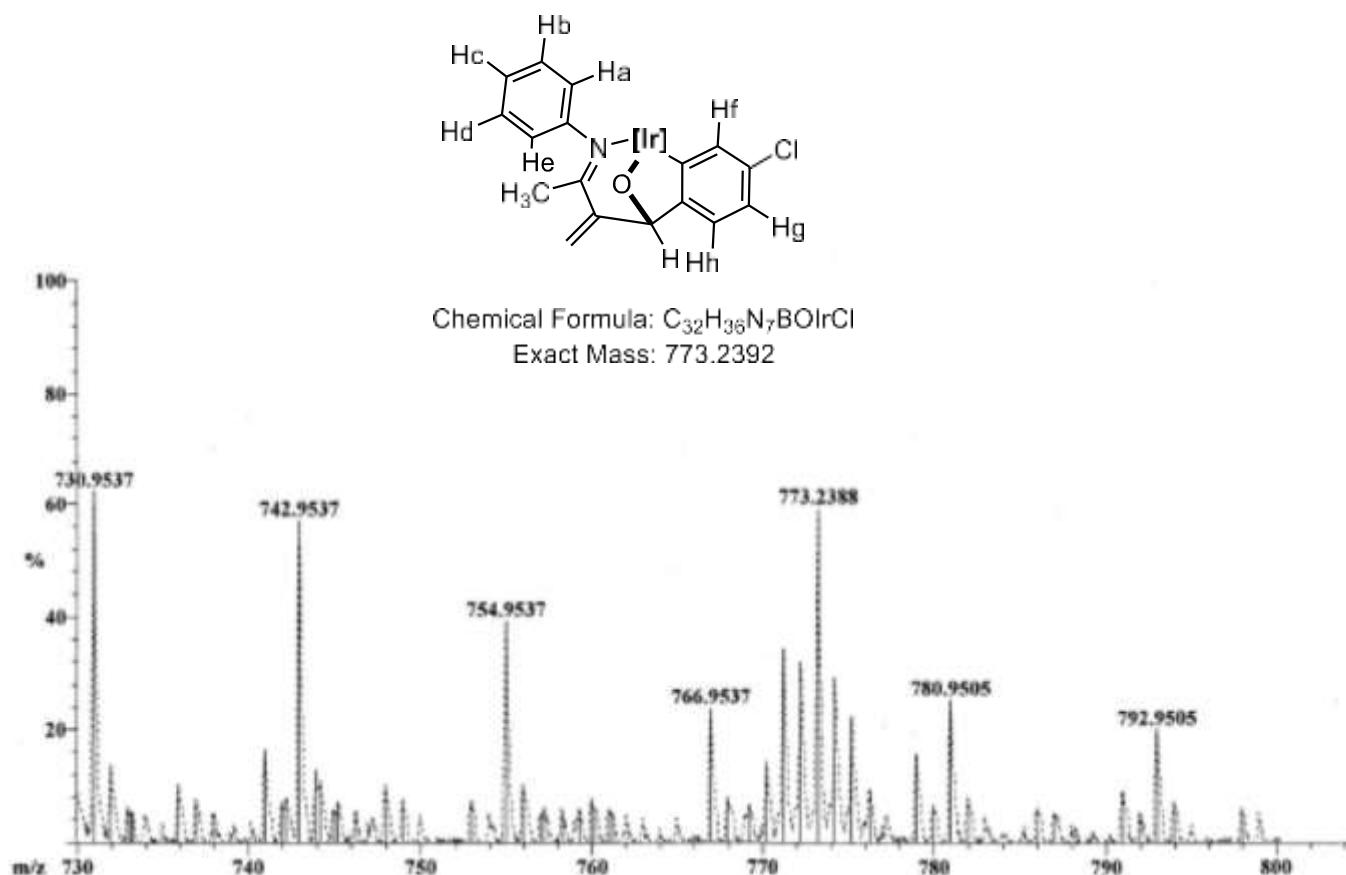


Figure S23. IR spectrum of **4i**.



MS Calcd: 773.2392 for $C_{32}H_{36}N_7BOIrCl$, observed: 773.2388

Figure S24. MS Spectra of complex 4i.

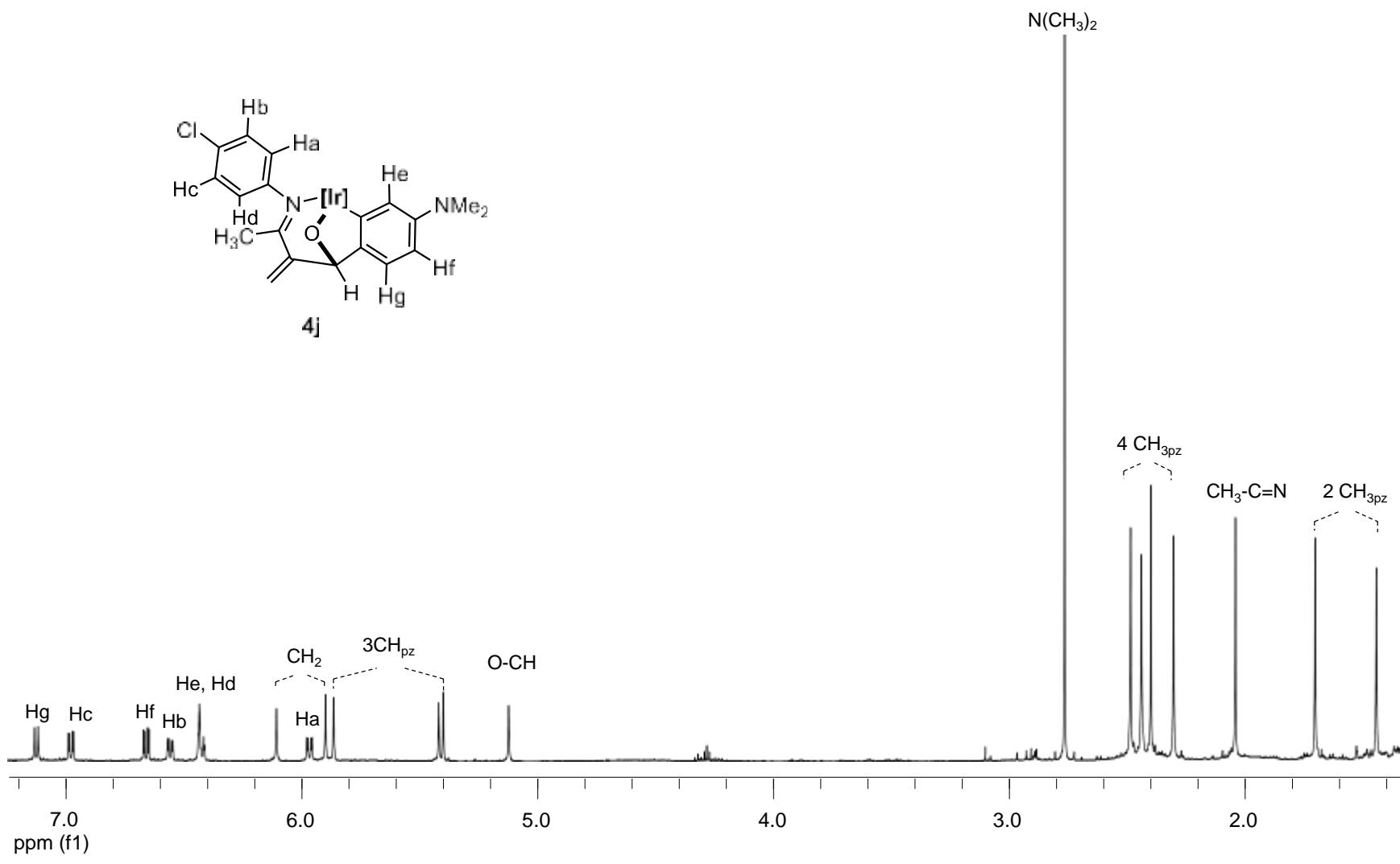


Figure S25. ^1H NMR (CDCl_3 , 25 °C, 400 MHz) spectrum of **4j**.

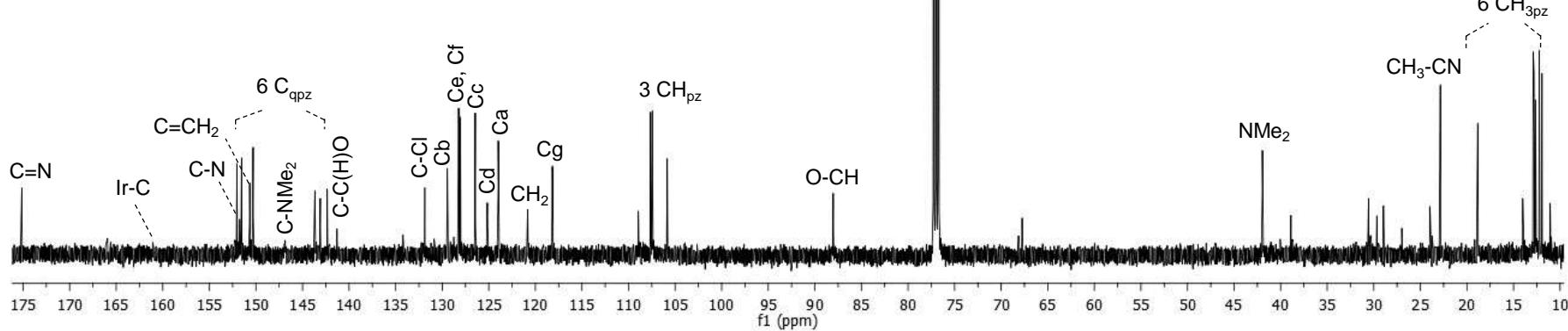
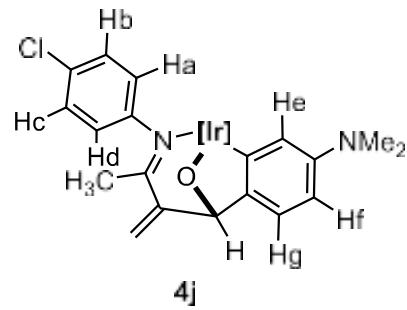


Figure S26. ^{13}C $\{^1\text{H}\}$ NMR (CDCl_3 , 25°C , 100.6 MHz) spectrum of **4j**.

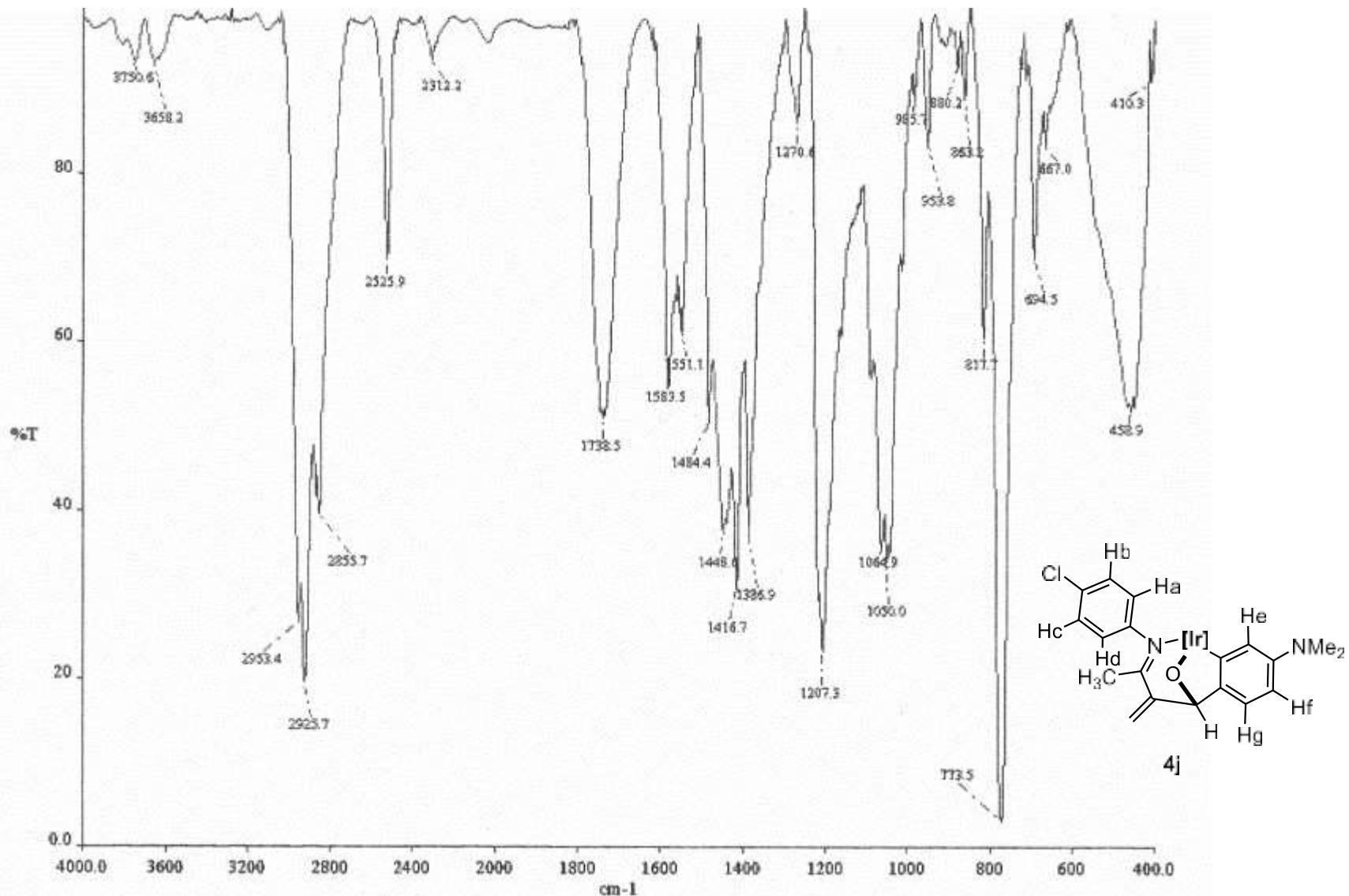
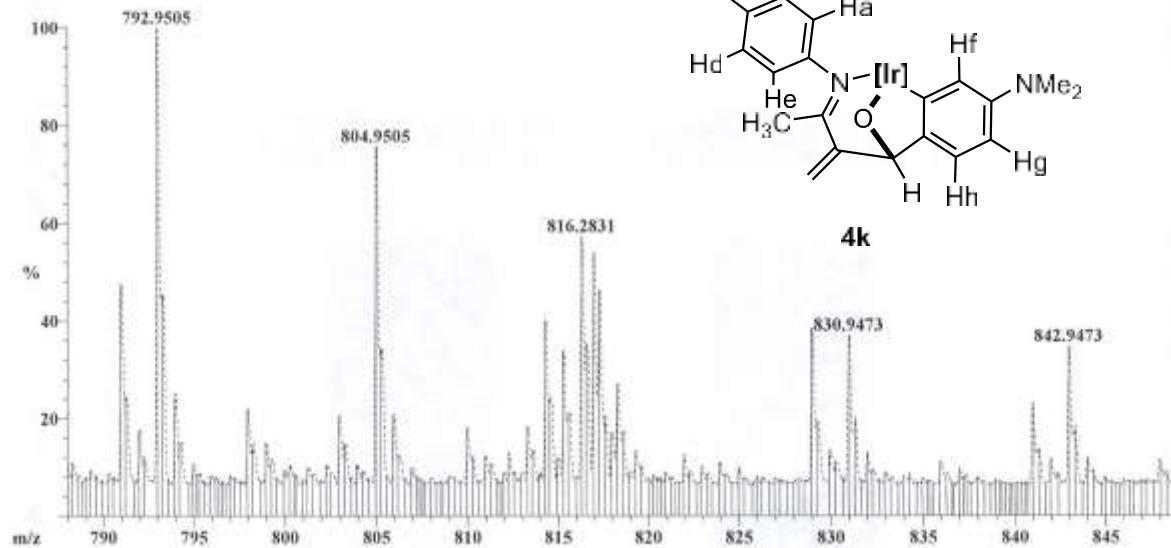


Figure S27. IR spectrum of **4j**.

Instrument: JEOL GCmate
Inlet: Direct Probe

Ionization mode: EI+

Scan: 40-43
Base: m/z 793; .4%FS TIC: 102680



MS Calcd: 816.2814 for $C_{34}H_{41}N_8BOClIr$, observed: 816.2831.

Figure S28. ESI-MS Spectra of complex **4j**.

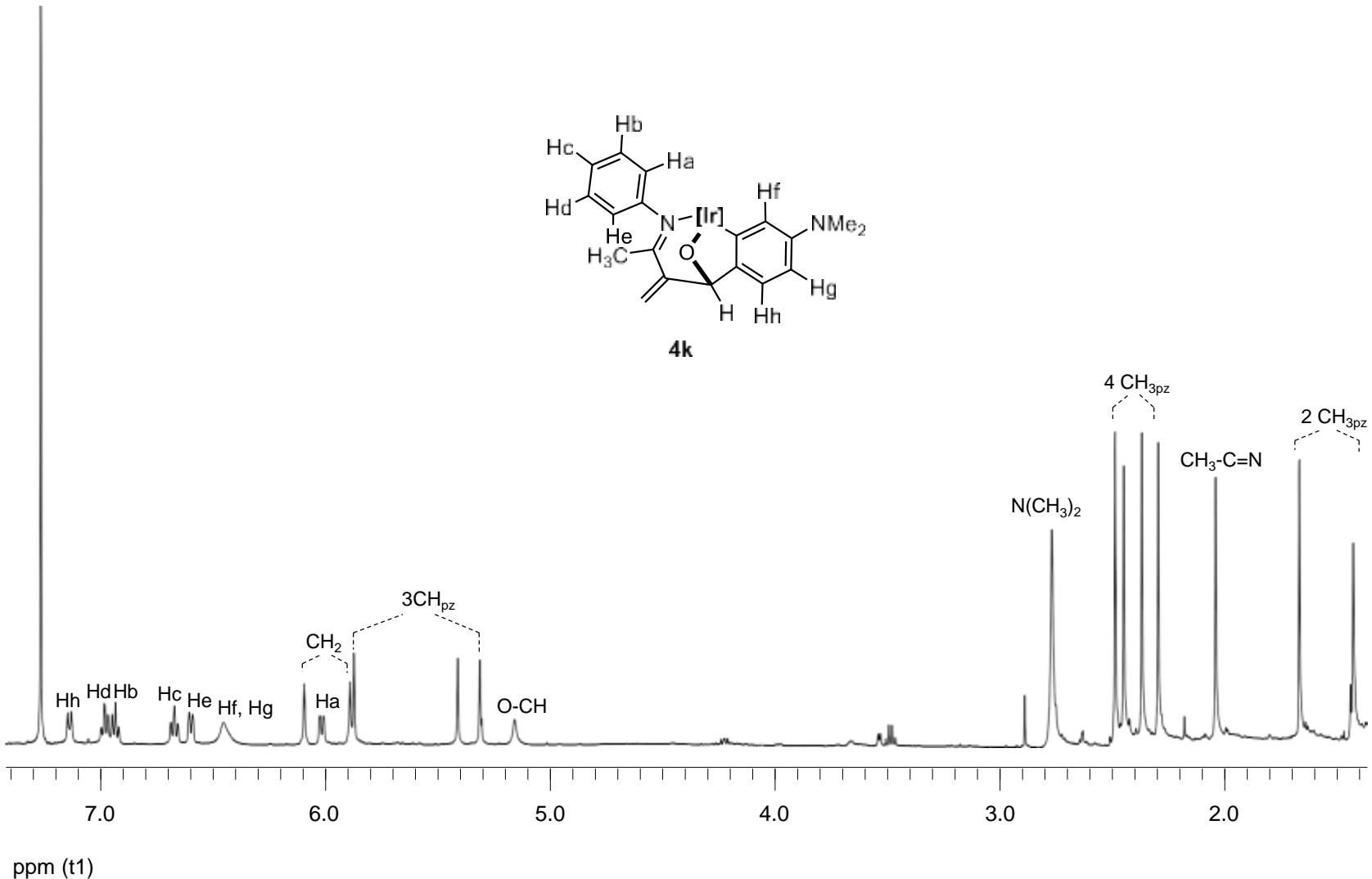


Figure S29. ^1H NMR (CDCl_3 , 25 °C, 500 MHz) spectrum of **4k**.

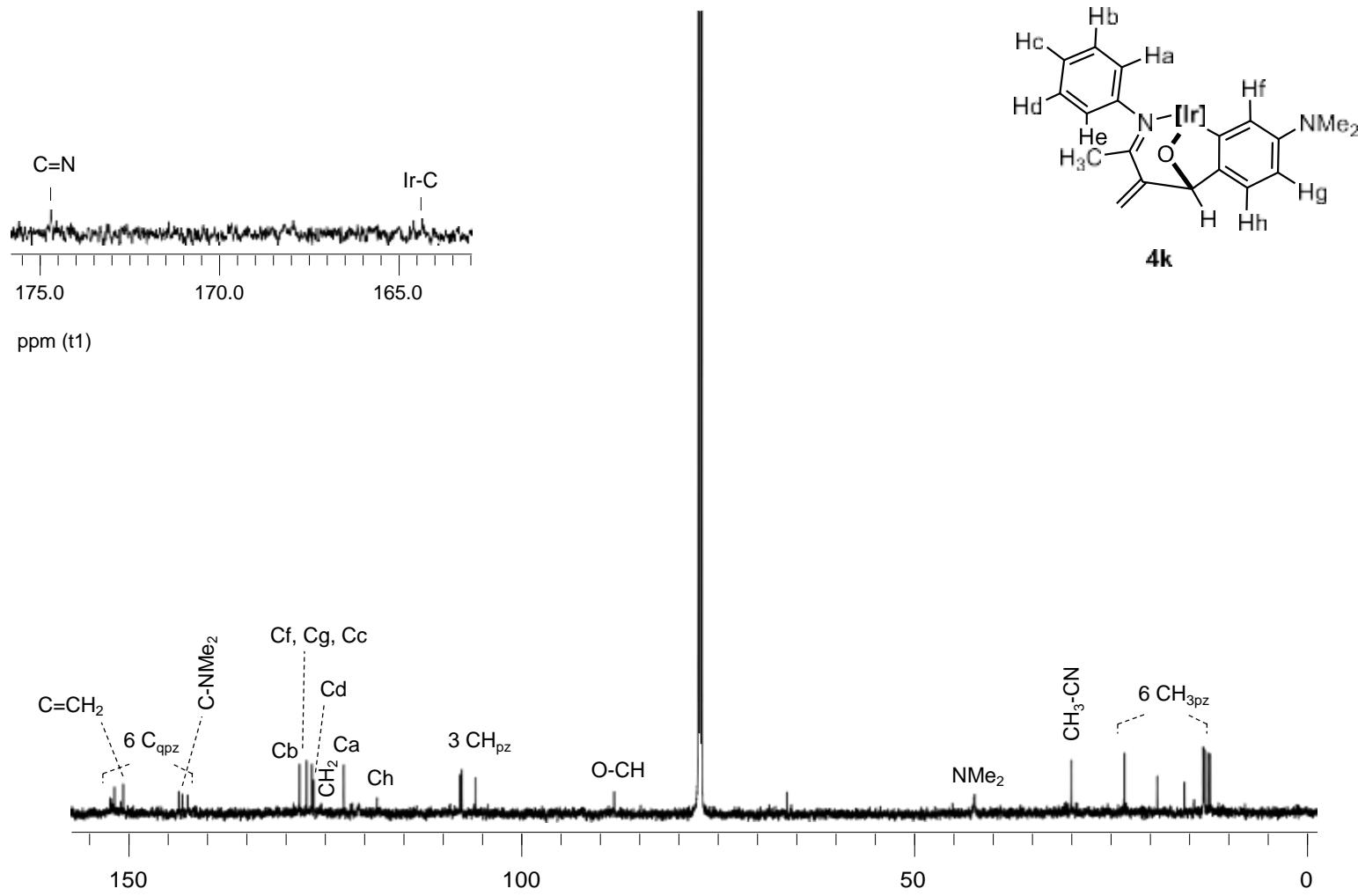


Figure S30. ^{13}C { ^1H } NMR (CDCl_3 , 25 °C, 125 MHz) spectrum of **4k**.

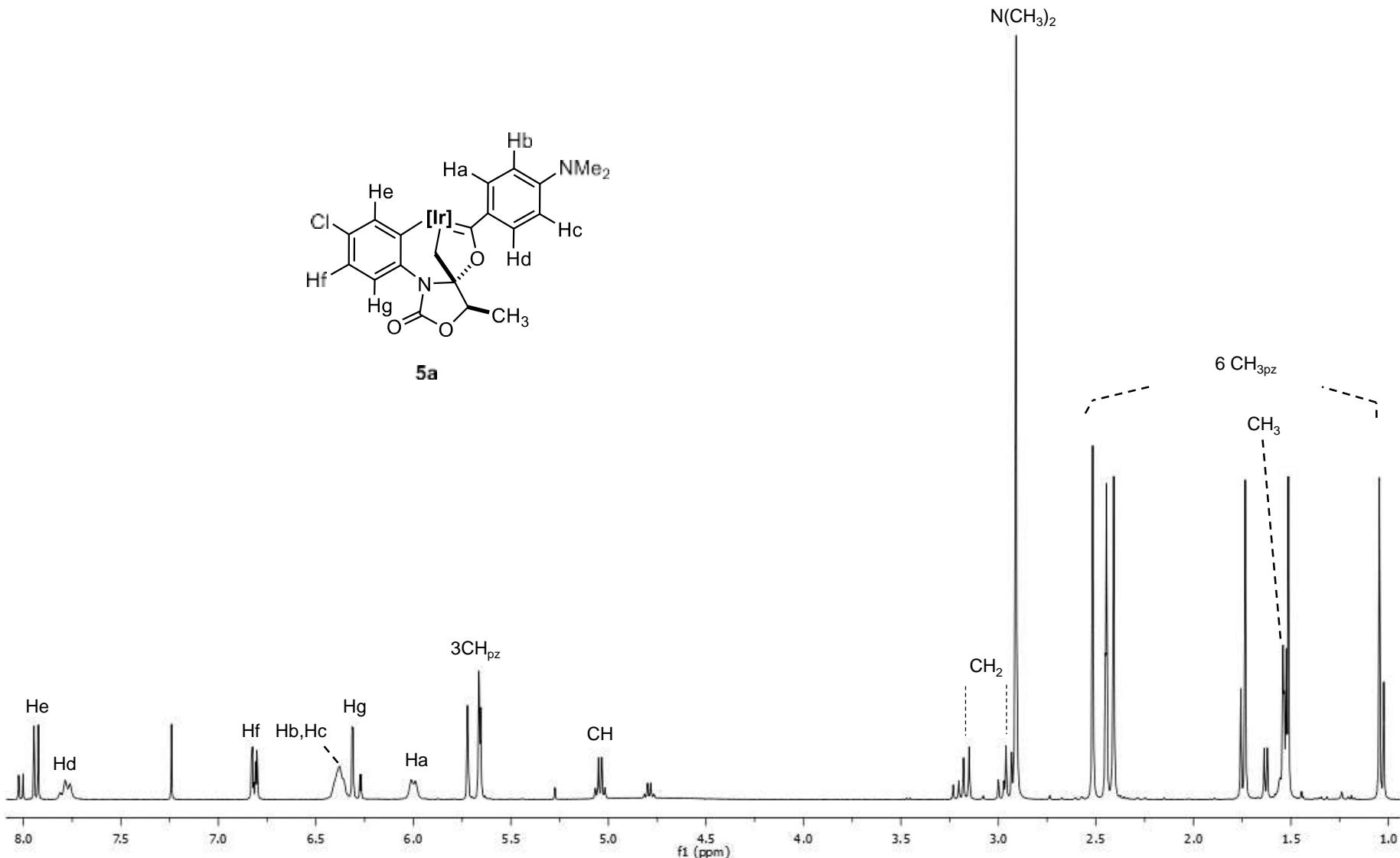
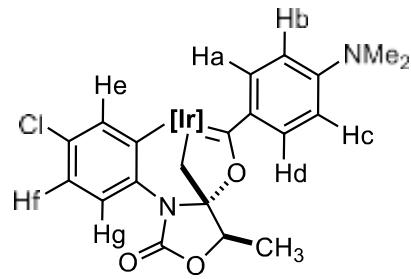


Figure S31. ^1H NMR (CDCl_3 , 25 °C, 400 MHz) spectrum of **5a**.

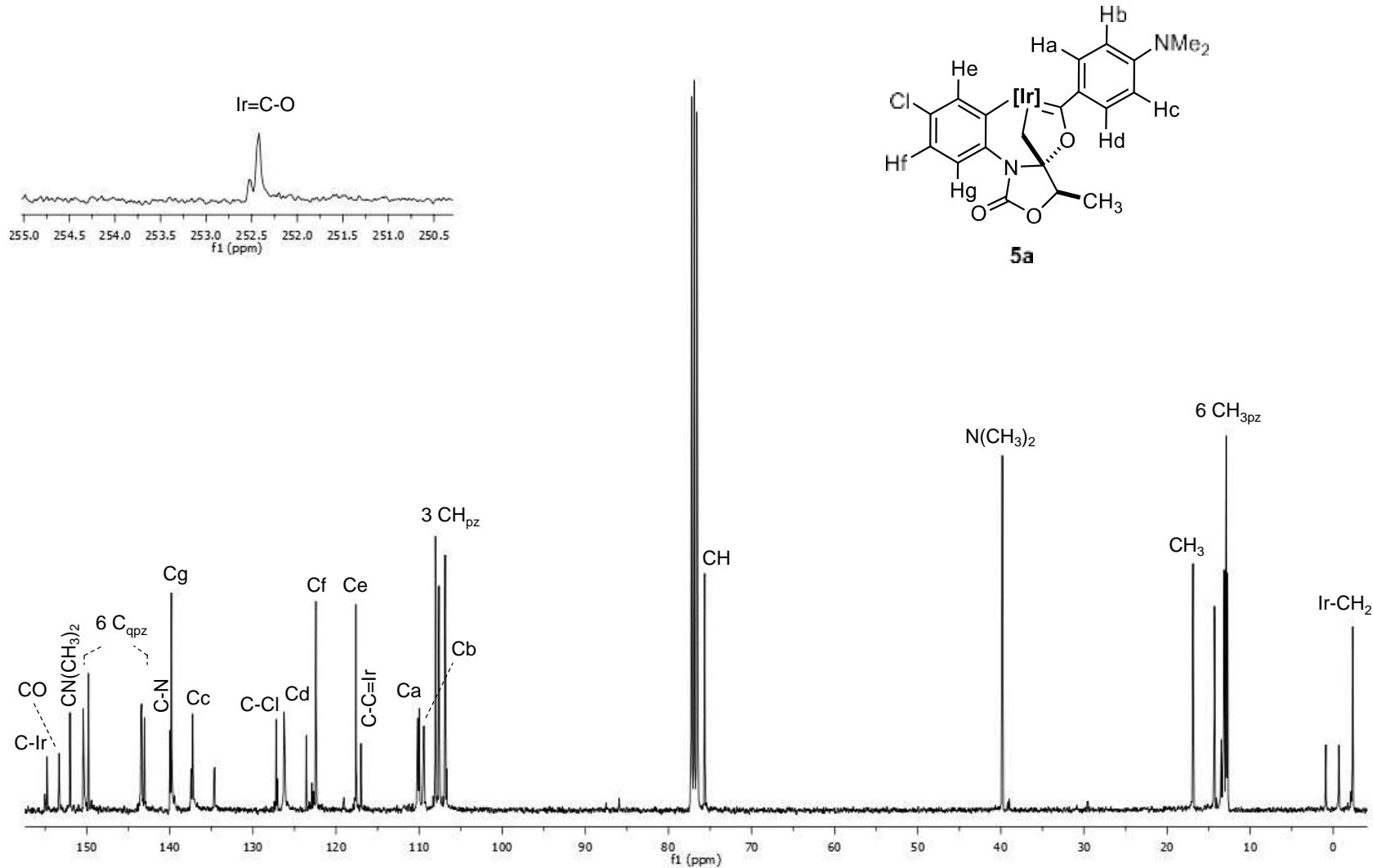


Figure S32. ^{13}C $\{\text{H}\}$ NMR (CDCl_3 , 25°C , 100.6 MHz) spectrum of **5a**.

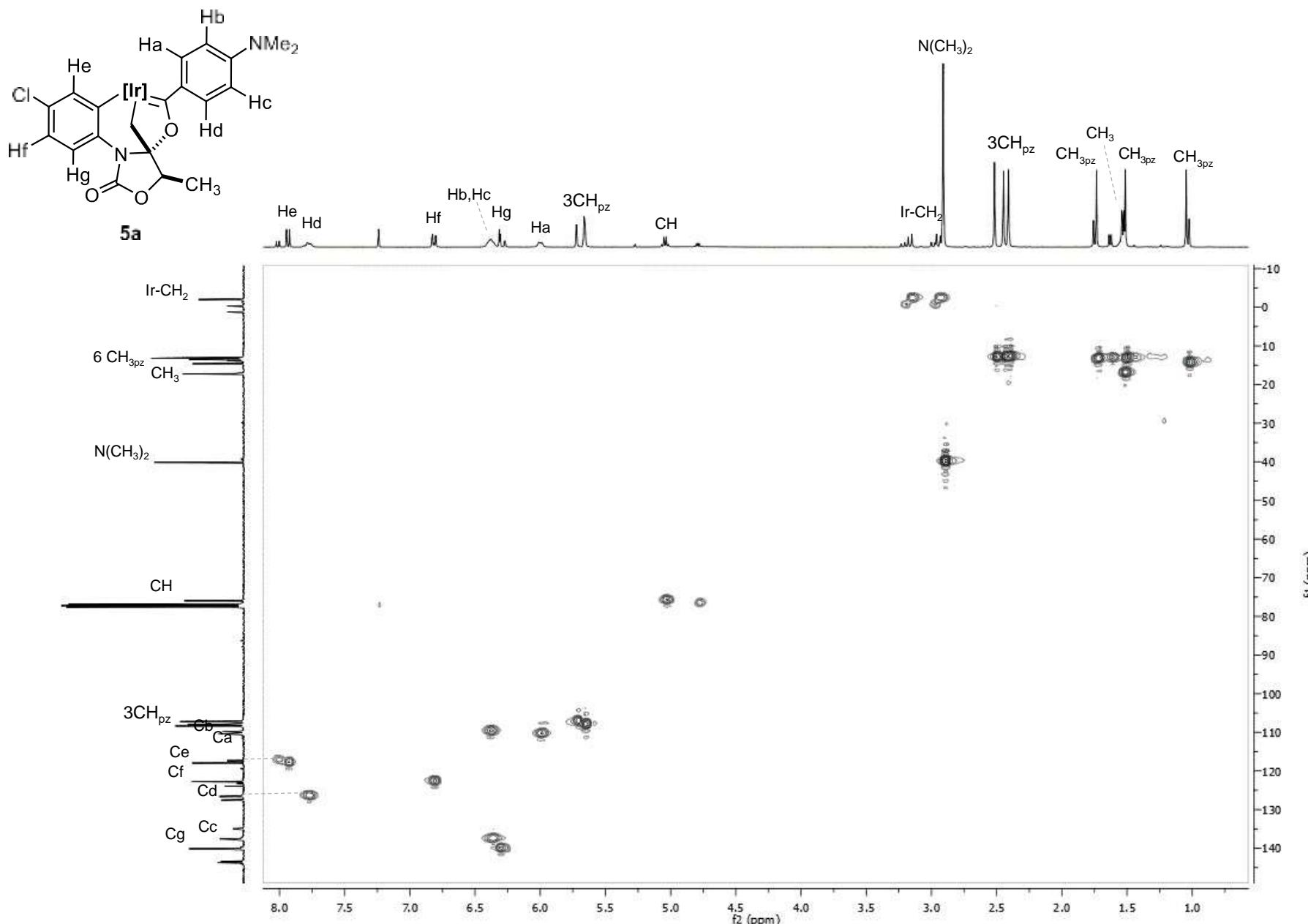


Figure S33. HMQC diagram of **5a**.

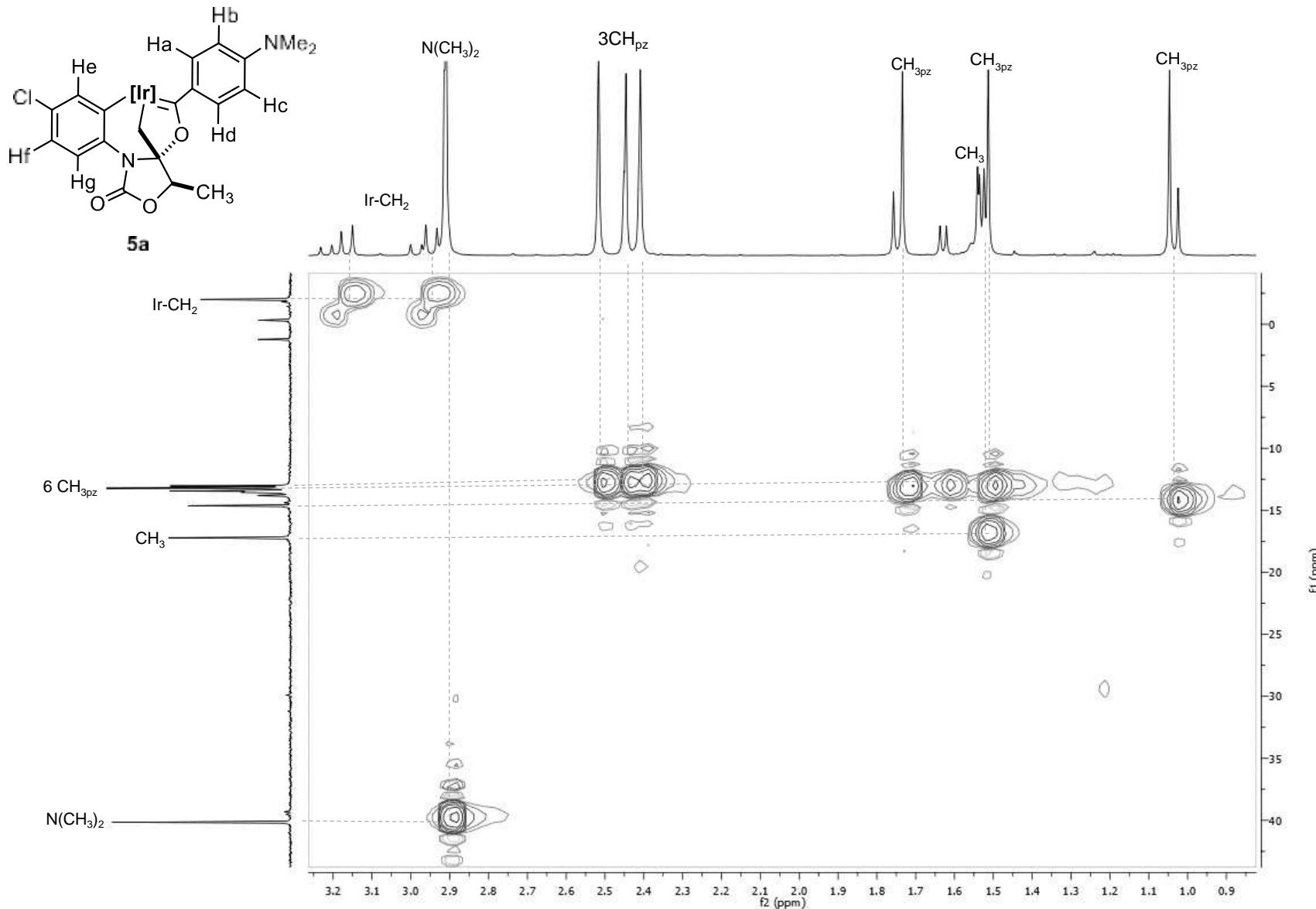


Figure S34. HMQC diagram of **5a**.

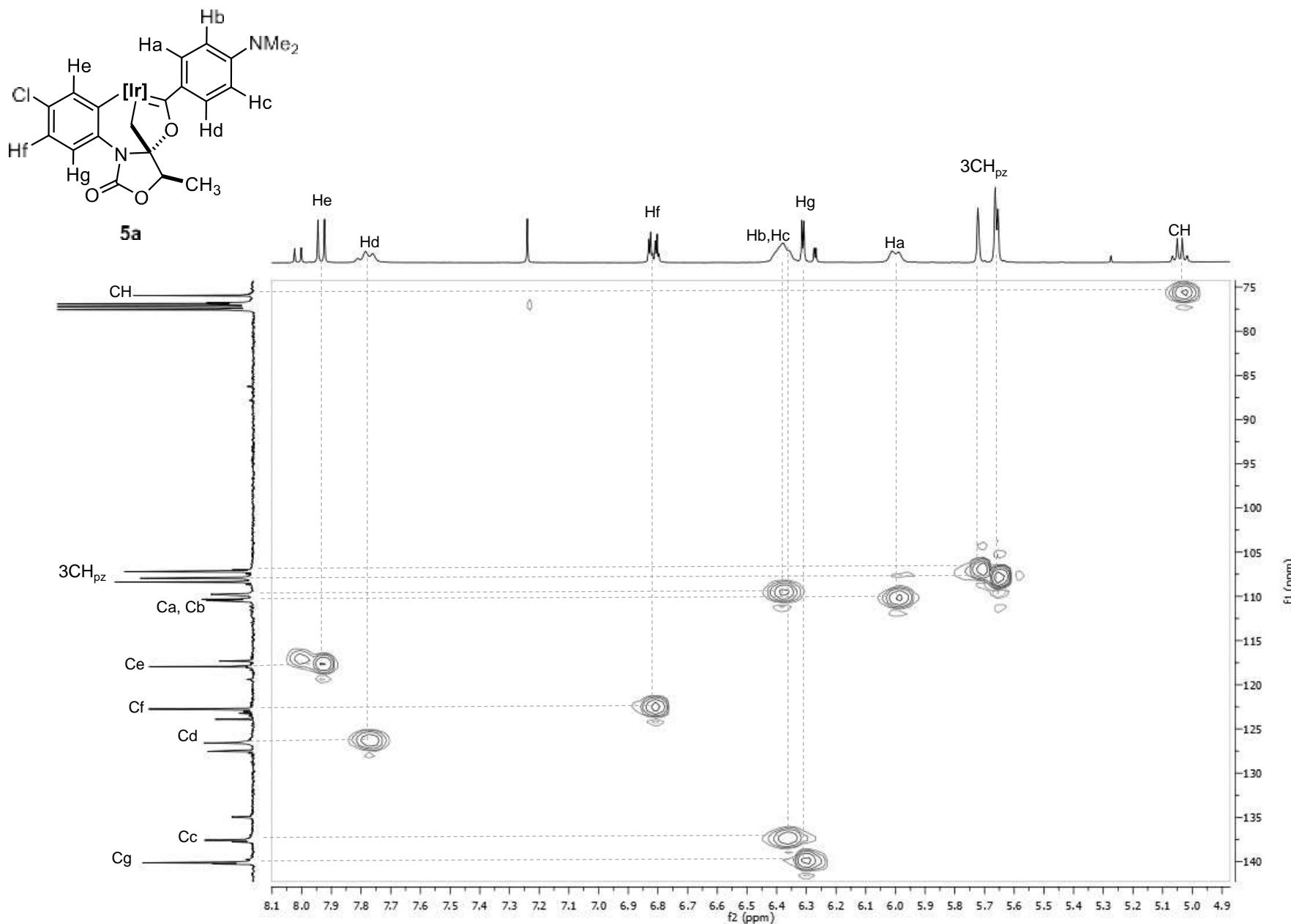


Figure S35. HMQC diagram of **5a**.

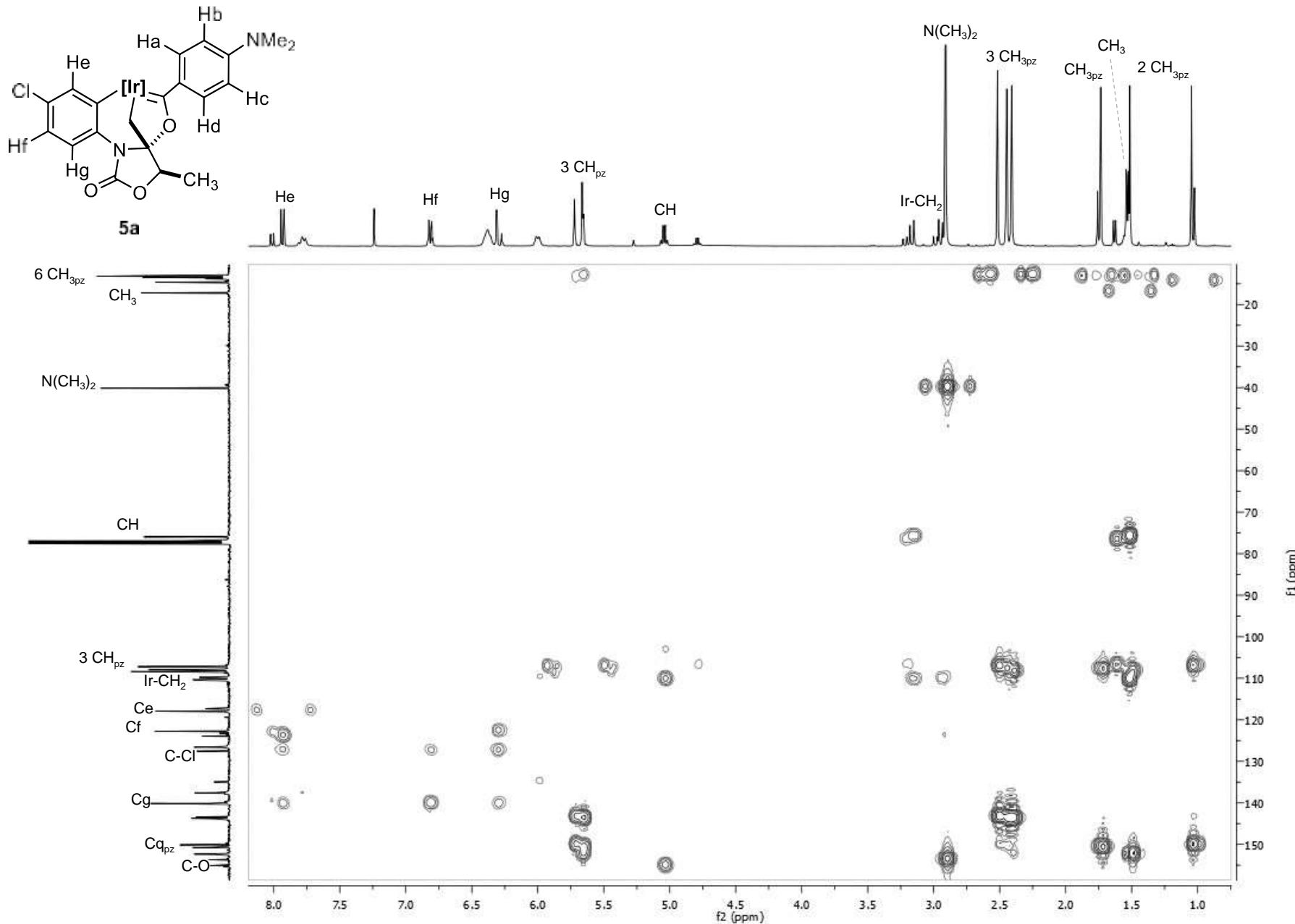


Figure S36. HMBC diagram of **5a**.

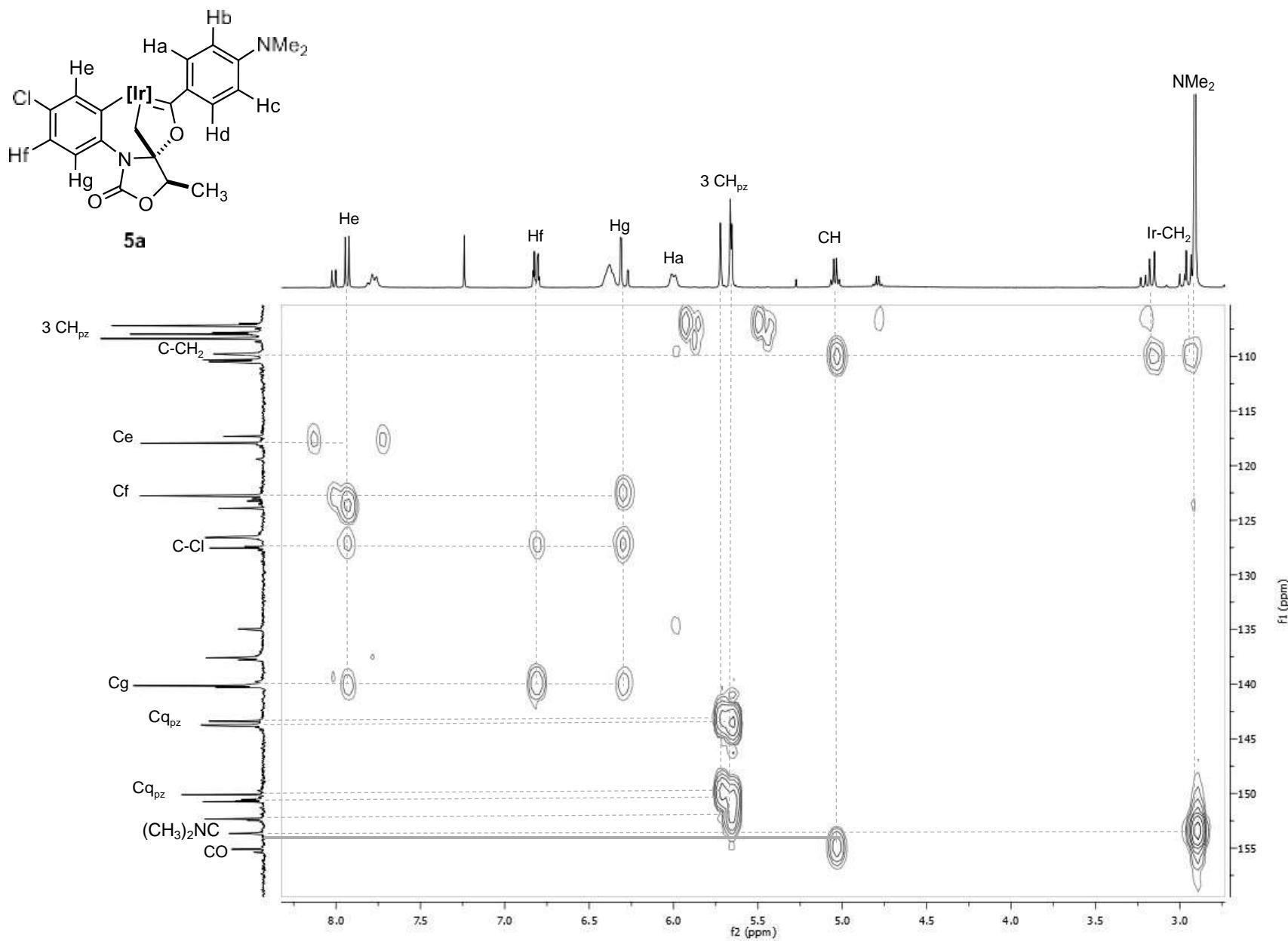


Figure S37. HMBC diagram of **5a**.

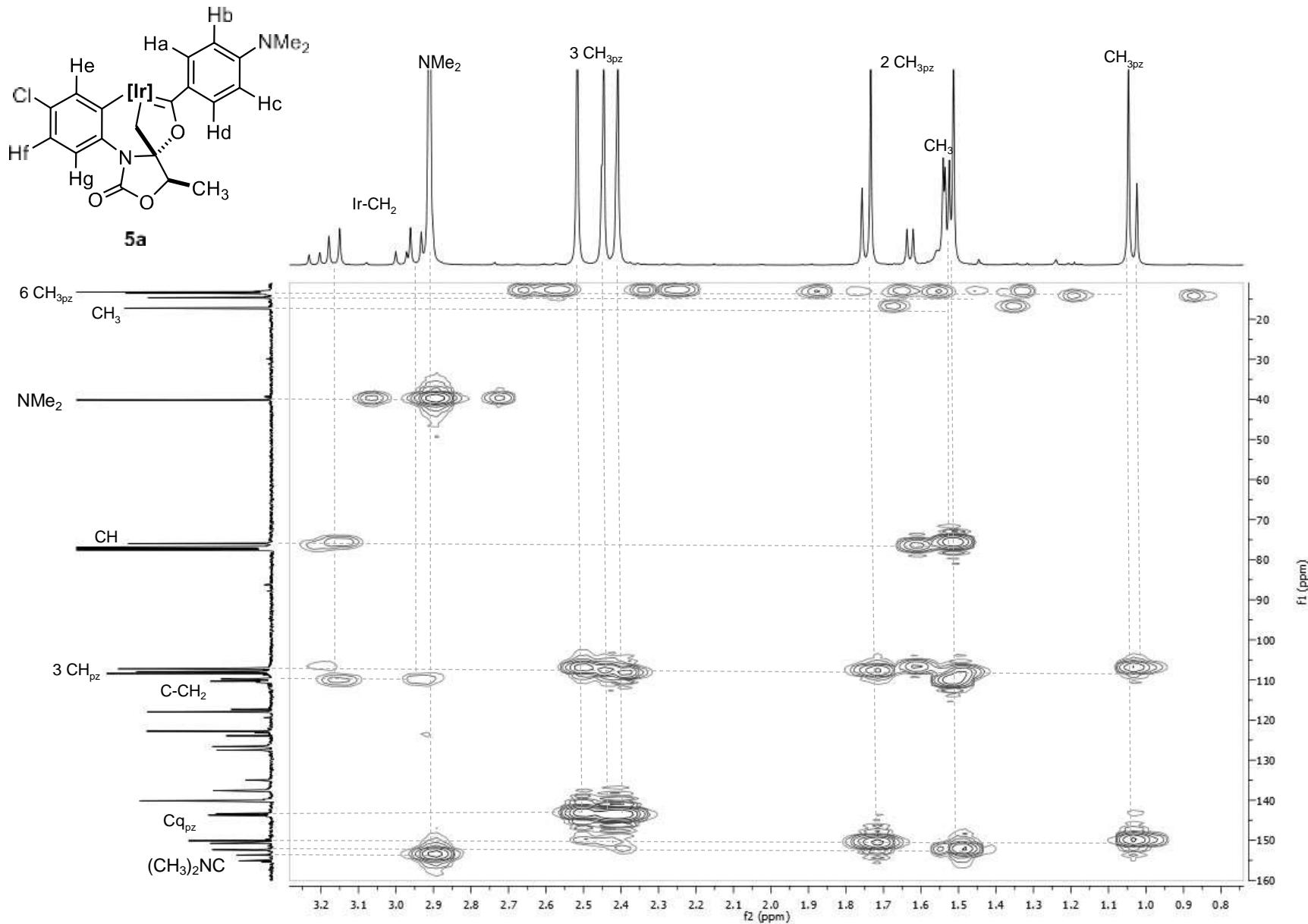


Figure S38. HMBC diagram of **5a**.

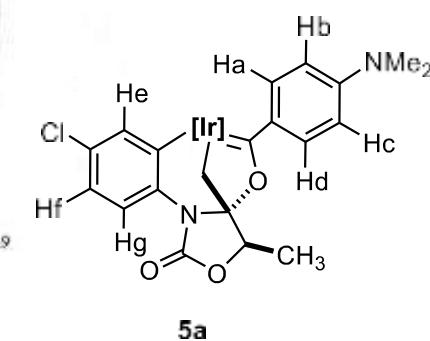
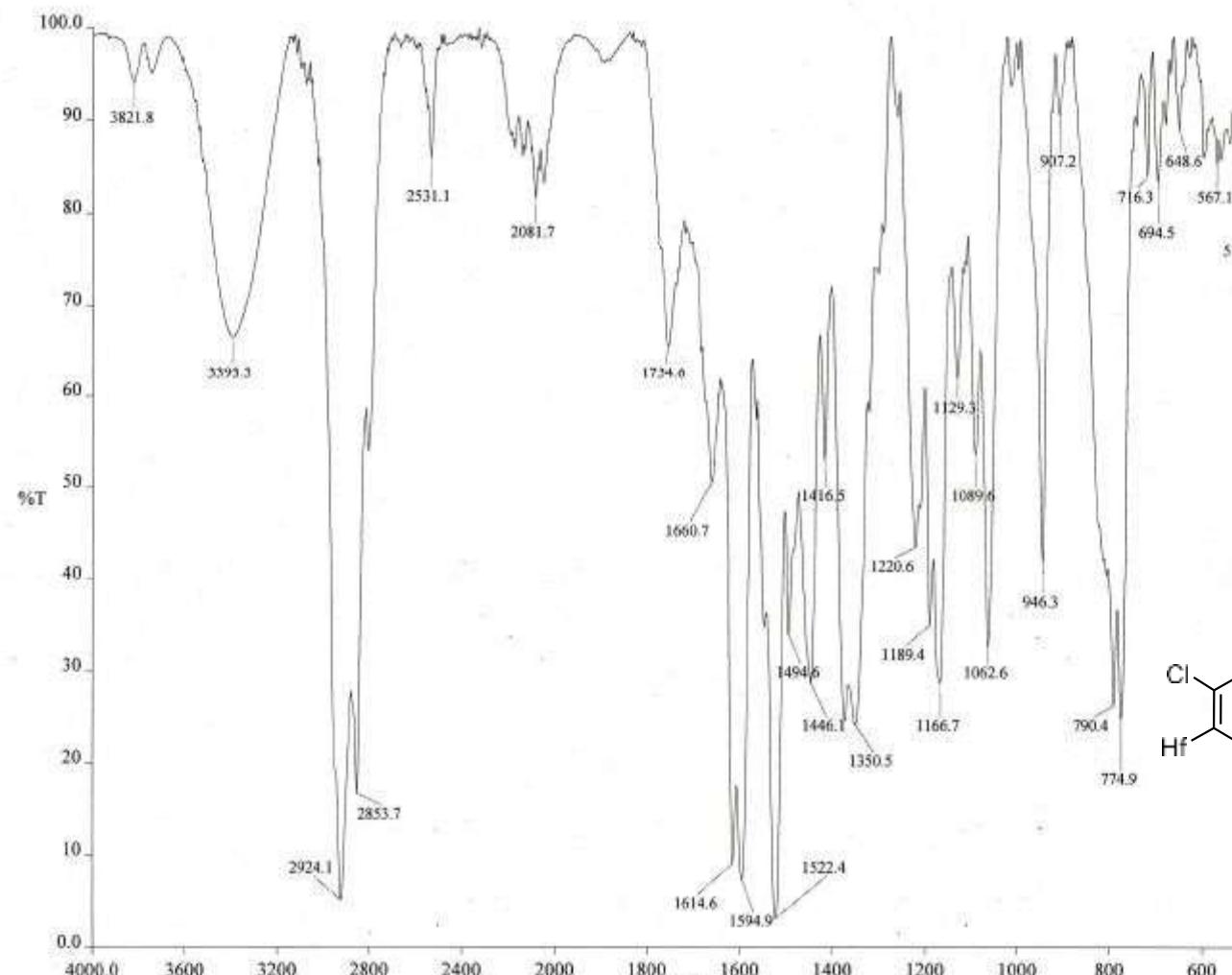


Figure S39. IR spectrum of **5a**.

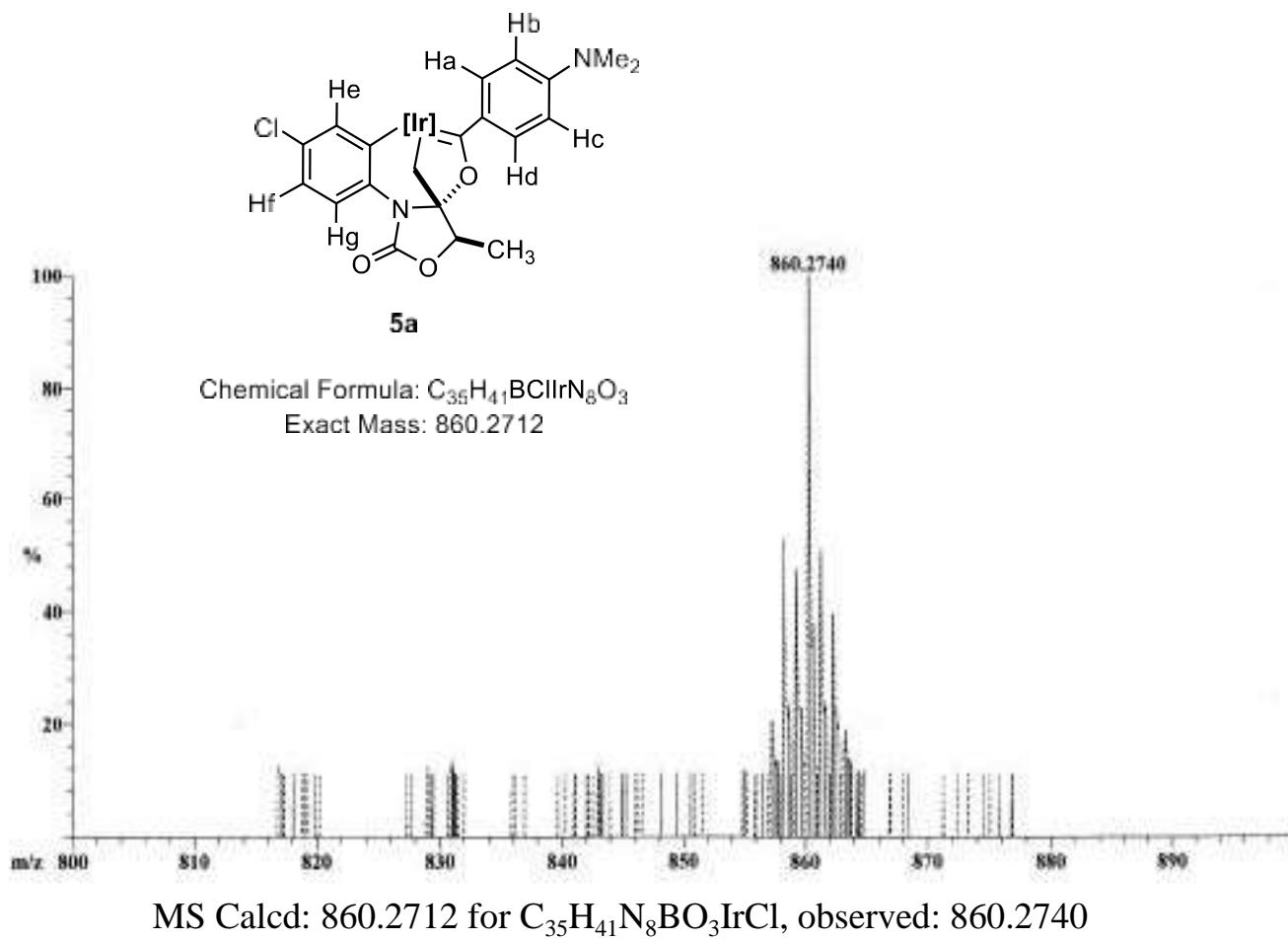


Figure S40. MS Spectra of complex **5a**.

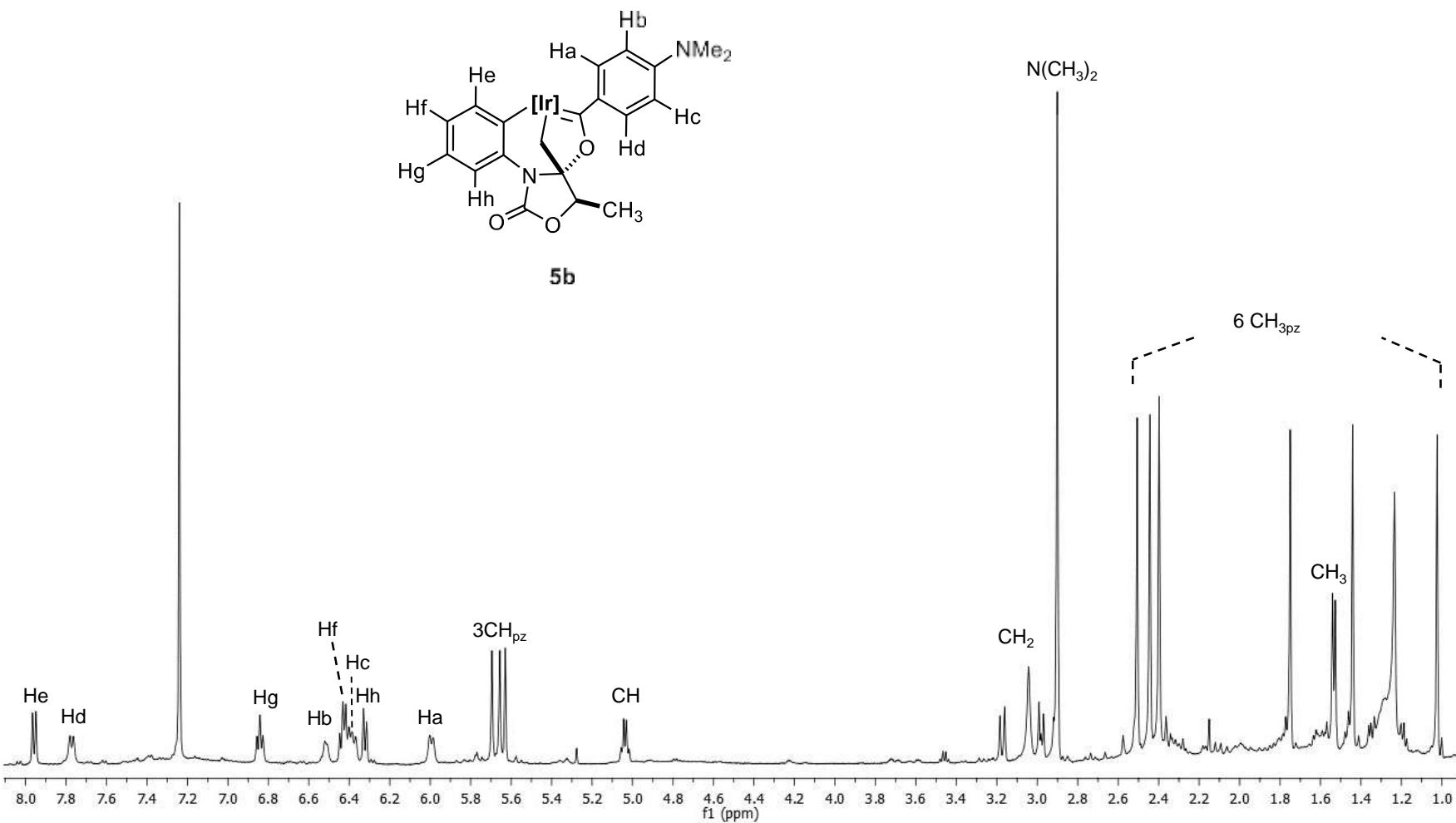


Figure S41. ^1H NMR (CDCl_3 , 25°C , 500 MHz) spectrum of **5b**.

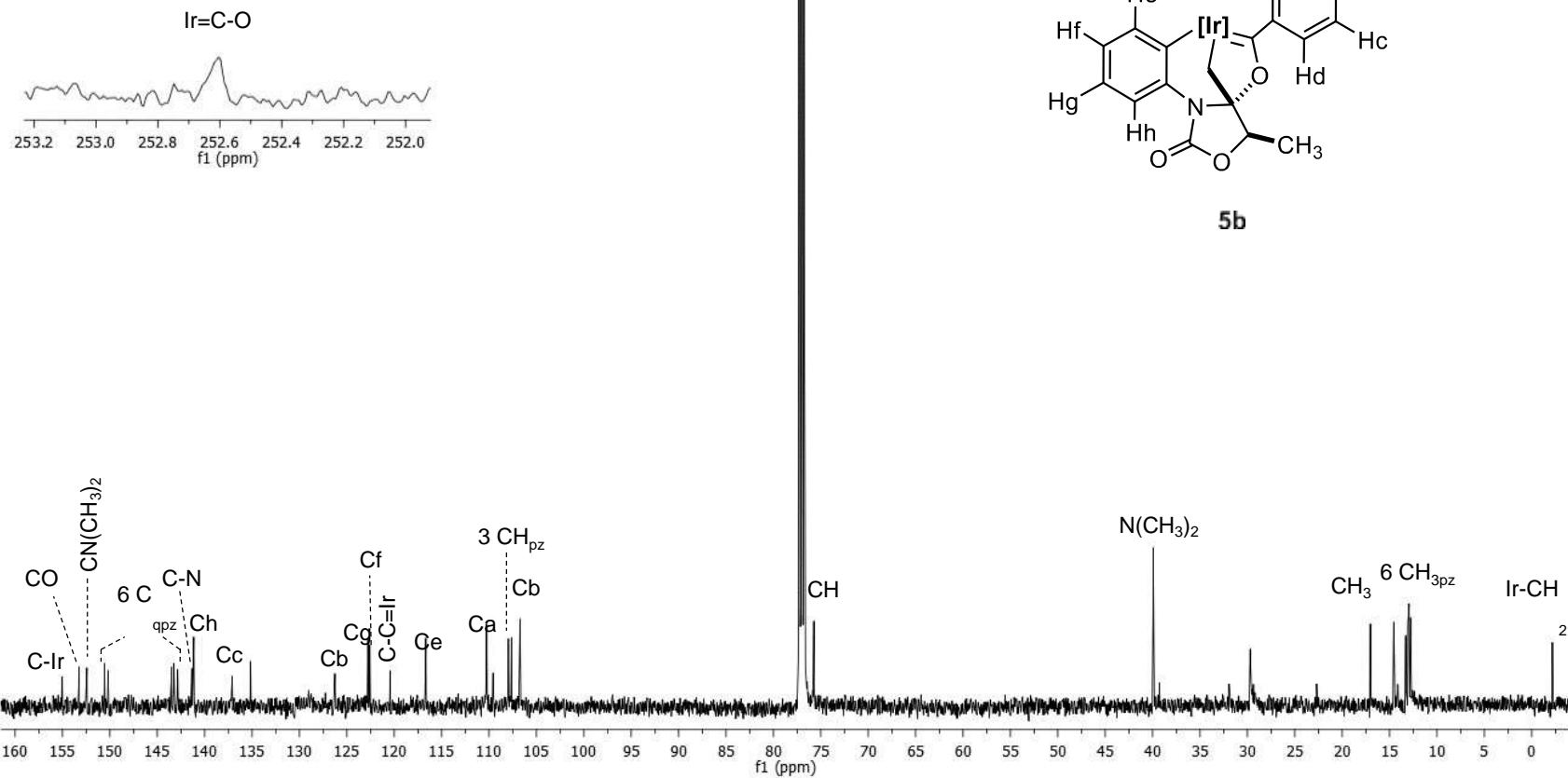


Figure S42. ^{13}C { ^1H } NMR (CDCl_3 , 25 °C, 125 MHz) spectrum of **5b**.

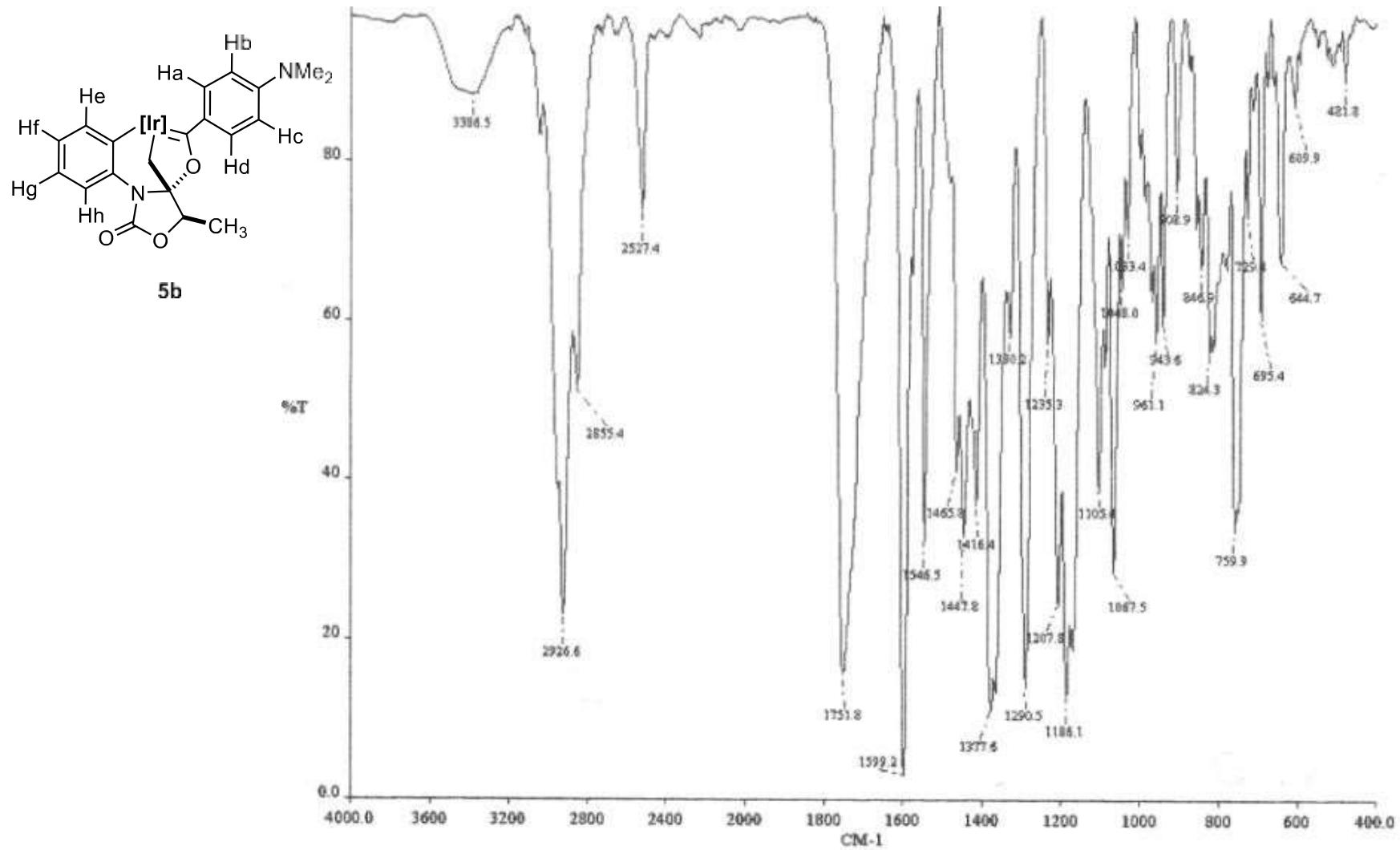
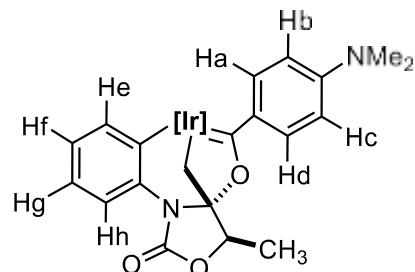
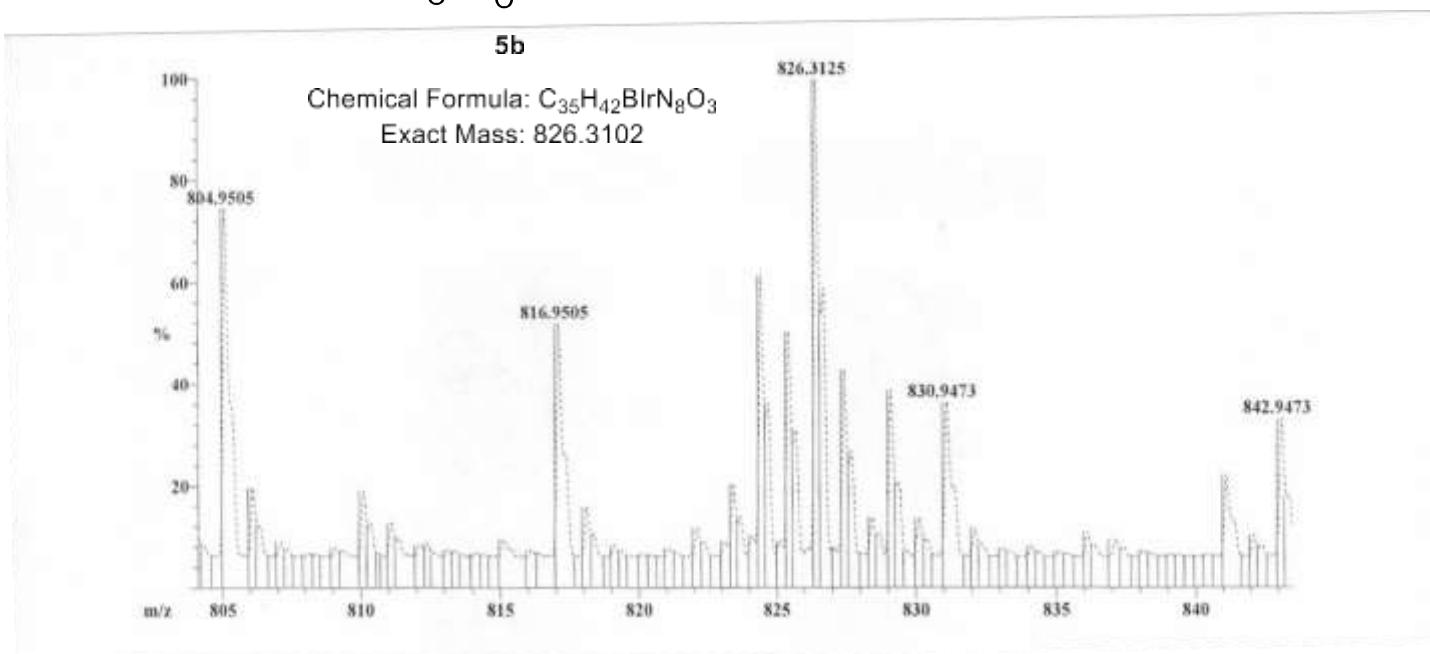


Figure S43. IR spectrum of **5b**.



5b

Chemical Formula: $C_{35}H_{42}BIrN_8O_3$
Exact Mass: 826.3102



MS Calcd: 826.3102 for $C_{35}H_{42}N_8BO_3Ir$, observed: 826.3125

Figure S44. MS Spectra of complex **5b**.

B. ^1H NMR Experiments: deuterium labeling of **4-d₁, **4-d**₅ and **5-d**₁**

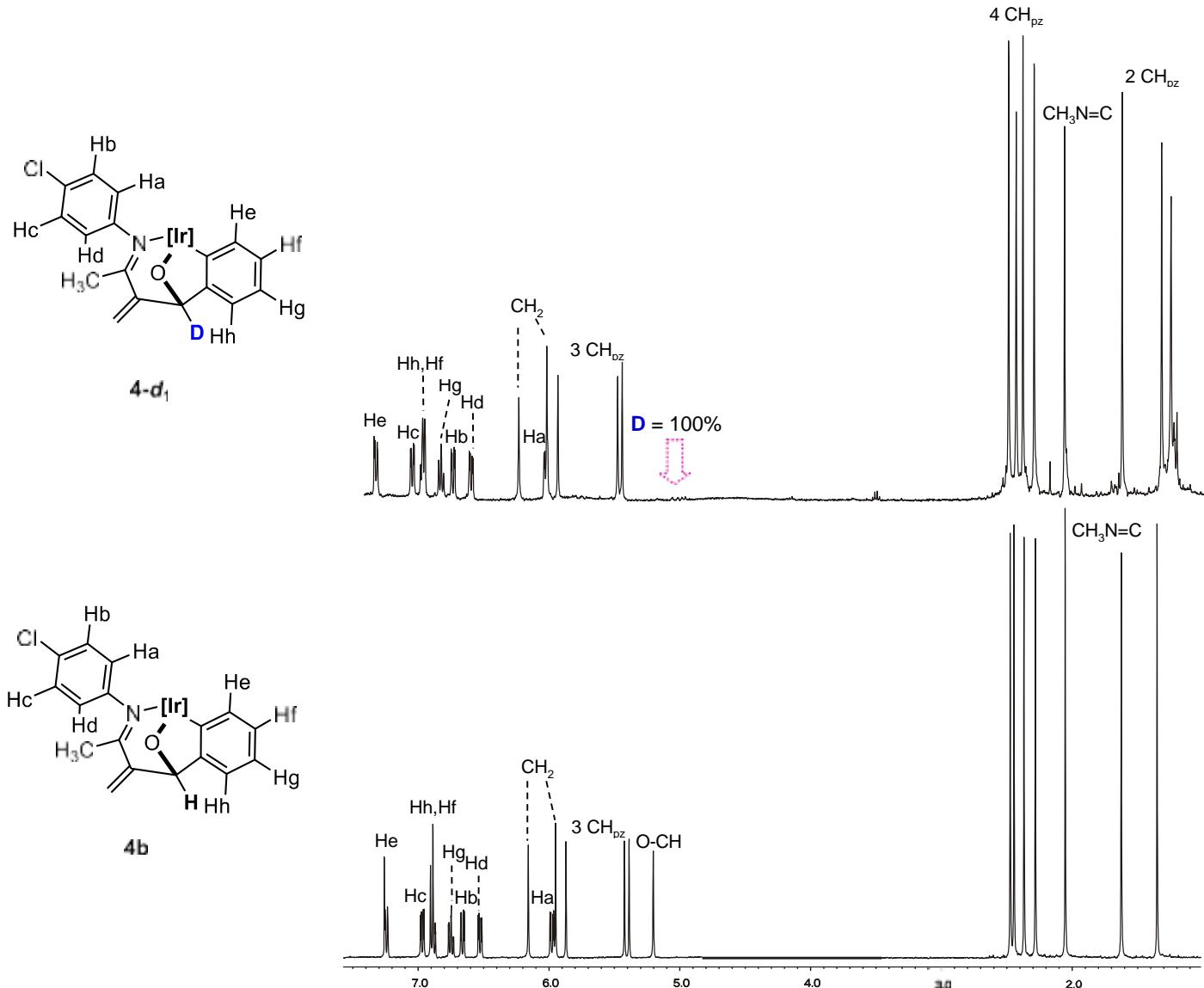


Figure S45. ^1H NMR (CDCl_3 , 25°C , 400 MHz) spectra of deuterium labeling in the compound **4-d**₁

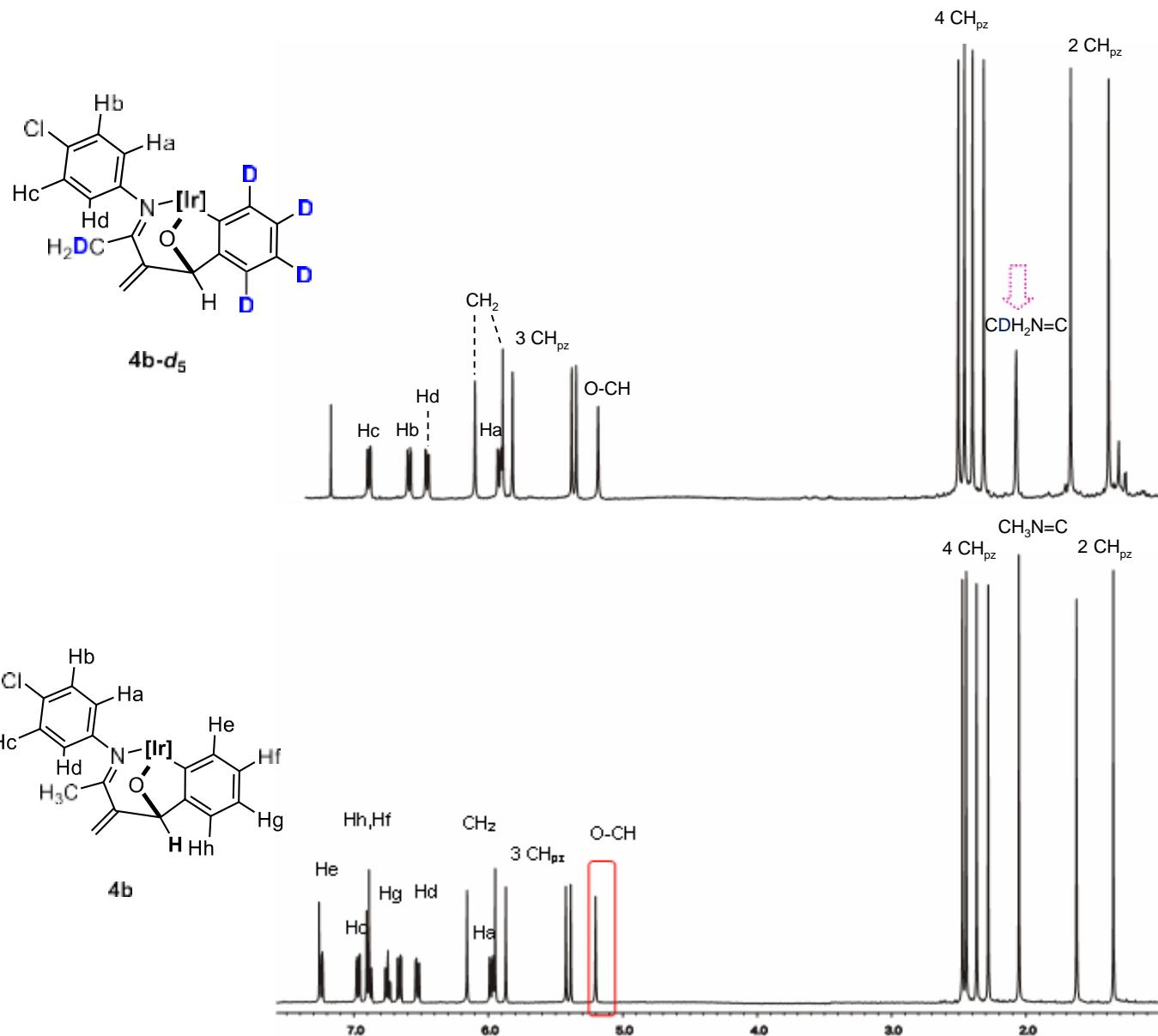


Figure S46. ^1H NMR (CDCl_3 , 25 °C, 400 MHz) spectra of deuterium labeling in the compound $\mathbf{4-d}_5$

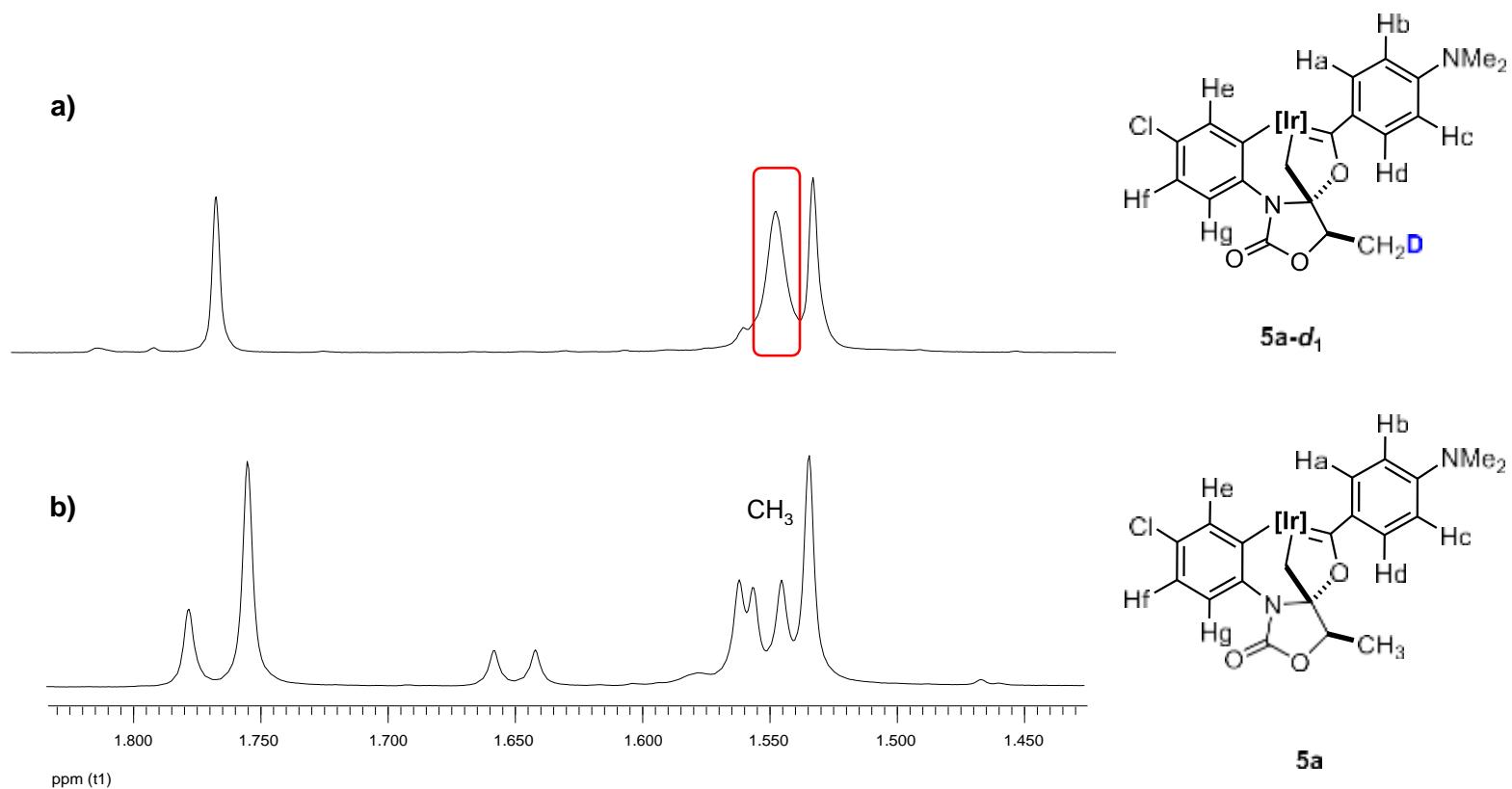
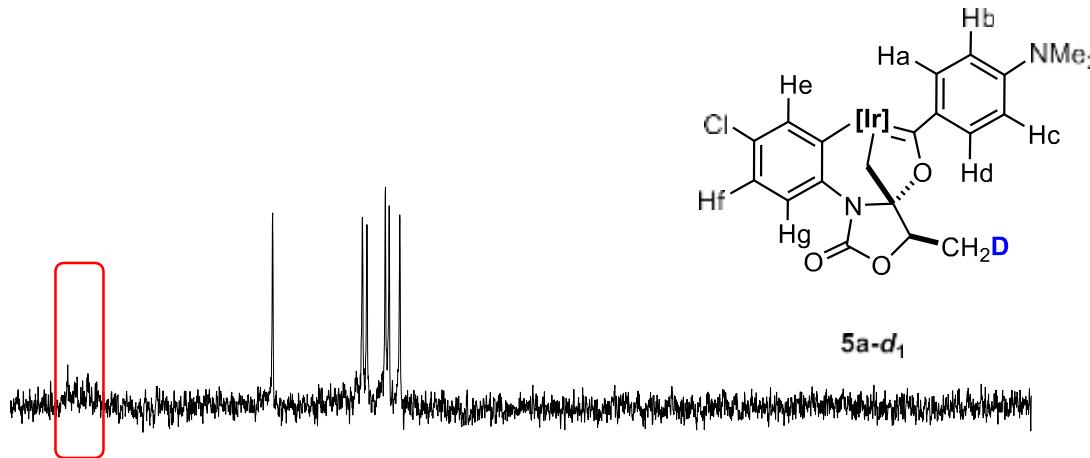


Figure S47. ^1H NMR (CDCl_3 , 25°C , 500 MHz) spectra of **a)** deuterium labeling in the compound **5-d₁** and **b)** compound **5a** (spectra at different vertical scales to optimize peak visibility)

d)



e)

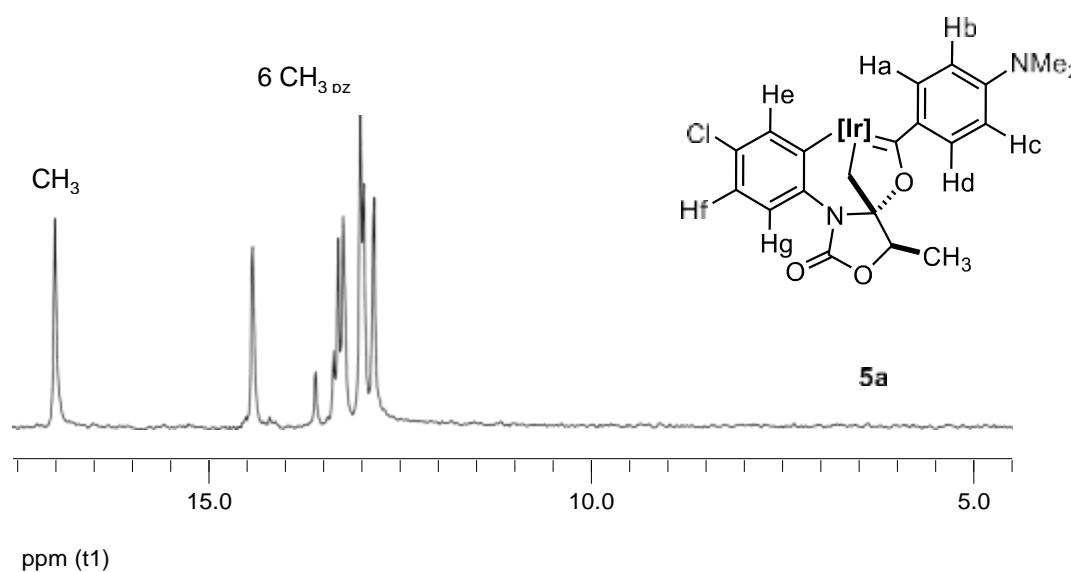
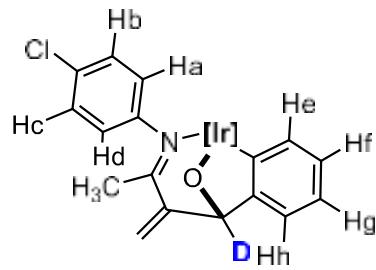


Figure S48. ¹³C {¹H} NMR (CDCl_3 , 25 °C, 125 MHz) spectra of **c**) deuterium labeling in the compound **5-d₁** and **d**) compound **5a** (spectra at different vertical scales to optimize peak visibility).



4b-d₁

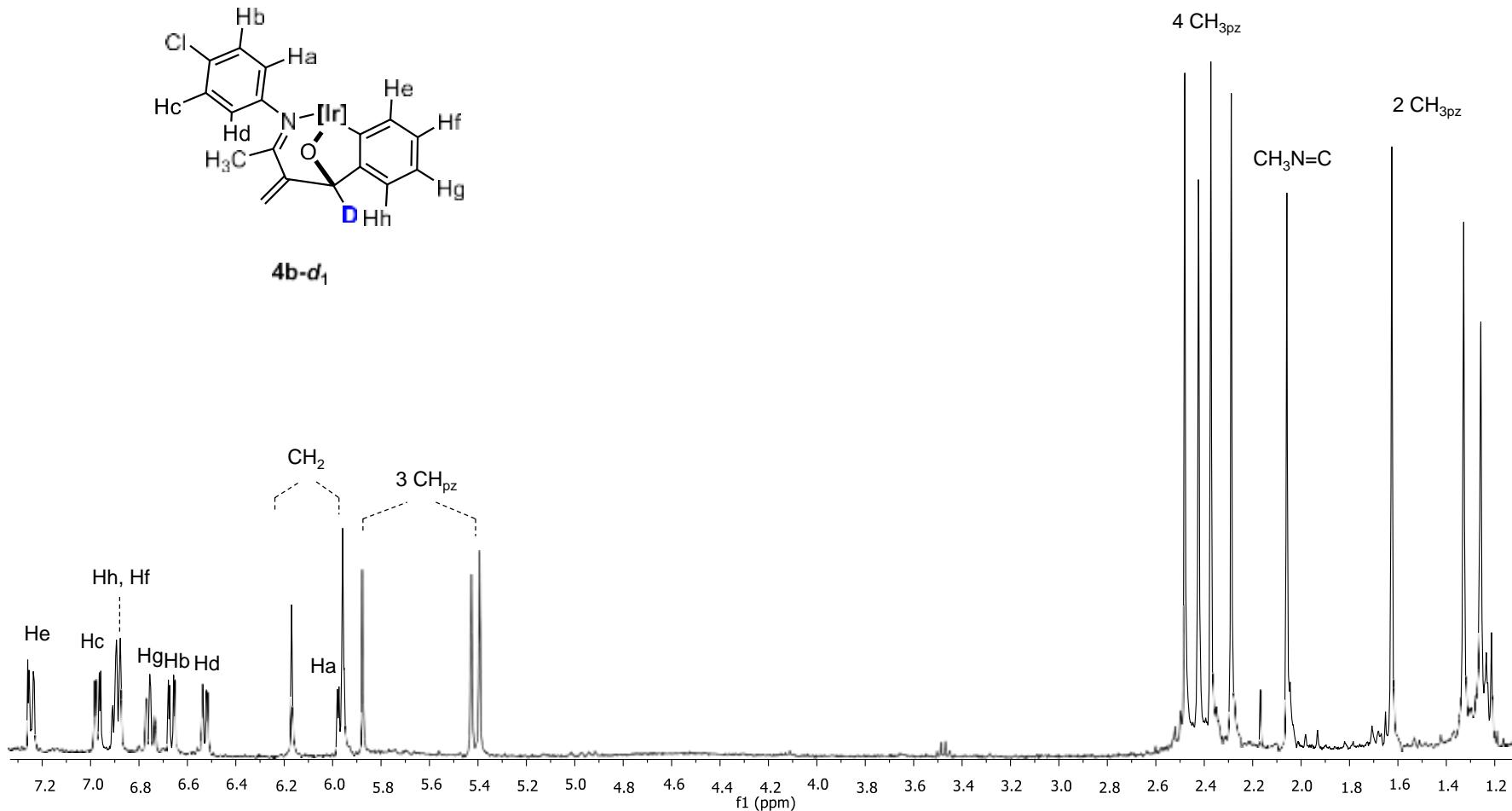
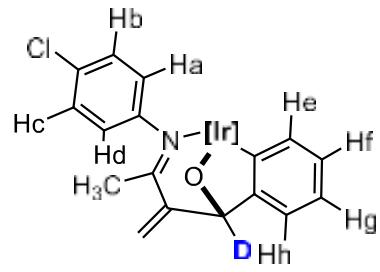


Figure S49. ¹H NMR (CDCl_3 , 25 °C, 500 MHz) spectrum of **4b-d₁**.



4b-d₁

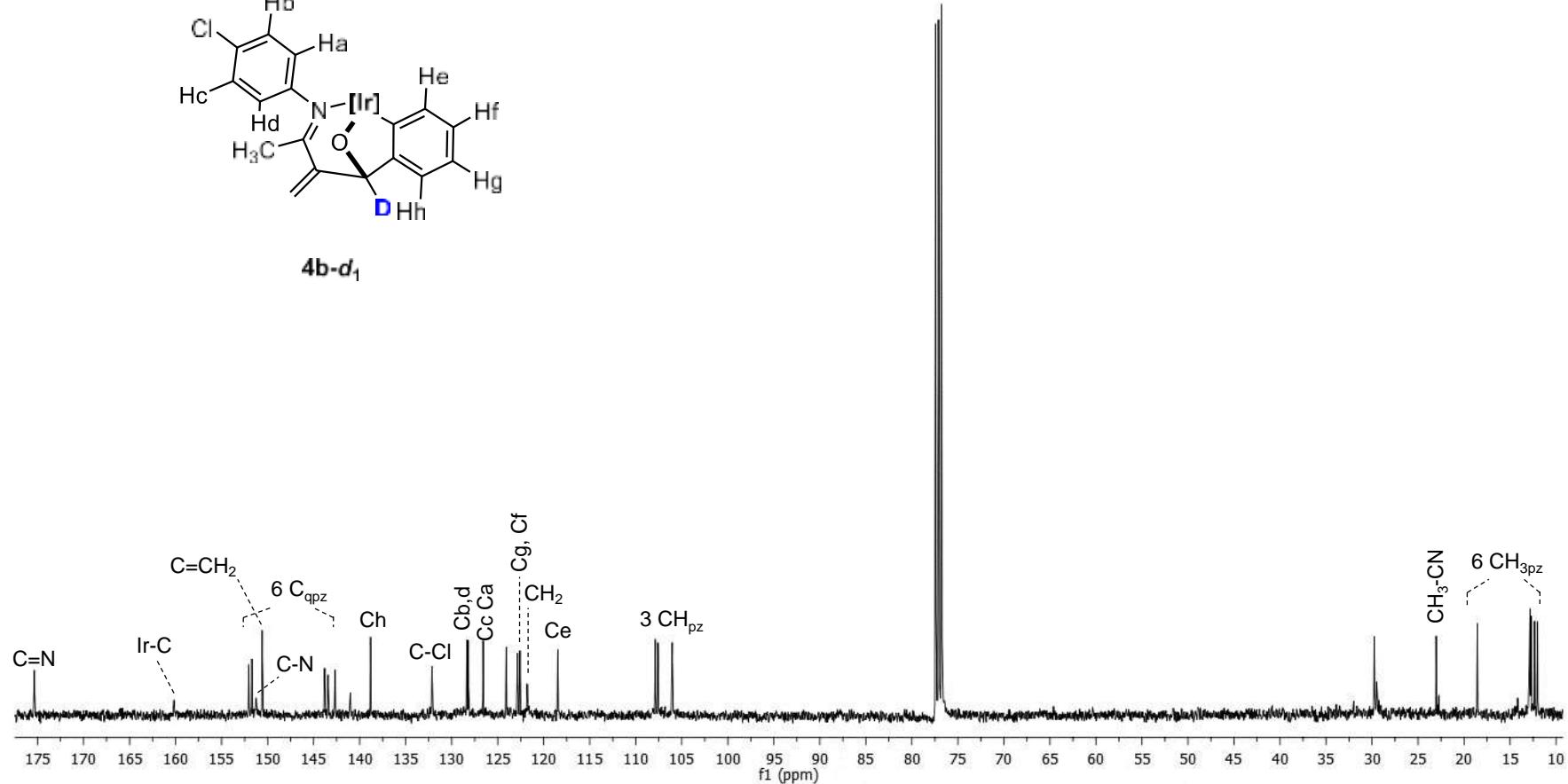


Figure S50. ^{13}C { ^1H } NMR (CDCl_3 , 25 °C, 125 MHz) spectrum of **4b-d₁**.

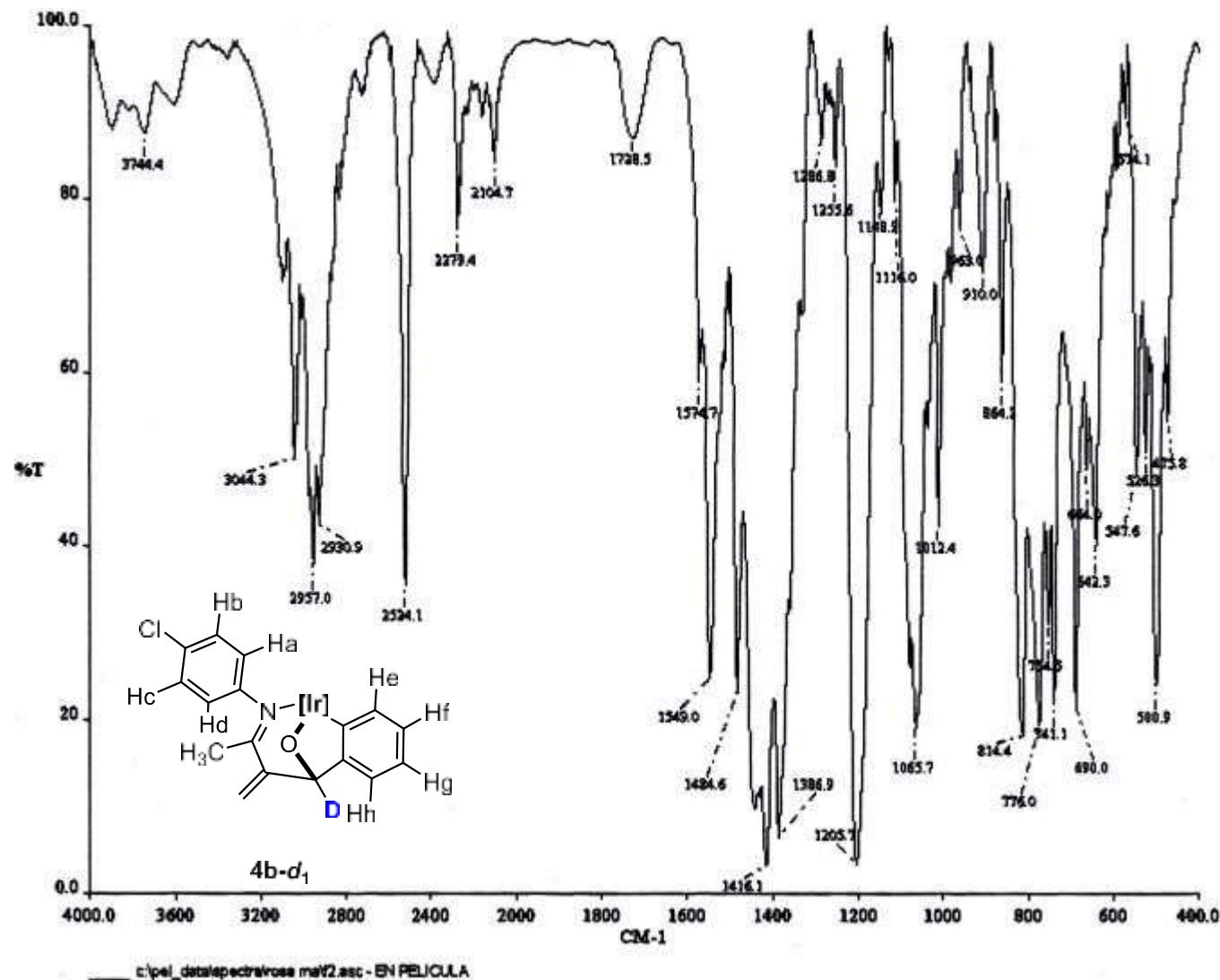


Figure S51. IR spectrum of **4b-d₁**.

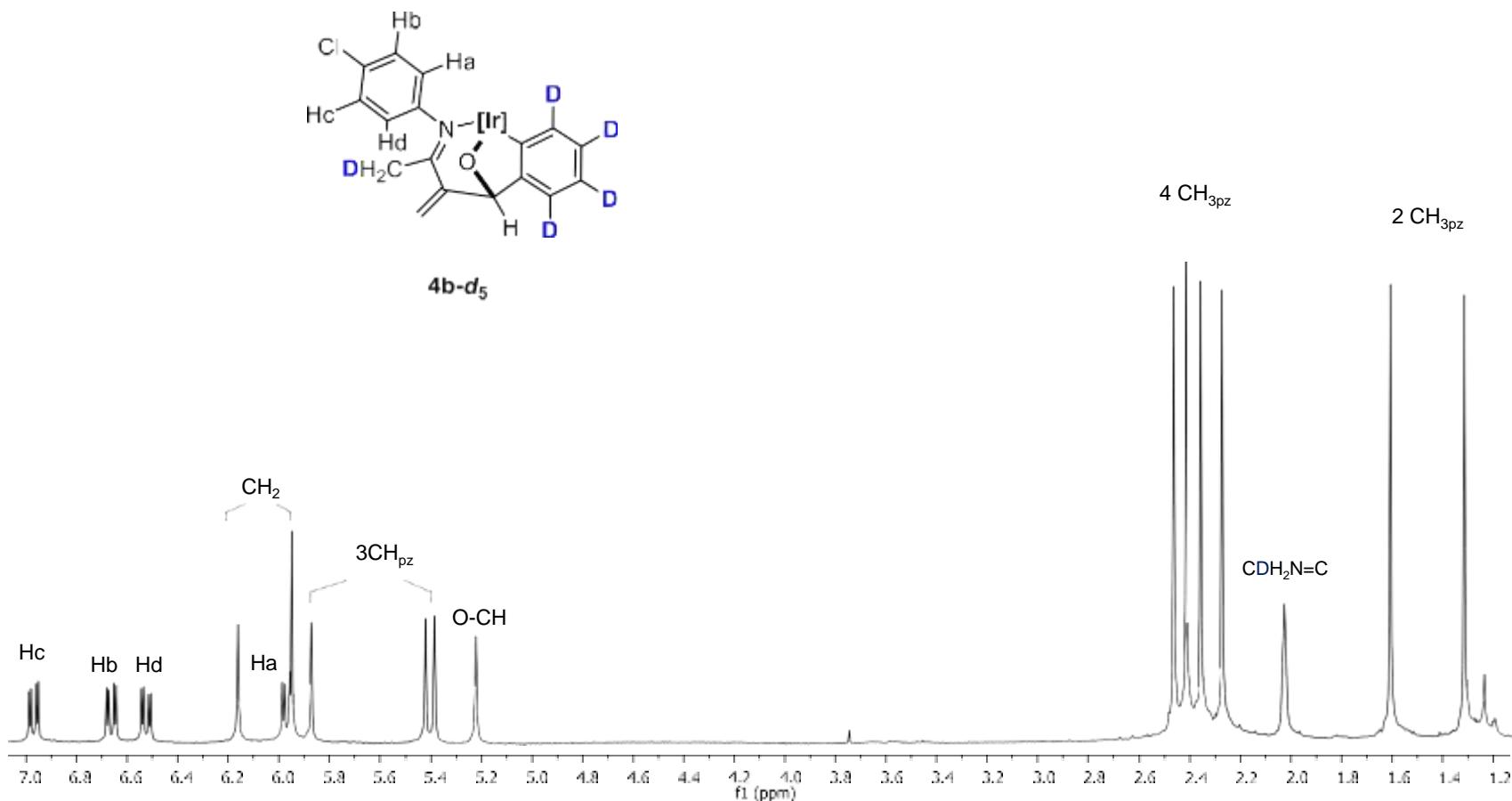


Figure S52. ^1H NMR (CDCl_3 , 25 °C, 400 MHz) spectrum of **4b-d₅**.

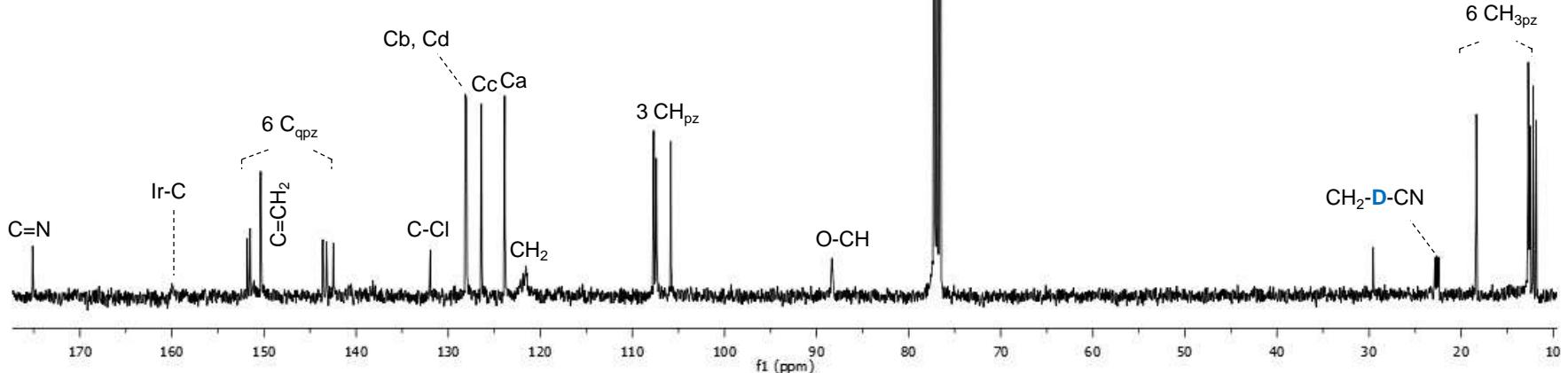
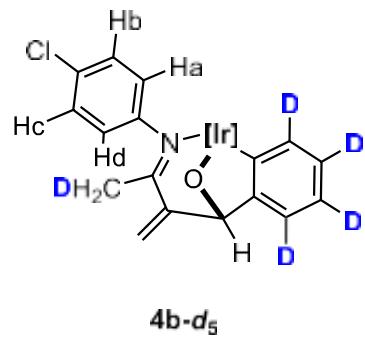


Figure S53. ^{13}C { ^1H } NMR (CDCl_3 , 25 °C, 100 .6 MHz) spectrum of **4b-d₅**.

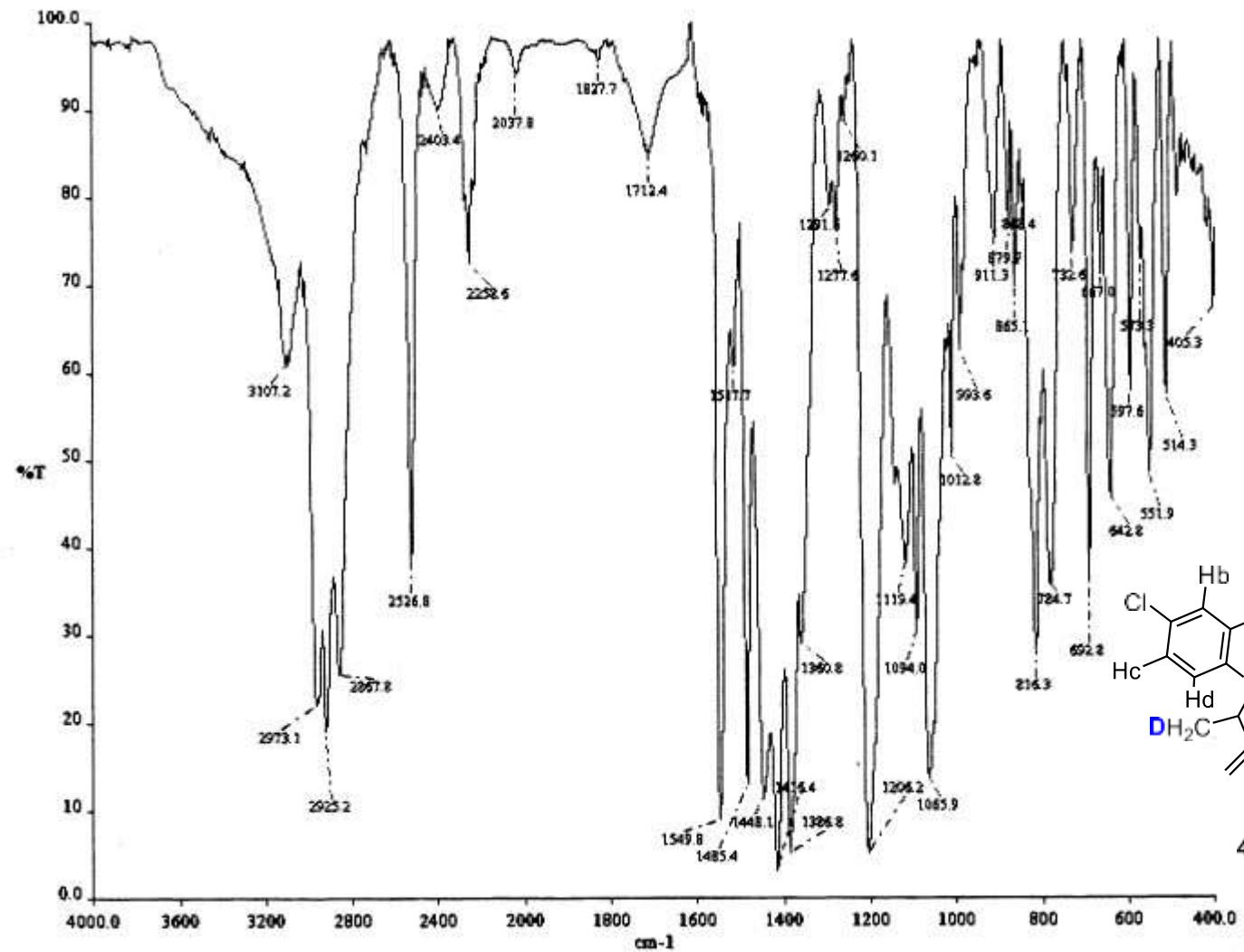


Figure S54. IR spectrum of **4b-d₅**.

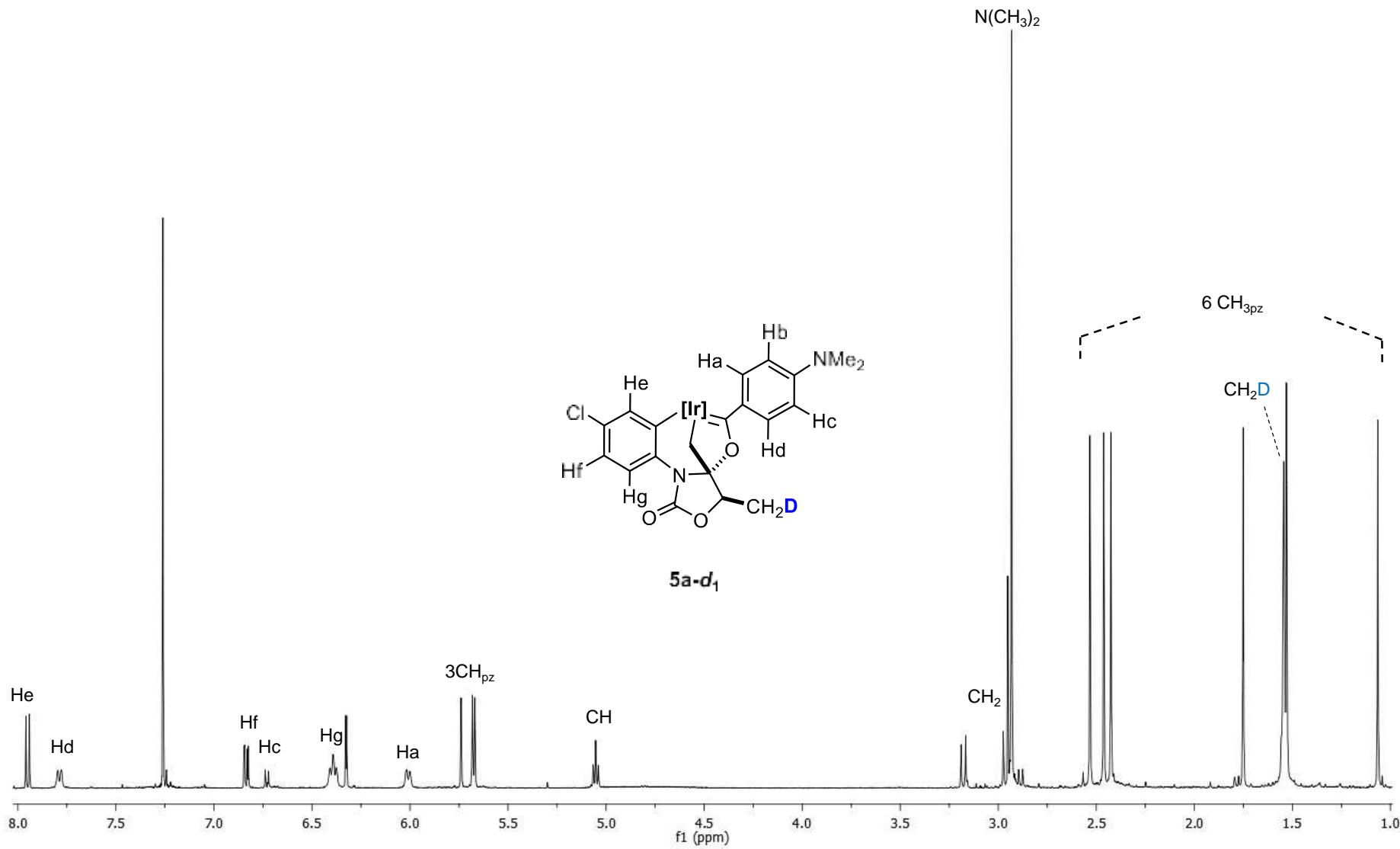


Figure S55. ^1H NMR (CDCl_3 , 25 °C, 500 MHz) spectrum of $\mathbf{5a-d}_1$.

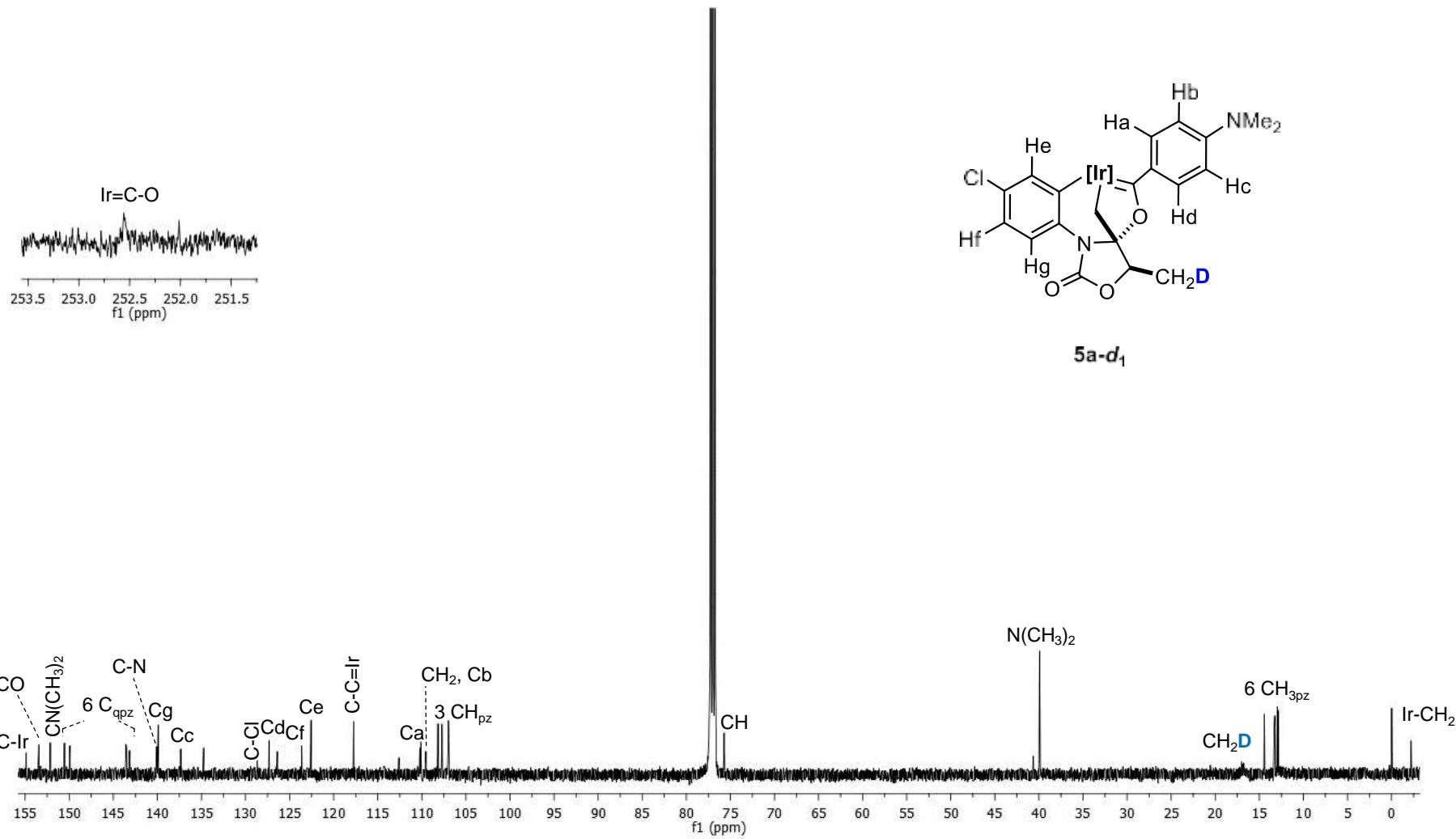


Figure S56. ^{13}C { ^1H } NMR (CDCl_3 , 25 °C, 125 MHz) spectrum of $\mathbf{5a-d}_1$.

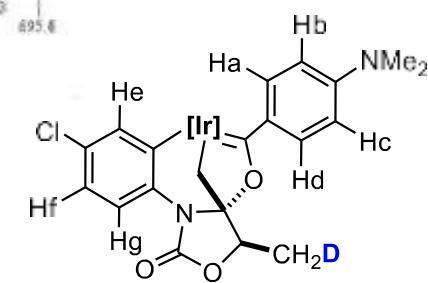
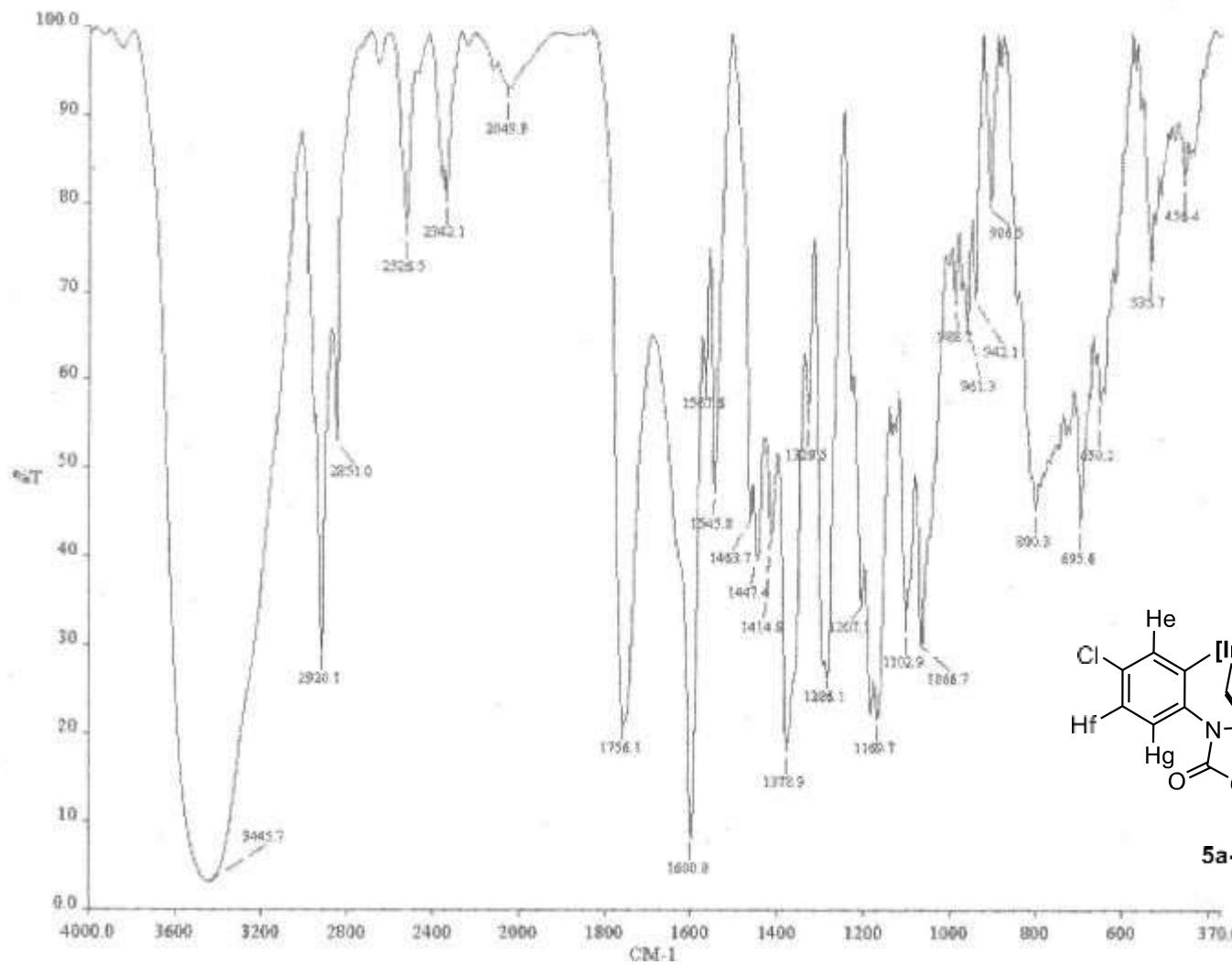


Figure S57. IR spectrum of **5a-d₁**.

C. NMR Experiments: key intermediates **6a**-**7a**.

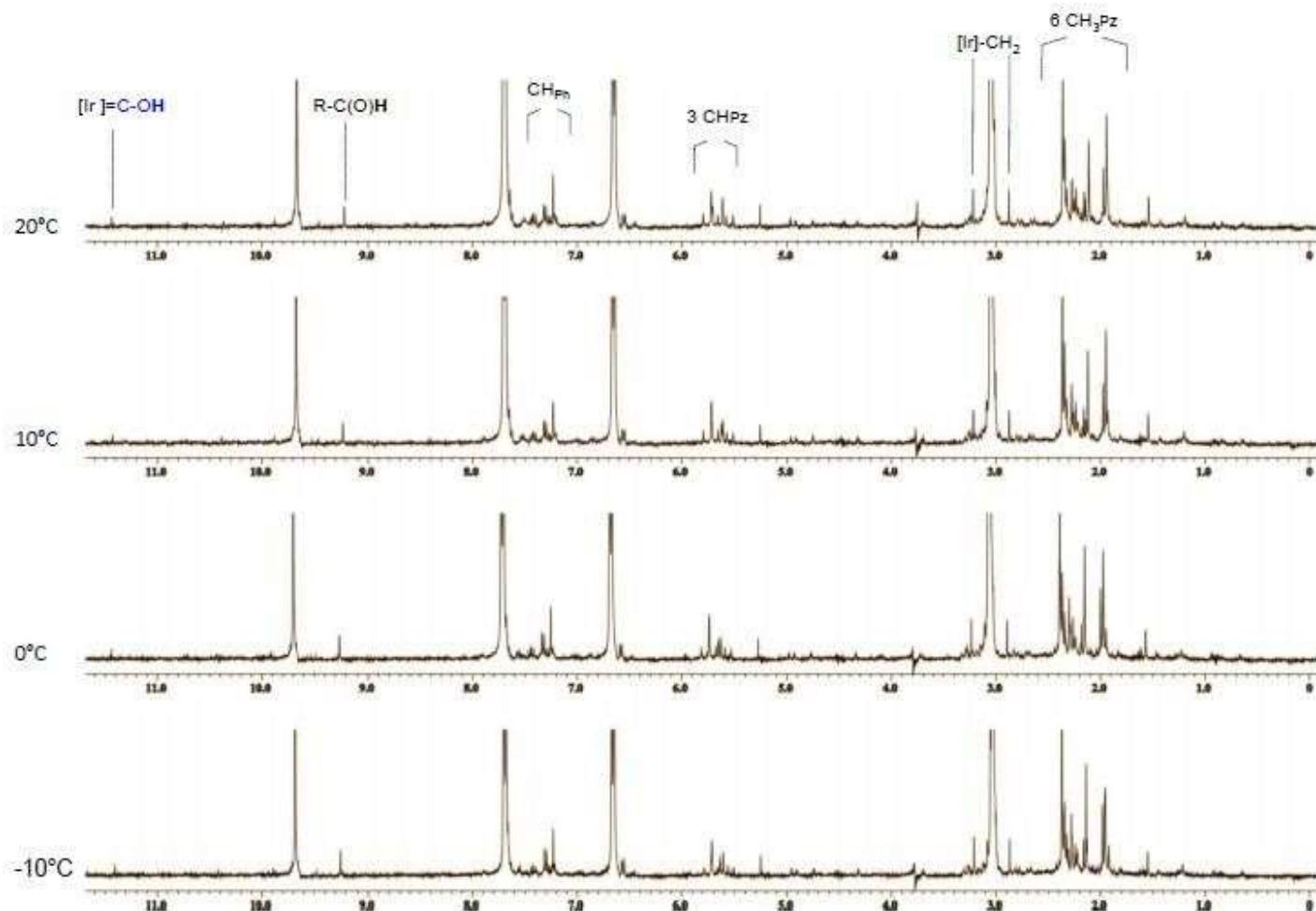


Figure S58. ¹H NMR spectra (CDCl_3 , 25 °C, 400 MHz) at variable temperature for the formation of aldehyde adduct **6a** and hydroxycarbene **7a**.

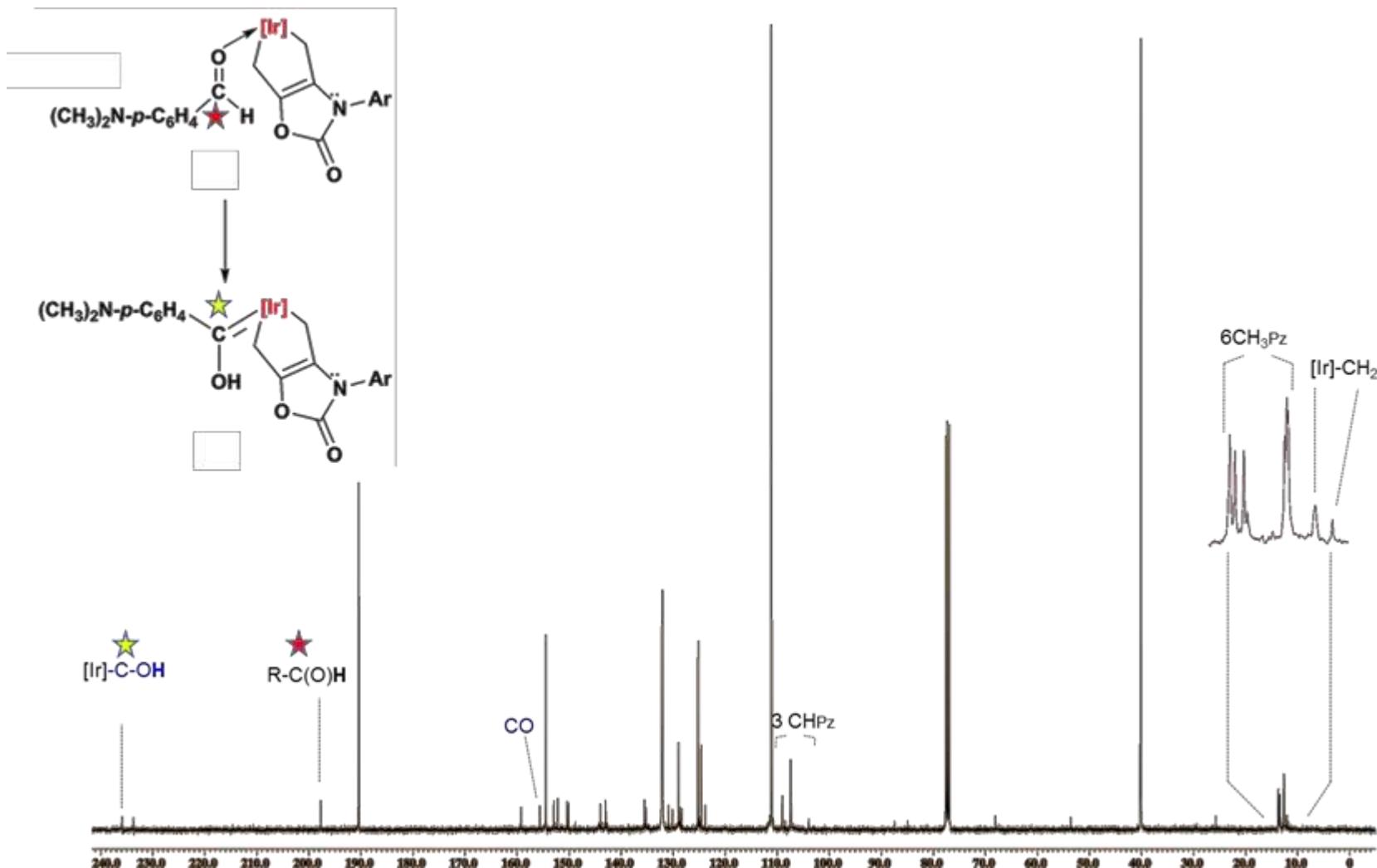


Figure S59. ^{13}C { ^1H } NMR (CDCl_3 , 25°C , 100.6 MHz) for the progress of the reaction with the aldehyde adduct **6a** and hydroxycarbene **7a**.

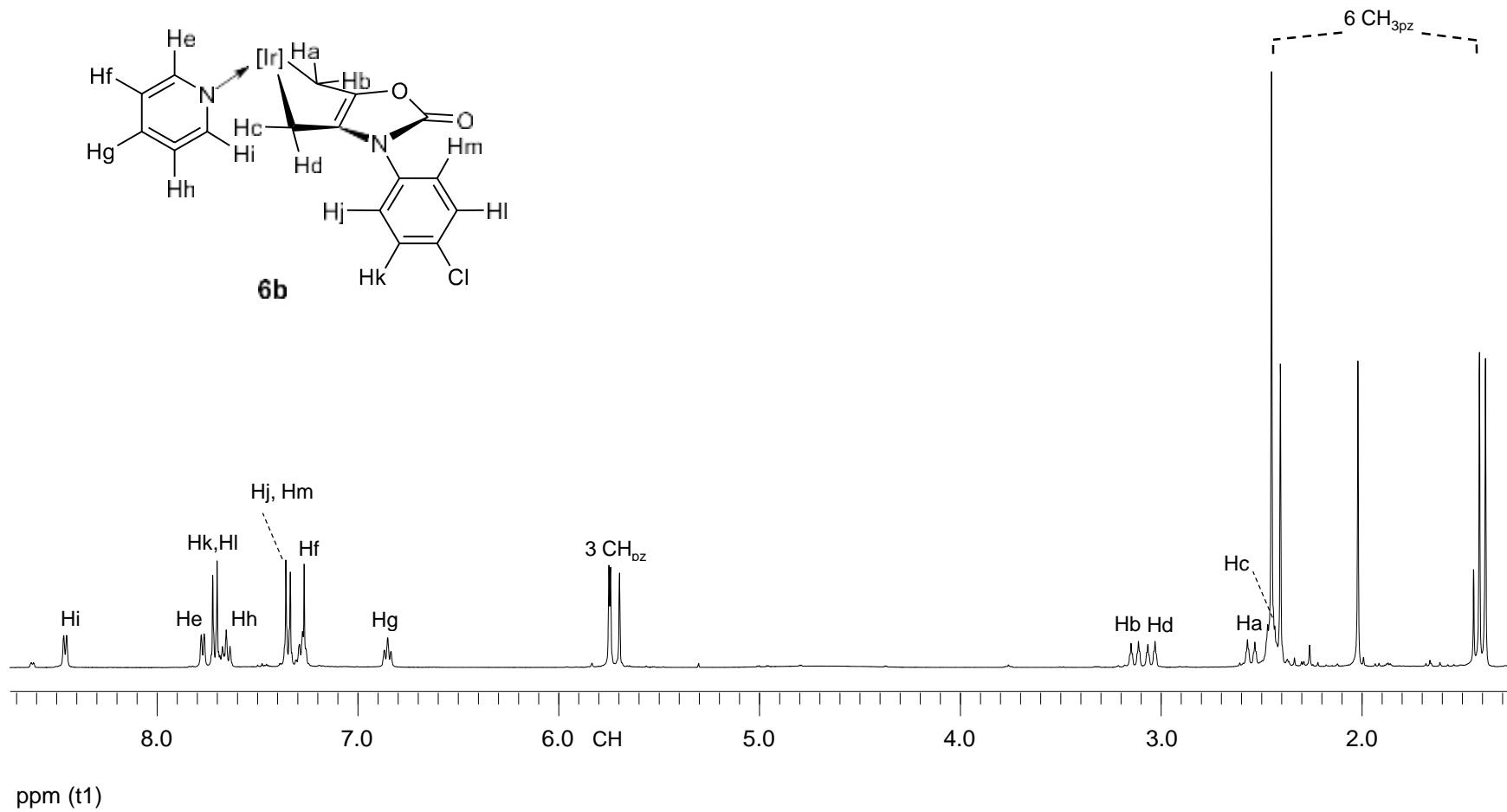
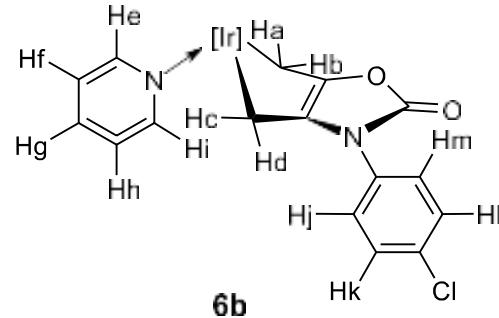


Figure S60. ^1H NMR (CDCl_3 , 25°C , 400 MHz) spectrum of **6b**.

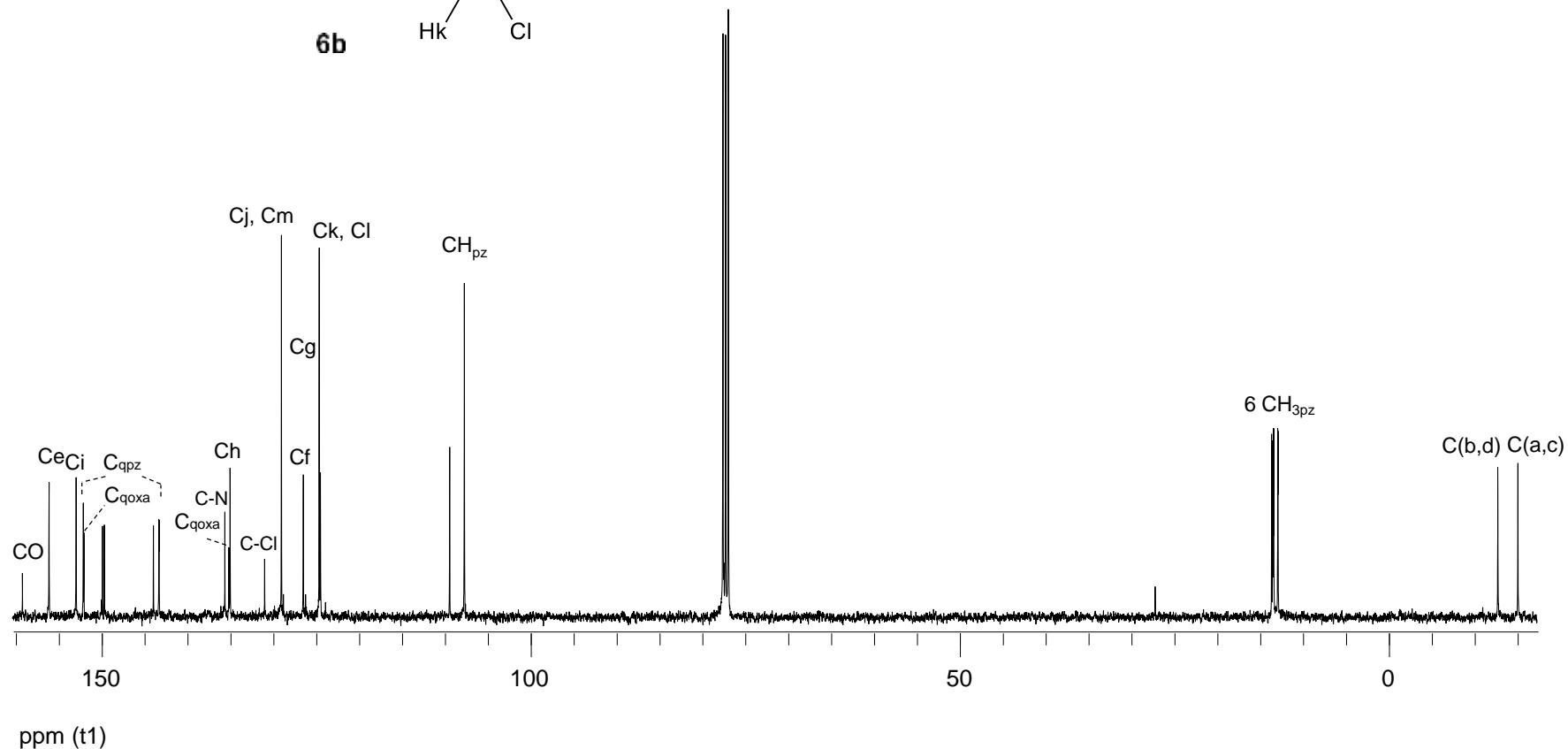
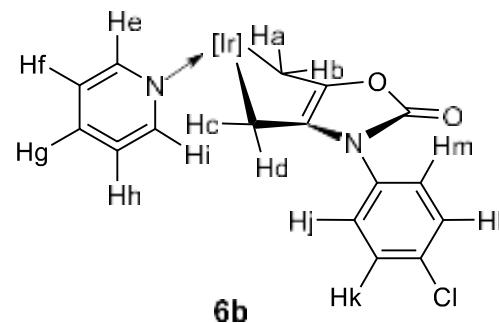


Figure S61. ^{13}C { ^1H } NMR (CDCl_3 , 25°C , 100.6 MHz) spectrum of **6b**.

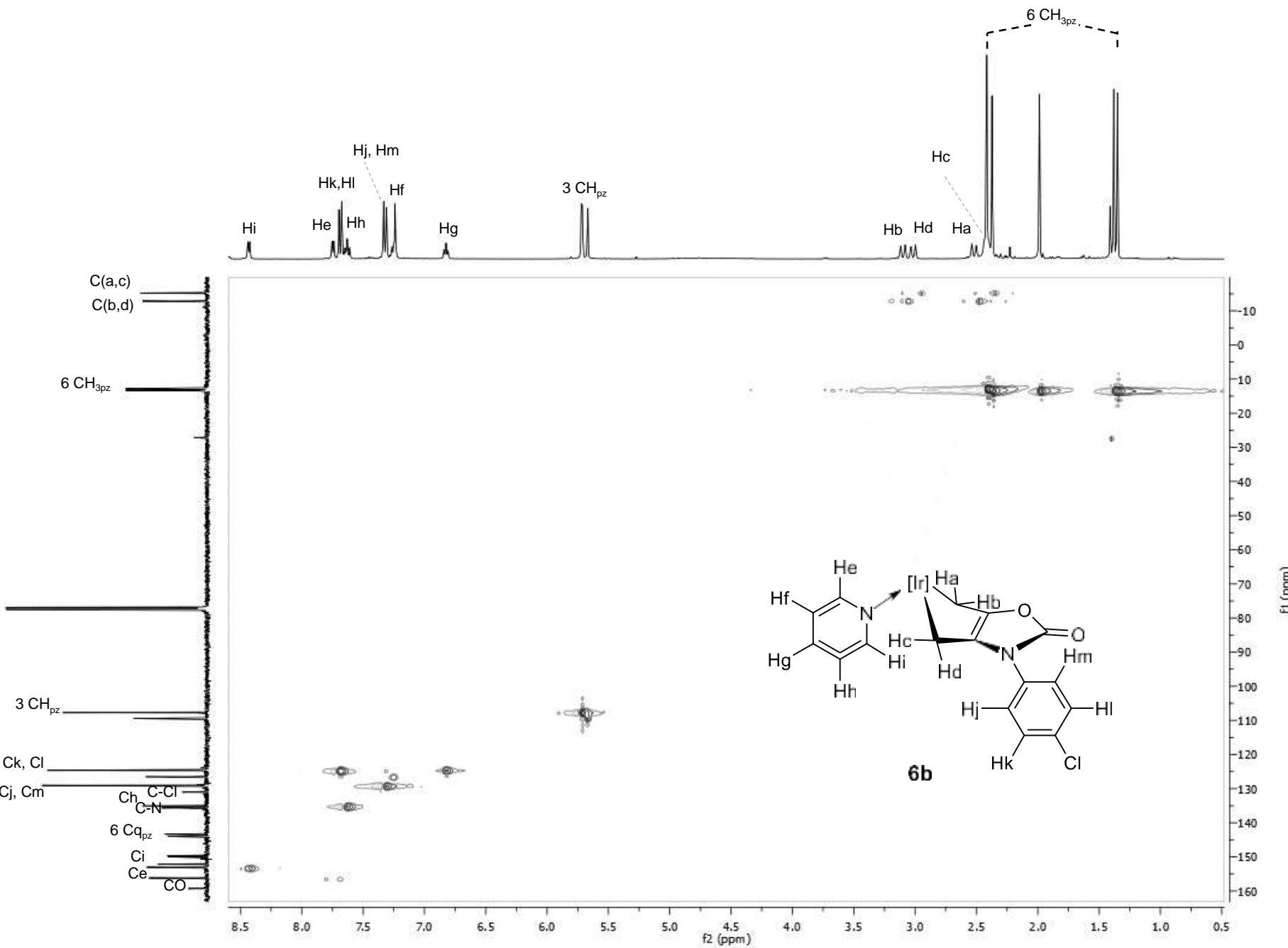


Figure S62. HMQC diagram of **6b**.

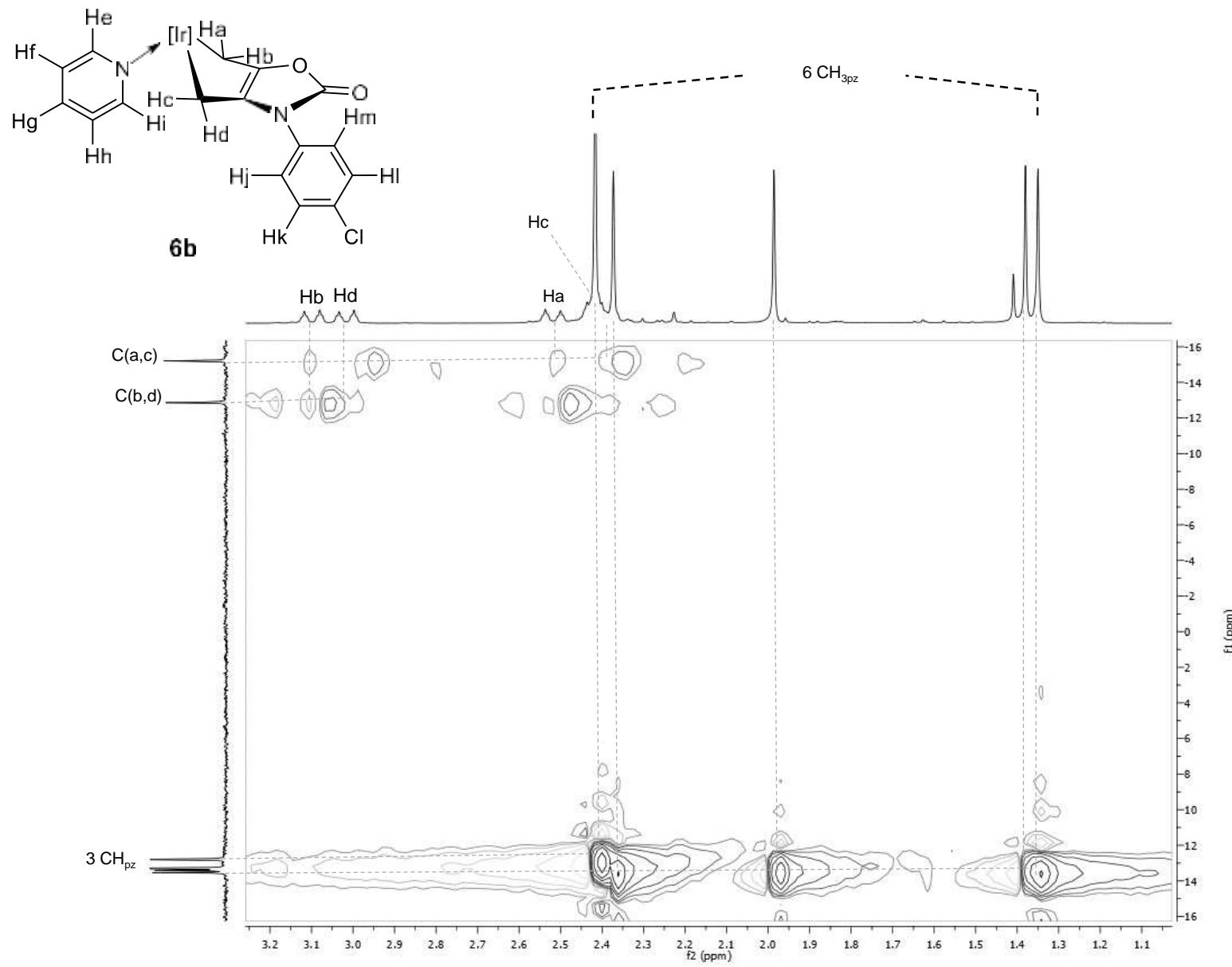


Figure S63. HMQC diagram of **6b**.

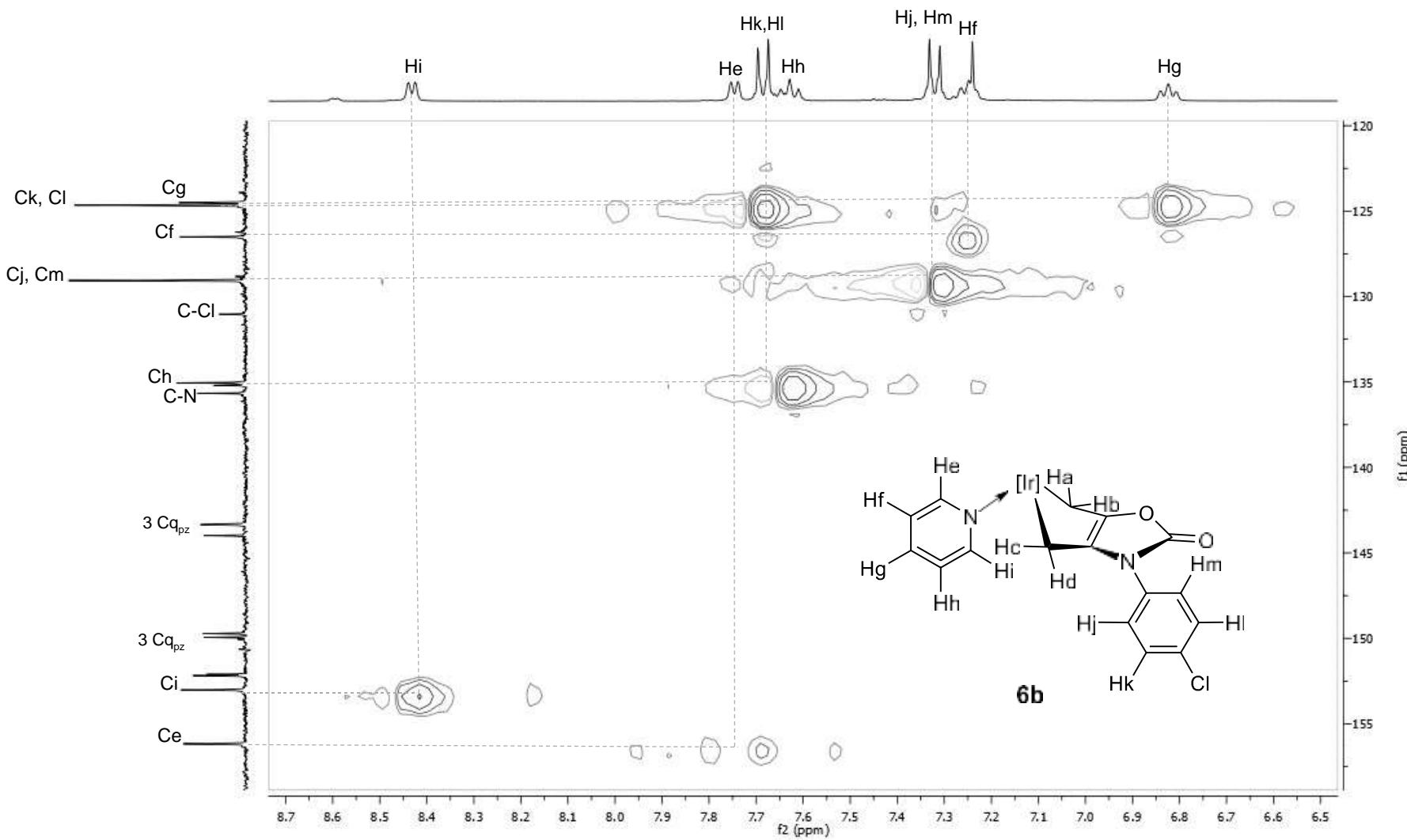


Figure S64. HMQC diagram of **6b**.

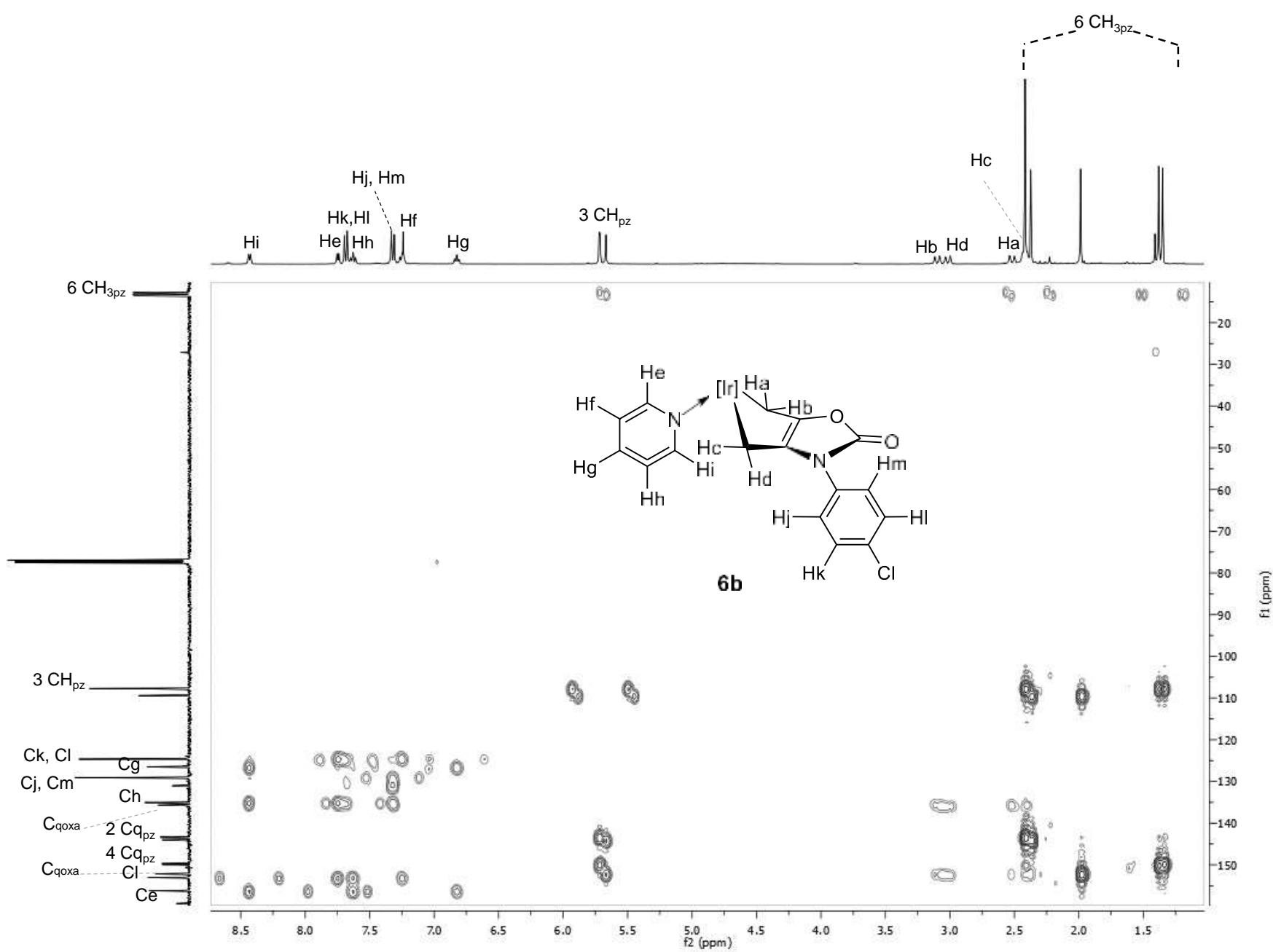


Figure S65. HMQC diagram of **6b**.

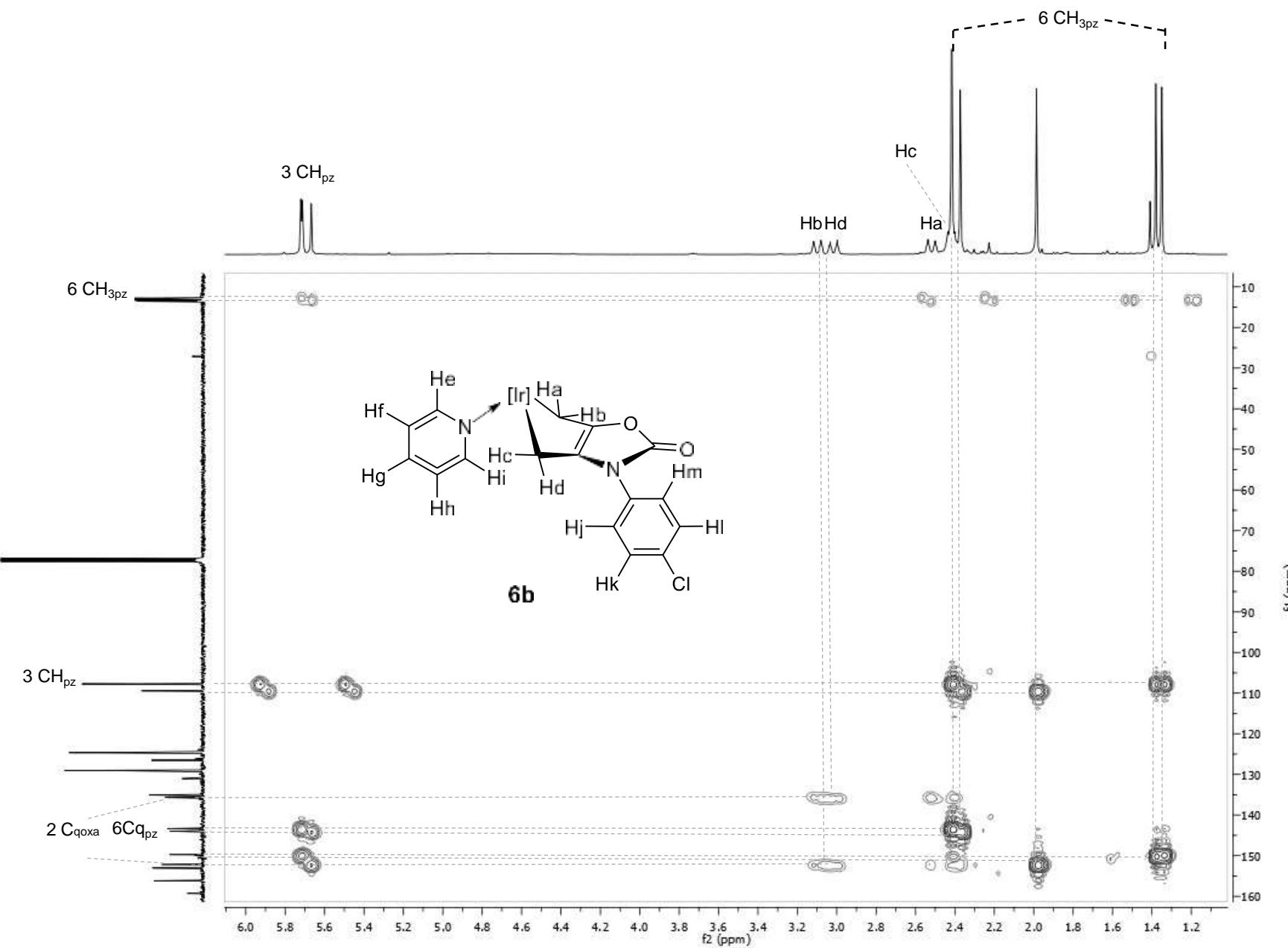


Figure S66. HMQC diagram of **6b**.

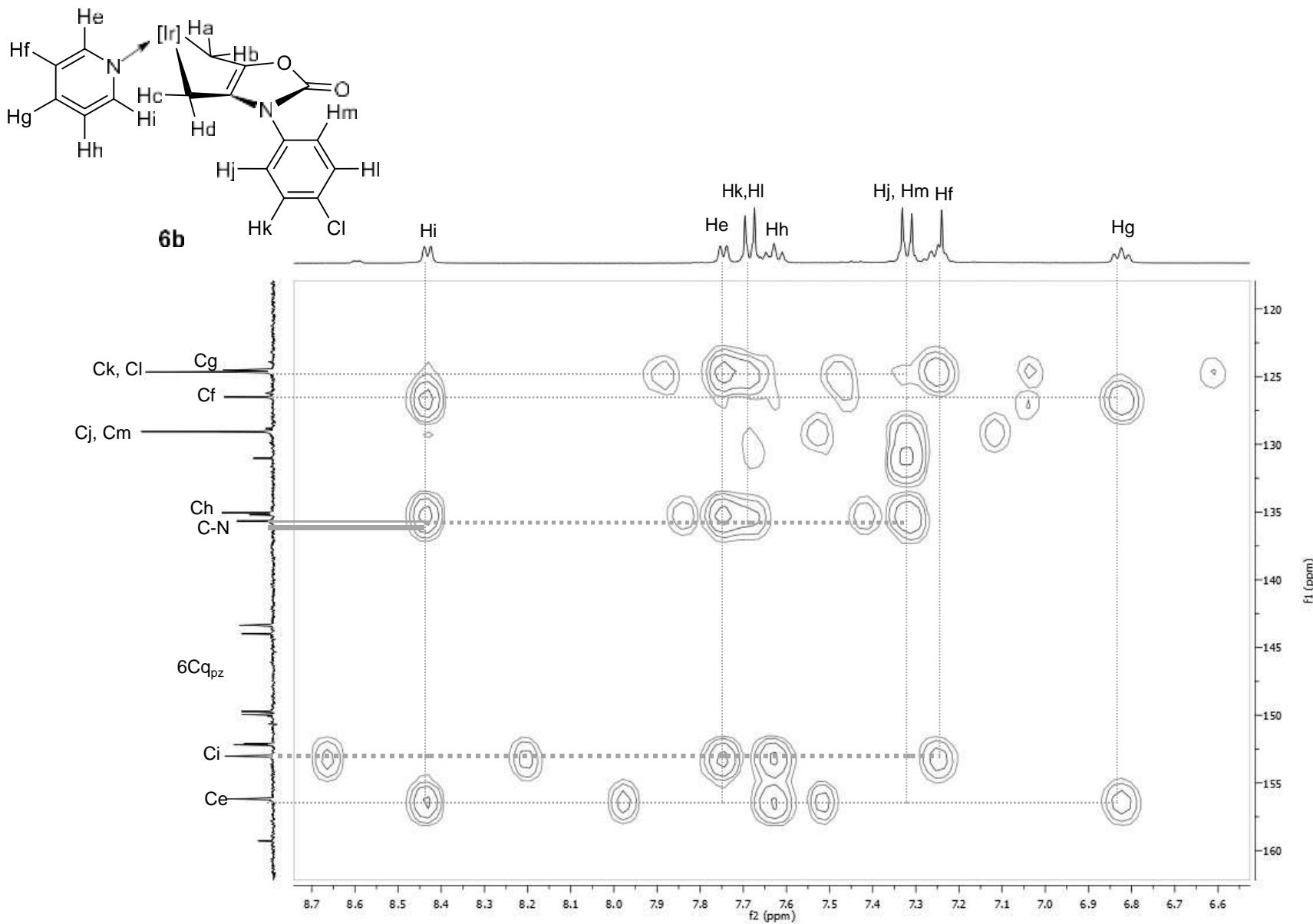


Figure S67. HMQC diagram of **6b**.

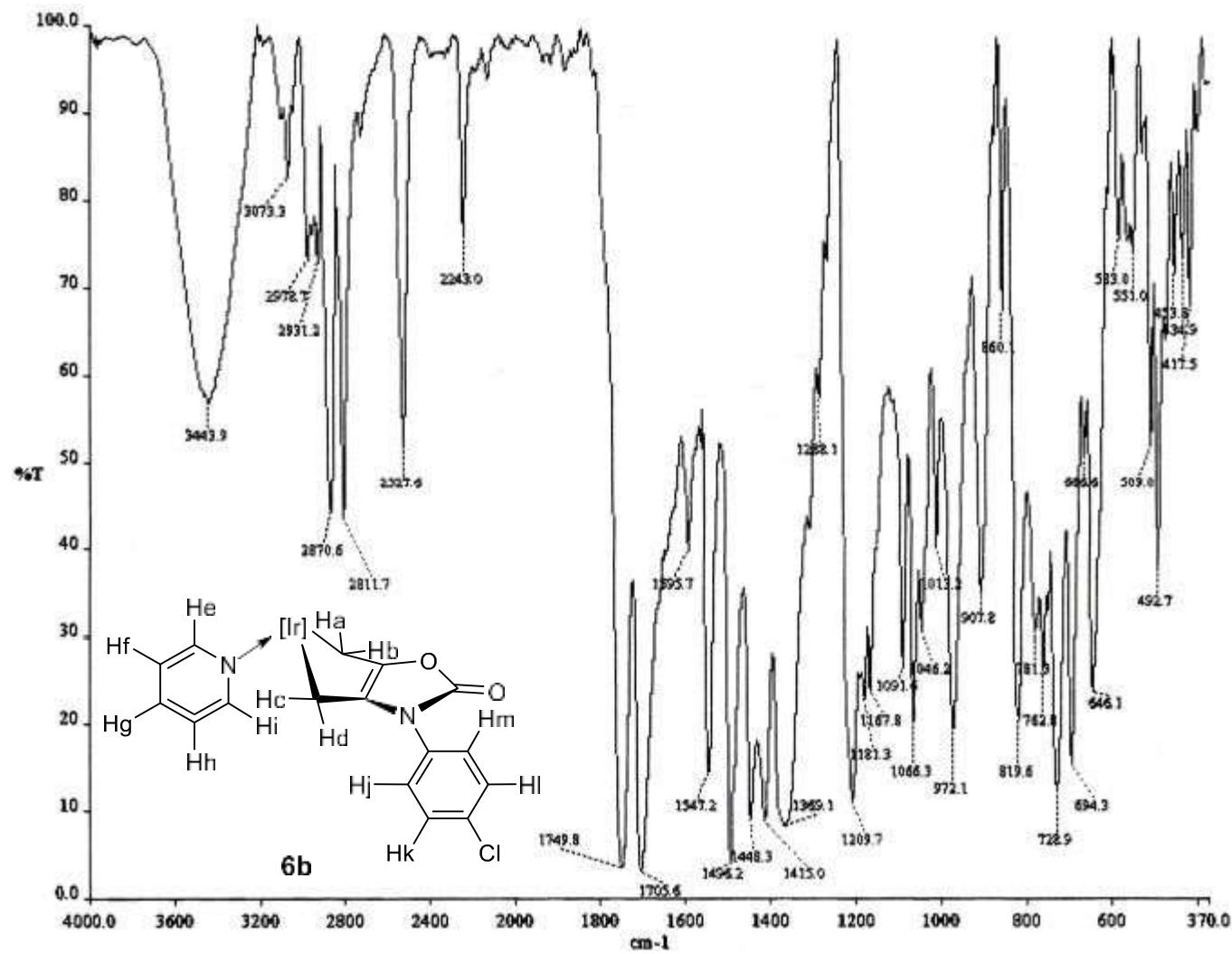


Figure S68. IR spectrum of **6b**.

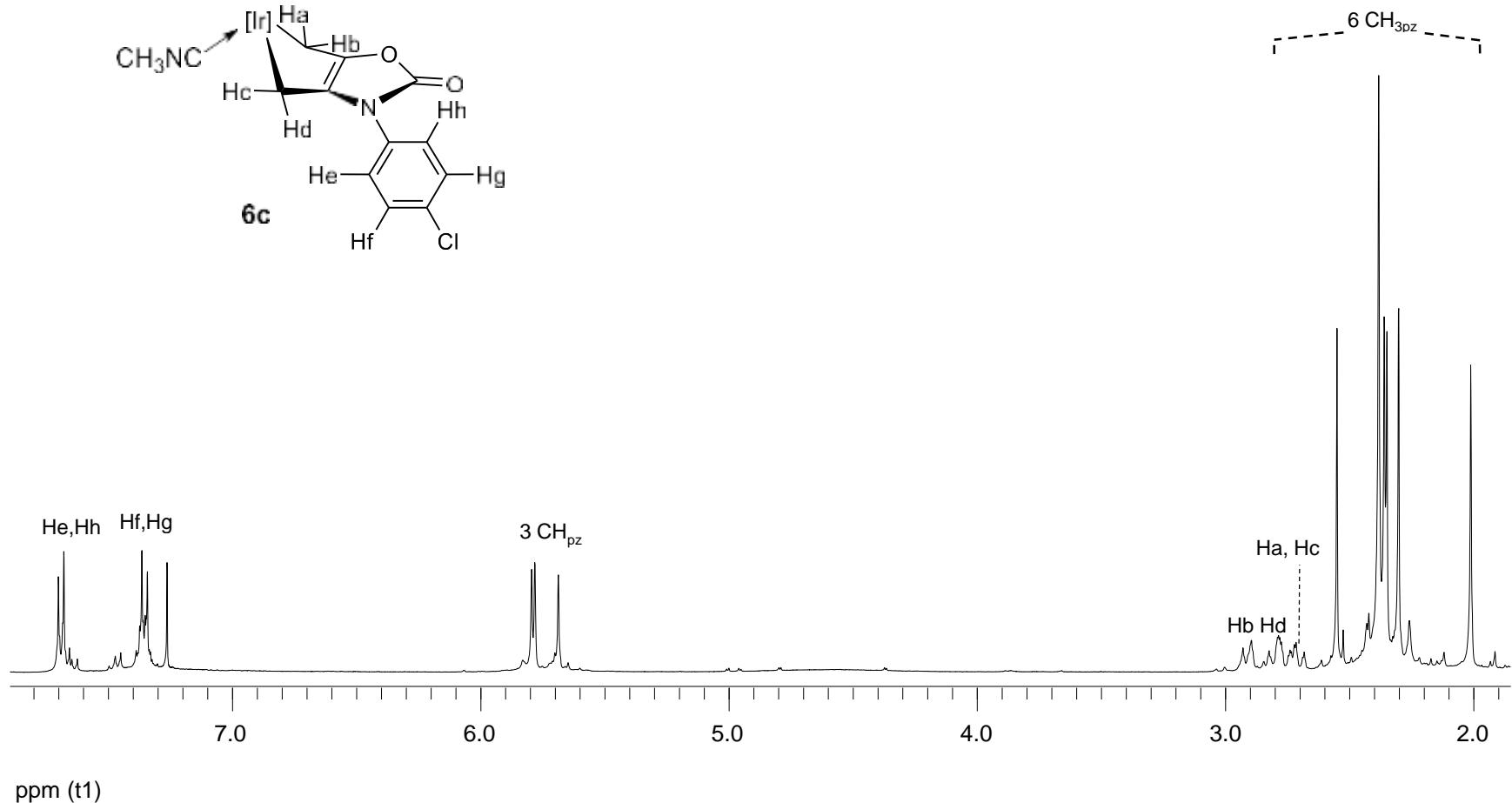
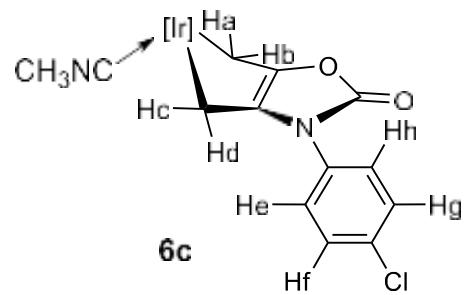


Figure S69. ^1H NMR (CDCl_3 , 25°C , 400 MHz) spectrum of **6c**.

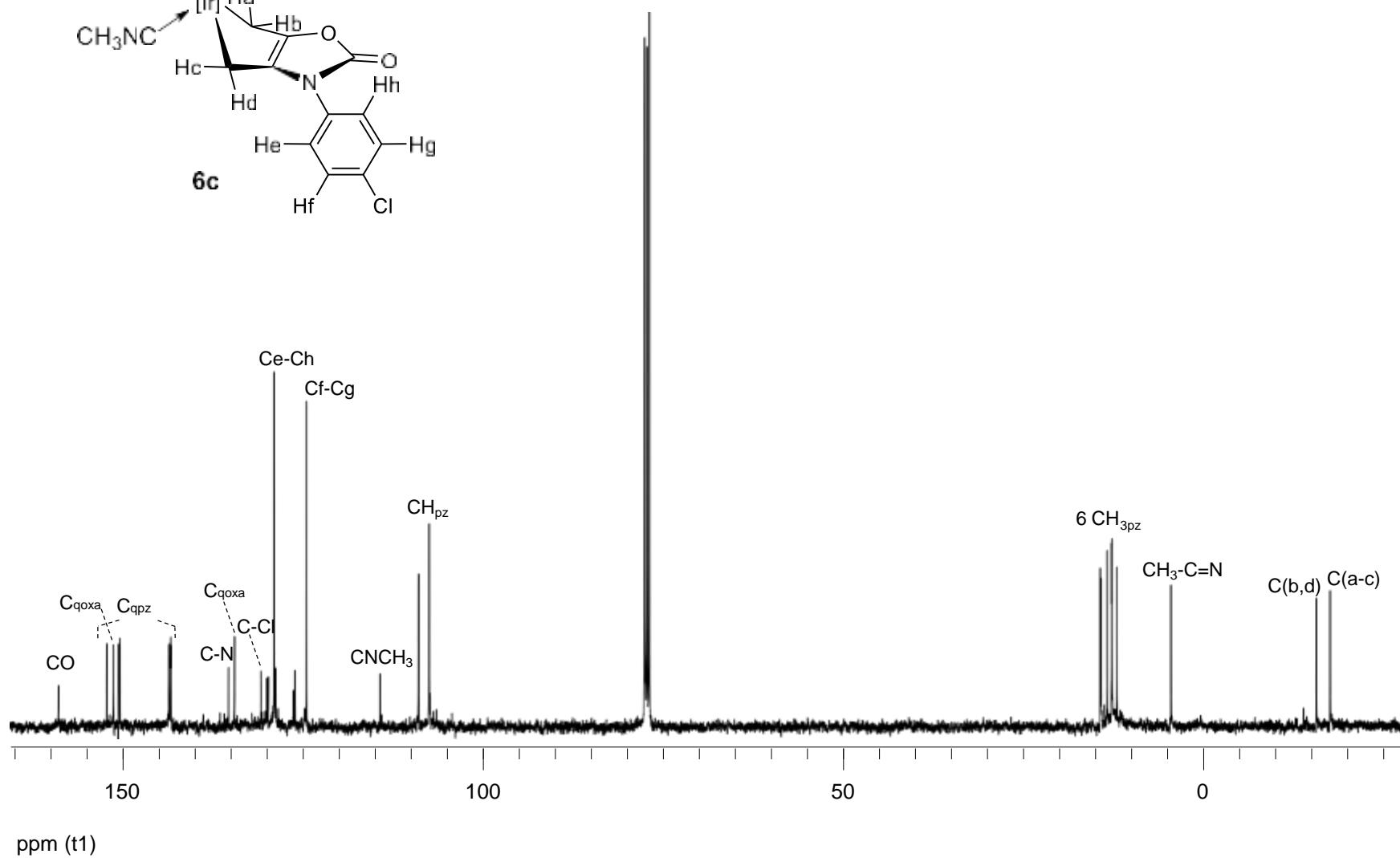
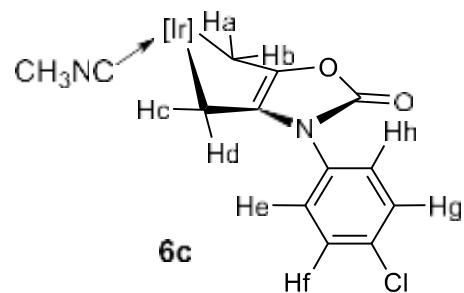


Figure S70. ^{13}C { ^1H } NMR (CDCl_3 , 25°C , 100.6 MHz) spectrum of **6c**.

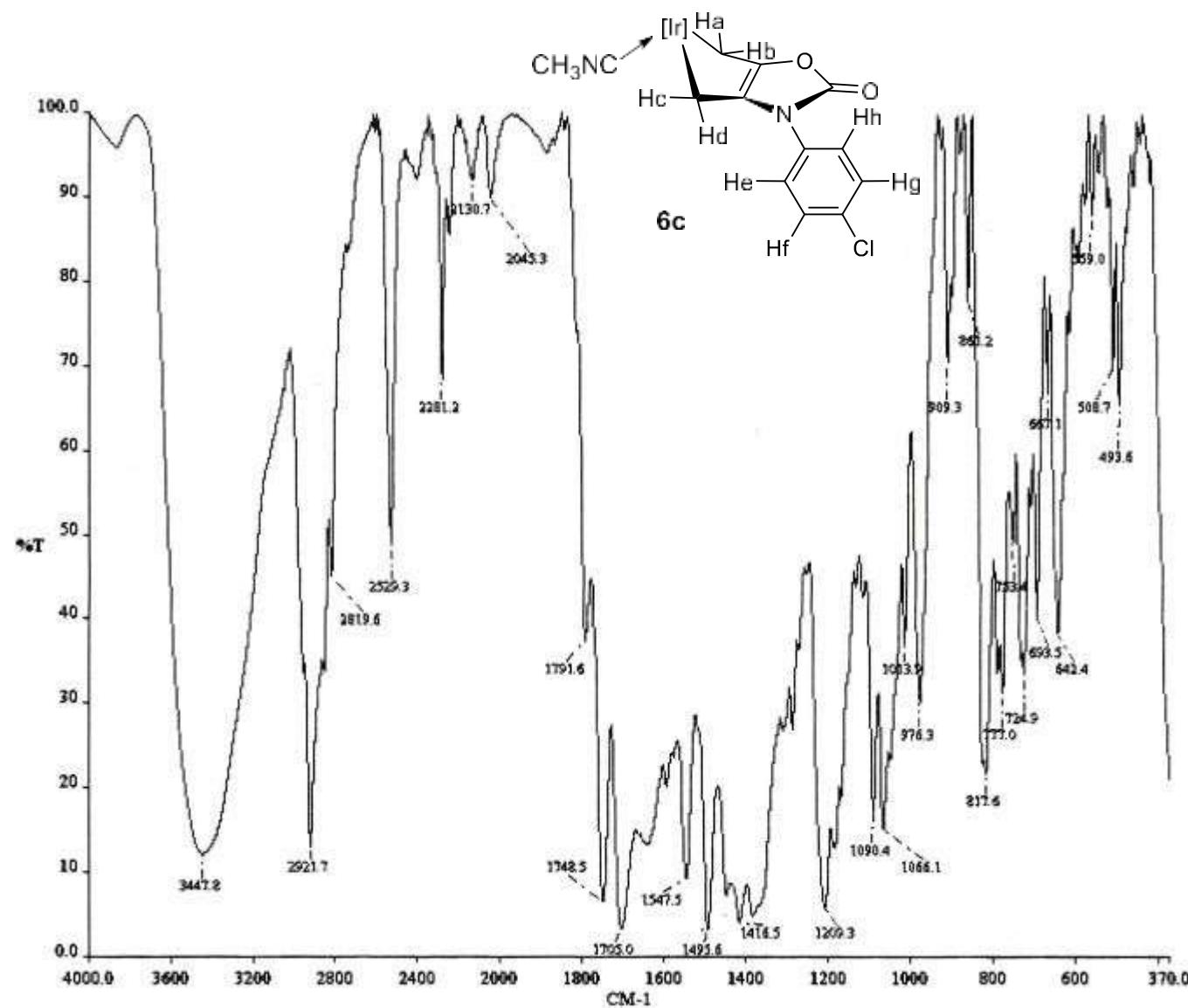


Figure S71. IR spectrum of **6c**.

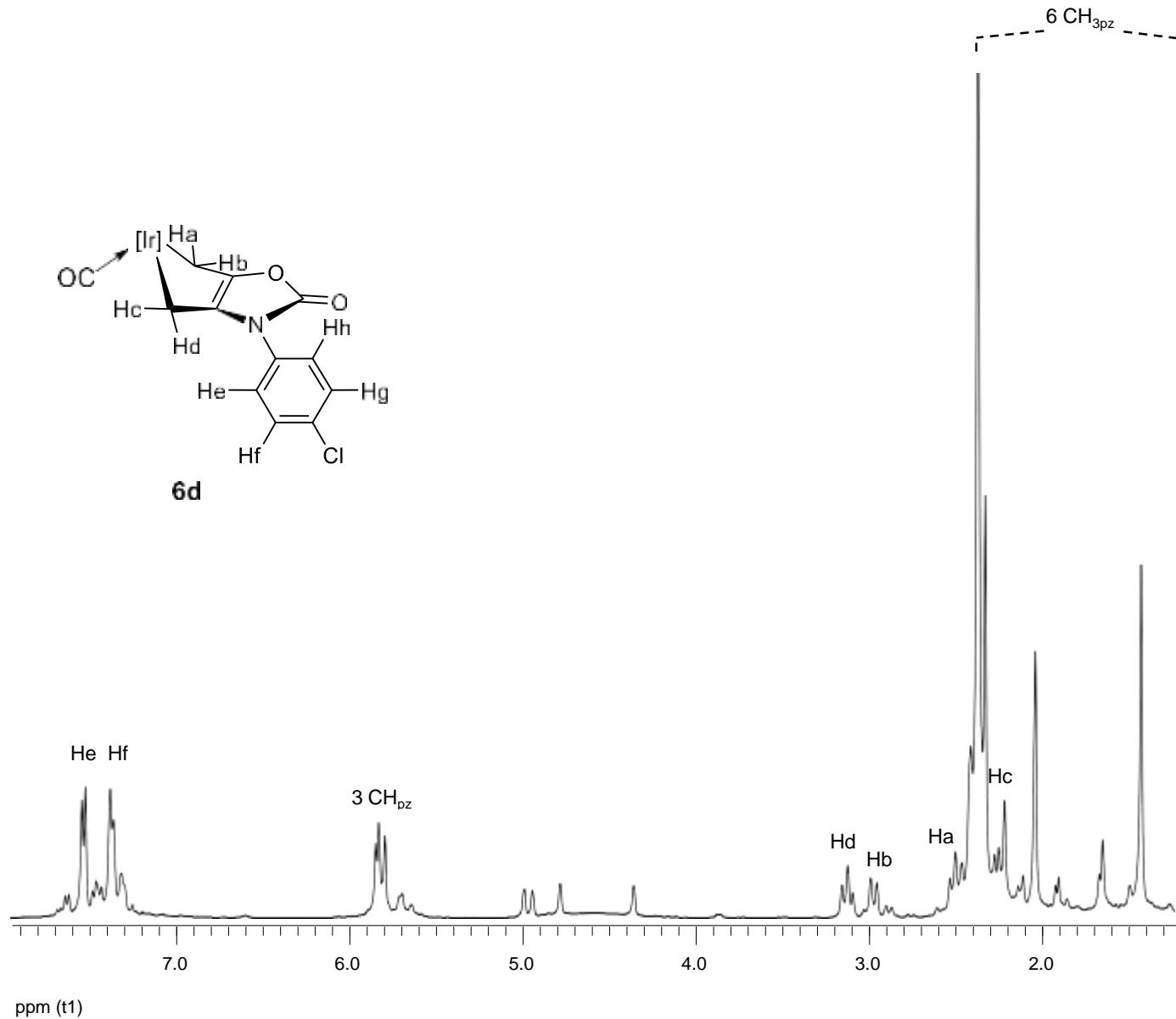
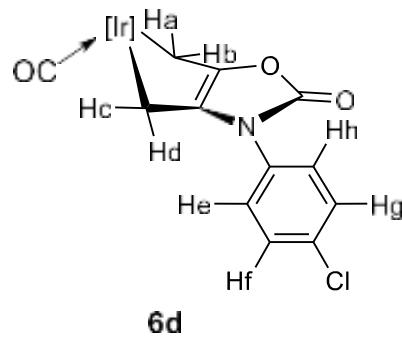


Figure S72. ^1H NMR (CDCl_3 , 25°C , 400 MHz) spectrum of **6d**.

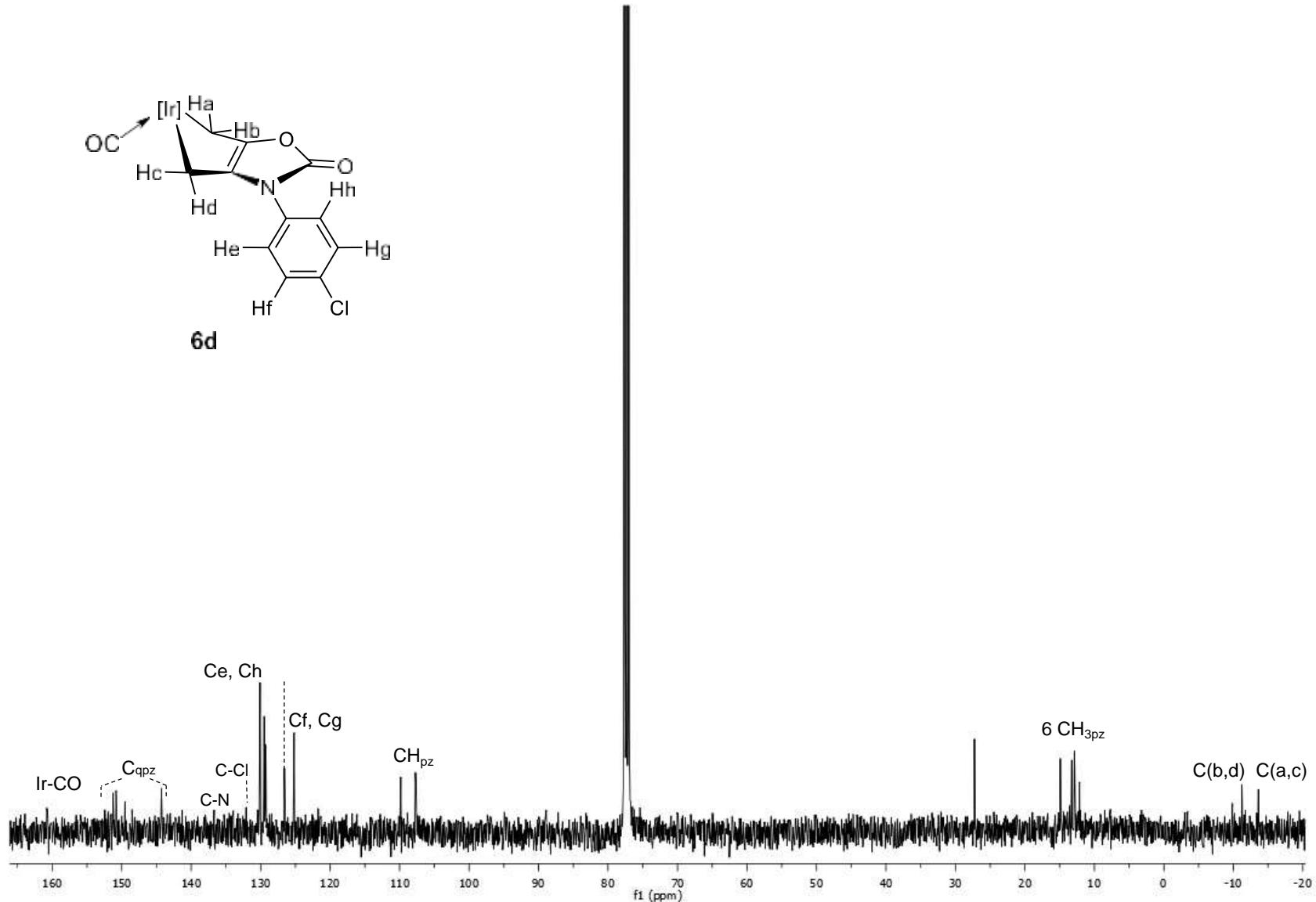
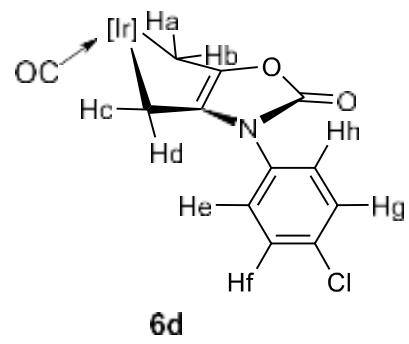


Figure S73. ^{13}C $\{\text{H}\}$ NMR (CDCl_3 , 25°C , 100.6 MHz) spectrum of **6d**.

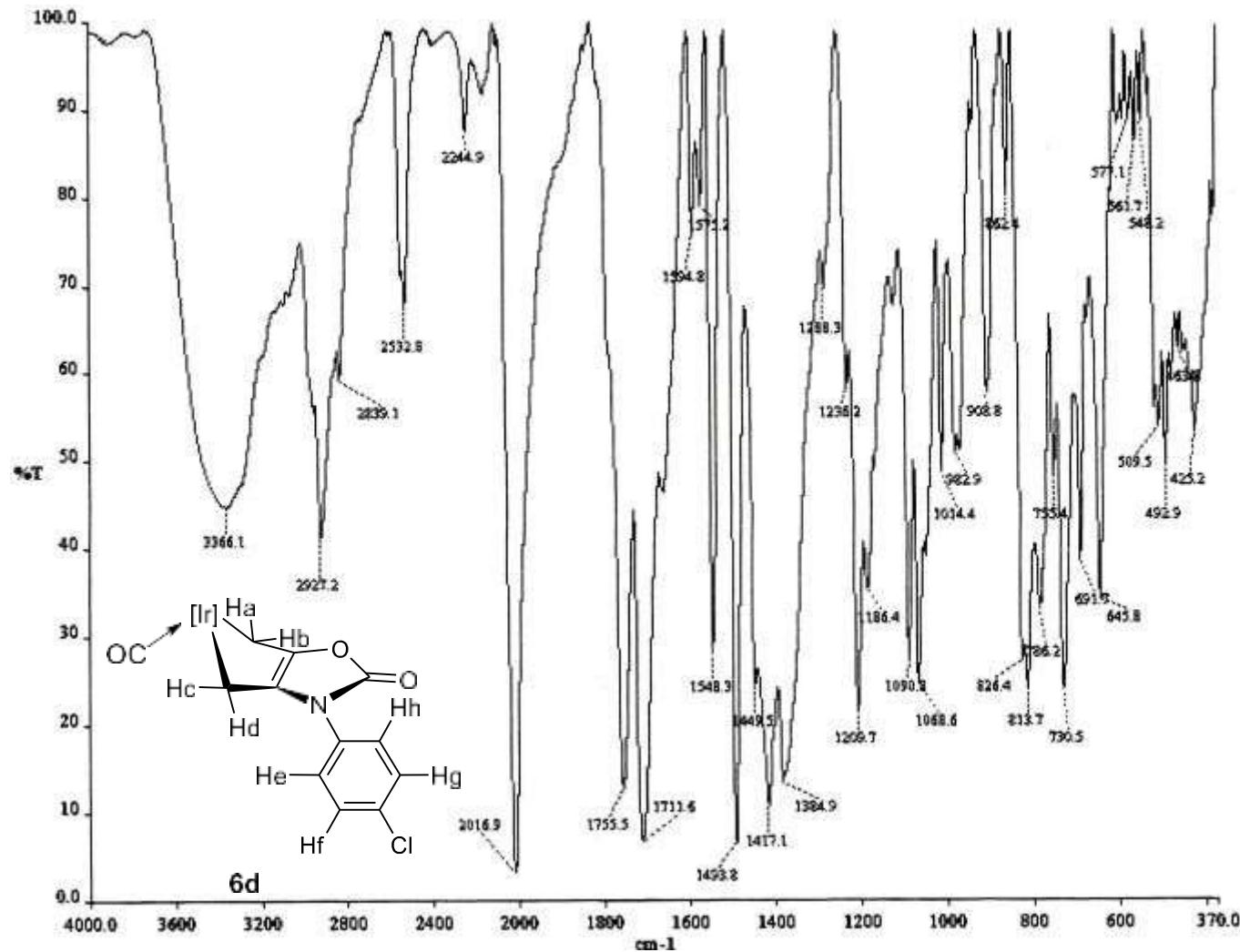


Figure S74. IR spectrum of **6d**.

Elemental Composition Report

Multiple Mass Analysis: 5 mass(es) processed

Tolerance = 15.0 PPM / DBE: min = -50.0, max = 50.0

Isotope cluster parameters: Separation = 1.0 Abundance = 1.0%

Monoisotopic Mass, Odd and Even Electron Ions

319 formula(e) evaluated with 2 results within limits (up to 50 closest results for each mass)

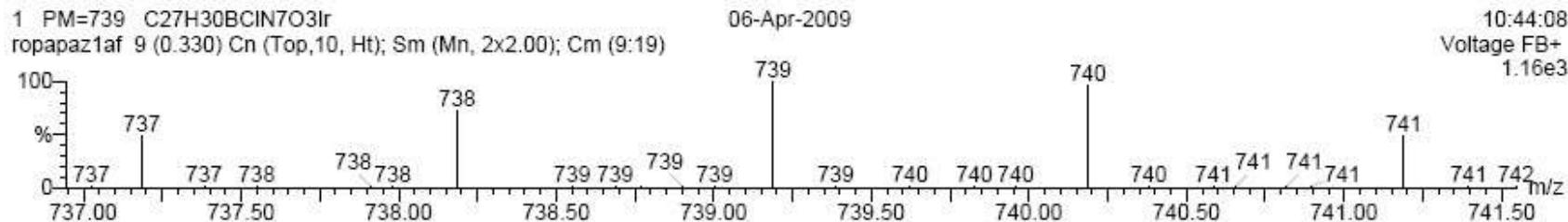
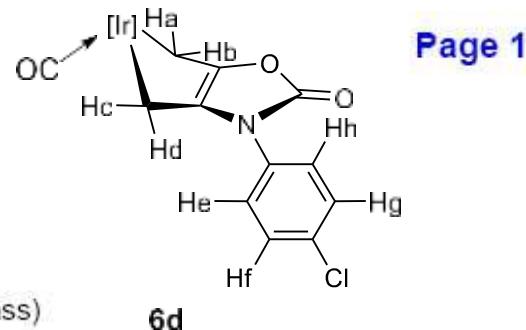


Figure S75. MS Spectra of complex **6d**.

DFT calculations data annex

Minimum 2'

Optimized coordinates at the VWN/3-21G/GEN-A2 level of theory

C	0.0000	0.0000	0.0000
O	0.0000	0.0000	1.2119
N	1.0494	0.0000	-0.9088
C	0.5932	-0.1723	-2.2193
C	-0.8342	-0.1697	-2.1323
O	-1.2064	-0.0214	-0.7879
C	-1.6453	-0.4489	-3.2938
C	1.1971	-0.4735	-3.5099
H	2.0193	-0.0912	-0.5989
H	-2.6854	-0.7655	-3.1090
H	2.2500	-0.8049	-3.5179
H	-1.4751	0.1624	-4.1978
H	0.8961	0.1615	-4.3629
Ir	-0.2117	-2.0118	-3.0248
N	-0.4329	-3.2869	-4.6094
C	-0.5828	-3.0598	-5.9329
C	-0.7440	-4.2828	-6.6085
C	-0.6797	-5.2678	-5.6246
N	-0.4948	-4.6599	-4.4205
B	-0.3560	-5.2246	-2.9998
N	-1.4663	-4.6141	-2.1321
C	-2.3654	-5.1794	-1.2767
C	-3.0321	-4.1587	-0.6038
C	-2.4831	-2.9564	-1.0889
N	-1.5415	-3.2342	-2.0203
N	0.9859	-4.7131	-2.4351
C	2.0562	-5.3821	-1.9219
C	3.0144	-4.4489	-1.5330
C	2.4615	-3.1925	-1.8399
N	1.2335	-3.3488	-2.3855
H	-0.8863	-4.4294	-7.6773
H	3.9861	-4.6500	-1.0867
H	-3.8076	-4.2656	0.1514
H	2.0578	-6.4696	-1.8729
H	-2.4590	-6.2615	-1.2058
H	-0.7536	-6.3521	-5.6936
H	-0.5655	-2.0353	-6.3047
H	2.8724	-2.1919	-1.7052
H	-2.6553	-1.9186	-0.7968
H	-0.4001	-6.4430	-2.9957

Transition state 2'- A'

Optimized coordinates at the VWN/3-21G/GEN-A2 level of theory

C	0.0000	0.0000	0.0000
O	0.0000	0.0000	1.2189
N	1.0462	0.0000	-0.9148
C	0.5652	-0.0218	-2.2263
C	-0.7925	-0.0234	-2.1453
O	-1.1838	-0.0015	-0.8021
C	-1.6651	-0.0261	-3.3319
C	1.2395	-0.0436	-3.5451
H	2.0226	-0.0192	-0.6150
H	-2.5112	-0.7480	-3.2529
H	-2.0707	0.9773	-3.6059
H	1.6079	0.9540	-3.8856
H	2.0800	-0.7762	-3.6026
Ir	-0.3187	-0.6571	-4.8014
N	-0.3829	1.0179	-5.7374
C	-0.3516	2.2931	-5.2862
C	-0.4344	3.1610	-6.3915
C	-0.5171	2.3480	-7.5200
N	-0.4861	1.0430	-7.1257
B	-0.5547	-0.2870	-7.9123
N	-1.7722	-1.0667	-7.3867
C	-2.8769	-1.5554	-8.0158
C	-3.7057	-2.1395	-7.0603
C	-3.0448	-1.9674	-5.8293
N	-1.8711	-1.3237	-6.0240
N	0.7186	-1.0839	-7.5784
C	1.7031	-1.5920	-8.3704
C	2.6579	-2.1946	-7.5541
C	2.1976	-2.0133	-6.2362
N	1.0208	-1.3461	-6.2472
H	-0.4353	4.2487	-6.3657
H	-0.5969	2.6013	-8.5759
H	3.5692	-2.6989	-7.8703
H	-4.6651	-2.6246	-7.2302
H	-2.9958	-1.4498	-9.0929
H	1.6557	-1.4866	-9.4530
H	-0.2784	2.4799	-4.2139
H	2.6382	-2.3193	-5.2864
H	-3.3417	-2.2608	-4.8215
H	-0.6453	-0.0811	-9.1099

Minimum A'

Optimized coordinates at the VWN/3-21G/GEN-A2 level of theory

C	0.0000	0.0000	0.0000
O	0.0000	0.0000	1.2161
N	1.0559	0.0000	-0.9149
C	0.5831	0.0066	-2.2248
C	-0.7868	0.0098	-2.1476
O	-1.1785	0.0261	-0.8093
C	-1.6473	0.0238	-3.3303
C	1.2469	-0.0180	-3.5437
H	2.0319	0.0277	-0.6112
H	-2.0989	1.0170	-3.5569
H	-2.4449	-0.7555	-3.2759
H	1.6752	0.9655	-3.8520
H	2.0436	-0.8003	-3.6208
Ir	-0.3116	-0.4978	-4.8653
N	-0.3343	1.3257	-5.5851
C	-0.2853	2.5331	-4.9765
C	-0.3811	3.5458	-5.9498
C	-0.4947	2.8902	-7.1738
N	-0.4690	1.5451	-6.9516
B	-0.5664	0.3316	-7.8993
N	-1.7823	-0.5093	-7.4675
C	-2.8709	-0.9632	-8.1516
C	-3.6421	-1.7364	-7.2865
C	-2.9609	-1.7214	-6.0526
N	-1.8401	-0.9796	-6.1635
N	0.6962	-0.5254	-7.6809
C	1.6627	-0.9463	-8.5446
C	2.5926	-1.6992	-7.8317
C	2.1341	-1.7044	-6.4999
N	0.9875	-0.9964	-6.4064
H	-0.3715	4.6203	-5.7799
H	-4.5752	-2.2460	-7.5184
H	3.4844	-2.1844	-8.2235
H	-3.0163	-0.7056	-9.1993
H	-0.5931	3.2810	-8.1851
H	1.6179	-0.6805	-9.5994
H	-3.1882	-2.2012	-5.1003
H	2.5470	-2.1800	-5.6098
H	-0.1940	2.5743	-3.8896
O	-0.6206	-2.3152	-3.9277
C	-0.0948	-2.4150	-2.7424
C	-0.8557	-2.8807	-1.6163
C	-0.2658	-2.8661	-0.3402
C	-1.0420	-3.1339	0.7854
C	-2.3953	-3.4555	0.6376
C	-2.9824	-3.4905	-0.6381
C	-2.2221	-3.1897	-1.7607
H	-0.5940	-3.0751	1.7836
H	-3.0049	-3.6684	1.5243
H	-4.0466	-3.7367	-0.7421
H	-2.6524	-3.1586	-2.7710
H	0.7945	-2.5972	-0.2410
H	0.9814	-2.2122	-2.5926
H	-0.6630	0.6870	-9.0614

Transition state A' - B'

Optimized coordinates at the VWN/3-21G/GEN-A2 level of theory

C	0.0000	0.0000	0.0000
O	0.0000	0.0000	1.2135
O	1.1282	0.0000	-0.8273
N	-1.1151	0.0142	-0.8866
C	-0.7108	0.0502	-2.1800
C	0.6966	0.1651	-2.1883
C	-1.4133	0.2159	-3.4523
C	1.4122	-0.3233	-3.3913
H	-2.0786	0.0334	-0.5370
H	1.4792	-1.4315	-3.4286
H	2.4117	0.1482	-3.5137
H	-2.0818	-0.6344	-3.7269
H	-2.0114	1.1646	-3.4608
Ir	0.1135	0.4101	-4.8574
N	-0.2746	-1.3625	-5.6361
C	-0.5233	-2.5672	-5.0716
C	-0.7147	-3.5273	-6.0836
C	-0.5656	-2.8451	-7.2884
N	-0.2979	-1.5360	-7.0157
B	-0.0212	-0.3255	-7.9289
N	-1.0604	0.7597	-7.5912
C	-1.9521	1.4379	-8.3676
C	-2.6274	2.3530	-7.5637
C	-2.0942	2.1874	-6.2703
N	-1.1485	1.2230	-6.2855
N	1.3683	0.2292	-7.5638
C	2.4788	0.4627	-8.3192
C	3.4610	1.0106	-7.4978
C	2.8820	1.0928	-6.2158
N	1.6193	0.6205	-6.2552
H	4.4651	1.3130	-7.7880
H	-0.9288	-4.5858	-5.9512
H	-3.3992	3.0551	-7.8732
H	-0.6266	-3.1938	-8.3179
H	2.4884	0.2233	-9.3811
H	-2.0372	1.2234	-9.4316
H	3.2869	1.4660	-5.2758
H	-0.5342	-2.6547	-3.9844
H	-2.3082	2.7164	-5.3409
O	0.7830	2.1120	-3.9257
C	0.6988	2.0897	-2.5830
C	1.8804	2.5591	-1.8454
C	3.0917	2.7104	-2.5332
C	4.2412	3.0971	-1.8489
C	1.8238	2.7862	-0.4644
C	2.9764	3.1659	0.2220
C	4.1851	3.3212	-0.4672
H	2.9352	3.3429	1.3034
H	5.0894	3.6216	0.0768
H	5.1881	3.2284	-2.3880
H	0.8742	2.6549	0.0735
H	3.0724	2.5359	-3.6174
H	-0.2747	2.3401	-2.1031
H	-0.0759	-0.6409	-9.1054

Minimum B'

Optimized coordinates at the VWN/3-21G/GEN-A2 level of theory

C	0.0000	0.0000	0.0000
O	0.0000	0.0000	1.2132
O	1.1428	0.0000	-0.7998
N	-1.1310	0.0515	-0.8525
C	-0.7576	0.2140	-2.1792
C	-1.4531	0.8025	-3.2454
H	-2.0558	0.2761	-0.4719
C	0.6784	-0.3212	-2.1684
C	0.3675	-1.7761	-2.4022
C	1.5004	0.1809	-3.3514
O	0.6888	-0.1567	-4.5236
C	2.8408	-0.5165	-3.4163
C	3.1983	-1.1672	-4.6008
C	4.4162	-1.8460	-4.6889
C	5.2778	-1.8794	-3.5874
C	4.9161	-1.2294	-2.4022
C	3.7030	-0.5423	-2.3137
H	6.2342	-2.4131	-3.6512
H	5.5850	-1.2587	-1.5335
H	4.6983	-2.3480	-5.6239
H	2.4764	-1.1202	-5.4283
H	3.3920	-0.0625	-1.3769
H	-2.5224	1.0364	-3.1237
H	-0.8671	1.3474	-4.0042
H	1.2048	-2.3817	-2.7923
H	-0.1670	-2.2380	-1.5488
H	1.6241	1.2846	-3.2890
Ir	-0.9667	-1.2160	-3.9161
N	-2.5613	-2.2225	-3.2372
C	-3.0619	-2.3863	-1.9908
C	-4.1665	-3.2579	-2.0423
C	-4.3025	-3.6212	-3.3795
N	-3.3291	-2.9928	-4.0994
B	-2.9115	-3.0972	-5.5747
N	-2.8906	-1.6855	-6.1894
C	-3.4254	-1.1932	-7.3416
C	-2.9514	0.1041	-7.5269
C	-2.1013	0.3581	-6.4334
N	-2.0708	-0.7208	-5.6248
N	-1.4516	-3.6045	-5.6015
C	-0.8617	-4.6457	-6.2495
C	0.5112	-4.5957	-6.0113
C	0.7216	-3.4698	-5.1949
N	-0.4671	-2.8777	-4.9465
H	1.2665	-5.2833	-6.3855
H	-3.1809	0.7754	-8.3519
H	-4.7802	-3.5886	-1.2073
H	-5.0134	-4.2846	-3.8686
H	-4.0940	-1.8017	-7.9486
H	-1.4586	-5.3425	-6.8361
H	-1.4828	1.2253	-6.1976
H	-2.5665	-1.8891	-1.1542
H	1.6394	-3.0321	-4.7925
H	-3.6494	-3.8421	-6.1952

Transition state B' - C'

Optimized coordinates at the VWN/3-21G/GEN-A2 level of theory

H	-0.1563	-2.5479	-1.7096
H	-0.4474	0.6859	2.6360
H	-4.6486	-1.0072	0.4889
H	-2.4730	-5.3613	-0.6390
H	-2.3744	-0.8283	2.1024
H	-2.2467	3.5125	1.2908
H	1.8207	4.8148	-2.1443
H	-1.1159	-3.4768	0.3338
H	-1.5795	-0.5728	-1.6138
H	1.7980	-3.4173	-3.4715
H	3.9081	2.9897	-2.2811
H	3.8683	-1.6113	-3.0809
H	-4.9274	-5.0526	-1.0274
H	-6.0063	-2.8713	-0.4448
H	5.4526	-0.1513	0.9014
H	4.5294	-0.8273	3.4280
H	-0.1620	3.4301	-0.8122
H	1.7746	-0.6055	3.1872
H	4.4210	0.4855	-1.5013
H	-1.4842	1.2757	-1.5761
H	0.0624	2.3837	2.1585
B	3.3139	0.4063	-1.0304
C	-1.9401	-1.0243	1.0982
C	3.9523	-0.5295	2.5567
C	-4.3278	-4.2368	-0.6137
C	-0.4145	1.4475	1.8428
C	-1.6591	1.5671	1.1142
C	4.4383	-0.1907	1.2917
C	-3.8599	2.3588	0.2387
C	-4.1712	-1.9608	0.2496
C	-4.9332	-3.0110	-0.2839
C	-2.9509	-4.4066	-0.4003
C	0.8267	-2.1286	-1.9137
C	-2.1834	-3.3556	0.1318
C	-1.4529	0.3348	-1.0173
C	1.8340	-2.5657	-2.7979
C	2.8859	-1.6653	-2.6182
C	-2.7844	-2.1255	0.4533
C	0.8388	3.1021	-1.0841
C	1.8575	3.7976	-1.7644
C	2.9178	2.8926	-1.8437
C	-1.9071	0.3151	0.3210
C	2.5515	-0.4103	2.4515
N	3.3816	0.1179	0.4934
N	2.2222	-0.0156	1.2045
N	1.2456	-1.0311	-1.2526
N	2.5121	-0.7487	-1.6854
N	1.2609	1.8571	-0.7718
N	2.5389	1.7322	-1.2428
N	-2.4059	2.6107	0.8344
O	-4.0453	1.1303	0.0636
O	-4.5045	3.3978	0.1146
O	-0.5561	-1.3468	1.1940
Ir	0.3781	0.2468	0.2157

Minimum C'

Optimized coordinates at the VWN/3-21G/GEN-A2 level of theory

C	0.0000	0.0000	0.0000
N	0.0000	0.0000	1.2893
C	1.1152	0.0000	-0.9797
C	-1.1538	0.5297	-0.8066
C	-1.5912	1.8382	-0.5659
H	0.9445	-0.2498	1.6622
C	-1.5556	-0.1415	-2.1387
O	-0.6466	0.4956	-3.0993
C	-2.9899	0.1709	-2.4885
C	-3.2486	0.9449	-3.6227
C	-4.5594	1.3089	-3.9431
C	-5.6163	0.8965	-3.1255
C	-4.0473	-0.2543	-1.6783
C	-5.3569	0.1120	-1.9950
H	-6.6472	1.1802	-3.3711
H	-6.1839	-0.2185	-1.3543
H	-4.7586	1.9108	-4.8398
H	-2.3735	1.2442	-4.2176
H	-3.8426	-0.8633	-0.7859
H	-2.4140	2.2427	-1.1726
H	-1.3181	2.3551	0.3667
H	2.1332	0.1227	-0.5648
H	1.0319	-0.7335	-1.8069
H	-1.3727	-1.2366	-2.0913
Ir	0.2857	1.7855	-1.8008
N	1.1929	2.9666	-0.4418
C	1.2664	2.9112	0.9080
C	2.0094	4.0133	1.3738
C	2.3768	4.7355	0.2413
N	1.8779	4.1010	-0.8576
B	1.9158	4.4524	-2.3544
N	0.4586	4.5999	-2.8409
C	-0.1894	5.6276	-3.4572
C	-1.4970	5.2277	-3.7235
C	-1.6000	3.9086	-3.2406
N	-0.4180	3.5318	-2.7083
N	2.5078	3.2460	-3.1137
C	3.5025	3.1391	-4.0387
C	3.5180	1.8317	-4.5222
C	2.4804	1.1590	-3.8497
N	1.8818	2.0174	-3.0005
H	4.1882	1.4180	-5.2727
H	-2.2756	5.8131	-4.2080
H	2.2448	4.2521	2.4087
H	4.1196	4.0003	-4.2903
H	2.9529	5.6532	0.1369
H	0.3250	6.5652	-3.6614
H	2.0952	0.1416	-3.9389
H	-2.4317	3.1991	-3.2547
H	0.7686	2.0837	1.4301
H	2.5576	5.4672	-2.5593

Transition state C' - D'

Optimized coordinates at the VWN/3-21G/GEN-A2 level of theory

C	0.0000	0.0000	0.0000
N	0.0000	0.0000	1.3031
C	1.1687	0.0000	-0.8854
C	-1.2619	0.3506	-0.7302
C	-2.2242	1.0344	-0.0813
H	0.9625	-0.1919	1.6645
C	-1.2943	0.1177	-2.2424
C	-2.6901	0.1445	-2.7890
C	-3.3729	-1.0411	-3.0713
C	-4.6942	-1.0012	-3.5228
C	-5.3383	0.2271	-3.6974
C	-4.6546	1.4175	-3.4252
C	-3.3339	1.3744	-2.9774
O	-0.5544	1.2440	-2.8404
Ir	0.7408	1.9662	-1.5179
N	2.6182	2.1765	-2.0255
C	3.4955	1.3045	-2.5782
C	4.6906	1.9834	-2.8695
C	4.4941	3.3024	-2.4660
N	3.2389	3.4196	-1.9511
B	2.4830	4.6207	-1.3369
N	2.0195	4.1546	0.0463
C	2.1102	4.7049	1.2887
C	1.4604	3.8652	2.1903
C	0.9708	2.7810	1.4383
N	1.3146	2.9578	0.1388
N	1.2369	4.8601	-2.2093
C	0.8713	5.8921	-3.0202
C	-0.2692	5.5126	-3.7271
C	-0.5618	4.2015	-3.3070
N	0.3436	3.8144	-2.3827
H	5.5837	1.5609	-3.3247
H	-0.8134	6.1048	-4.4599
H	1.3508	4.0132	3.2625
H	1.4492	6.8145	-3.0409
H	5.1548	4.1670	-2.5045
H	2.6274	5.6510	1.4390
H	3.1967	0.2700	-2.7454
H	-1.3207	3.4861	-3.6251
H	-3.1471	1.3365	-0.5918
H	-5.2227	-1.9364	-3.7452
H	-6.3761	0.2580	-4.0522
H	-2.0569	1.2989	0.9712
H	-5.1574	2.3834	-3.5658
H	-2.8588	-2.0028	-2.9363
H	-2.7700	2.2907	-2.7562
H	0.3849	1.8867	1.7151
H	2.1398	-0.0857	-0.3600
H	1.1027	-0.6478	-1.7844
H	-0.8056	-0.8470	-2.5015
H	3.1921	5.6101	-1.2848

Minimum D'

Optimized coordinates at the VWN/3-21G/GEN-A2 level of theory

C	0.0000	0.0000	0.0000
N	0.0000	0.0000	1.3033
C	1.2063	0.0000	-0.8476
C	-1.3017	0.1693	-0.7042
C	-2.4427	0.1054	-0.0047
C	-1.2460	0.4394	-2.1873
C	-2.5948	0.6886	-2.7881
C	-3.2208	-0.2524	-3.6074
C	-4.4954	0.0043	-4.1210
C	-5.1425	1.2058	-3.8200
C	-4.5122	2.1542	-3.0044
C	-3.2415	1.8958	-2.4916
O	-0.4400	1.6637	-2.4195
Ir	1.1967	1.9961	-1.4731
N	1.5405	2.9166	0.2612
C	0.9501	2.7549	1.4712
C	1.3732	3.7933	2.3201
C	2.2380	4.5881	1.5707
N	2.3424	4.0569	0.3225
B	3.1199	4.4957	-0.9293
N	2.0808	4.8441	-2.0079
C	1.8517	5.9639	-2.7491
C	0.7290	5.7395	-3.5463
C	0.2985	4.4334	-3.2440
N	1.1176	3.8985	-2.3140
N	3.8937	3.2390	-1.3716
C	5.2180	3.0079	-1.5825
C	5.3899	1.6564	-1.8767
C	4.1063	1.0857	-1.8290
N	3.1992	2.0451	-1.5291
H	0.9699	-0.1455	1.6689
H	6.3239	1.1451	-2.0994
H	0.2807	6.4314	-4.2562
H	1.0796	3.9388	3.3573
H	5.9402	3.8189	-1.5040
H	2.4969	6.8356	-2.6553
H	2.7900	5.4888	1.8338
H	3.7731	0.0633	-2.0068
H	-0.5298	3.8272	-3.6148
H	-6.1423	1.4071	-4.2245
H	-4.9836	-0.7379	-4.7646
H	-5.0190	3.0988	-2.7684
H	-3.4180	0.2450	-0.4838
H	-2.7183	2.6172	-1.8493
H	-2.7036	-1.1925	-3.8438
H	-2.3677	-0.0669	1.0765
H	0.2786	1.8929	1.6377
H	2.1277	-0.2480	-0.2799
H	1.1165	-0.6134	-1.7746
H	-0.7332	-0.3961	-2.7155
H	3.8697	5.4299	-0.7051

Transition state D' - E'

Optimized coordinates at the VWN/3-21G/GEN-A2 level of theory

C	0.0000	0.0000	0.0000
N	0.0000	0.0000	1.3067
C	1.2004	0.0000	-0.8480
C	-1.2920	0.0627	-0.7383
C	-2.2724	-0.7870	-0.4029
H	0.9777	-0.1692	1.6472
C	-1.5339	1.0999	-1.8215
O	-0.3622	1.5724	-2.5697
Ir	1.1641	2.0226	-1.3814
N	3.0380	1.8639	-1.9282
C	3.7259	0.8456	-2.4969
C	5.0099	1.3009	-2.8408
C	5.0650	2.6366	-2.4484
N	3.8707	2.9787	-1.8911
N	1.9900	2.8115	0.2521
C	1.6638	2.6323	1.5568
C	2.3784	3.5625	2.3343
C	3.1497	4.3067	1.4424
N	2.9109	3.8510	0.1812
B	3.3882	4.2835	-1.2174
N	2.1566	4.8066	-1.9722
C	1.8534	6.0141	-2.5275
C	0.5429	5.9614	-3.0002
C	0.0753	4.6655	-2.7033
N	1.0547	3.9730	-2.0862
C	-2.0696	2.3854	-1.2126
C	-3.0414	3.1444	-1.8646
C	-1.3792	2.9384	-0.1261
C	-1.6284	4.2469	0.2870
C	-3.3124	4.4533	-1.4414
C	-2.5991	5.0100	-0.3752
H	5.7971	0.7244	-3.3220
H	2.3412	3.6690	3.4164
H	-0.0053	6.7579	-3.4989
H	5.8671	3.3693	-2.5214
H	2.5863	6.8189	-2.5450
H	3.8502	5.1221	1.6146
H	3.2431	-0.1219	-2.6352
H	-0.8933	4.1864	-2.8661
H	-2.1346	-1.4807	0.4343
H	-2.7990	6.0406	-0.0583
H	-4.0728	5.0481	-1.9633
H	0.9275	1.8610	1.8226
H	-1.0437	4.6717	1.1148
H	-3.2291	-0.8034	-0.9424
H	-3.5626	2.7185	-2.7332
H	-2.2622	0.6987	-2.5548
H	-0.6272	2.3261	0.4011
H	1.0854	-0.5742	-1.7923
H	2.1323	-0.2486	-0.2965
H	4.2798	5.1126	-1.1730

Minimum E'

Optimized coordinates at the VWN/3-21G/GEN-A2 level of theory

C	0.0000	0.0000	0.0000
N	0.0000	0.0000	1.2977
C	1.2095	0.0000	-0.8602
C	-1.3052	0.1275	-0.7036
C	-2.3297	-0.6705	-0.3750
C	-1.4758	1.2364	-1.7239
O	-0.3974	1.2869	-2.7057
C	-1.4656	2.5807	-1.0423
C	-2.5033	3.5095	-1.1065
C	-2.3205	4.8080	-0.6113
C	-1.0869	5.2021	-0.0743
C	-0.0292	4.2919	-0.0285
C	-0.2230	2.9916	-0.5114
H	0.9806	-0.1297	1.6502
H	-0.9528	6.2241	0.2999
H	-3.1500	5.5251	-0.6546
H	-2.2157	-1.4269	0.4102
H	-3.4586	3.2179	-1.5621
H	0.9681	4.5754	0.3397
H	-3.3058	-0.5812	-0.8715
Ir	1.2736	1.9065	-1.7295
N	2.3175	1.1591	-3.2375
C	2.0640	0.1206	-4.0591
C	3.0565	0.0776	-5.0549
C	3.9057	1.1538	-4.7982
N	3.4531	1.8119	-3.6953
B	3.8313	3.1801	-3.0831
N	2.6119	4.0973	-3.2970
C	2.4384	5.2519	-4.0013
C	1.0929	5.6094	-3.9335
C	0.4674	4.6099	-3.1610
N	1.3875	3.7024	-2.7783
N	4.0236	2.9883	-1.5679
C	5.0732	3.2618	-0.7420
C	4.7220	2.8955	0.5552
C	3.4145	2.3806	0.4669
N	2.9911	2.4419	-0.8175
H	3.1376	-0.6414	-5.8674
H	5.3355	2.9812	1.4499
H	0.6219	6.4753	-4.3940
H	4.7911	1.5045	-5.3262
H	5.9924	3.6910	-1.1372
H	3.2788	5.7308	-4.5012
H	1.1601	-0.4690	-3.8977
H	2.7533	1.9642	1.2300
H	-0.5744	4.4704	-2.8620
H	1.1240	-0.6947	-1.7201
H	-2.4363	1.0848	-2.2597
H	2.1448	-0.1769	-0.2812
H	0.4887	2.1667	-0.0584
H	4.8351	3.6339	-3.6031

Transition state E' - F'

Optimized coordinates at the VWN/3-21G/GEN-A2 level of theory

C	0.0000	0.0000	0.0000
N	0.0000	0.0000	1.2894
C	1.3102	0.0000	-0.7021
C	2.3744	0.5067	-0.0621
C	-1.2432	0.0857	-0.8372
C	1.4456	-0.6319	-2.0684
O	0.4128	-0.1593	-2.9900
C	1.3221	-2.1296	-1.9447
C	2.3851	-3.0049	-1.7207
C	2.1478	-4.3826	-1.6465
C	0.8499	-4.8824	-1.8031
C	-0.2188	-4.0040	-2.0321
C	0.0153	-2.6294	-2.1014
H	-0.9713	0.0613	1.6776
Ir	-1.2971	-1.1811	-2.6597
N	-1.1812	-1.9529	-4.5338
C	-0.1297	-2.4476	-5.2168
C	-0.5571	-2.8301	-6.5008
C	-1.9205	-2.5354	-6.5535
N	-2.2942	-2.0036	-5.3583
B	-3.6344	-1.4438	-4.8336
N	-3.9585	-2.2070	-3.5405
C	-5.0043	-3.0218	-3.2242
C	-4.7695	-3.5749	-1.9682
C	-3.5305	-3.0566	-1.5497
N	-3.0408	-2.2236	-2.4988
N	-3.3813	0.0362	-4.5013
C	-3.8096	1.1745	-5.1141
C	-3.0775	2.2484	-4.6110
C	-2.1831	1.6922	-3.6773
N	-2.3766	0.3589	-3.6008
H	0.0514	-3.2609	-7.2928
H	-3.1663	3.2951	-4.8951
H	-5.4103	-4.2652	-1.4233
H	-4.5916	1.1372	-5.8708
H	-2.6467	-2.6629	-7.3548
H	-5.8335	-3.1499	-3.9182
H	-2.9549	-3.2340	-0.6402
H	0.8470	-2.4820	-4.7320
H	-1.3808	2.1566	-3.1015
H	2.2517	0.8862	0.9592
H	2.9835	-5.0699	-1.4689
H	3.3688	0.5204	-0.5269
H	0.6701	-5.9640	-1.7517
H	3.4017	-2.6074	-1.5990
H	-1.2429	-4.3777	-2.1908
H	-1.2182	0.9946	-1.4678
H	-2.1673	0.0731	-0.2207
H	2.4380	-0.3514	-2.4821
H	-1.3330	-1.4392	-1.0625
H	-4.5243	-1.5700	-5.6560

Minimum F'

Optimized coordinates at the VWN/3-21G/GEN-A2 level of theory

C	-0.1688	0.2427	-0.1304
N	-0.2225	0.4551	1.1466
C	1.1709	0.1047	-0.7754
C	1.3071	0.1169	-2.1232
H	-1.2117	0.5206	1.4411
C	-1.3984	0.1178	-1.0156
C	2.4129	-0.0776	0.0900
O	2.2904	-1.2955	0.8557
C	2.7973	1.0828	0.9833
C	2.9365	2.3998	0.5182
C	3.3686	3.4119	1.3920
C	3.6707	3.0946	2.7286
C	3.5357	1.7730	3.1902
C	3.0959	0.7382	2.3341
Ir	2.7708	-1.2095	2.7378
N	4.3802	-1.5114	3.9677
C	5.6557	-1.0773	3.8666
C	6.4378	-1.6869	4.8680
C	5.5531	-2.5059	5.5744
N	4.3181	-2.3868	5.0178
B	2.9473	-3.0084	5.3992
N	2.4568	-3.8928	4.2249
C	2.0827	-5.2013	4.1793
C	1.6945	-5.4979	2.8702
N	2.3226	-3.3315	2.9869
C	1.8632	-4.2896	2.1599
N	1.9715	-1.8118	5.5598
C	1.1548	-1.4331	6.5792
C	0.4822	-0.2686	6.1987
N	1.8428	-0.9198	4.5298
C	0.9459	0.0201	4.8991
H	5.7102	-3.1615	6.4276
H	5.9209	-0.3623	3.0910
H	7.4986	-1.5447	5.0536
H	0.6954	0.8189	4.2039
H	-0.2409	0.2959	6.7807
H	1.1115	-2.0187	7.4941
H	2.1200	-5.8208	5.0724
H	1.6833	-4.0510	1.1130
H	1.3409	-6.4508	2.4855
H	0.4603	0.2478	-2.8008
H	3.4694	4.4403	1.0340
H	2.2920	0.0070	-2.5860
H	4.0095	3.8791	3.4127
H	3.7722	1.5437	4.2352
H	2.6980	2.6401	-0.5239
H	-1.4381	0.9288	-1.7609
H	-2.3123	0.1710	-0.4060
H	-1.3973	-0.8366	-1.5660
H	3.2478	-0.2561	-0.6166
H	3.0269	-3.6461	6.4195

Transition state F'- 4'

Optimized coordinates at the VWN/3-21G/GEN-A2 level of theory

C	0.0000	0.0000	0.0000
N	0.0000	0.0000	1.2969
C	1.3087	0.0000	-0.7209
C	1.3608	0.0957	-2.0717
H	-0.9728	-0.0054	1.6437
C	-1.2737	-0.0083	-0.8306
C	2.6132	-0.1171	0.0696
O	2.5811	-1.3332	0.8317
C	2.9186	1.0768	0.9551
C	3.0802	2.3761	0.4497
C	3.4180	3.4313	1.3143
C	3.5994	3.1743	2.6850
C	3.4359	1.8717	3.1902
C	3.0810	0.7975	2.3447
Ir	2.7210	-1.1372	2.7809
N	4.3471	-1.4871	3.9124
C	5.6313	-1.0973	3.7540
C	6.4378	-1.7688	4.6938
C	5.5603	-2.5770	5.4208
N	4.3012	-2.3942	4.9393
B	2.9393	-3.0152	5.3655
N	2.3990	-3.8669	4.1891
C	2.0325	-5.1756	4.1008
C	1.6191	-5.4233	2.7886
N	2.2368	-3.2596	2.9783
C	1.7676	-4.1873	2.1220
N	1.9742	-1.8227	5.6000
C	1.1562	-1.5041	6.6394
C	0.4704	-0.3297	6.3174
N	1.8328	-0.8859	4.6123
C	0.9284	0.0245	5.0315
H	5.7365	-3.2678	6.2414
H	5.8804	-0.3687	2.9870
H	7.5122	-1.6756	4.8248
H	0.6697	0.8570	4.3809
H	-0.2564	0.1990	6.9279
H	1.1217	-2.1335	7.5253
H	2.0916	-5.8299	4.9674
H	1.5747	-3.9079	1.0879
H	1.2636	-6.3635	2.3747
H	0.4678	0.2006	-2.6924
H	3.5423	4.4442	0.9209
H	2.3206	0.0762	-2.5957
H	3.8654	3.9919	3.3625
H	3.5754	1.6903	4.2612
H	2.9384	2.5689	-0.6200
H	-1.3541	0.9028	-1.4460
H	-2.1546	-0.0570	-0.1740
H	-1.3011	-0.8721	-1.5146
H	3.4209	-0.2199	-0.6844
H	3.0627	-3.6815	6.3628

Minimum 4'

Optimized coordinates at the VWN/3-21G/GEN-A2 level of theory

C	0.0000	0.0000	0.0000
N	0.0000	0.0000	1.3114
C	1.2359	0.0000	-0.7748
Ir	1.5281	0.0145	2.5624
C	1.1968	-0.1550	-2.1158
C	-1.3098	-0.0409	-0.7340
C	2.1667	1.7442	1.7773
C	2.2548	3.0019	2.3841
C	2.8242	4.0800	1.6920
C	3.3162	3.9033	0.3931
C	3.2447	2.6457	-0.2186
C	2.6730	1.5759	0.4696
C	2.5555	0.1684	-0.0566
O	2.6242	-0.7714	1.0580
H	-0.9412	-0.0199	1.7583
N	3.0899	0.0069	3.8307
C	4.3804	0.3592	3.6665
C	5.0709	0.1603	4.8769
C	4.1269	-0.3283	5.7797
N	2.9262	-0.4186	5.1424
B	1.5326	-0.8857	5.6114
N	1.1234	-2.0724	4.7210
C	0.8972	-3.3874	4.9981
C	0.6921	-4.0601	3.7946
C	0.8145	-3.0820	2.7871
N	1.0682	-1.8827	3.3490
N	0.5549	0.2780	5.3498
C	-0.2250	1.0123	6.1939
C	-0.8389	2.0249	5.4609
C	-0.3869	1.8691	4.1361
N	0.4539	0.8083	4.0680
H	6.1257	0.3452	5.0684
H	0.4932	-5.1220	3.6635
H	-1.5208	2.7851	5.8367
H	4.2234	-0.6188	6.8246
H	-0.2803	0.7635	7.2526
H	0.9072	-3.7503	6.0246
H	0.7800	-3.1570	1.6993
H	4.7051	0.7210	2.6899
H	-0.5643	2.4656	3.2396
H	3.7695	4.7458	-0.1429
H	0.2595	-0.2787	-2.6704
H	2.1276	-0.1695	-2.6949
H	2.8943	5.0649	2.1722
H	3.6441	2.4983	-1.2316
H	1.8893	3.1187	3.4167
H	-2.1593	-0.0372	-0.0235
H	-1.3979	0.8315	-1.4085
H	-1.3700	-0.9550	-1.3563
H	3.3695	-0.0625	-0.7771
H	1.5414	-1.1957	6.7902

Minimum 2''

Optimized coordinates at the VWN/3-21G/GEN-A2 level of theory

C	0.0000	0.0000	0.0000
O	0.0000	0.0000	1.2193
N	1.0661	0.0000	-0.9068
C	2.4209	0.0106	-0.5041
C	3.4330	-0.2105	-1.4515
C	4.7726	-0.1379	-1.0700
C	5.1205	0.1381	0.2546
C	4.1074	0.3245	1.1990
C	2.7641	0.2611	0.8338
C	0.5699	0.2050	-2.2191
C	-0.8561	0.2120	-2.1053
C	-1.6986	0.5482	-3.2263
O	-1.2064	0.0387	-0.7573
C	1.1189	0.5452	-3.5330
H	3.1675	-0.4424	-2.4879
H	1.9564	0.3799	1.5627
H	6.1742	0.1928	0.5512
H	5.5524	-0.3110	-1.8221
H	4.3620	0.5235	2.2471
H	2.1668	0.8767	-3.5846
H	-2.7277	0.8672	-2.9922
H	-1.5615	-0.0207	-4.1626
H	0.7691	-0.0647	-4.3863
Ir	-0.2278	2.0785	-2.9293
N	-0.4921	3.4214	-4.4453
C	-0.7126	3.2496	-5.7677
C	-0.8663	4.5021	-6.3881
C	-0.7275	5.4455	-5.3713
N	-0.5026	4.7865	-4.2021
B	-0.2789	5.2900	-2.7681
N	-1.3712	4.6746	-1.8791
C	-2.2269	5.2297	-0.9747
C	-2.9075	4.2020	-0.3261
C	-2.4145	3.0059	-0.8812
N	-1.4897	3.2945	-1.8258
N	1.0683	4.7208	-2.2852
C	2.1720	5.3377	-1.7778
C	3.1090	4.3623	-1.4472
C	2.5125	3.1310	-1.7778
N	1.2766	3.3479	-2.2882
H	4.0958	4.5161	-1.0164
H	-3.6575	4.3003	0.4555
H	-1.0538	4.6946	-7.4425
H	2.2078	6.4221	-1.6897
H	-2.2834	6.3101	-0.8553
H	-0.7717	6.5334	-5.3953
H	-0.7441	2.2403	-6.1782
H	-2.6189	1.9624	-0.6348
H	2.8900	2.1123	-1.6592
H	-0.2905	6.5082	-2.7157

Transition state 2''- A''

Optimized coordinates at the VWN/3-21G/GEN-A2 level of theory

C	0.0000	0.0000	0.0000
O	0.0000	0.0000	1.2248
N	1.0688	0.0000	-0.9146
C	2.4195	-0.0584	-0.5138
C	3.4241	-0.3379	-1.4536
C	4.7591	-0.3864	-1.0559
C	5.1125	-0.1671	0.2778
C	4.1072	0.0902	1.2135
C	2.7687	0.1446	0.8321
C	0.5481	0.0763	-2.2262
C	-0.8071	0.0822	-2.1211
O	-1.1802	0.0222	-0.7731
C	-1.7114	0.1392	-3.2803
C	1.1681	0.2161	-3.5694
H	3.1532	-0.5334	-2.4965
H	1.9609	0.3093	1.5526
H	6.1633	-0.2068	0.5874
H	4.3651	0.2512	2.2677
H	5.5318	-0.6093	-1.8026
H	2.0081	0.9486	-3.5830
H	-2.5860	0.8112	-3.1219
H	1.5352	-0.7459	-4.0026
H	-2.0757	-0.8586	-3.6214
Ir	-0.4223	0.9490	-4.7088
N	-0.4965	-0.5943	-5.8500
C	-0.4393	-1.9170	-5.5711
C	-0.5443	-2.6344	-6.7776
C	-0.6663	-1.6822	-7.7874
N	-0.6372	-0.4397	-7.2267
B	-0.7338	0.9787	-7.8366
N	-1.9423	1.6747	-7.1878
C	-3.0578	2.2450	-7.7216
C	-3.8605	2.7026	-6.6787
C	-3.1723	2.3698	-5.4967
N	-2.0077	1.7525	-5.8017
N	0.5414	1.7392	-7.4331
C	1.4986	2.3646	-8.1728
C	2.4643	2.8712	-7.3053
C	2.0392	2.5107	-6.0126
N	0.8724	1.8299	-6.0864
H	-0.5337	-3.7161	-6.8944
H	3.3598	3.4290	-7.5725
H	-4.8203	3.2091	-6.7613
H	-0.7723	-1.7962	-8.8649
H	1.4267	2.4017	-9.2585
H	-3.2024	2.2812	-8.8001
H	-0.3320	-2.2436	-4.5360
H	2.4979	2.6964	-5.0405
H	-3.4432	2.5320	-4.4526
H	-0.8520	0.9235	-9.0480

Minimum A''

Optimized coordinates at the VWN/3-21G/GEN-A2 level of theory

C	0.0000	0.0000	0.0000
O	0.0000	0.0000	1.2269
N	1.0676	0.0000	-0.9158
C	2.4185	-0.0076	-0.5135
C	3.4464	-0.0652	-1.4685
C	4.7806	-0.0723	-1.0650
C	5.1165	-0.0233	0.2897
C	4.0917	0.0306	1.2379
C	2.7536	0.0383	0.8522
C	0.5317	0.0100	-2.2330
C	-0.8131	0.0080	-2.1175
O	-1.1819	-0.0037	-0.7646
C	-1.7348	0.0329	-3.2608
C	1.1340	0.0483	-3.5888
H	3.1979	-0.1083	-2.5334
H	6.1669	-0.0287	0.6037
H	1.9332	0.0720	1.5771
H	4.3338	0.0677	2.3076
H	5.5684	-0.1185	-1.8279
H	-2.3975	-0.8632	-3.3174
H	-2.3466	0.9656	-3.2930
H	1.7682	-0.8408	-3.8186
H	1.7171	0.9825	-3.7690
Ir	-0.4750	-0.0013	-4.9270
N	-0.4498	-1.9676	-4.8578
C	-0.3252	-2.8439	-3.8364
C	-0.3702	-4.1532	-4.3467
C	-0.5287	-4.0221	-5.7270
N	-0.5769	-2.6976	-6.0385
B	-0.7436	-1.9623	-7.3846
N	-1.9962	-1.0681	-7.2845
C	-3.1336	-1.0043	-8.0320
C	-3.9633	-0.0238	-7.4899
C	-3.2688	0.4881	-6.3760
N	-2.0768	-0.1417	-6.2538
N	0.4763	-1.0374	-7.5764
C	1.3946	-0.9380	-8.5782
C	2.3015	0.0677	-8.2471
C	1.8841	0.5578	-6.9937
N	0.7777	-0.1093	-6.5891
O	-0.5059	1.9832	-5.0242
C	-0.6437	2.6338	-6.1194
H	-0.2986	-5.0796	-3.7809
H	-4.9503	0.2692	-7.8435
H	3.1617	0.3928	-8.8294
H	-0.6118	-4.7766	-6.5074
H	-3.2755	-1.6645	-8.8862
H	1.3423	-1.5921	-9.4472
H	-3.5598	1.2372	-5.6376
H	2.3202	1.3203	-6.3460
H	-0.2177	-2.4429	-2.8244
H	-0.6519	3.7331	-6.0680
H	-0.7520	2.0915	-7.0761
H	-0.8440	-2.7529	-8.3067

Transition state A''- B''

Optimized coordinates at the VWN/3-21G/GEN-A2 level of theory

C	0.0000	0.0000	0.0000
O	0.0000	0.0000	1.2261
N	1.0689	0.0000	-0.9173
C	2.4214	-0.0077	-0.5145
C	3.4477	-0.0737	-1.4703
C	4.7819	-0.0801	-1.0671
C	5.1178	-0.0231	0.2872
C	4.0941	0.0378	1.2359
C	2.7560	0.0453	0.8505
C	0.5370	0.0242	-2.2298
C	-0.8129	0.0153	-2.1178
O	-1.1817	-0.0015	-0.7653
C	-1.7275	0.0449	-3.2613
C	1.1436	0.0829	-3.5805
H	3.2004	-0.1231	-2.5352
H	1.9372	0.0837	1.5768
H	6.1683	-0.0279	0.6006
H	4.3369	0.0806	2.3052
H	5.5690	-0.1323	-1.8301
H	-2.3517	-0.8737	-3.3777
H	1.7463	-0.8165	-3.8480
H	1.7433	1.0079	-3.7406
H	-2.4071	0.9359	-3.2296
Ir	-0.4493	0.1566	-4.9200
N	-0.3961	-1.8031	-5.0164
C	-0.3300	-2.7445	-4.0481
C	-0.2087	-4.0107	-4.6492
C	-0.2097	-3.7850	-6.0248
N	-0.3153	-2.4449	-6.2485
B	-0.4430	-1.6165	-7.5456
N	0.6971	-0.5909	-7.5919
C	1.6358	-0.3123	-8.5406
C	2.4077	0.7572	-8.0920
C	1.8845	1.1018	-6.8295
N	0.8515	0.2862	-6.5301
N	-1.7829	-0.8563	-7.4313
C	-2.9385	-0.9987	-8.1381
C	-3.9358	-0.2555	-7.5111
C	-3.3201	0.3287	-6.3895
N	-2.0124	-0.0252	-6.3396
H	-0.1372	-4.9702	-4.1419
H	-4.9751	-0.1567	-7.8182
H	-0.1513	-4.4802	-6.8605
H	3.2413	1.2271	-8.6104
H	-2.9691	-1.6256	-9.0277
H	1.6867	-0.8922	-9.4607
H	-3.7448	0.9438	-5.5949
H	2.1713	1.8818	-6.1224
H	-0.3666	-2.4227	-3.0043
H	-0.4329	-2.3362	-8.5287
O	-0.2261	2.2066	-4.5294
C	-1.4463	2.5775	-4.7397
H	-1.9614	2.3083	-5.6831
H	-1.9448	3.2276	-3.9942

Minimum B''

Optimized coordinates at the VWN/3-21G/GEN-A2 level of theory

C	0.0000	0.0000	0.0000
O	0.0000	0.0000	1.2264
N	1.0671	0.0000	-0.9176
C	2.4201	0.0001	-0.5179
C	3.4459	-0.0084	-1.4762
C	4.7808	-0.0106	-1.0753
C	5.1183	-0.0043	0.2798
C	4.0952	0.0050	1.2310
C	2.7564	0.0072	0.8477
C	0.5303	0.0057	-2.2298
C	-0.8140	-0.0006	-2.1166
O	-1.1837	-0.0098	-0.7658
C	-1.7370	-0.0001	-3.2605
C	1.1392	0.0287	-3.5801
H	3.1999	-0.0096	-2.5427
H	6.1692	-0.0044	0.5915
H	1.9380	0.0147	1.5755
H	5.5672	-0.0150	-1.8407
H	4.3390	0.0123	2.3009
H	1.7026	0.9614	-3.7932
H	1.7515	-0.8702	-3.8209
H	-2.3817	0.9089	-3.2695
H	-2.3731	-0.9170	-3.3134
Ir	-0.4724	-0.0078	-4.9309
N	-0.3276	-1.9916	-4.7811
C	-0.2540	-2.7976	-3.6979
C	-0.0546	-4.1196	-4.1240
C	-0.0239	-4.0709	-5.5195
N	-0.1798	-2.7810	-5.9157
B	-0.3487	-2.1457	-7.3121
N	0.7193	-1.0615	-7.5022
C	1.6195	-0.8334	-8.5012
C	2.2930	0.3543	-8.2218
C	1.7526	0.8247	-7.0078
N	0.8065	-0.0348	-6.5768
N	-1.7342	-1.4640	-7.2790
C	-2.8589	-1.6739	-8.0165
C	-3.8824	-0.8809	-7.4991
C	-3.3144	-0.1952	-6.4101
N	-2.0164	-0.5461	-6.2784
H	0.0454	-5.0019	-3.4957
H	-4.9084	-0.8156	-7.8560
H	3.0745	0.8204	-8.8188
H	-2.8531	-2.3773	-8.8474
H	1.7140	-1.5275	-9.3347
H	0.0875	-4.8647	-6.2563
H	1.9548	1.7192	-6.4162
H	-3.7580	0.5092	-5.7049
H	-0.3322	-2.3419	-2.7068
H	-0.2908	-2.9863	-8.1912
C	-1.2335	1.9182	-5.4641
O	-0.0404	2.0504	-4.8444
H	-1.2708	1.9654	-6.5723
H	-2.1556	2.1494	-4.8926

Transition state B''- C''

Optimized coordinates at the VWN/3-21G/GEN-A2 level of theory

C	0.0000	0.0000	0.0000
O	0.0000	0.0000	1.2257
N	1.0667	0.0000	-0.9175
C	0.5332	-0.0206	-2.2308
C	-0.8133	-0.0289	-2.1165
C	2.4199	0.0249	-0.5181
C	3.4405	0.1511	-1.4734
C	4.7760	0.1636	-1.0748
C	5.1176	0.0570	0.2752
C	4.0987	-0.0562	1.2244
C	2.7594	-0.0723	0.8430
O	-1.1839	-0.0157	-0.7667
C	-1.7334	-0.0746	-3.2608
C	1.1422	-0.0595	-3.5816
H	3.1863	0.2514	-2.5333
H	1.9438	-0.1426	1.5704
H	6.1690	0.0695	0.5855
H	5.5594	0.2656	-1.8367
H	4.3463	-0.1319	2.2907
H	-2.3441	-1.0083	-3.3022
H	1.7084	0.8632	-3.8353
H	1.7698	-0.9617	-3.7662
H	-2.4140	0.8095	-3.2961
Ir	-0.4587	-0.1382	-4.9321
C	-0.6107	1.9399	-5.7864
O	0.5687	2.3078	-5.5134
H	-1.0448	1.9227	-6.8120
N	-0.4269	-2.0879	-4.7800
C	-0.3255	-2.8755	-3.6858
C	-0.3733	-4.2197	-4.0962
C	-0.5137	-4.1960	-5.4830
N	-0.5461	-2.8986	-5.8979
B	-0.7004	-2.2531	-7.2918
N	0.5266	-1.3585	-7.5083
C	1.4907	-1.3725	-8.4708
C	2.4245	-0.3833	-8.1721
C	1.9734	0.2208	-6.9825
N	0.8277	-0.3699	-6.5778
N	-1.9694	-1.3803	-7.2298
C	-3.1276	-1.4243	-7.9452
C	-4.0118	-0.4878	-7.4128
C	-3.3265	0.1102	-6.3381
N	-2.0908	-0.4267	-6.2289
H	-0.5934	-5.0059	-6.2058
H	-5.0249	-0.2747	-7.7487
H	-3.2428	-2.1237	-8.7718
H	-0.3138	-5.0978	-3.4569
H	3.3165	-0.1286	-8.7408
H	1.4436	-2.0851	-9.2925
H	-3.6537	0.8701	-5.6258
H	2.3749	1.0502	-6.4017
H	-0.2309	-2.3985	-2.7064
H	-1.3472	1.7880	-4.9084
H	-0.7935	-3.0978	-8.1639

Minimum C''

Optimized coordinates at the VWN/3-21G/GEN-A2 level of theory

C	0.0000	0.0000	0.0000
O	0.0000	0.0000	1.2250
N	1.0642	0.0000	-0.9174
C	2.4162	0.0689	-0.5192
C	3.4180	0.3497	-1.4608
C	4.7532	0.4073	-1.0646
C	5.1091	0.1970	0.2696
C	4.1059	-0.0602	1.2077
C	2.7674	-0.1241	0.8279
C	0.5367	-0.0345	-2.2333
C	-0.8110	-0.0349	-2.1184
O	-1.1844	-0.0126	-0.7703
C	-1.7447	-0.1594	-3.2492
C	1.1637	-0.2055	-3.5666
H	3.1460	0.5433	-2.5036
H	1.9612	-0.2872	1.5507
H	6.1598	0.2460	0.5784
H	5.5232	0.6331	-1.8131
H	4.3654	-0.2112	2.2631
H	-2.4400	0.6989	-3.3549
H	-2.3224	-1.1112	-3.2483
H	1.7655	0.6643	-3.9115
H	1.7657	-1.1413	-3.6404
Ir	-0.4339	-0.4012	-4.9044
H	-0.6605	1.1612	-4.4998
C	0.1407	1.2222	-6.0437
O	1.2461	1.7555	-6.0225
H	-0.6479	1.4509	-6.8143
N	-0.6136	-2.4100	-4.4368
C	-0.5155	-3.0559	-3.2557
C	-0.7974	-4.4208	-3.4488
C	-1.0618	-4.5634	-4.8113
N	-0.9568	-3.3418	-5.4034
B	-1.0013	-2.8931	-6.8780
N	-2.0746	-1.8036	-7.0275
C	-3.1692	-1.7448	-7.8364
C	-3.8458	-0.5550	-7.5791
C	-3.1015	0.0913	-6.5738
N	-2.0304	-0.6621	-6.2379
N	0.3856	-2.2766	-7.1516
C	1.4039	-2.6864	-7.9568
C	2.5208	-1.8912	-7.7004
C	2.1254	-0.9906	-6.6949
N	0.8382	-1.2271	-6.3639
H	3.4953	-1.9532	-8.1801
H	-0.8009	-5.2040	-2.6934
H	-4.7617	-0.2029	-8.0501
H	-1.3067	-5.4454	-5.4004
H	1.2630	-3.5179	-8.6453
H	-3.3877	-2.5540	-8.5316
H	2.6565	-0.1732	-6.2053
H	-3.2799	1.0378	-6.0610
H	-0.2577	-2.4808	-2.3623
H	-1.2229	-3.8288	-7.6257

Transition state C''- D''

Optimized coordinates at the VWN/3-21G/GEN-A2 level of theory

C	0.0000	0.0000	0.0000
O	0.0000	0.0000	1.2244
N	1.0677	0.0000	-0.9158
C	2.4208	-0.0425	-0.5157
C	3.4360	-0.2727	-1.4569
C	4.7711	-0.2980	-1.0563
C	5.1150	-0.1035	0.2831
C	4.1001	0.1069	1.2202
C	2.7620	0.1375	0.8358
C	0.5357	0.0554	-2.2250
C	-0.8140	0.0660	-2.1228
O	-1.1808	0.0158	-0.7729
C	-1.7595	0.0718	-3.2501
C	1.1898	0.1062	-3.5544
H	1.9491	0.2729	1.5568
H	3.1836	-0.4518	-2.5071
H	6.1655	-0.1233	0.5954
H	4.3503	0.2514	2.2787
H	5.5509	-0.4794	-1.8067
H	1.9179	0.9374	-3.6688
H	1.6780	-0.8429	-3.8657
H	-2.3795	0.9958	-3.2855
H	-2.4064	-0.8366	-3.2519
Ir	-0.5160	-0.0970	-4.9376
C	-0.9767	1.6418	-5.8391
O	-0.2224	2.5855	-6.1077
H	0.2062	1.1788	-4.2593
N	-2.0513	-0.8638	-6.0510
C	-3.3611	-0.5429	-6.1308
C	-3.9903	-1.3771	-7.0716
C	-2.9909	-2.2247	-7.5493
N	-1.8184	-1.9074	-6.9360
B	-0.4388	-2.6110	-6.9603
N	0.6280	-1.5709	-7.3264
C	1.5001	-1.5058	-8.3717
C	2.1847	-0.2944	-8.3001
C	1.6755	0.3655	-7.1646
N	0.7447	-0.4123	-6.5730
N	-0.1996	-3.0970	-5.5197
C	-0.0307	-4.3462	-5.0042
C	0.0271	-4.2467	-3.6151
C	-0.1253	-2.8768	-3.3266
N	-0.2595	-2.1822	-4.4786
H	2.9451	0.0716	-8.9869
H	-5.0400	-1.3702	-7.3582
H	0.1514	-5.0593	-2.9022
H	0.0300	-5.2132	-5.6598
H	-3.0317	-3.0378	-8.2721
H	1.5657	-2.3213	-9.0901
H	1.8614	1.3617	-6.7582
H	-3.7647	0.2506	-5.4998
H	-0.1598	-2.3380	-2.3774
H	-2.0433	1.6267	-6.2183
H	-0.4391	-3.5386	-7.7502

Minimum D''

Optimized coordinates at the VWN/3-21G/GEN-A2 level of theory

C	0.0000	0.0000	0.0000
O	0.0000	0.0000	1.2221
N	1.0709	0.0000	-0.9080
C	2.4105	0.1462	-0.4914
C	3.3568	0.7483	-1.3331
C	4.6835	0.8667	-0.9201
C	5.0748	0.4093	0.3402
C	4.1174	-0.1447	1.1952
C	2.7909	-0.2769	0.7919
C	0.5620	-0.0905	-2.2215
C	-0.7906	-0.0899	-2.1412
O	-1.1707	-0.0221	-0.7904
C	-1.7550	-0.2432	-3.2373
C	1.2896	-0.4492	-3.4605
H	2.0128	-0.6486	1.4654
H	3.0435	1.1810	-2.2899
H	6.1174	0.5067	0.6648
H	5.4126	1.3452	-1.5859
H	4.4050	-0.4776	2.2003
H	1.5236	-1.5339	-3.5298
H	2.2352	0.1109	-3.6165
H	-2.5513	-0.9779	-2.9786
H	-2.2005	0.7307	-3.5415
Ir	-0.6409	-1.0836	-4.8013
C	-0.7591	0.5053	-5.9338
O	0.0878	1.4268	-5.9473
N	-2.2684	-1.8312	-5.6158
C	-3.4773	-1.2909	-5.8875
C	-4.2969	-2.2694	-6.4768
C	-3.5219	-3.4259	-6.5437
N	-2.2919	-3.1599	-6.0238
B	-1.0584	-4.0704	-5.8108
N	-0.7614	-4.0959	-4.3034
C	-0.7387	-5.1233	-3.4088
C	-0.5075	-4.5969	-2.1398
C	-0.3991	-3.2046	-2.3210
N	-0.5464	-2.8998	-3.6316
N	0.1235	-3.4177	-6.5475
C	0.9306	-3.8715	-7.5468
C	1.7985	-2.8442	-7.9127
C	1.4648	-1.7532	-7.0873
N	0.4578	-2.1044	-6.2588
H	-5.3266	-2.1482	-6.8067
H	2.5663	-2.8770	-8.6832
H	-0.4370	-5.1459	-1.2030
H	-3.7564	-4.4209	-6.9186
H	0.8274	-4.8865	-7.9269
H	-0.8936	-6.1498	-3.7367
H	-3.6714	-0.2475	-5.6354
H	1.8582	-0.7356	-7.0448
H	-0.2535	-2.4004	-1.5974
H	0.7635	0.0461	-4.4023
H	-1.6443	0.5342	-6.6442
H	-1.2761	-5.1904	-6.2388

Minimum E''

Optimized coordinates at the VWN/3-21G/GEN-A2 level of theory

C	0.0000	0.0000	0.0000
O	0.0000	0.0000	1.2060
O	1.0893	0.0000	-0.8218
C	0.6678	0.0348	-2.2154
C	-0.8015	0.0425	-2.1574
N	-1.1967	0.0095	-0.8910
C	-2.5175	-0.0256	-0.3637
C	-2.7601	0.4384	0.9371
C	-4.0633	0.4218	1.4299
C	-5.1151	-0.0599	0.6461
C	-4.8592	-0.5429	-0.6413
C	-3.5640	-0.5276	-1.1519
C	-1.5239	0.1367	-3.4139
C	1.1782	1.2630	-2.9465
H	-1.9249	0.7677	1.5604
H	-3.3625	-0.9368	-2.1473
H	-5.6750	-0.9491	-1.2510
H	-4.2543	0.7843	2.4469
H	-6.1362	-0.0735	1.0446
H	0.6435	2.2037	-2.7262
H	-2.4392	0.7689	-3.3521
H	2.2652	1.3980	-2.7472
H	-1.8261	-0.8893	-3.7427
Ir	-0.1935	0.8401	-4.8855
C	0.5385	-0.9680	-5.1559
O	1.0945	-1.6998	-4.2877
N	-1.5550	0.4704	-6.2771
C	-2.2706	-0.6408	-6.5779
C	-3.0726	-0.3792	-7.6983
C	-2.7996	0.9400	-8.0638
N	-1.8815	1.4527	-7.2028
B	-1.1547	2.8210	-7.1858
N	0.3455	2.5124	-7.3230
C	1.2486	2.8706	-8.2759
C	2.4567	2.2287	-8.0074
C	2.2300	1.4623	-6.8528
N	0.9542	1.6372	-6.4347
N	-1.4157	3.4628	-5.8155
C	-2.0312	4.6243	-5.4669
C	-2.0938	4.6897	-4.0747
C	-1.4881	3.5082	-3.6158
N	-1.0692	2.7658	-4.6688
H	3.3800	2.3005	-8.5793
H	-3.7594	-1.0670	-8.1875
H	-2.5218	5.4905	-3.4748
H	0.9690	3.5499	-9.0801
H	-3.1902	1.5459	-8.8806
H	-2.3853	5.3203	-6.2261
H	-2.1487	-1.5529	-5.9909
H	2.8978	0.7895	-6.3112
H	-1.3378	3.1519	-2.5947
H	1.4008	1.0683	-4.1110
H	0.4427	-1.3731	-6.2032
H	0.9972	-0.8789	-2.8498
H	-1.5475	3.5287	-8.0927

Transition state E''- F''

Optimized coordinates at the VWN/3-21G/GEN-A2 level of theory

C	0.0000	0.0000	0.0000
O	0.0000	0.0000	1.2049
O	1.0908	0.0000	-0.8308
N	-1.2004	0.0832	-0.8695
C	-0.8270	0.2284	-2.1316
C	-2.5168	0.0751	-0.3426
C	-2.7875	0.6330	0.9110
C	-4.1010	0.6210	1.3799
C	-5.1225	0.0520	0.6145
C	-4.8311	-0.5333	-0.6240
C	-3.5259	-0.5264	-1.1067
C	-1.4895	0.7312	-3.3093
C	0.6155	-0.1413	-2.2133
C	1.3723	0.5682	-3.2991
H	-1.9708	1.0377	1.5148
H	-6.1510	0.0442	0.9942
H	-4.3250	1.0578	2.3604
H	-5.6251	-1.0195	-1.2035
H	-3.2608	-1.0361	-2.0435
H	1.1733	1.6496	-3.3812
H	-2.5790	0.5618	-3.3661
H	0.5625	-1.2308	-2.4454
H	2.4685	0.4040	-3.2035
H	-1.2935	1.8389	-3.3577
Ir	-0.3594	0.1131	-4.9669
C	-0.7714	-1.7510	-4.4622
O	-0.8722	-2.2153	-3.2988
N	-1.9927	0.0447	-6.0885
C	-3.2156	-0.4969	-5.8723
C	-4.0204	-0.2696	-6.9979
C	-3.2204	0.4286	-7.9045
N	-1.9929	0.6167	-7.3519
B	-0.6987	1.2477	-7.9223
N	0.3688	0.1430	-7.8792
C	1.0730	-0.4611	-8.8744
C	1.8135	-1.5060	-8.3234
C	1.5112	-1.5035	-6.9521
N	0.6421	-0.5011	-6.6805
N	-0.2919	2.3913	-6.9831
C	-0.1620	3.7244	-7.2166
C	0.1390	4.3567	-6.0110
C	0.1749	3.3328	-5.0509
N	-0.0802	2.1357	-5.6351
H	-5.0535	-0.5806	-7.1403
H	0.3083	5.4200	-5.8507
H	2.4827	-2.1851	-8.8485
H	-0.2944	4.1320	-8.2179
H	-3.4381	0.7971	-8.9062
H	0.9949	-0.1114	-9.9031
H	1.8566	-2.1629	-6.1539
H	-3.4207	-1.0268	-4.9407
H	0.3707	3.4057	-3.9792
H	-0.9935	-2.4204	-5.3437
H	1.3353	-0.0459	-4.3369
H	-0.8780	1.6502	-9.0551

Minimum F''

Optimized coordinates at the VWN/3-21G/GEN-A2 level of theory

C	0.0000	0.0000	0.0000
O	0.0000	0.0000	1.2123
N	1.0885	0.0000	-0.8926
C	0.6483	-0.1873	-2.2224
C	2.4367	-0.1959	-0.4819
C	2.7484	-0.5039	0.8480
C	4.0782	-0.7266	1.2039
C	5.0994	-0.6474	0.2546
C	4.7836	-0.3201	-1.0663
C	3.4599	-0.0875	-1.4363
O	-1.1884	-0.0816	-0.7558
C	-0.8574	0.1441	-2.1466
C	-1.6844	-0.7132	-3.0720
C	0.9160	-1.4977	-2.9265
H	1.9415	-0.5395	1.5860
H	6.1411	-0.8226	0.5467
H	4.3152	-0.9634	2.2481
H	5.5798	-0.2198	-1.8142
H	3.2200	0.2292	-2.4589
H	-1.6179	-1.7872	-2.8371
H	1.9974	-1.7235	-2.9991
H	-0.9908	1.2177	-2.3901
H	0.4029	-2.3213	-2.3857
H	-2.7566	-0.4132	-3.0704
Ir	0.0312	-1.1123	-4.7666
C	0.9027	0.5661	-4.4275
O	1.2047	0.9042	-3.1743
N	1.6246	-1.7145	-5.7894
C	2.9519	-1.5431	-5.5724
C	3.6649	-2.1933	-6.5882
C	2.7040	-2.7658	-7.4243
N	1.4694	-2.4736	-6.9390
B	0.0557	-2.8566	-7.4440
N	-0.7016	-1.5445	-7.6778
C	-1.2707	-1.0214	-8.7968
C	-1.7658	0.2454	-8.4901
C	-1.4594	0.4538	-7.1361
N	-0.8164	-0.6309	-6.6402
N	-0.6176	-3.6296	-6.2981
C	-1.0713	-4.9066	-6.2296
C	-1.4651	-5.1694	-4.9155
C	-1.2125	-3.9900	-4.2033
N	-0.7067	-3.0473	-5.0386
H	-1.8748	-6.0995	-4.5262
H	-2.2804	0.9300	-9.1618
H	4.7460	-2.2441	-6.7008
H	-1.2828	-1.5815	-9.7310
H	2.8153	-3.3608	-8.3300
H	-1.0789	-5.5453	-7.1122
H	-1.6616	1.3174	-6.5005
H	-1.3560	-3.7835	-3.1414
H	3.3043	-0.9797	-4.7063
H	1.3188	1.2801	-5.1659
H	-1.5597	-0.4032	-4.2274
H	0.1221	-3.5268	-8.4551

Transition state F''- G''

Optimized coordinates at the VWN/3-21G/GEN-A2 level of theory

H	-2.4153	1.5252	-1.2469
H	1.5855	-2.6064	-2.0273
H	2.8205	4.2645	-2.1963
H	0.0202	-0.1160	3.1841
H	-3.1961	3.8294	-0.8243
H	5.5256	-1.6442	-0.4387
H	-6.6431	2.2595	1.2295
H	0.6298	2.6165	-2.0845
H	-5.8038	-0.0550	0.8522
H	4.2905	0.6499	3.4504
H	-1.2930	-0.6855	1.6008
H	-0.8670	-4.1845	0.2358
H	4.9210	0.7296	0.8218
H	-5.3239	4.2128	0.4159
H	-0.9561	-2.8506	1.4282
H	0.0884	-2.6789	-0.0173
H	2.0451	0.2661	4.9867
H	4.6853	3.0682	-0.5711
H	-2.0031	-2.7987	-1.4732
H	-1.6242	0.8224	0.6890
H	4.1983	-3.4518	-2.0299
H	0.0132	0.0990	-2.7973
B	3.7618	0.5097	0.5690
C	2.1161	0.2632	3.9047
C	3.2649	0.4610	3.1448
C	-5.6906	2.1044	0.7138
C	-1.2093	-0.2184	0.6014
C	-2.0082	-2.4892	-0.4109
C	-5.2292	0.8132	0.5220
C	-0.3117	-0.1552	-1.7687
C	-2.0841	-0.9430	-0.3968
C	4.4748	-1.6926	-0.7101
C	-4.0152	0.5890	-0.1354
C	3.7837	-2.5955	-1.5094
C	2.4502	-2.1839	-1.5212
C	-3.3029	1.6907	-0.6302
C	2.7197	3.3406	-1.6375
C	1.5972	2.5118	-1.6007
C	-0.8738	-3.0888	0.3540
C	3.6762	2.7526	-0.8204
C	-3.7629	2.9836	-0.4237
C	-4.1810	-1.8693	0.1154
C	1.0768	0.0624	2.9998
C	-4.9542	3.1956	0.2582
N	1.5648	0.1335	1.7336
N	2.9194	0.3810	1.8387
N	3.5869	-0.7752	-0.2544
N	2.3385	-1.0774	-0.7453
N	1.8654	1.4664	-0.7826
N	3.1499	1.6132	-0.3063
N	-3.4769	-0.7036	-0.2690
O	-1.5932	-0.5428	-1.7859
O	-3.2746	-2.9143	0.1704
O	-5.3515	-1.9777	0.4139
Ir	0.6934	-0.0364	-0.1457

Minimum G''

Optimized coordinates at the VWN/3-21G/GEN-A2 level of theory

C	0.0000	0.0000	0.0000
O	0.0000	0.0000	1.2145
O	1.1140	0.0000	-0.8026
N	-1.1421	0.0229	-0.8547
C	-2.4407	0.2101	-0.3763
C	-2.6732	0.9146	0.8118
C	-3.9816	1.1342	1.2441
C	-5.0857	0.6554	0.5185
C	-4.8653	-0.0845	-0.6357
C	-3.5480	-0.3079	-1.0928
C	-0.7659	0.0150	-2.2298
C	-1.7206	0.7690	-3.1145
C	0.7151	0.4033	-2.1639
C	0.9082	1.8952	-2.2835
H	-1.8137	1.2344	1.4078
H	-6.1037	0.8313	0.8840
H	-4.1432	1.6844	2.1796
H	-5.6915	-0.5185	-1.2198
H	1.3126	-0.1768	-2.8832
H	1.9655	2.1501	-2.1025
H	0.6219	2.2394	-3.2932
H	-2.0007	1.7307	-2.6407
H	0.2828	2.4113	-1.5294
H	-1.2766	0.9638	-4.1148
Ir	-3.3611	-0.4955	-3.3167
C	-1.9141	-1.7621	-3.3467
O	-0.7438	-1.4423	-2.7930
N	-3.3171	-0.3757	-5.3240
C	-2.3000	-0.4427	-6.2161
C	-2.8189	-0.3393	-7.5147
C	-4.1994	-0.2055	-7.3622
N	-4.4974	-0.2287	-6.0363
B	-5.8509	-0.1260	-5.2998
N	-5.7415	1.0723	-4.3429
C	-6.4570	2.2202	-4.2219
C	-5.8917	2.9883	-3.2002
C	-4.8018	2.2446	-2.7236
N	-4.7117	1.0831	-3.4142
N	-6.0108	-1.4009	-4.4523
C	-7.0110	-2.3215	-4.4065
C	-6.6840	-3.2856	-3.4533
C	-5.4373	-2.8986	-2.9359
N	-5.0256	-1.7567	-3.5406
H	-2.2616	-0.3614	-8.4492
H	-6.2253	3.9649	-2.8553
H	-7.2690	-4.1613	-3.1775
H	-4.9883	-0.0967	-8.1052
H	-7.8820	-2.2307	-5.0546
H	-7.3117	2.4186	-4.8678
H	-1.2720	-0.5632	-5.8701
H	-4.0871	2.4632	-1.9274
H	-4.8141	-3.3812	-2.1799
H	-1.8667	-2.7334	-3.8817
H	-3.3853	-1.3463	-1.5803
H	-6.7682	0.0048	-6.0864

Minimum 5''

Optimized coordinates at the VWN/3-21G/GEN-A2 level of theory

C	0.0000	0.0000	0.0000
O	0.0000	0.0000	1.2216
O	1.1722	0.0000	-0.7502
N	-1.0861	0.0247	-0.8851
C	-2.4503	0.0025	-0.4827
C	-2.7648	0.3311	0.8457
C	-4.0918	0.3428	1.2703
C	-5.1163	0.0257	0.3758
C	-4.7924	-0.3231	-0.9381
C	-3.4640	-0.3494	-1.4012
C	-0.6410	-0.1213	-2.2305
C	-1.5439	0.4774	-3.2695
C	0.8158	0.3145	-2.1399
C	0.9676	1.8036	-2.3425
H	-1.9370	0.5201	1.5356
H	-6.1638	0.0328	0.7022
H	-4.3188	0.5956	2.3131
H	-5.5849	-0.5920	-1.6530
H	1.4465	-0.2870	-2.8128
H	2.0081	2.1072	-2.1400
H	0.6969	2.0747	-3.3783
H	-1.8549	1.4952	-2.9533
H	0.2917	2.3286	-1.6407
H	-1.0331	0.5222	-4.2590
Ir	-3.1523	-0.8302	-3.3609
C	-1.7636	-2.0563	-2.9903
O	-0.5700	-1.6406	-2.5291
N	-3.0319	-1.1262	-5.4402
C	-1.9918	-1.2933	-6.2860
C	-2.4689	-1.4722	-7.5978
C	-3.8578	-1.4038	-7.5014
N	-4.1894	-1.1968	-6.1967
B	-5.5577	-1.0379	-5.5089
N	-5.5654	0.3334	-4.8070
C	-6.3957	1.4056	-4.9161
C	-5.9640	2.3898	-4.0254
C	-4.8344	1.8508	-3.3836
N	-4.5906	0.6113	-3.8598
N	-5.6741	-2.1235	-4.4228
C	-6.6282	-3.0717	-4.2028
C	-6.3051	-3.7600	-3.0349
C	-5.1133	-3.1746	-2.5665
N	-4.7279	-2.1909	-3.4086
H	-1.8806	-1.6332	-8.4990
H	-6.4100	3.3690	-3.8636
H	-6.8596	-4.5781	-2.5796
H	-4.6300	-1.4866	-8.2643
H	-7.4654	-3.1856	-4.8901
H	-7.2295	1.3953	-5.6165
H	-0.9737	-1.2794	-5.8934
H	-4.1953	2.2524	-2.5955
H	-4.5224	-3.3712	-1.6703
H	-1.7462	-3.1475	-3.2012
H	-6.4671	-1.1268	-6.3159

Minimum 7''

Optimized coordinates at the VWN/3-21G/GEN-A2 level of theory

C	-3.7169	-2.0320	0.3995
O	-4.8024	-2.5736	0.5447
N	-3.3963	-0.6828	0.1691
O	-2.4935	-2.7348	0.4116
C	-1.9950	-0.5617	0.0201
C	-4.3695	0.3309	0.0902
C	-5.7313	0.0009	0.0825
C	-6.6862	1.0030	-0.0037
C	-6.3138	2.3414	-0.0807
C	-4.9621	2.6683	-0.0602
C	-3.9947	1.6762	0.0275
C	-1.4696	-1.8079	0.1722
C	-0.0298	-2.0830	0.1820
C	-1.0734	0.5840	-0.1787
O	-0.7303	-1.1424	-2.6268
C	0.4380	-0.6552	-2.1941
Ir	0.8342	-0.2611	-0.3908
N	1.7106	1.5724	-0.7907
C	1.4023	2.6005	-1.6098
N	2.8728	1.9250	-0.1165
C	3.2645	3.1605	-0.5297
C	2.3581	3.6181	-1.4755
B	3.4811	0.9570	0.9058
N	3.7751	-0.3671	0.1905
C	4.9305	-1.0699	0.0431
C	4.6590	-2.2186	-0.6861
N	2.7461	-1.0546	-0.4418
C	3.2858	-2.1745	-0.9681
N	2.4310	0.6907	1.9917
C	2.4271	0.8748	3.3373
C	1.1972	0.4601	3.8363
N	1.2093	0.1573	1.6086
C	0.4649	0.0186	2.7259
H	5.3632	-2.9914	-0.9761
H	0.5173	2.5469	-2.2407
H	0.8741	0.4754	4.8720
H	2.3843	4.5668	-2.0015
H	-0.5438	-0.3891	2.6567
H	2.6582	-2.8781	-1.5113
H	4.1572	3.6266	-0.1222
H	5.8618	-0.7053	0.4671
H	3.2927	1.2864	3.8488
H	-7.7450	0.7271	-0.0091
H	-4.6489	3.7155	-0.1076
H	0.3298	-2.3308	1.2051
H	-7.0722	3.1259	-0.1497
H	-6.0003	-1.0552	0.1676
H	-2.9380	1.9470	0.0580
H	-1.0464	1.2463	0.7157
H	-1.3471	1.2081	-1.0567
H	1.1275	-0.5174	-3.0553
H	0.2473	-2.9278	-0.4838
H	-1.3447	-1.2638	-1.7878
H	4.4934	1.4193	1.3838