Supporting information

for

A Rollover Ir(III) Complex of 2-(6-bromopyridin-2-yl)imidazo[1,2-a]pyridine

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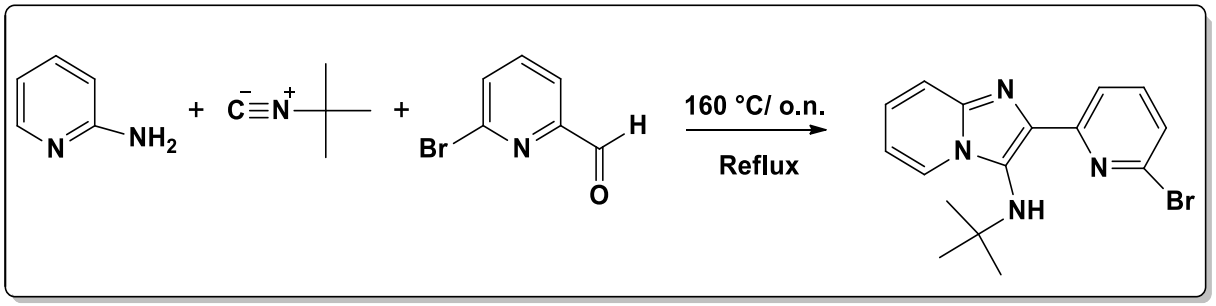
Ec. S.1. Synthesis of L_1

The new synthesis of bromine 2-(Pyridin-2-yl)imidazo[1,2-a]pyridine ligand (**L_1**) is obtained through a metal and solvent free multicomponent Groebke-Blackburn-Bienayme reaction. In a Schlenk Tube with Young's Tap is added tert-Butyl isocyanide (5.37 mmol), 2-amine pyridine (5.37 mmol) and 6-bromo-2-pyridinecarboxaldehyde (5.37 mmol), the mixture is stirred at 160 °C in reflux, o.n. The product is obtained as brown oil in quantitively yield (see equation). The ligand (**L_1**) is very soluble in commune organic solvents.



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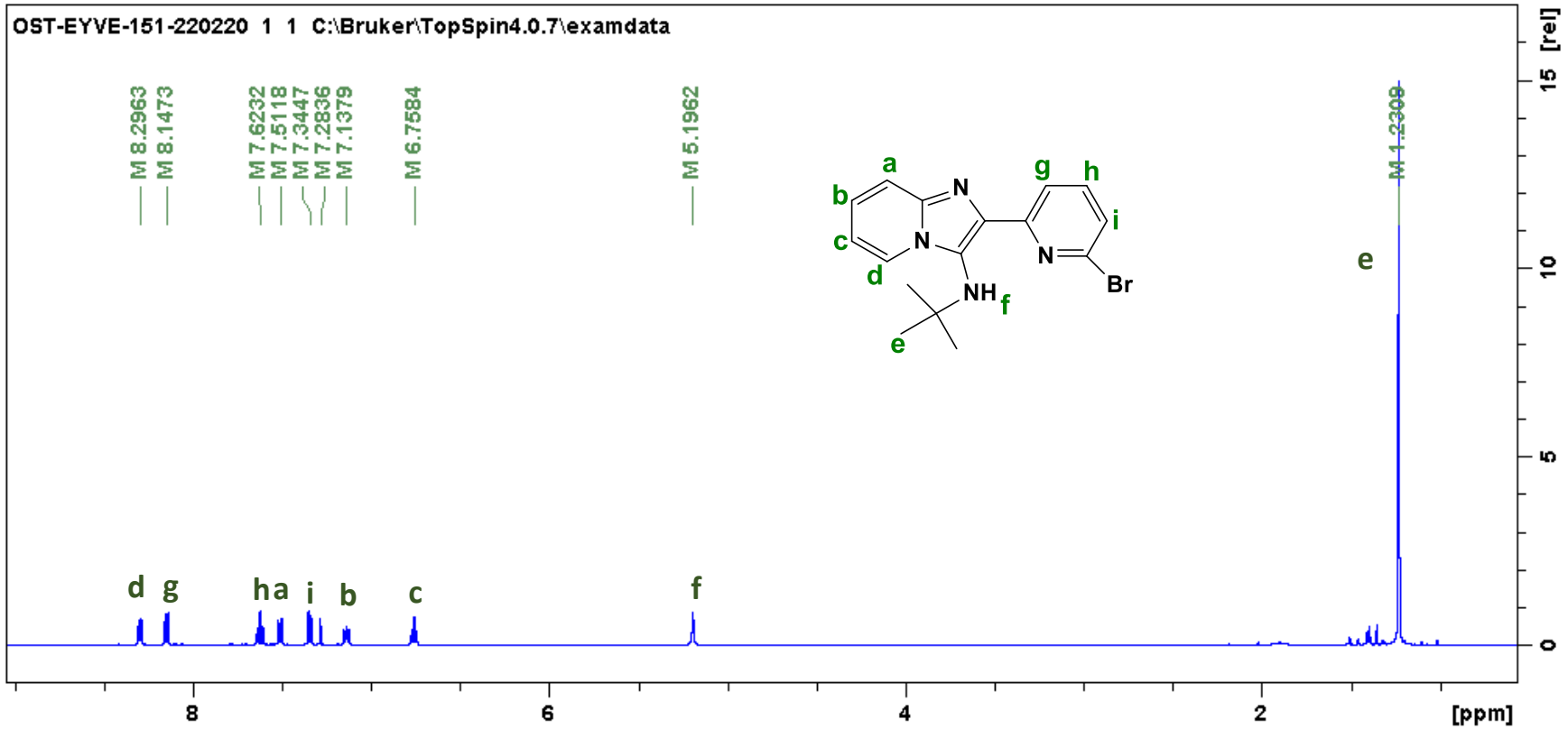
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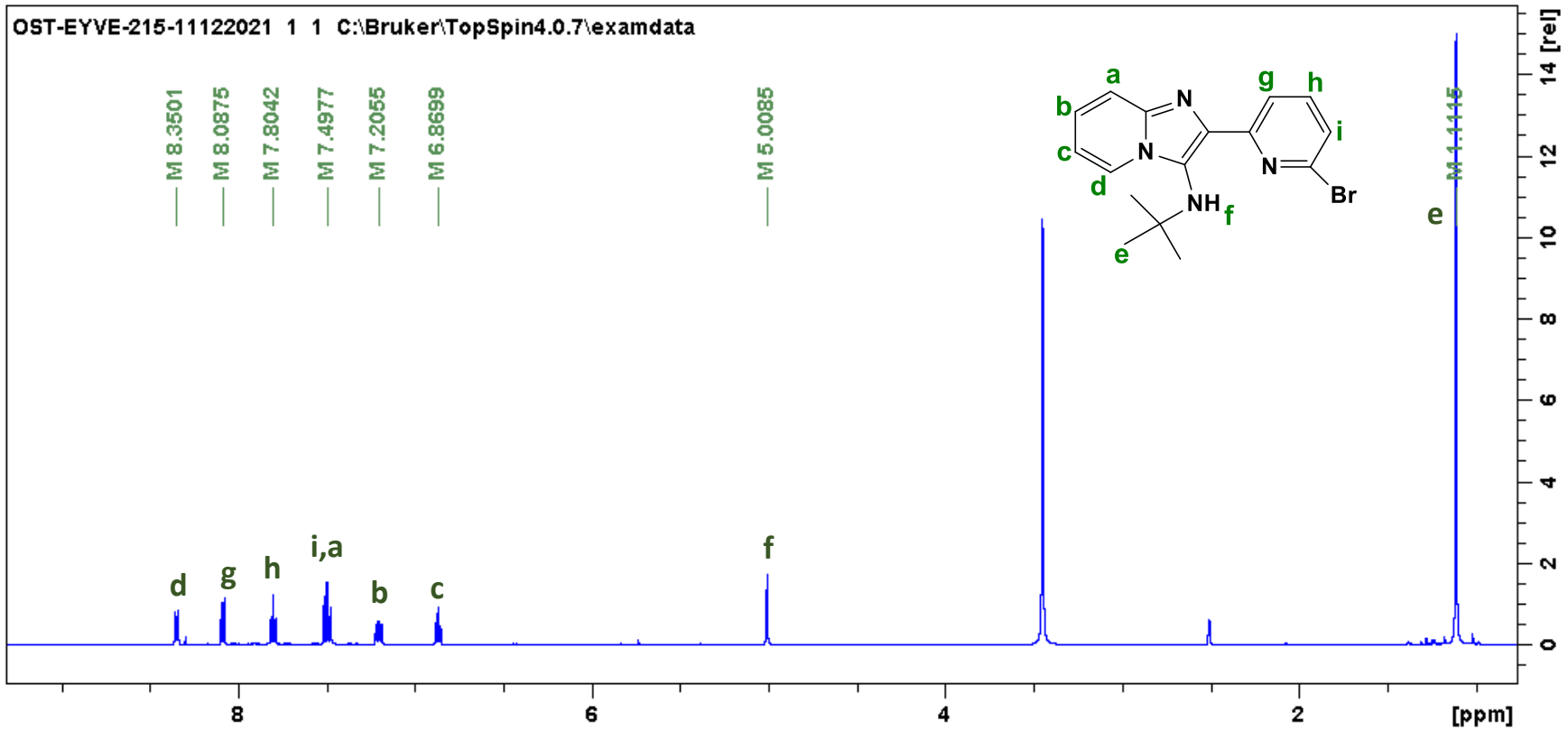
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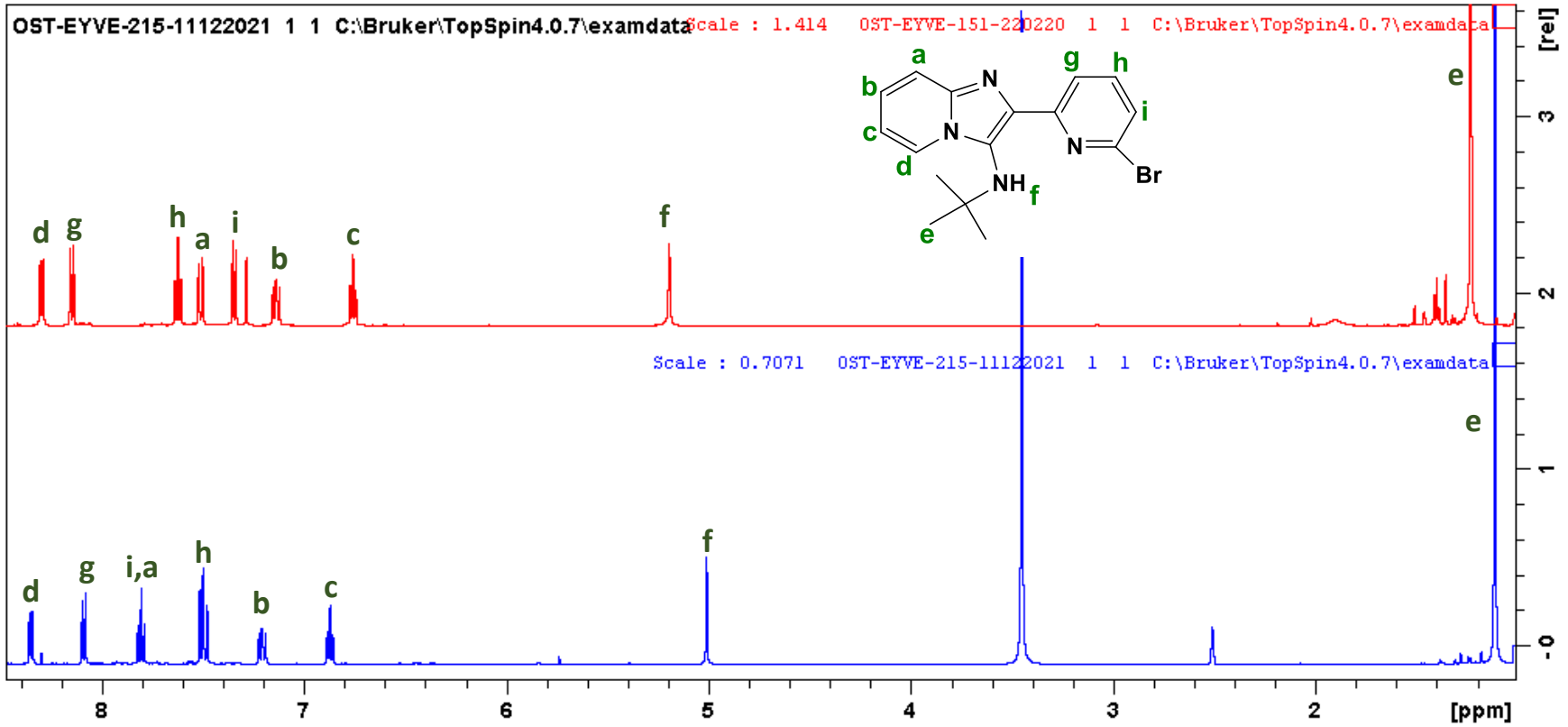

Fig. S .1. a) ^{1}H NMR spectrum of ligand **L$_1$** in ***a)*** $CDCl_3$, ***b)*** $(CD_3)_2SO$ and ***c)*** merge.

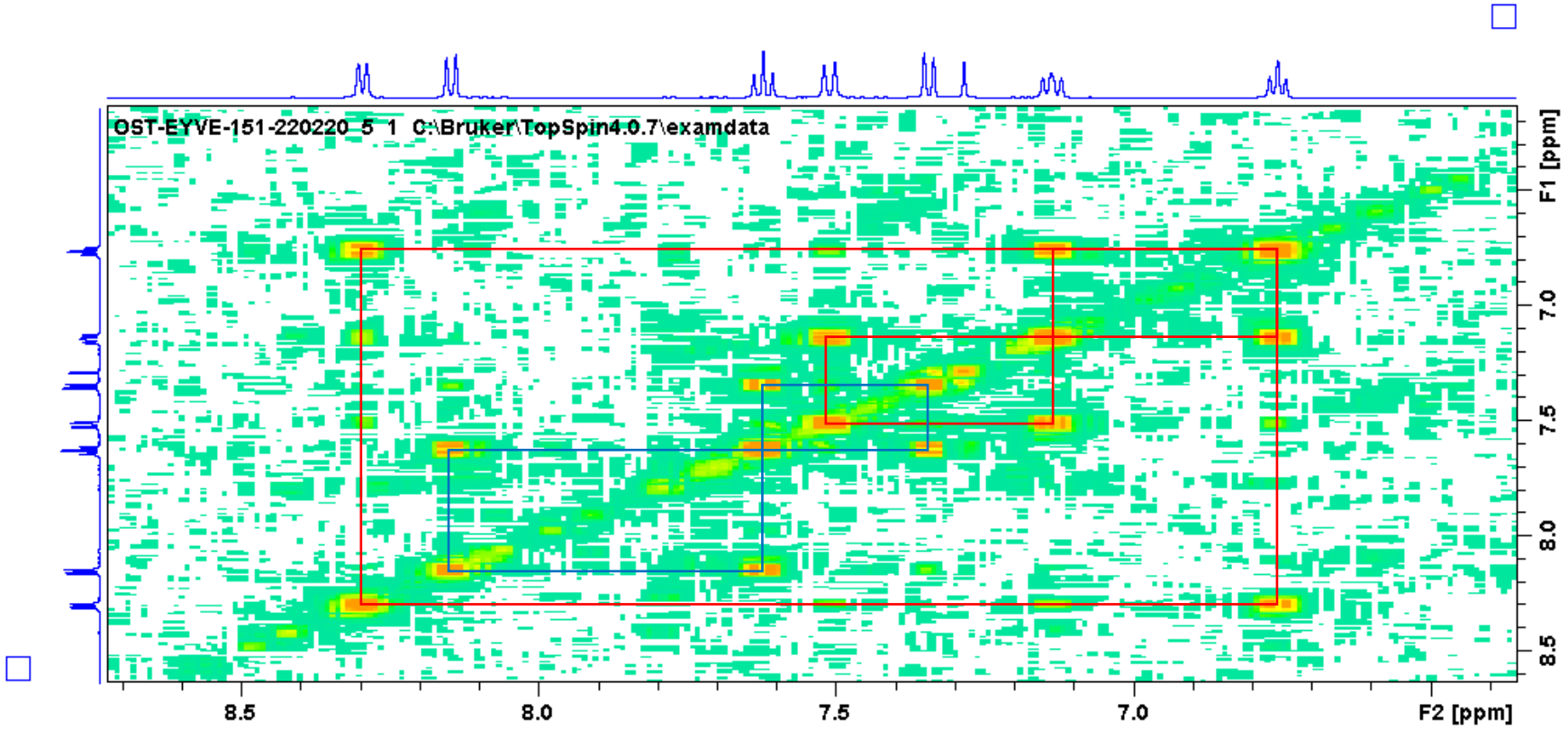

Fig. S.2. COSY spectrum of ligand **L**$_1$ in $CDCl_3$.

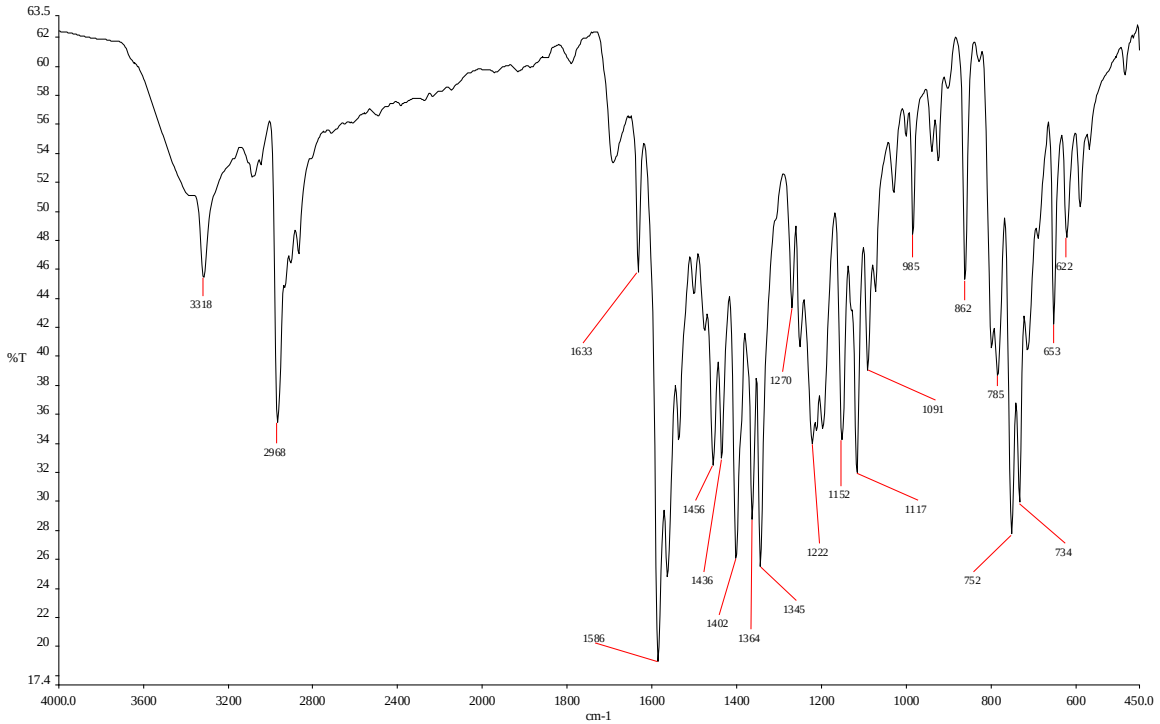

Fig. S.3. Infrared spectrum of ligand **L_1** in KBr.

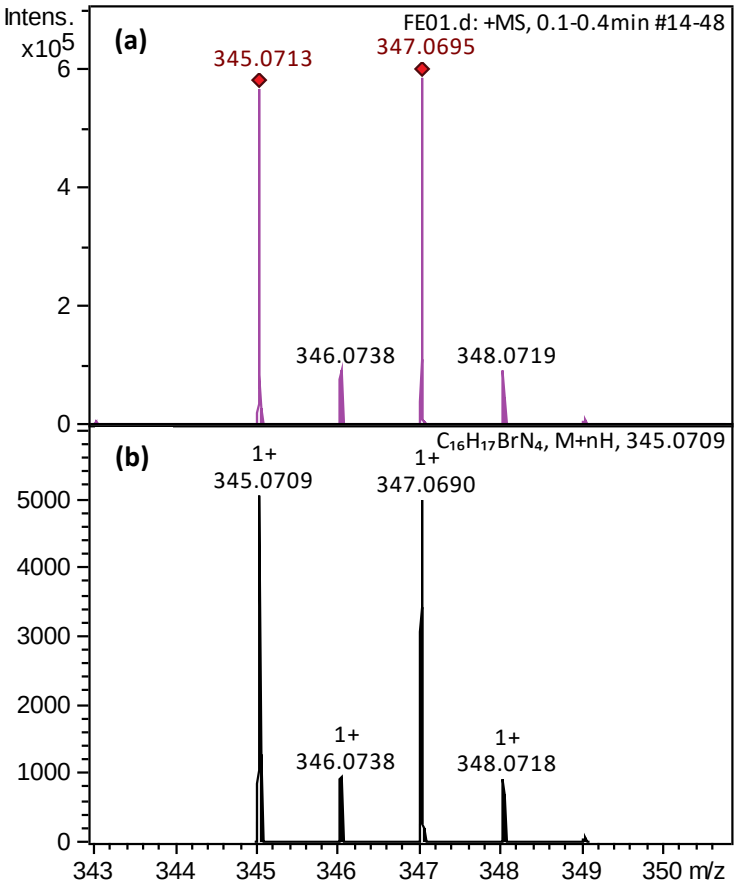

Fig. S.4a. ***(a)*** Experimental mass spectrum of ligand **L_1** dissolved in acetonitrile.
(b) In-silico calculated isotopic patterns of two ions (*m/z* values correspond to monoisotopic ions).

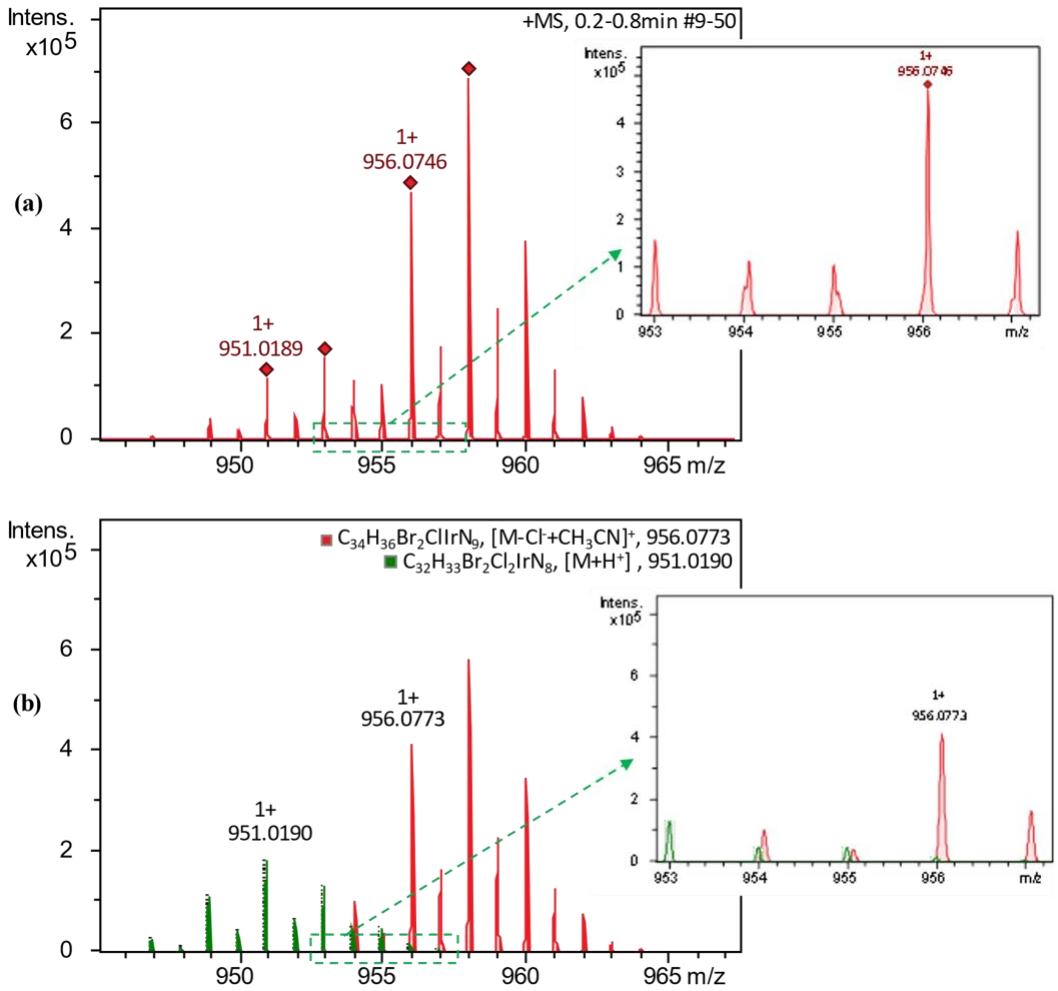

Figure S.4b. ***(a)*** Experimental mass spectrum of complex **1** dissolved in acetonitrile, showing overlapped isotopic patterns of $[M+H^+]$ and $[M\text{-}Cl^- + CH_3CN]^+$. ***(b)*** In-silico calculated isotopic patterns of two ions (*m/z* values correspond to monoisotopic ions).

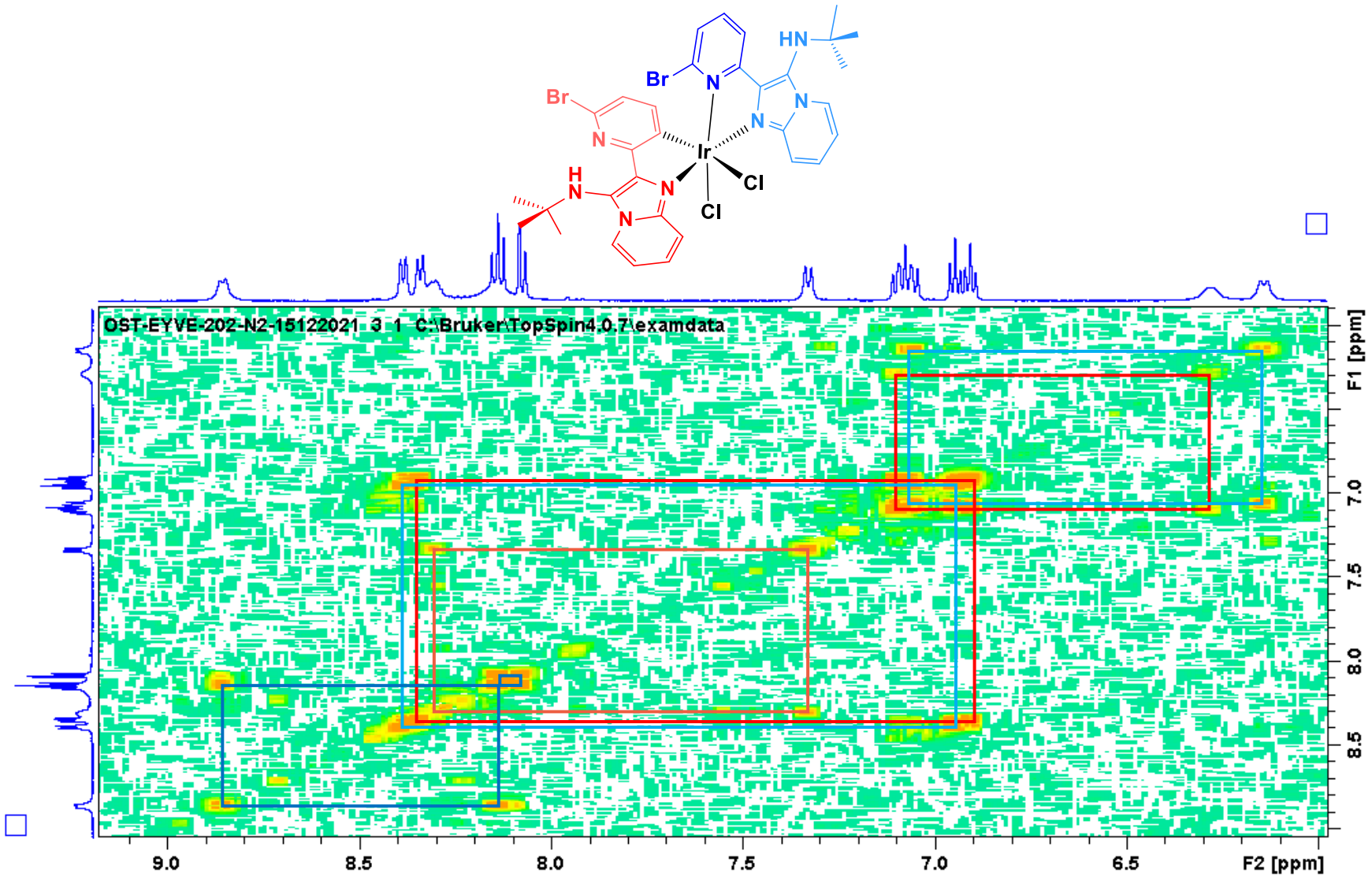

Fig. S.5. COSY spectrum of complex **1** in $(CD_3)_2SO$.

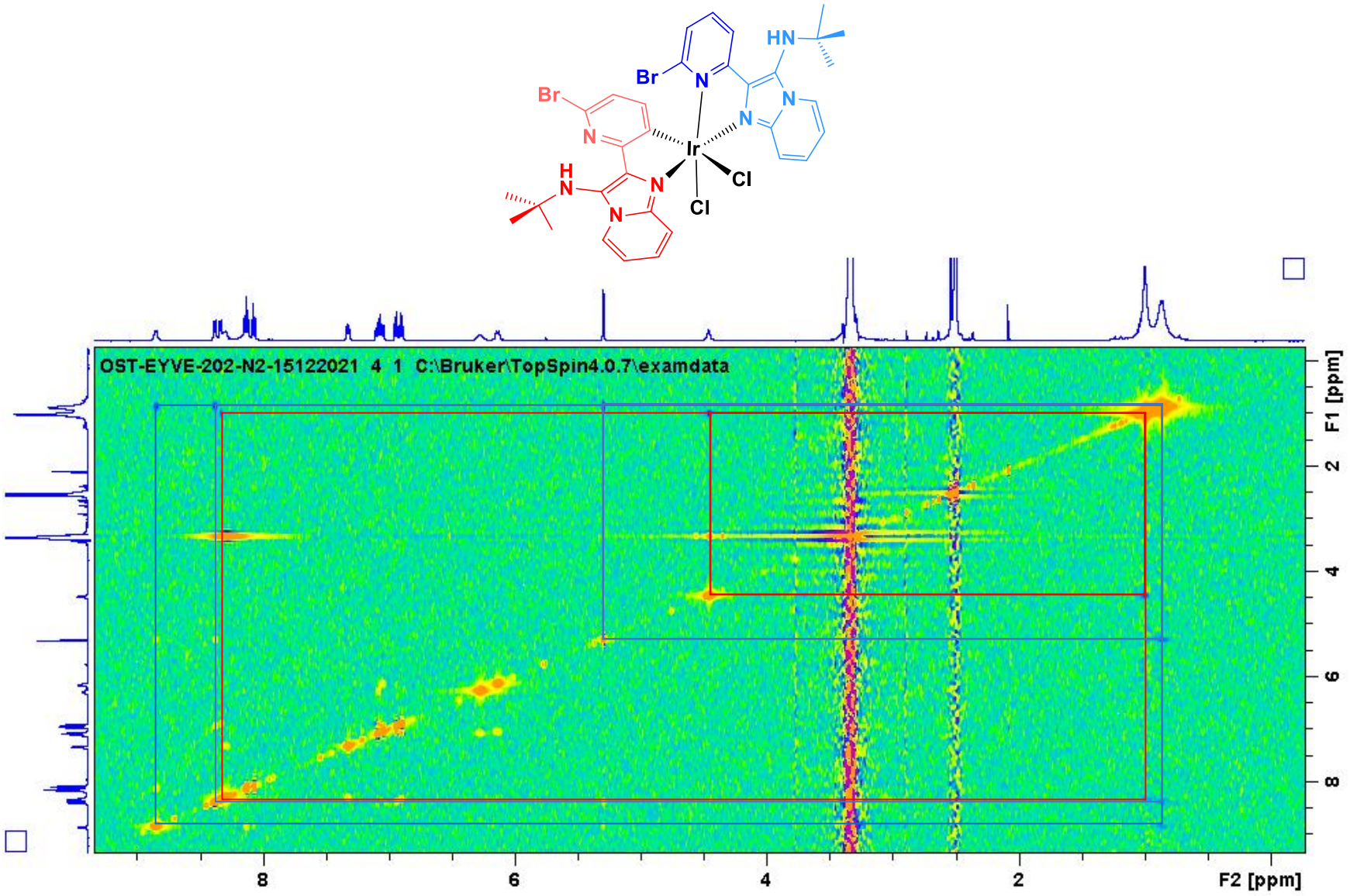

Fig. S.6. NOESY spectrum of complex **1** in $(CD_3)_2SO$.

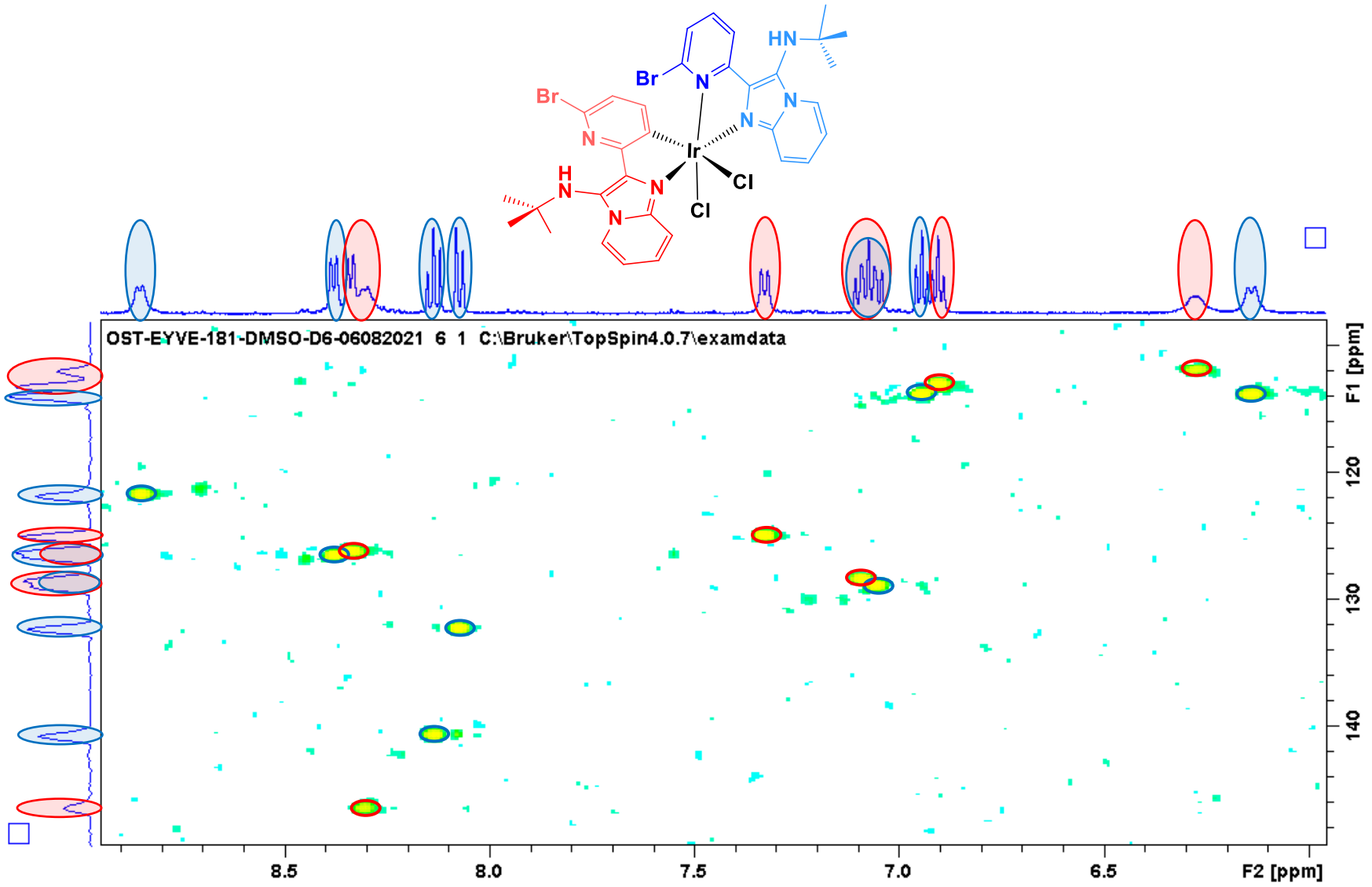

Fig. S.7. HSQC spectrum of complex **1** in $(CD_3)_2SO$.

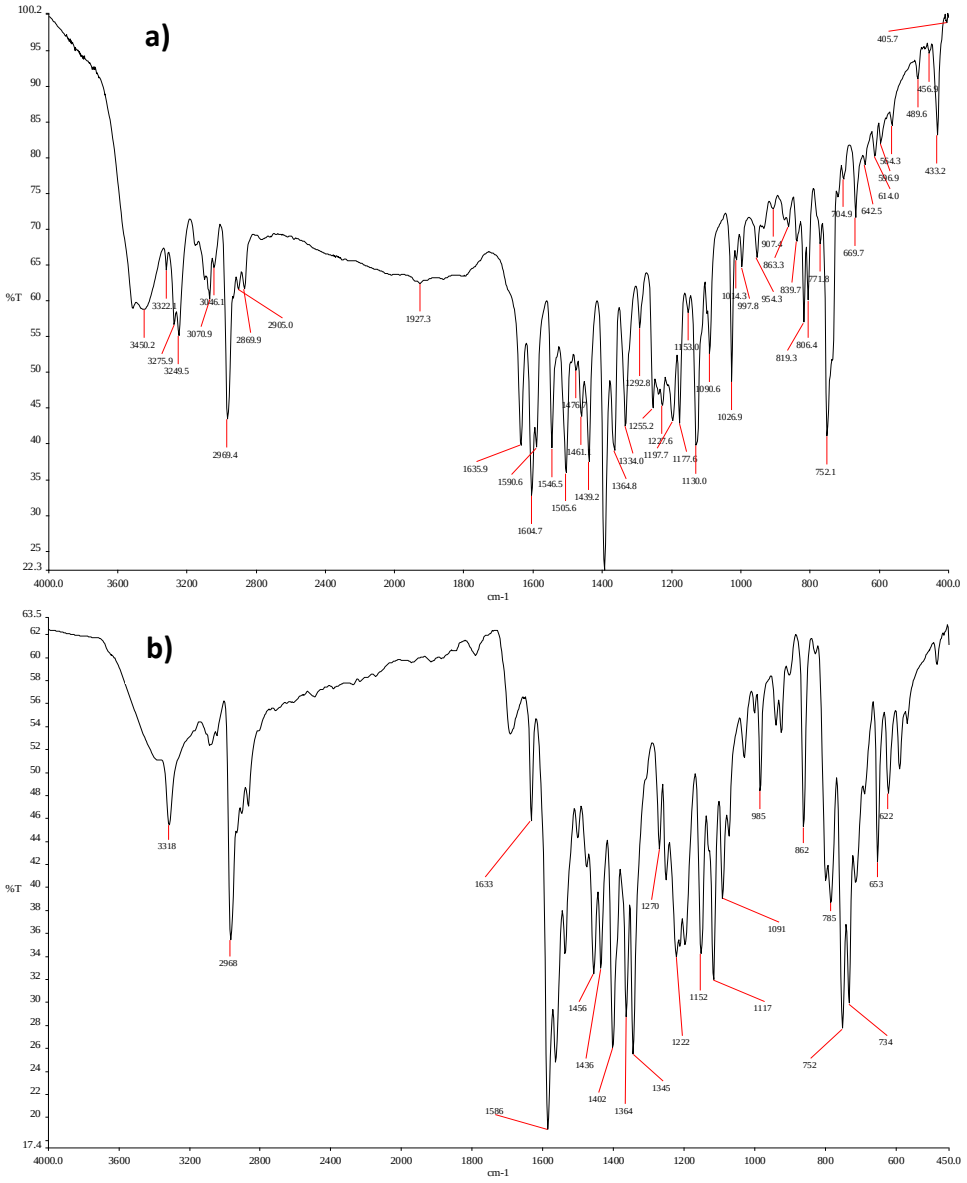

Fig. S.8. (a) Comparative IR spectrum of complex **1** and (b) **L_1**, in KBr.

A comparative analysis between IR spectrum of ligand **L_1** and rollover complex **1**, give a strong suggestion about two different coordination of κ^2-C,N- and κ^2-N,N-donor modes coming from ligand fragments according to vibration frequency of NH bonds between 3450 to 3249 cm^{-1}.

Table S.1. ADMET properties of the ligand $\mathbf{L_1}$ and complex **1.**

ADMET Characteristics	**Compound**	
	$\mathbf{L_1}$	**Complex 1**
Molecular weight	345.24	952.6
Log P	4.37	6.9
H bond acceptor	4	5
H bond donor	1	2
Rotatable bonds	2	2
Absorption		
Oral bioavailability	+	+
Blood brain barrier	+	+
Intestinal absorption	+	+
CaCo-2 permeability	+	-
P-glycoprotein substrate	-	-
P-glycoprotein inhibitor	-	+
Distribution and Metabolism		
CYP3A4 substrate	+	+
CYP2C9 substrate	-	-
CYP2D6 substrate	-	-
CYP3A4 inhibition	+	-
CYP2C9 inhibition	+	-
CYP2D6 inhibition	+	-
CYP inhibitory promiscuity	+	+
Excretion and Toxicity		
Human Ether-a-go-go-Related Gene Inhibition	-	+
Carcinogenicity (binary)	-	-
Fish toxicity	+	+
Acute oral toxicity	III	III
Hepatoxicity	+	+

Biological assays

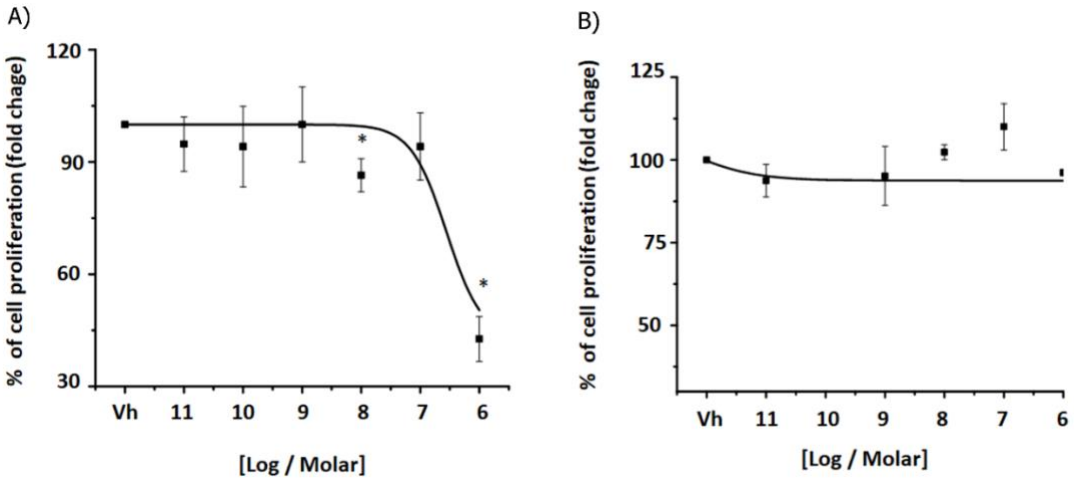

Fig. S.9. Antiproliferative effect of ligand $\mathbf{L_1}$ and complex **1** in cancer cells. Triple-negative breast cancer cells HCC1937 were incubated in the presence of a) $\mathbf{L_1}$ and b) complex **1** at different concentrations for 72 hours. Cell proliferation was evaluated by the Sulforhodamine method. Results are shown as the mean ± standard deviation (S.D) of triplicate determinations of three independent experiments. Data from vehicle-treated cells (V) were normalized to 100%. *p < 0.001 vs the vehicle.

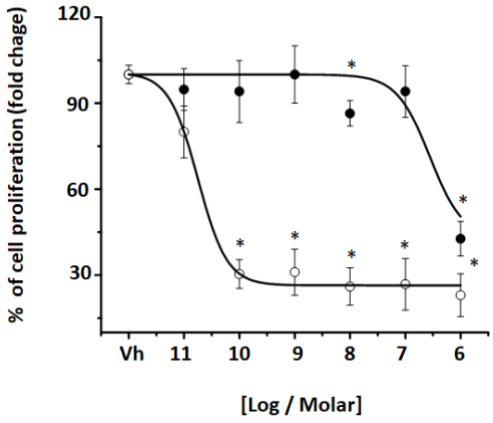

Fig1 S.10. Antiproliferative effect of $\mathbf{L_1}$ and cabaxitazel in cancer cells. Triple-negative breast cancer cells HCC1937 were incubated in the presence of $\mathbf{L_1}$ (•) and cabazitaxel (○) at different concentrations for 72 hours. Cell proliferation was evaluated by the Sulforhodamine method. Results are shown as the mean ± standard deviation (S.D) of triplicate determinations of three independent experiments. Data from vehicle-treated cells (V) were normalized to 100%. *p < 0.001 vs the vehicle.

Computational methodology

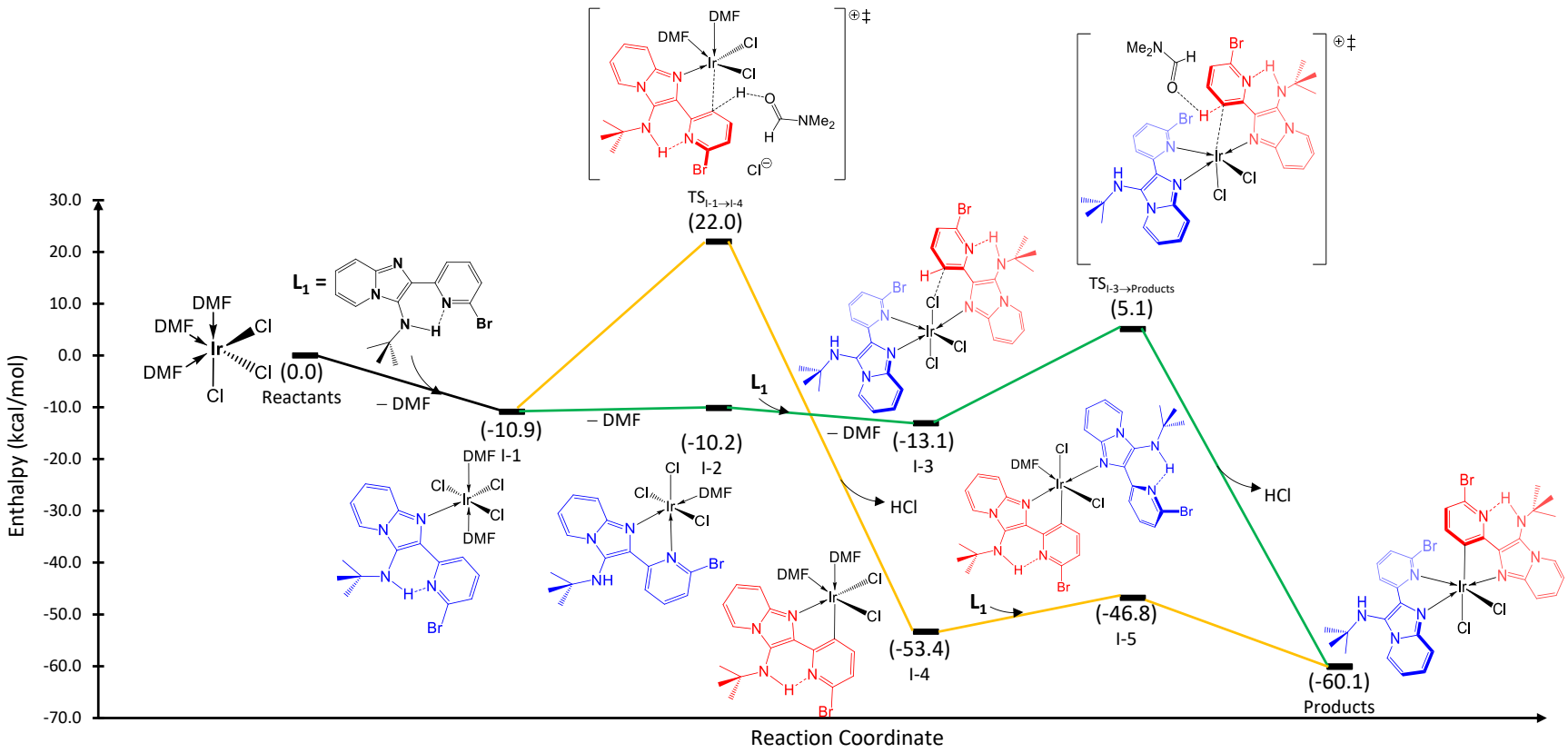

Fig. S.11. Proposed reaction mechanism (energies in the enthalpy scale), with thermal corrections at 298.15K, calculated at the SMD(DCE):ωB97X-D/def2-tzvpp//ωB97X-D/def2-svpp level.

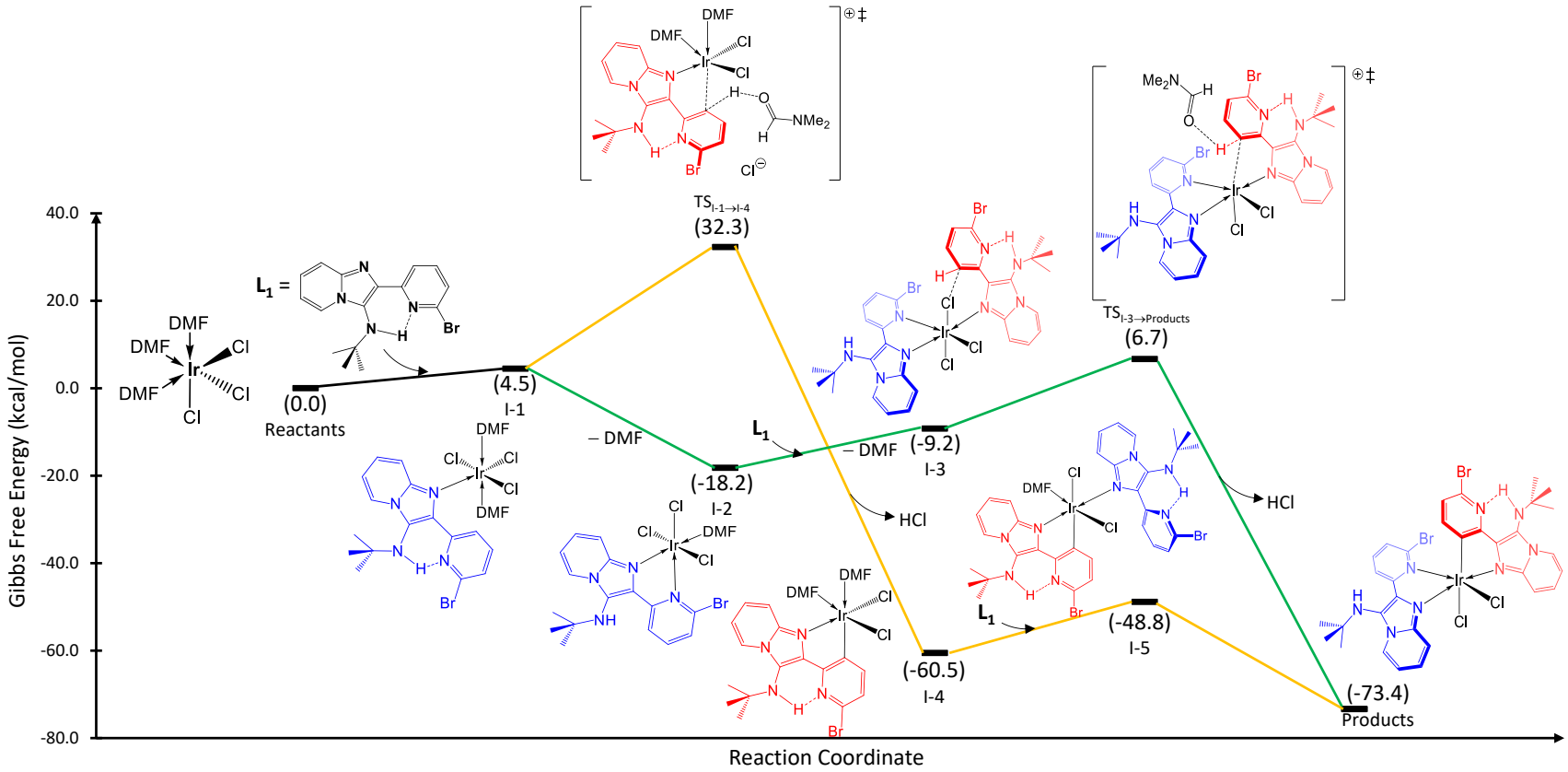

Fig. S.12. Proposed reaction mechanism (energies in the Gibbs free energy scale), with entropic corrections at 298.15K, calculated at the SMD(DCE):ωB97X-D/def2-tzvpp//ωB97X-D/def2-svpp level.

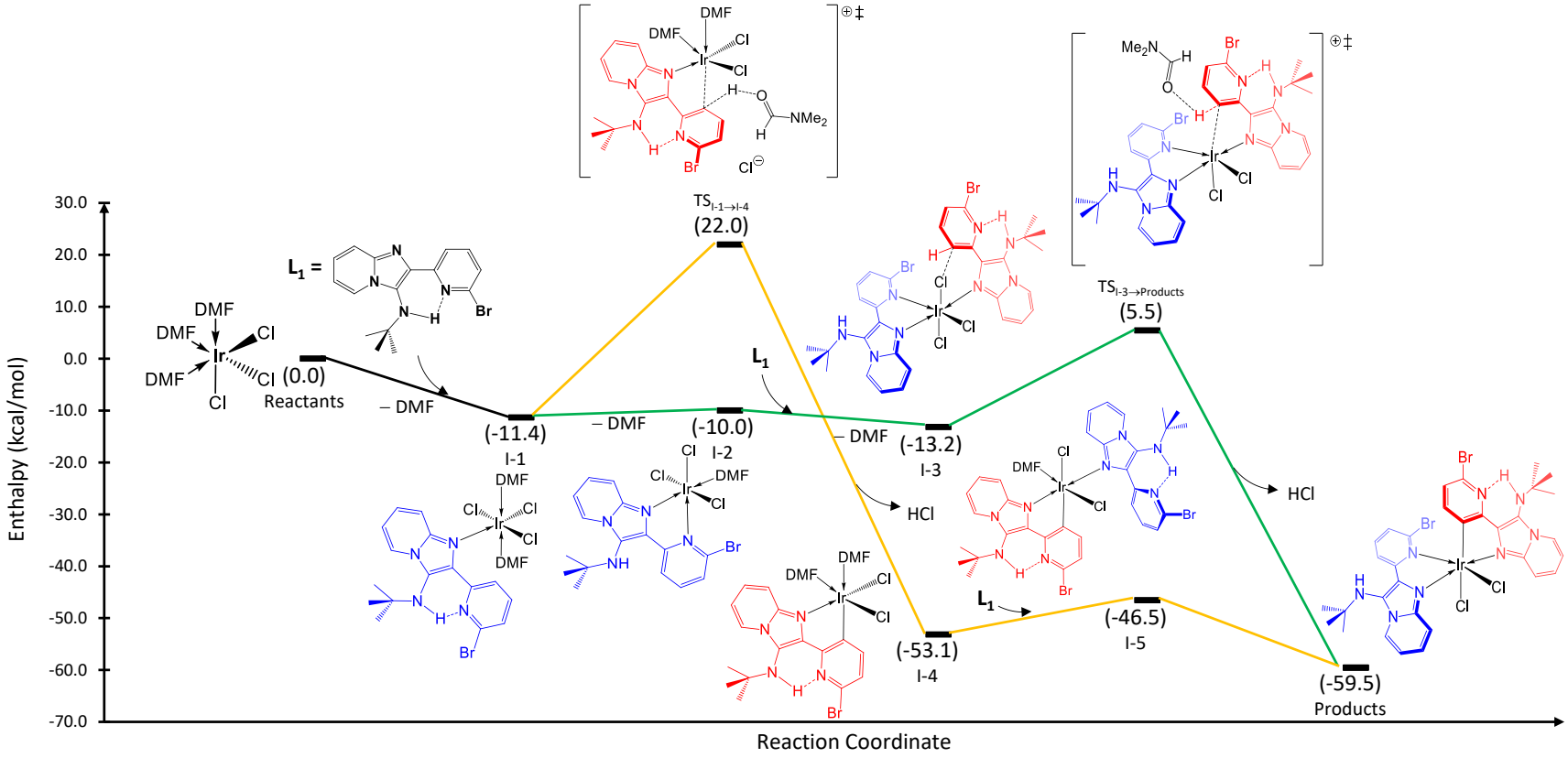

Fig. S.13. Proposed reaction mechanism (energies in the enthalpy scale), with thermal corrections at 368.15K, calculated at the SMD(DCE):ωB97X-D/def2-tzvpp//ωB97X-D/def2-svpp level.

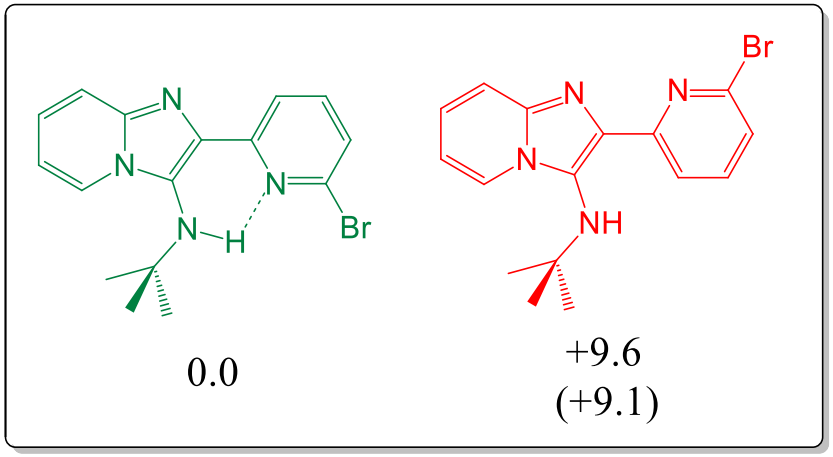

Fig. S.14. Structural stability of our ligand **L₁** calculated at the ωB97X-D/def2-svpp level. Energy values (enthalpy; in parenthesis, Gibbs free energy) are in kcal/mol.

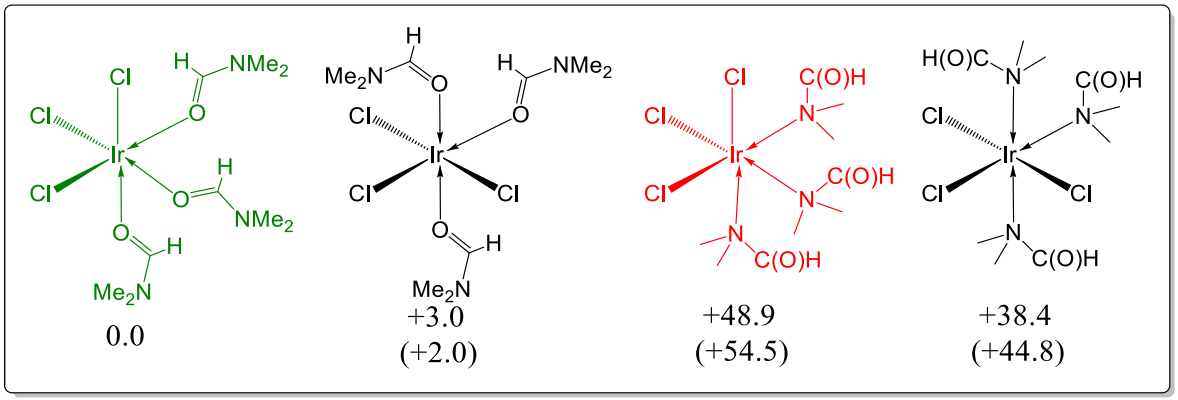

Fig. S.15. Conformation study of the reactant showing two coordination modes of DMF. Values are in kcal/mol calculated at the ωB97X-D/def2-svpp level.

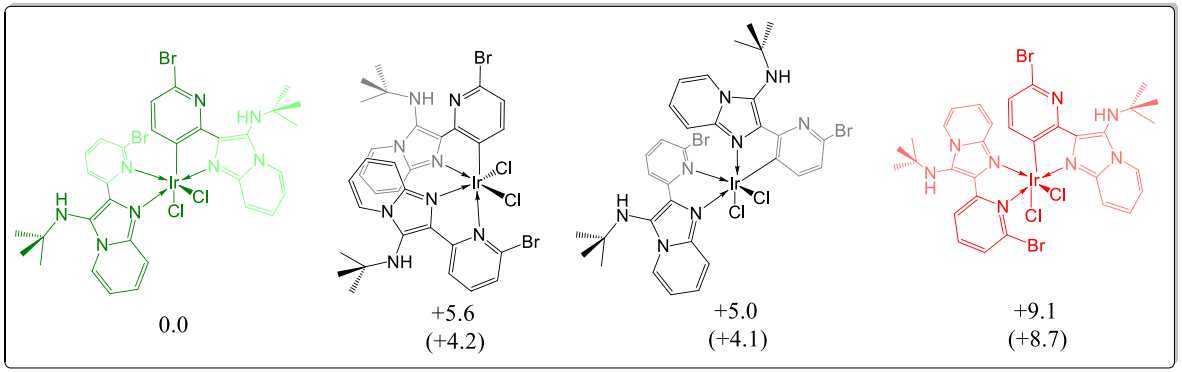

Fig. S.16. Conformation study of the potential reaction products. Values are in kcal/mol calculated at the ωB97X-D/def2-svpp level.

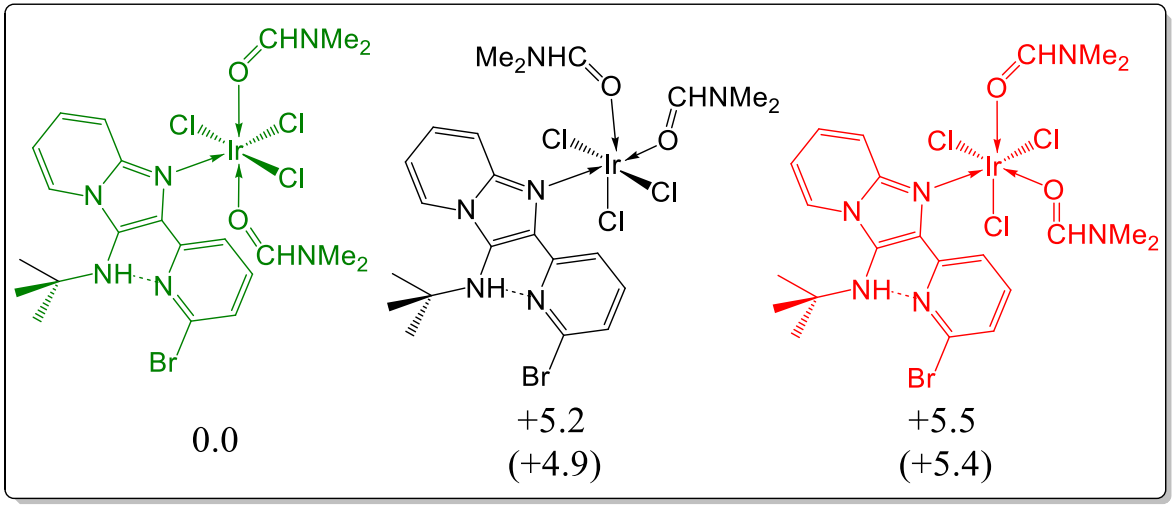

Fig. S.17. Conformation study of intermediate **I-1**. Values are in kcal/mol calculated at the ωB97X-D/def2-svpp level.

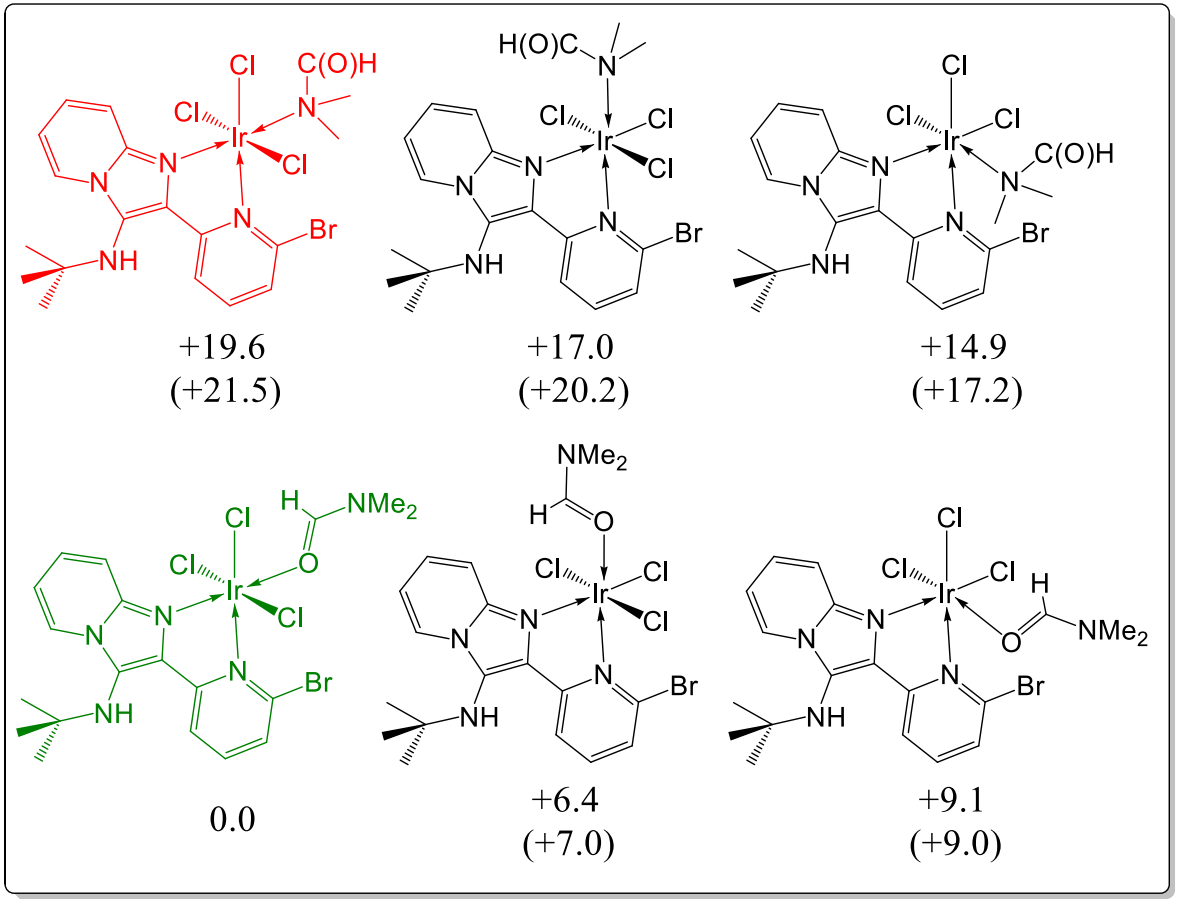

Fig. S.18. Conformation study of intermediate **I-2**. Values are in kcal/mol calculated at the ωB97X-D/def2-svpp level.

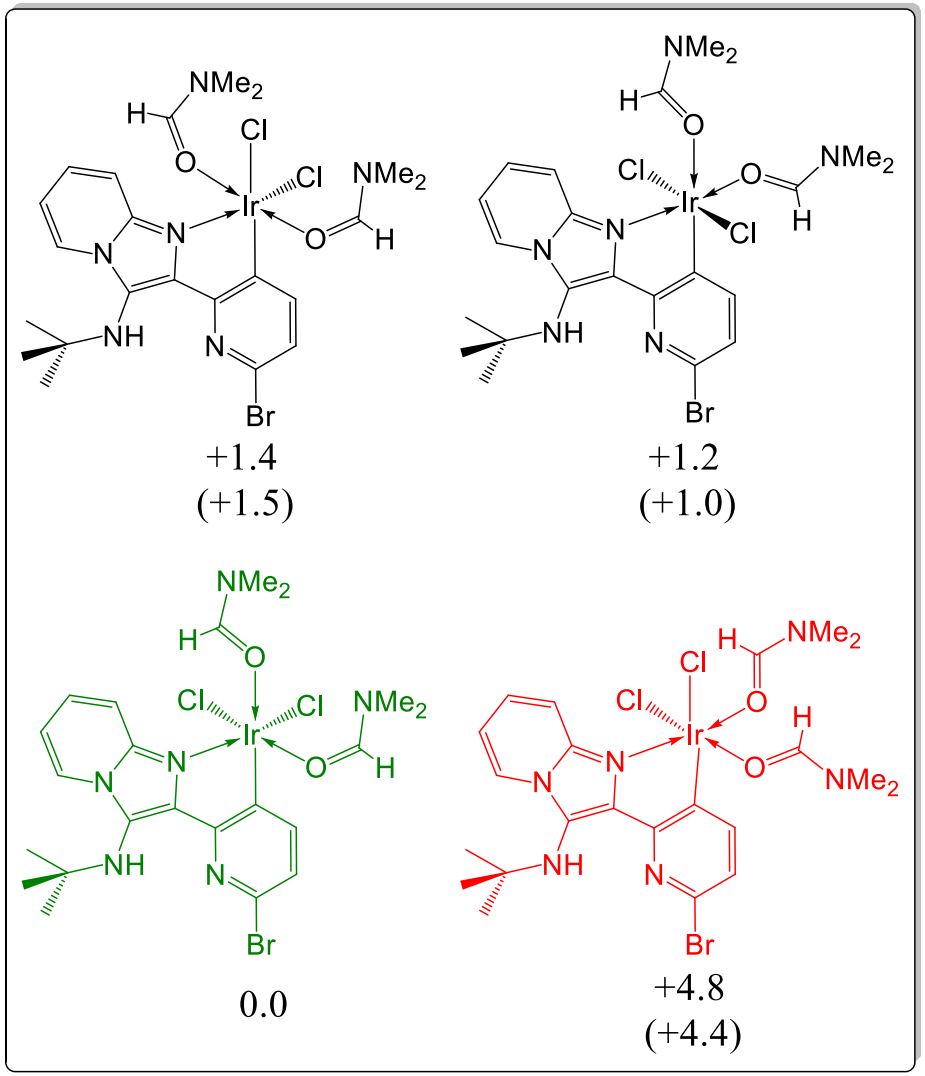

Fig. S.19. Conformation study of intermediate **I-4**. Values are in kcal/mol calculated at the ωB97X-D/def2-svpp level.

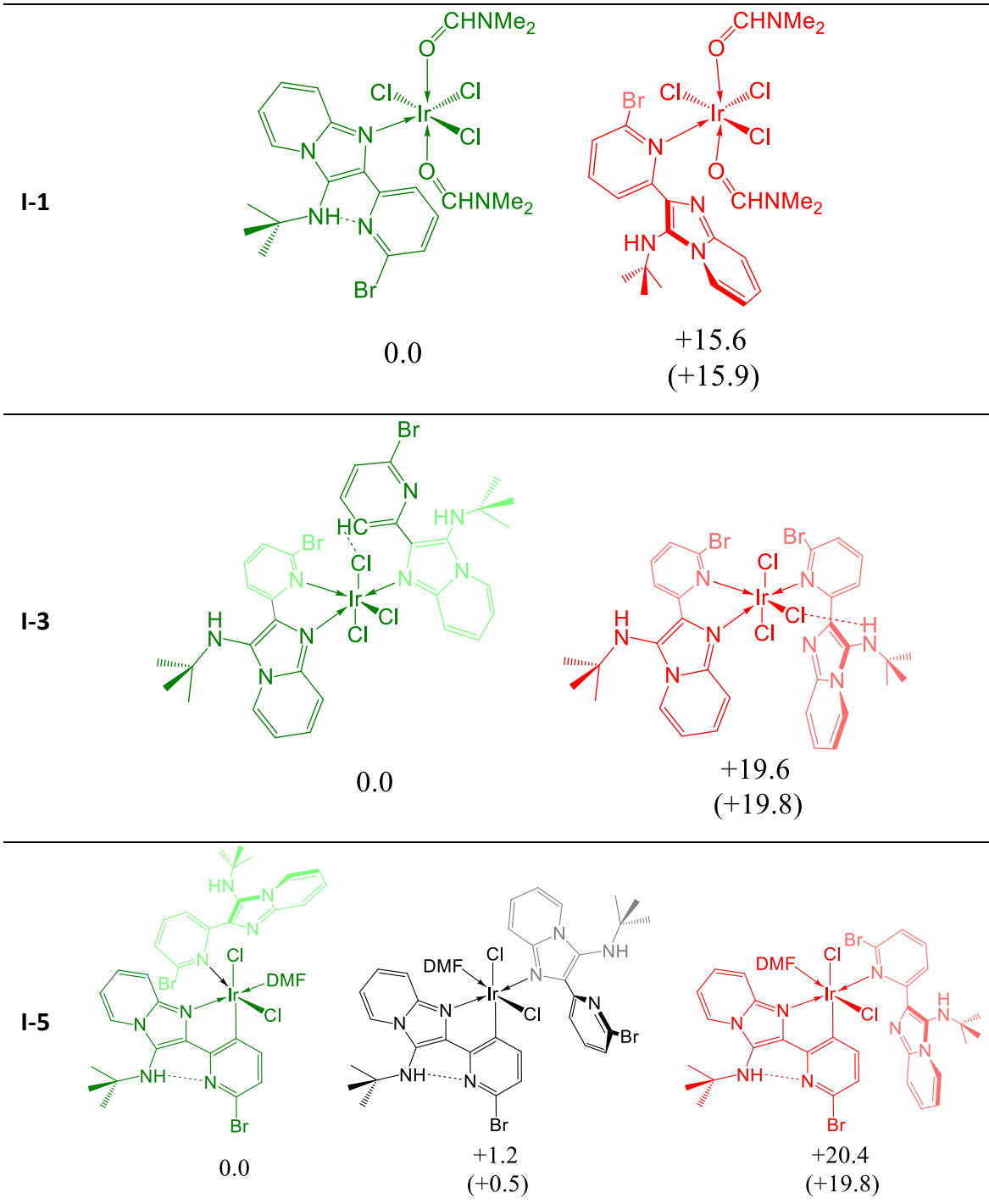

Fig. S.20. Conformation study of two coordination modes (via either pyridine or 3-azaindolizine nitrogen) for the indicated intermediates. Values are in kcal/mol calculated at the ωB97X-D/def2-svpp level.

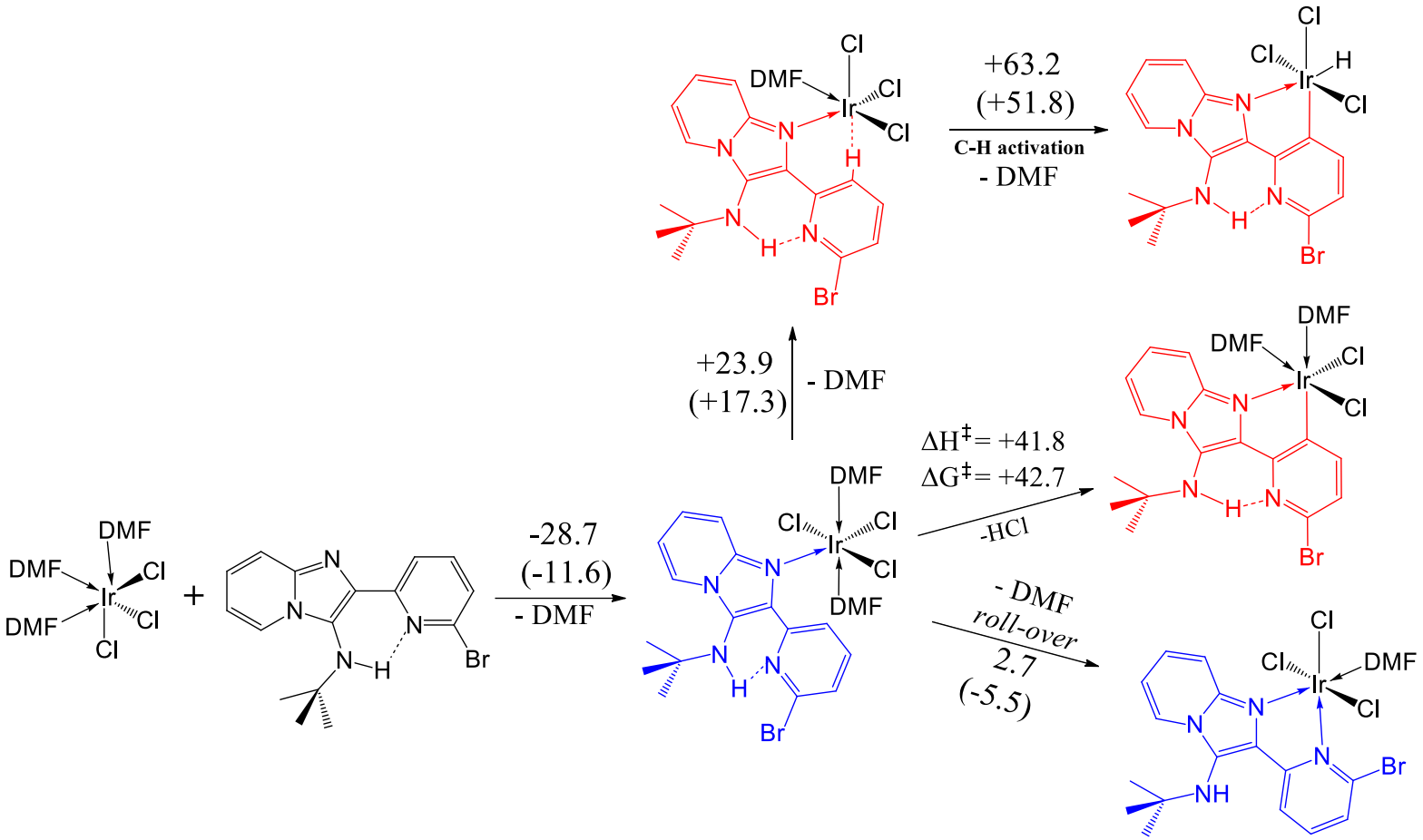

Fig. S.21. Different reaction pathways from coordination of our ligand into the Ir(III) complex calculated in electronic energies at the ωB97X-D/def2-svpp level (energy values are shown in kcal/mol). It can be seen that the oxidative addition route through the Ir(IV) complex (upper side) is the highest in energy.

NMR complementary spectrums of ligand L_1 in $CDCl_3$ and $(CD_3)_2SO$

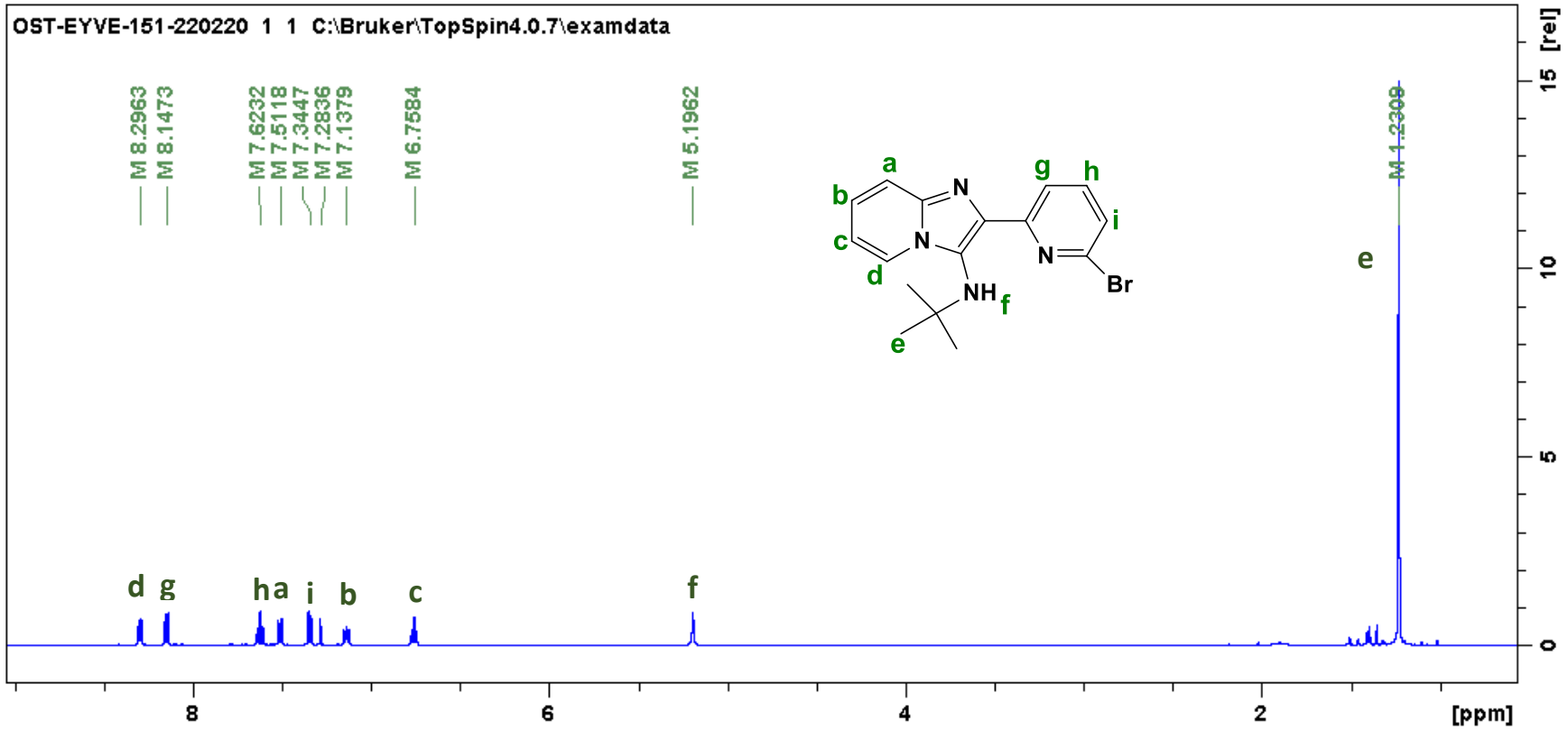

Fig. S.22. ^1H NMR spectrum of ligand **L_1** in $CDCl_3$.

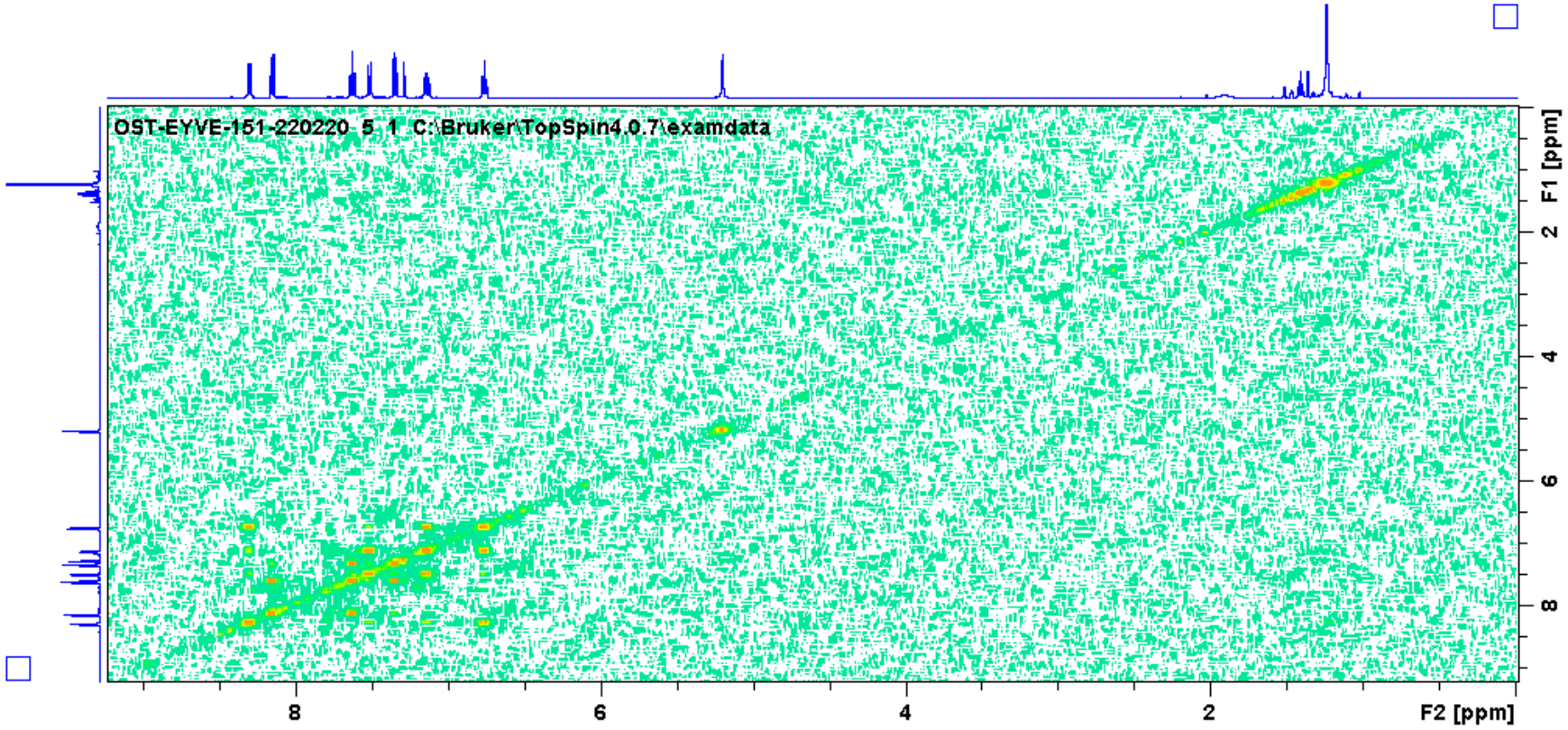

Fig. S.23. COSY spectrum of ligand **L1** in $CDCl_3$.

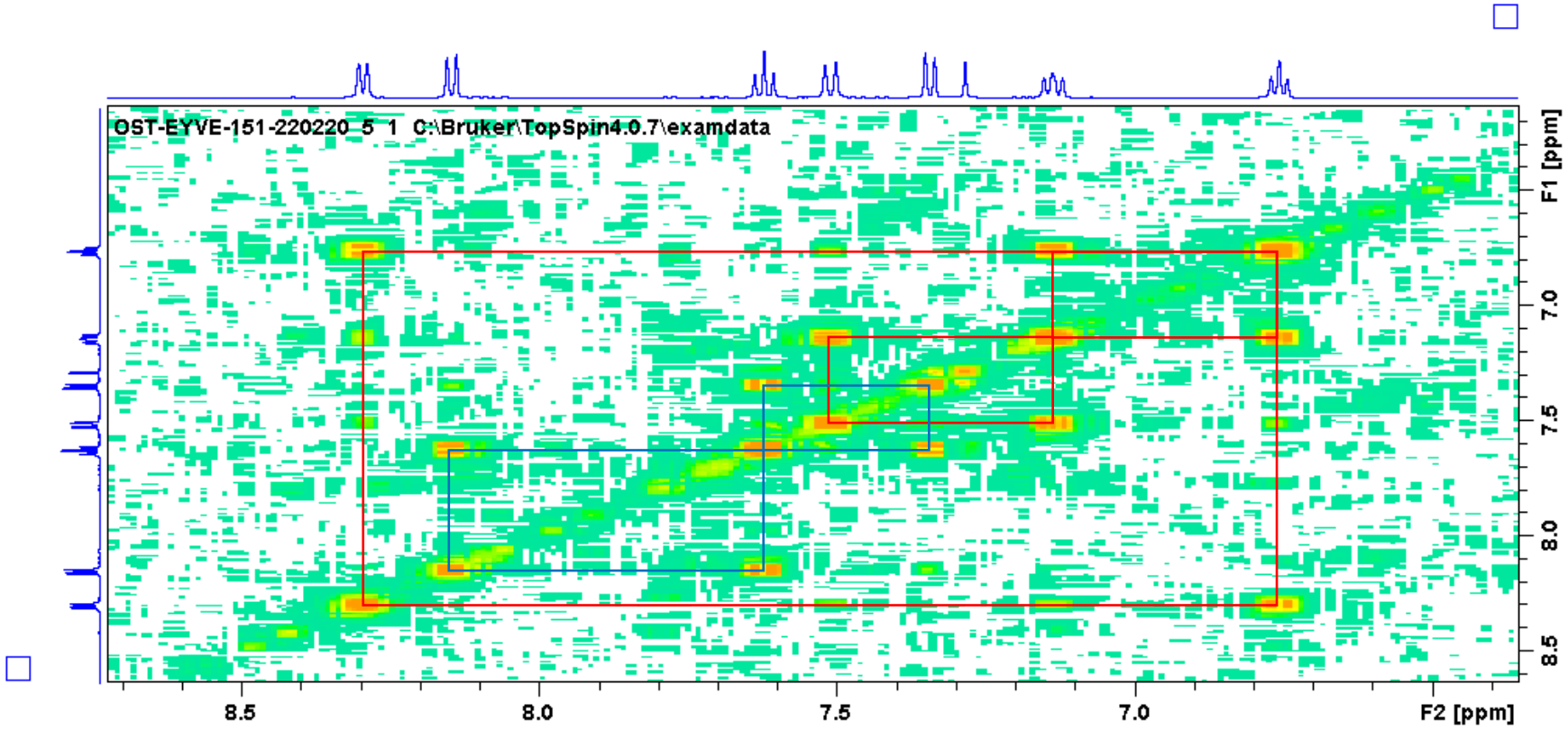

Fig. S.24. COSY spectrum of ligand **L1** in $CDCl_3$.

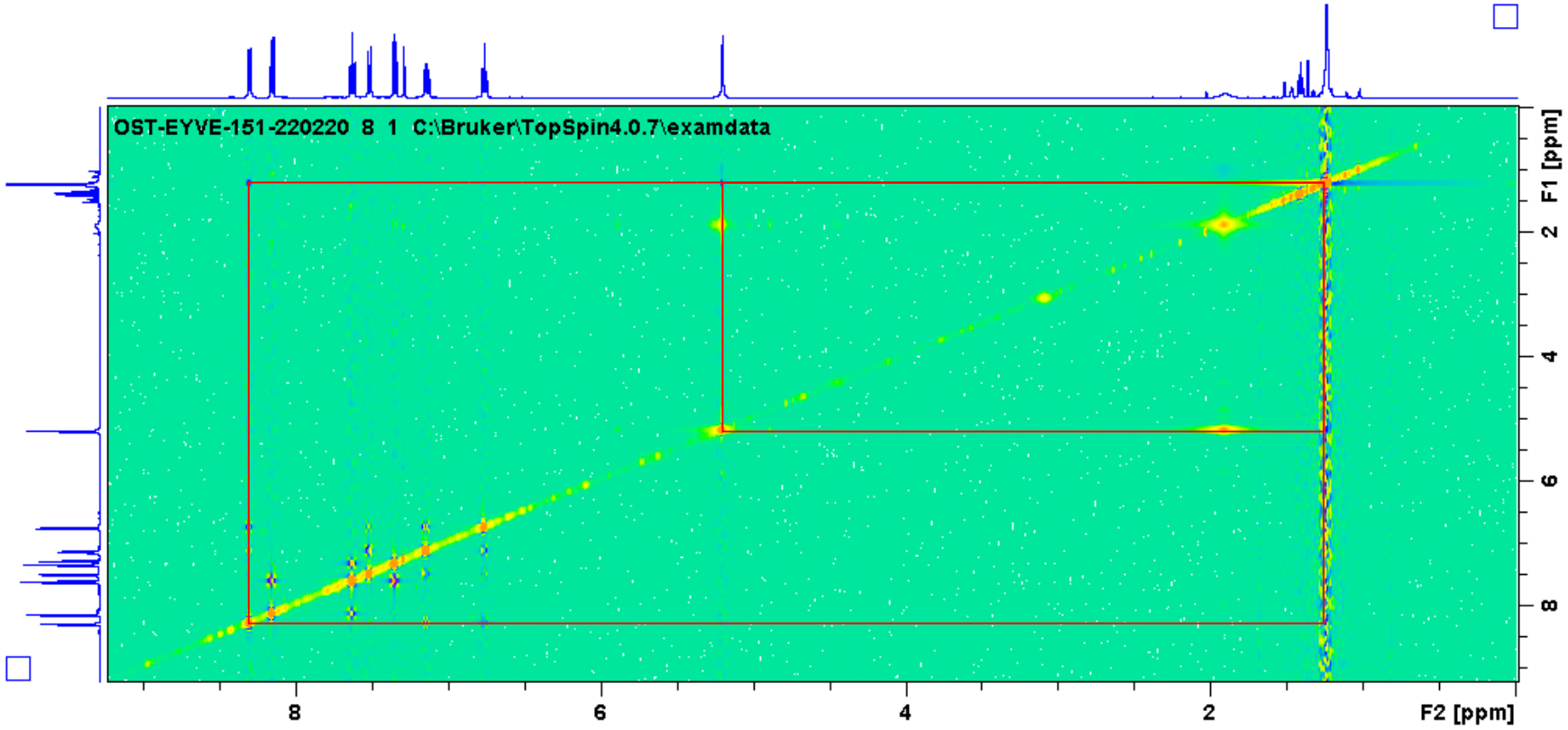

Fig. S.25. NOESY spectrum of ligand **L**$_1$ in $CDCl_3$.

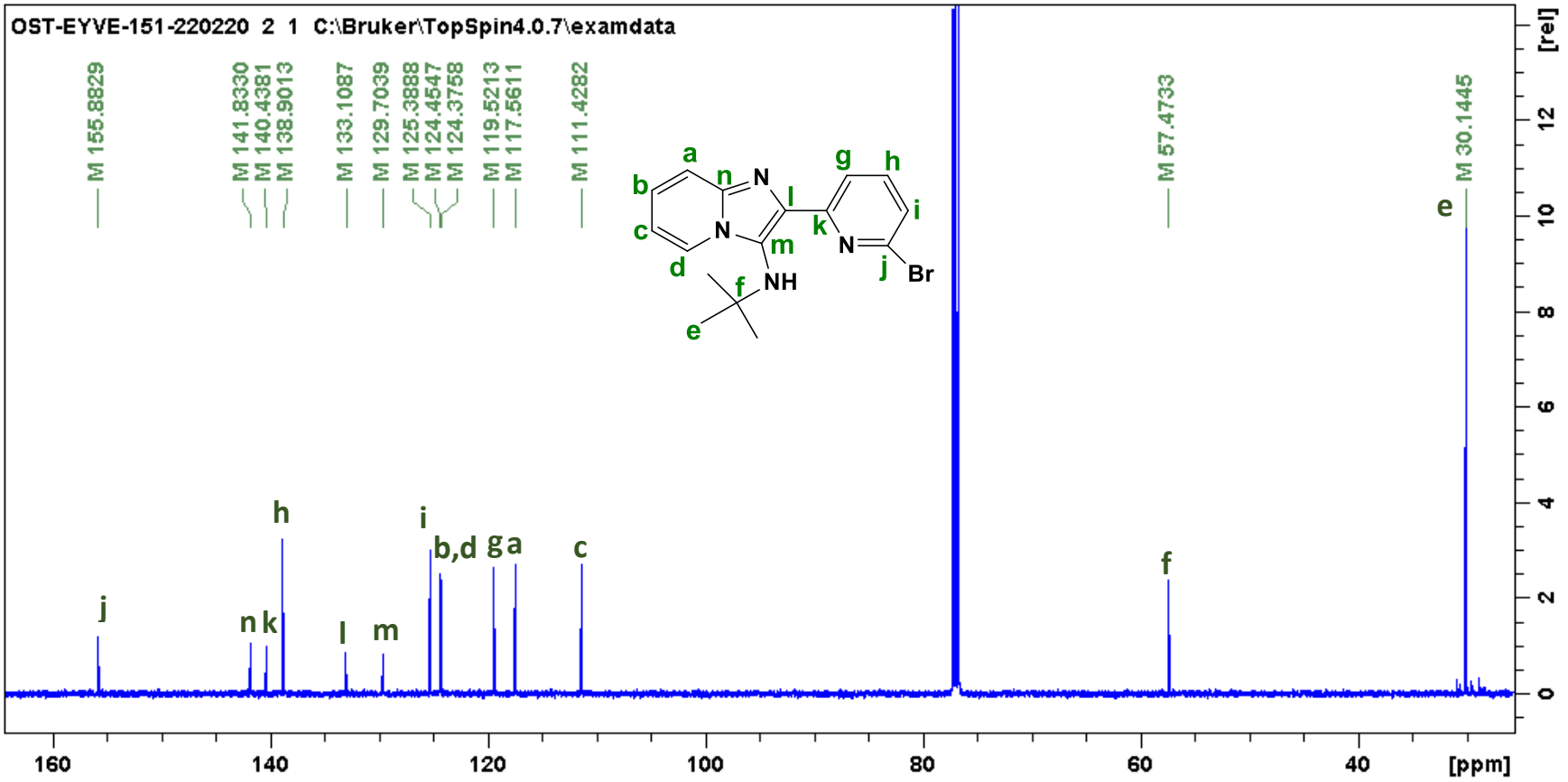

Fig. S.26. $^{13}C\{^{1}H\}$ NMR spectrum of ligand **L_1** in $CDCl_3$.

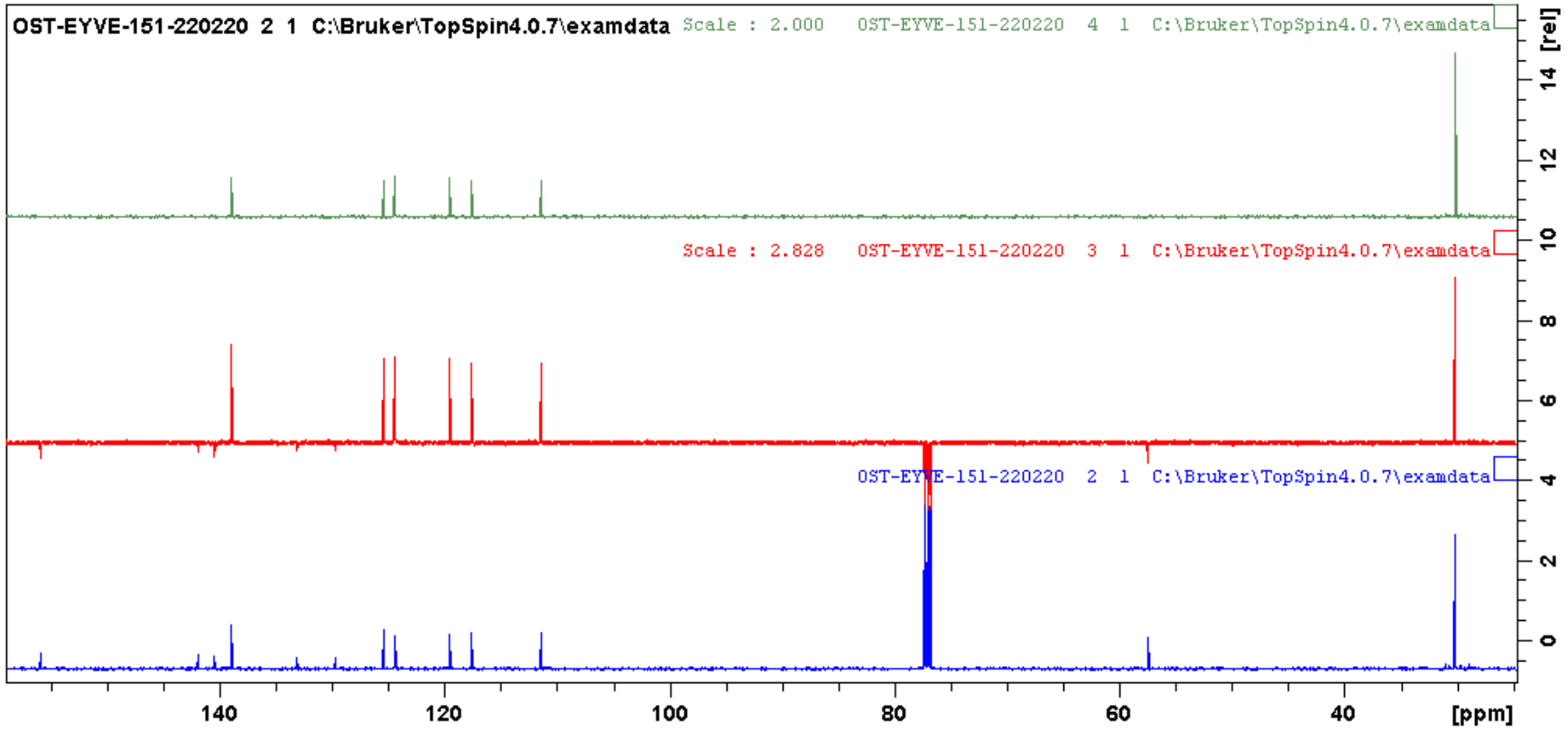

Fig. S.27. $^{13}C\{^{1}H\}$ NMR spectrum of ligand $\mathbf{L_1}$ in $CDCl_3$.

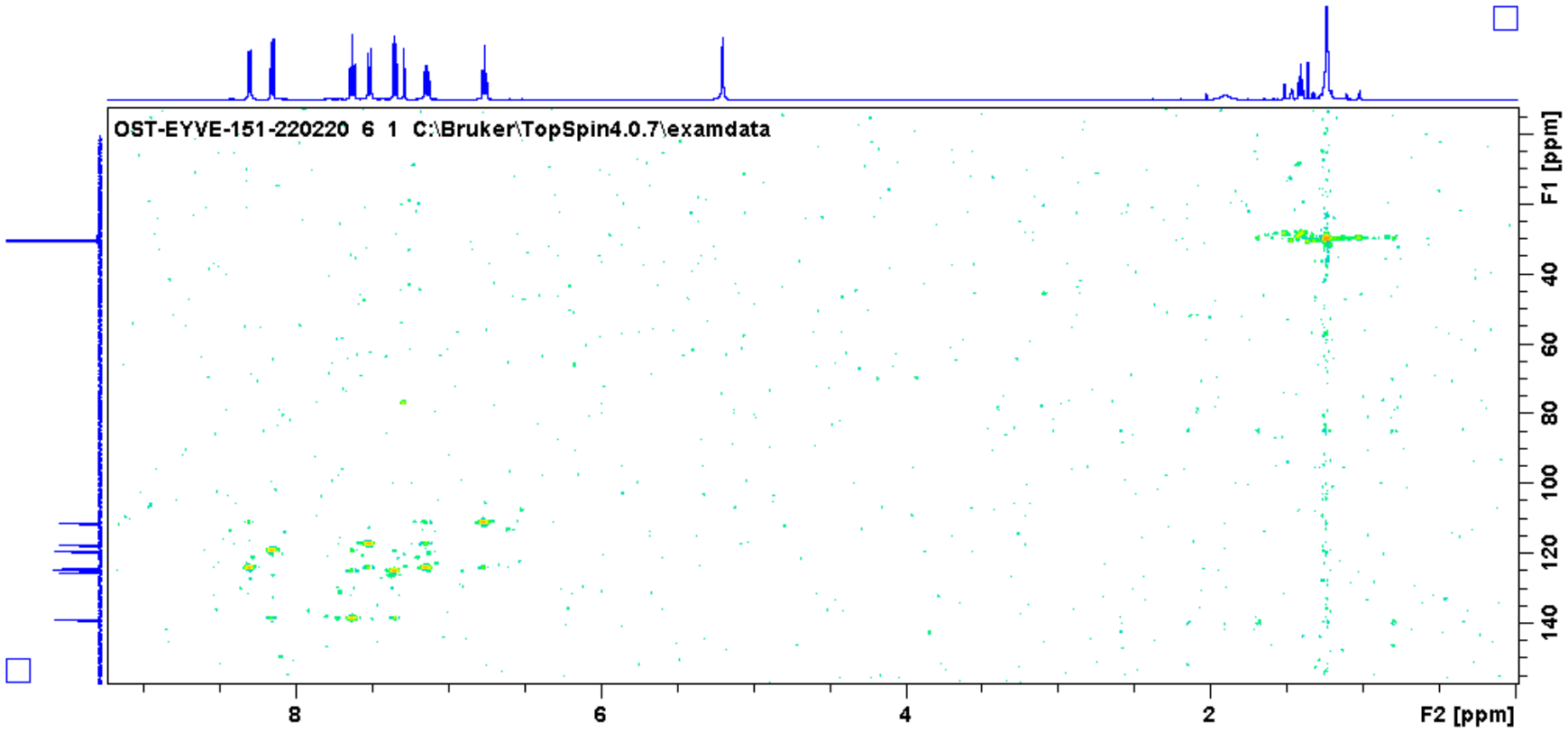

Fig. S.28. HSQC spectrum of ligand **L_1** in $CDCl_3$.

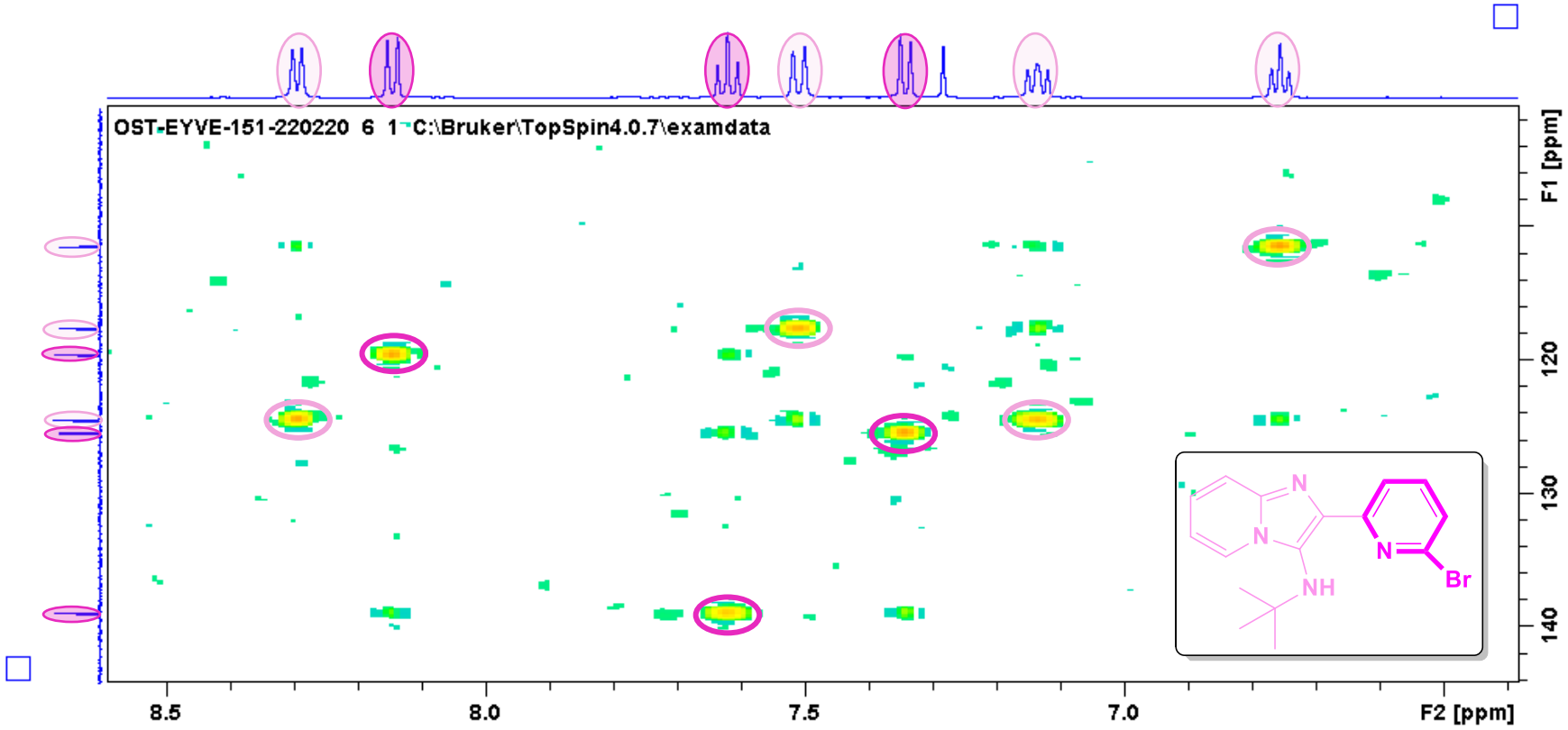

Fig. S.29. HSQC spectrum of ligand **L**$_1$ in $CDCl_3$.

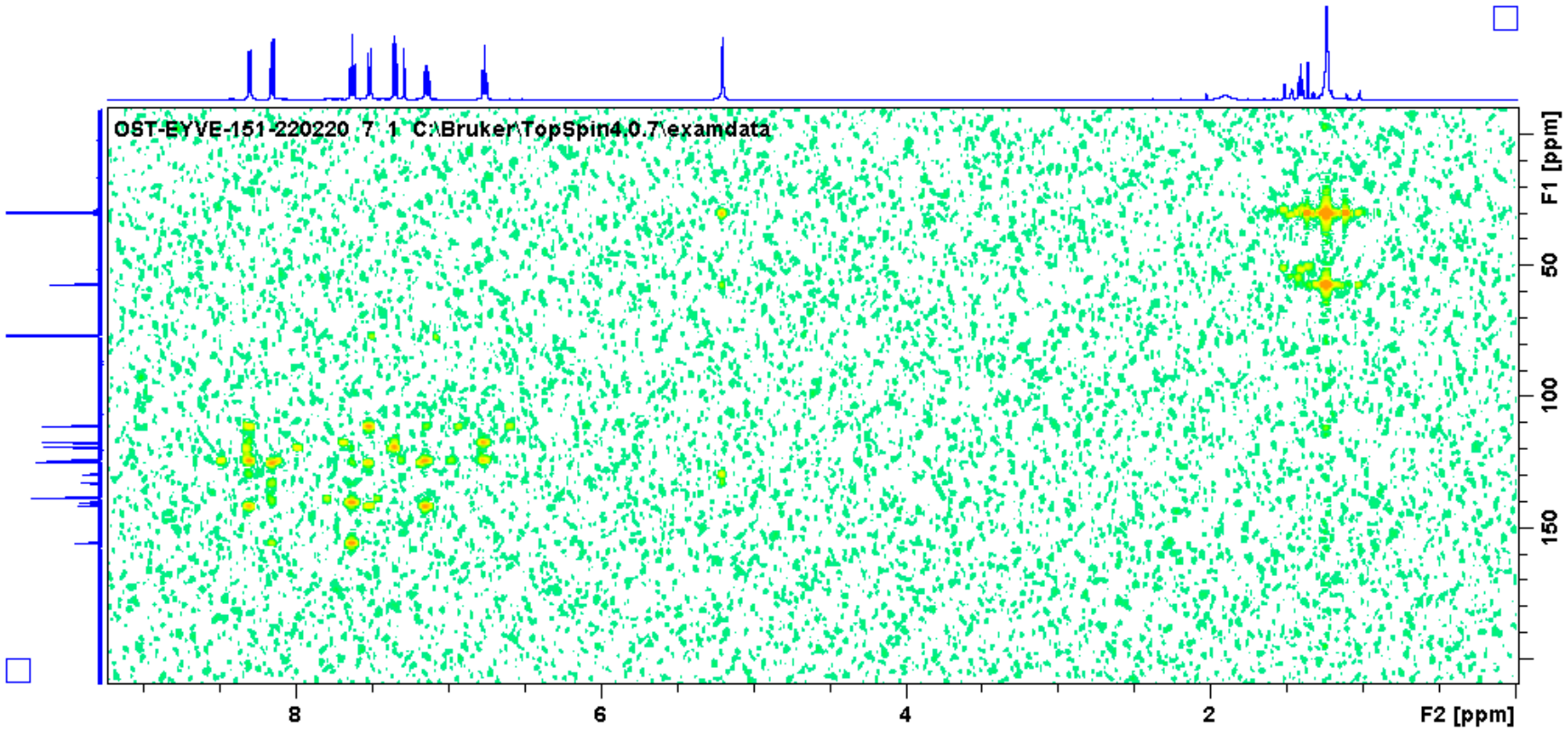

Fig. S.30. HMBC spectrum of ligand **L1** in $CDCl_3$..

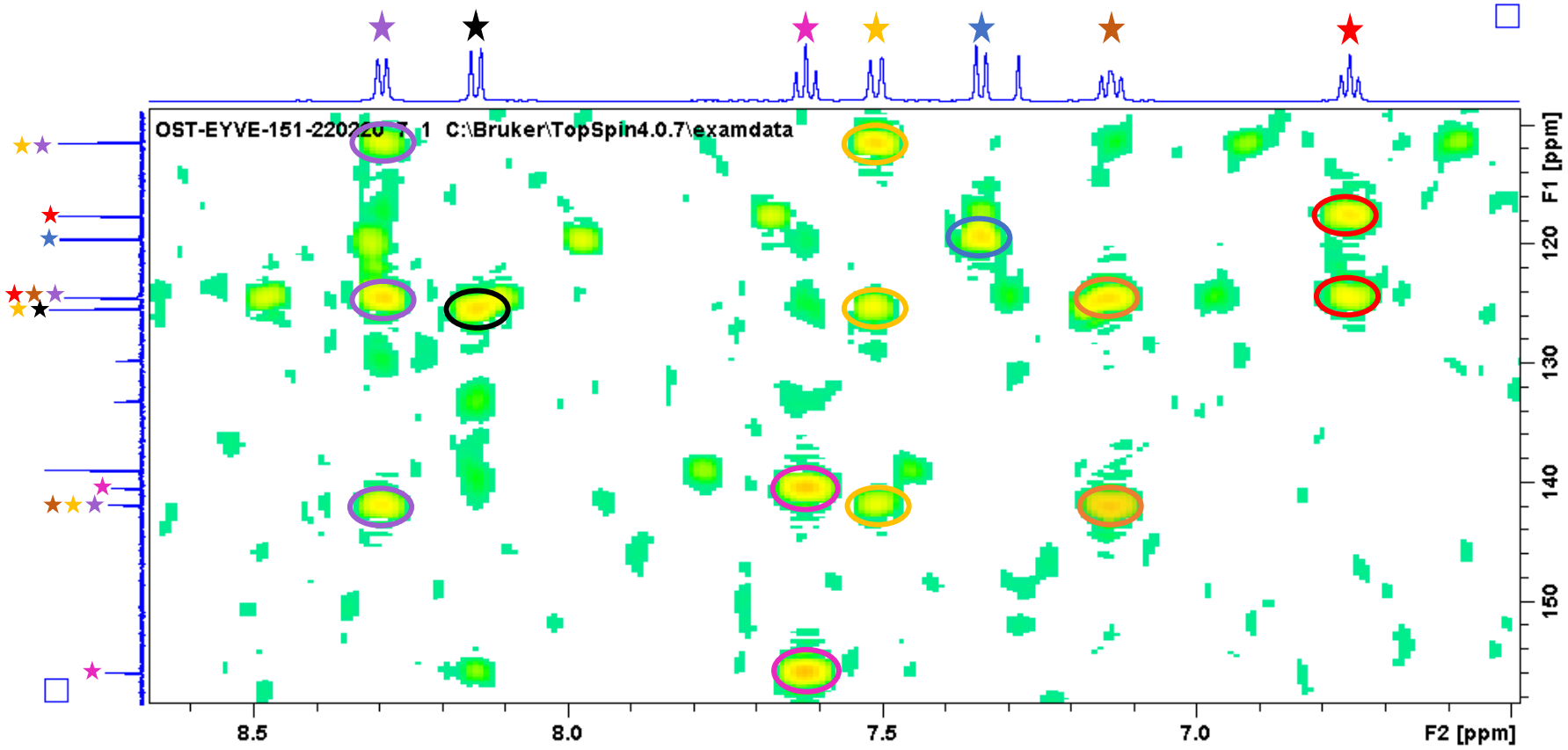

Fig. S.31. HMBC spectrum of ligand $\mathbf{L_1}$ in $CDCl_3$.

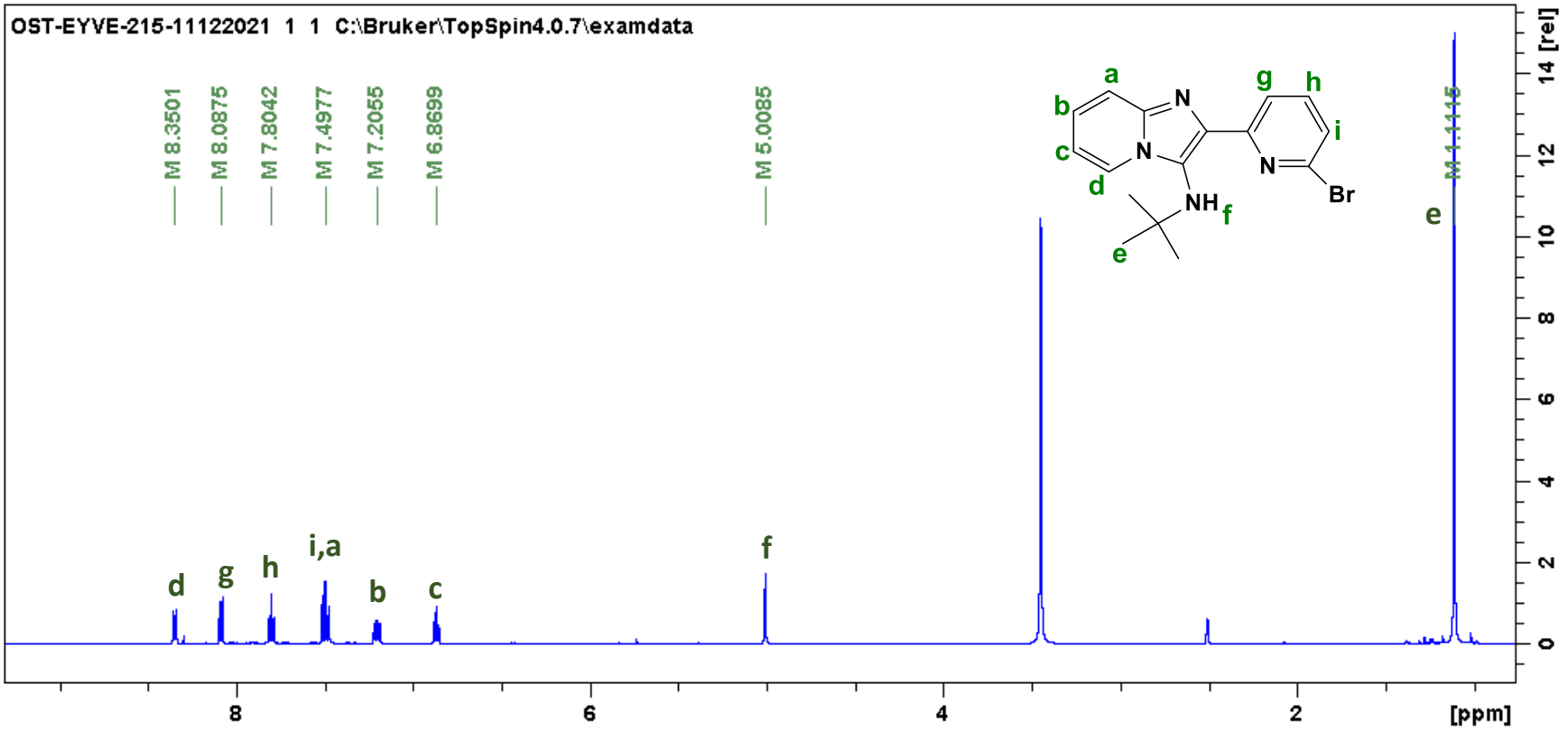

Fig. S.32. ^{1}H NMR spectrum of ligand **L$_1$** in $(CD_3)_2SO$.

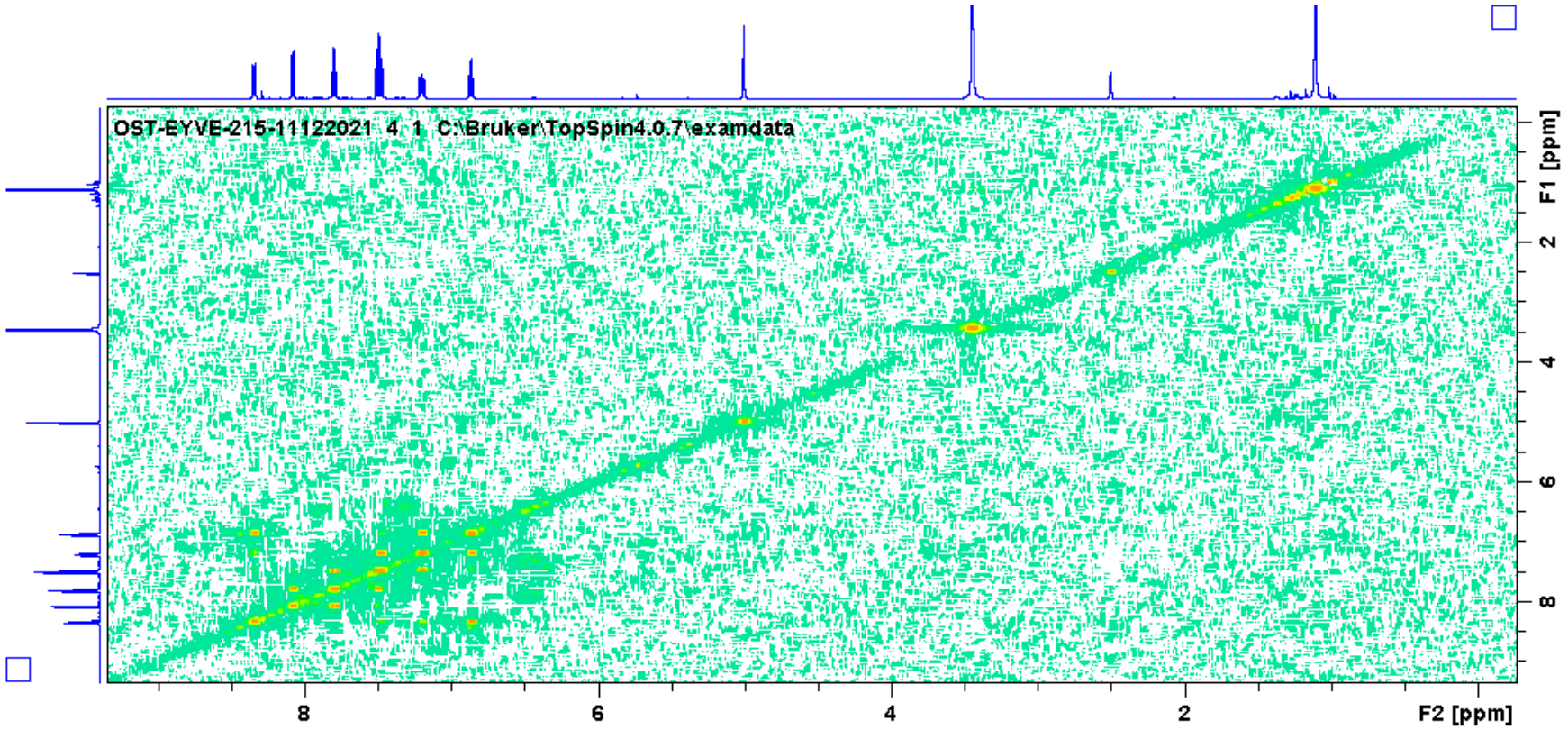

Fig. S.33. COSY spectrum of ligand **L**$_1$ in $(CD_3)_2SO$.

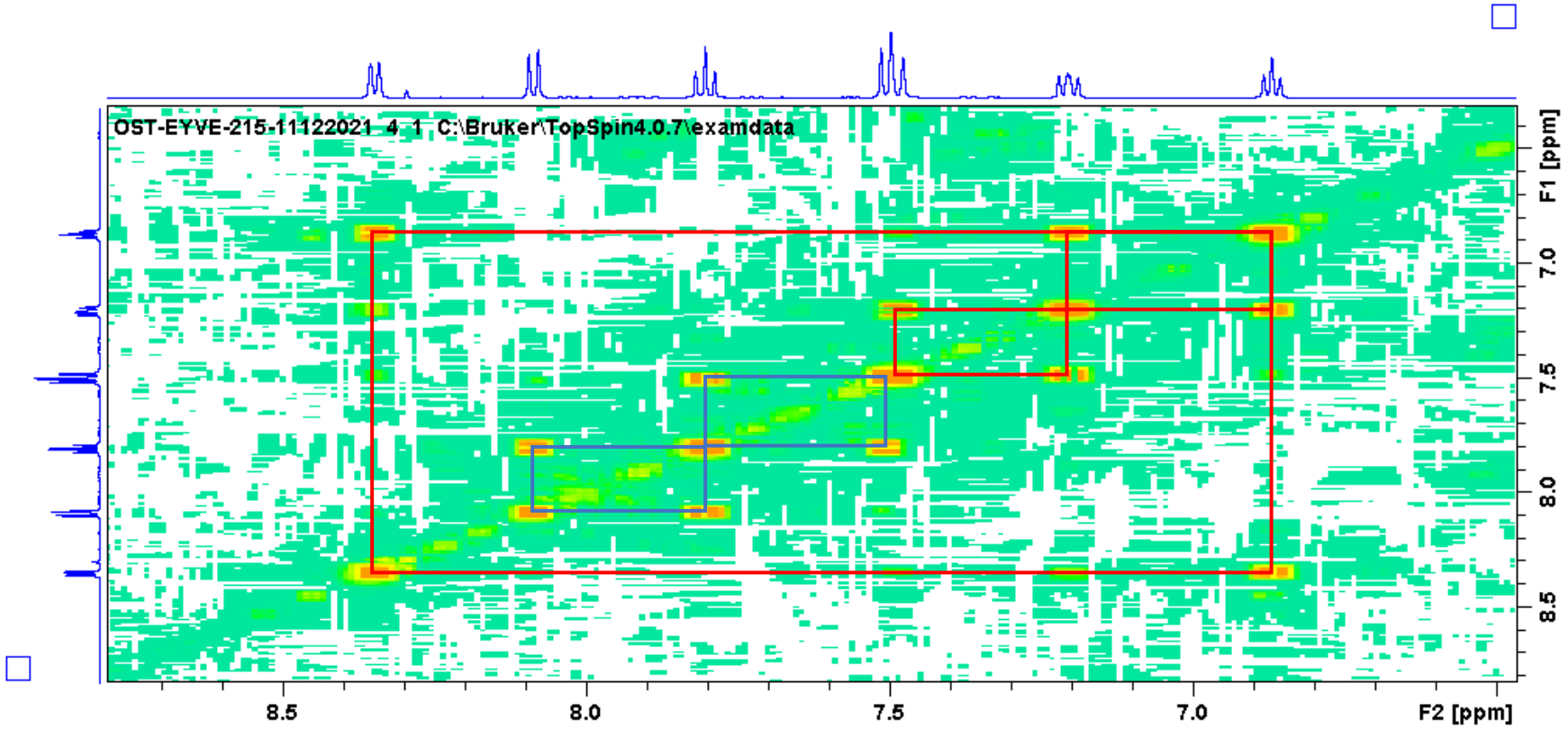

Fig. S.34. COSY spectrum of ligand $\mathbf{L_1}$ in $(CD_3)_2SO$.

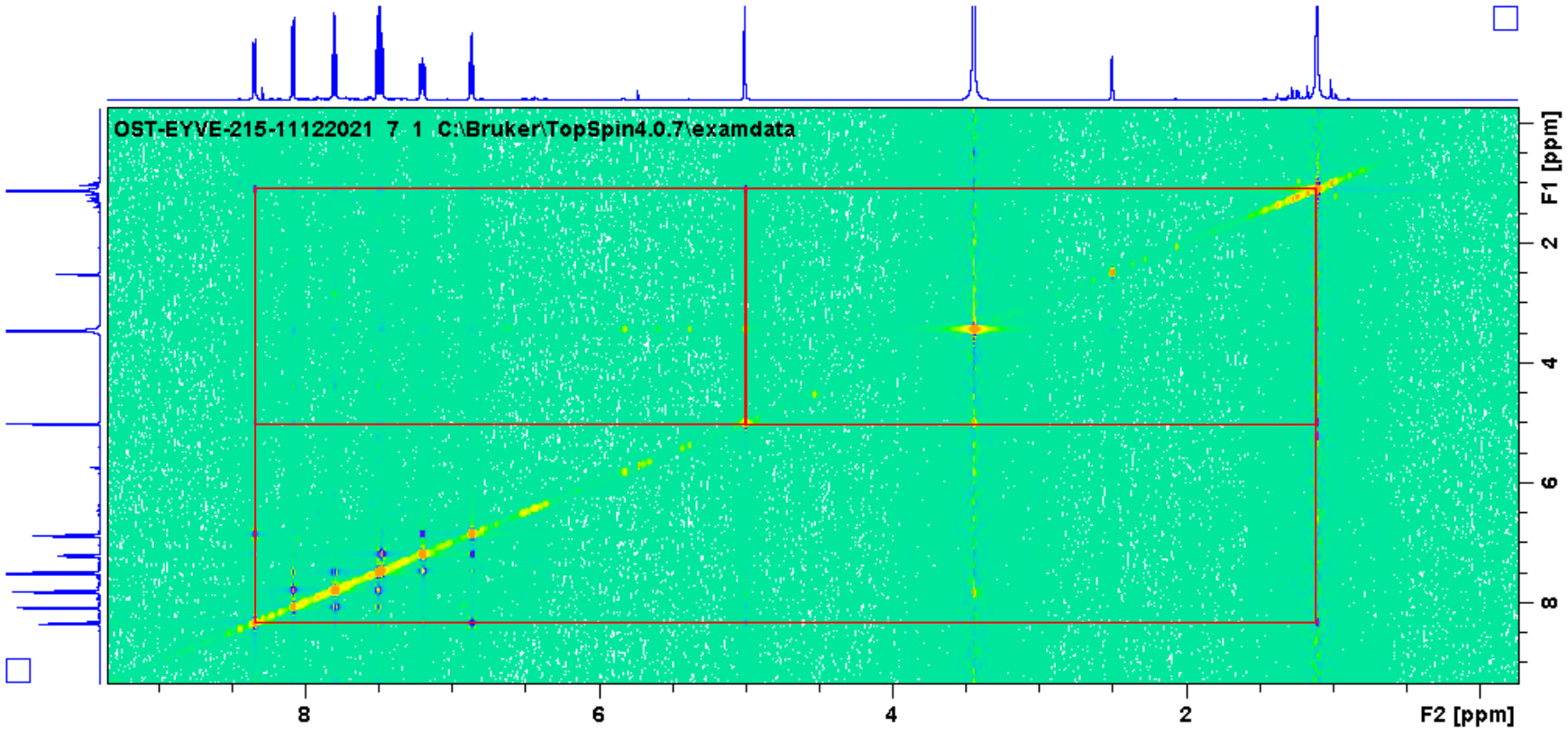

Fig. S.35. NOESY spectrum of ligand **L₁** in $(CD_3)_2SO$.

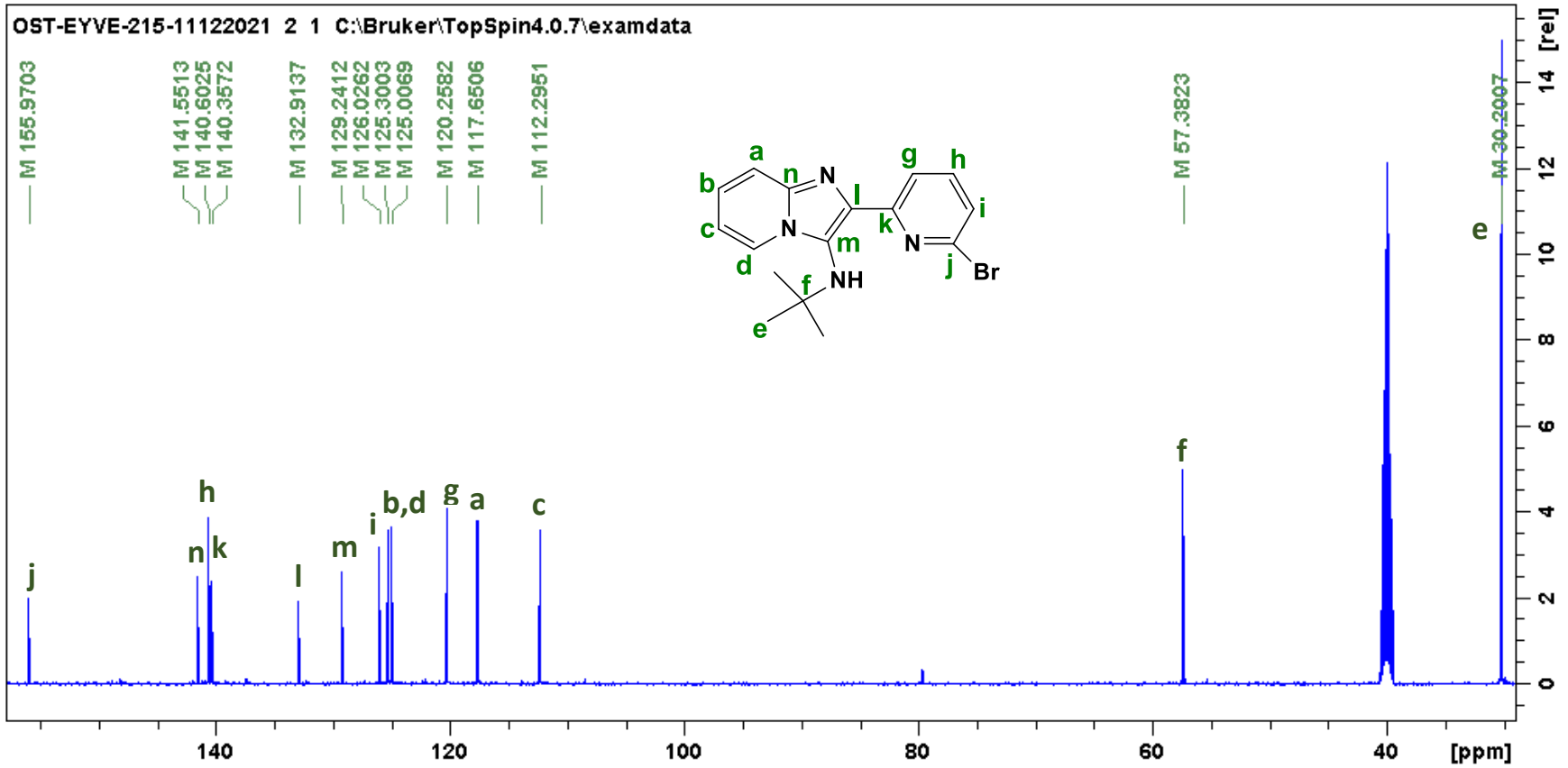

Fig. S.36. $^{13}C\{^{1}H\}$ NMR spectrum of ligand **L_1** in $(CD_3)_2SO$.

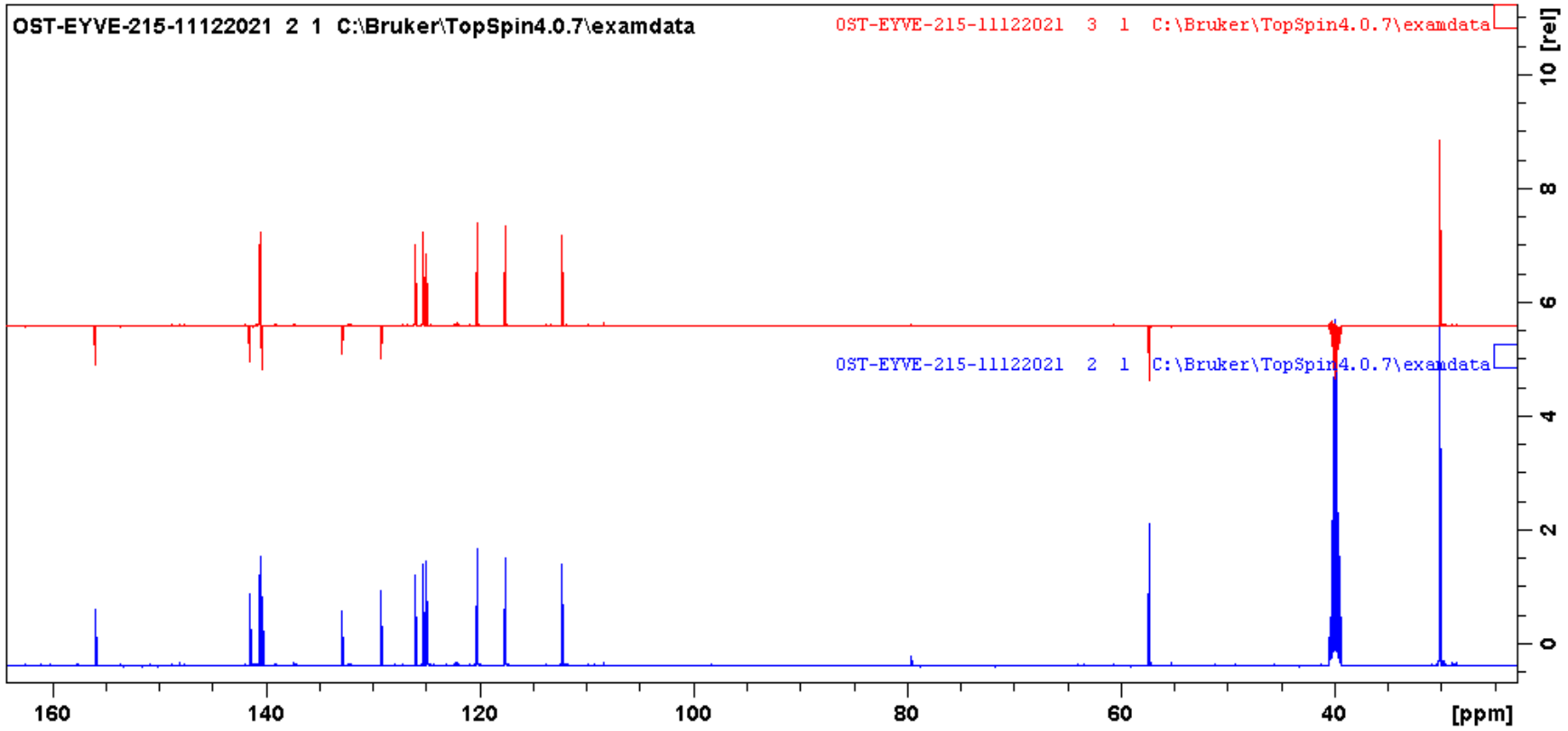

Fig. S.37. $^{13}C\{^{1}H\}$ NMR spectrum of ligand **L_1** in $(CD_3)_2SO$.

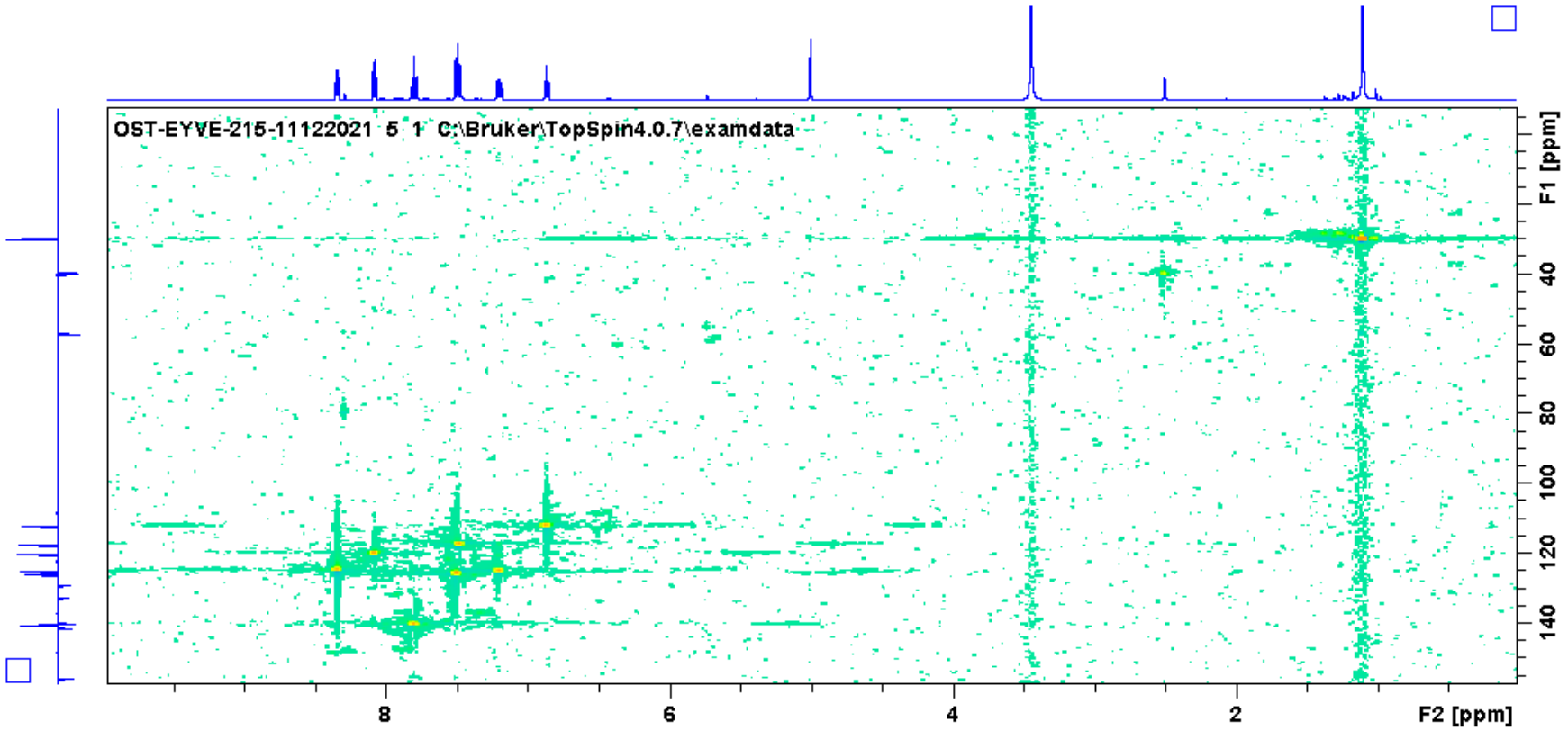

Fig. S.38. HSQC spectrum of ligand **L**$_1$ in $(CD_3)_2SO$.

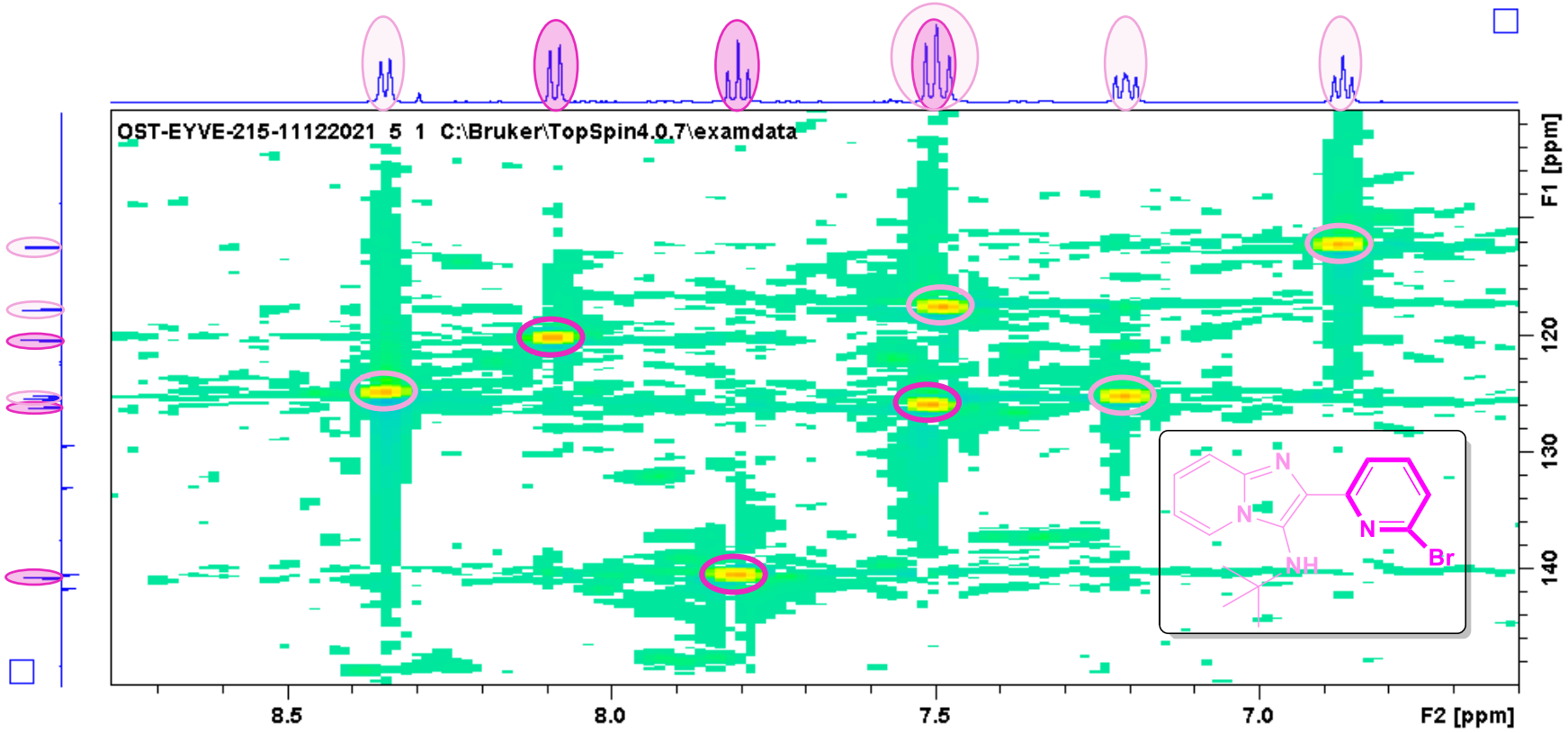

Fig. S.39. HSQC spectrum of ligand **L**$_1$ in $(CD_3)_2SO$.

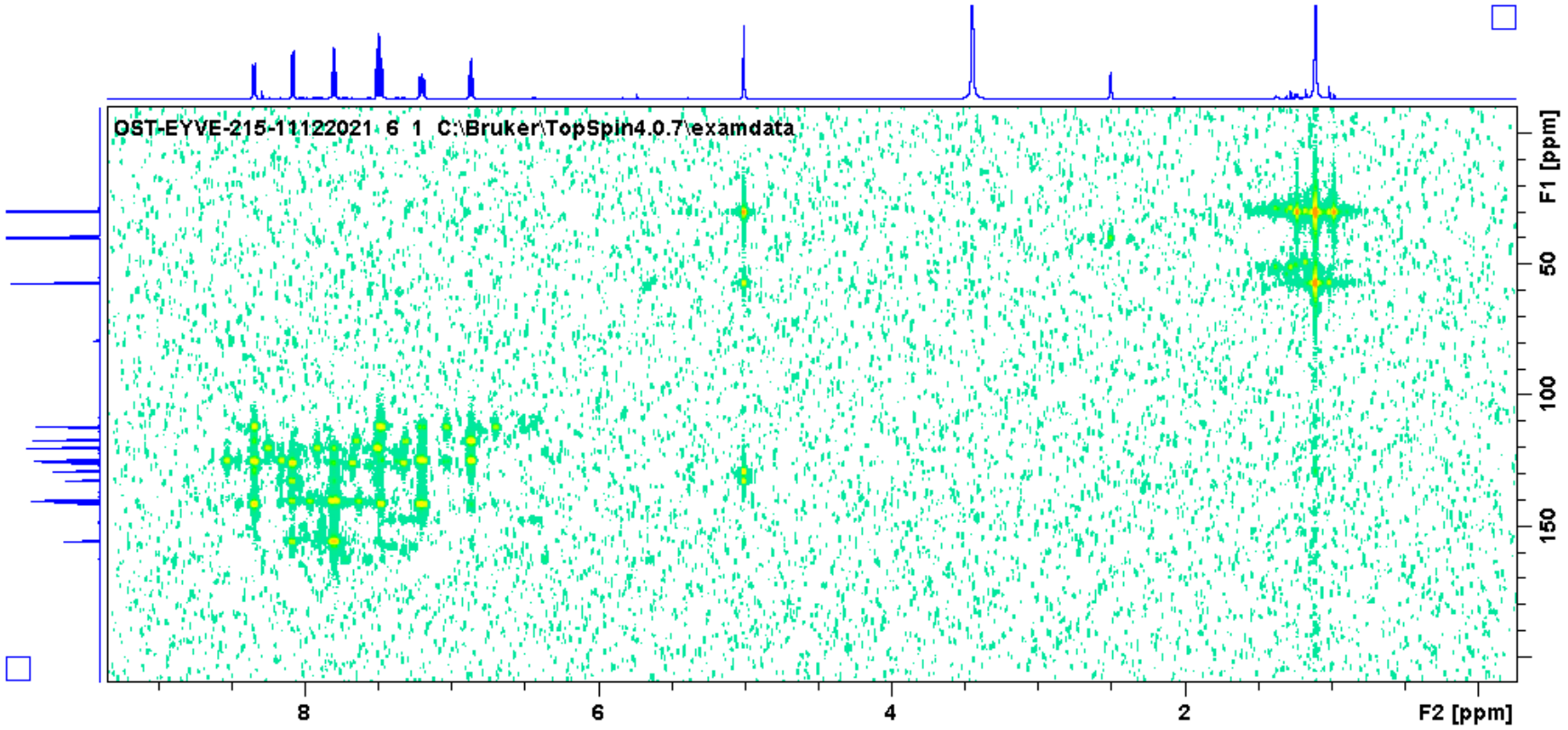

Fig. S.40. HMBC spectrum of ligand **L_1** in $(CD_3)_2SO$.

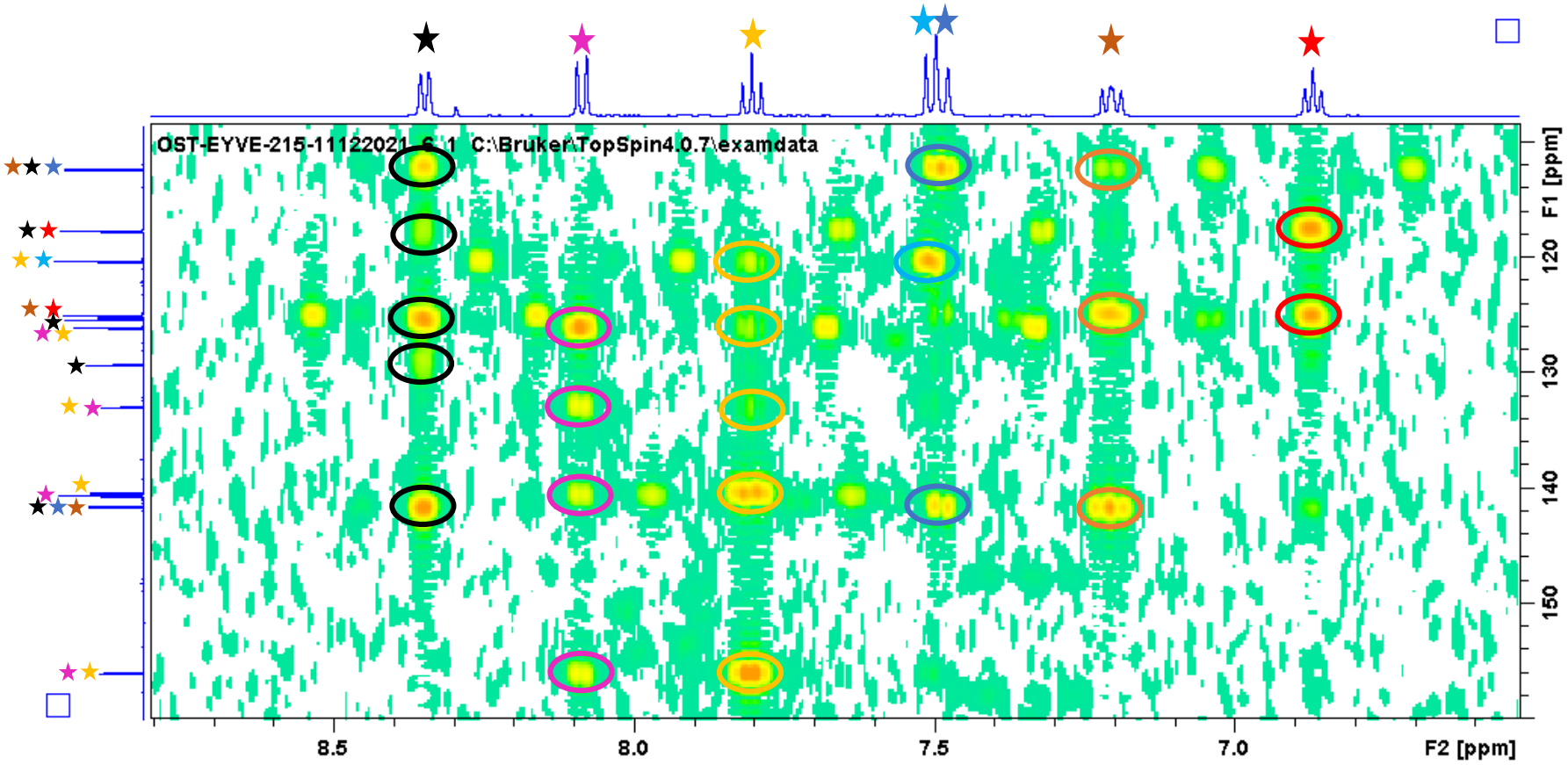

Fig. S.41. HMBC spectrum of ligand **L**$_1$ in $(CD_3)_2SO$.

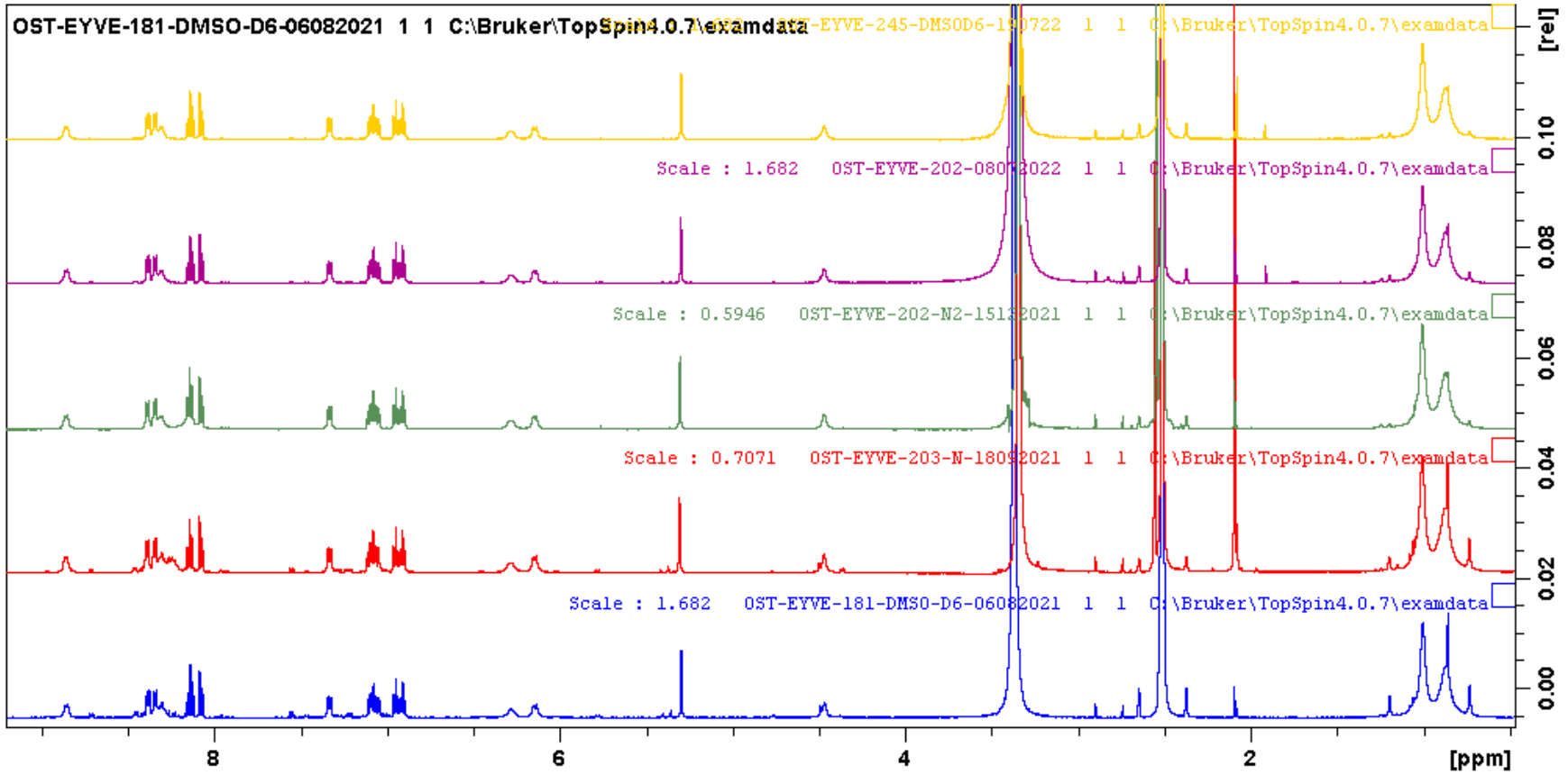

Fig. S.42. ^{1}H RMN spectrum of complex **1** in $(CD_3)_2SO$. Comparison of 5 independent reactions.

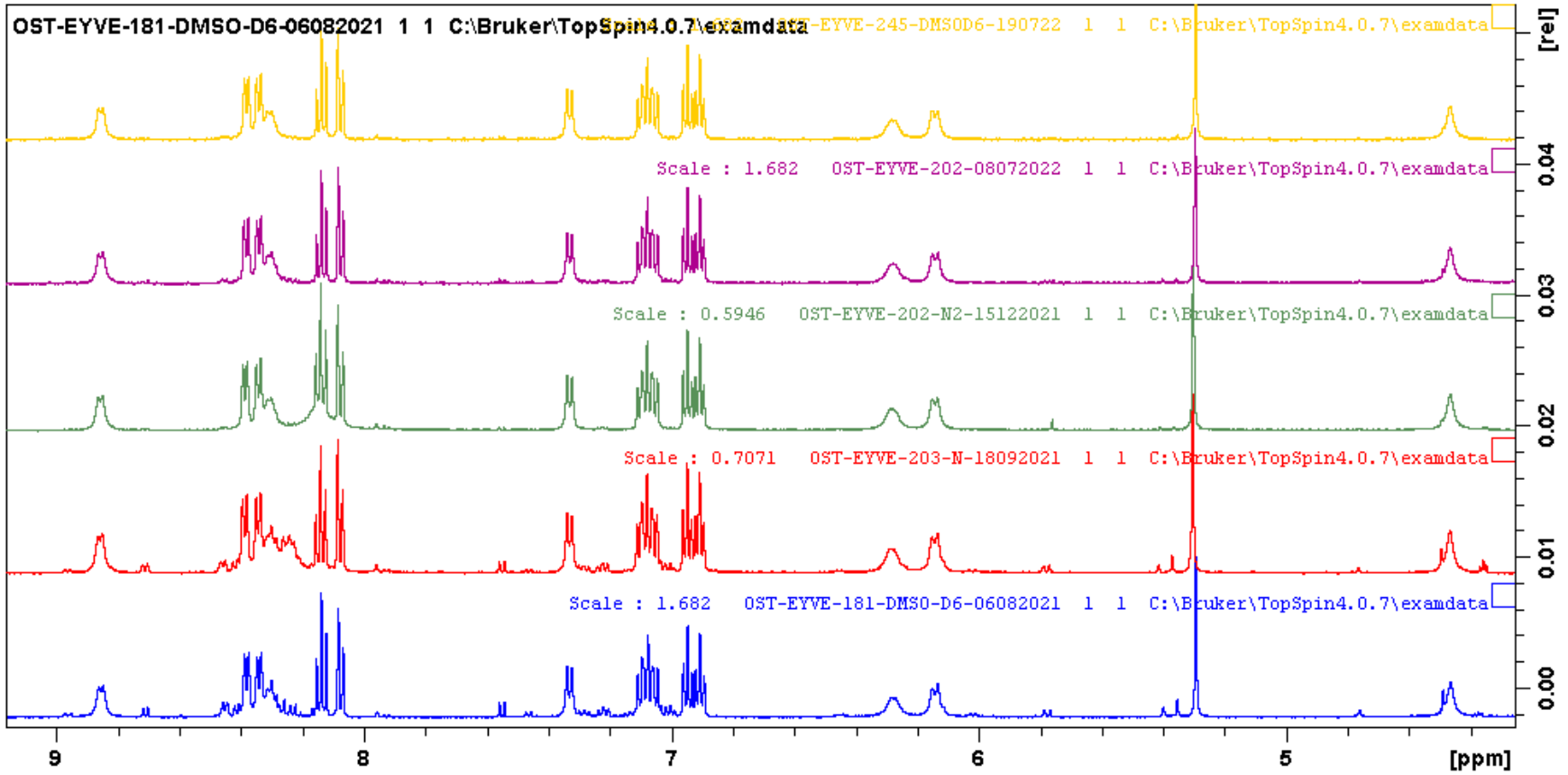

Fig. S.43. ^{1}H RMN spectrum of complex **1** in $(CD_3)_2SO$. Comparison of 5 independent reactions.

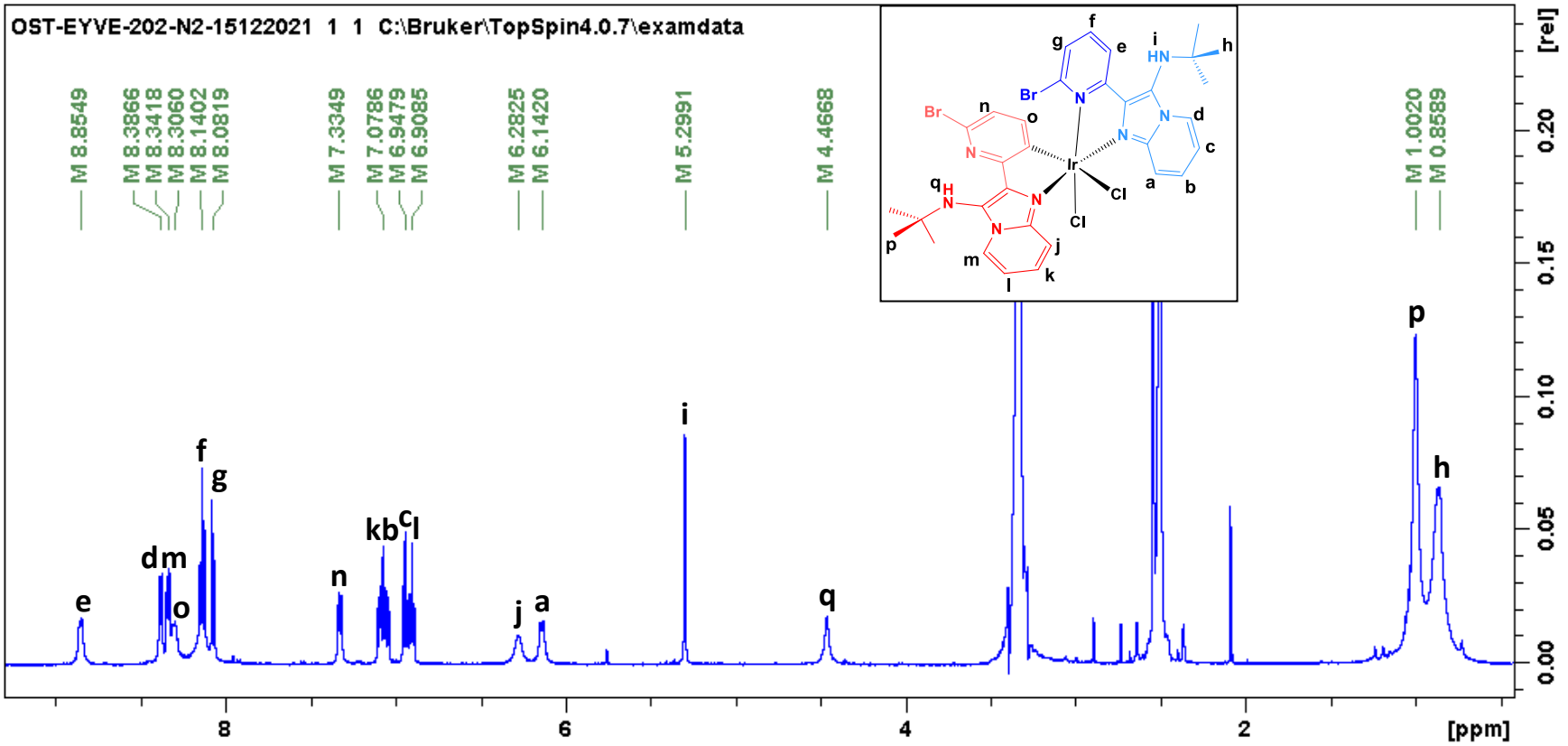

Fig. S.44. ^{1}H NMR spectrum of complex **1** in $(CD_3)_2SO$.

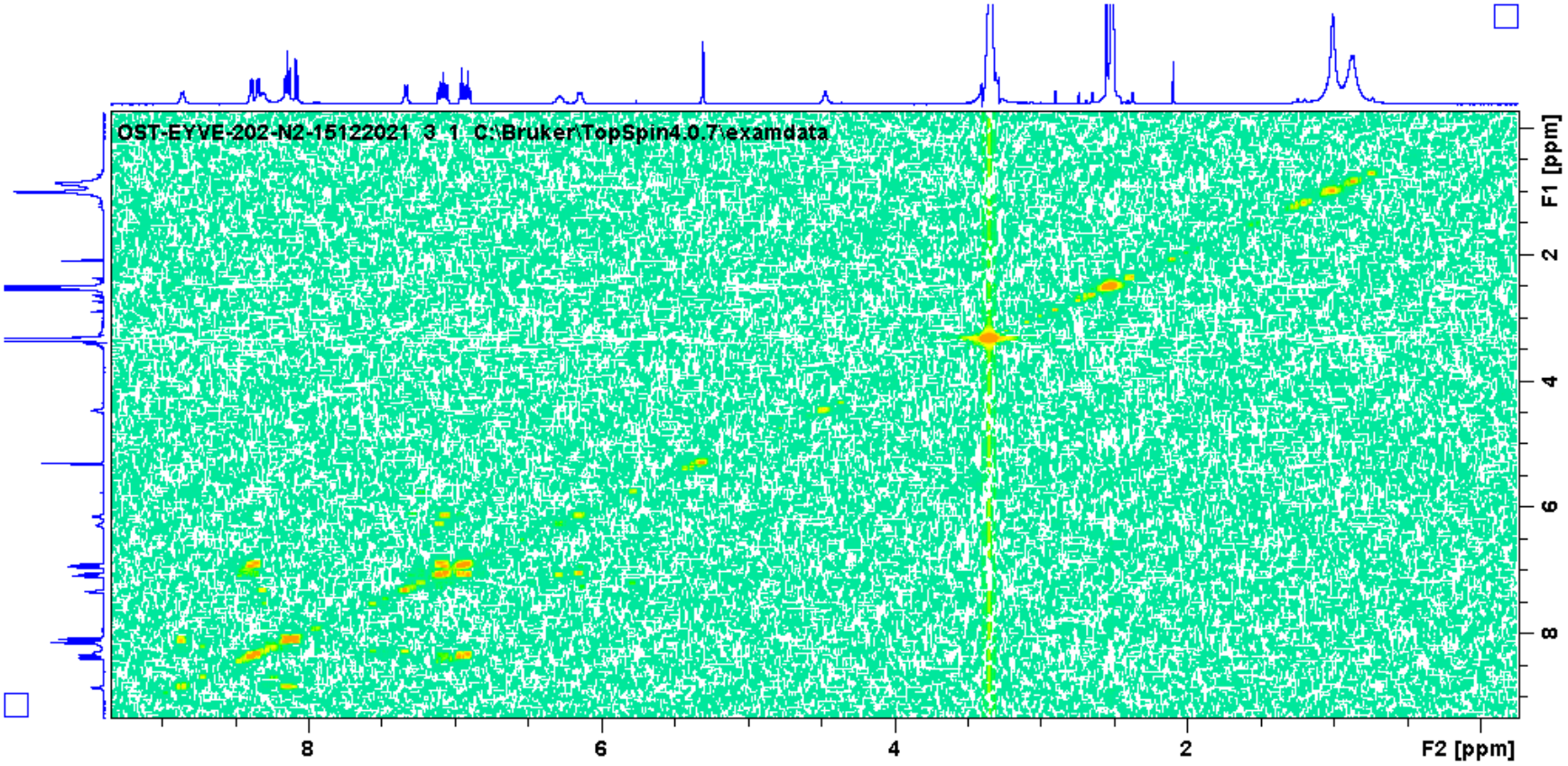

Fig. S.45. COSY spectrum of complex **1** in $(CD_3)_2SO$.

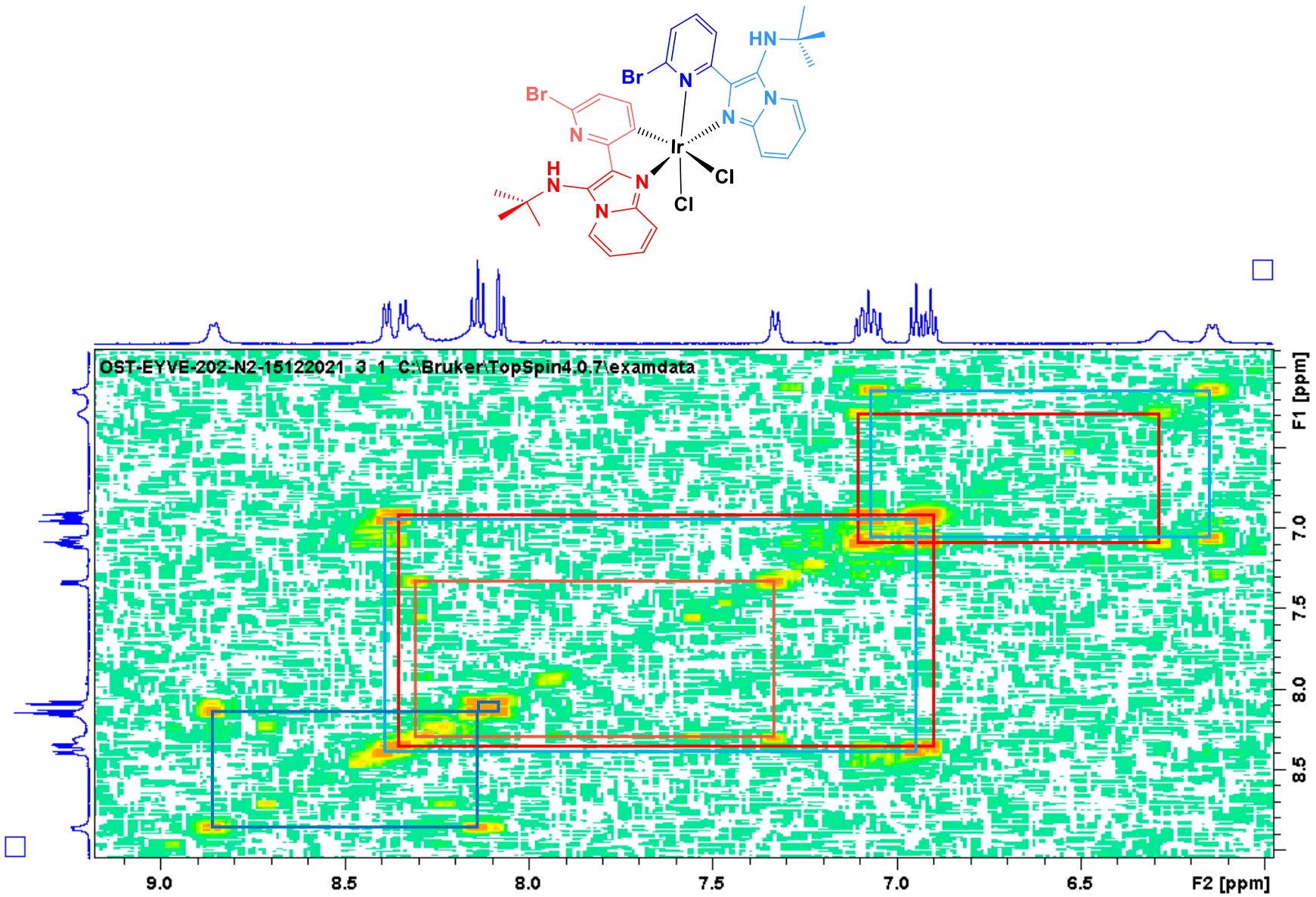

Fig. S.46. COSY spectrum of complex **1** in $(CD_3)_2SO$.

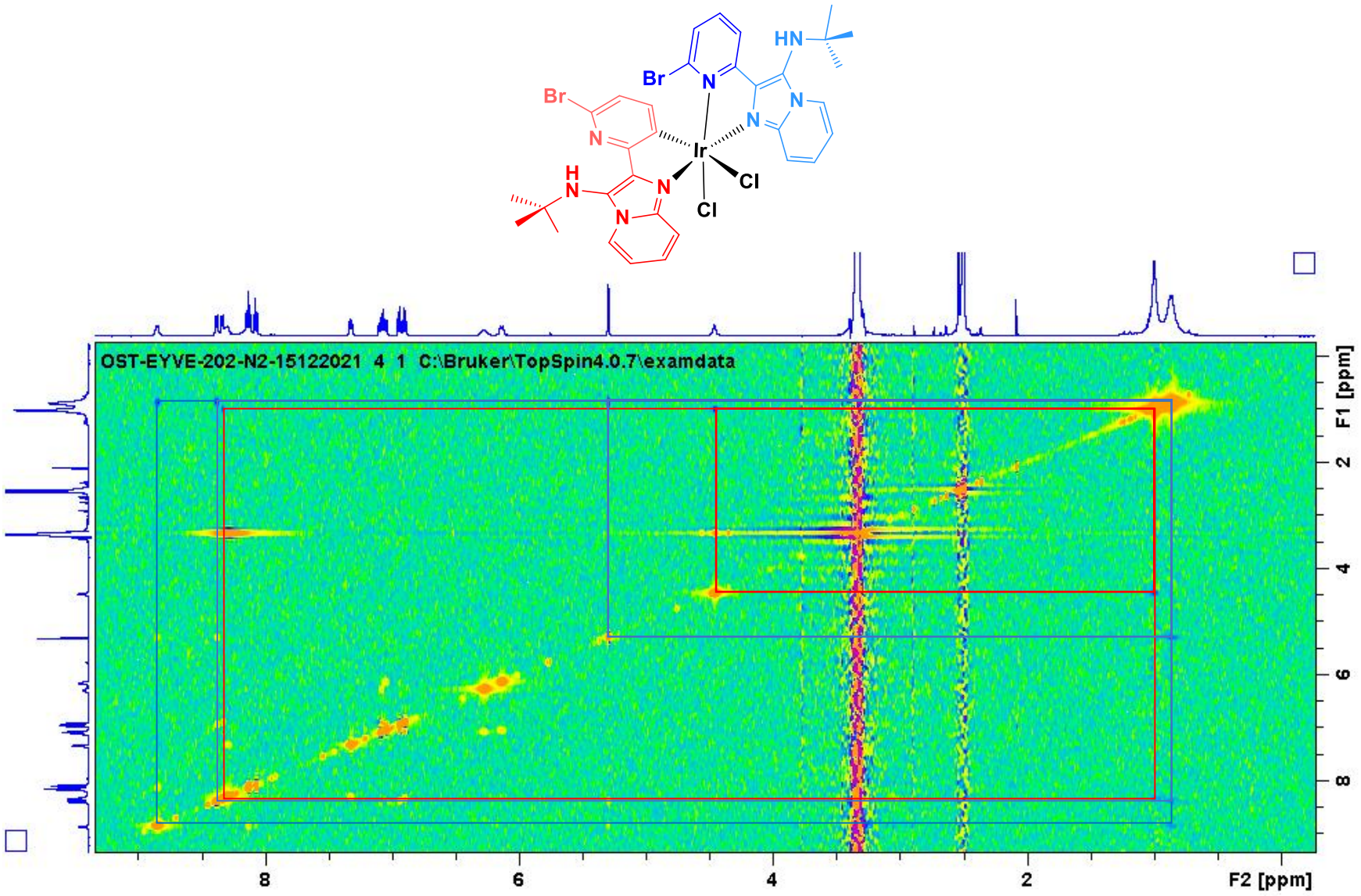

Fig. S.47. NOESY spectrum of complex **1** in $(CD_3)_2SO$.

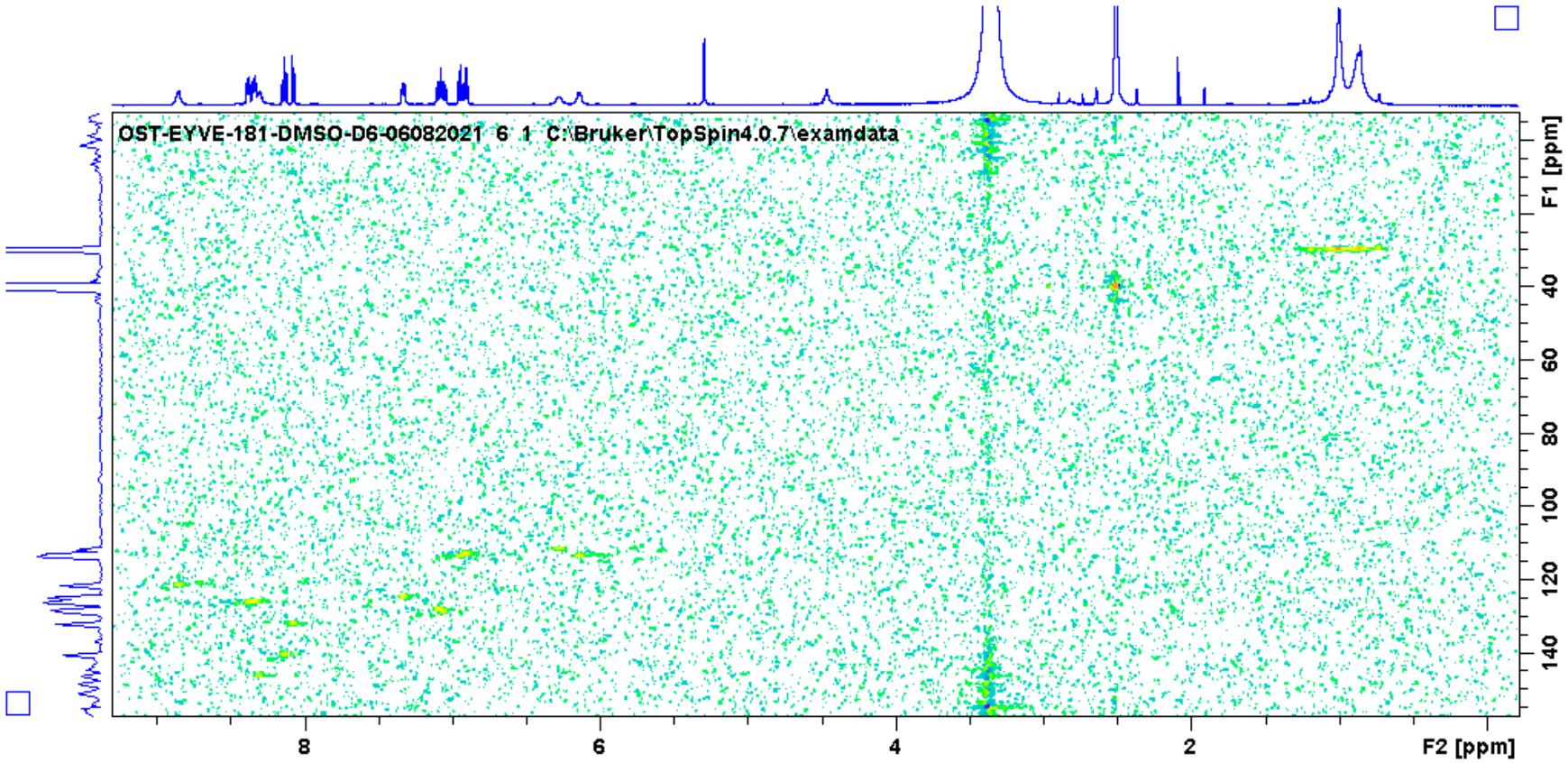

Fig. S.48. HSQC spectrum of complex **1** in $(CD_3)_2SO$.

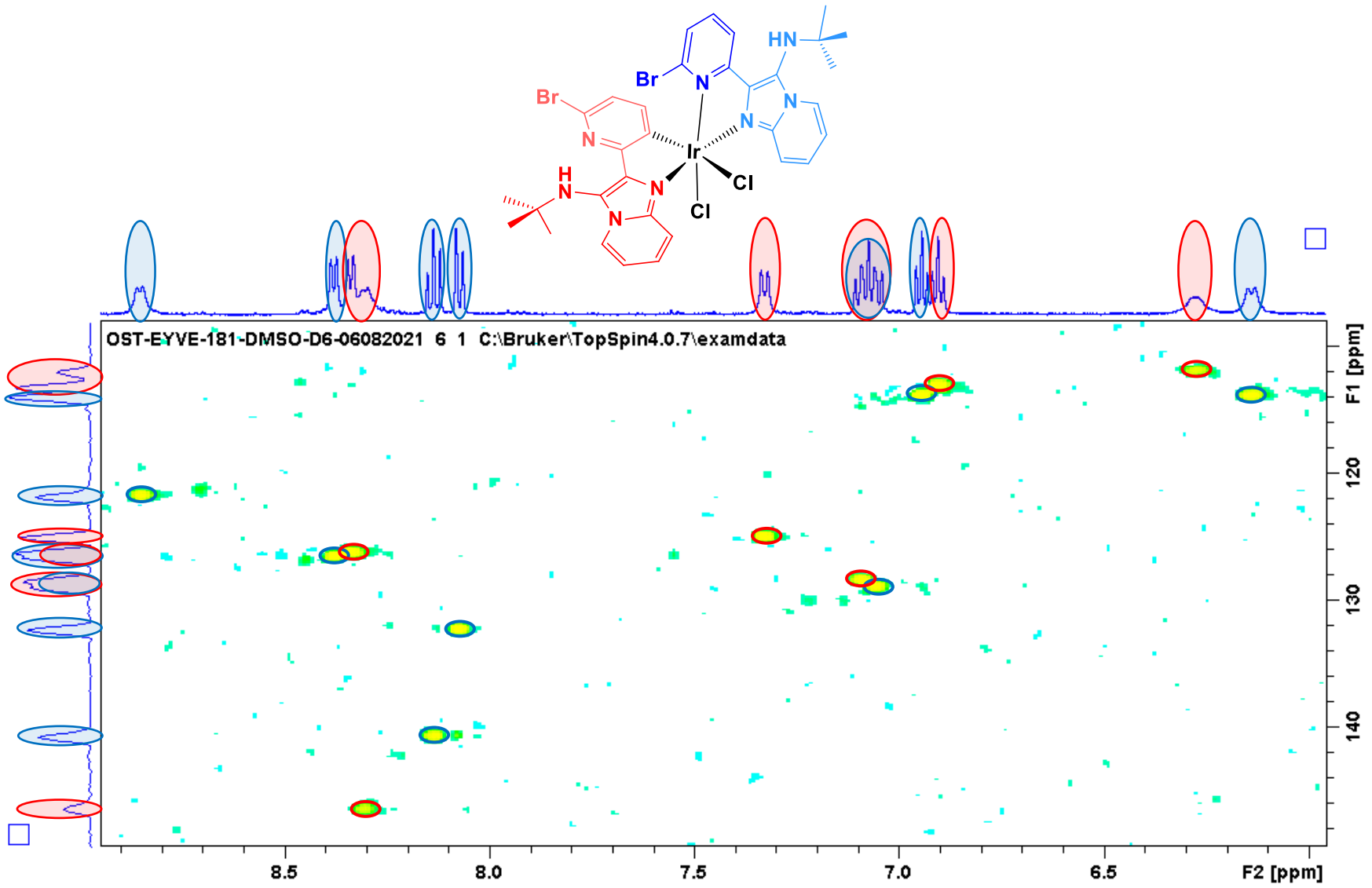

Fig. S.49. HSQC spectrum of complex **1** in $(CD_3)_2SO$.

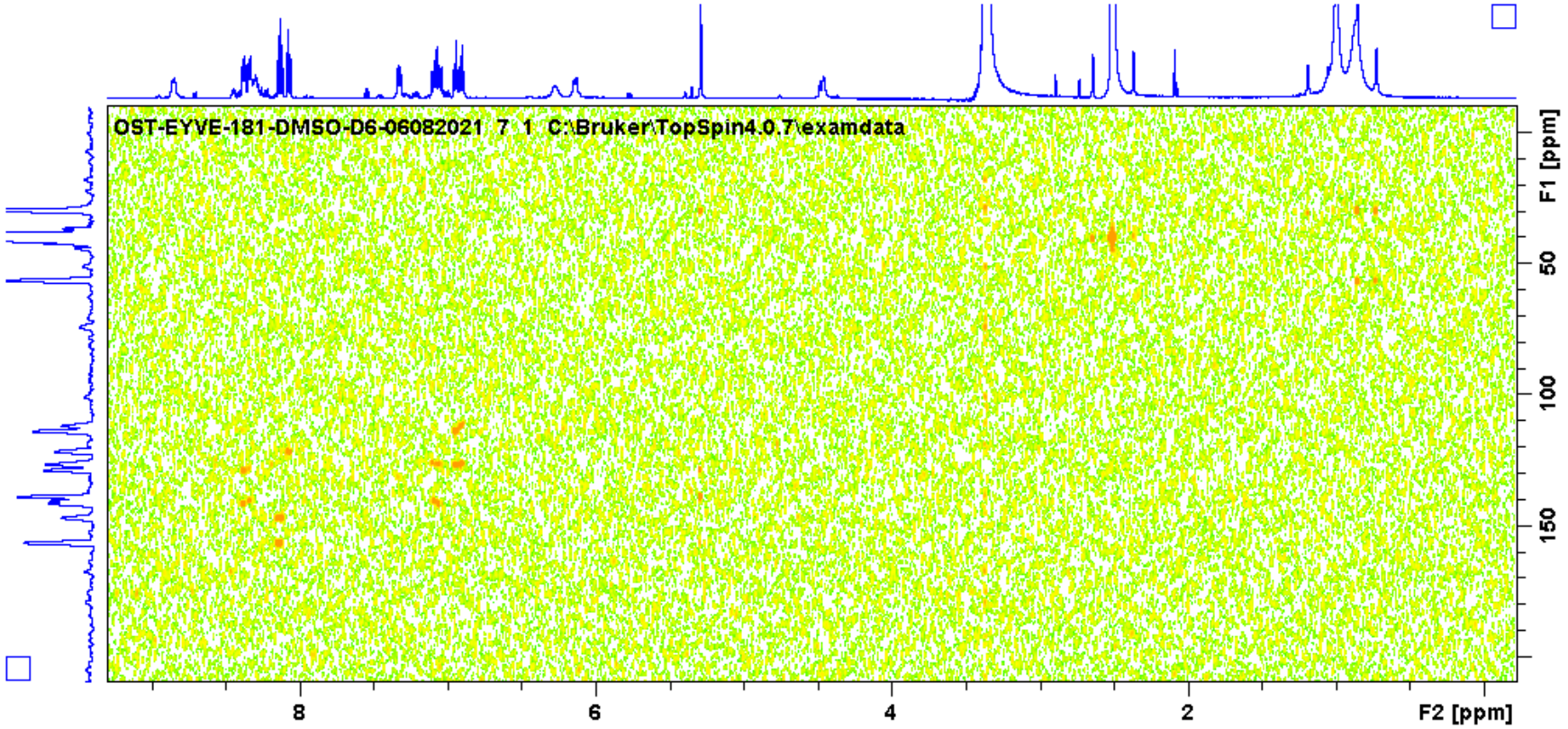

Fig. S.50. HMBC spectrum of complex **1** in $(CD_3)_2SO$.

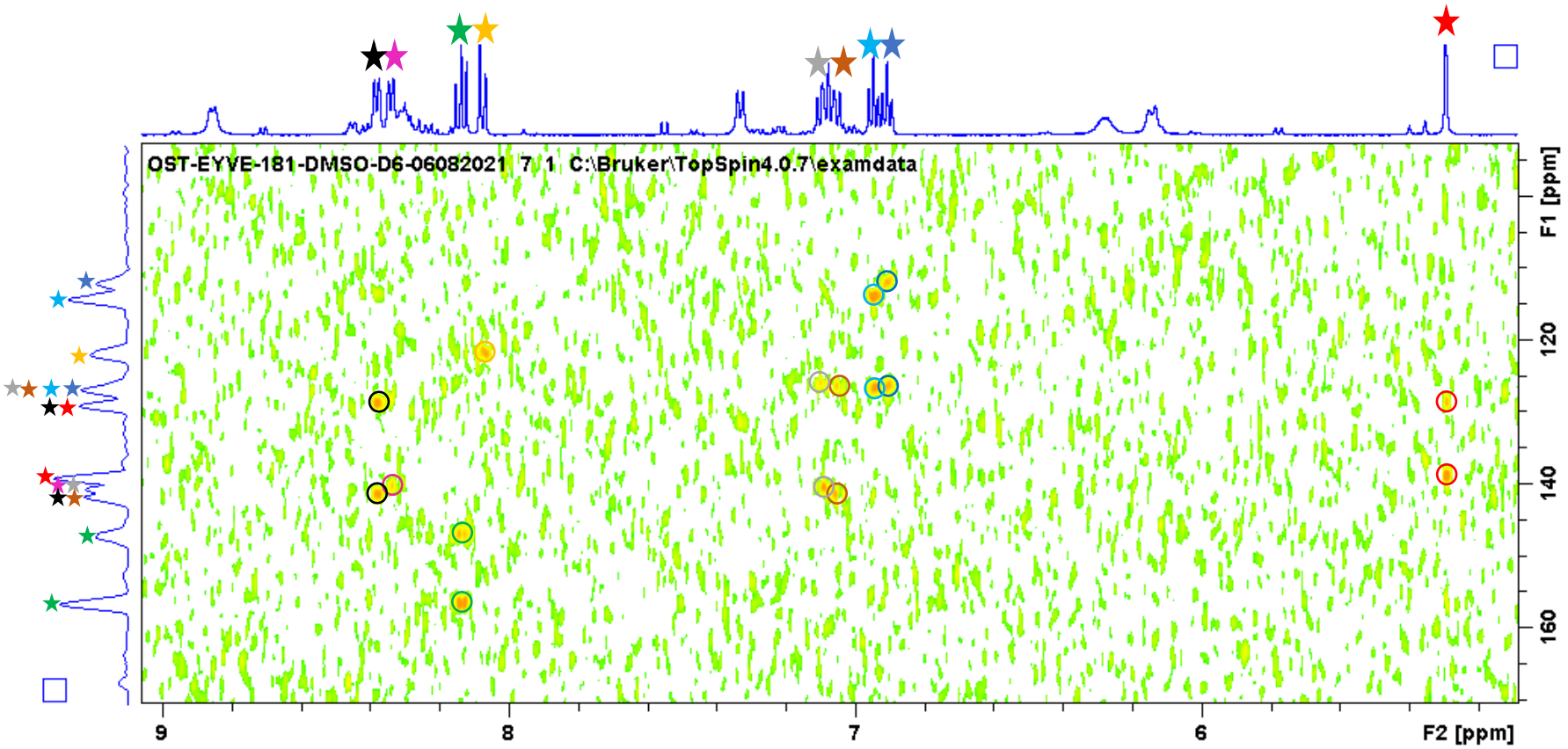

Fig. S.51. HMBC spectrum of complex **1** in $(CD_3)_2SO$.

Table S.2. Cartesian coordinates (x-y-z format) for all the species investigated to propose our reaction mechanism calculated at the ωB97X-D/def2-svpp level.

$IrCl_3$_3DMF (conf1)			
E(scf) = -2229.44305368 a.u.			
Ir	0.003231	0.002049	-0.433064
Cl	1.276925	-1.533049	-1.696383
Cl	-1.961132	-0.328210	-1.701090
Cl	0.703935	1.874172	-1.689821
H	2.842064	0.648554	2.778839
H	4.528933	0.036967	2.893724
C	3.876198	0.806397	2.444286
H	4.221611	1.802040	2.775177
N	3.916870	0.716920	1.000108
O	1.702225	0.301448	0.815955
C	5.194103	0.908503	0.349328
H	5.922834	0.154127	0.695820
H	5.595578	1.913634	0.570090
H	5.076235	0.808556	-0.739971
C	2.811137	0.472659	0.291586
H	2.937228	0.424147	-0.801914
H	-2.008548	2.119425	2.772678
H	-2.335397	3.883353	2.892278
C	-2.664034	2.933293	2.434608
H	-3.701204	2.725889	2.752762
N	-2.592389	3.020467	0.991499
O	-1.113664	1.319666	0.812170
C	-3.398332	4.027622	0.337238
H	-3.120902	5.036297	0.691918
H	-4.470397	3.862220	0.545924
H	-3.241430	3.981623	-0.750745
C	-1.817750	2.192111	0.285777
H	-1.831490	2.328829	-0.807301
H	-0.871088	-2.782983	2.768944
H	-2.244911	-3.937918	2.877425
C	-1.250403	-3.757116	2.431976
H	-0.561937	-4.553841	2.765687
N	-1.340470	-3.747058	0.987352
O	-0.589612	-1.622499	0.808774
C	-1.809913	-4.948706	0.333695
H	-2.831888	-5.198806	0.670201
H	-1.144570	-5.800241	0.563051
H	-1.825776	-4.798893	-0.756148

$IrCl_3$_3DMF (conf2)			
E(scf) = -2229.43959134 a.u.			
Ir	-0.084504	-0.226060	0.061138
Cl	-0.369955	-2.518639	-0.407242
Cl	0.282590	-0.689037	2.374195
Cl	-0.429513	0.358328	-2.256329
H	3.810580	-0.242959	-1.623074
H	5.367219	-0.378259	-0.729327
C	4.515753	-0.941026	-1.152105
H	4.895554	-1.645472	-1.912074
N	3.822730	-1.672260	-0.110911
O	1.960272	-0.413092	-0.283464
C	4.526775	-2.758882	0.535101
H	5.436128	-2.385705	1.038781
H	4.820985	-3.521241	-0.207453
H	3.875620	-3.230851	1.285653
C	2.573259	-1.363737	0.232017
H	2.100358	-1.980888	1.012396
H	0.376656	3.553058	2.033426
H	1.605042	4.845442	1.795655
C	0.671408	4.404620	1.404498
H	-0.122385	5.172381	1.429863
N	0.874645	3.934161	0.048753
O	0.191090	1.839244	0.531899
C	1.327934	4.889573	-0.936897
H	2.299308	5.322915	-0.638913
H	0.597035	5.710779	-1.047474
H	1.447186	4.393692	-1.912173
C	0.614265	2.665030	-0.282181
H	0.778627	2.384476	-1.338307
H	-3.925728	0.263776	1.772898
H	-5.408023	0.817912	0.916804
C	-4.765878	-0.052920	1.139782
H	-5.363660	-0.810354	1.675431
N	-4.239403	-0.621544	-0.085041
O	-2.123221	-0.018757	0.398589
C	-5.172641	-1.244646	-0.997569
H	-5.922481	-0.512062	-1.345575
H	-5.697802	-2.079437	-0.500564
H	-4.634156	-1.639573	-1.871911

C	-0.992736	-2.667971	0.280995	C	-2.935414	-0.577087	-0.355739
H	-1.088400	-2.752283	-0.813366	H	-2.606018	-1.059306	-1.289529

$IrCl_3$_3DMF (conf3)

E(scf) = -2229.36643552 a.u.

Ir	0.548285	0.006901	0.006112
Cl	2.016434	-1.708057	-0.596581
Cl	1.977782	1.437611	-1.165412
Cl	1.951918	0.360988	1.841527
N	-0.714349	1.944774	0.855061
C	-0.106545	3.180567	0.311802
H	-0.163231	3.188040	-0.784214
H	-0.631989	4.061418	0.724534
H	0.954841	3.207359	0.587577
C	-0.673965	1.999283	2.330142
H	-1.296855	2.839224	2.684550
H	-1.065882	1.072291	2.762628
H	0.367071	2.121709	2.645418
C	-2.054967	1.815304	0.388775
H	-2.173345	2.069412	-0.682274
O	-2.969449	1.474374	1.079971
N	-0.657276	-1.735854	1.248057
C	-0.572287	-3.040649	0.560736
H	-0.968088	-2.968744	-0.458151
H	0.479721	-3.339028	0.509433
H	-1.169795	-3.786858	1.113000
C	-0.052220	-1.864912	2.593624
H	-0.141006	-0.922670	3.149209
H	-0.556034	-2.679285	3.146255
H	1.016516	-2.085972	2.483599
C	-2.013548	-1.311883	1.363017
H	-2.160288	-0.512029	2.114234
O	-2.910638	-1.771407	0.719560
N	-0.634359	-0.236210	-2.129574
C	-0.585506	1.015505	-2.911997
H	-1.017242	1.844229	-2.340783
H	0.461422	1.246750	-3.132984
H	-1.168658	0.892060	-3.841474
C	0.008451	-1.315723	-2.913243
H	-0.490491	-1.403528	-3.895878
H	1.070398	-1.075709	-3.047716
H	-0.049652	-2.270421	-2.375289

$IrCl_3$_3DMF (conf4)

E(scf) = -2229.38326574 a.u.

Ir	0.029712	-0.321819	0.018109
Cl	-0.211578	-0.335963	2.405592
Cl	0.180246	-2.663566	0.148694
Cl	0.273033	-0.303284	-2.378622
N	-2.178045	-0.573299	-0.383866
C	-2.485128	-1.926978	-0.943329
H	-2.292179	-2.705537	-0.198329
H	-3.547170	-1.937835	-1.244891
H	-1.840264	-2.102611	-1.814127
C	-2.708887	0.400735	-1.373497
H	-3.807927	0.327000	-1.399206
H	-2.427042	1.429220	-1.142772
H	-2.277324	0.149063	-2.348491
C	-2.869053	-0.491235	0.895287
H	-2.616540	-1.340762	1.557365
O	-3.640076	0.375455	1.165487
N	-0.142062	2.095115	0.332748
C	-1.402469	2.477602	1.007296
H	-2.284492	2.194926	0.432952
H	-1.431191	1.964938	1.977058
H	-1.420234	3.571642	1.152307
C	0.955310	2.570618	1.209245
H	1.933591	2.458183	0.734079
H	0.800386	3.639734	1.439046
H	0.919045	1.989577	2.140667
C	-0.024012	2.646063	-0.979582
H	1.015920	2.610498	-1.366713
O	-0.938121	3.105768	-1.595635
N	2.351809	-0.389325	0.093109
C	2.883973	-0.358169	1.470381
H	2.614722	0.579486	1.966004
H	2.438087	-1.193111	2.025381
H	3.983347	-0.450322	1.444193
C	2.875913	-1.612147	-0.597320
H	3.970347	-1.507331	-0.710816
H	2.643550	-2.489673	0.012572
H	2.391413	-1.720909	-1.577357

C	-1.981898	-0.591994	-1.828302	C	2.854301	0.693353	-0.717657
H	-2.098678	-1.649083	-1.520019	H	2.556400	0.582301	-1.778299
O	-2.902931	0.166817	-1.905339	O	3.525596	1.587893	-0.294875

ligand (conf1)

E(scf) = -3411.94463394 a.u.

N	2.646306	-0.825651	-0.277939
C	4.013864	-0.764815	-0.211569
C	4.727878	-1.911573	-0.035732
C	4.054816	-3.166891	0.075349
C	2.689811	-3.226109	0.001890
C	0.483240	-0.509884	-0.497039
C	1.698938	0.168382	-0.482495
H	4.461565	0.225391	-0.304223
H	5.816945	-1.856636	0.019478
H	4.638503	-4.080033	0.216201
H	2.135135	-4.162800	0.078001
C	1.945665	-2.029500	-0.181980
N	0.646442	-1.841361	-0.295370
N	1.994697	1.523311	-0.595799
H	2.728076	1.732949	-1.268036
C	2.044111	2.406547	0.591437
C	3.183707	2.025309	1.551494
H	3.194210	2.689266	2.433674
H	3.064906	0.988802	1.912593
H	4.167393	2.114107	1.055983
C	2.264894	3.824595	0.058216
H	2.299060	4.552755	0.885850
H	3.222463	3.898637	-0.490428
H	1.450053	4.110763	-0.628014
C	0.708007	2.337150	1.336716
H	-0.124924	2.633174	0.678717
H	0.505121	1.317906	1.707136
H	0.726418	3.015979	2.206387
C	-0.855637	0.083392	-0.703054
C	-1.036536	1.201398	-1.526764
C	-2.321474	1.711330	-1.689284
H	-0.173980	1.661797	-2.010684
C	-3.085146	-0.009766	-0.243702
C	-3.387849	1.100802	-1.035738
H	-2.496084	2.581975	-2.328064
H	-4.412136	1.464693	-1.133205

ligand (conf2)

E(scf) = -3411.96106444 a.u.

N	2.720603	-0.097539	-0.367813
C	3.725963	0.746395	-0.765467
C	5.006322	0.285579	-0.796993
C	5.294251	-1.066628	-0.429309
C	4.284013	-1.917829	-0.076121
C	0.835873	-1.127419	0.056382
C	1.360778	0.121856	-0.262026
H	3.411767	1.748574	-1.056026
H	5.805371	0.956125	-1.119237
H	6.328763	-1.419222	-0.447769
H	4.458706	-2.962432	0.186802
C	2.943382	-1.442638	-0.062813
N	1.812130	-2.068979	0.185988
N	0.785691	1.363787	-0.518978
H	-0.128574	1.198547	-0.938147
C	0.612071	2.334333	0.598697
C	-0.177341	1.732929	1.772262
H	-0.281912	2.472465	2.585399
H	-1.185692	1.427501	1.449468
H	0.334947	0.845344	2.183314
C	1.976073	2.816040	1.099966
H	1.840830	3.543264	1.918708
H	2.582359	1.981839	1.494672
H	2.541564	3.314613	0.294702
C	-0.165244	3.511801	0.004252
H	0.379738	3.942743	-0.852730
H	-1.160710	3.184206	-0.346525
H	-0.316955	4.300219	0.760966
C	-0.582660	-1.471633	0.197663
C	-0.976167	-2.716500	0.704097
C	-2.335571	-2.988327	0.813523
H	-0.209951	-3.436304	0.995945
C	-2.759385	-0.828488	-0.075121
C	-3.268160	-2.028111	0.421943
H	-2.677430	-3.949394	1.208444
H	-4.343001	-2.199327	0.498245

N	-1.883133	-0.502586	-0.078271	N	-1.481976	-0.556512	-0.194845
Br	-4.508647	-0.880198	0.675824	Br	-3.968004	0.537080	-0.621495

I-1 (conf1)

E(scf) = -5393.14561782 a.u.

Ir	1.618709	-0.284836	-0.546273
Cl	2.226305	1.280462	-2.201963
Cl	3.230787	-1.845481	-1.329341
Cl	-0.039199	-1.236895	-1.915522
C	0.337049	2.446099	0.121293
C	-0.805496	4.542580	-0.171170
C	0.400420	5.185763	-0.103498
C	1.589335	4.439225	0.127363
C	1.543090	3.080050	0.225337
C	-1.207762	0.956563	0.164952
C	-1.873019	2.179821	0.016573
H	-1.745909	5.067436	-0.339982
H	0.455650	6.270862	-0.221258
H	2.555423	4.938387	0.217453
H	2.399067	2.439054	0.412610
N	-0.845204	3.135144	-0.023912
N	0.138498	1.112480	0.184377
N	-3.247661	2.418213	-0.107724
H	-3.668696	1.642191	-0.615604
C	-4.055965	2.727253	1.092151
C	-3.915900	1.656670	2.189302
H	-4.522461	1.921115	3.073635
H	-4.255272	0.671686	1.825340
H	-2.865784	1.558566	2.516030
C	-3.645194	4.089102	1.658916
H	-4.272300	4.348097	2.529634
H	-2.593093	4.085074	1.993601
H	-3.767634	4.877862	0.897254
C	-5.509953	2.784403	0.614322
H	-5.623119	3.542073	-0.179449
H	-5.825993	1.807335	0.205427
H	-6.187863	3.038723	1.446873
C	-1.902749	-0.320099	0.401294
C	-1.534582	-1.159886	1.453717
C	-2.284288	-2.310426	1.676181
H	-0.674062	-0.906863	2.071420
C	-3.701134	-1.625571	-0.101762
C	-3.390673	-2.575526	0.874474

I-1 (conf2)

E(scf) = -5393.14556881 a.u.

Ir	1.479160	-0.156777	0.036535
Cl	1.947393	0.362041	-2.271288
Cl	1.405649	-0.575176	2.392777
Cl	0.258776	-2.057993	-0.612225
C	-0.249517	2.287460	-0.512903
C	-1.711950	4.001949	-1.375538
C	-0.622524	4.788538	-1.626063
C	0.675247	4.315439	-1.283310
C	0.844503	3.076090	-0.741671
C	-1.565253	0.677528	0.065623
C	-2.397272	1.705537	-0.407614
H	-2.731492	4.301824	-1.619625
H	-0.740948	5.771689	-2.088181
H	1.559400	4.931255	-1.456571
H	1.801974	2.661194	-0.451983
N	-1.524632	2.727731	-0.787609
N	-0.255718	1.028859	-0.015887
N	-3.791342	1.726635	-0.552820
H	-4.097618	0.796295	-0.834031
C	-4.638382	2.217870	0.556317
C	-4.374251	1.477268	1.879244
H	-5.025706	1.867200	2.681231
H	-4.572371	0.396640	1.774803
H	-3.326244	1.602699	2.202629
C	-4.403988	3.717479	0.759950
H	-5.052560	4.101729	1.566127
H	-3.357340	3.925685	1.043601
H	-4.633400	4.274856	-0.164373
C	-6.084794	1.976060	0.114077
H	-6.284973	2.490337	-0.841209
H	-6.273235	0.896652	-0.030865
H	-6.795510	2.345488	0.872980
C	-2.134085	-0.585539	0.588034
C	-1.773472	-1.152173	1.809492
C	-2.466221	-2.278495	2.240561
H	-0.939687	-0.743617	2.382008
C	-3.797591	-2.117789	0.285566
C	-3.505576	-2.792521	1.470067

H	-2.019095	-2.997251	2.485740	H	-2.193552	-2.758420	3.184443
H	-4.009867	-3.463011	1.014918	H	-4.076064	-3.671158	1.776090
N	-2.999805	-0.543374	-0.331154	N	-3.150310	-1.062403	-0.142319
Br	-5.266530	-1.867559	-1.152524	Br	-5.260392	-2.708630	-0.782710
O	1.245147	-1.739839	0.975267	O	3.200074	-1.372598	0.032752
H	0.811509	-3.145072	-0.435331	H	2.694567	-2.271524	-1.730010
C	0.987643	-2.901158	0.624673	C	3.339065	-2.249561	-0.837683
N	0.866990	-3.907100	1.494003	N	4.266906	-3.198774	-0.742413
C	1.080038	-3.706158	2.910822	C	5.115251	-3.293663	0.429339
H	1.361408	-2.658381	3.082318	H	4.763923	-2.570279	1.178018
H	0.159452	-3.937846	3.476698	H	5.054387	-4.311753	0.850226
H	1.888615	-4.366105	3.271561	H	6.166843	-3.078861	0.167235
C	0.526568	-5.240257	1.046331	C	4.432709	-4.191928	-1.782670
H	0.401572	-5.245594	-0.046550	H	3.691912	-4.025595	-2.578861
H	1.324391	-5.954908	1.314747	H	5.444863	-4.131416	-2.220324
H	-0.418316	-5.574400	1.511039	H	4.284413	-5.204820	-1.369684
O	3.197266	0.441963	0.728438	O	2.885453	1.364546	0.657366
C	4.330212	0.541806	0.223611	C	4.024545	1.378137	0.171177
H	4.458355	0.588290	-0.869960	H	4.205628	1.015996	-0.857657
N	5.440860	0.630559	0.953882	N	5.078452	1.834092	0.845289
C	6.738374	0.759386	0.324921	C	6.379968	1.953401	0.225232
H	7.236203	1.689725	0.650681	H	6.707483	3.007950	0.204932
H	7.380421	-0.098363	0.591794	H	7.127553	1.363647	0.783866
H	6.621371	0.782509	-0.768639	H	6.335131	1.580175	-0.809267
C	5.397964	0.547809	2.399250	C	4.928032	2.251267	2.228735
H	4.356184	0.401478	2.714328	H	4.003053	1.812184	2.630761
H	6.009878	-0.303227	2.746350	H	5.793138	1.892692	2.810210
H	5.792562	1.475951	2.849230	H	4.874493	3.351858	2.306529

I-1 (conf3)

E(scf) = -5393.15513862 a.u.

Ir	-1.720703	-0.499369	-0.106247
Cl	-1.938788	-0.005849	2.248825
Cl	-3.154322	-2.380472	0.143036
Cl	-1.650348	-0.887252	-2.463969
C	-0.570398	2.322462	0.384552
C	0.465923	4.218304	1.447144
C	-0.772278	4.770031	1.630284
C	-1.925796	4.089610	1.148622
C	-1.811462	2.874245	0.541793
C	1.049619	1.025573	-0.169015
C	1.649219	2.148650	0.423344

I-1 (conf4)

E(scf) = -5393.12871257 a.u.

Ir	0.947048	0.754581	-0.432171
Cl	2.397959	1.594748	1.313874
Cl	1.934094	2.299690	-1.912488
Cl	-0.408456	0.004818	-2.231629
C	-4.144222	0.404059	-0.256764
C	-4.651835	-1.279727	-1.901625
C	-5.796313	-0.597189	-2.211135
C	-6.123037	0.609088	-1.516724
C	-5.288923	1.092435	-0.553865
C	-2.291110	-0.144956	0.597860
C	-2.582150	-1.176697	-0.323924

H	1.381992	4.693518	1.798712	H	-4.352639	-2.195326	-2.414285
H	-0.881255	5.729322	2.142199	H	-6.462911	-0.962040	-2.996574
H	-2.919642	4.525665	1.263205	H	-7.036340	1.158100	-1.754339
H	-2.640545	2.298121	0.139721	H	-5.447528	2.007312	0.018578
N	0.574693	2.970291	0.787907	N	-3.799920	-0.777770	-0.885165
N	-0.302250	1.122121	-0.165687	N	-3.245524	0.790082	0.645844
N	3.007116	2.410043	0.651331	N	-1.852313	-2.314189	-0.674191
H	3.474933	1.531950	0.867714	H	-0.908754	-2.075477	-0.970968
C	3.791085	3.153239	-0.361330	C	-1.980904	-3.577057	0.059537
C	3.697172	2.523037	-1.762153	C	-1.773395	-3.424894	1.577458
H	4.287624	3.105438	-2.491157	H	-1.897044	-4.394949	2.090895
H	4.085798	1.489970	-1.759529	H	-0.760165	-3.051116	1.800093
H	2.652631	2.496096	-2.118509	H	-2.506987	-2.719828	2.005567
C	3.310940	4.605908	-0.425664	C	-3.373846	-4.168883	-0.195140
H	3.918477	5.179371	-1.146882	H	-3.497204	-5.132421	0.330101
H	2.258090	4.669170	-0.751475	H	-4.162544	-3.483878	0.163717
H	3.402042	5.087835	0.562720	H	-3.527530	-4.335628	-1.274974
C	5.243595	3.112413	0.122861	C	-0.907973	-4.510955	-0.507921
H	5.325272	3.550149	1.132233	H	-1.038941	-4.629024	-1.597166
H	5.612782	2.071343	0.167553	H	0.100423	-4.097724	-0.322805
H	5.900989	3.675674	-0.561038	H	-0.962386	-5.506125	-0.034559
C	1.843220	-0.058034	-0.781751	C	-1.208402	-0.170515	1.592024
C	1.577256	-0.561456	-2.056345	C	-1.555122	-0.013433	2.934621
C	2.481862	-1.461409	-2.610436	C	-0.628256	-0.321705	3.919103
H	0.661085	-0.279125	-2.578950	H	-2.571961	0.302616	3.172488
C	3.779214	-1.259053	-0.636228	C	0.868226	-0.960671	2.176963
C	3.624978	-1.823866	-1.900716	C	0.586703	-0.876149	3.535015
H	2.296998	-1.878949	-3.604005	H	-0.870644	-0.201111	4.978308
H	4.364531	-2.517046	-2.305362	H	1.310869	-1.240783	4.263911
N	2.935209	-0.416615	-0.091233	N	0.053759	-0.502847	1.215608
Br	5.311571	-1.718446	0.401102	Br	2.424833	-1.917386	1.707320
O	-0.120559	-1.769818	0.263858	O	-0.448378	2.175213	0.173520
H	-0.866781	-2.344583	2.074574	H	0.913719	3.689641	0.082748
C	-0.131548	-2.503073	1.270119	C	-0.108917	3.361723	0.323711
N	0.738719	-3.492027	1.433271	N	-0.945489	4.295432	0.765054
C	1.716415	-3.809665	0.411335	C	-2.321032	3.985912	1.106283
H	1.496813	-3.218308	-0.487825	H	-2.520843	2.916268	0.934219
H	2.735530	-3.575256	0.765359	H	-2.505255	4.227565	2.168232
H	1.657195	-4.884295	0.167629	H	-3.002697	4.590920	0.482266
C	0.750524	-4.284898	2.644222	C	-0.512088	5.667849	0.916317
H	-0.040134	-3.939322	3.326534	H	0.546967	5.763283	0.634241
H	0.575157	-5.348855	2.407783	H	-1.112612	6.333431	0.271346
H	1.725262	-4.189847	3.153897	H	-0.629663	5.993131	1.965027

O	-3.452839	0.601832	-0.549661	O	2.329566	-0.634148	-1.115976
C	-4.506515	0.291731	0.044874	C	3.530325	-0.331866	-1.197660
H	-4.484485	-0.101306	1.073657	H	3.917887	0.590152	-0.735627
N	-5.694316	0.445206	-0.523513	N	4.411725	-1.109543	-1.822730
C	-6.915344	0.147493	0.194746	C	5.814102	-0.759298	-1.877382
H	-7.576372	1.031449	0.214969	H	6.428486	-1.544411	-1.401998
H	-7.449665	-0.686690	-0.291954	H	6.140055	-0.641272	-2.925713
H	-6.678805	-0.142094	1.229369	H	5.983205	0.190456	-1.348394
C	-5.793408	0.836724	-1.918947	C	3.988549	-2.325283	-2.490071
H	-4.812718	0.695740	-2.396043	H	2.892338	-2.386223	-2.453749
H	-6.541267	0.199899	-2.418998	H	4.319773	-2.306702	-3.542628
H	-6.101131	1.893466	-2.010382	H	4.424779	-3.209630	-1.992596

I-1_DMF

E(scf) = -5641.45465544 a.u.

Ir	1.51975	-1.085636	-0.005748
Cl	1.628592	-1.219937	-2.415120
Cl	2.773557	-3.100873	0.198408
Cl	1.575914	-0.826361	2.383431
N	-0.40026	2.440469	-1.424890
C	-0.319731	3.531507	-2.247187
C	0.898697	3.931243	-2.702199
C	2.066273	3.206739	-2.322922
C	1.973375	2.099091	-1.525582
C	-1.047541	0.770951	-0.158909
C	-1.519865	1.866017	-0.851213
H	-1.272697	3.998051	-2.492072
H	0.966153	4.797706	-3.362610
H	3.043908	3.535052	-2.685111
H	2.838961	1.515385	-1.224422
C	0.697875	1.692966	-1.062785
N	0.318704	0.658219	-0.304278
N	-2.799193	2.355928	-1.082700
H	-3.424518	1.564511	-1.225058
C	-3.42728	3.323701	-0.139627
C	-3.492157	2.772533	1.293068
H	-4.005958	3.491871	1.954838
H	-4.053507	1.822323	1.327685
H	-2.475839	2.614195	1.690698
C	-2.639975	4.635941	-0.136658
H	-3.102824	5.345297	0.570739
H	-1.602241	4.470014	0.198969

I-2 (conf1)

E(scf) = -5144.93599925 a.u.

Ir	-0.761002	-0.535640	0.017871
Cl	0.086385	-0.075099	2.218789
Cl	-1.175986	-2.814570	0.561408
Cl	-1.595665	-0.869090	-2.203524
N	3.312218	-1.245559	-0.669393
C	4.406295	-2.057186	-0.834265
C	4.225834	-3.398155	-0.981247
C	2.910625	-3.952276	-0.967031
C	1.815836	-3.146772	-0.812080
C	1.887844	0.410569	-0.495702
C	3.239147	0.142918	-0.537090
H	5.377194	-1.562845	-0.838343
H	5.099297	-4.039939	-1.111427
H	2.779703	-5.030175	-1.086994
H	0.785949	-3.508218	-0.775867
C	2.025721	-1.754820	-0.664958
N	1.170569	-0.746223	-0.532777
N	4.322675	0.989897	-0.368876
H	5.056822	0.874167	-1.063305
C	4.868339	1.237414	0.995464
C	5.507228	-0.026077	1.593998
H	5.927108	0.186557	2.592101
H	4.761225	-0.830646	1.713212
H	6.332263	-0.395787	0.958375
C	5.928681	2.329163	0.831889
H	6.384963	2.574700	1.805159
H	6.739922	1.999936	0.155999

H	-2.645534	5.105512	-1.135487
C	-4.840701	3.557094	-0.679415
H	-4.803733	3.937964	-1.714497
H	-5.42431	2.617875	-0.675941
H	-5.378342	4.288570	-0.052883
C	-1.949729	-0.064989	0.655893
C	-1.706604	-0.363236	1.997953
C	-2.698882	-1.017719	2.717978
H	-0.745312	-0.114116	2.450205
C	-4.014277	-1.035209	0.746487
C	-3.898002	-1.360777	2.095149
H	-2.539724	-1.258239	3.772620
H	-4.704976	-1.866965	2.627751
N	-3.093174	-0.414406	0.047665
Br	-5.606406	-1.515590	-0.189031
O	-0.221727	-2.225360	0.078768
H	-0.567251	-2.265843	-1.930230
C	-0.847901	-2.612743	-0.922268
N	-1.87457	-3.450600	-0.836697
C	-2.284805	-4.012914	0.434791
H	-1.709876	-3.535446	1.239912
H	-3.361757	-3.832643	0.590611
H	-2.096287	-5.101102	0.444667
C	-2.634625	-3.823686	-2.011540
H	-2.185215	-3.369329	-2.906935
H	-2.636138	-4.920833	-2.133120
H	-3.675777	-3.468957	-1.916927
O	3.388147	-0.135827	0.036168
C	4.325005	-0.725395	-0.545652
H	4.150446	-1.286242	-1.477389
N	5.571356	-0.665774	-0.096668
C	6.657589	-1.294471	-0.818236
H	7.443952	-0.556249	-1.053080
H	7.097057	-2.106415	-0.213519
H	6.280005	-1.723214	-1.758266
C	5.855178	-0.072095	1.197121
H	4.917069	-0.005648	1.766416
H	6.567173	-0.714776	1.740091
H	6.29383	0.935320	1.084129
H	1.245904	5.047475	0.964301
H	2.829582	5.248630	1.791794
C	2.244326	4.608927	1.104820
H	2.763088	4.572916	0.128991
H	5.481599	3.246789	0.413356
C	3.749579	1.723322	1.922137
H	3.319200	2.673199	1.565305
H	2.928408	0.990614	2.015899
H	4.159780	1.895605	2.931391
C	1.125613	1.653704	-0.508032
C	1.726031	2.894440	-0.690056
C	0.918380	4.019298	-0.790687
H	2.813340	2.943712	-0.761340
C	-0.988392	2.578023	-0.580858
C	-0.458593	3.860653	-0.742288
H	1.355907	5.011658	-0.926084
H	-1.136326	4.709204	-0.841564
N	-0.224000	1.492753	-0.433771
Br	-2.857413	2.438095	-0.629433
O	-2.721000	-0.256415	0.758092
C	-3.647496	-0.969269	0.350185
H	-3.524645	-1.611261	-0.537129
N	-4.847294	-0.979586	0.934613
H	-4.169363	0.306993	2.421673
C	-5.100783	-0.195030	2.125985
H	-5.437670	-0.853876	2.945315
H	-5.882588	0.560833	1.931113
C	-5.917670	-1.810576	0.431264
H	-6.226772	-2.547550	1.193703
H	-5.579594	-2.353159	-0.464270
H	-6.794092	-1.194420	0.161308

N	2.093598	3.281751	1.648201
O	-0.189742	3.339501	1.671956
C	3.289552	2.522467	1.925738
H	3.890508	3.006496	2.719782
H	3.910263	2.440918	1.015264
H	3.015207	1.501845	2.238510
C	0.863618	2.765385	1.890242
H	0.909991	1.736022	2.304177

I-2 (conf2)

E(scf) = -5144.91859915 a.u.

Ir	-0.988423	-0.050546	-0.043507
Cl	0.005094	-0.268905	2.155259
Cl	-3.087921	0.469873	0.975755
Cl	-1.861306	-0.004198	-2.256308
C	1.458123	-1.681872	-1.086788
C	3.615150	-2.685347	-1.360754
C	2.987805	-3.835583	-1.759858
C	1.564596	-3.898517	-1.831232
C	0.809617	-2.813766	-1.497868
C	1.825223	0.348190	-0.488937
C	3.097154	-0.232762	-0.599460
H	4.702412	-2.612293	-1.305314
H	3.578317	-4.713228	-2.034367
H	1.063844	-4.808412	-2.165653
H	-0.278840	-2.741112	-1.532445
N	2.833251	-1.556622	-1.007045
N	0.867506	-0.543962	-0.753998
N	4.329097	0.378968	-0.315350
H	5.031052	0.150796	-1.016037
C	4.899794	0.217550	1.048666
C	5.237482	-1.251065	1.353407
H	5.701059	-1.348186	2.350271
H	4.328828	-1.877346	1.344473
H	5.951746	-1.653906	0.611469
C	6.178694	1.058985	1.075005
H	6.664875	0.997095	2.063092
H	6.906093	0.703817	0.321347
H	5.952273	2.117389	0.861606
C	3.908873	0.737274	2.094314
H	3.711921	1.813157	1.957492
H	2.941987	0.204814	2.060124

I-2 (conf3)

E(scf) = -5144.91549829 a.u.

Ir	0.741366	-0.445829	-0.615230
Cl	-0.788732	0.080816	-2.332973
Cl	2.577082	0.114004	-2.007761
Cl	1.059187	-2.673700	-1.387129
C	-1.790776	-1.838125	0.712443
C	-4.057482	-2.403810	1.263750
C	-3.703902	-3.726618	1.226082
C	-2.366370	-4.102853	0.916237
C	-1.419621	-3.153931	0.663716
C	-1.726008	0.307883	0.689573
C	-3.062200	-0.009926	0.961760
H	-5.075858	-2.085828	1.492311
H	-4.449559	-4.499324	1.428850
H	-2.079742	-5.154577	0.866821
H	-0.382919	-3.337854	0.368992
N	-3.077085	-1.418665	0.991286
N	-0.980937	-0.796963	0.525561
N	-4.135862	0.883468	1.122120
H	-4.742239	0.596478	1.887599
C	-4.960213	1.224506	-0.070302
C	-5.653118	-0.014296	-0.659887
H	-6.290186	0.266876	-1.516041
H	-4.913484	-0.749062	-1.021312
H	-6.300064	-0.502707	0.092014
C	-6.011460	2.224424	0.418558
H	-6.658835	2.546148	-0.414432
H	-6.661555	1.775733	1.192876
H	-5.527637	3.116980	0.850473
C	-4.083460	1.870668	-1.146493
H	-3.650006	2.820446	-0.792588
H	-3.257773	1.210423	-1.465885

H	4.331052	0.598197	3.104025	H	-4.694409	2.092155	-2.037972
C	1.331484	1.701318	-0.243403	C	-1.002716	1.577440	0.624097
C	2.186678	2.791706	-0.188022	C	-1.587041	2.765831	1.045984
C	1.636249	4.064540	-0.090612	C	-0.808701	3.915428	1.082000
H	3.260965	2.609123	-0.245365	H	-2.635944	2.747655	1.346538
C	-0.547759	3.056543	-0.206534	C	1.064455	2.578954	0.395335
C	0.258260	4.198303	-0.117072	C	0.539469	3.818291	0.772534
H	2.276034	4.948647	-0.030430	H	-1.238010	4.873049	1.387329
H	-0.220215	5.177745	-0.093186	H	1.205819	4.678975	0.841912
N	-0.030746	1.819180	-0.204624	N	0.303427	1.488995	0.245554
Br	-2.376263	3.342937	-0.426274	Br	2.930978	2.494899	0.229853
O	-1.731989	-2.014276	0.076123	O	2.124706	-0.838998	0.967141
C	-2.326356	-2.375043	1.110751	C	3.201626	-1.390218	0.690580
H	-2.129561	-1.887905	2.077919	H	3.345859	-1.896085	-0.277111
N	-3.195498	-3.379350	1.100896	N	4.235949	-1.412287	1.531917
H	-3.309429	-3.328851	-0.978551	H	3.206163	-0.235266	2.904963
C	-3.593261	-3.994950	-0.151031	C	4.178637	-0.736470	2.811353
H	-3.105193	-4.977452	-0.282628	H	4.299418	-1.462197	3.635166
H	-4.686599	-4.136197	-0.154511	H	4.984480	0.015463	2.877354
C	-3.823320	-3.839669	2.320979	C	5.472445	-2.074542	1.175940
H	-3.435783	-3.268460	3.177461	H	5.376553	-2.533444	0.180688
H	-4.916319	-3.695017	2.266504	H	6.304042	-1.348319	1.150344
H	-3.613567	-4.911271	2.484684	H	5.714521	-2.863602	1.909705

I-2 (conf4)

E(scf) = -5144.89911379 a.u.

Ir	-0.827436	-0.657102	0.170175
Cl	0.403608	-0.085600	2.182737
Cl	-0.616365	-2.961875	0.634396
Cl	-1.933632	-1.172168	-1.875812
N	-2.677532	-0.672455	1.493099
C	-2.867130	0.680657	2.068041
H	-3.097801	1.405368	1.279719
H	-3.700587	0.666460	2.793040
H	-1.935358	0.968473	2.574816
C	-2.564907	-1.635196	2.617131
H	-3.453989	-1.533861	3.263117
H	-2.507500	-2.653817	2.225381
H	-1.648799	-1.399996	3.174264
C	-3.794238	-1.022681	0.636157
H	-4.013917	-0.236501	-0.109907
O	-4.411385	-2.034630	0.743682

I-2 (conf5)

E(scf) = -5144.90051722 a.u.

Ir	1.043344	0.437324	0.285015
Cl	-0.007276	-0.257569	2.345854
Cl	3.178639	0.039446	1.239443
Cl	1.948794	1.140162	-1.815772
N	1.129122	2.512724	1.192051
C	1.930839	2.548967	2.447066
H	2.971124	2.278465	2.237272
H	1.863215	3.562922	2.880617
H	1.515599	1.804973	3.140345
C	-0.235397	2.981273	1.512587
H	-0.182877	3.956551	2.025900
H	-0.822977	3.116340	0.600890
H	-0.701875	2.227777	2.161078
C	1.776774	3.340362	0.200745
H	2.855275	3.108833	0.106300
O	1.204471	4.189287	-0.415564

N	3.163038	-0.945631	-1.013678	N	-3.003299	0.843285	-1.101168
C	4.262155	-1.770977	-1.347798	C	-4.055226	1.659532	-1.586240
C	4.027819	-3.060527	-1.749201	C	-3.768793	2.920174	-2.040117
C	2.696625	-3.551196	-1.849575	C	-2.424696	3.393365	-2.052398
C	1.636363	-2.754716	-1.526914	C	-1.413579	2.612567	-1.575875
C	1.635507	0.584720	-0.547729	C	-1.521002	-0.655088	-0.418959
C	3.016303	0.410339	-0.644916	C	-2.889972	-0.495135	-0.670407
H	5.271221	-1.359716	-1.284543	H	-5.070657	1.259729	-1.595985
H	4.863900	-3.713920	-2.010366	H	-4.568334	3.561119	-2.419414
H	2.500593	-4.566491	-2.197392	H	-2.178456	4.372880	-2.464899
H	0.583996	-3.032154	-1.585968	H	-0.350247	2.860941	-1.605872
C	1.895219	-1.485416	-1.088263	C	-1.731686	1.384365	-1.061473
N	0.982137	-0.568561	-0.773753	N	-0.862067	0.501094	-0.580108
N	4.027031	1.350237	-0.392623	N	-3.896824	-1.459051	-0.516293
H	4.808510	1.214501	-1.029385	H	-4.574302	-1.414308	-1.274540
C	4.532367	1.472363	1.007523	C	-4.604564	-1.537590	0.790280
C	4.768327	0.100824	1.657970	C	-5.364094	-0.236768	1.097755
H	5.212018	0.224325	2.660687	H	-5.909991	-0.318100	2.053308
H	3.818330	-0.448244	1.777338	H	-4.670246	0.617766	1.180112
H	5.460055	-0.515884	1.056776	H	-6.103715	-0.013766	0.306742
C	5.848834	2.247088	0.913056	C	-5.593820	-2.699574	0.669292
H	6.260093	2.435425	1.918427	H	-6.149621	-2.835447	1.612046
H	6.607687	1.678483	0.343493	H	-6.333161	-2.514779	-0.132120
H	5.694336	3.218733	0.412603	H	-5.063307	-3.638762	0.438030
C	3.527599	2.258099	1.855300	C	-3.602234	-1.819538	1.912618
H	3.401619	3.284230	1.470655	H	-3.102407	-2.791499	1.769815
H	2.543823	1.758081	1.884004	H	-2.820061	-1.044434	1.985687
H	3.889337	2.327775	2.895507	H	-4.130053	-1.853385	2.880609
C	0.767197	1.753763	-0.429195	C	-0.657895	-1.830015	-0.281206
C	1.271753	3.044651	-0.532440	C	-1.154837	-3.123332	-0.312089
C	0.377959	4.100988	-0.644834	C	-0.251878	-4.178120	-0.400321
H	2.354152	3.176917	-0.558445	H	-2.235613	-3.266771	-0.303118
C	-1.395313	2.488950	-0.679698	C	1.526389	-2.563967	-0.554904
C	-0.977084	3.819081	-0.753334	C	1.095606	-3.896617	-0.549811
H	0.734168	5.132232	-0.710170	H	-0.602082	-5.213517	-0.403503
H	-1.712183	4.604188	-0.934437	H	1.831368	-4.687675	-0.698224
N	-0.567581	1.476291	-0.412059	N	0.679920	-1.550664	-0.328637
Br	-3.190155	2.169969	-1.153276	Br	3.301666	-2.265735	-1.046985

I-2 (conf6)

E(scf) = -5144.90427488 a.u.

Ir	0.982825	-0.711842	-0.426286

I-3 (conf1)

E(scf) = -8308.61098228 a.u.

Ir	-0.690640	0.287196	-0.221973

Cl	-0.098477	-0.080256	-2.410859	Cl	-1.522854	0.016260	2.032843
Cl	3.081444	-0.549199	-1.507990	Cl	0.460011	2.225017	0.515611
Cl	1.110985	-2.987962	-1.094202	Cl	-0.257606	0.675972	-2.554965
N	1.937288	-1.413207	1.594444	C	-3.043584	2.373543	-0.281405
C	3.274342	-1.996519	1.358823	C	-5.119726	3.488846	0.179294
H	3.919680	-1.254971	0.869517	C	-4.442684	4.679825	0.182236
H	3.707679	-2.335875	2.317498	C	-3.041295	4.707764	-0.060920
H	3.161391	-2.840979	0.665191	C	-2.352423	3.554145	-0.297070
C	1.039923	-2.381208	2.245325	C	-3.553321	0.296351	-0.487946
H	1.463738	-2.691419	3.217284	C	-4.757543	0.931032	-0.176464
H	0.060388	-1.918365	2.417702	H	-6.194951	3.434462	0.356819
H	0.946238	-3.249957	1.580581	H	-4.976768	5.614810	0.368261
C	2.001375	-0.175728	2.288218	H	-2.493892	5.651559	-0.063462
H	2.890140	0.421452	1.990329	H	-1.276352	3.469335	-0.465139
O	1.186400	0.196392	3.083430	N	-4.404848	2.291211	-0.060104
N	-3.165776	-1.043516	0.614874	N	-2.532714	1.167924	-0.520162
C	-4.325649	-1.847889	0.733538	N	-6.008643	0.322989	0.016091
C	-4.211141	-3.206975	0.615706	H	-6.757008	0.886489	-0.382049
C	-2.940127	-3.794658	0.365367	C	-6.378810	-0.102221	1.394381
C	-1.822410	-3.019638	0.264142	C	-6.435012	1.090788	2.361549
C	-1.519947	0.434965	0.557519	H	-6.751712	0.763891	3.366916
C	-2.912443	0.338013	0.684053	H	-5.445129	1.568253	2.462400
H	-5.286307	-1.362318	0.910434	H	-7.159650	1.848987	2.012162
H	-5.095591	-3.842989	0.700968	C	-7.762717	-0.745981	1.276456
H	-2.838025	-4.873078	0.234221	H	-8.107802	-1.112450	2.257810
H	-0.820012	-3.374897	0.008029	H	-8.510835	-0.018833	0.909423
C	-1.949419	-1.664648	0.413197	H	-7.736577	-1.596169	0.573727
N	-0.956737	-0.768931	0.382208	C	-5.366997	-1.126761	1.915837
N	-3.835737	1.391940	0.791530	H	-5.353020	-2.030609	1.283714
H	-4.536870	1.207493	1.505658	H	-4.343707	-0.713717	1.964218
C	-4.486260	1.899946	-0.446633	H	-5.647060	-1.433998	2.937738
C	-5.436200	0.858595	-1.060327	C	-3.224271	-1.073479	-0.870732
H	-5.950126	1.273157	-1.944501	C	-4.206450	-1.981896	-1.250976
H	-4.886035	-0.040477	-1.386691	C	-3.813356	-3.201352	-1.785644
H	-6.212064	0.554557	-0.333751	H	-5.252020	-1.689647	-1.136193
C	-5.281649	3.139999	-0.028063	C	-1.532799	-2.488269	-1.563726
H	-5.796744	3.584489	-0.896147	C	-2.459427	-3.451541	-1.965010
H	-6.050504	2.885056	0.724576	H	-4.555451	-3.941320	-2.095622
H	-4.612701	3.900849	0.408703	H	-2.104970	-4.374488	-2.425291
C	-3.424237	2.284193	-1.481158	N	-1.894784	-1.343990	-0.969185
H	-2.776488	3.096139	-1.112454	Br	0.270003	-2.855191	-1.938205
H	-2.779351	1.431744	-1.757708	C	1.017504	-1.875979	1.136893
H	-3.918197	2.639804	-2.400856	C	2.397836	-3.331048	2.482940

C	-0.628167	1.592186	0.574831
C	-1.114049	2.826224	0.990974
C	-0.254904	3.914012	1.017111
H	-2.165720	2.893092	1.274248
C	1.490905	2.438433	0.273656
C	1.063782	3.716618	0.647909
H	-0.603635	4.900855	1.331431
H	1.788649	4.530894	0.660526
N	0.669573	1.378289	0.215918
Br	3.328160	2.310747	-0.076645
C	1.295574	-4.078850	2.788964
C	0.033464	-3.718063	2.240828
C	-0.090043	-2.623696	1.438357
C	2.384504	-0.419300	0.326135
C	3.166588	-1.288695	1.100991
H	3.389781	-3.543143	2.882583
H	1.373948	-4.938624	3.458883
H	-0.865264	-4.291412	2.474070
H	-1.041292	-2.270682	1.058330
N	2.261253	-2.218306	1.618278
N	1.075810	-0.772820	0.352752
N	4.540683	-1.238898	1.375513
H	4.815738	-0.262354	1.471446
C	5.491844	-1.946151	0.490536
C	5.284982	-3.458474	0.614752
H	6.005300	-3.999211	-0.023189
H	5.433123	-3.786012	1.657881
H	4.269342	-3.752800	0.296497
C	5.351883	-1.533546	-0.985334
H	6.074305	-2.083259	-1.614273
H	4.338419	-1.752127	-1.364729
H	5.538752	-0.453726	-1.115851
C	6.888810	-1.572301	0.995069
H	7.060306	-0.484812	0.897168
H	6.998810	-1.843048	2.058772
H	7.669422	-2.091825	0.413457
C	2.996799	0.706713	-0.411724
C	2.797794	0.924752	-1.771478
C	3.499426	1.958723	-2.383790
H	2.079324	0.325107	-2.327166
C	4.559925	2.362444	-0.300458
C	4.402270	2.713422	-1.642235
H	3.341304	2.172392	-3.444325
H	4.975834	3.530457	-2.083098
N	3.895440	1.404471	0.296155
Br	5.851747	3.288163	0.748954

I-3 (conf2)

E(scf) = -8308.57740851 a.u.

Ir	0.273297	-1.154833	-0.118733
Cl	-0.853074	0.635362	-1.356830
Cl	0.797766	-1.959936	-2.291680

I-3_DMF

E(scf) = -8556.92435293 a.u.

Ir	0.798958	0.372215	0.009953
Cl	1.816862	0.876650	-2.128529
Cl	-0.256334	2.490500	-0.031661

Cl	0.869104	-3.124763	1.092002	Cl	0.175078	-0.039347	2.290960
C	-2.423050	-2.435004	-1.002774	N	4.526613	2.142025	0.780806
C	-4.687897	-2.594483	-1.774431	C	5.354808	3.214380	0.995665
C	-4.278965	-3.545169	-2.673611	C	4.817284	4.403930	1.380773
C	-2.917206	-3.951277	-2.719011	C	3.40696	4.530520	1.559067
C	-1.998381	-3.396592	-1.875527	C	2.577721	3.462384	1.352586
C	-2.480320	-1.025106	0.621645	C	3.624394	0.182703	0.407909
C	-3.788907	-1.073495	0.145081	C	4.83712	0.834683	0.402282
H	-5.728798	-2.273011	-1.707262	H	6.420088	3.042802	0.840806
H	-5.000961	-4.000054	-3.356361	H	5.479051	5.255465	1.550169
H	-2.584703	-4.713127	-3.425560	H	2.988163	5.491976	1.865223
H	-0.932468	-3.625536	-1.845827	H	1.491283	3.501658	1.449683
N	-3.734152	-2.016297	-0.904938	C	3.157047	2.232787	0.956288
N	-1.667950	-1.820741	-0.095116	N	2.614125	1.047564	0.708795
N	-4.880523	-0.292896	0.558385	N	6.086023	0.405093	-0.018316
H	-5.745174	-0.826710	0.510687	H	6.847889	0.707270	0.583265
C	-5.070774	1.030321	-0.106308	C	6.433819	0.516509	-1.467344
C	-4.987792	0.924263	-1.636914	C	6.187079	1.931790	-2.011802
H	-5.195779	1.903597	-2.101258	H	6.459305	1.983897	-3.079730
H	-3.978554	0.610230	-1.954905	H	5.119664	2.202612	-1.930950
H	-5.725874	0.201185	-2.028989	H	6.791459	2.684468	-1.475817
C	-6.459843	1.515002	0.316331	C	7.916277	0.153979	-1.571225
H	-6.660990	2.517117	-0.097291	H	8.245208	0.175634	-2.623107
H	-7.250580	0.835809	-0.054094	H	8.544759	0.870783	-1.010230
H	-6.536204	1.568706	1.416165	H	8.099653	-0.857631	-1.169717
C	-4.007613	2.019874	0.380124	C	5.590989	-0.474153	-2.276775
H	-4.082280	2.183369	1.468098	H	5.776007	-1.511794	-1.952727
H	-2.987045	1.677641	0.133303	H	4.512114	-0.252871	-2.191121
H	-4.147932	2.993986	-0.119058	H	5.85519	-0.397601	-3.345236
C	-1.845593	-0.370230	1.762417	C	3.260496	-1.220366	0.241494
C	-2.594549	0.152020	2.808247	C	4.200121	-2.245341	0.298912
C	-1.930208	0.560688	3.958308	C	3.754693	-3.559703	0.308928
H	-3.679657	0.189896	2.700456	H	5.257292	-1.982753	0.357062
C	0.123542	-0.143525	2.935232	C	1.505941	-2.725750	0.266598
C	-0.557511	0.387202	4.033988	C	2.387562	-3.806431	0.314007
H	-2.481765	0.974950	4.806433	H	4.46471	-4.389722	0.348211
H	0.002556	0.645560	4.933159	H	1.989483	-4.820220	0.370956
N	-0.489086	-0.461425	1.793154	N	1.923091	-1.458053	0.167489
Br	1.955819	-0.456879	3.185461	Br	-0.323734	-3.128043	0.411519
C	-0.181768	3.237713	1.068008	N	-2.039205	-0.954714	-2.856323
C	-0.935908	4.594903	-0.760222	C	-2.227372	-1.475855	-4.108220
C	-1.896412	5.119180	0.061754	C	-1.202615	-2.134387	-4.714415
C	-1.983674	4.708535	1.426583	C	0.046531	-2.260506	-4.042037

C	-1.124866	3.765356	1.903253
C	1.360398	2.015861	0.327127
C	1.035412	2.860264	-0.750356
H	-0.865749	4.879674	-1.810100
H	-2.610972	5.849877	-0.326158
H	-2.743437	5.125690	2.090041
H	-1.123068	3.359413	2.915929
N	-0.017449	3.639658	-0.247419
N	0.658240	2.265230	1.427103
N	1.527270	2.689950	-2.047938
H	0.908291	2.121043	-2.621757
C	2.351591	3.656660	-2.765199
C	3.591879	3.986697	-1.926977
H	4.235525	4.715435	-2.449998
H	3.301113	4.424586	-0.955296
H	4.176551	3.071669	-1.734208
C	2.779210	2.968811	-4.066381
H	3.442104	3.620702	-4.660778
H	3.307886	2.026760	-3.844117
H	1.898026	2.724704	-4.687338
C	1.607251	4.963900	-3.098088
H	0.678505	4.746951	-3.655721
H	1.344985	5.511760	-2.176332
H	2.230516	5.632430	-3.718864
C	2.473446	1.035665	0.298556
C	3.705945	1.594494	0.619647
C	4.850602	0.815176	0.592430
H	3.737067	2.649512	0.892618
C	3.449002	-1.005930	-0.130638
C	4.713940	-0.498782	0.192250
H	5.828860	1.225296	0.856057
H	5.575794	-1.161589	0.113195
N	2.314235	-0.276963	-0.035806
Br	3.531295	-2.781108	-0.735136

C	0.242028	-1.683986	-2.816421
C	-2.237752	0.070049	-0.922247
C	-2.950097	-0.303085	-2.041739
H	-3.214267	-1.304566	-4.536361
H	-1.347273	-2.551401	-5.712767
H	0.866253	-2.801254	-4.521318
H	1.206781	-1.722540	-2.318077
C	-0.827213	-0.981754	-2.203068
N	-0.925281	-0.332911	-1.031963
N	-4.25968	-0.064052	-2.444302
H	-4.509352	0.885643	-2.167961
C	-5.343628	-1.004796	-2.059691
C	-5.095811	-2.373797	-2.699148
H	-5.887921	-3.080497	-2.398570
H	-5.100061	-2.307661	-3.800172
H	-4.130384	-2.801410	-2.374165
C	-5.462502	-1.175075	-0.536868
H	-6.294869	-1.856488	-0.288190
H	-4.538726	-1.599645	-0.109169
H	-5.653674	-0.208488	-0.041588
C	-6.635715	-0.397481	-2.612831
H	-6.835034	0.584021	-2.145814
H	-6.558312	-0.251688	-3.703644
H	-7.497438	-1.053060	-2.401342
C	-2.908898	0.731118	0.215033
C	-2.872444	0.202515	1.501558
C	-3.671884	0.780239	2.484177
H	-2.241203	-0.653532	1.728531
C	-4.463519	2.279292	0.819580
C	-4.484538	1.859583	2.151251
H	-3.669643	0.351996	3.490645
H	-5.134041	2.342447	2.883496
N	-3.722865	1.742344	-0.117855
Br	-5.630450	3.687142	0.277783
H	-2.620895	-4.128177	3.943588
H	-1.173314	-4.692430	3.035820
C	-1.531459	-4.268627	3.993016
H	-1.291244	-4.983939	4.802079
N	-0.920730	-2.986294	4.242465
O	-2.902414	-1.846503	4.268447
C	0.518347	-2.925288	4.294546
H	0.956699	-3.314898	3.356473
H	0.912109	-3.520611	5.140720

H	0.845758	-1.880062	4.397394
C	-1.691036	-1.872490	4.360237
H	-1.091576	-0.957945	4.555060

I-4 (conf1)

E(scf) = -4932.51780279 a.u.

Ir	1.353923	-0.609365	-0.276292
Cl	1.85367	-0.571734	-2.571940
Cl	2.454439	-2.728458	0.048860
N	-0.666177	3.131013	-0.488438
C	-0.710491	4.496905	-0.576161
C	0.453713	5.204482	-0.534321
C	1.704106	4.527567	-0.403562
C	1.752789	3.159873	-0.351906
C	-1.072649	0.976424	-0.499907
C	-1.702311	2.200706	-0.502112
H	-1.70554	4.925412	-0.695268
H	0.41652	6.292682	-0.613244
H	2.627755	5.110018	-0.358181
H	2.675657	2.583940	-0.264975
C	0.535439	2.443143	-0.420979
N	0.284249	1.142300	-0.436601
N	-3.04079	2.576530	-0.553715
H	-3.540375	1.918952	-1.151299
C	-3.783618	2.718058	0.730676
C	-3.737636	1.431304	1.569505
H	-4.310317	1.560600	2.504861
H	-4.158916	0.582444	1.007101
H	-2.69732	1.172079	1.836102
C	-3.196596	3.877074	1.540912
H	-3.741204	3.983971	2.494506
H	-2.133631	3.703461	1.785200
H	-3.28113	4.831019	0.993504
C	-5.230331	3.036157	0.345632
H	-5.27307	3.941686	-0.283358
H	-5.678876	2.198656	-0.218400
H	-5.845091	3.201418	1.246559
C	-1.519213	-0.406558	-0.614885
C	-0.473814	-1.356048	-0.578705
C	-0.870531	-2.689852	-0.745903
C	-3.139886	-1.949379	-0.923276
C	-2.219289	-3.000328	-0.917627

I-4 (conf2)

E(scf) = -4932.51657880 a.u.

Ir	-1.488756	-0.248466	-0.218871
Cl	-3.578245	1.177644	-0.024818
Cl	-2.839895	-1.903679	-1.294604
C	-0.104864	2.266514	1.201975
C	1.350276	3.884930	2.221370
C	0.260692	4.687345	2.431562
C	-1.031083	4.271010	1.996454
C	-1.203544	3.060703	1.390535
C	1.173134	0.621090	0.659063
C	2.033981	1.582405	1.196581
H	2.352229	4.163582	2.549304
H	0.376949	5.648324	2.939097
H	-1.904492	4.907786	2.147843
H	-2.153039	2.646081	1.027621
N	1.181059	2.637773	1.569517
N	-0.105122	1.043135	0.668087
N	3.422795	1.486530	1.368053
H	3.656433	0.496222	1.431442
C	4.306506	2.090497	0.338973
C	3.930361	1.644513	-1.083956
H	4.619226	2.085712	-1.826058
H	3.978216	0.546044	-1.169933
H	2.903489	1.961462	-1.339868
C	4.250128	3.617442	0.431949
H	4.964756	4.069124	-0.277900
H	3.246047	4.000790	0.180574
H	4.511238	3.953835	1.450196
C	5.721087	1.606933	0.672506
H	5.991406	1.891197	1.703896
H	5.787478	0.507134	0.585959
H	6.458689	2.044563	-0.021595
C	1.370645	-0.722668	0.125764
C	0.207361	-1.347501	-0.365211
C	0.391957	-2.639098	-0.875170
C	2.718539	-2.477508	-0.339510
C	1.660004	-3.219704	-0.869115

H	-0.115308	-3.480572	-0.742869	H	-0.464023	-3.187212	-1.279155
H	-2.553274	-4.031552	-1.050874	H	1.828210	-4.223477	-1.265302
N	-2.814489	-0.685761	-0.787166	N	2.592306	-1.267352	0.150185
Br	-4.996941	-2.334882	-1.133859	Br	4.469942	-3.232111	-0.312885
O	3.395045	0.342047	0.120898	O	-1.883272	-1.131551	1.627833
H	4.2066	-0.912654	-1.262254	H	-3.894528	-1.089560	1.292789
C	4.35567	-0.157081	-0.471261	C	-3.056591	-1.408979	1.932547
N	5.631192	0.170175	-0.221165	N	-3.362259	-2.078565	3.041090
C	5.966521	1.141308	0.796585	C	-2.331234	-2.544432	3.947820
H	5.046603	1.433032	1.321727	H	-1.347162	-2.340206	3.505339
H	6.677311	0.704794	1.520582	H	-2.411482	-2.025518	4.919336
H	6.430235	2.036661	0.343794	H	-2.442278	-3.629907	4.112628
C	6.718127	-0.435933	-0.956950	C	-4.739927	-2.352638	3.390993
H	6.318155	-1.152740	-1.689907	H	-5.409865	-1.958022	2.612809
H	7.30056	0.332214	-1.497013	H	-4.903501	-3.440751	3.480792
H	7.396735	-0.976115	-0.272759	H	-4.995267	-1.875857	4.353818
O	0.890346	-0.509747	1.821437	O	-1.064619	0.642445	-2.054723
C	0.659649	-1.536163	2.472947	C	-1.975983	0.826485	-2.879673
H	0.941155	-2.526152	2.070573	H	-3.017972	0.563758	-2.639780
N	0.086146	-1.517473	3.678228	N	-1.748597	1.352567	-4.080922
C	-0.161003	-2.741569	4.409069	C	-2.831993	1.581332	-5.013221
H	0.352251	-2.719130	5.386581	H	-2.926381	2.658042	-5.239652
H	-1.243465	-2.876871	4.581450	H	-2.649206	1.035833	-5.955444
H	0.213883	-3.601821	3.834546	H	-3.779026	1.228168	-4.578921
C	-0.355086	-0.274001	4.276511	C	-0.411150	1.729889	-4.494487
H	-0.125719	0.550194	3.587854	H	0.300253	1.441809	-3.708970
H	-1.443987	-0.307612	4.457221	H	-0.149406	1.213155	-5.433902
H	0.161398	-0.105177	5.237784	H	-0.354406	2.820407	-4.658676

I-4 (conf3)

E(scf) = -4932.51647962 a.u.

Ir	1.168813	-0.137452	-0.086246
Cl	1.561329	-0.248475	-2.443431
Cl	0.902334	0.025974	2.295403
C	-0.254963	2.615325	-0.228668
C	-1.735164	4.502255	-0.308736
C	-0.641353	5.322864	-0.236549
C	0.668091	4.768333	-0.123580
C	0.846878	3.416874	-0.123576
C	-1.532824	0.883596	-0.329647
C	-2.405607	1.975786	-0.317710
H	-2.750450	4.890407	-0.397158

I-4 (conf4)

E(scf) = -4932.51005925 a.u.

Ir	1.497620	0.354176	-0.199347
Cl	3.143125	2.157720	0.401244
Cl	2.113636	0.389053	-2.465491
C	-0.540033	2.709523	-0.550196
C	-2.432441	4.164916	-0.816132
C	-1.573788	5.231636	-0.781324
C	-0.175506	5.023535	-0.605531
C	0.333150	3.762038	-0.496676
C	-1.357551	0.713701	-0.596953
C	-2.465394	1.558595	-0.683017
H	-3.506887	4.282837	-0.960239

H	-0.766968	6.408033	-0.265710	H	-1.958650	6.248222	-0.895860
H	1.542279	5.416110	-0.038135	H	0.514944	5.867652	-0.564080
H	1.800537	2.894377	-0.033958	H	1.388034	3.496605	-0.349979
N	-1.556044	3.096599	-0.279895	N	-1.913203	2.854125	-0.681881
N	-0.251781	1.287877	-0.285368	N	-0.213101	1.418294	-0.509679
N	-3.806826	1.956075	-0.348857	N	-3.816442	1.193834	-0.784096
H	-4.098641	1.106017	-0.829378	H	-3.861858	0.280530	-1.234238
C	-4.532028	2.019948	0.947543	C	-4.614954	1.128528	0.465190
C	-4.027121	0.965504	1.946492	C	-3.912375	0.310670	1.563644
H	-4.592382	1.024122	2.893359	H	-4.542373	0.253348	2.469357
H	-4.144870	-0.048615	1.529227	H	-3.708091	-0.713796	1.209117
H	-2.957753	1.112785	2.180062	H	-2.949518	0.774013	1.844553
C	-4.385833	3.417475	1.555005	C	-4.891928	2.544863	0.976486
H	-4.981912	3.494171	2.480732	H	-5.543066	2.511615	1.867433
H	-3.336272	3.633435	1.819270	H	-3.958251	3.058203	1.264777
H	-4.739499	4.187631	0.847701	H	-5.395994	3.144079	0.198944
C	-6.002836	1.754886	0.613756	C	-5.933051	0.449116	0.083045
H	-6.370908	2.492070	-0.120337	H	-6.429187	1.004755	-0.730973
H	-6.129819	0.744133	0.184994	H	-5.752912	-0.585200	-0.262336
H	-6.626336	1.816309	1.521906	H	-6.616739	0.403748	0.947799
C	-1.683694	-0.563753	-0.371970	C	-1.165639	-0.732138	-0.639349
C	-0.465364	-1.268611	-0.268162	C	0.181946	-1.137784	-0.538729
C	-0.574674	-2.660608	-0.349760	C	0.397433	-2.517122	-0.636085
C	-2.946246	-2.426232	-0.568198	C	-1.962817	-2.835415	-0.860918
C	-1.826565	-3.258088	-0.494705	C	-0.681375	-3.388444	-0.797107
H	0.316957	-3.294052	-0.316837	H	1.415856	-2.916003	-0.588501
H	-1.936356	-4.342559	-0.559776	H	-0.538210	-4.468213	-0.878142
N	-2.888832	-1.116240	-0.521159	N	-2.211686	-1.547973	-0.795500
Br	-4.675908	-3.204551	-0.753983	Br	-3.468644	-3.990242	-1.041619
O	3.077696	1.143449	0.116374	O	3.098373	-0.993899	0.165933
H	3.840272	0.429427	-1.627226	H	4.389216	0.248117	-0.804371
C	3.997037	1.001988	-0.692662	C	4.218940	-0.712905	-0.295857
N	5.218453	1.526336	-0.521656	N	5.267588	-1.527809	-0.191401
C	5.539886	2.295847	0.662401	C	5.165215	-2.817450	0.457746
H	4.695152	2.237419	1.362938	H	4.153117	-2.931980	0.867622
H	6.444831	1.886004	1.144080	H	5.358720	-3.627591	-0.267661
H	5.727328	3.353363	0.402219	H	5.902777	-2.889940	1.276155
C	6.248039	1.371577	-1.525358	C	6.551780	-1.159923	-0.750436
H	5.867046	0.763686	-2.360001	H	6.481592	-0.169025	-1.222548
H	6.559300	2.354847	-1.921525	H	7.320566	-1.121708	0.041201
H	7.135006	0.870826	-1.097711	H	6.864130	-1.894387	-1.513451
O	2.539658	-1.757289	0.123862	O	0.891489	0.329286	1.861453
C	2.624286	-2.430449	1.160361	C	0.787873	-0.714759	2.509320

H	2.031425	-2.159152	2.053033	H	1.188697	-1.669260	2.122770
N	3.422683	-3.494286	1.261618	N	0.193468	-0.781360	3.702250
C	3.524723	-4.237682	2.499769	C	0.075512	-2.031280	4.420961
H	3.271011	-5.298948	2.332339	H	0.573118	-1.961283	5.404242
H	4.550793	-4.180477	2.904619	H	-0.987668	-2.283027	4.580314
H	2.828876	-3.821897	3.243901	H	0.544224	-2.843280	3.844558
C	4.240239	-3.923738	0.143908	C	-0.404111	0.398376	4.298201
H	3.967981	-3.334806	-0.742954	H	-0.232640	1.255918	3.633858
H	5.311615	-3.775920	0.369197	H	-1.489624	0.246001	4.429768
H	4.064690	-4.994293	-0.057659	H	0.053829	0.598947	5.282211

I-5 (conf1)

E(scf) = -8096.24895834 a.u.

N	4.604612	1.107952	0.173894
C	5.769814	0.819714	-0.484596
C	6.595226	1.840921	-0.847210
C	6.237571	3.194303	-0.547367
C	5.051967	3.476723	0.074334
C	2.640518	1.105077	1.128927
C	3.623516	0.249359	0.641116
H	5.941597	-0.239629	-0.681807
H	7.527434	1.616273	-1.369423
H	6.917061	4.003050	-0.828397
H	4.736943	4.495771	0.305295
C	4.185352	2.408671	0.437605
N	3.00057	2.415443	1.013108
N	3.767356	-1.115543	0.472397
H	2.939547	-1.563087	0.061377
C	4.316815	-1.963399	1.556649
C	3.274702	-2.172340	2.665803
H	3.660224	-2.850332	3.447773
H	3.012624	-1.212969	3.147018
H	2.357172	-2.614635	2.243141
C	4.656433	-3.309899	0.910483
H	5.035469	-4.022321	1.663704
H	3.75865	-3.743274	0.437394
H	5.425315	-3.178888	0.129345
C	5.576058	-1.327877	2.150462
H	6.37219	-1.219138	1.394887
H	5.36479	-0.333183	2.581659
H	5.967338	-1.966415	2.960505
C	1.413043	0.727779	1.835079

I-5 (conf2)

E(scf) = -8096.23944083 a.u.

Ir	-0.004757	0.799693	-1.052420
Cl	0.332348	2.962882	-1.937549
Cl	-1.154087	0.109035	-3.178756
C	2.615129	0.002817	-2.653001
C	4.823057	-0.539685	-3.432345
C	4.292528	-0.768117	-4.674326
C	2.893980	-0.616549	-4.896452
C	2.065655	-0.224308	-3.885549
C	2.870154	0.557617	-0.587332
C	4.143126	0.177549	-1.017102
H	5.890335	-0.627989	-3.226756
H	4.943616	-1.056295	-5.503632
H	2.461284	-0.796114	-5.882095
H	0.980346	-0.073294	-3.955388
N	3.964786	-0.151582	-2.374400
N	1.961566	0.429380	-1.572214
N	5.326734	0.148895	-0.264795
H	5.243745	0.845953	0.473754
C	5.721209	-1.137706	0.361017
C	4.549128	-1.819241	1.090299
H	4.881742	-2.757635	1.568765
H	4.139284	-1.152955	1.868291
H	3.736857	-2.064493	0.382113
C	6.276858	-2.085333	-0.705900
H	6.650582	-3.013574	-0.239396
H	5.499813	-2.368799	-1.436772
H	7.110744	-1.607456	-1.247893
C	6.820352	-0.792704	1.369806
H	7.654748	-0.275753	0.865785

C	0.998689	1.526426	2.905062	H	6.428003	-0.129786	2.162279
C	-0.045669	1.094244	3.705275	H	7.211119	-1.704748	1.851956
H	1.521369	2.467624	3.078897	C	2.334493	1.053676	0.675788
C	-0.102652	-0.902161	2.400452	C	0.935418	1.249727	0.687896
C	-0.563617	-0.182201	3.495191	C	0.410043	1.637805	1.928398
H	-0.412567	1.710105	4.530487	C	2.619207	1.637078	2.844251
H	-1.297969	-0.624270	4.169350	C	1.250047	1.842543	3.024479
N	0.752974	-0.407455	1.494744	H	-0.668894	1.767645	2.059850
Br	-0.613981	-2.713472	2.292270	H	0.854402	2.145774	3.996095
Ir	0.151689	-0.557271	-0.726590	N	3.156029	1.245949	1.711553
Cl	1.335758	-2.794495	-1.001336	Br	3.808395	1.893009	4.309381
Cl	-0.600072	-0.514175	-2.950589	O	-0.043068	-1.282591	-0.528970
N	-3.75684	-2.068225	-0.198898	C	0.549629	-1.820248	0.412056
C	-4.693862	-3.066860	-0.181308	H	0.893460	-1.241796	1.287198
C	-4.309825	-4.342859	-0.464456	N	0.823548	-3.123709	0.445515
C	-2.945832	-4.628822	-0.771046	C	1.502665	-3.725822	1.573141
C	-1.999977	-3.638972	-0.746333	H	0.851837	-4.476206	2.054140
C	-2.637936	-0.195408	-0.007906	H	2.434760	-4.213115	1.239052
C	-3.913551	-0.702025	0.025979	H	1.759600	-2.952640	2.312629
H	-5.705112	-2.752449	0.074690	C	0.443638	-3.989575	-0.652907
H	-5.056807	-5.138705	-0.450206	H	-0.073009	-3.391134	-1.416344
H	-2.65455	-5.652380	-1.019803	H	1.342683	-4.456367	-1.092207
H	-0.93826	-3.799793	-0.952261	H	-0.232029	-4.782582	-0.287513
C	-2.416926	-2.327056	-0.421974	C	-2.482858	2.424451	-0.113293
N	-1.734563	-1.196279	-0.262557	C	-4.576520	3.607656	0.008039
N	-5.157078	-0.111552	0.221764	C	-3.886766	4.764242	0.252711
H	-5.048478	0.654783	0.884104	C	-2.469302	4.731812	0.357114
C	-5.896749	0.395137	-0.974157	C	-1.783612	3.567823	0.167757
C	-5.048359	1.364605	-1.810173	C	-3.024133	0.363904	-0.405030
H	-5.624091	1.723320	-2.681170	C	-4.235060	1.058387	-0.324522
H	-4.743443	2.235903	-1.208111	H	-5.662861	3.571716	-0.078265
H	-4.133	0.874839	-2.186954	H	-4.417963	5.711802	0.371813
C	-6.338014	-0.779884	-1.850982	H	-1.901920	5.638040	0.574902
H	-6.897794	-0.403891	-2.724020	H	-0.700310	3.485031	0.194837
H	-5.472928	-1.346857	-2.236934	N	-3.858336	2.399338	-0.145461
H	-6.997271	-1.467595	-1.294653	N	-1.963458	1.192562	-0.318260
C	-7.127064	1.117943	-0.421097	N	-5.554260	0.591738	-0.441987
H	-7.729149	0.437783	0.205553	H	-5.632371	-0.099765	-1.183209
H	-6.828289	1.986220	0.193976	C	-6.316866	0.147878	0.745289
H	-7.759363	1.492128	-1.243742	C	-5.682566	-1.077014	1.423223
C	-2.075921	1.145350	0.060258	H	-6.307838	-1.430067	2.262198
C	-0.731864	1.218299	-0.355465	H	-5.575689	-1.909445	0.703804
C	-0.171466	2.499552	-0.355145	H	-4.680585	-0.841563	1.818637

C	-2.245283	3.358219	0.470513	C	-6.416268	1.292202	1.756582
C	-0.929921	3.592394	0.063745	H	-6.987973	0.965513	2.642009
H	0.870383	2.648584	-0.651342	H	-5.418090	1.612427	2.102130
H	-0.510497	4.600246	0.084041	H	-6.930604	2.163233	1.317275
N	-2.816880	2.176643	0.474751	C	-7.716560	-0.210359	0.235913
Br	-3.313623	4.826538	1.055152	H	-8.179016	0.657916	-0.262855
H	2.489805	-1.209315	-2.611257	H	-7.670285	-1.040799	-0.492678
C	2.567265	-0.128564	-2.401989	H	-8.367285	-0.531328	1.066899
O	1.889338	0.389443	-1.501366	C	-2.936765	-1.113486	-0.482432
N	3.438405	0.571172	-3.126535	C	-3.323615	-1.799761	-1.632420
C	4.256491	-0.065114	-4.134563	C	-3.386657	-3.190427	-1.581223
H	4.048925	0.367325	-5.129171	H	-3.532311	-1.245773	-2.547936
H	5.327149	0.078494	-3.903689	C	-2.670387	-3.049684	0.677666
H	4.041210	-1.143565	-4.166489	C	-3.062761	-3.847504	-0.398411
H	4.612709	2.274093	-2.764113	H	-3.687259	-3.763416	-2.462826
C	3.562759	2.006649	-2.971148	H	-3.114469	-4.933978	-0.307299
H	2.932364	2.331682	-2.132892	N	-2.607707	-1.742352	0.650607
H	3.233745	2.516229	-3.894205	Br	-2.213814	-3.896817	2.325172

I-5 (conf3)

E(scf) = -8096.22673006 a.u.

Ir	-0.324539	-0.668287	0.344082
Cl	-0.389128	1.518850	1.232487
Cl	-1.921168	-1.508884	2.093220
C	1.781027	-0.843568	2.659513
C	3.655388	-0.636165	4.147532
C	2.868650	-1.123885	5.157474
C	1.503986	-1.442043	4.909473
C	0.970714	-1.302950	3.660634
C	2.515654	-0.163454	0.748024
C	3.582835	0.015533	1.624715
H	4.705093	-0.379804	4.293202
H	3.286041	-1.268184	6.157254
H	0.857496	-1.800654	5.712237
H	-0.069268	-1.508107	3.376362
N	3.096428	-0.460157	2.859289
N	1.447039	-0.697953	1.373582
N	4.847453	0.552963	1.348699
H	5.049944	0.384753	0.364195
C	5.053252	2.004983	1.607007
C	3.974141	2.870240	0.935347
H	4.152358	3.940486	1.140311

Product (conf1)

E(scf) = -7848.00855402 a.u.

N	4.138188	1.729892	-1.202382
C	5.02321	2.358904	-2.039429
C	4.564994	2.927251	-3.188701
C	3.177659	2.864089	-3.516014
C	2.291462	2.237971	-2.682363
C	3.107986	0.707807	0.436807
C	4.362771	1.096195	0.021851
H	6.067306	2.365000	-1.724774
H	5.272191	3.426482	-3.853719
H	2.822933	3.318448	-4.444074
H	1.22684	2.127822	-2.895428
C	2.787395	1.658520	-1.489823
N	2.170404	1.018698	-0.502337
N	5.615987	0.811131	0.538463
H	6.259205	1.597280	0.514897
C	6.274743	-0.478404	0.157975
C	6.12954	-0.781168	-1.340810
H	6.641677	-1.727742	-1.583349
H	5.066867	-0.906824	-1.614829
H	6.578251	0.010638	-1.965834
C	7.749022	-0.323816	0.535377

H	3.982353	2.720579	-0.157364	H	8.296381	-1.258387	0.331036
H	2.963902	2.617888	1.303825	H	8.231748	0.481251	-0.049983
C	5.062458	2.271289	3.113992	H	7.857304	-0.089705	1.608981
H	5.289918	3.333487	3.308480	C	5.646757	-1.630820	0.948810
H	4.080236	2.056657	3.568687	H	5.754321	-1.470925	2.034653
H	5.829067	1.654973	3.614766	H	4.578324	-1.754414	0.698018
C	6.427074	2.337136	1.017608	H	6.151664	-2.577347	0.690124
H	7.207205	1.704989	1.475366	C	2.627048	0.083922	1.663829
H	6.435973	2.165672	-0.074294	C	3.419611	0.013395	2.804309
H	6.680251	3.396369	1.193522	C	2.880879	-0.523538	3.964120
C	2.301085	0.134815	-0.660223	H	4.443259	0.385383	2.748906
C	0.968545	-0.027891	-1.097863	C	0.818915	-0.818249	2.773425
C	0.776377	0.213236	-2.464403	C	1.558781	-0.943938	3.950807
C	3.102070	0.724541	-2.691206	H	3.476457	-0.601806	4.877110
C	1.842506	0.599808	-3.278136	H	1.081809	-1.357981	4.839681
H	-0.206770	0.100973	-2.926014	N	1.331563	-0.335712	1.635707
H	1.699778	0.798638	-4.342257	Br	-0.981991	-1.337308	2.876141
N	3.339838	0.488086	-1.422305	Ir	0.483875	-0.172595	-0.345184
Br	4.589152	1.248746	-3.758921	Cl	2.154538	-2.007199	-0.910265
O	0.120837	-2.711739	-0.169349	Cl	-0.2181	0.090763	-2.606670
C	1.087624	-3.130174	-0.810643	N	-2.973363	-2.640791	-0.541857
H	1.728395	-2.453110	-1.404240	C	-3.631754	-3.828758	-0.716796
N	1.431539	-4.418491	-0.841483	C	-2.907752	-4.962615	-0.932490
C	2.548557	-4.882361	-1.637025	C	-1.481855	-4.905836	-0.976321
H	3.300435	-5.372800	-0.994557	C	-0.820216	-3.724758	-0.769827
H	2.207539	-5.606963	-2.397188	C	-2.384868	-0.573907	-0.121096
H	3.025224	-4.032217	-2.148414	C	-3.489109	-1.365393	-0.325206
C	0.680845	-5.402663	-0.083732	H	-4.718389	-3.771298	-0.653934
H	-0.011697	-4.878622	0.589681	H	-3.431184	-5.910932	-1.068866
H	0.103184	-6.054898	-0.762036	H	-0.91492	-5.818893	-1.174590
H	1.375608	-6.023311	0.507128	H	0.268023	-3.614704	-0.797497
C	-2.388735	3.862866	-0.851436	C	-1.590511	-2.563802	-0.522374
C	-3.479733	4.397027	1.229107	N	-1.239195	-1.314481	-0.244387
C	-3.197244	5.717315	1.009681	N	-4.854983	-1.102779	-0.344858
C	-2.504174	6.115111	-0.176752	H	-5.06045	-0.400700	0.364904
C	-2.104795	5.181654	-1.085147	C	-5.458369	-0.658908	-1.637513
C	-2.478801	1.763773	-1.033179	C	-4.81234	0.633470	-2.160058
C	-3.172263	2.044547	0.167849	H	-5.299895	0.951893	-3.098094
H	-3.984975	4.038844	2.127783	H	-4.90882	1.444713	-1.420043
H	-3.486241	6.474563	1.742735	H	-3.73719	0.489272	-2.367462
H	-2.278416	7.167172	-0.361967	C	-5.304498	-1.761822	-2.687670
H	-1.558441	5.384123	-2.007170	H	-5.755633	-1.434235	-3.639536
N	-3.082614	3.436897	0.265224	H	-4.241531	-1.983991	-2.887231

N	-2.027624	2.863680	-1.648380
N	-3.747251	1.214858	1.131507
H	-3.111147	0.486309	1.464540
C	-5.126242	0.724167	1.004153
C	-5.489763	0.115711	2.363484
H	-6.508774	-0.309604	2.347694
H	-4.778714	-0.687634	2.623456
H	-5.435688	0.886317	3.150994
C	-6.068912	1.887591	0.685047
H	-7.112267	1.529973	0.637577
H	-6.005529	2.668002	1.462551
H	-5.823808	2.351077	-0.286692
C	-5.257689	-0.357378	-0.083879
H	-4.994021	0.048236	-1.077723
H	-4.584570	-1.200652	0.145447
H	-6.290983	-0.744452	-0.143602
C	-2.410666	0.479924	-1.735706
C	-2.816187	0.485626	-3.077252
C	-2.985179	-0.711698	-3.746282
H	-3.004382	1.451325	-3.547408
C	-2.457039	-1.816315	-1.688039
C	-2.866383	-1.889657	-3.014610
H	-3.281666	-0.737292	-4.798316
H	-3.121752	-2.858508	-3.444688
N	-2.078664	-0.667407	-1.088428
Br	-2.656821	-3.419946	-0.715042
H	-5.810954	-2.690360	-2.374294
C	-6.941159	-0.421233	-1.342801
H	-7.411501	-1.339208	-0.950814
H	-7.067738	0.380636	-0.592844
H	-7.474543	-0.111826	-2.257526
C	-2.191031	0.831025	0.212070
C	-0.843758	1.252854	0.185751
C	-0.629395	2.588204	0.539455
C	-2.982931	2.843128	0.869030
C	-1.706508	3.407181	0.884928
H	0.383679	3.003847	0.544167
H	-1.563535	4.454979	1.157557
N	-3.231740	1.593284	0.553318
Br	-4.486756	3.923492	1.327704

Product (conf2)

E(scf) = -7847.99950224 a.u.

N	4.583435	1.198458	-0.694362
C	5.682463	1.695965	-1.344805
C	5.50756	2.461466	-2.457650
C	4.193346	2.734576	-2.942537
C	3.09444	2.247329	-2.288491
C	3.142666	0.268822	0.667736
C	4.499478	0.402765	0.449679
H	6.654472	1.440151	-0.921975
H	6.384792	2.854091	-2.975324
H	4.068989	3.330819	-3.849585
H	2.068155	2.386485	-2.632530
C	3.296051	1.466591	-1.124446
N	2.425907	0.899125	-0.301419

Product (conf3)

E(scf) = -7847.99872279 a.u.

N	2.727435	2.341078	1.658592
C	2.933067	3.522266	2.323773
C	1.871794	4.328807	2.600730
C	0.556485	3.938051	2.211093
C	0.349183	2.754527	1.556663
C	2.862257	0.355473	0.727976
C	3.638611	1.346450	1.297229
H	3.963879	3.748452	2.594974
H	2.04105	5.270461	3.126090
H	-0.291449	4.585903	2.444797
H	-0.641899	2.417874	1.254805
C	1.465216	1.929849	1.270258
N	1.554145	0.741879	0.681066

N	5.589176	-0.194415	1.066012	N	5.014561	1.456064	1.416199
H	6.36647	0.441518	1.221751	H	5.341531	1.698426	2.348370
C	6.043582	-1.541390	0.602002	C	5.82285	2.100887	0.344071
C	6.114603	-1.633629	-0.929510	C	5.626788	3.625741	0.322187
H	6.460579	-2.636755	-1.231706	H	6.267994	4.088064	-0.447792
H	5.117495	-1.481771	-1.379454	H	4.581577	3.888450	0.084429
H	6.820176	-0.896351	-1.350981	H	5.896693	4.077905	1.294360
C	7.428723	-1.749469	1.217201	C	7.284206	1.772124	0.661181
H	7.815035	-2.750570	0.965470	H	7.955003	2.217802	-0.092198
H	8.153768	-1.006169	0.835216	H	7.579265	2.171510	1.649436
H	7.384878	-1.662046	2.316956	H	7.444889	0.680761	0.667874
C	5.075688	-2.613766	1.112160	C	5.43487	1.526132	-1.020800
H	5.019869	-2.606686	2.213419	H	5.640392	0.445285	-1.079565
H	4.064313	-2.471694	0.692482	H	4.366654	1.675824	-1.255541
H	5.42368	-3.610907	0.792105	H	6.024865	2.024895	-1.807863
C	2.399241	-0.415365	1.724937	C	3.219106	-0.984483	0.249310
C	3.014359	-0.729006	2.933186	C	4.500015	-1.505993	0.421555
C	2.26596	-1.319578	3.939784	C	4.759802	-2.798330	-0.018532
H	4.075779	-0.506033	3.047730	H	5.262476	-0.887549	0.896457
C	0.364547	-1.185083	2.483578	C	2.466901	-2.949685	-0.682672
C	0.916563	-1.545961	3.714468	C	3.73153	-3.538099	-0.583951
H	2.721468	-1.586918	4.896575	H	5.75687	-3.233524	0.089633
H	0.27512	-1.988236	4.477432	H	3.882667	-4.560167	-0.933576
N	1.078684	-0.653297	1.482755	N	2.211156	-1.703561	-0.297020
Br	-1.484936	-1.455648	2.314504	Br	1.069862	-4.022149	-1.330911
Ir	0.517937	-0.173962	-0.572528	Ir	0.362913	-0.259559	-0.701139
Cl	1.968549	-2.000456	-1.201915	Cl	1.851791	0.677708	-2.339505
Cl	0.23891	0.527846	-2.819897	Cl	-0.891496	-1.439287	-2.347985
N	-2.122642	3.048629	0.301553	N	-2.490872	-1.994594	1.962490
C	-2.390223	4.369802	0.538842	C	-2.925367	-2.911179	2.881287
C	-1.361134	5.223911	0.805120	C	-2.062354	-3.866122	3.329828
C	-0.017369	4.744744	0.827498	C	-0.71855	-3.899698	2.851308
C	0.254863	3.430239	0.553631	C	-0.27778	-2.965244	1.952318
C	-2.165613	0.927135	-0.256097	C	-2.230832	-0.291225	0.611794
C	-2.989111	2.000799	0.000667	C	-3.176344	-0.938102	1.371266
H	-3.44087	4.651321	0.474763	H	-3.959647	-2.791262	3.203527
H	-1.578194	6.278013	0.987388	H	-2.409329	-4.595125	4.064414
H	0.797204	5.438215	1.050637	H	-0.036126	-4.672412	3.213470
H	1.26386	3.015746	0.531537	H	0.744835	-2.940052	1.576583
C	-0.824086	2.563678	0.263500	C	-1.183129	-1.977660	1.500487
N	-0.855506	1.282582	-0.074921	N	-1.028167	-0.942766	0.685190
N	-4.366073	2.169993	-0.095117	N	-4.527963	-0.703374	1.596905
H	-4.702366	1.581762	-0.856723	H	-4.677382	0.304958	1.619121

C	-5.216988	1.922069	1.103467
C	-4.945687	0.548951	1.734499
H	-5.629808	0.373175	2.583133
H	-5.081815	-0.252688	0.990804
H	-3.909876	0.488886	2.113129
C	-4.981107	3.019056	2.144984
H	-5.618836	2.843447	3.028128
H	-3.932985	3.028136	2.493743
H	-5.229185	4.014193	1.737616
C	-6.662032	1.986659	0.602094
H	-6.858493	2.955486	0.111686
H	-6.858335	1.179904	-0.127049
H	-7.370678	1.863512	1.438236
C	-2.383012	-0.439005	-0.713313
C	-1.203038	-1.195389	-0.872821
C	-1.391492	-2.510884	-1.310666
C	-3.753091	-2.126205	-1.324467
C	-2.680041	-2.996033	-1.532073
H	-0.523464	-3.154114	-1.479340
H	-2.852559	-4.021904	-1.864476
N	-3.623787	-0.879549	-0.937311
Br	-5.535111	-2.752524	-1.601321

C	-5.503802	-1.302347	0.635389
C	-5.219538	-0.878681	-0.813396
H	-5.970255	-1.316741	-1.494198
H	-5.257064	0.218471	-0.912909
H	-4.222156	-1.214314	-1.149222
C	-5.458263	-2.828792	0.740189
H	-6.18626	-3.272602	0.040209
H	-4.463142	-3.224389	0.470803
H	-5.714075	-3.168804	1.758459
C	-6.878989	-0.792276	1.072185
H	-7.079315	-1.064056	2.122790
H	-6.936386	0.307488	0.979865
H	-7.671572	-1.222124	0.436843
C	-2.239005	0.917911	-0.197345
C	-1.050269	1.139014	-0.921044
C	-1.019990	2.310075	-1.689234
C	-3.215172	2.834356	-0.887998
C	-2.112624	3.175487	-1.676926
H	-0.138141	2.535621	-2.294703
H	-2.115711	4.094454	-2.267096
N	-3.289861	1.743928	-0.162492
Br	-4.725493	3.998647	-0.839238

Product (conf4)

E(scf) = -7847.99407638 a.u.

N	2.293596	1.201571	2.717383
C	2.372897	1.956670	3.860410
C	1.354706	1.912508	4.763163
C	0.221344	1.076372	4.529687
C	0.145573	0.312106	3.398282
C	2.62892	0.103029	0.847294
C	3.208958	1.047324	1.673676
H	3.274042	2.557795	3.979180
H	1.423049	2.515212	5.670690
H	-0.580721	1.038386	5.270169
H	-0.682676	-0.363829	3.188815
C	1.210018	0.376238	2.467200
N	1.40994	-0.262170	1.323280
N	4.380868	1.769483	1.529104
H	5.017174	1.715973	2.320648
C	4.399848	3.096463	0.861764
C	3.874488	4.207361	1.786270

$TS_{I\text{-}1 \rightarrow I\text{-}4}$

E(scf) = -5641.38166250 a.u.

ν_{min} = -890.0 cm^{-1}

Ir	-1.728509	-0.942753	0.193231
Cl	-3.573224	-1.256869	1.707437
Cl	-2.583769	-2.651072	-1.259555
Cl	3.611676	0.982822	-2.400088
N	0.169925	1.956745	2.712128
C	0.218699	2.816236	3.781594
C	-0.933108	3.126910	4.437550
C	-2.174952	2.550428	4.028835
C	-2.22303	1.660240	2.990935
C	0.586813	0.576184	1.072503
C	1.197636	1.481225	1.906114
H	1.210934	3.177677	4.049477
H	-0.890578	3.806193	5.291133
H	-3.089602	2.806998	4.568984
H	-3.12839	1.138780	2.672752
C	-1.016238	1.345351	2.320837

H	3.958035	5.193707	1.298273	N	-0.757637	0.504435	1.327694
H	2.810755	4.048954	2.033998	N	2.521757	1.865918	2.009468
H	4.456169	4.250216	2.725500	H	3.088397	1.074169	1.705422
C	5.861851	3.373448	0.499380	C	2.990964	3.097829	1.289099
H	5.964487	4.358835	0.014794	C	2.218535	3.326494	-0.014600
H	6.5014	3.375853	1.401297	H	2.575967	4.252955	-0.497468
H	6.244776	2.603323	-0.191323	H	2.407064	2.495436	-0.719646
C	3.541342	3.050178	-0.404205	H	1.133321	3.436787	0.167766
H	3.894534	2.275412	-1.104579	C	2.851835	4.317082	2.206711
H	2.481642	2.845471	-0.176240	H	3.326387	5.198317	1.741689
H	3.589764	4.024495	-0.918353	H	1.792265	4.574330	2.382013
C	3.105729	-0.605476	-0.338388	H	3.340249	4.132501	3.179487
C	4.405318	-0.457220	-0.806179	C	4.466685	2.847739	0.961946
C	4.825186	-1.242570	-1.873877	H	5.030992	2.594123	1.877423
H	5.0621	0.256849	-0.307626	H	4.563523	2.033737	0.219967
C	2.657348	-2.288510	-1.858787	H	4.91625	3.751174	0.517607
C	3.947667	-2.177379	-2.394934	C	1.108151	-0.296809	0.033604
H	5.836353	-1.146396	-2.277516	C	0.155045	-0.739937	-0.918695
H	4.241174	-2.847629	-3.203467	C	0.648297	-1.651072	-1.876741
N	2.212177	-1.479375	-0.887608	H	-0.458836	0.279165	-1.472682
Br	1.600068	-3.668315	-2.526480	C	2.778647	-1.547181	-0.811044
Ir	0.238257	-1.292907	-0.018833	C	1.97371	-2.053184	-1.841625
Cl	0.713307	-3.397693	1.228080	H	-0.029821	-2.042176	-2.640927
Cl	-1.226321	-2.279571	-1.650932	H	2.390476	-2.737373	-2.582040
N	-3.638639	-0.724323	1.590321	N	2.368198	-0.714223	0.120361
C	-4.722006	-1.086035	2.346377	Br	4.547511	-2.188763	-0.642209
C	-4.671283	-2.241151	3.067420	O	-0.54303	-2.265491	1.301639
C	-3.502306	-3.059014	3.031202	H	-0.494425	-3.744395	-0.100389
C	-2.404728	-2.683317	2.302172	C	-0.033573	-3.278738	0.787627
C	-2.15649	0.307472	0.351676	N	1.074998	-3.834497	1.256464
C	-3.462954	0.385569	0.768524	C	1.803511	-3.243431	2.366088
H	-5.561102	-0.391325	2.319340	H	1.899542	-3.978022	3.183836
H	-5.5342	-2.529159	3.671269	H	2.807351	-2.935694	2.026458
H	-3.484356	-3.996112	3.593310	H	1.255579	-2.361792	2.723219
H	-1.474901	-3.258830	2.230999	C	1.676509	-4.976418	0.597681
C	-2.470937	-1.467460	1.582123	H	1.030587	-5.316812	-0.225290
N	-1.564994	-0.823429	0.850786	H	2.662287	-4.694666	0.186915
N	-4.49273	1.278199	0.493278	H	1.808067	-5.805201	1.314159
H	-4.095244	2.211736	0.398468	O	-2.872711	0.429951	-0.846654
C	-5.341745	1.001379	-0.707609	C	-4.060239	0.191024	-1.131617
C	-4.507111	0.916608	-1.994518	H	-4.60194	-0.644047	-0.660483
H	-5.162617	0.720985	-2.861087	N	-4.728905	0.941104	-2.001104
H	-3.966725	1.860644	-2.172119	C	-6.132006	0.709008	-2.270182

H	-3.76391	0.100862	-1.941865
C	-6.107306	-0.310134	-0.515177
H	-6.743233	-0.500550	-1.396122
H	-5.421953	-1.169830	-0.416506
H	-6.761648	-0.268583	0.372078
C	-6.326121	2.169899	-0.792861
H	-6.912167	2.251594	0.138607
H	-5.791202	3.123814	-0.951733
H	-7.021739	2.031579	-1.637704
C	-1.331236	1.114413	-0.536164
C	-0.122674	0.493934	-0.919665
C	0.653214	1.232083	-1.820588
C	-0.971474	2.983263	-1.754275
C	0.235922	2.492817	-2.252407
H	1.593784	0.827933	-2.210336
H	0.827438	3.079638	-2.958387
N	-1.743896	2.324108	-0.922213
Br	-1.575748	4.706505	-2.305693

$TS_{I\text{-}3 \rightarrow Products}$

E(scf) = -8556.89565370 a.u.

ν_{min} = -556.8 cm^{-1}

Ir	0.074918	-0.515632	-1.113378
Cl	0.729097	-2.295219	-2.596447
Cl	-0.773131	0.737650	-2.954210
Cl	3.431339	2.465348	1.739322
N	3.888481	1.330408	-1.231951
C	4.690995	2.414431	-1.465689
C	4.268784	3.384824	-2.320034
C	2.986056	3.283493	-2.933040
C	2.152427	2.238274	-2.643199
C	2.878887	-0.383252	-0.329710
C	4.083808	0.284664	-0.335844
H	5.626505	2.440290	-0.911597
H	4.910079	4.248319	-2.504809
H	2.655955	4.062509	-3.624723
H	1.149723	2.126013	-3.058303
C	2.608017	1.251320	-1.735960
N	1.997267	0.200994	-1.188237
N	5.206361	0.119364	0.447961
H	5.294551	0.887689	1.120628
H	-6.731316	1.592653	-1.987689
H	-6.287343	0.504539	-3.343633
H	-6.485397	-0.157373	-1.691495
C	-4.066422	2.029853	-2.695877
H	-2.980653	1.941924	-2.538316
H	-4.291762	1.965478	-3.773855
H	-4.420589	3.004580	-2.314369
H	-1.140319	3.947309	-4.103283
H	-1.363735	3.689390	-2.340293
C	-0.645365	3.990325	-3.115727
H	-0.321428	5.027068	-2.929415
N	0.510369	3.118215	-3.071664
O	-0.650140	1.439545	-2.105351
C	1.761785	3.604435	-3.637625
H	2.033429	4.559336	-3.155821
H	1.644440	3.771927	-4.723105
H	2.561456	2.861735	-3.445932
C	0.426388	1.900417	-2.554765
H	1.386670	1.324996	-2.522401

I-6 (conf1)

E(scf) = -5144.85393469 a.u.

Ir	-1.869085	-0.455479	-0.418313
Cl	-2.137544	0.511044	-2.535975
Cl	-2.972475	-2.426847	-1.077779
Cl	-3.859045	0.498454	0.279533
N	-1.591341	-1.444690	1.686505
C	-2.902992	-1.761553	2.292054
H	-3.461423	-0.833768	2.450870
H	-3.454083	-2.406759	1.594508
H	-2.742074	-2.274677	3.256886
C	-0.787978	-2.672233	1.527093
H	-0.723373	-3.213003	2.488547
H	-1.272363	-3.306174	0.770825
H	0.228489	-2.419445	1.193241
C	-0.885361	-0.435542	2.415375
H	0.208160	-0.456134	2.209600
O	-1.397115	0.346848	3.156158
C	-0.611024	2.385875	0.408938
C	0.706244	4.282840	1.079975
C	-0.454669	4.979426	1.285845
C	-1.711637	4.361995	1.033654

C	6.437302	-0.548518	-0.005256
C	7.320984	0.360422	-0.878291
H	8.268508	-0.144459	-1.136264
H	6.813807	0.619385	-1.823472
H	7.571547	1.294151	-0.343673
C	7.210191	-0.934137	1.261408
H	8.162916	-1.429246	1.007732
H	7.442384	-0.037743	1.864017
H	6.616507	-1.621191	1.888534
C	6.072719	-1.804201	-0.804787
H	5.466128	-2.503948	-0.206215
H	5.498919	-1.551526	-1.713068
H	6.990194	-2.329199	-1.120103
C	2.377974	-1.431731	0.538753
C	3.197971	-2.038967	1.489295
C	2.666006	-3.011816	2.317817
H	4.230476	-1.698064	1.561875
C	0.5551	-2.652583	1.242506
C	1.323562	-3.335510	2.184318
H	3.285397	-3.510543	3.067843
H	0.851896	-4.093105	2.810605
N	1.049165	-1.716126	0.424140
Br	-1.266711	-3.105488	1.234167
N	-4.088891	-1.523182	-1.137272
C	-5.172624	-2.261707	-1.537754
C	-4.964623	-3.434282	-2.196917
C	-3.634989	-3.877043	-2.474106
C	-2.553616	-3.126932	-2.099946
C	-2.71667	0.010909	-0.402100
C	-4.054505	-0.305522	-0.472204
H	-6.143921	-1.822360	-1.310841
H	-5.82539	-4.019476	-2.526287
H	-3.483875	-4.818349	-3.008064
H	-1.516654	-3.390240	-2.322170
C	-2.788376	-1.907370	-1.419180
N	-1.955346	-0.986172	-0.952427
N	-5.208057	0.360507	-0.080745
H	-5.092963	1.354771	-0.278494
C	-5.670096	0.196615	1.326833
C	-5.923568	-1.284738	1.616141
H	-6.270209	-1.410213	2.655687
H	-6.698117	-1.697412	0.948261
H	-5.001801	-1.882259	1.500582
C	-1.780906	3.070247	0.602099
C	0.819702	0.854719	-0.063739
C	1.587072	1.959157	0.310572
H	1.691858	4.710066	1.266817
H	-0.421563	6.008952	1.650529
H	-2.643897	4.907606	1.188044
H	-2.698690	2.512521	0.404861
N	0.632783	2.948855	0.616565
N	-0.503934	1.110976	0.022748
N	2.979164	2.070577	0.404829
H	3.358136	1.180289	0.723605
C	3.740733	2.525242	-0.784769
C	3.449952	1.655072	-2.019249
H	4.051081	1.986359	-2.883678
H	3.695556	0.597168	-1.818919
H	2.385855	1.714102	-2.308973
C	3.395889	3.984451	-1.090573
H	3.978290	4.341016	-1.957142
H	2.326472	4.104249	-1.336957
H	3.632271	4.628469	-0.226308
C	5.219176	2.409508	-0.404476
H	5.432650	3.007163	0.497734
H	5.488651	1.358230	-0.194019
H	5.864214	2.764349	-1.225752
C	1.263836	-0.492017	-0.444998
C	0.543428	-1.258708	-1.369147
C	0.930862	-2.584040	-1.584014
H	-0.225034	-0.801821	-2.014341
C	2.729930	-2.198344	-0.073040
C	2.048058	-3.078332	-0.925114
H	0.354573	-3.211644	-2.268261
H	2.396834	-4.102518	-1.066161
N	2.348545	-0.965967	0.182792
Br	4.300152	-2.794412	0.796619

C	-4.644801	0.749412	2.329400
H	-5.019167	0.642036	3.362466
H	-3.682948	0.211027	2.259553
H	-4.449146	1.817800	2.137981
C	-6.979467	0.981787	1.431617
H	-6.809916	2.054747	1.229863
H	-7.715459	0.606087	0.700846
H	-7.408254	0.893636	2.444309
C	-2.034090	1.238399	-0.022067
C	-0.619344	1.165164	0.078315
C	0.044318	2.401215	0.266874
H	-0.295418	0.413830	1.039158
C	-2.082709	3.472522	0.303315
C	-0.688487	3.575231	0.369622
H	1.135316	2.442358	0.405912
H	-0.201101	4.538181	0.529951
N	-2.748876	2.354813	0.101651
Br	-3.128690	5.035993	0.531796
H	0.455232	-0.562967	5.793804
H	-0.210752	-1.309444	4.298524
C	0.711602	-1.033047	4.827695
H	1.308026	-1.941212	5.026499
N	1.471789	-0.113214	4.009186
O	-0.095817	-0.030813	2.376532
C	2.776246	0.308055	4.490499
H	3.444720	-0.568809	4.573301
H	2.676311	0.771602	5.487580
H	3.212157	1.040234	3.785482
C	1.005204	0.322981	2.841465
H	1.686151	1.025431	2.304090

I-6 (conf2)

E(scf) = -5144.87254315 a.u.

Ir	-1.882066	-0.028251	-0.511676
Cl	-2.633358	1.496671	-2.126062
Cl	-3.167344	-1.825156	-1.353173
Cl	-3.504902	0.509371	1.046804
C	-0.481946	2.556070	0.675833
C	0.922160	4.226917	1.678193
C	-0.199165	4.973783	1.922667
C	-1.480311	4.505784	1.508983
C	-1.613103	3.299040	0.889386

I-6 (conf3)

E(scf) = -5144.87168657 a.u.

Ir	-1.569966	-0.150244	-0.055374
Cl	-2.095634	-1.196526	2.053397
Cl	-1.044712	0.970145	-2.082757
Cl	-3.086656	-1.503537	-1.189637
C	0.387513	-2.550643	-0.435139
C	2.191279	-4.096206	-0.803409
C	1.266927	-5.096533	-0.938426
C	-0.121033	-4.812905	-0.790212
C	-0.550393	-3.543036	-0.543042

C	0.857978	1.011890	0.013918	C	1.340982	-0.648058	-0.110079
C	1.684911	1.982474	0.587651	C	2.392125	-1.549069	-0.298510
H	1.920242	4.548884	1.977081	H	3.262531	-4.265705	-0.913995
H	-0.116803	5.935514	2.434931	H	1.588438	-6.116467	-1.163007
H	-2.375997	5.104633	1.681556	H	-0.866022	-5.605212	-0.879214
H	-2.547574	2.856122	0.541595	H	-1.591292	-3.231268	-0.441133
N	0.788962	2.982218	1.016349	N	1.749228	-2.781614	-0.519982
N	-0.440910	1.354411	0.103114	N	0.143440	-1.258112	-0.219585
N	3.076538	1.964100	0.747470	N	3.769092	-1.296387	-0.306798
H	3.374002	1.004735	0.918376	H	3.924358	-0.360014	-0.678071
C	3.931973	2.550932	-0.312180	C	4.534731	-1.442634	0.955884
C	3.692611	1.883061	-1.676677	C	3.986086	-0.532413	2.067677
H	4.359793	2.308945	-2.446205	H	4.567995	-0.652829	2.998092
H	3.887052	0.797853	-1.617932	H	4.037589	0.527367	1.764142
H	2.651937	2.030132	-2.015781	H	2.932965	-0.774252	2.296870
C	3.667952	4.054307	-0.420104	C	4.502796	-2.899818	1.421842
H	4.330550	4.502544	-1.179937	H	5.104991	-3.017094	2.338862
H	2.626686	4.262910	-0.721377	H	3.475448	-3.229163	1.655157
H	3.861457	4.553644	0.544488	H	4.919841	-3.566743	0.648202
C	5.376639	2.310702	0.135197	C	5.973783	-1.040475	0.620843
H	5.556296	2.775782	1.119128	H	6.372579	-1.677940	-0.186104
H	5.586181	1.228865	0.221867	H	6.019226	0.011278	0.284209
H	6.088769	2.733866	-0.593357	H	6.624315	-1.139056	1.506412
C	1.165608	-0.268250	-0.632324	C	1.343843	0.782685	0.184744
C	0.322701	-0.747922	-1.648033	C	0.231500	1.353831	0.820476
C	0.504793	-2.051459	-2.106718	C	0.171442	2.740268	0.944198
H	-0.406502	-0.083128	-2.157979	H	-0.492528	0.727734	1.408851
C	2.369069	-2.194312	-0.632553	C	2.335922	2.811762	-0.045238
C	1.549680	-2.806431	-1.586769	C	1.243173	3.500514	0.495246
H	-0.179358	-2.466432	-2.850550	H	-0.702954	3.212358	1.397893
H	1.734407	-3.832408	-1.908730	H	1.250207	4.588720	0.572266
N	2.188076	-0.981711	-0.155907	N	2.387718	1.509806	-0.214539
Br	3.832562	-3.167980	0.079243	Br	3.867862	3.792568	-0.570663
O	-1.033364	-1.378963	0.905984	O	-3.168627	1.192724	0.202945
H	-2.778685	-2.355207	1.307083	H	-4.388675	-0.201586	1.061385
C	-1.690314	-2.272974	1.460121	C	-4.273003	0.800550	0.617242
N	-1.126036	-3.181960	2.251958	N	-5.361981	1.561114	0.565754
C	0.306627	-3.184983	2.483342	C	-5.324212	2.876732	-0.044628
H	0.752259	-2.301302	2.006667	H	-4.352359	3.011084	-0.538994
H	0.511949	-3.158012	3.567164	H	-6.130407	2.959574	-0.792892
H	0.761610	-4.096131	2.056247	H	-5.462342	3.661683	0.720002
C	-1.910875	-4.224844	2.878940	C	-6.625486	1.099716	1.101931
H	-2.972311	-4.104013	2.616203	H	-6.504592	0.094778	1.533024

H	-1.572269	-5.218932	2.537853
H	-1.809513	-4.173576	3.977022
H	-6.980294	1.783535	1.892782
H	-7.387374	1.054698	0.304465

Ir(V) complex

E(scf) = -4896.52858782 a.u.

Ir	1.884625	-1.226322	0.053217
Cl	3.780179	-0.396660	1.090761
Cl	1.126648	-0.964156	2.381514
Cl	2.431088	-1.602885	-2.124578
C	0.247461	2.952356	-0.641367
C	0.453976	4.337579	-0.859006
C	1.732580	4.821787	-0.924578
C	2.844791	3.941382	-0.769769
C	2.648073	2.606073	-0.583871
C	-0.317045	0.828661	-0.406024
C	-0.876729	2.109584	-0.533602
H	-0.419200	4.978738	-0.982243
H	1.909071	5.885526	-1.100407
H	3.866361	4.324120	-0.802321
H	3.428034	1.855717	-0.445309
N	1.362602	2.135130	-0.539089
N	1.024493	0.861841	-0.415234
N	-2.225797	2.470770	-0.560491
H	-2.761256	1.687694	-0.931929
C	-2.870118	2.911125	0.706392
C	-2.719534	1.856511	1.815876
H	-3.192121	2.204058	2.750909
H	-3.201128	0.909303	1.519250
H	-1.657000	1.645923	2.032951
C	-2.269580	4.239084	1.172054
H	-2.795828	4.594383	2.074170
H	-1.202446	4.134350	1.432746
H	-2.370677	5.009458	0.388461
C	-4.351504	3.106474	0.372171
H	-4.471162	3.854340	-0.429957
H	-4.805581	2.157871	0.032218
H	-4.909508	3.446930	1.260685
C	-0.917145	-0.481247	-0.231799
C	-0.076054	-1.552175	0.156758
C	-0.665932	-2.800141	0.407316
H	2.315880	-2.682196	0.414662
C	-2.743421	-1.836170	-0.263332

Dimethylformamide (DMF)

E(scf) = -248.237485716 a.u.

H	0.604683	1.819815	-0.000243
H	-0.953254	1.787743	-0.896979
C	-0.420075	1.421588	0.000031
H	-0.952570	1.787517	0.897562
N	-0.345701	-0.020544	-0.000267
O	1.943029	-0.094429	0.000070
C	-1.584684	-0.755860	0.000069
H	-2.189221	-0.518692	-0.895692
H	-2.188964	-0.518186	0.895874
H	-1.379324	-1.838543	0.000398
C	0.866519	-0.643177	-0.000048
H	0.763764	-1.755729	0.000082

C	-2.018811	-2.964034	0.152090
H	-0.066567	-3.630504	0.786049
H	-2.514416	-3.925122	0.298240
N	-2.223410	-0.643700	-0.449532
Br	-4.605268	-1.996292	-0.542061