Supporting Information for:

Cyclometalated Osmium-Amine Electronic Communication through the *para*-Oligophenylene Wire

Jun-Jian Shen, Jiang-Yang Shao, Zhong-Liang Gong, and Yu-Wu Zhong*

Beijing National Laboratory for Molecular Sciences, CAS Key Laboratory of Photochemistry, Institute of Chemistry, Chinese Academy of Sciences, Beijing 100190, China.

*Email: zhongyuwu@iccas.ac.cn

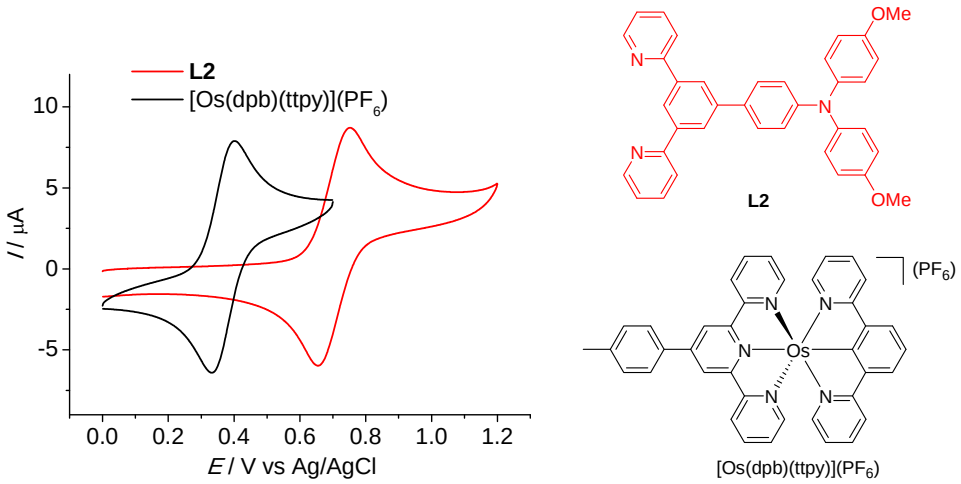

Figure S1. CVs (left) and chemical structures (right) of **L2** and [Os(dpb)(ttpy)](PF_6).

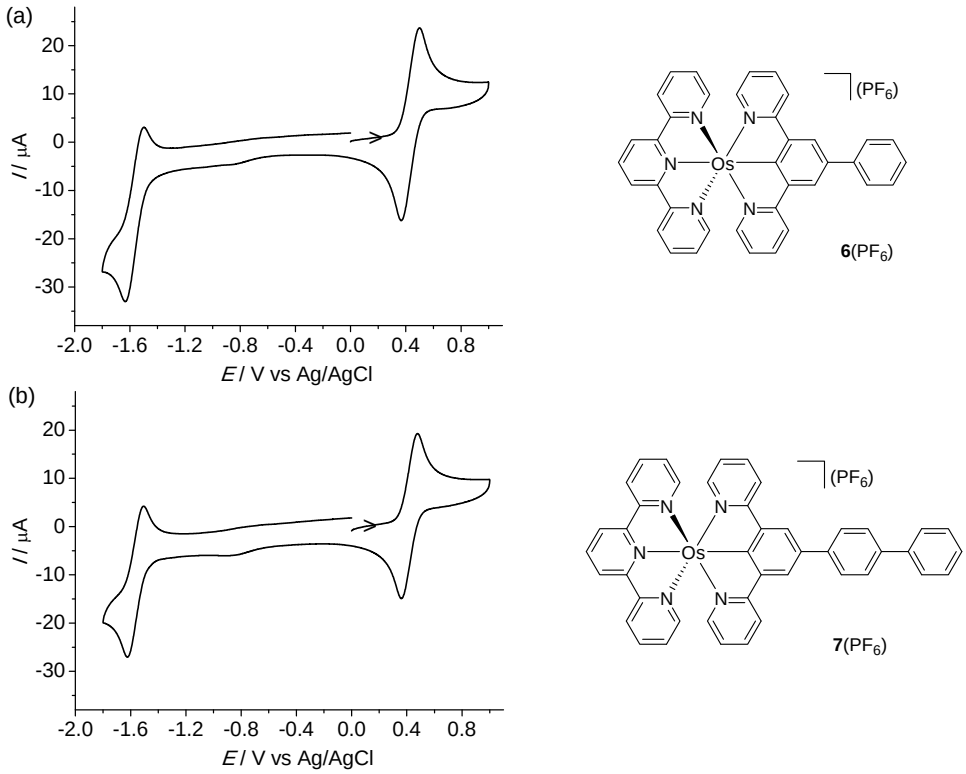

Figure S2. CVs of **6**(PF_6) (a) and **7**(PF_6) (b).

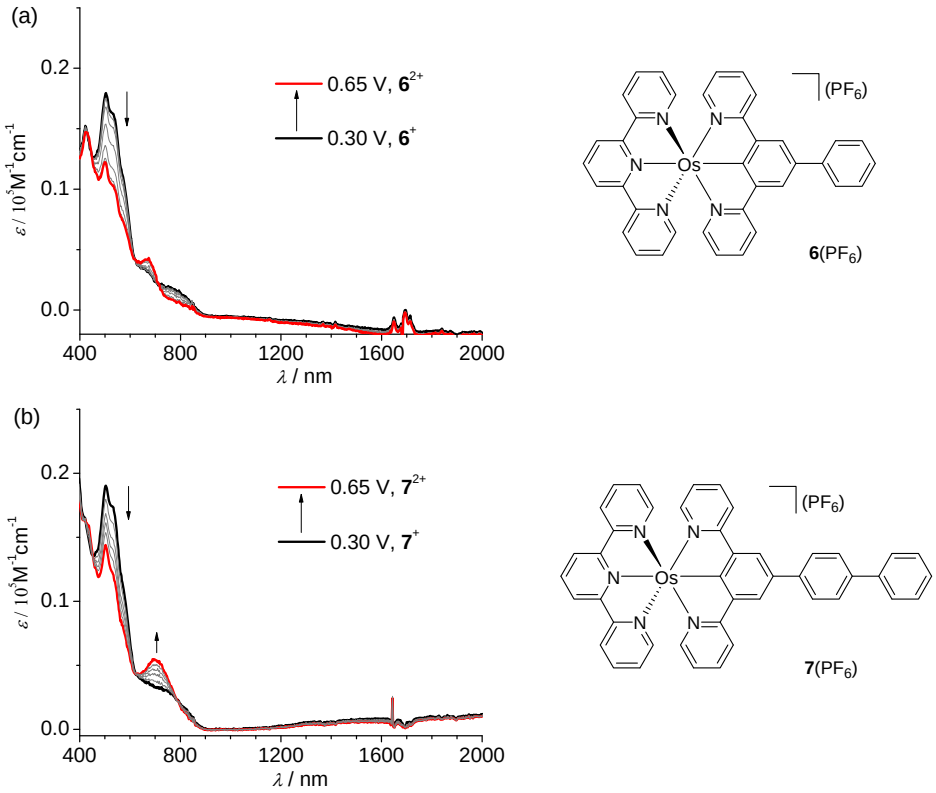

Figure S3. Absorption spectral changes of **6**(PF_6) (a) and **7**(PF_6) (b) in CH_2Cl_2 upon stepwise oxidative electrolysis at an ITO glass electrode. The applied potential was referenced versus Ag/AgCl.

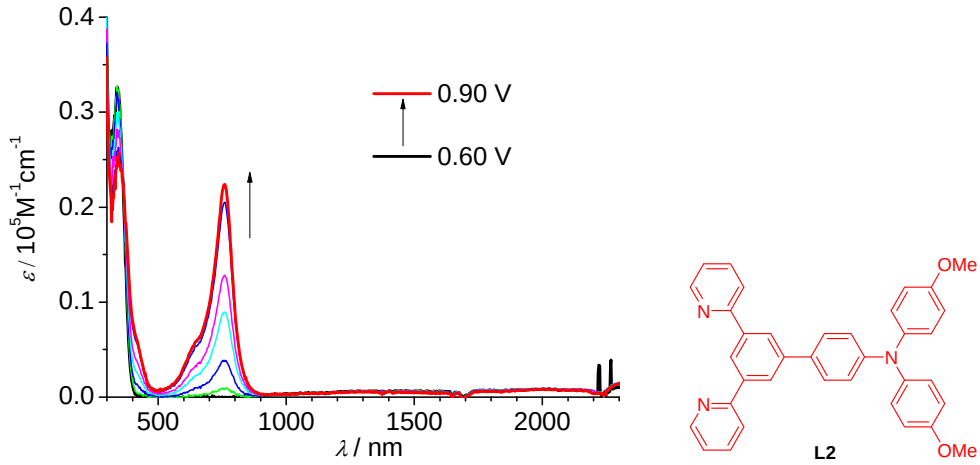

Figure S4. Absorption spectral changes of ligand **L2** upon oxidative electrolysis in 0.1 M Bu_4NClO_4/CH_2Cl_2 by stepwise electrolysis using an ITO glass electrode. The applied potential was referenced versus Ag/AgCl.

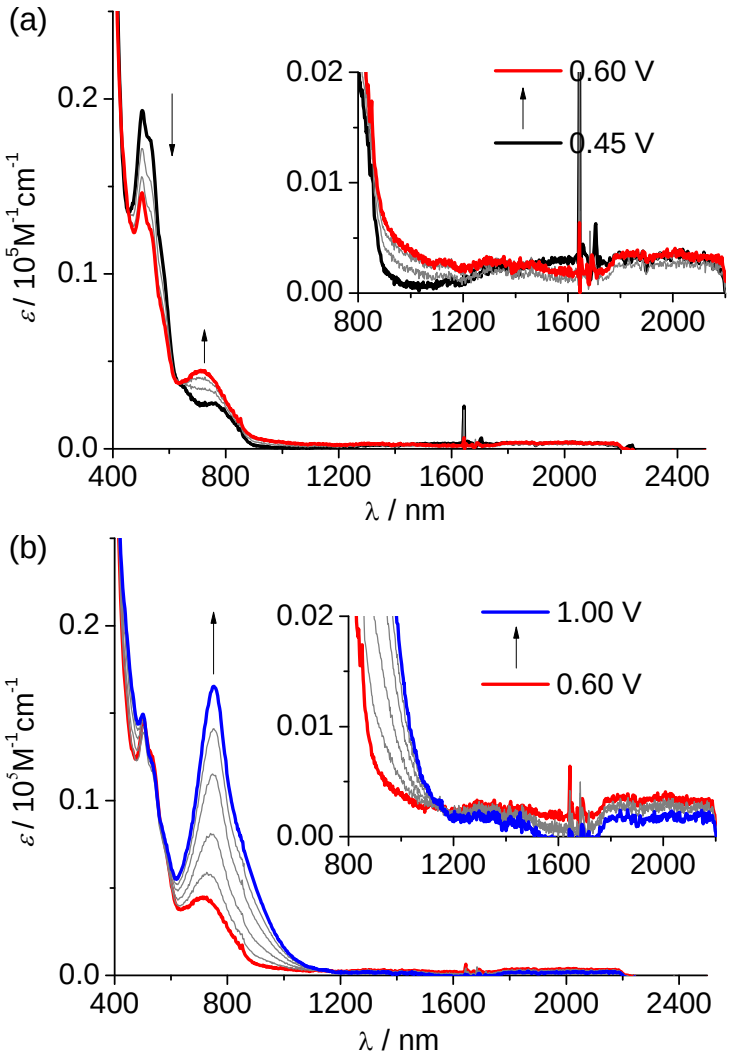

Figure S5. Absorption spectral changes of **5**(PF_6) upon single- (a) and double-oxidation (b) in CH_2Cl_2 by stepwise oxidative electrolysis at an ITO glass electrode. The applied potential was referenced versus Ag/AgCl.

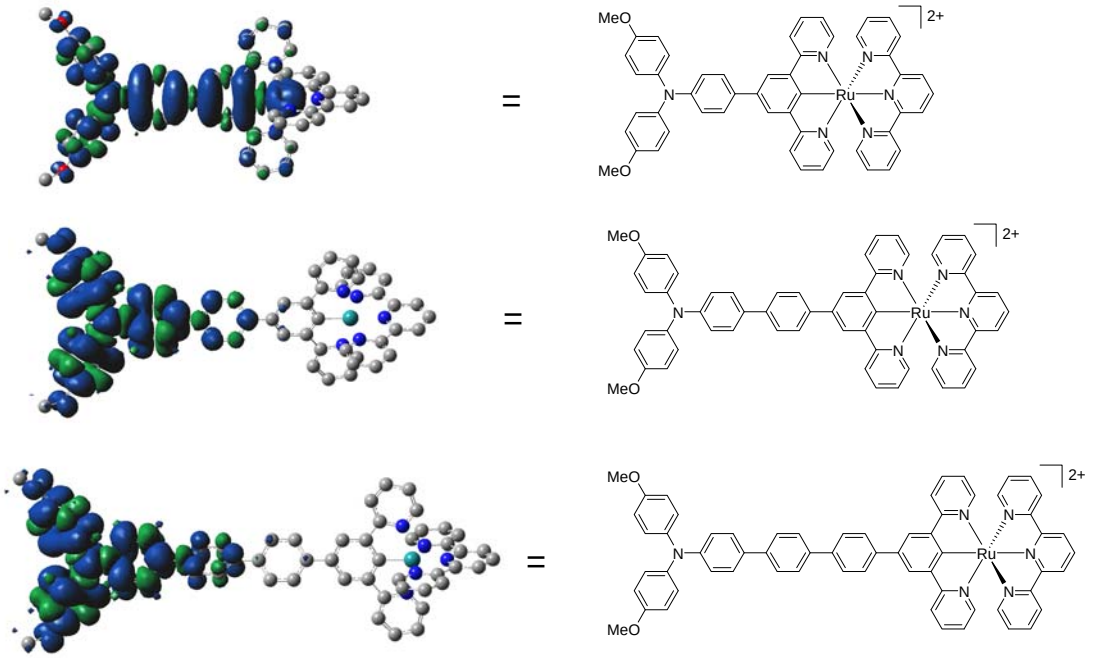

Figure S6. DFT-calculated spin density distributions of ruthenium-amine series compounds by using the UCAM-B3LYP functional.

Cartesian coordinates for the DFT-optimized structure of $\mathbf{1}^{2+}$ by UB3LYP:

Charge = 2 multiplicity = 2

O	12.15569635	-3.42553833	9.07137464
O	6.56799228	0.56434514	15.58686205
N	10.77187959	6.72921602	7.05563589
N	8.63001118	7.82312335	6.07008247
N	6.70773857	6.26568840	6.86625806
N	8.59336353	6.90350441	9.19592481
N	9.01112029	4.59544336	5.74182192
N	9.18430741	1.02186228	10.67507730
C	11.84472047	6.10744710	7.59406400
H	11.63406871	5.21089752	8.16253446
C	13.14179148	6.57776761	7.43600056
H	13.96258096	6.03559980	7.89183326
C	13.35646001	7.73888431	6.69359366
C	12.26008656	8.38759106	6.13462696
H	12.39977904	9.29096245	5.55301333
C	10.97443387	7.87605054	6.32056006
C	9.76286187	8.50004313	5.76207432
C	9.69128483	9.66148310	4.98931629
H	10.58506250	10.21737623	4.73289628
C	8.44133784	10.10033694	4.54890609
C	7.28677638	9.38778559	4.87798821
H	6.31845213	9.73200248	4.53502262
C	7.40724136	8.23204480	5.65303587
C	6.32103277	7.34615134	6.10482714
C	4.97583820	7.55957752	5.79852543
H	4.69131141	8.41527634	5.19804296
C	4.00620972	6.67670000	6.26286375
C	4.40695617	5.58491049	7.03281348
H	3.69036004	4.86813720	7.41767848
C	5.75679679	5.41414081	7.31118415
H	6.11016580	4.58061555	7.90402280
C	8.43317655	8.20267150	9.51716456
H	8.39106743	8.89668693	8.68599564
C	8.32660264	8.64604757	10.83027625
H	8.19982621	9.70422348	11.02919451
C	8.38681698	7.70914243	11.86237038
H	8.30780070	8.01951849	12.89922626
C	8.55036042	6.36431957	11.54288078
H	8.59891169	5.61678257	12.32676909
C	8.65338149	5.96687550	10.20810965
C	8.82586057	4.58188312	9.74233942
C	8.91633914	3.43977145	10.51953231
H	8.87857171	3.48110630	11.60230765
C	9.09688585	2.17302394	9.89454975
C	9.18625552	2.07615311	8.47657639
H	9.29685627	1.09373022	8.03169258
C	9.09449264	3.22076479	7.70300747
C	8.91190644	4.49018198	8.32318463
C	9.14244129	3.31282640	6.23529838
C	9.30590488	2.23509839	5.36217402
H	9.40908296	1.23362748	5.76473471
C	9.33575863	2.44666754	3.98677957
H	9.46160693	1.61016879	3.30703835
C	9.20145831	3.74740488	3.50044826
H	9.21845188	3.96225538	2.43791803

C	9.04262914	4.78801956	4.40816121
H	8.93594177	5.81266637	4.07235795
C	9.96158100	-0.09466844	10.24797427
C	11.26284532	0.08798225	9.76004538
H	11.68552437	1.08654761	9.71502234
C	12.02943910	-1.00099618	9.35079832
H	13.03532541	-0.83060638	8.98678428
C	11.49948730	-2.29810758	9.43578265
C	10.19555645	-2.48311297	9.93385259
H	9.79718912	-3.49101712	9.98808167
C	9.43573772	-1.39706322	10.33485051
H	8.42772603	-1.54794455	10.70672855
C	13.48433432	-3.31141400	8.55942417
H	13.50509780	-2.71163299	7.64225707
H	13.80309450	-4.32993108	8.33625901
H	14.15875532	-2.87119187	9.30276210
C	8.49478750	0.92850520	11.91986496
C	9.15440874	0.42658362	13.05700453
H	10.19683368	0.13348611	12.98993158
C	8.48117510	0.31944012	14.26239776
H	8.98223658	-0.05794466	15.14783136
C	7.13231494	0.71012350	14.36417510
C	6.46925728	1.20812287	13.23147216
H	5.42732288	1.50084945	13.27697415
C	7.14957384	1.30961806	12.01992804
H	6.62538092	1.67181278	11.14134088
C	5.20031112	0.93824396	15.76044558
H	4.54187521	0.33910478	15.12110506
H	5.05081149	2.00303753	15.54810347
H	4.97066979	0.73956543	16.80762819
H	2.95990458	6.83889192	6.02722176
H	8.36668914	10.99999721	3.94789672
H	14.35699576	8.13296202	6.55149502
Os	8.77332227	6.09535333	7.23433111

Cartesian coordinates for the DFT-optimized structure of $\mathbf{1}^{2+}$ by UCAM-B3LYP:

Charge = 2 multiplicity = 2

O	11.71286585	-3.58546793	8.89974504
O	6.99190940	0.69777254	15.76072953
N	10.75143339	6.81772145	7.14369214
N	8.62827653	7.83953631	6.05597572
N	6.72962836	6.21669330	6.76009330
N	8.47012524	6.90943305	9.17861590
N	9.13614678	4.63166293	5.74124146
N	9.19296015	1.06688170	10.65295589
C	11.80650175	6.23258296	7.73497940
H	11.59729211	5.32859592	8.29124587
C	13.08886148	6.74663050	7.64542319
H	13.90296009	6.23359120	8.14258120
C	13.29819167	7.91037002	6.91924019
C	12.21399470	8.52029024	6.30532160
H	12.35120713	9.42894457	5.73322152
C	10.94883392	7.96239121	6.42600873
C	9.74312673	8.54559576	5.80511337
C	9.67483773	9.69669318	5.02894253
H	10.56001591	10.28112383	4.81342282
C	8.43791248	10.08866620	4.52896101
C	7.29736474	9.34167557	4.80245836
H	6.33663800	9.65036964	4.41085484
C	7.42321743	8.19905748	5.58385965
C	6.34542123	7.27393870	5.98611707
C	5.01860348	7.44222431	5.61532305
H	4.73246663	8.28670585	5.00159366
C	4.06409750	6.52646398	6.03331042
C	4.46324632	5.45477215	6.81921828
H	3.75580590	4.71336502	7.16984562
C	5.79943075	5.33400369	7.16094544
H	6.15524249	4.51464861	7.77110506
C	8.24715011	8.19237905	9.49220115
H	8.22218544	8.88933375	8.66321133
C	8.05692714	8.62306609	10.79553646
H	7.88078261	9.67345468	10.99258709
C	8.09811284	7.68622625	11.81888826
H	7.95356617	7.98623075	12.85086211
C	8.32746509	6.35392902	11.50386709
H	8.36279492	5.60329353	12.28415074
C	8.51266152	5.97623627	10.18083083
C	8.76029139	4.59621942	9.72007895
C	8.85351797	3.46321602	10.49538273
H	8.75621323	3.50110794	11.57326551
C	9.10540825	2.20480850	9.88110875
C	9.26429197	2.12238251	8.46969920
H	9.43753328	1.15009842	8.02565012
C	9.16942890	3.26132752	7.70311039
C	8.91505414	4.51378124	8.31427376
C	9.28753058	3.36289568	6.23556239
C	9.53036901	2.29726631	5.37934164
H	9.64847121	1.30024803	5.78627260
C	9.61977531	2.51387539	4.01111569
H	9.80877948	1.68479275	3.33826739
C	9.46339406	3.80315906	3.52130371
H	9.52420362	4.02069555	2.46198337

C	9.22373112	4.83070957	4.41961258
H	9.09516544	5.85161207	4.08075876
C	9.86031378	-0.10673250	10.18013946
C	11.18914336	-0.05066750	9.77276283
H	11.72133136	0.89451075	9.80527601
C	11.84596552	-1.19380692	9.32766655
H	12.88030135	-1.12142499	9.01677656
C	11.16990682	-2.41418109	9.30607401
C	9.83644714	-2.47373277	9.72846434
H	9.32650056	-3.43047263	9.70505566
C	9.18764768	-1.33161111	10.15755068
H	8.15323925	-1.38182999	10.48046898
C	13.06363396	-3.58787497	8.46832943
H	13.20448041	-2.93799454	7.59789461
H	13.28895393	-4.61714762	8.19106288
H	13.73837469	-3.27204422	9.27117842
C	8.60557197	1.00170082	11.95561496
C	9.38315296	0.62860731	13.05531789
H	10.43710682	0.41132364	12.91832538
C	8.81267792	0.53385097	14.31049992
H	9.40410266	0.24560079	15.17252076
C	7.45378446	0.81631108	14.49403033
C	6.67345053	1.18910248	13.39909566
H	5.61828194	1.40326652	13.51070364
C	7.25278881	1.27036739	12.13666343
H	6.64073404	1.54328181	11.28315271
C	5.61801058	0.95141057	16.00311976
H	4.98085308	0.26063585	15.44049289
H	5.35208272	1.98263891	15.74679302
H	5.46696001	0.79423604	17.07060182
H	3.02592117	6.65072337	5.74769150
H	8.36223876	10.98282710	3.92131242
H	14.28934680	8.33986879	6.83003567
Os	8.77500579	6.10564498	7.23264224

Cartesian coordinates for the DFT-optimized structure of $\mathbf{2}^{2+}$ by UB3LYP:

Charge = 2 multiplicity = 2

N	0.48755158	-1.26615305	1.64741165
N	-0.41231245	1.61657294	1.17018673
N	-2.02444361	-0.03238163	-0.02760481
N	-0.43587833	-1.69361337	-1.23966965
N	0.47971231	1.18262220	-1.72602000
C	4.83288815	-0.05665675	-0.06018108
C	4.10785900	0.67265112	-1.04344029
H	4.66019064	1.19522439	-1.81769278
C	2.72000230	0.67889182	-1.04221793
C	2.72460566	-0.77747615	0.94246822
C	4.11244129	-0.78088248	0.93017216
H	4.66869252	-1.30747928	1.69887030
C	1.82423283	1.36295763	-1.98540003
C	2.23136183	2.14513373	-3.06975471
H	3.29024976	2.27882017	-3.26141519
C	1.28650594	2.74663157	-3.89499284
H	1.60270964	3.35366814	-4.73721348
C	-0.06918937	2.55670481	-3.62131314
H	-0.84213850	3.00526578	-4.23516763
C	-0.42667456	1.77162338	-2.53224838
H	-1.46656831	1.59800520	-2.28178092
C	1.83322183	-1.45550041	1.89413182
C	2.24528716	-2.24051793	2.97456980
H	3.30501122	-2.38113290	3.15641390
C	1.30421575	-2.83604626	3.80841505
H	1.62424665	-3.44532484	4.64756524
C	-0.05269449	-2.63727755	3.54731878
H	-0.82280943	-3.08101922	4.16819812
C	-0.41515176	-1.84948274	2.46186496
H	-1.45617339	-1.66888451	2.22119738
C	0.44609482	-2.52056257	-1.84477205
H	1.49152690	-2.29312633	-1.68099107
C	0.05026213	-3.59589616	-2.62914521
H	0.80444482	-4.22437826	-3.08929059
C	-1.31174131	-3.84114795	-2.80631153
H	-1.65430047	-4.67243920	-3.41312502
C	-2.22913207	-2.99727156	-2.18895599
H	-3.29262331	-3.16507923	-2.31103658
C	-1.78274508	-1.92861619	-1.40884978
C	-2.68650320	-0.99004159	-0.72324459
C	-4.08315745	-1.00411462	-0.73082898
H	-4.63033731	-1.76143792	-1.27934847
C	-4.77042717	-0.02116821	-0.01609152
C	-4.06921865	0.95611297	0.69283000
H	-4.60562555	1.71791588	1.24579070
C	-2.67283812	0.93060502	0.67354707
C	-1.75577499	1.86190133	1.35140016
C	-2.18690416	2.93361394	2.13584537
H	-3.24793659	3.10948843	2.26752494
C	-1.25758812	3.77018425	2.74527714
H	-1.58835981	4.60381386	3.35541385
C	0.10085718	3.51453633	2.55584264
H	0.86396012	4.13701721	3.00938283
C	0.48135929	2.43646169	1.76764661
H	1.52347107	2.20093244	1.59440695

C	6.29469287	-0.06210933	-0.06775325
C	7.03864025	-1.12538949	0.50423837
C	7.04057624	0.99537475	-0.64793675
C	8.41912452	-1.13825628	0.49929167
H	6.52107098	-1.98603867	0.91403881
C	8.42106750	0.99677114	-0.65953492
H	6.52529588	1.86036495	-1.05142884
C	9.14838501	-0.07400771	-0.08490664
H	8.95001238	-1.98890240	0.91074918
H	8.95404551	1.84303156	-1.07730278
C	11.27417453	-0.75129741	0.92731773
C	10.93666072	-0.57610805	2.28285873
C	12.35735395	-1.57577616	0.59291662
C	11.66017726	-1.22277730	3.27111112
H	10.11662803	0.08050685	2.55448755
C	13.09078213	-2.22445530	1.58300206
H	12.62061740	-1.72066399	-0.44962822
C	12.74440546	-2.05454997	2.93329935
H	11.41480576	-1.08670785	4.31935728
H	13.91717686	-2.86215168	1.29371298
C	11.26701195	0.58139384	-1.12663207
C	12.36700534	1.39007564	-0.80865220
C	10.90590907	0.41256934	-2.47695423
C	13.09390644	2.02940782	-1.80956757
H	12.64888002	1.52991367	0.22969694
C	11.62271733	1.05024112	-3.47581430
H	10.07280146	-0.23235257	-2.73645662
C	12.72387359	1.86613729	-3.15439445
H	13.93375270	2.65494578	-1.53270874
H	11.35896179	0.91884930	-4.52018458
N	10.54091261	-0.08052865	-0.09433667
O	13.38626835	-2.63711357	3.97405210
O	13.35738729	2.44073808	-4.20462506
C	14.50255924	-3.48680914	3.70402969
H	14.85573341	-3.82801072	4.67752180
H	14.20528815	-4.35093648	3.09887915
H	15.30349234	-2.93858406	3.19511538
C	14.49129036	3.27219407	-3.95174419
H	14.83412255	3.60902100	-4.93044092
H	14.21775822	4.14017136	-3.34091955
H	15.29139392	2.71050508	-3.45640473
H	-5.85493546	-0.01673510	-0.01162015
C	2.00929117	-0.04688702	-0.04645739
Os	0.05836401	-0.04013006	-0.03709385

Cartesian coordinates for the DFT-optimized structure of $\mathbf{2}^{2+}$ by UCAM-B3LYP:

Charge = 2 multiplicity = 2

N	0.49620809	-1.12441306	1.74893357
N	-0.39987828	1.70661228	1.01532709
N	-2.02286956	-0.02744228	-0.02257816
N	-0.44531219	-1.78630866	-1.08854931
N	0.48369448	1.02944892	-1.83559084
C	4.81862401	-0.06938908	-0.07165055
C	4.10505596	0.56579392	-1.11364068
H	4.66519615	1.01780227	-1.92466879
C	2.72111108	0.57585249	-1.10728829
C	2.72834552	-0.69692645	0.98921937
C	4.11227779	-0.69890381	0.97868084
H	4.67833034	-1.15501503	1.78327374
C	1.81809563	1.18020262	-2.10753881
C	2.23106716	1.85659530	-3.24670844
H	3.28934414	1.96798072	-3.44919290
C	1.28836768	2.38555155	-4.11862304
H	1.60651968	2.91488125	-5.00990181
C	-0.06003339	2.22684727	-3.83228859
H	-0.83059218	2.62232313	-4.48254200
C	-0.41808527	1.54272202	-2.68121848
H	-1.45839536	1.39517735	-2.41767186
C	1.83243800	-1.29140195	2.00168748
C	2.25353595	-1.97397393	3.13417538
H	3.31318127	-2.09837858	3.32128707
C	1.31716446	-2.49285326	4.01887031
H	1.64168921	-3.02710964	4.90489661
C	-0.03317817	-2.31783813	3.75192246
H	-0.79904602	-2.70501559	4.41262838
C	-0.39941406	-1.62800748	2.60684275
H	-1.44159501	-1.46772494	2.35862434
C	0.43607881	-2.65271187	-1.61500831
H	1.48173798	-2.41328228	-1.47517956
C	0.03974970	-3.78947223	-2.29885827
H	0.79212962	-4.45480932	-2.70400153
C	-1.31538637	-4.04712723	-2.44716365
H	-1.65918447	-4.92815110	-2.97659722
C	-2.23064018	-3.15605030	-1.90525908
H	-3.29329471	-3.33503837	-2.00709293
C	-1.78020444	-2.03100505	-1.23019326
C	-2.68085862	-1.03074797	-0.62470581
C	-4.07053720	-1.04516837	-0.62871525
H	-4.62165877	-1.84302332	-1.10945422
C	-4.74675189	-0.00684281	0.00215798
C	-4.04356384	1.02116129	0.62026970
H	-4.57368230	1.82712499	1.11097481
C	-2.65458282	0.98582480	0.59086783
C	-1.72809899	1.97263010	1.17923819
C	-2.14913812	3.10618857	1.85908174
H	-3.20695322	3.30244663	1.97820915
C	-1.21081158	3.98388897	2.38307888
H	-1.53151986	4.87152009	2.91595680
C	0.13733922	3.70442979	2.21234360
H	0.90704780	4.35861849	2.60281150
C	0.50389731	2.56006796	1.52460198
H	1.54306645	2.30384965	1.36741244

C	6.29021894	-0.07420517	-0.07944150
C	7.02281557	-1.13784272	0.46785846
C	7.02360421	0.98530339	-0.63359611
C	8.40496553	-1.15121037	0.45894909
H	6.50276721	-1.99926027	0.87472997
C	8.40584132	0.99128554	-0.63708018
H	6.50459282	1.84958896	-1.03566407
C	9.13264664	-0.08179077	-0.09208796
H	8.93238306	-2.00461440	0.86725005
H	8.93409568	1.84190624	-1.05005948
C	11.26373920	-0.87947069	0.82938719
C	11.04443915	-0.76142592	2.20601126
C	12.23947680	-1.76234964	0.37877053
C	11.77429328	-1.52200575	3.10136063
H	10.29365570	-0.06812567	2.57086050
C	12.99347294	-2.51755900	1.27311645
H	12.41987227	-1.85808767	-0.68692989
C	12.75825027	-2.40419714	2.64262594
H	11.60948922	-1.43750040	4.17014329
H	13.74863819	-3.19161318	0.88888268
C	11.26038448	0.70709483	-1.02885995
C	12.24204305	1.58629565	-0.58394350
C	11.03143611	0.59115676	-2.40408483
C	12.99242184	2.33997320	-1.48260809
H	12.42997527	1.68036883	0.48060100
C	11.75769637	1.35028386	-3.30359025
H	10.27594245	-0.09933988	-2.76450640
C	12.74756861	2.22882354	-2.85060553
H	13.75237842	3.01114840	-1.10281232
H	11.58540346	1.26742083	-4.37131960
N	10.52509534	-0.08536318	-0.09769894
O	13.42644455	-3.09716949	3.59968304
O	13.41153964	2.92065535	-3.81142182
C	14.43472528	-4.00294038	3.18786440
H	14.83593763	-4.44368338	4.10024149
H	14.02434531	-4.79562209	2.55250202
H	15.23871078	-3.48833937	2.65003897
C	14.42513246	3.82311916	-3.40540831
H	14.82142251	4.26376678	-4.31998004
H	14.02127042	4.61621888	-2.76640687
H	15.23127764	3.30565449	-2.87359940
H	-5.83037867	0.00126428	0.01210577
C	2.02986883	-0.05741791	-0.05473036
Os	0.08726316	-0.04442427	-0.04027416

Cartesian coordinates for the DFT-optimized structure of **3**$^{2+}$ by UB3LYP:

Charge = 2 multiplicity = 2

N	0.49471325	-1.36277422	1.56430799
N	-0.40454886	1.53713237	1.26317477
N	-2.01443959	-0.03895285	-0.02849834
N	-0.42937893	-1.62734282	-1.33562024
N	0.48644949	1.26663180	-1.64684919
C	4.84144782	-0.06320338	-0.06487133
C	4.12280454	0.71653933	-1.00058286
H	4.67842707	1.28590537	-1.74051366
C	2.72719582	0.72443998	-0.99780237
C	2.73202828	-0.83602711	0.89108987
C	4.12762300	-0.83796253	0.87863344
H	4.68727976	-1.41133263	1.61240957
C	1.83340655	1.46083029	-1.89559693
C	2.23799311	2.30660196	-2.93545809
H	3.29735560	2.44989993	-3.11847434
C	1.29507518	2.95478374	-3.72370165
H	1.61121080	3.60941467	-4.52977074
C	-0.06254605	2.74970789	-3.46105978
H	-0.83530601	3.23342335	-4.04814805
C	-0.41942741	1.90402365	-2.42035515
H	-1.45978626	1.71684988	-2.18075623
C	1.84290963	-1.56617208	1.79858306
C	2.25287014	-2.41456199	2.83420089
H	3.31313790	-2.56502880	3.00587501
C	1.31407430	-3.05622454	3.63262363
H	1.63437115	-3.71290510	4.43537599
C	-0.04485848	-2.84194860	3.38451478
H	-0.81454099	-3.32034431	3.97994461
C	-0.40713437	-1.99390456	2.34760013
H	-1.44871839	-1.79955361	2.11929074
C	0.45057598	-2.42116021	-1.98796821
H	1.49615880	-2.20233448	-1.81118236
C	0.05457506	-3.45045266	-2.83082879
H	0.80787378	-4.05321804	-3.32594965
C	-1.30863956	-3.68522050	-3.02135052
H	-1.65157336	-4.48163030	-3.67326495
C	-2.22479703	-2.87665314	-2.35803638
H	-3.28857831	-3.03713921	-2.48873336
C	-1.77823740	-1.85240810	-1.51874094
C	-2.68090640	-0.95518706	-0.78107474
C	-4.07739233	-0.96612128	-0.78826973
H	-4.62518048	-1.68886162	-1.38155531
C	-4.76540163	-0.02763438	-0.01597208
C	-4.06270048	0.90512182	0.75000887
H	-4.59907595	1.63244261	1.34811216
C	-2.66647707	0.88271468	0.73006976
C	-1.74979847	1.77254958	1.45936793
C	-2.18026694	2.79951763	2.30371911
H	-3.24146024	2.96818017	2.44476327
C	-1.25151212	3.60032820	2.95888997
H	-1.58200717	4.39881581	3.61467753
C	0.10794871	3.35503855	2.75519568
H	0.87065416	3.95142910	3.24358548
C	0.48779201	2.32341450	1.90775573
H	1.52986234	2.09642128	1.72078783

C	6.31946672	-0.06819687	-0.07286086
C	7.05390818	-1.20985388	0.31000349
C	7.05729570	1.06858338	-0.46363612
C	8.44220728	-1.21353821	0.30819519
H	6.52896609	-2.12143646	0.57856301
C	8.44551893	1.06307701	-0.47665820
H	6.53555244	1.98361734	-0.72663878
C	9.17780028	-0.07763813	-0.08811729
H	8.96226829	-2.12818845	0.57564707
H	8.96871499	1.97430284	-0.74961917
H	-5.84995252	-0.02315494	-0.01109825
C	2.01697619	-0.05330376	-0.04948096
C	10.65107149	-0.08233868	-0.09578293
C	11.38266274	0.72973767	-0.99096616
C	11.38678630	-0.89895665	0.79186037
C	12.76738075	0.72742283	-1.00751190
H	10.85657054	1.36296544	-1.69743797
C	12.77159453	-0.90486672	0.79442467
H	10.86409221	-1.52905678	1.50362816
C	13.48367364	-0.09073433	-0.11003689
H	13.30313757	1.36983705	-1.69741144
H	13.31050933	-1.55046321	1.47887780
C	15.60729068	-0.18303667	1.09981362
C	15.16027528	0.51698192	2.24248416
C	16.77406306	-0.96550375	1.18513770
C	15.86378331	0.43183846	3.42756431
H	14.27797848	1.14430067	2.18043494
C	17.48162495	-1.05473513	2.37629551
H	17.10999282	-1.52699951	0.32041854
C	17.03228759	-0.35487265	3.51142159
H	15.54161380	0.97916419	4.30700618
H	18.36615531	-1.67807858	2.41905678
C	15.59638888	-0.00911474	-1.33966164
C	16.76622277	0.76751799	-1.43566736
C	15.13506052	-0.70632434	-2.47835258
C	17.46297431	0.85375397	-2.63340471
H	17.11305290	1.32694755	-0.57391553
C	15.82774952	-0.62410356	-3.66998785
H	14.25025578	-1.32924652	-2.40819650
C	16.99936012	0.15675337	-3.76455200
H	18.35020792	1.47263683	-2.68422932
H	15.49453803	-1.16936003	-4.54659520
O	17.64117650	-0.37002765	4.71266320
O	17.59689098	0.16936812	-4.97150984
C	18.84258809	-1.13222474	4.87516325
H	19.14649257	-0.98140690	5.91081790
H	18.65832608	-2.19695772	4.69638142
H	19.62890796	-0.77180562	4.20342310
C	18.80066751	0.92535739	-5.14508949
H	19.09422494	0.77300952	-6.18350214
H	18.62355882	1.99101993	-4.96463799
H	19.59127097	0.56087774	-4.48061472
N	14.89353180	-0.09447007	-0.11665689
Os	0.04604372	-0.04655179	-0.03885337

Cartesian coordinates for the DFT-optimized structure of $\mathbf{3}^{2+}$ by UCAM-B3LYP:

Charge = 2 multiplicity = 2

N	0.50176793	-1.26037351	1.66289976
N	-0.40760587	1.61493295	1.14618535
N	-2.01803192	-0.03980908	-0.02961428
N	-0.42950016	-1.70561059	-1.21949235
N	0.49301271	1.16405736	-1.74563774
C	4.82297741	-0.06167754	-0.06202227
C	4.11624677	0.64882921	-1.05460481
H	4.68002997	1.16175697	-1.82613850
C	2.73024880	0.65780910	-1.04948145
C	2.73539860	-0.76783029	0.94575689
C	4.12144175	-0.76772745	0.93738884
H	4.68940252	-1.28443646	1.70331160
C	1.82785239	1.33683569	-2.00163812
C	2.24324863	2.10146173	-3.08226209
H	3.30192091	2.22983189	-3.27219520
C	1.30197639	2.69704952	-3.91203359
H	1.62185345	3.29548803	-4.75778484
C	-0.04682826	2.51553287	-3.64236775
H	-0.81611775	2.96092117	-4.26104518
C	-0.40719132	1.74230365	-2.54978178
H	-1.44786954	1.57403865	-2.30064011
C	1.83787032	-1.44132443	1.90638617
C	2.25868157	-2.20856100	2.98307043
H	3.31827973	-2.34325821	3.16322105
C	1.32158366	-2.79865533	3.82143304
H	1.64568790	-3.39913601	4.66412119
C	-0.02855745	-2.60906682	3.56427022
H	-0.79471111	-3.05001413	4.18998145
C	-0.39441286	-1.83339289	2.47525181
H	-1.43633221	-1.65871714	2.23587666
C	0.45858081	-2.52382325	-1.80798185
H	1.50257128	-2.29143522	-1.64551834
C	0.07013680	-3.60500608	-2.58077240
H	0.82724085	-4.23337889	-3.03328876
C	-1.28312722	-3.85531093	-2.75590159
H	-1.62046224	-4.69299326	-3.35519444
C	-2.20505605	-3.01331919	-2.15038023
H	-3.26651073	-3.18673289	-2.27276246
C	-1.76243143	-1.94398015	-1.38582436
C	-2.66928488	-0.99737574	-0.70821752
C	-4.05876467	-1.01761895	-0.71876648
H	-4.60386984	-1.78140188	-1.25807478
C	-4.74210501	-0.03018800	-0.01782434
C	-4.04579646	0.95237429	0.67715441
H	-4.58085236	1.71994956	1.22114141
C	-2.65663769	0.92228331	0.65459623
C	-1.73732737	1.86248634	1.32429425
C	-2.16575632	2.93475050	2.09281413
H	-3.22486119	3.11548653	2.22452883
C	-1.23273172	3.77025961	2.69028816
H	-1.55899351	4.61017951	3.29257720
C	0.11716854	3.51056781	2.50324402
H	0.88261540	4.13357716	2.94908259
C	0.49126060	2.42681980	1.72697651
H	1.53210881	2.18717013	1.55518780

C	6.30166758	-0.06633394	-0.06942080
C	7.02351663	-1.19861410	0.32724110
C	7.02645218	1.06141070	-0.47359840
C	8.40954080	-1.20350647	0.31487855
H	6.49645122	-2.10305419	0.61405088
C	8.41251970	1.05746995	-0.47600379
H	6.50211685	1.96918265	-0.75484185
C	9.13717391	-0.07536096	-0.08452403
H	8.93606317	-2.11042337	0.59350746
H	8.94181008	1.96102863	-0.76022861
H	-5.82577922	-0.02637437	-0.01318314
C	2.04236531	-0.05283128	-0.04852174
C	10.61696146	-0.08014566	-0.09271306
C	11.34318310	0.62580950	-1.05820205
C	11.34930933	-0.79087672	0.86460695
C	12.72852384	0.62910390	-1.06918905
H	10.81641578	1.17818087	-1.83020942
C	12.73463166	-0.80317917	0.86009773
H	10.82760851	-1.33985878	1.64244911
C	13.45575981	-0.08936996	-0.10857695
H	13.25532858	1.19086419	-1.83144390
H	13.26628096	-1.36833284	1.61645287
C	15.59416729	-0.31115046	1.08278270
C	15.33539729	0.44652399	2.23076291
C	16.60742398	-1.26384476	1.12679525
C	16.06189494	0.24013630	3.38955769
H	14.55499711	1.20011384	2.20937257
C	17.35946862	-1.46348972	2.28187482
H	16.81941091	-1.85611604	0.24269437
C	17.08413272	-0.71362641	3.42402394
H	15.86451892	0.82302073	4.28291993
H	18.14392727	-2.20995035	2.27811220
C	15.58244580	0.11934420	-1.32321906
C	16.60139136	1.06541917	-1.37766002
C	15.30630032	-0.63581955	-2.46879723
C	17.34223316	1.26083280	-2.54066750
H	16.82682097	1.65574794	-0.49558850
C	16.02165795	-0.43352938	-3.63523302
H	14.52115273	-1.38419492	-2.43944520
C	17.04976981	0.51346693	-3.68018888
H	18.13150335	2.00219499	-2.54490024
H	15.81077319	-1.01452948	-4.52673526
O	17.74736047	-0.83187164	4.60422968
O	17.70107698	0.62807818	-4.86737325
C	18.79449032	-1.78113621	4.68758394
H	19.18736442	-1.71043215	5.70175320
H	18.42728719	-2.79842974	4.51152542
H	19.59443799	-1.55783963	3.97278903
C	18.75331070	1.57068156	-4.96146274
H	19.13490232	1.49797994	-5.97979033
H	18.39450466	2.59020927	-4.78105456
H	19.55938418	1.34194435	-4.25532113
N	14.85698671	-0.09390001	-0.11630980
Os	0.09410448	-0.04679877	-0.03928198

Cartesian coordinates for the DFT-optimized structure of **4**$^{2+}$ by UB3LYP:

Charge = 2 multiplicity = 2

N	0.45991804	-1.51367579	1.43262452
N	-0.45490920	1.39647432	1.40556623
N	-2.05310943	-0.06090461	-0.03063272
N	-0.45816335	-1.50949240	-1.47929733
N	0.44037377	1.40575484	-1.51360153
C	4.80242855	-0.04310031	-0.05863405
C	4.08169126	0.81531743	-0.91731797
H	4.63597512	1.45655379	-1.59770847
C	2.68366053	0.81606521	-0.91513024
C	2.69522036	-0.91242292	0.81587830
C	4.09322078	-0.90493750	0.80618602
H	4.65645748	-1.54356762	1.48166103
C	1.78763145	1.62921292	-1.73970759
C	2.18932911	2.57258184	-2.69416242
H	3.24844558	2.73705504	-2.86007448
C	1.24525164	3.28859261	-3.41885323
H	1.55965162	4.01879552	-4.15798309
C	-0.11220550	3.05298038	-3.17998872
H	-0.88622677	3.58701250	-3.72001326
C	-0.46692839	2.11038463	-2.22590516
H	-1.50750401	1.89734230	-2.00954460
C	1.81012767	-1.73015380	1.64776785
C	2.22447164	-2.67135234	2.59893213
H	3.28575185	-2.83026995	2.75613658
C	1.29006490	-3.39216239	3.33134800
H	1.61425561	-4.12066661	4.06791929
C	-0.07049423	-3.16357550	3.10358132
H	-0.83729092	-3.70155337	3.64996056
C	-0.43788745	-2.22291374	2.15237527
H	-1.48132204	-2.01532328	1.94459572
C	0.42720337	-2.23298563	-2.20284993
H	1.47150592	-2.02644396	-2.00411736
C	0.03855094	-3.17960734	-3.14043270
H	0.79600091	-3.72804218	-3.68955588
C	-1.32320623	-3.40358420	-3.35478884
H	-1.66048157	-4.13625800	-4.08030308
C	-2.24496823	-2.66789287	-2.61881273
H	-3.30748511	-2.82241795	-2.76589959
C	-1.80605467	-1.72483830	-1.68502870
C	-2.71462757	-0.90710577	-0.86707384
C	-4.11094761	-0.92564092	-0.87621845
H	-4.65429654	-1.59263151	-1.53536804
C	-4.80572539	-0.06857723	-0.01979187
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C	-2.71272788	0.78168765	0.81093465
C	-1.80231762	1.60450172	1.62171015
C	-2.23911954	2.54525635	2.55880059
H	-3.30129318	2.69407486	2.71404885
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H	-1.65132862	4.01694912	4.01560700
C	0.04555955	3.06938704	3.06274510
H	0.80423790	3.62197158	3.60598063
C	0.43208870	2.12481156	2.12222661
H	1.47592184	1.92397674	1.91534361

C	6.28569325	-0.03969203	-0.06539223
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C	8.41376691	-1.21803201	0.13749307
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C	8.40629752	1.14832335	-0.28918678
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C	9.14113549	-0.03321584	-0.07956926
H	8.94228026	-2.14920615	0.31994003
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C	10.62198987	-0.02994739	-0.08725090
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C	11.35336818	-1.14159130	-0.54822705
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C	15.67709736	1.17418129	-0.29923525
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C	17.06296542	1.18475499	-0.31138251
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C	17.06983504	-1.21735371	0.06994412
H	15.16005499	-2.14890104	0.23212809
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H	17.59903827	2.11786021	-0.44481047
H	17.61105922	-2.14825869	0.19780596
C	19.90121178	-0.81727832	0.78296370
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C	21.07851304	-1.47966154	0.38276101
C	20.14032322	-1.75422657	3.00196900
H	18.54933383	-0.44146448	2.43596765
C	21.78190825	-2.27429081	1.27617450
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H	19.80915626	-1.86301171	4.02912614
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H	18.52215163	0.41503369	-2.69188814
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H	22.65168520	2.77722418	-1.23473091
H	19.76150422	1.84008225	-4.29793382
N	19.19097082	-0.01199145	-0.13124048
O	21.92194538	-3.16089790	3.54385096
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C	23.13327094	-3.85542192	3.22207969
H	23.42865228	-4.36601787	4.13829499
H	22.96330588	-4.59044416	2.42839460

H	23.91771806	-3.15356055	2.92043605
C	23.08762533	3.84262143	-3.52473189
H	23.37275572	4.35319859	-4.44420028
H	22.92349397	4.57789517	-2.73004906
H	23.87679281	3.14304979	-3.23013843
Os	0.00090999	-0.05523709	-0.03867363

Cartesian coordinates for the DFT-optimized structure of **4**$^{2+}$ by UCAM-B3LYP:

Charge = 2 multiplicity = 2

N	0.47802057	-1.42421728	1.53869292
N	-0.44599293	1.48186769	1.29993044
N	-2.04606994	-0.06140531	-0.03095372
N	-0.44724041	-1.59379238	-1.37567449
N	0.45812701	1.31738742	-1.62107465
C	4.79356683	-0.04273872	-0.05920346
C	4.08420762	0.75732035	-0.97874314
H	4.64526868	1.34588732	-1.69652059
C	2.69793863	0.75867981	-0.97383787
C	2.70958307	-0.85412667	0.87309709
C	4.09581587	-0.84613031	0.86632380
H	4.66575185	-1.43209725	1.57922142
C	1.79231340	1.52206403	-1.85673580
C	2.20457722	2.38971993	-2.85777553
H	3.26269914	2.54262517	-3.03189928
C	1.26075966	3.05580584	-3.62893230
H	1.57809257	3.73446841	-4.41279666
C	-0.08721802	2.84018600	-3.38139706
H	-0.85824862	3.33749808	-3.95685785
C	-0.44463775	1.96388326	-2.36854366
H	-1.48494076	1.76626003	-2.13989572
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H	3.30021726	-2.63509102	2.92651799
C	1.30584868	-3.15825415	3.54002636
H	1.63300930	-3.83522380	4.32130845
C	-0.04518513	-2.94941735	3.30362958
H	-0.80891376	-3.45051260	3.88551249
C	-0.41531957	-2.07504762	2.29367096
H	-1.45845285	-1.88254702	2.07369094
C	0.44624921	-2.34779361	-2.03738890
H	1.48893497	-2.12612929	-1.85280793
C	0.06469698	-3.35366457	-2.90893804
H	0.82578244	-3.93261065	-3.41729126
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H	-1.61884557	-4.37393608	-3.78422638
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H	-3.27442338	-2.98571379	-2.56785793
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C	-2.69150155	-0.95078052	-0.80161429
C	-4.08084975	-0.97804096	-0.81552509
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C	-4.08004895	0.84133978	0.77161587
H	-4.62007934	1.54609152	1.39053819
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C	-1.77721456	1.70166235	1.50181652

C	-2.21214735	2.69441266	2.36735715
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H	0.82867173	3.83049667	3.32919446
C	0.44802941	2.24230003	1.95349730
H	1.49056738	2.02760509	1.76006567
C	6.27314181	-0.03941407	-0.06565307
C	6.99898709	-1.20377751	0.21135922
C	6.99139779	1.12810618	-0.34909915
C	8.38531337	-1.19977175	0.20464290
H	6.47537197	-2.13179658	0.41712247
C	8.37773910	1.13010513	-0.35489857
H	6.46194129	2.05383780	-0.55019353
C	9.10507333	-0.03327666	-0.07843291
H	8.91748375	-2.11629212	0.43698637
H	8.90380722	2.04890607	-0.59207755
H	-5.85395003	-0.07445696	-0.01407350
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C	10.58680588	-0.03016340	-0.08535050
C	11.30978329	1.08483987	0.35215070
C	11.31023806	-1.14215236	-0.52972138
C	12.69689545	1.08649428	0.34735050
H	10.78163391	1.95346202	0.73272554
C	12.69731852	-1.13796891	-0.53823973
H	10.78212615	-2.01297488	-0.90528246
H	13.22589352	1.95627139	0.72372626
H	13.22633422	-2.00550660	-0.91972275
C	13.42254425	-0.02419888	-0.09896333
C	14.90368046	-0.02104784	-0.10638477
C	15.62861482	1.14016596	-0.39515651
C	15.63643797	-1.17920559	0.17479042
C	17.01450496	1.15106971	-0.39874169
H	15.10006486	2.05798882	-0.63383390
C	17.02233159	-1.18440030	0.16362891
H	15.11425348	-2.09920678	0.41902417
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H	17.54190422	2.07106662	-0.62269361
H	17.55584820	-2.10223533	0.38189399
C	19.87958462	-0.91242489	0.69275532
C	19.59313050	-1.03332412	2.05762400
C	20.91648273	-1.67300292	0.16030144
C	20.31610468	-1.90162629	2.85553822
H	18.79381853	-0.44095743	2.49053796
C	21.66515037	-2.53266499	0.96044838
H	21.15021249	-1.58853091	-0.89586642
C	21.36255232	-2.65554386	2.31523613
H	20.09649062	-2.00033981	3.91332579
H	22.46830745	-3.10415630	0.51223694
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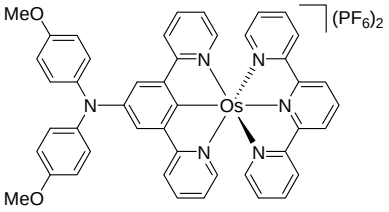
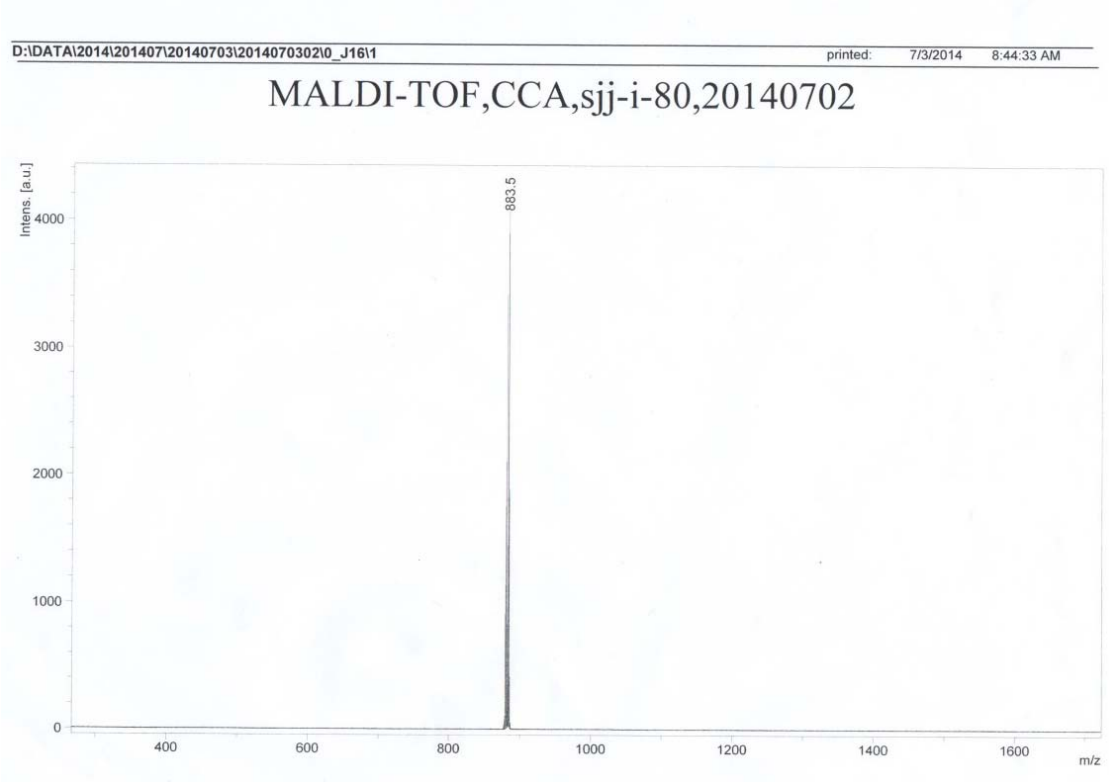
C	20.90756434	1.65394498	-0.44071170
C	19.56322362	1.00960039	-2.32162232
C	21.64378727	2.51569890	-1.25011012
H	21.15437087	1.57048368	0.61256117
C	20.27373166	1.87992367	-3.12846628
H	18.76054069	0.41468444	-2.74467959
C	21.32430042	2.63729008	-2.60113543

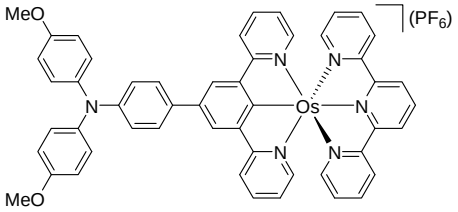
H	22.45058128	3.08975643	-0.81179741
H	20.04094098	1.97769358	-4.18352154
N	19.14522307	-0.01224888	-0.12919832
O	22.02011675	-3.46890745	3.18367047
O	21.96853171	3.45256664	-3.47772921
C	23.09013083	-4.24975944	2.68446500
H	23.47355223	-4.81613668	3.53310326
H	22.75052476	-4.94541596	1.90884422
H	23.88979766	-3.62000277	2.27850517
C	23.04162348	4.23749940	-2.99173132
H	23.41228547	4.80544691	-3.84497795
H	22.70897673	4.93174475	-2.21184588
H	23.84873456	3.61082563	-2.59585666
Os	0.06538917	-0.05460065	-0.03965277

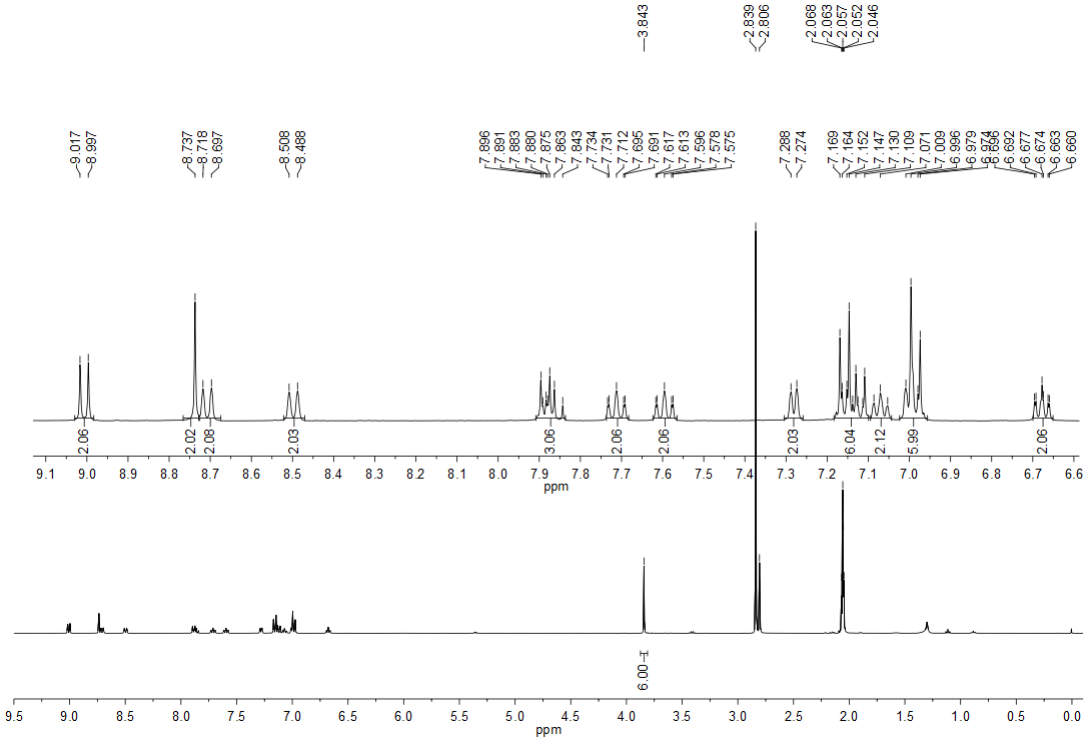
MALDI-TOF mass spectrum of complex **1**$(PF_6)_2$:

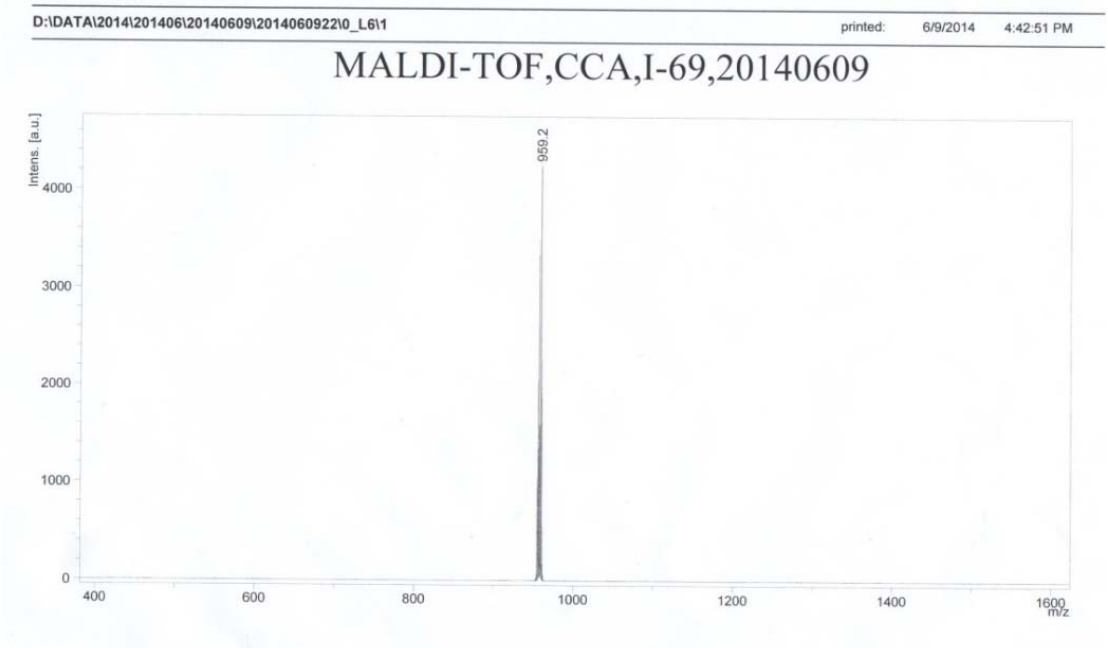




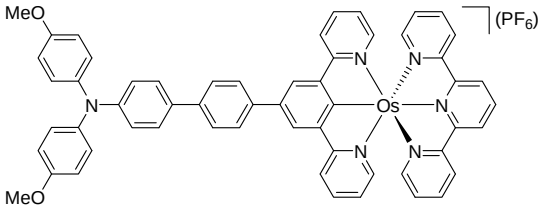
^{1}H NMR and MALDI-TOF mass spectra of complex **2**(PF_6):

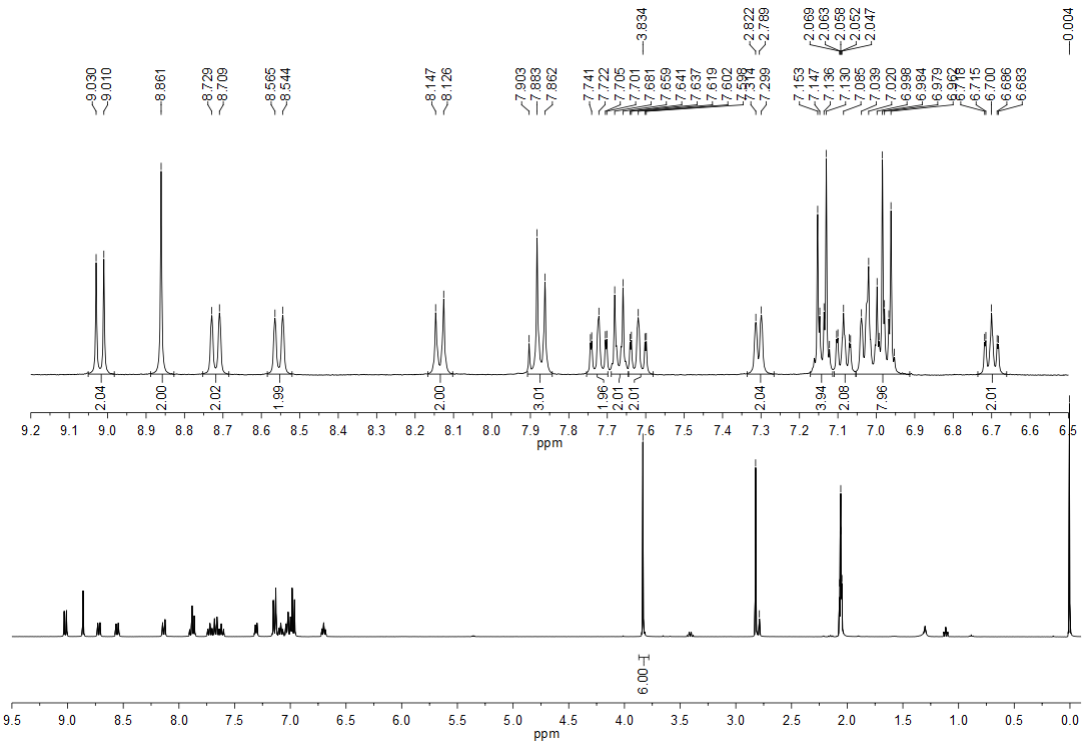


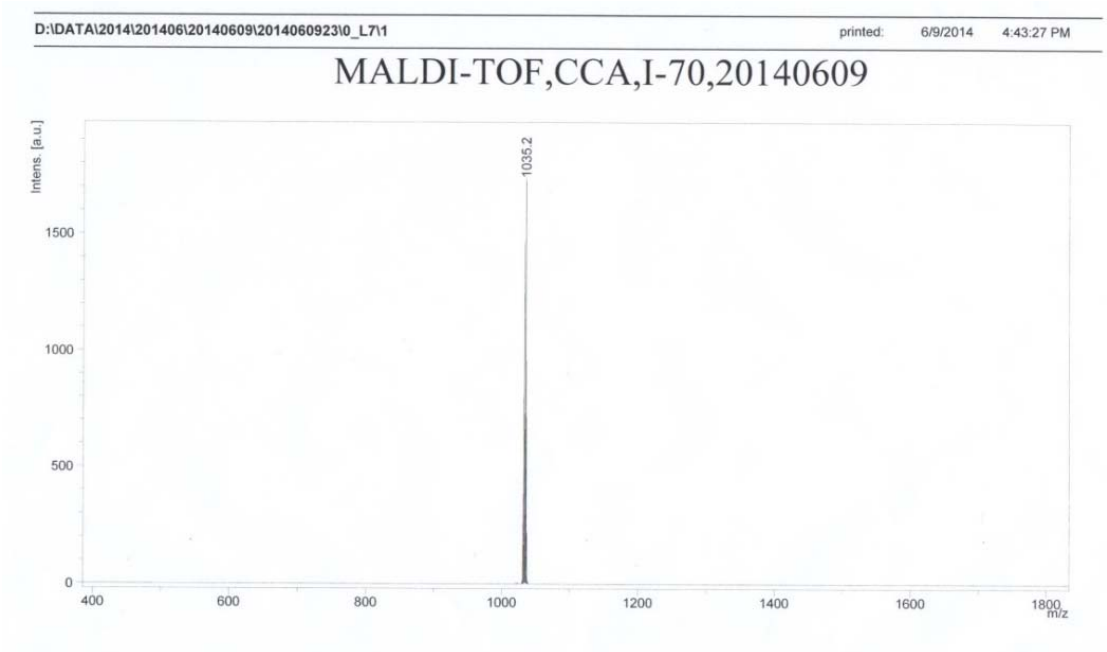




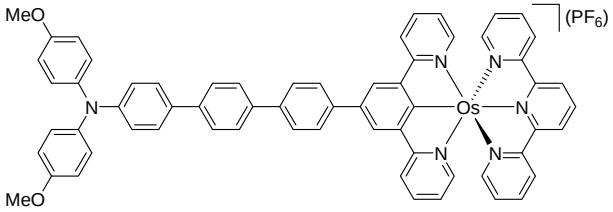
^{1}H NMR and MALDI-TOF mass spectra of complex **3**(PF_6):

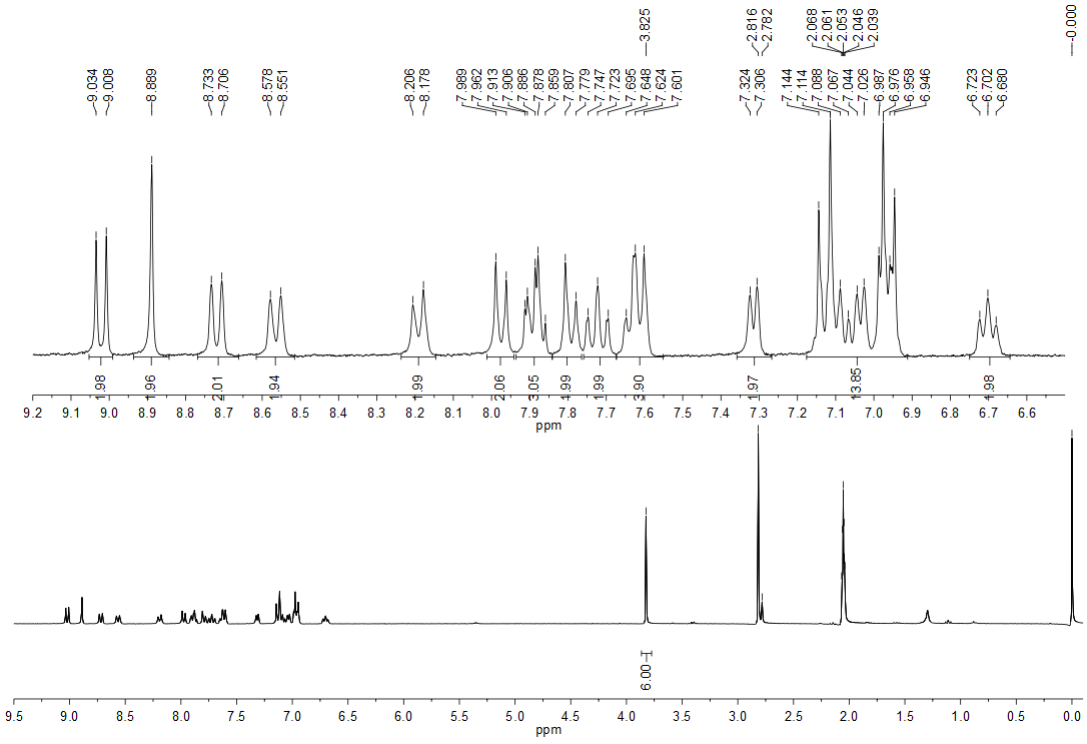


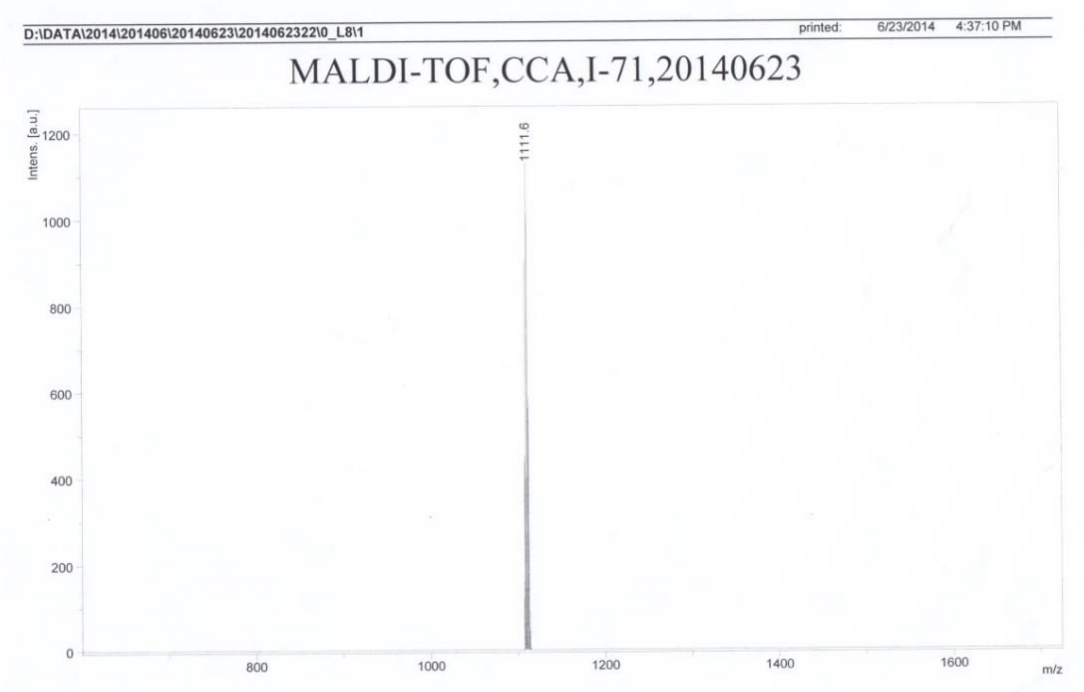




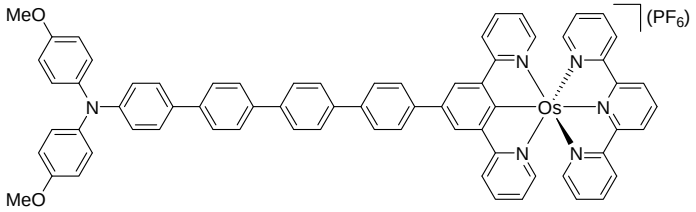
^{1}H NMR and MALDI-TOF mass spectra of complex **4**(PF_6):

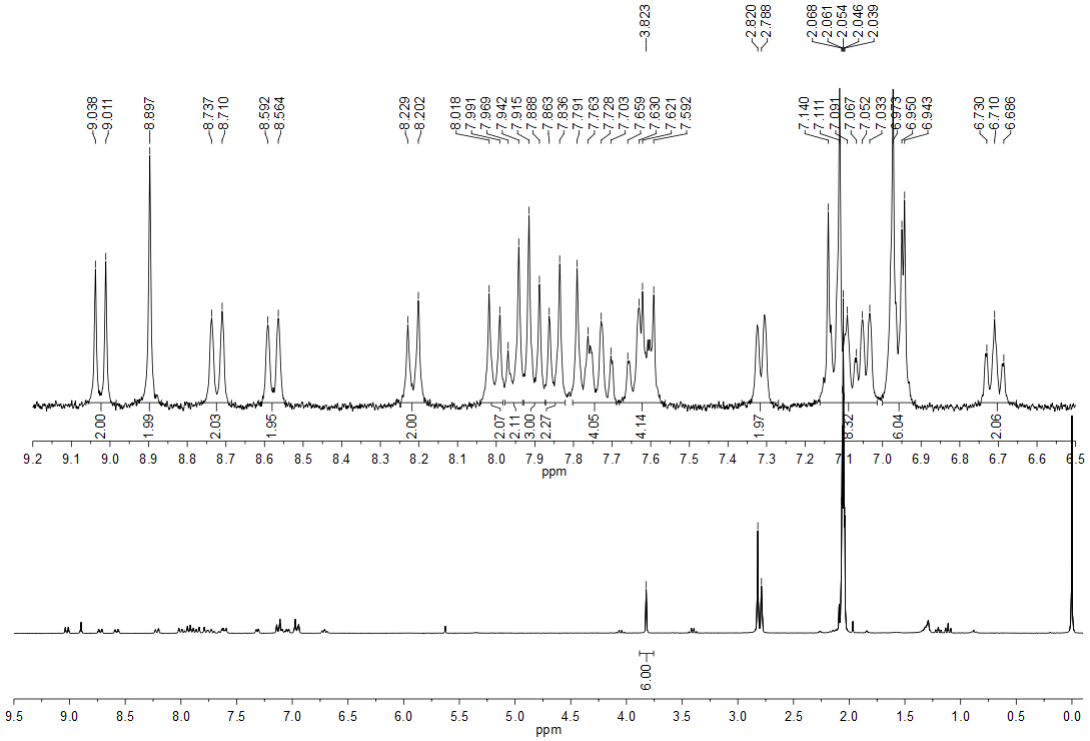


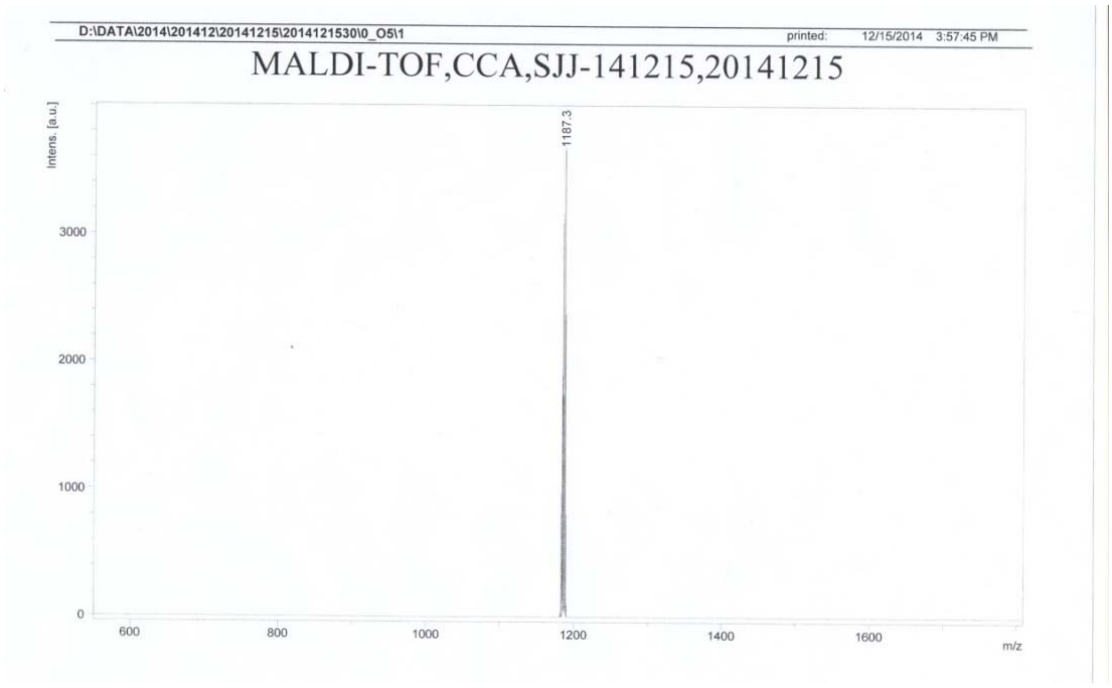




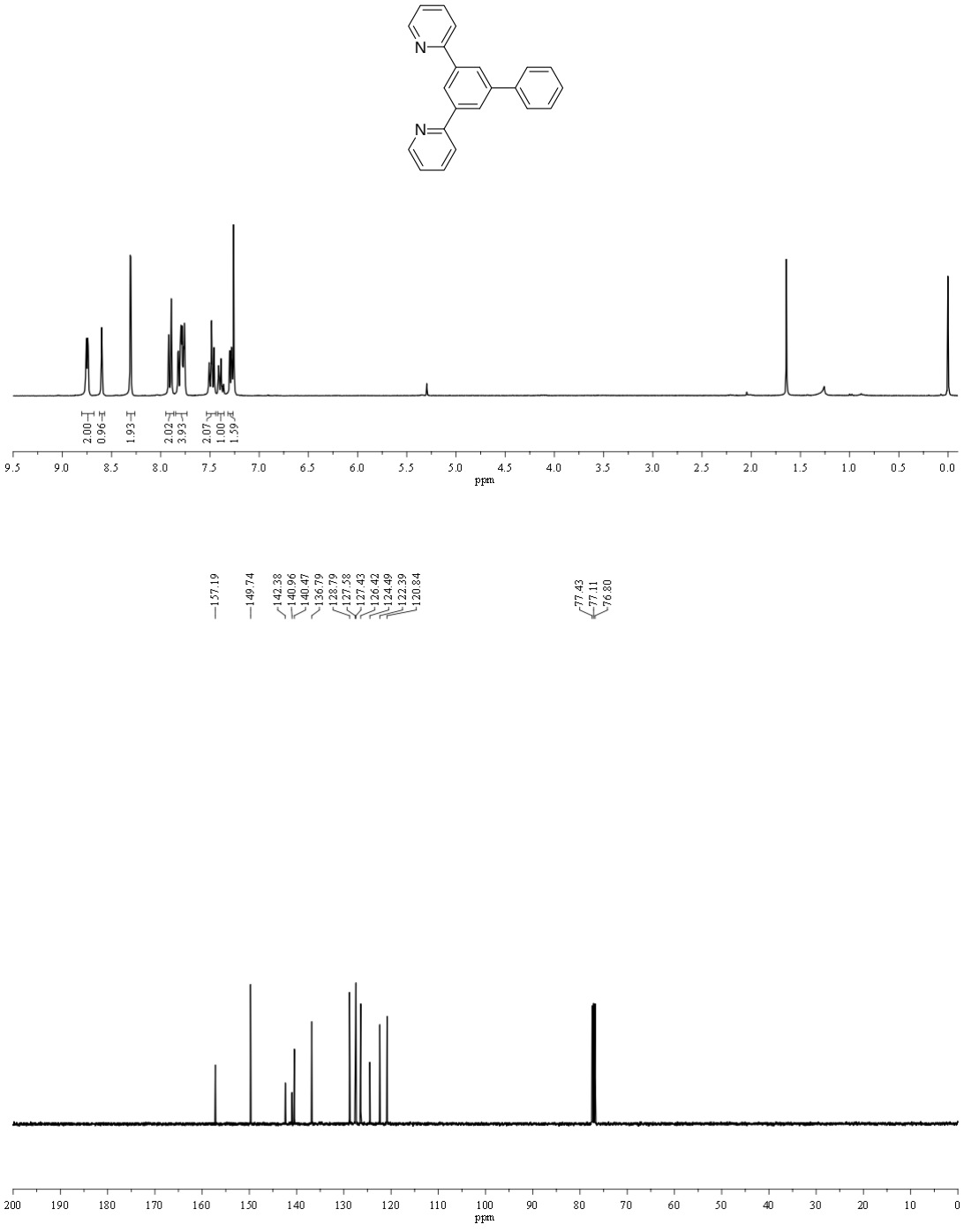
^{1}H NMR and MALDI-TOF mass spectra of complex **5**(PF_6):



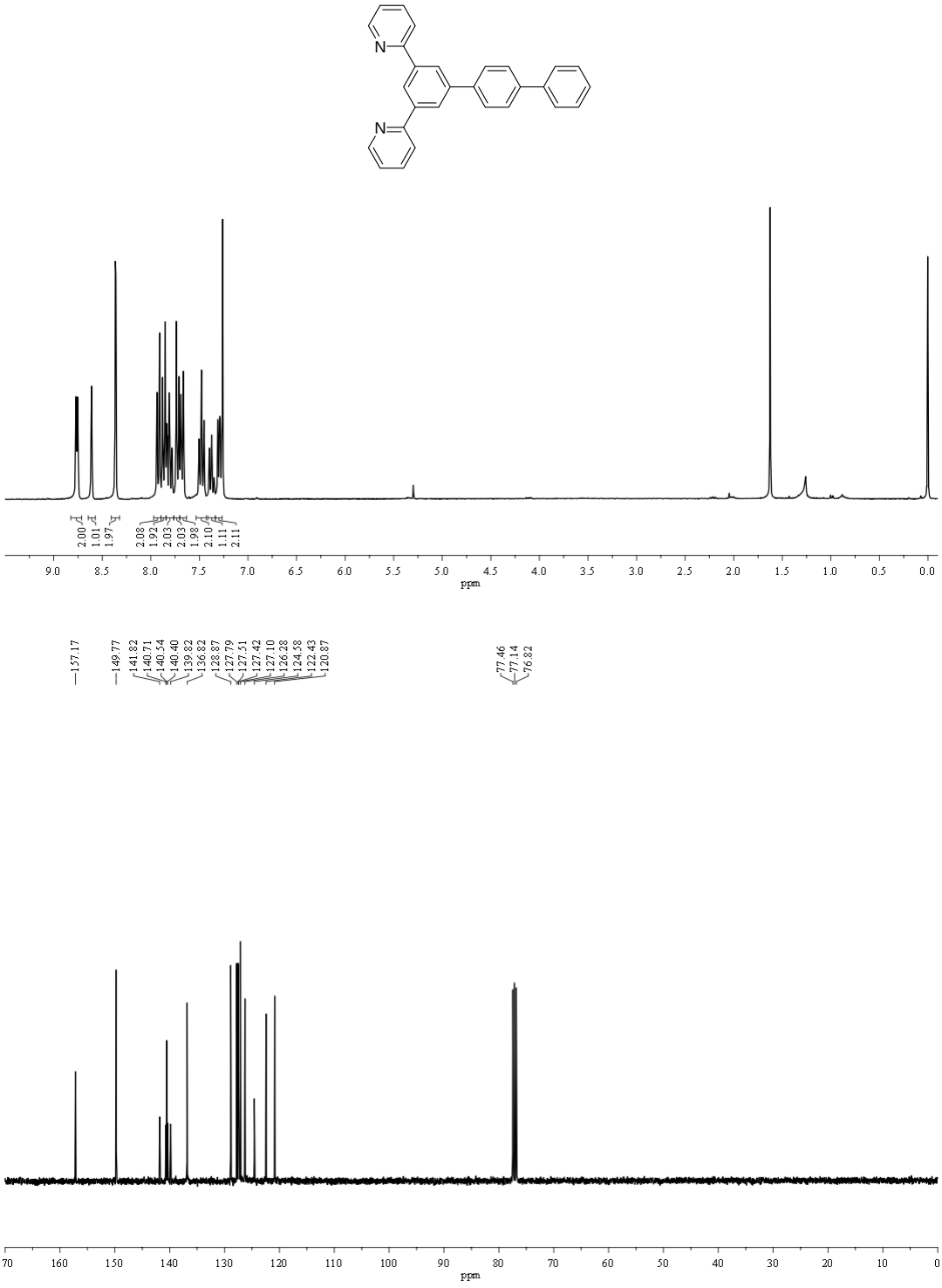




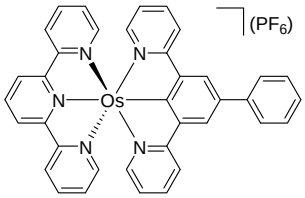
^{1}H and ^{13}C NMR spectra of ligand **L6**:

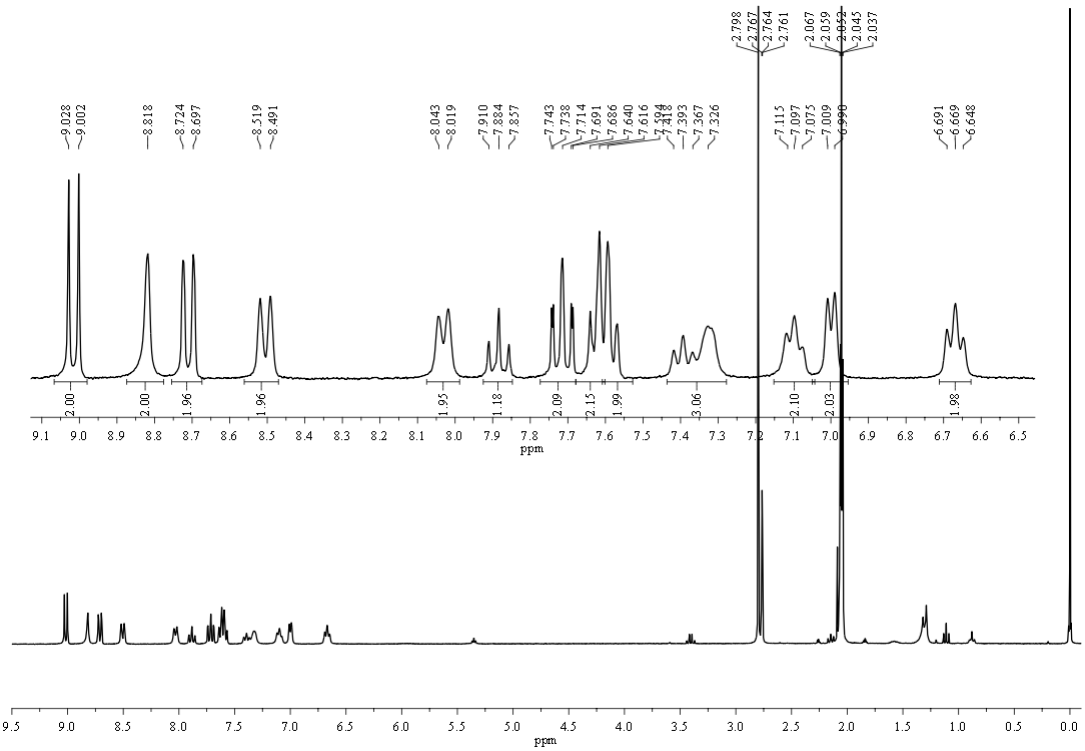


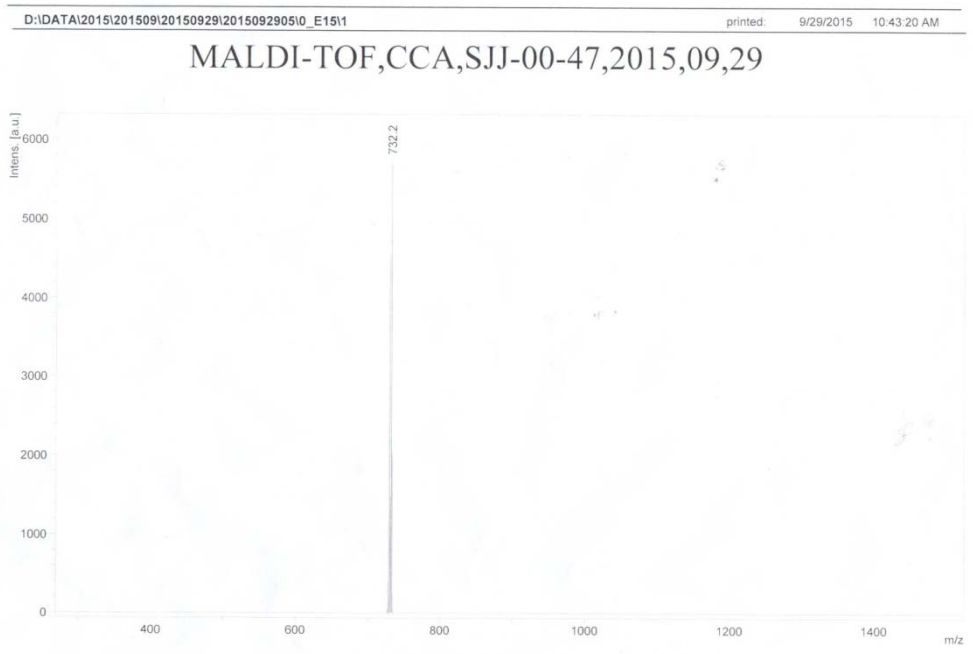
^{1}H and ^{13}C NMR spectra of ligand **L7**:



^{1}H NMR and MALDI-TOF mass spectra of complex **6**(PF_6):







^{1}H NMR and MALDI-TOF mass spectra of complex **7**(PF_6):