Supporting Information for:

Synthesis and Electronic Coupling Studies of Cyclometalated Diruthenium Complexes Bridged by 3,3',5,5'-Tetrakis(benzimidazol-2-yl)-biphenyl

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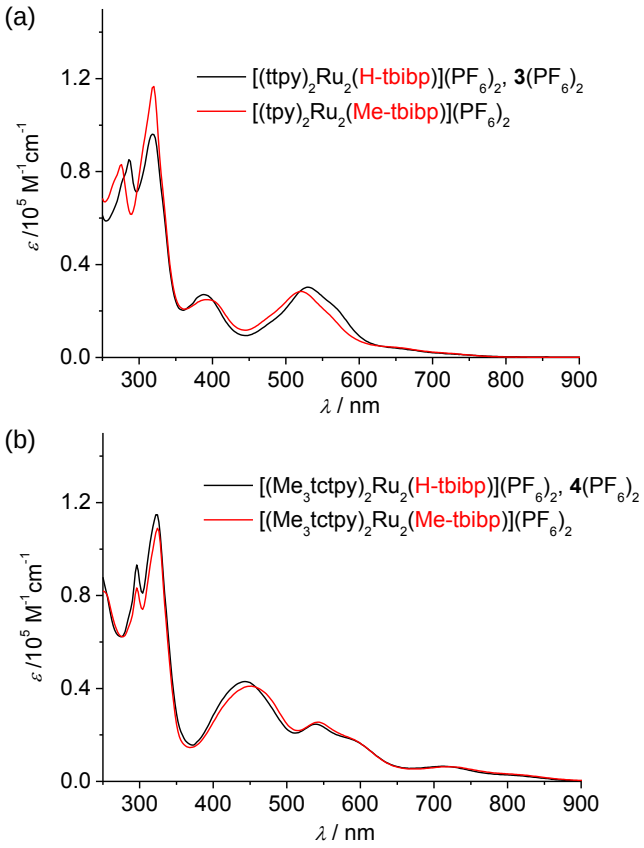

Figure S1. A comparison of the absorption spectra of diruthenium complexes with H-tbibp or Me-tbibp bridging ligand.

Table S1. TDDFT Results with UCAM-B3LYP.[a]

Comp.	*Exci.*	λ (nm)	$\tilde{\nu}$ (cm^{-1})	*f*	Major contribution
$\mathbf{3}^{3+}$	D_1	-2332	4288	-1.0456	H(β)→ L(β) (100%)
	D_7	593	16863	0.0507	H-7(β)→ L(β) (77%)
	D_9	557	17953	0.0818	H-6(β)→ L(β) (85%)
$\mathbf{4}^{3+}$	D_1	-2693	3713	-1.0426	H(β)→ L(β) (100%)
	D_7	622	16077	0.0495	H-7(β)→ L(β) (76%)
	D_9	580	17241	0.0693	H-6(β)→ L(β) (85%)
$\mathbf{5}^{3+}$	D_1	-2613	3827	-1.0239	H(β)→ L(β) (100%)
	D_7	618	16181	0.0400	H-8(β)→ L(β) (65%)
	D_9	567	17636	0.0756	H-7(β)→ L(β) (53%)

[a]Calculated on the level of UCAM-B3LYP/LanL2DZ/6-31G*/CH_3CN.

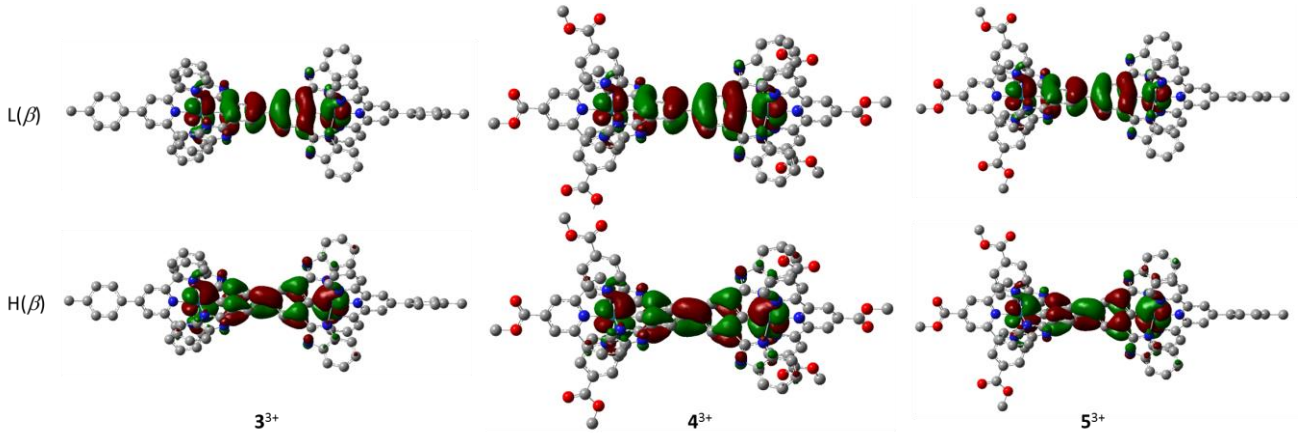

Figure S2. Highest occupied (below) and lowest unoccupied (upper) β spin orbitals of $\mathbf{3}^{3+}$ – $\mathbf{5}^{3+}$ calculated on the level of UCAM-B3LYP/LanL2DZ/6-31G*/CH_3CN.

Table S2. TDDFT Results with UBLYP35.[a]

Comp.	*Exci.*	λ (nm)	$\tilde{\nu}$ (cm^{-1})	f	Major contribution
$\mathbf{3}^{3+}$	D_1	3543	2822	0	--[b]
	D_3	1310	7633	0.5970	H(β)→ L(β) (91%)
	D_6	692	14451	0.0176	H-6(β)→ L(β) (78%)
	D_7	649	15408	0.0414	H-3(β)→ L(β) (40%); H-8(β)→ L(β) (34%)
$\mathbf{4}^{3+}$	D_1	6865	1457	0.9109	H(β)→ L(β) (100%)
	D_2	1728	5787	0.0011	H-1(β)→ L(β) (84%)
	D_7	746	13405	0.0508	H-7(β)→ L(β) (77%)
$\mathbf{5}^{3+}$	D_1	3570	2801	0.0006	--[b]
	D_3	770	12987	0.1961	H(β)→ L(β) (76%)
	D_6	596	16778	0.0275	H-6(β)→ L(β) (44%)
	D_9	582	17182	0.0229	H-5(β)→ L(β) (30%); H-6(β)→ L(β) (35%)

[a]Calculated on the level of UBLYP35/LanL2DZ/6-31G*/CH_3CN. [b]The information has not been provided since the corresponding oscillator strength is zero or negligible.

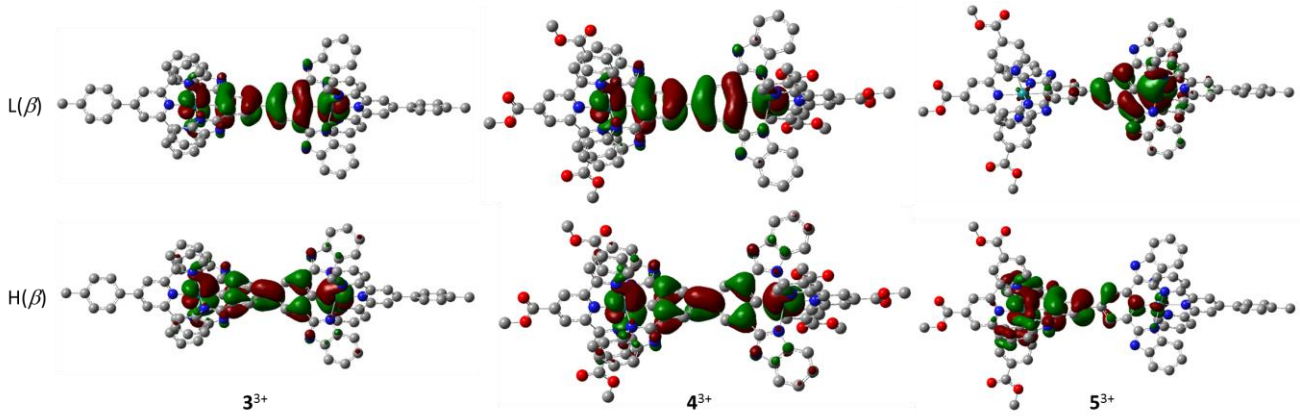

Figure S3. Highest occupied (below) and lowest unoccupied (upper) β spin orbitals of $\mathbf{3}^{3+}$ – $\mathbf{5}^{3+}$ calculated on the level of UBLYP35/LanL2DZ/6-31G*/CH_3CN.

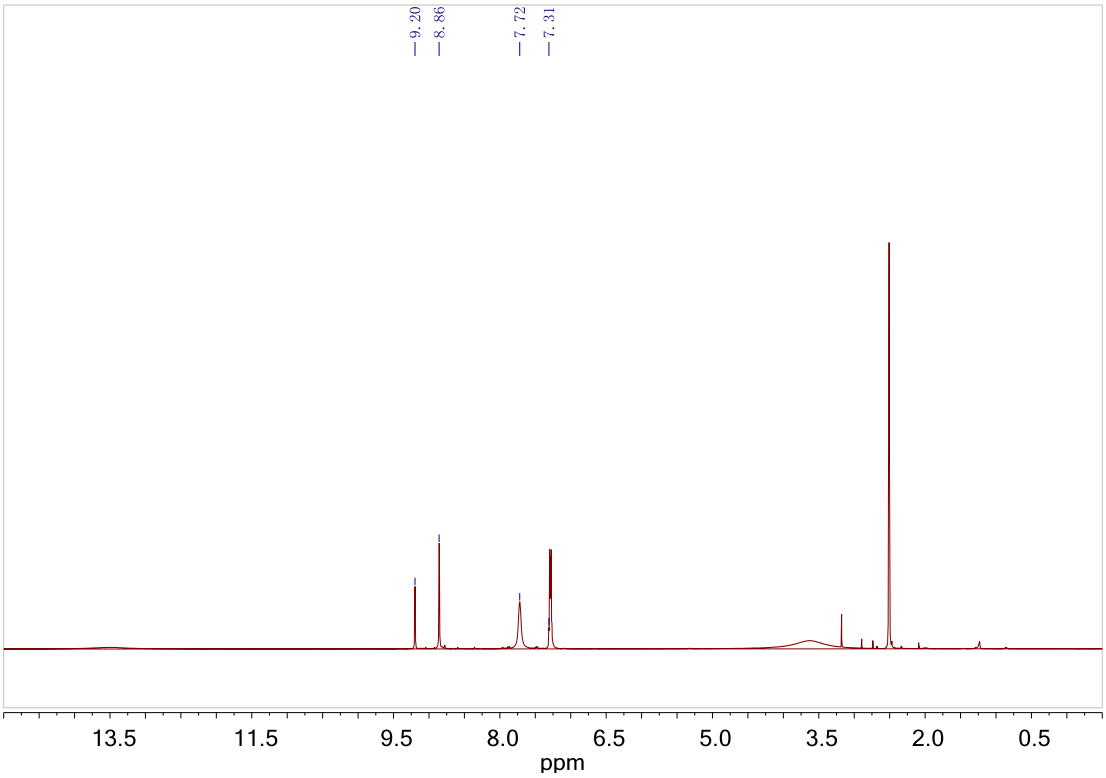

Figure S4. ^{1}H NMR spectrum of H-tbibp in d_6-DMSO.

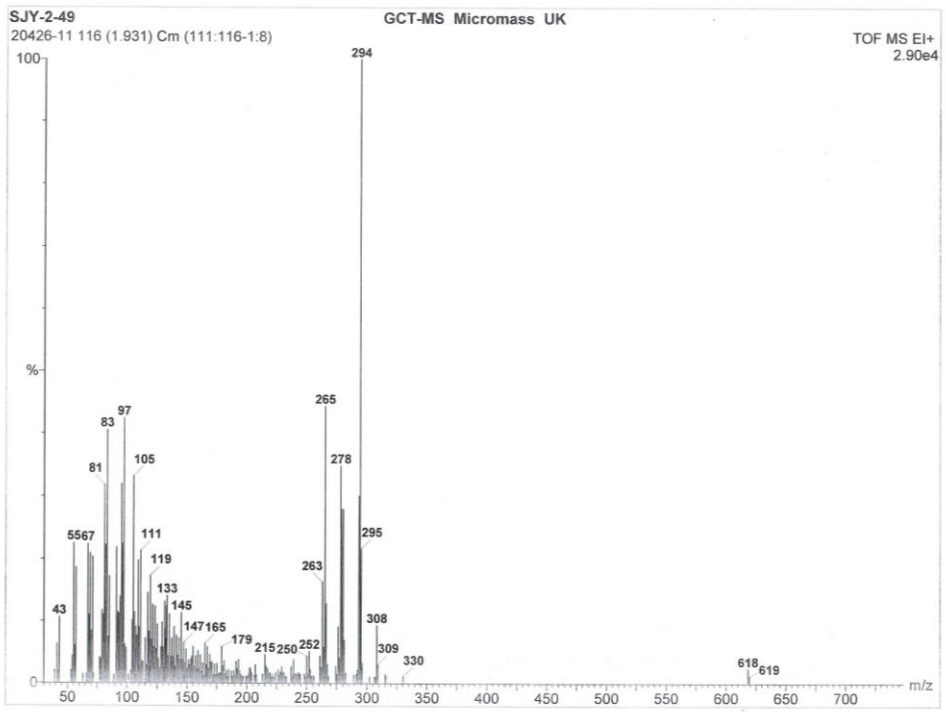

Figure S5. EI mass spectrum of H-tbibp

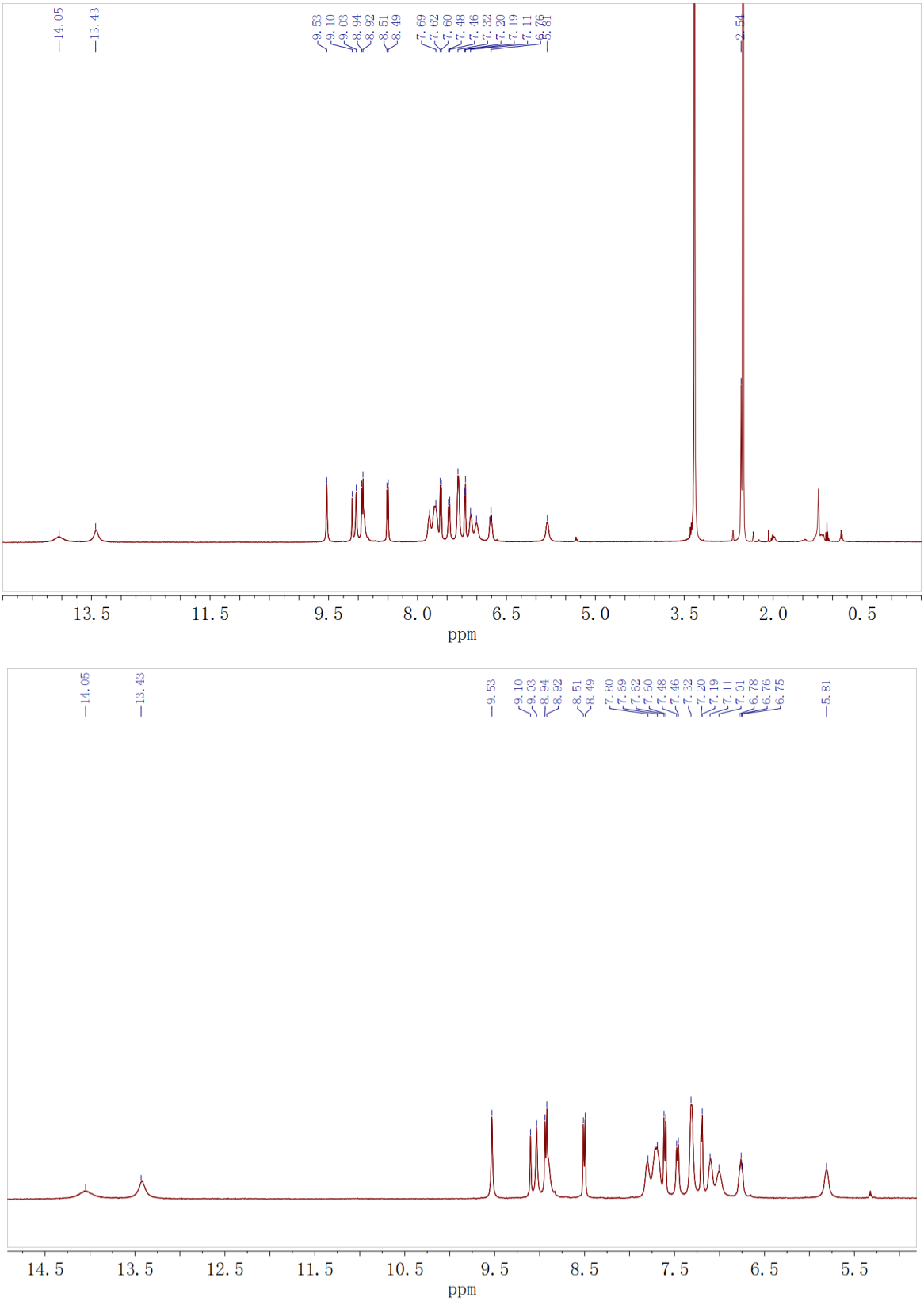

Figure S6. Full-scale (upper) and enlarged (below) ^{1}H NMR spectrum of **1**(PF_6) in d_6-DMSO.

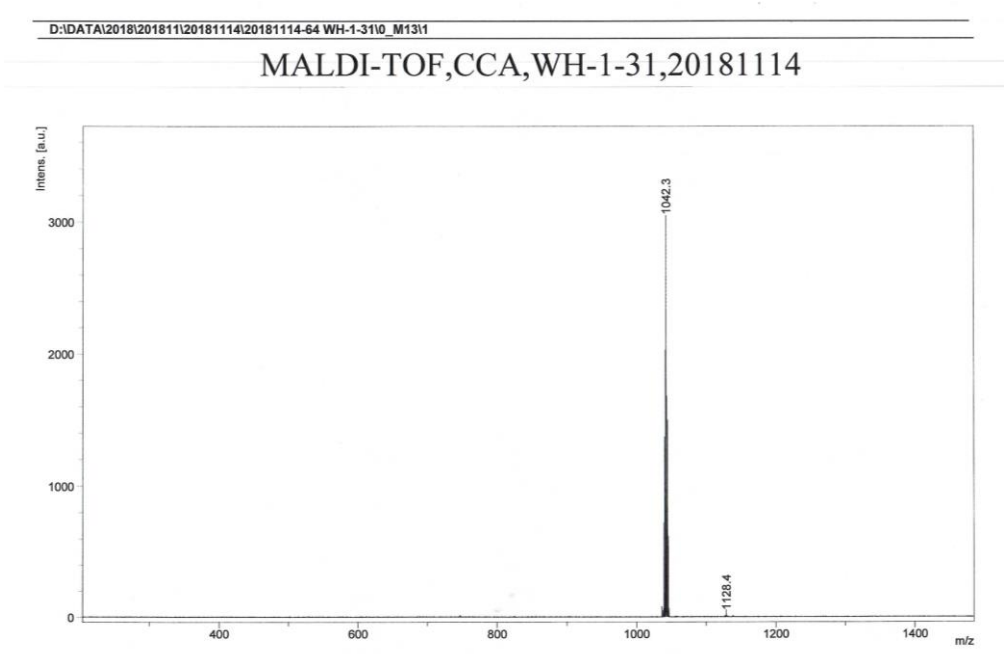

Figure S7. MALDI-TOF mass spectrum of **1**(PF_6).

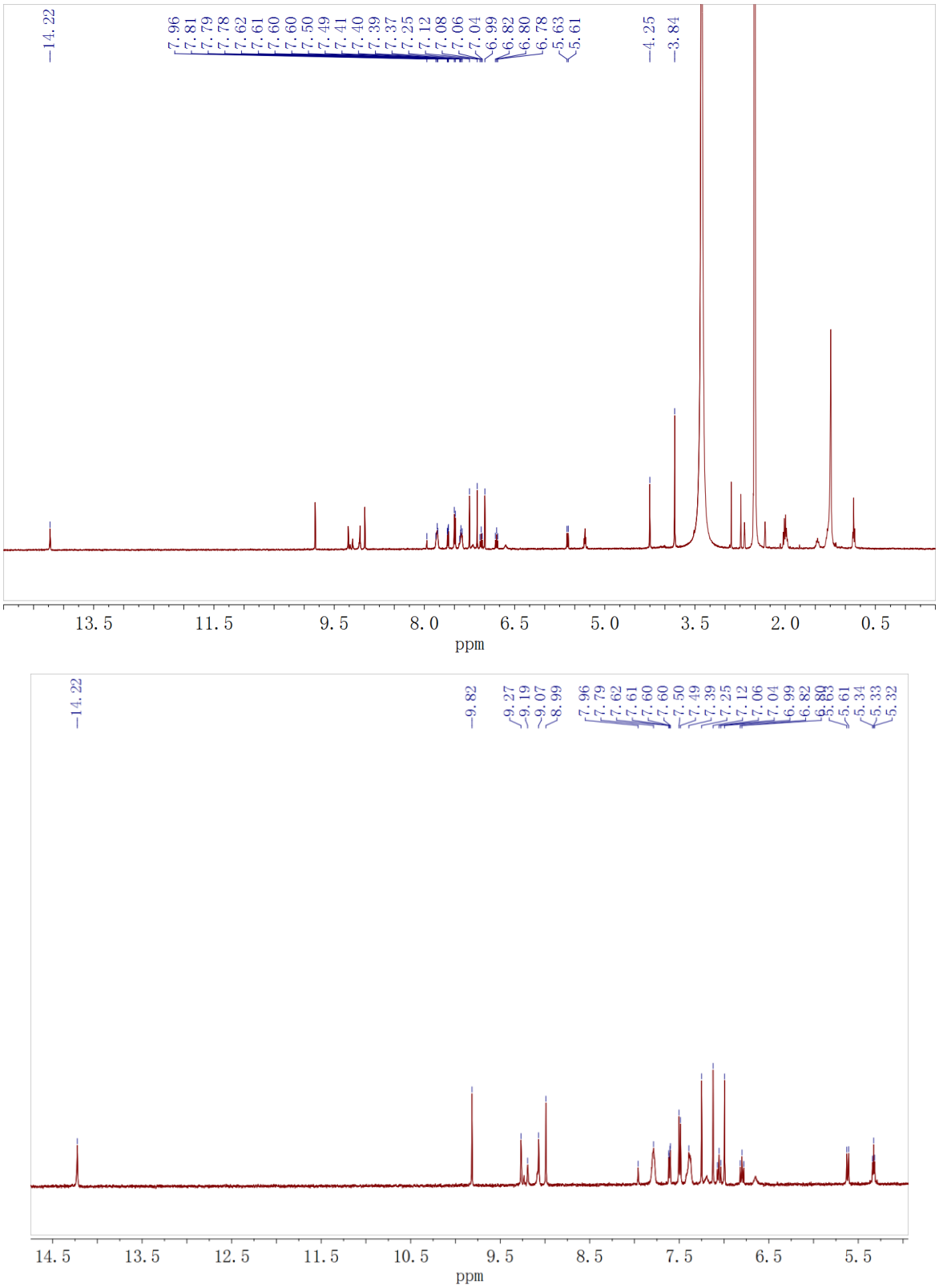

Figure S8. Full-scale (upper) and enlarged (below) ^{1}H NMR spectrum of **2**(PF_6) in d_6-DMSO.

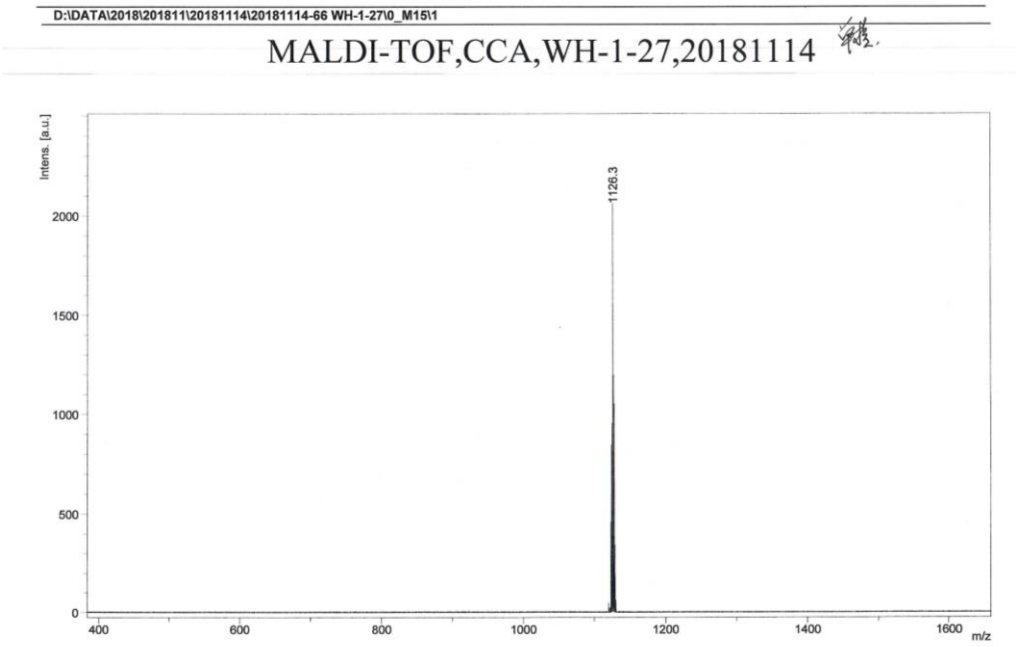

Figure S9. MALDI-TOF mass spectrum of **2**(PF_6).

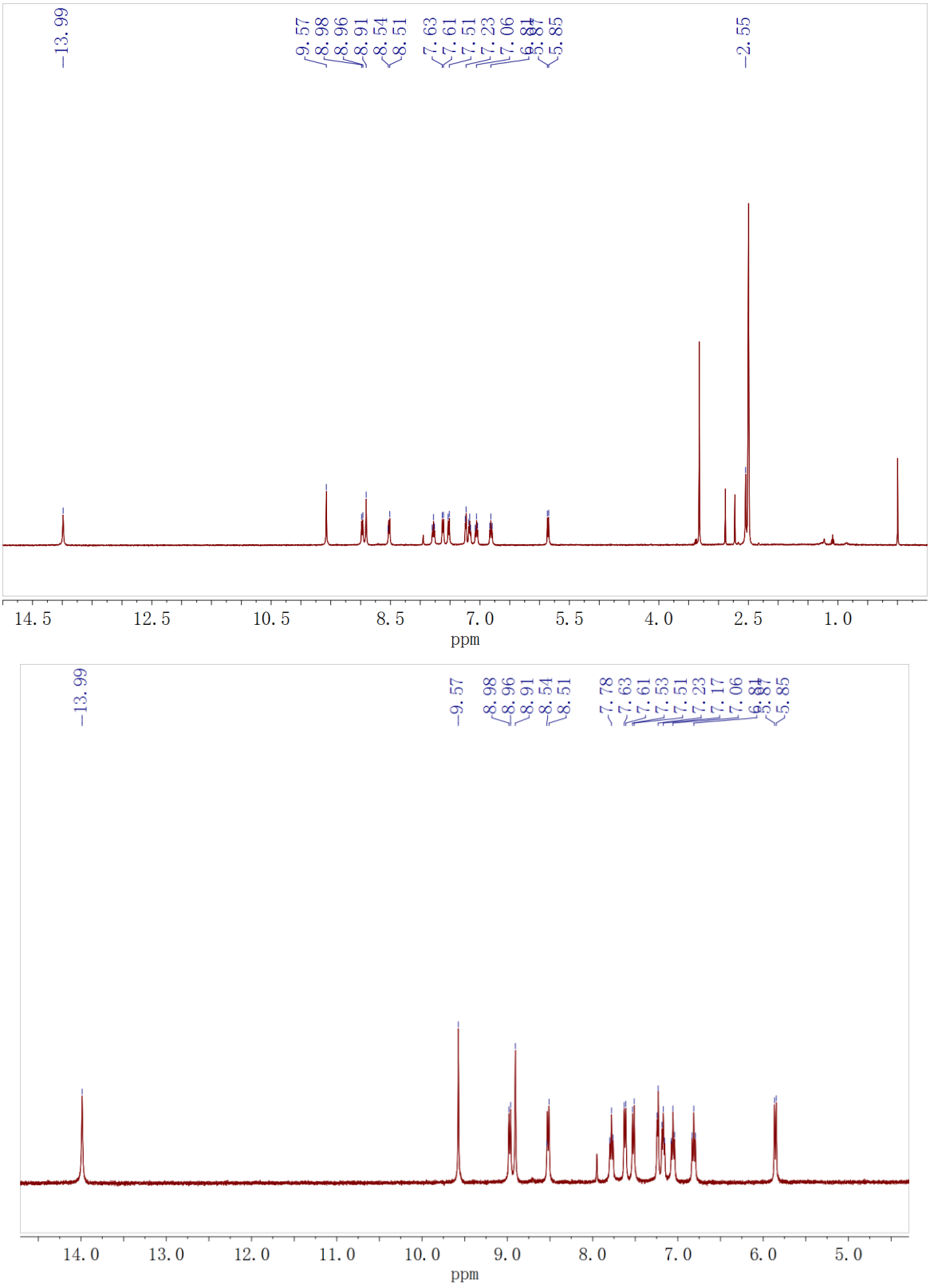

Figure S10. Full-scale (upper) and enlarged (below) ^{1}H NMR spectrum of **3**$(PF_6)_2$ in d_6-DMSO.

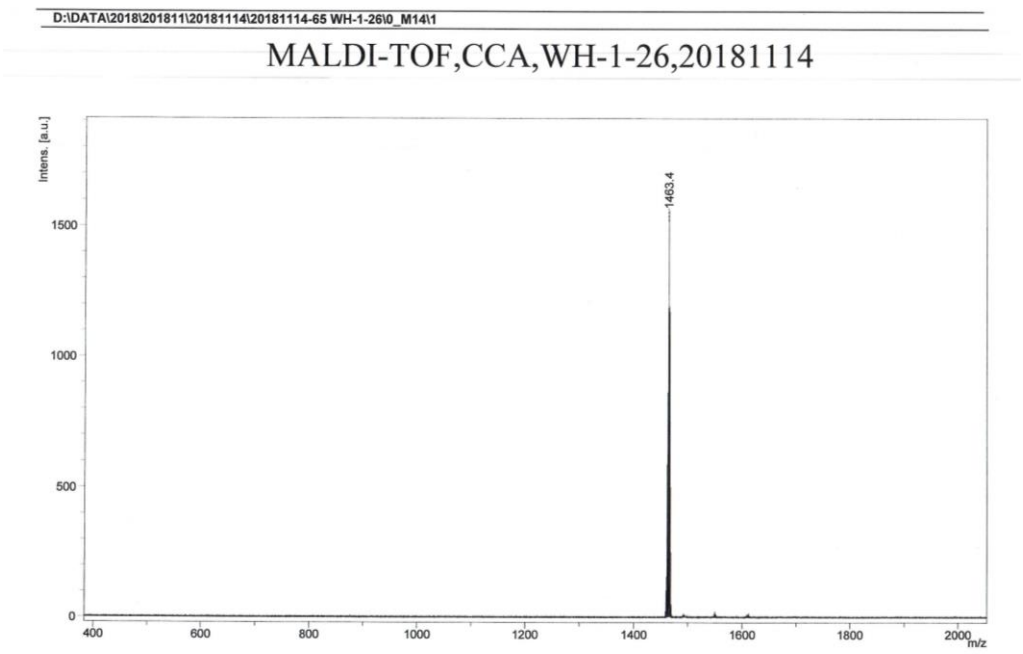

Figure S11. MALDI-TOF mass spectrum of **3**$(PF_6)_2$.

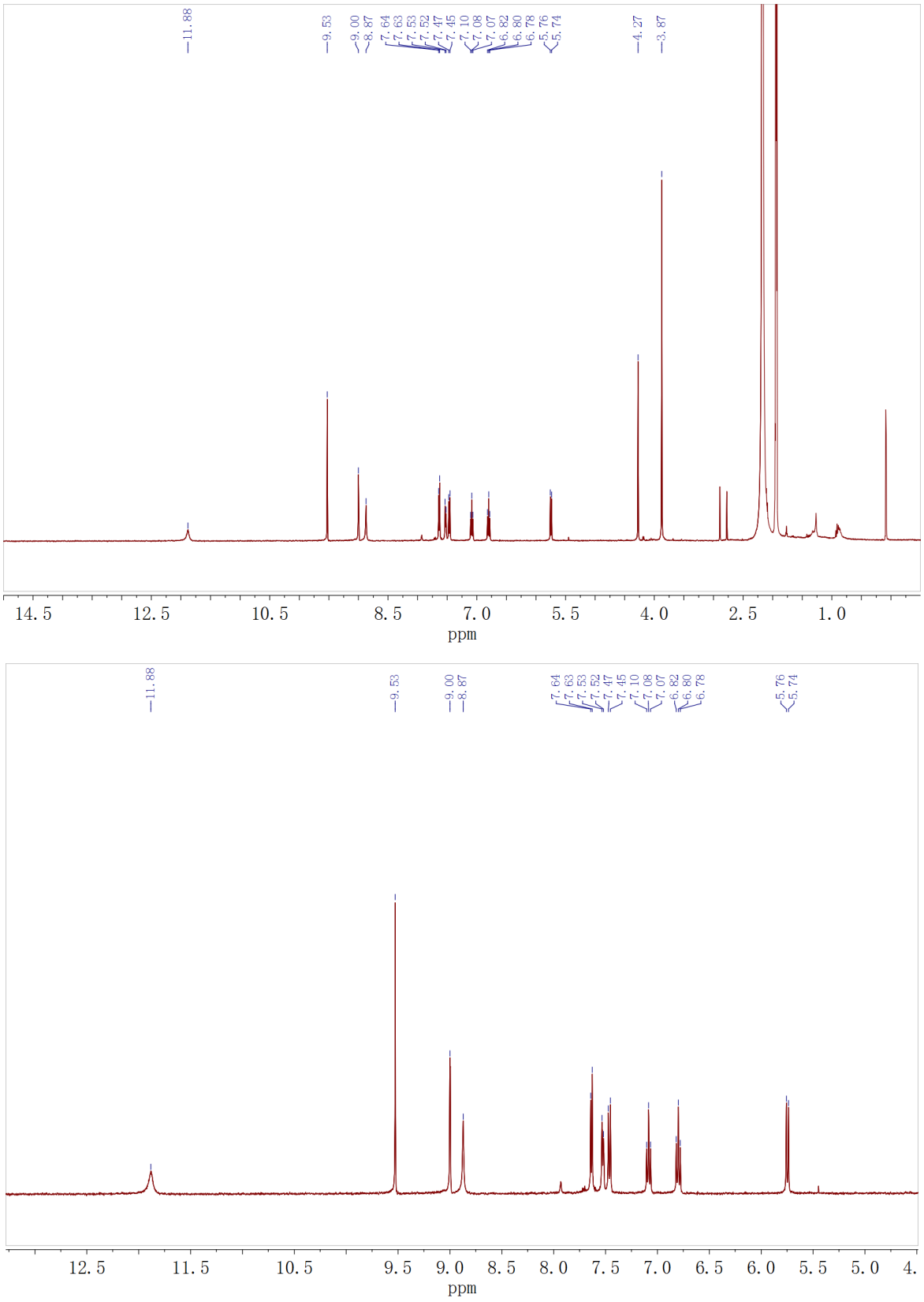

Figure S12. ^{1}H NMR spectrum of **4**$(PF_6)_2$ in d_6-DMSO.

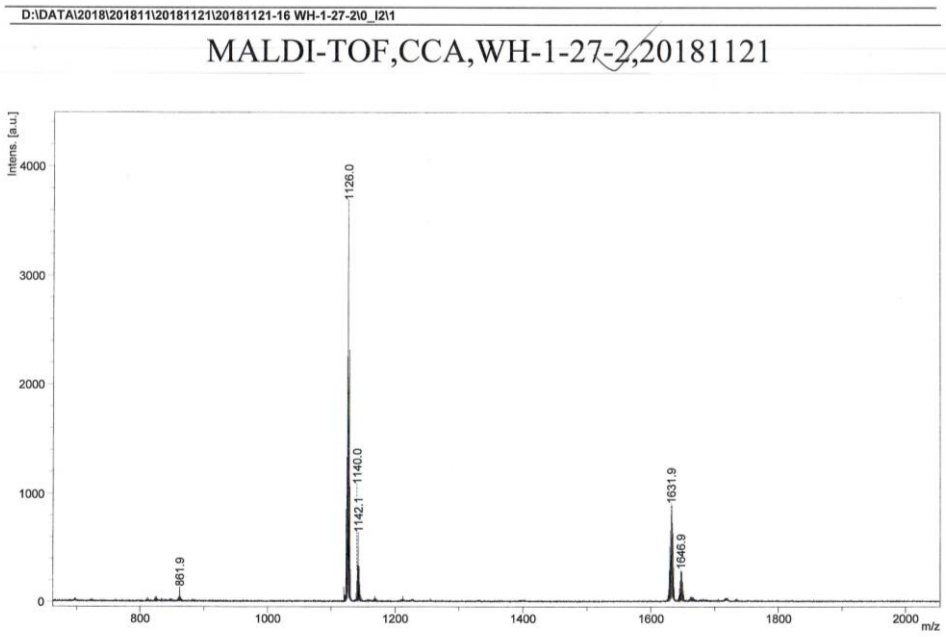

Figure S13. MALDI-TOF mass spectrum of **4**$(PF_6)_2$.

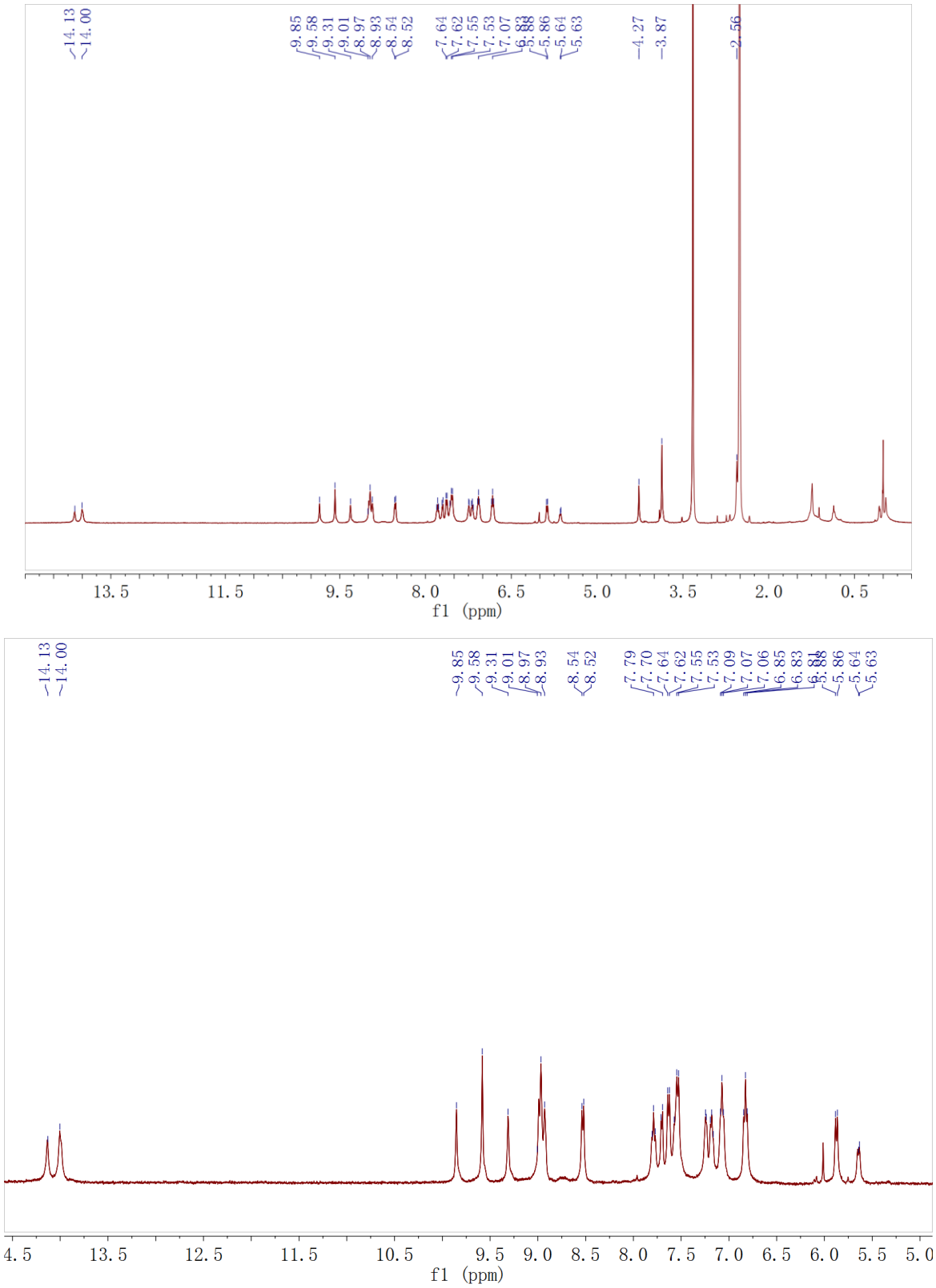

Figure S14. ^{1}H NMR spectrum of **5**$(PF_6)_2$ in d_6-DMSO.

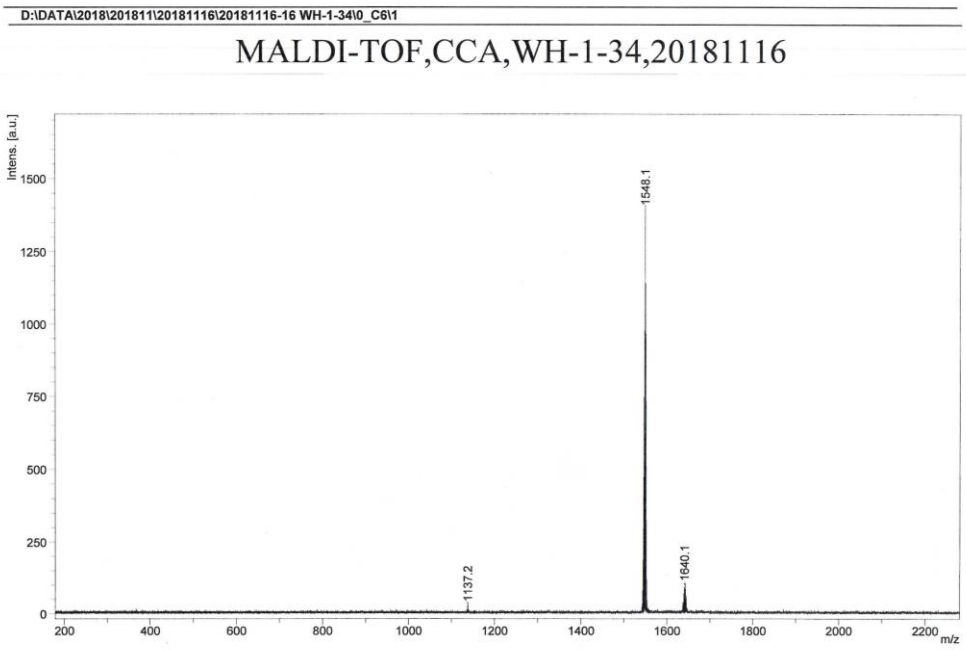

Figure S15. MALDI-TOF mass spectrum of **5**$(PF_6)_2$.

Cartesian coordinates of DFT-optimized structure of $\mathbf{3}^{3+}$ with UB3LYP:
Charge = 3; multiplicity=2

Ru	-5.51219910	0.08702942	-0.01532166
N	-5.09045541	-0.28286628	-2.10108798
N	-3.52667632	-0.59137681	-3.66591959
N	-5.03703590	0.44001439	2.06445421
N	-3.43035509	0.67716157	3.59824558
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C	-7.09303591	-0.50155804	-3.64443091
C	-7.42718981	-0.72268723	-4.97726391
C	-6.43716209	-0.91777997	-5.96650576
C	-5.08046902	-0.89810649	-5.65313557
C	-4.74522807	-0.67544920	-4.31433682
C	-3.76820198	-0.35679055	-2.35235894
C	-2.84104420	-0.17925616	-1.24271611
C	-3.55067080	0.04483095	-0.03334964
C	-2.81147442	0.23004204	1.16461042
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C	-4.63079983	0.82156191	4.26947492
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C	-5.64370589	0.66955946	3.28770072
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H	-8.47665254	-0.74612093	-5.26733472
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H	-8.33497099	1.08099978	5.29291943
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C	-6.98081202	-4.54240872	0.78856362
C	-5.19033538	-2.97361806	0.49460265
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C	-7.87651389	-3.48760826	0.62611812
N	-6.04876896	-1.94852793	0.33569469
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C	5.05704204	1.28578227	-5.60991787
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H	8.97007572	3.55242530	0.86071732
C	7.41195479	1.07171540	-4.97573250
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C	5.21439434	2.85150823	0.66441956
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C	8.31679608	0.95079714	0.21396950

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C	12.63304296	0.59499879	0.82585547

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H	12.10697611	1.25049129	1.51899331
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H	14.55173500	-1.75347733	-1.58104027
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H	16.66989510	-0.60368294	-0.95985453
H	16.67650500	0.65670905	0.29751218
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H	-14.52612414	-1.32801438	1.56473823
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H	-16.63012928	0.59222970	-0.82435112
H	-16.63653471	-0.66698832	0.43424292

Cartesian coordinates of DFT-optimized structure of **4**$^{3+}$ with UB3LYP:
Charge = 3; multiplicity=2

Ru	-5.50585511	0.10223656	-0.02583742
N	-5.09004765	-0.27988996	-2.10586539
N	-3.54007561	-0.59947209	-3.68055122
N	-5.02022941	0.47163392	2.04497366
N	-3.41125799	0.72613574	3.57190192
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C	-7.10686569	-0.51317639	-3.62772516
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C	-2.79952388	0.25872404	1.14048244
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C	-1.44818438	-0.20623311	-1.28456541
C	-3.69169988	0.48830726	2.26763145
C	-4.61061397	0.87448555	4.24415985
C	-4.90552464	1.13080877	5.58641463
C	-6.25237784	1.22020743	5.92781243
C	-7.27192354	1.05984378	4.96241734
C	-6.97818085	0.80477001	3.62632463
C	-5.62592538	0.71145450	3.26660419
H	-7.86264855	-0.35628614	-2.86035475
H	-8.50420103	-0.77339198	-5.23614726
H	-6.78525161	-1.12814142	-6.97869346
H	-4.35171536	-1.08040353	-6.41555965
H	-0.85682262	0.39867968	2.04975980
H	-0.92161142	-0.41609012	-2.21447590
H	-4.11652768	1.25393406	6.32655765
H	-6.52703766	1.41873616	6.96270178
H	-8.31247858	1.13833545	5.27405530
H	-7.76395916	0.68198011	2.88349899
H	-4.81978265	-5.05003283	0.79756793
C	-5.56252640	-4.26245219	0.69978909
C	-6.93002609	-4.52982293	0.79918174
C	-5.15081082	-2.95332387	0.47089744
H	-4.09568056	-2.70445881	0.39002449
C	-7.83099533	-3.47264533	0.66449711
N	-6.01438498	-1.92916868	0.33741761
H	-8.89904616	-3.66544005	0.73885454

C	-7.35942781	-2.18249578	0.43242067
C	-8.25471560	-1.01700386	0.27182616
H	-10.19784499	-1.94375806	0.53768492
C	-9.64938976	-1.02502362	0.34712620
N	-7.59691653	0.13307426	0.03620014
N	-5.97309360	2.14387674	-0.37865387
H	-4.03818262	2.85140633	-0.58740586
C	-8.23007600	1.30907956	-0.13510615
C	-10.33219383	0.18547942	0.17406221
C	-5.08762400	3.13499390	-0.59724885
C	-7.31154664	2.44157168	-0.37884442
C	-9.62215168	1.36733237	-0.07016766
C	-5.47537535	4.45018877	-0.82392077
C	-7.76076425	3.74300942	-0.60093791
H	-4.72595565	5.21931166	-0.99614115
H	-10.16397166	2.30106859	-0.20234214
C	-6.83608056	4.76434458	-0.82711560
H	-8.82652977	3.95722478	-0.59866070
C	1.47498194	-0.37202057	1.09984056
H	4.85098837	4.91439197	1.12523217
C	6.96443838	4.41233484	1.05500564
C	5.59707591	4.14224637	0.95621094
H	6.77193809	1.53919346	-6.94458989
C	6.46783363	1.28696199	-5.92981155
H	4.34400539	1.43496849	-6.36538020
C	5.11123172	1.23233959	-5.61985746
C	7.87013212	3.37569424	0.82521944
H	8.93791693	3.57058377	0.89757818
C	7.45938495	1.02290115	-4.95838317
H	8.50864332	1.07698759	-5.24500777
C	5.19080534	2.85125429	0.63461880
C	4.77759252	0.90391653	-4.30273913
H	4.13626446	2.60105659	0.55036189
C	7.12677027	0.69600086	-3.64706334
N	3.55955344	0.76291467	-3.66287893
C	7.40335937	2.10254565	0.50559411
C	5.76467190	0.63723839	-3.31947794
N	6.05814302	1.84553235	0.41235737
H	10.24524435	1.88433118	0.53042314
H	7.89054852	0.49224810	-2.89887831
C	3.80234910	0.43103806	-2.37099231
N	5.12547346	0.34584699	-2.12648027
C	9.69963710	0.97428953	0.29535047
C	8.30410165	0.95850251	0.25083514

C	2.87983076	0.17017259	-1.27535517
C	1.49030852	0.20427719	-1.28235585
Ru	5.56703192	-0.16017644	-0.07680732
C	10.38834864	-0.21650934	0.03033304
C	3.59710424	-0.13386396	-0.08832777
N	7.64943462	-0.18127352	-0.04270145
C	0.75900432	-0.06300133	-0.09093284
C	2.86336763	-0.40547192	1.09615295
C	8.28846917	-1.33949923	-0.29997263
C	9.68201787	-1.38796133	-0.27032752
N	5.09312688	-0.65793351	1.96758462
C	3.76612738	-0.69944482	2.19919236
N	6.03211062	-2.17377035	-0.55631837
H	7.84482469	-0.90243676	2.76794453
C	5.71072127	-0.97294198	3.16637619
C	7.37278896	-2.46244954	-0.59320863
C	7.06661822	-1.08007063	3.50769859
H	10.22813425	-2.30639491	-0.47295596
N	3.49917582	-1.02434402	3.48800885
C	4.70539139	-1.20757900	4.13934365
C	5.15040780	-3.15796494	-0.81824219
H	4.09957948	-2.88246133	-0.77811850
C	7.37433109	-1.42150266	4.82141441
C	7.82645240	-3.74714439	-0.89169892
H	8.41816057	-1.51321031	5.11812422
C	5.01402759	-1.54993834	5.45894350
C	6.36464158	-1.65264487	5.78239547
H	8.89338518	-3.95413172	-0.91444827
C	5.54240883	-4.45582390	-1.12304758
H	4.23261225	-1.72737361	6.19611101
C	6.90496399	-4.76101203	-1.16058297
H	6.64955617	-1.91750532	6.79952309
H	4.79535988	-5.21934832	-1.32734259
H	0.92801778	-0.61119829	2.01049232
H	0.95622816	0.47040862	-2.19346923
C	-7.24822603	6.18355194	-1.07390148
O	-6.45261470	7.08539216	-1.27229602
O	-8.57461844	6.34004029	-1.05122612
C	-7.47782524	-5.90306392	1.04304150
O	-8.66880738	-6.13916011	1.15274152
O	-6.51581143	-6.82599762	1.12236574
C	-11.82649328	0.27108751	0.24477300
O	-12.44576967	1.31120895	0.09877482
O	-12.39457320	-0.91422401	0.48505337

C	-6.95081132	-8.18599416	1.35450578
H	-7.59992649	-8.51583616	0.53710218
H	-6.03488361	-8.77893292	1.38577794
H	-7.48809118	-8.24994242	2.30612525
C	-13.83825245	-0.92660696	0.57207582
H	-14.27332098	-0.58534683	-0.37266318
H	-14.10499737	-1.96672181	0.76834380
H	-14.16966108	-0.27935194	1.39034397
C	-9.06526042	7.68117642	-1.28161389
H	-10.15251487	7.60264228	-1.22527541
H	-8.68371356	8.35700583	-0.50961210
H	-8.75130151	8.02978172	-2.27067202
H	2.60028700	0.89034519	-4.09848303
H	2.53184703	-1.12096951	3.91369519
H	-2.43910226	0.78719144	3.99498199
H	-2.58464388	-0.70108043	-4.13287152
C	7.50554942	5.76650274	1.39698788
O	8.69679546	6.00948305	1.48835056
O	6.53676976	6.66633579	1.58824626
C	11.88380370	-0.29137691	0.05854877
O	12.50863768	-1.31485037	-0.16338548
O	12.44882927	0.88367402	0.35331772
C	7.32175648	-6.16253228	-1.48520798
O	6.52955422	-7.05652385	-1.72874028
O	8.64911527	-6.31516229	-1.47414694
C	6.96562543	8.00659402	1.92255850
H	7.58238866	8.41466234	1.11545851
H	6.04538466	8.58259382	2.03622259
H	7.53510080	7.99555279	2.85739769
C	13.89400276	0.90424205	0.40380979
H	14.15796246	1.93394942	0.65195877
H	14.25182183	0.21482089	1.17519924
H	14.30701158	0.62081587	-0.56950391
C	9.14375312	-7.64131445	-1.77168585
H	10.23085104	-7.56212625	-1.71294154
H	8.76569228	-8.35611385	-1.03378550
H	8.82968473	-7.94172641	-2.77640964

Cartesian coordinates of DFT-optimized structure of $\mathbf{5}^{3+}$ with UB3LYP:
Charge = 3; multiplicity=2

Ru	-5.55804527	0.09717161	-0.02937927
N	-5.12906763	-0.45960515	-2.07012683
N	-3.58950068	-0.89634740	-3.62946082
N	-5.01714391	0.65663619	1.98361959
N	-3.39078552	1.07560873	3.45713539
C	-5.78812789	-0.79167870	-3.24345903
C	-7.15518191	-0.87821399	-3.54062429
C	-7.51214572	-1.24640531	-4.83552137
C	-6.53848975	-1.52338636	-5.81977486
C	-5.17584682	-1.44038733	-5.53966790
C	-4.81900259	-1.07137457	-4.24007783
C	-3.80875420	-0.53328129	-2.34000450
C	-2.86591901	-0.23346503	-1.27378091
C	-3.55843369	0.09098963	-0.08521738
C	-2.80375882	0.39961860	1.06885672
C	-1.40753105	0.38116731	1.04352221
C	-0.72322373	0.05409867	-0.15027944
C	-1.46879697	-0.25124047	-1.31278896
C	-3.68414172	0.71345031	2.18239256
C	-4.58332283	1.26909266	4.13200403
C	-4.86413316	1.64597432	5.44779802
C	-6.20832410	1.74951509	5.80067251
C	-7.23728799	1.48555990	4.87068496
C	-6.95610998	1.10939388	3.55949435
C	-5.60837490	1.00097738	3.18950633
H	-7.90614152	-0.66398149	-2.78234894
H	-8.56659923	-1.32278234	-5.09695284
H	-6.85947374	-1.80822109	-6.82064796
H	-4.42184526	-1.65293474	-6.29592119
H	-0.83760747	0.64200048	1.93522929
H	-0.94589802	-0.52863236	-2.22814296
H	-4.06736691	1.84898664	6.16163003
H	-6.47085073	2.04096148	6.81656636
H	-8.27495182	1.57888124	5.18788620
H	-7.74989040	0.90710308	2.84289221
H	-4.74326552	-4.93698532	1.30486785
C	-5.49965268	-4.17561193	1.13327217
C	-6.86243280	-4.45293309	1.28106524
C	-5.11439357	-2.89317068	0.75913958
H	-4.06508384	-2.63695632	0.63565560
C	-7.78243882	-3.43050170	1.04460813
N	-5.99430344	-1.89860216	0.53091024
H	-8.84594433	-3.63098762	1.15408355

C	-7.33587366	-2.16394181	0.67180066
C	-8.25293619	-1.03609077	0.40745111
H	-10.17575358	-1.96589570	0.77345425
C	-9.64549533	-1.05988167	0.49259994
N	-7.61369759	0.10127420	0.05765331
N	-6.03246480	2.09085590	-0.55979066
H	-4.11531648	2.81129467	-0.85266738
C	-8.27469998	1.24710634	-0.21951329
C	-10.35449537	0.11558750	0.20806573
C	-5.16937156	3.07625684	-0.87728995
C	-7.37833764	2.36712402	-0.57332677
C	-9.66670005	1.28253398	-0.15186960
C	-5.58107877	4.35841823	-1.21727761
C	-7.85183772	3.63706671	-0.90464305
H	-4.84764422	5.12167677	-1.46652008
H	-10.22736535	2.18878153	-0.36887363
C	-6.94822793	4.64980962	-1.23199926
H	-8.92096870	3.83327314	-0.90792622
C	1.47622395	-0.36834723	0.98519940
H	4.98444932	4.97016319	1.06999109
C	7.07649933	4.38686906	1.13776251
C	5.71472862	4.17539722	0.92930332
H	6.77571319	2.10068467	-6.89862672
C	6.46738896	1.77698602	-5.90563720
H	4.34576665	1.96782172	-6.33463654
C	5.11000022	1.70728993	-5.60422700
C	7.96323287	3.33082410	0.93626045
H	9.03200009	3.47182302	1.08613155
C	7.45551614	1.43765265	-4.95368581
H	8.50563113	1.50725092	-5.23363105
C	5.28469673	2.91272904	0.53087187
C	4.77107485	1.28626298	-4.31504178
H	4.23218150	2.70173311	0.35751257
C	7.11853294	1.01812655	-3.67076791
N	3.54975151	1.10801280	-3.69080430
C	7.47740613	2.08524720	0.53661379
C	5.75484116	0.94338868	-3.35217205
N	6.13573104	1.88701490	0.34390674
H	10.28867260	1.76408487	0.68821485
H	7.87930853	0.75765870	-2.93731722
C	3.78512481	0.68365365	-2.42678485
N	5.10918501	0.57209053	-2.18651136
C	9.73609190	0.87635999	0.38906510
C	8.34671703	0.91725584	0.27579282

C	2.86210225	0.35145440	-1.35266996
C	1.46415341	0.38653074	-1.34500285
Ru	5.55092705	-0.08707633	-0.20055157
C	10.42350082	-0.31416506	0.08391887
C	3.57165856	-0.03625915	-0.19746022
N	7.66627574	-0.16930768	-0.12502752
C	0.75669632	0.02629121	-0.17561817
C	2.86698584	-0.39570024	0.97078925
C	8.28369515	-1.31929718	-0.44270087
C	9.67049303	-1.42492972	-0.34242009
N	5.10968592	-0.73587860	1.81800900
C	3.78169045	-0.77528432	2.04703094
N	6.02646287	-2.04286827	-0.91141842
H	7.86013570	-1.06795411	2.60726328
C	5.72365288	-1.13651022	2.99456947
C	7.35353135	-2.38050573	-0.88652759
C	7.07636725	-1.28306015	3.33072020
H	10.16767310	-2.36395077	-0.57481716
N	3.51082496	-1.18002785	3.30730565
C	4.71409695	-1.42146021	3.94816743
C	5.12304982	-2.94940072	-1.32947966
H	4.08503022	-2.62539841	-1.33516029
C	7.37460737	-1.71378083	4.62076538
C	7.77244875	-3.65254572	-1.27875572
H	8.41640179	-1.83785027	4.91290586
C	5.01200663	-1.85324920	5.24326063
C	6.36017135	-1.99457872	5.56254746
H	8.83082082	-3.90512523	-1.25461688
C	5.48537754	-4.23233406	-1.73012138
H	4.22520029	-2.06802051	5.96455828
C	6.83225376	-4.59002907	-1.70229413
H	6.63885932	-2.32893082	6.56068947
H	4.71544616	-4.92904224	-2.05657176
H	0.92682586	-0.67220289	1.87556000
H	0.91417124	0.71278690	-2.22703083
C	-7.38646480	6.03341409	-1.59571057
O	-6.61045801	6.92712503	-1.88975712
O	-8.71559993	6.17554157	-1.55964830
C	-7.38110789	-5.79774632	1.68280307
O	-8.56713402	-6.05089286	1.81273676
O	-6.39863810	-6.68258678	1.88218272
C	-11.84658995	0.17730449	0.27742731
O	-12.49203474	1.18392186	0.03411755
O	-12.39140359	-0.99136316	0.63594060

C	-6.80650315	-8.01299331	2.27441734
H	-7.43942259	-8.45547682	1.49851386
H	-5.87859614	-8.57719135	2.38543579
H	-7.35271255	-7.97392854	3.22234084
C	-13.83330867	-1.02295686	0.73021879
H	-14.27872690	-0.78209191	-0.24032480
H	-14.07976514	-2.04436755	1.02635344
H	-14.17622315	-0.30714875	1.48422670
C	-9.22805179	7.48595954	-1.89256596
H	-10.31284923	7.40093087	-1.80539177
H	-8.83921177	8.23023576	-1.19024024
H	-8.94047343	7.75292851	-2.91455613
H	7.44861297	5.36188583	1.45016085
H	7.15172802	-5.58525774	-2.00918432
H	2.59141546	1.27385115	-4.11883407
H	2.53902558	-1.29064345	3.72665602
H	-2.41641866	1.19137762	3.85608376
H	-2.63948192	-1.02238316	-4.08051947
C	11.89807196	-0.39545072	0.20240696
C	12.64732382	-1.23287137	-0.64330719
C	12.58954470	0.36469547	1.16328861
C	14.03451429	-1.30339597	-0.53049262
H	12.14789554	-1.81325744	-1.41810614
C	13.97580282	0.28469195	1.27327160
H	12.03881157	1.00910869	1.84756619
C	14.72560301	-0.55137376	0.43131537
H	14.59254763	-1.94916255	-1.20865712
H	14.48579385	0.88000947	2.03096881
C	16.22547771	-0.65334691	0.57202772
H	16.49745179	-1.39058212	1.34226246
H	16.69355710	-0.97247417	-0.36677441
H	16.66471186	0.30602001	0.87220250