Supporting Information for

Ruthenium(II) Bipyridyl Complexes with Cyclometalated NHC Ligands

David Schleicher[†], Hendrik Leopold[†], Horst Borrmann[#], Thomas Strassner[†,]*

†Physikalische Organische Chemie, Technische Universität Dresden, 01069 Dresden, Germany; thomas.strassner@chemie.tu-dresden.de

 # Max-Planck-Institut für Chemische Physik fester Stoffe, 01187 Dresden, Germany; horst.borrmann@cpfs.mpg.de

Figure S1. ^{1}H NMR spectrum of complex **4** in chloroform

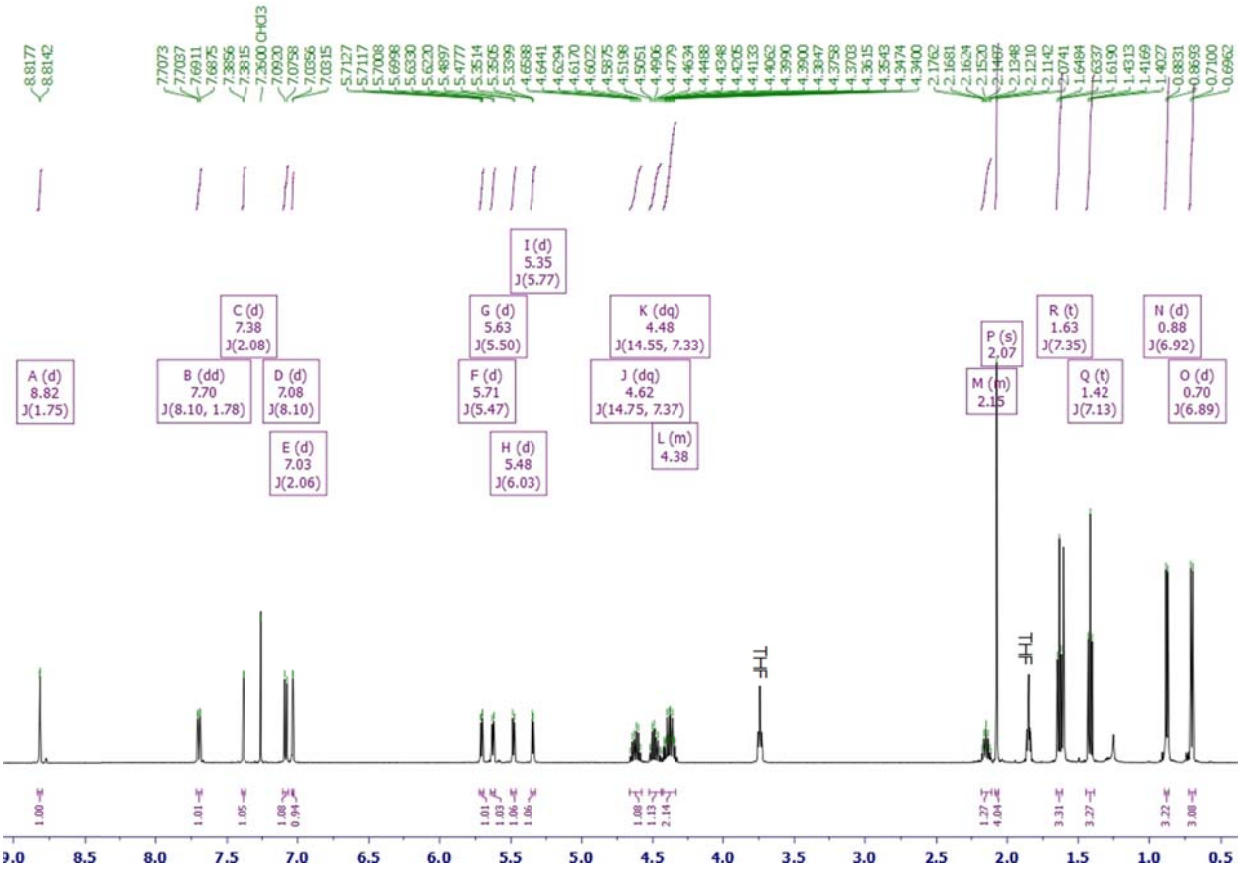


Figure S2. ^{13}C NMR spectrum of complex **4** in chloroform

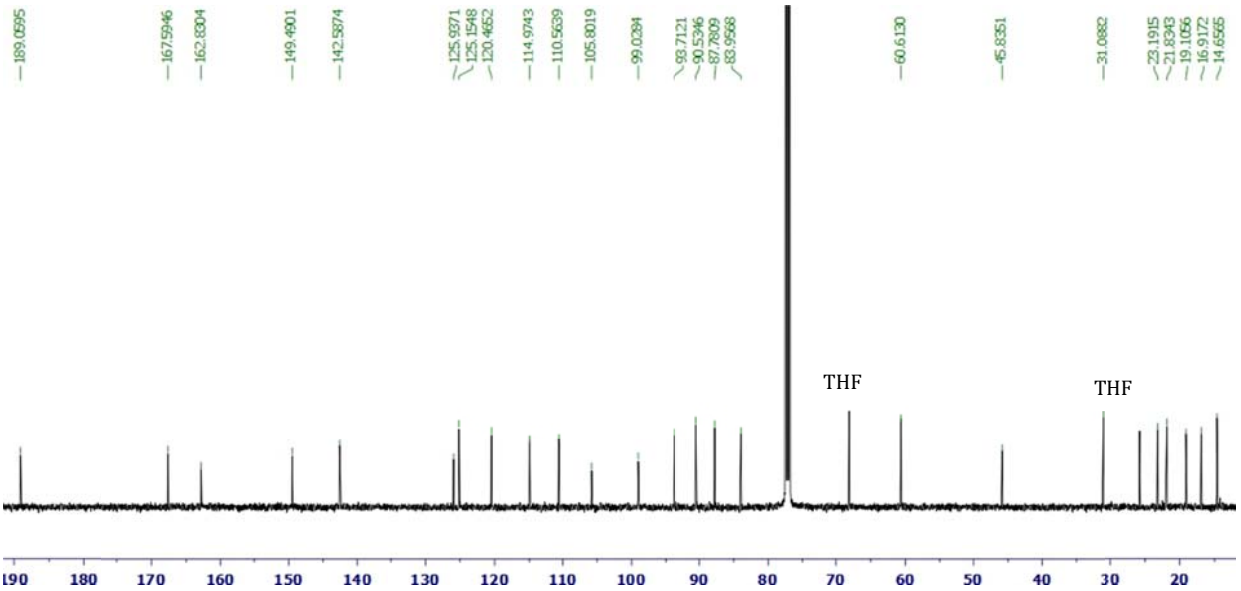


Figure S3. ^{1}H NMR spectrum of complex **5** in $CDCl_3$

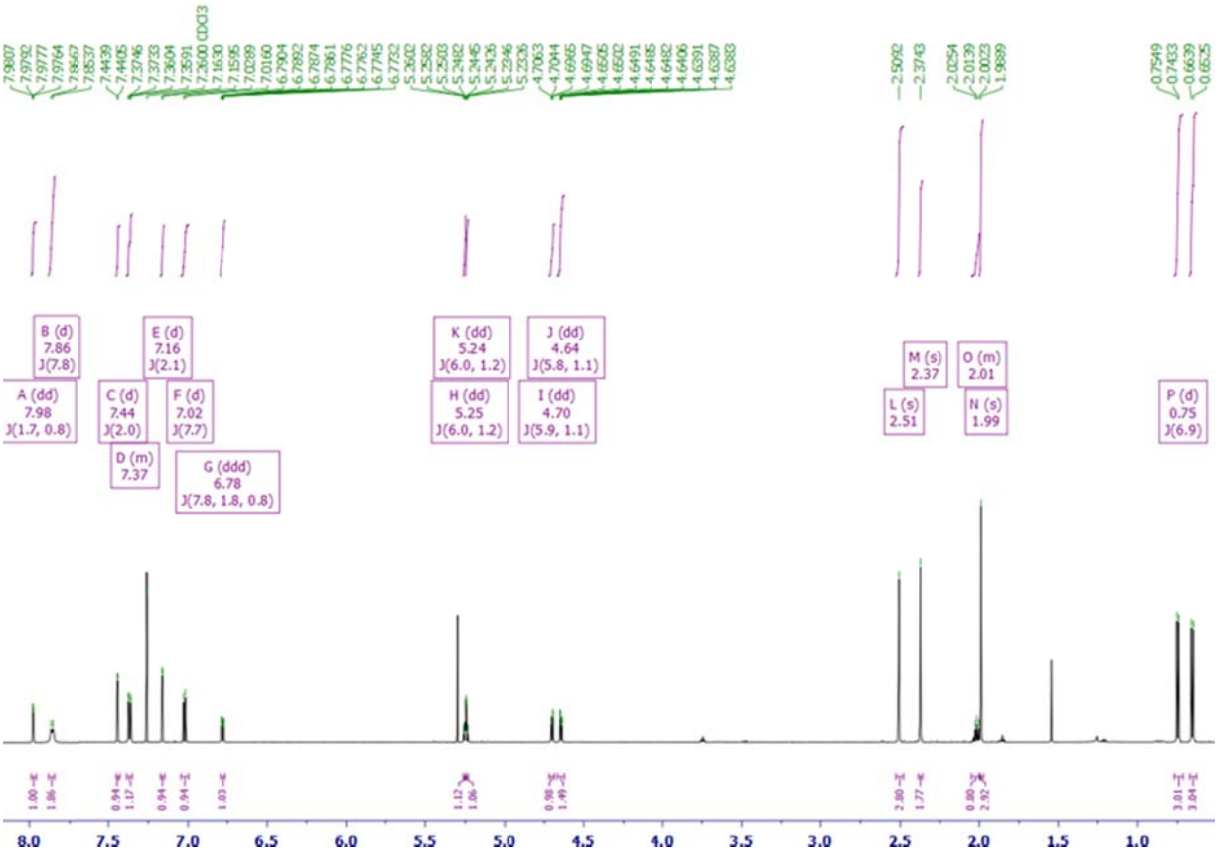


Figure S4. ^{13}C NMR spectrum of complex **5** in $CDCl_3$

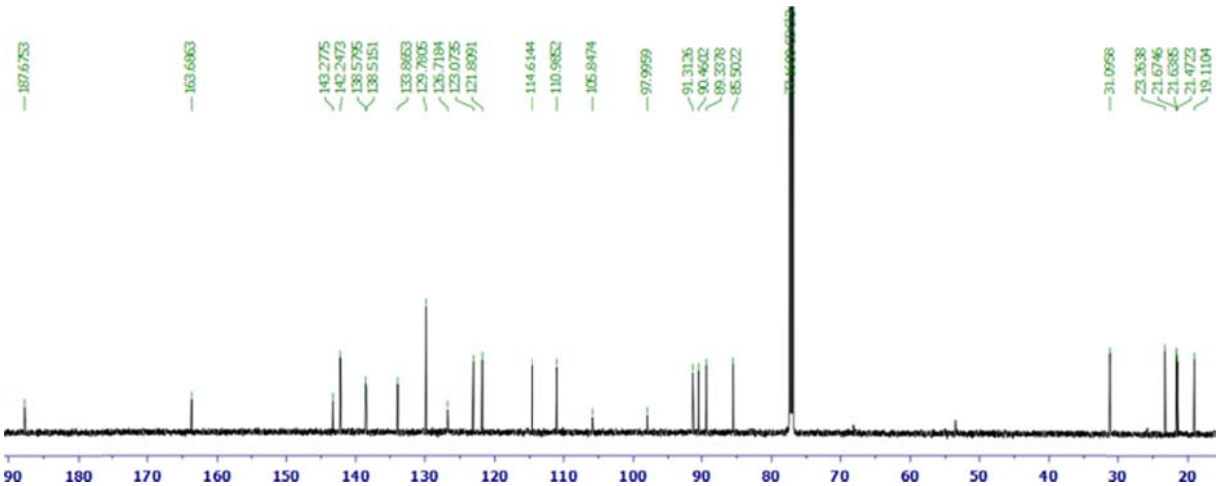


Figure S5. ^{1}H NMR spectrum of complex **6** in $CDCl_3$

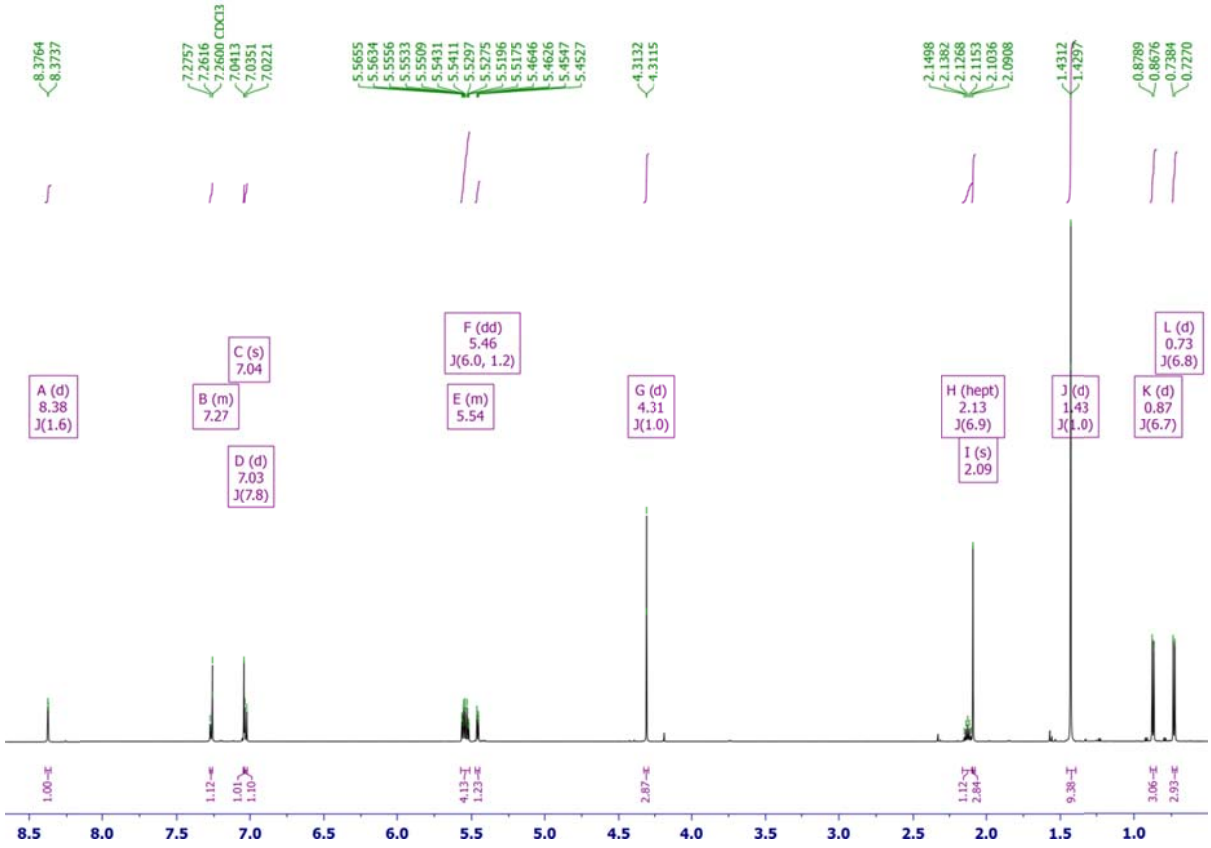


Figure S6. ^{13}C NMR spectrum of complex **6** in $CDCl_3$

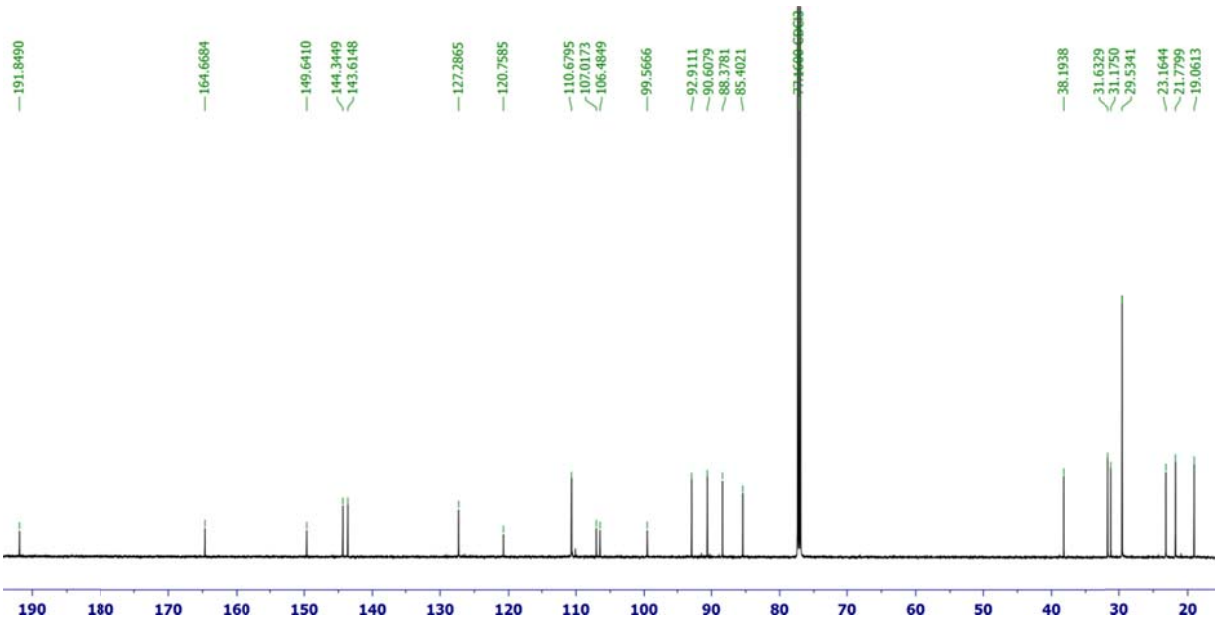


Table S1. Crystallographic details for complex **5**.

Chemical formula	$C_{27}H_{29}ClN_2Ru$
M_r	518.04
Crystal system, space group	Triclinic, P_{-1}
Temperature (K)	295
a, b, c (Å)	7.8688 (5), 12.2572 (11), 13.7691 (13)
α, β, γ (°)	113.513 (3), 96.555 (3), 91.984 (2)
V (Å^3)	1205.10 (18)
Z	2
F(000)	532
D_x (Mg m^{-3})	1.428
Radiation type	Mo Kα
μ (mm^{-1})	0.78
Crystal size (mm)	0.45 × 0.30 × 0.21
Diffractometer	Rigaku Saturn724+ (1x1 bin mode)
Absorption correction	Multi-scan R.H. Blessing, Acta Cryst. (1995), A51, 33-38
T_{min}, T_{max}	0.721, 0.854
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	33100, 7522, 7030
R_{int}	0.022
$(\sin \theta/\lambda)_{max}$ (Å^{-1})	0.724
R[$F^2 > 2\sigma(F^2)$], $wR(F^2)$, S	0.028, 0.075, 1.06
No. of reflections	7522
No. of parameters	358
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.61, −0.61

Table S2. Crystallographic details for complex **6**.

Chemical formula	$C_{25}H_{30}ClN_3Ru \cdot C_3H_6O$
M_r	567.12
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	198
a, b, c (Å)	15.3160 (16), 12.3740 (3), 16.444 (2)
β (°)	120.477 (8)
V (Å^3)	2685.9 (5)
Z	4
F(000)	1176
D_x (Mg m^{-3})	1.402
Radiation type	Mo Kα
μ (mm^{-1})	0.71
Crystal size (mm)	0.41 × 0.25 × 0.17
Diffractometer	KappaCCD diffractometer
Absorption correction	Multi-scan *SADABS* 2.10.(Sheldrick,Bruker AXS Inc.,2002)
T_{min}, T_{max}	0.760, 0.889
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	59470, 5509, 3770
R_{int}	0.110
$(\sin \theta/\lambda)_{max}$ (Å^{-1})	0.626
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.041, 0.137, 1.05
No. of reflections	5509
No. of parameters	316
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.62, −0.87

Figure S7. ^{1}H NMR spectrum of complex **11** in CD_3CN

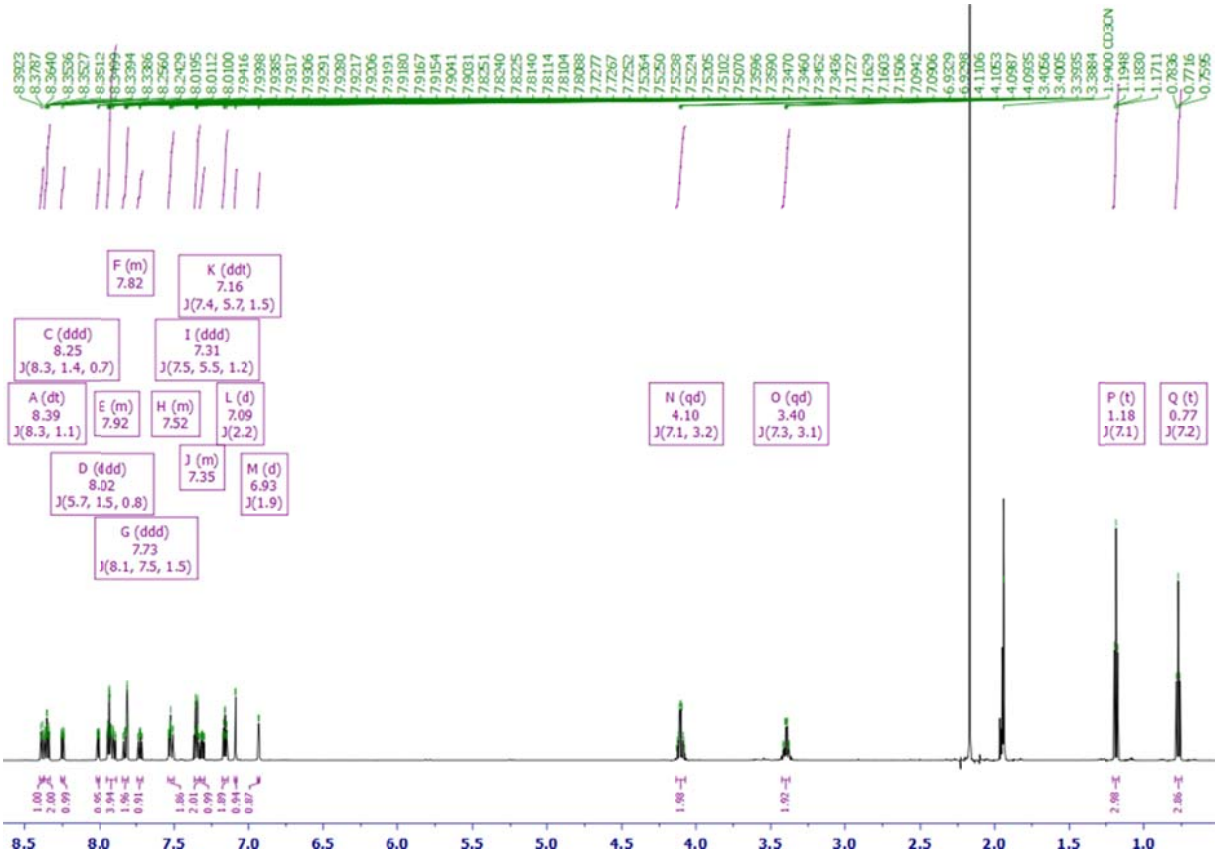


Figure S8. ^{13}C NMR spectrum of complex **11** in CD_3CN

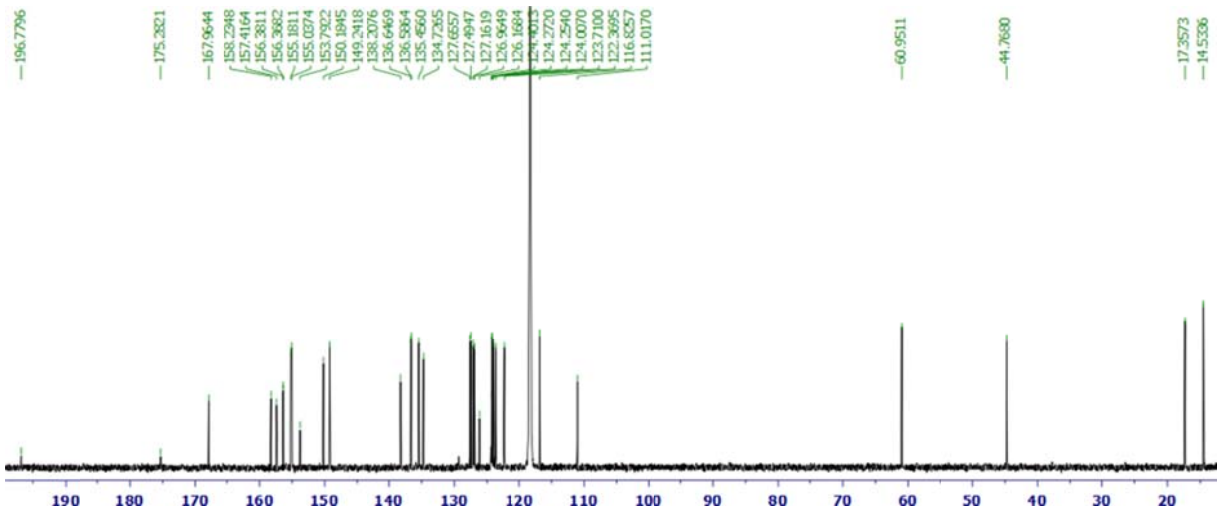


Figure S9. ^{1}H NMR spectrum of complex **12** in CD_3CN

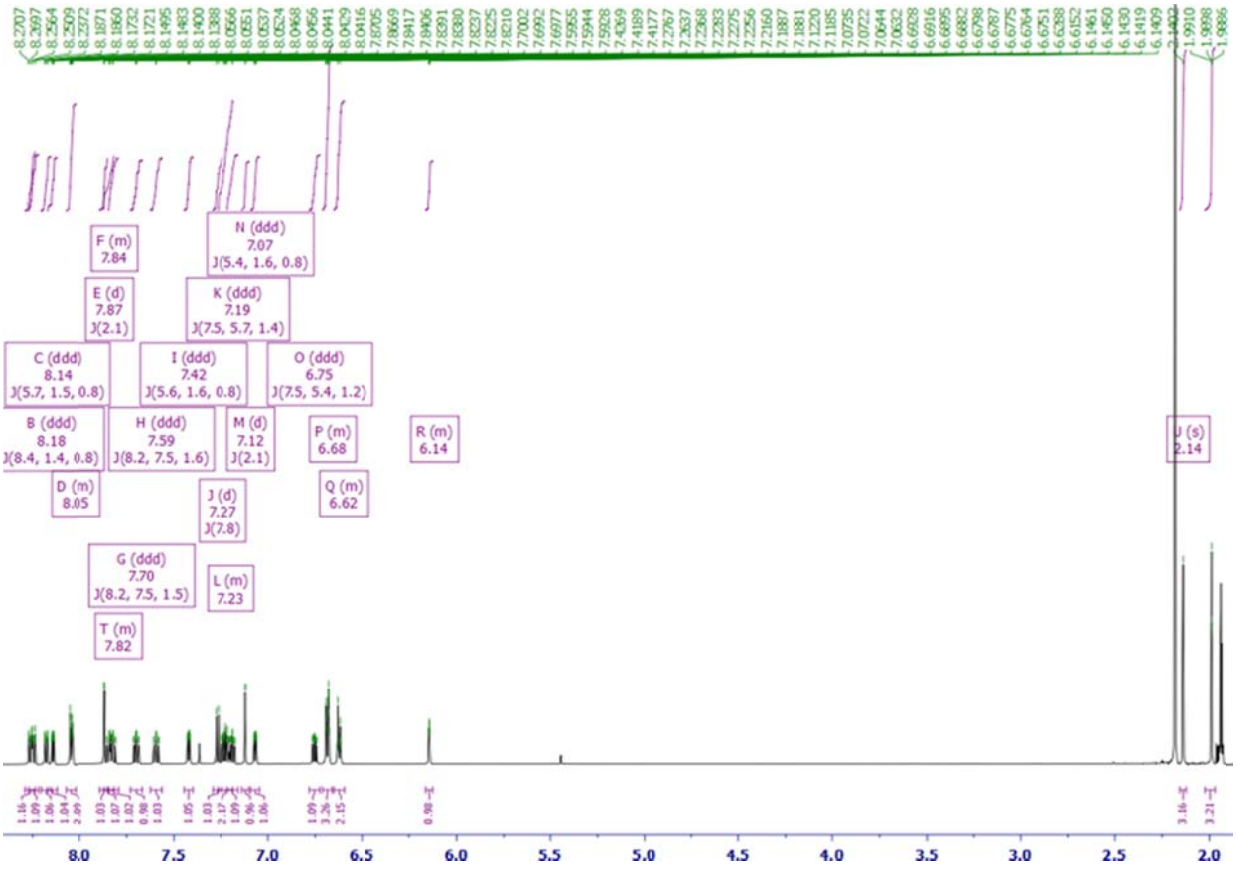


Figure S10. ^{13}C NMR spectrum of complex **12** in CD_3CN

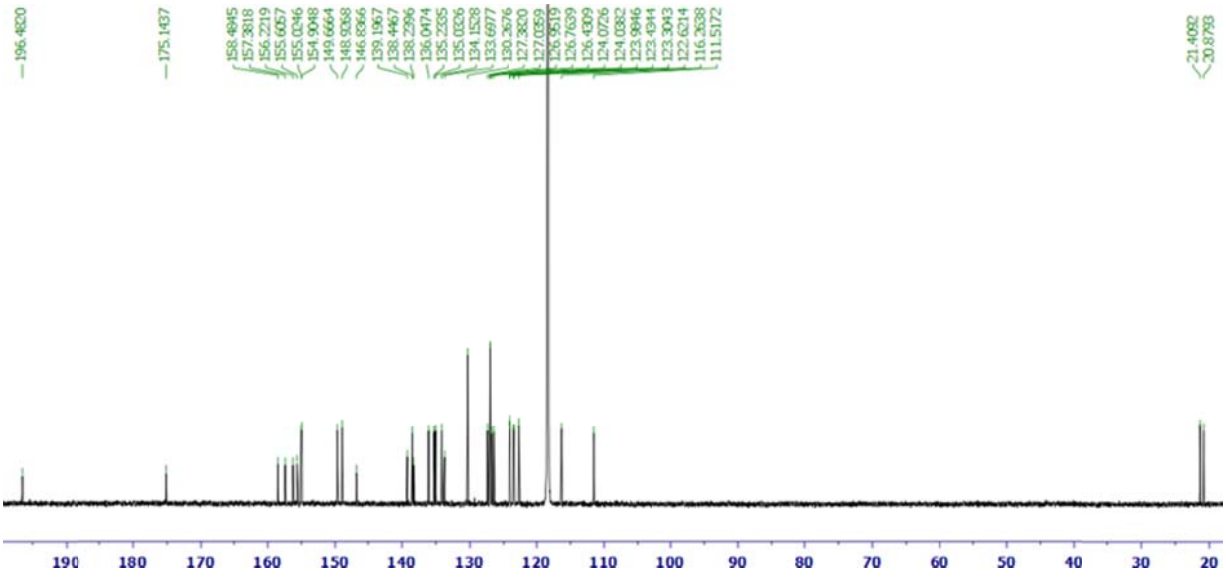


Figure S11. ^{1}H NMR spectrum of complex **13** in CD_3CN

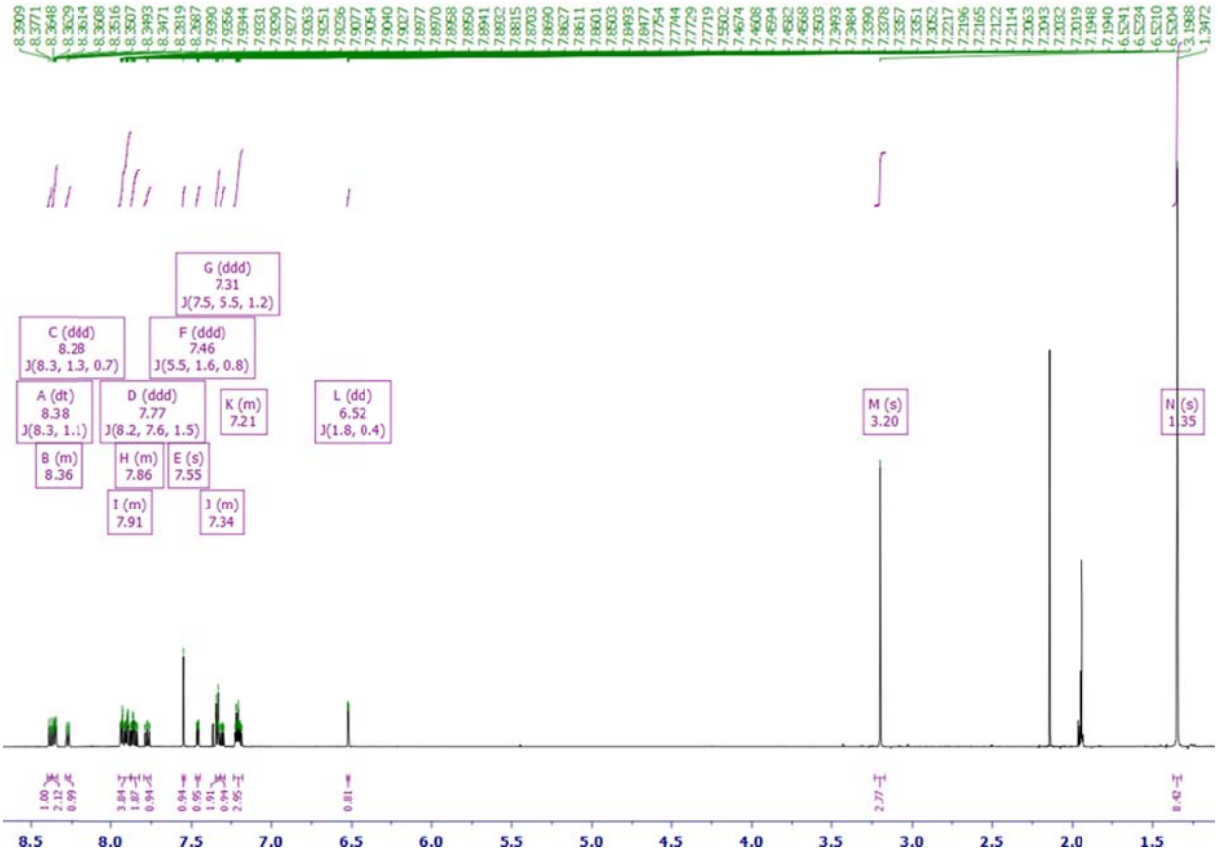


Figure S12. ^{13}C NMR spectrum of complex **13** in CD_3CN

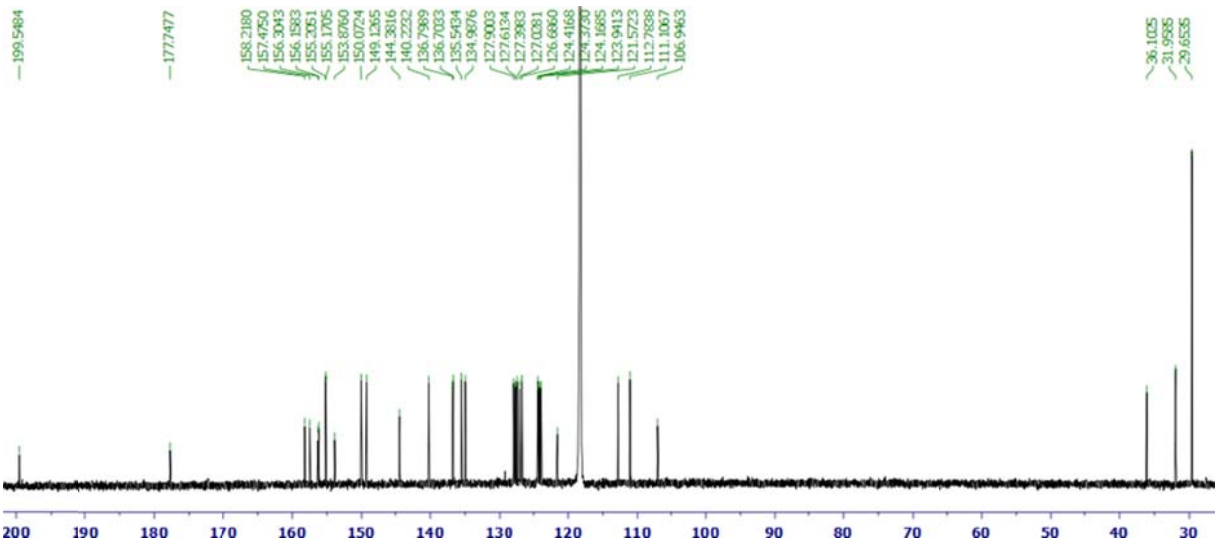


Figure S13. ^{1}H NMR spectrum of complex **14** in CD_3CN

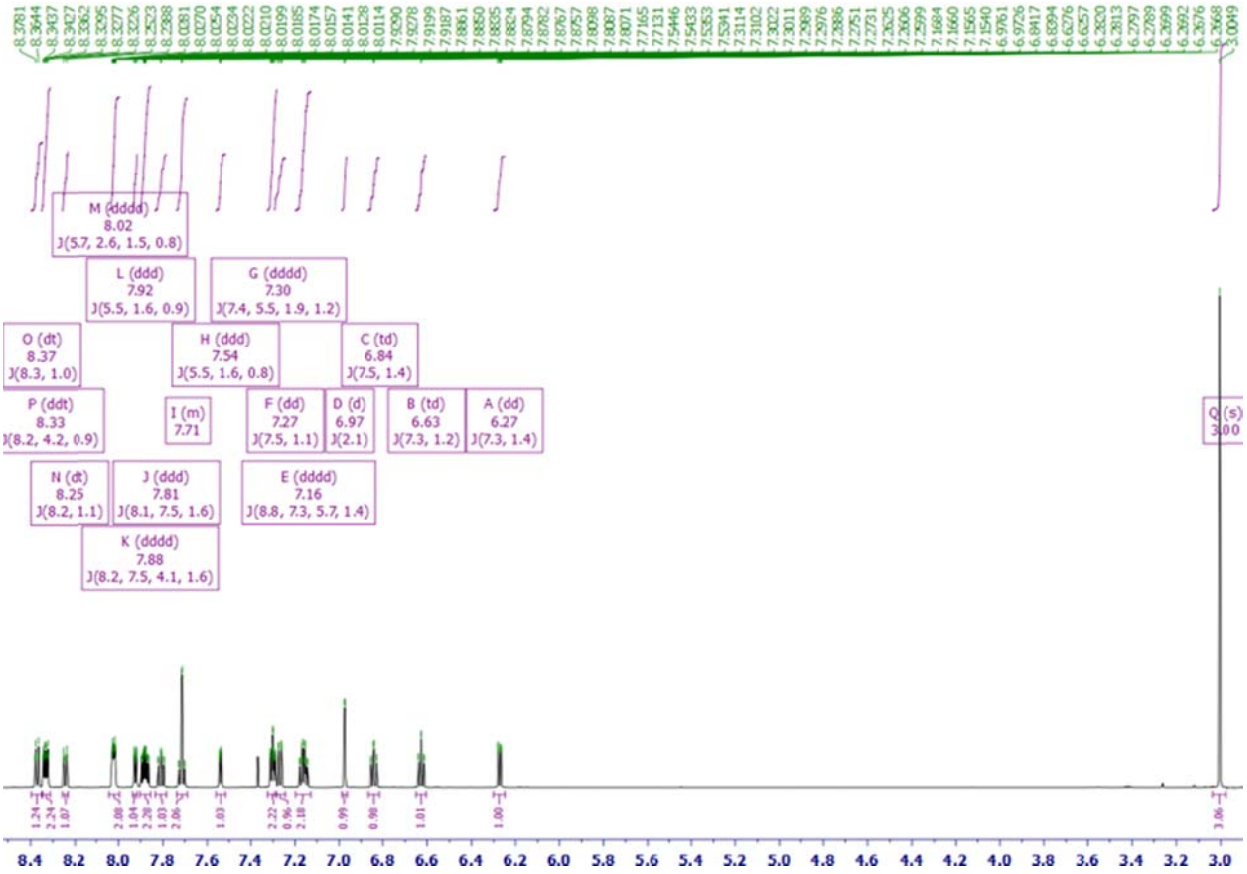


Figure S14. ^{13}C NMR spectrum of complex **14** in CD_3CN

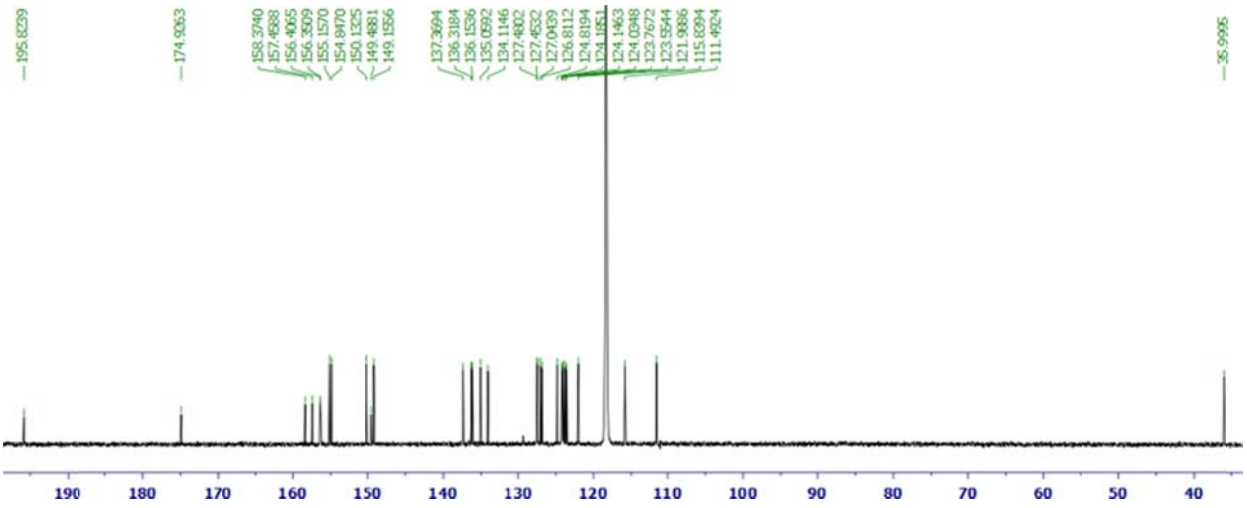


Figure S15. ^{1}H NMR spectrum of complex **15** in CD_3CN

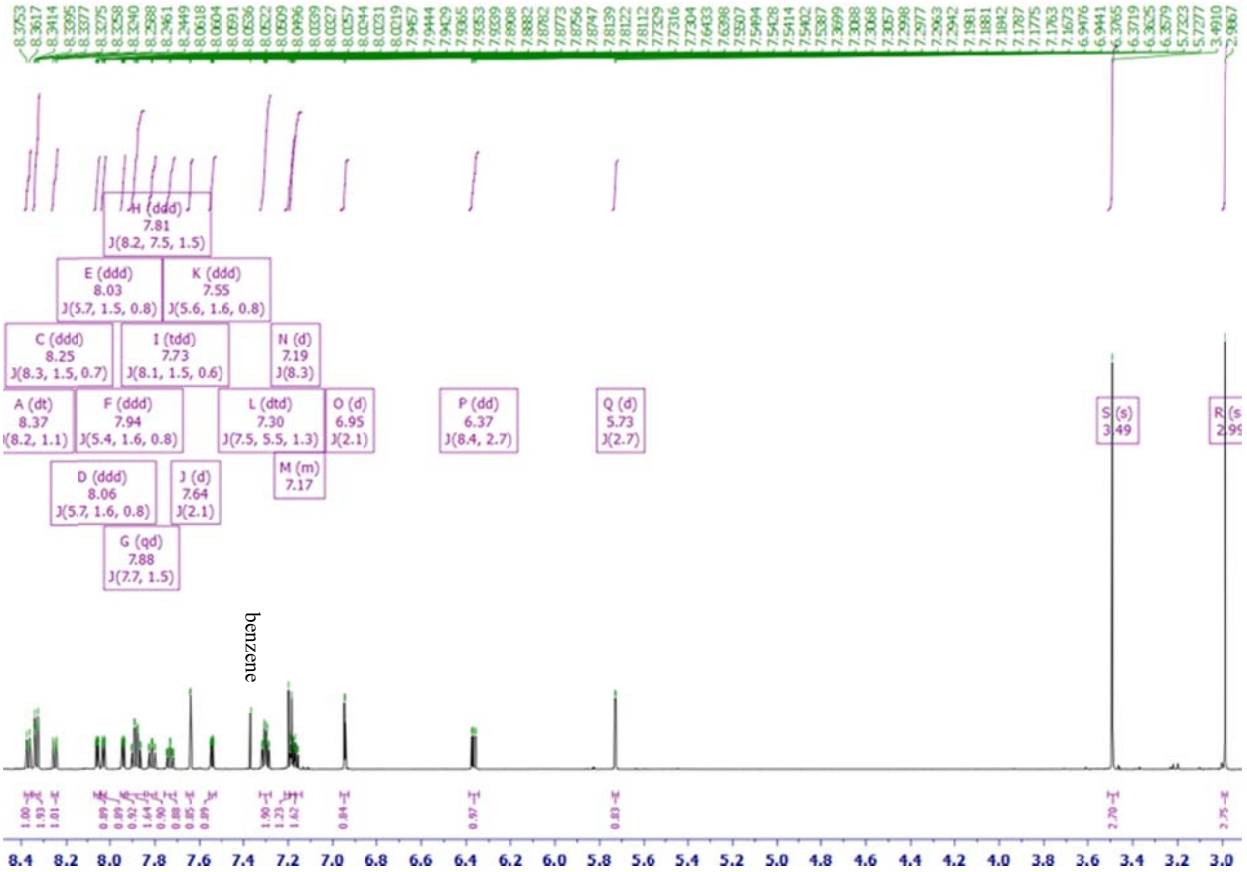


Figure S16. ^{13}C NMR spectrum of complex **15** in CD_3CN

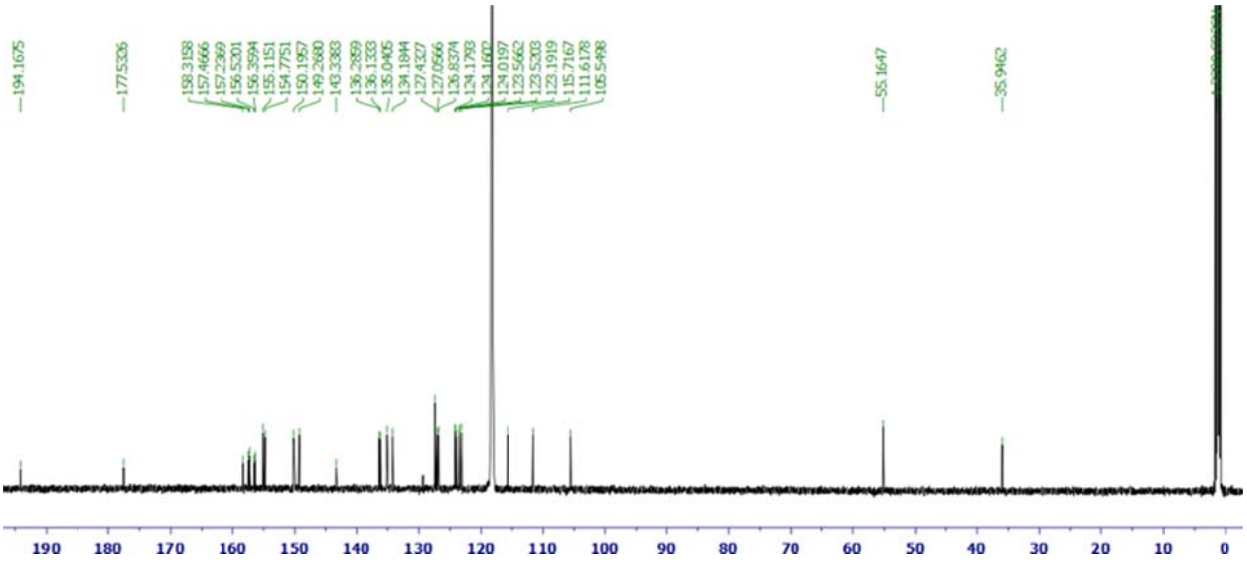


Figure S17. ^{1}H NMR spectrum of complex **16** in DMSO-d_6

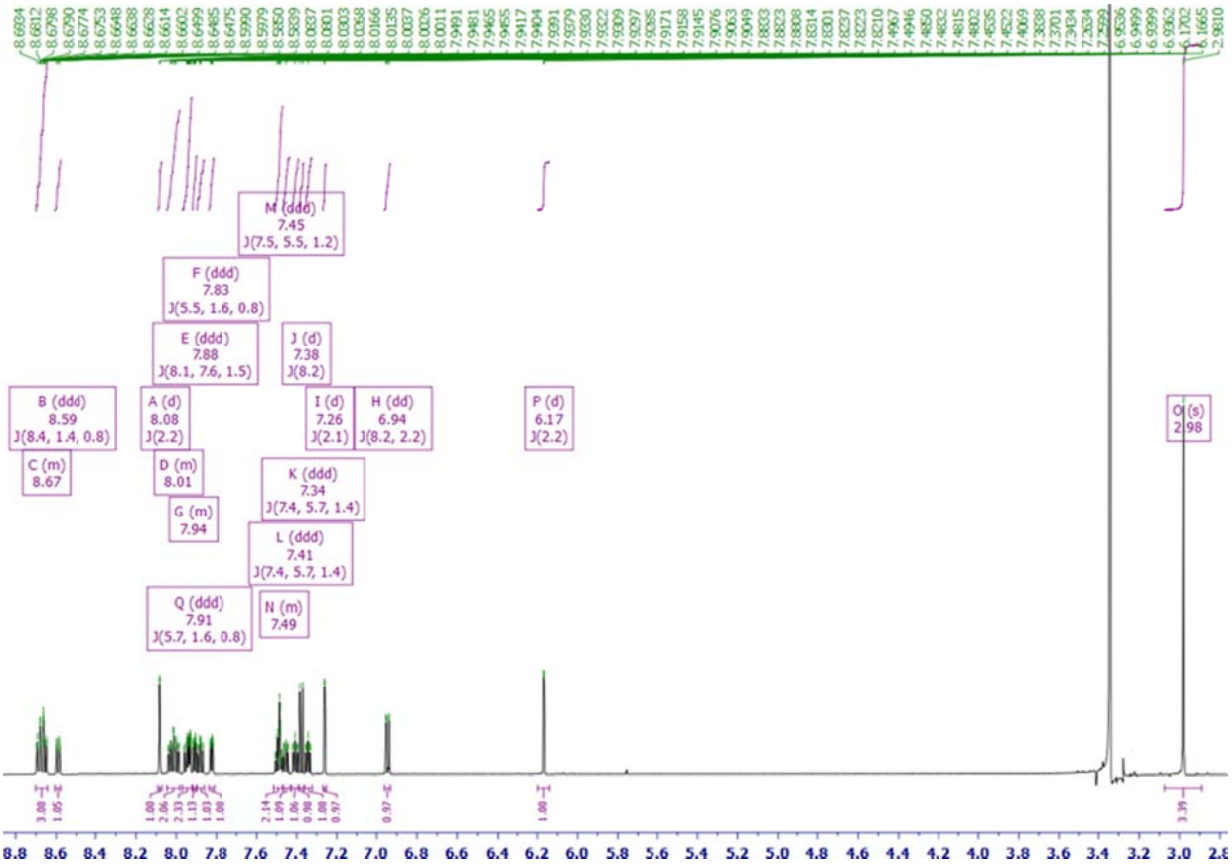


Figure S18. ^{13}C NMR spectrum of complex **16** in DMSO-d_6

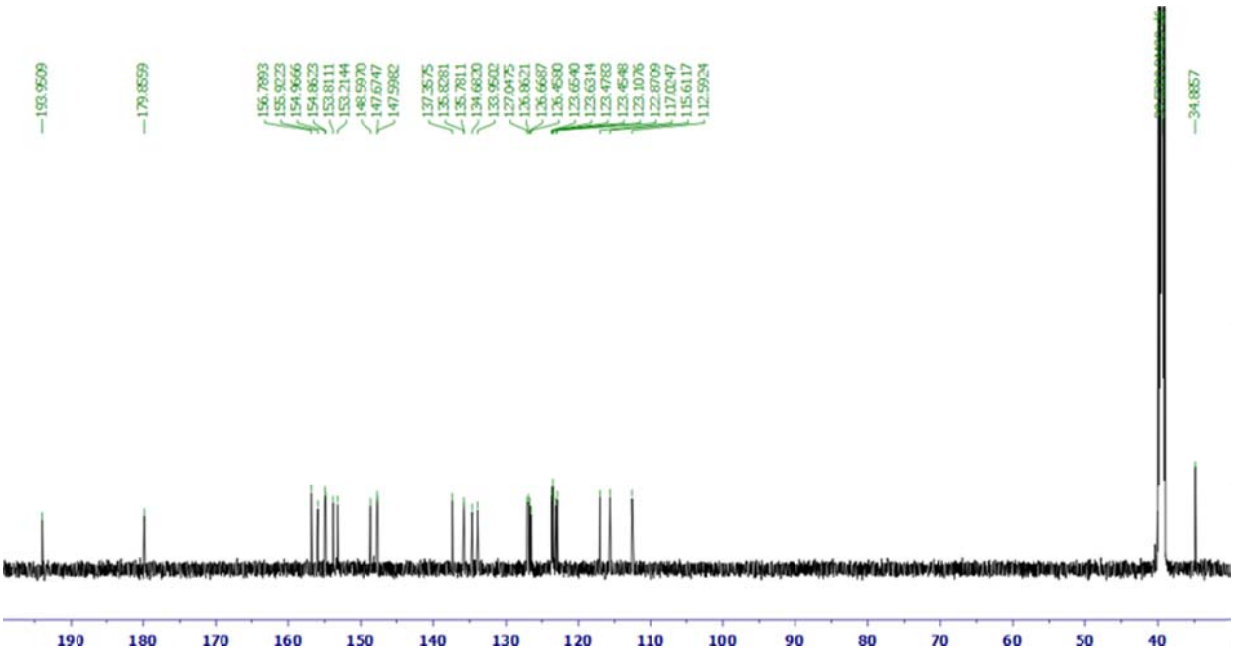


Figure S19. ^{1}H NMR spectrum of complex **17** in DMSO-d_6

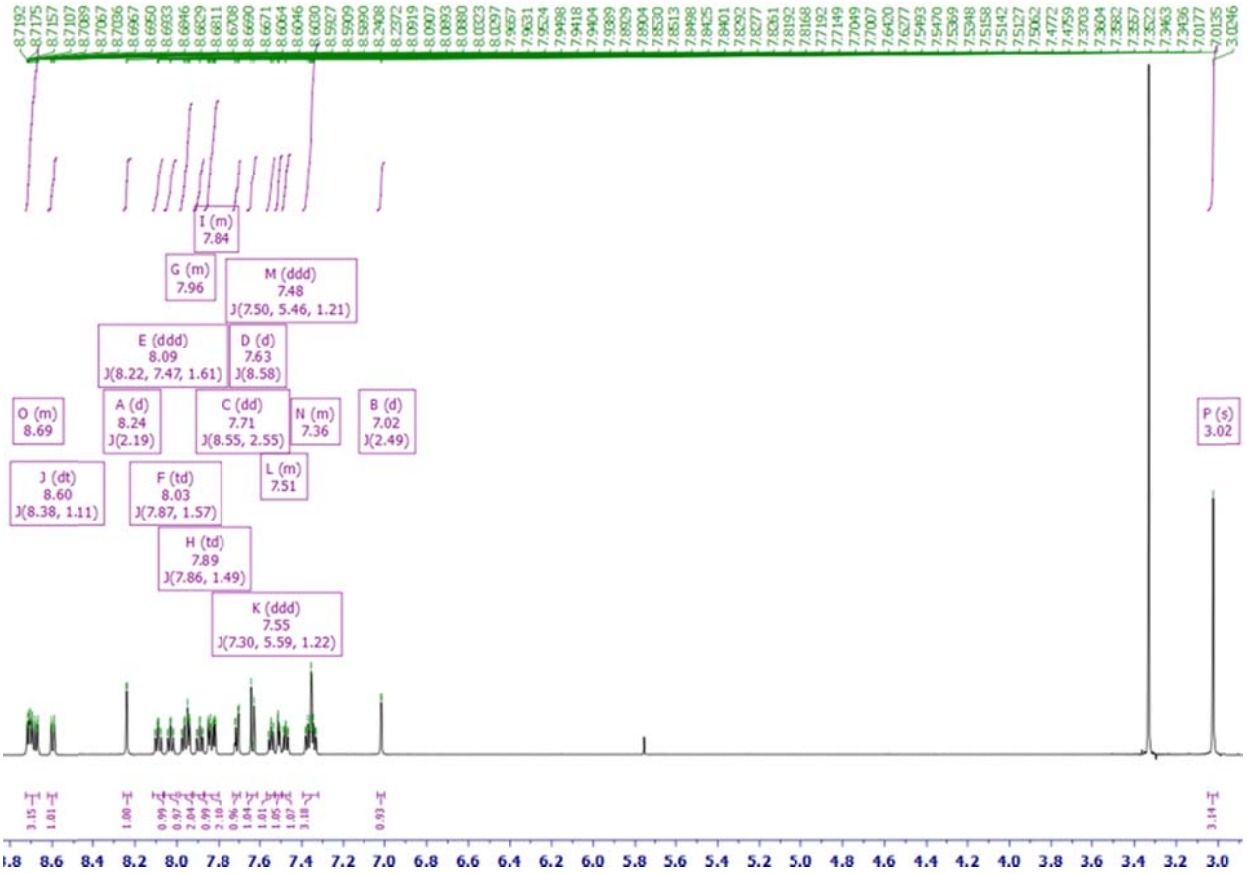


Figure S20. ^{13}C NMR spectrum of complex **17** in DMSO-d_6

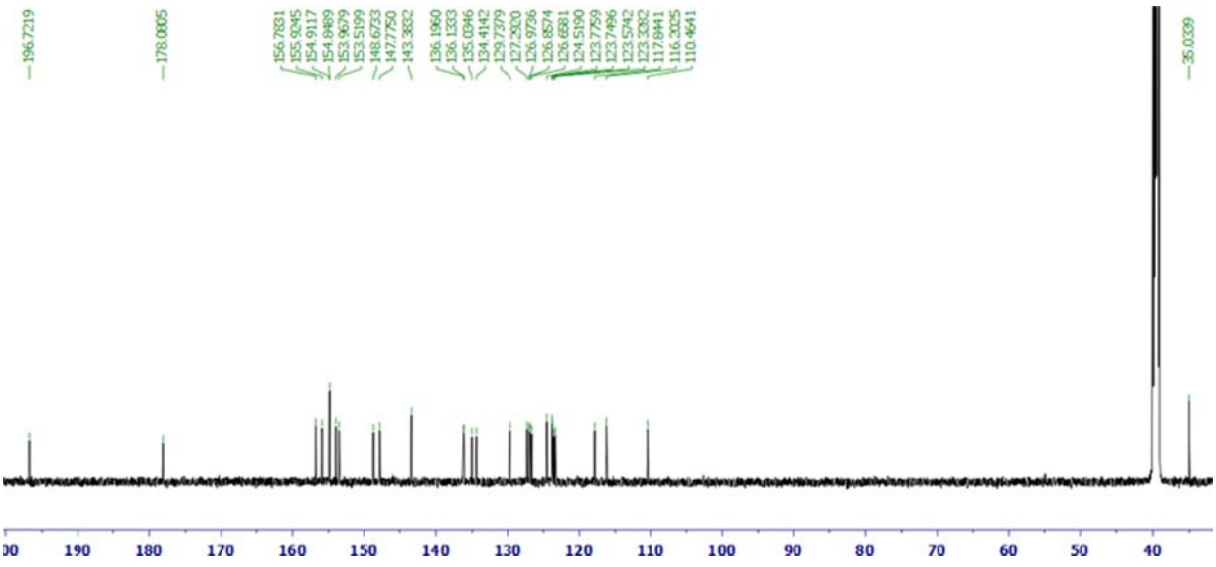


Table S3. Crystallographic details for complex **12**.

Chemical formula	$C_{37}H_{31}N_6Ru{\cdot}F_6P{\cdot}CH_2Cl_2$
M_r	890.66
Crystal system, space group	Monoclinic, $P2_1/n$
Temperature (K)	198
a, b, c (Å)	13.898 (2), 18.543 (4), 14.3820 (14)
β (°)	95.655 (10)
V (Å^3)	3688.4 (10)
Z	4
F(000)	1800
D_x (Mg m^{-3})	1.604
Radiation type	Mo Kα
μ (mm $^{-1}$)	0.68
Crystal size (mm)	0.41 × 0.20 × 0.14
Diffractometer	Bruker KappaCCD diffractometer
Absorption correction	Multi-scan *SADABS* 2.10.(Sheldrick,Bruker AXS Inc.,2002)
T_{min}, T_{max}	0.014, 0.190
No. of measured, independent and observed [i > 2σ(i)] reflections	86927, 7555, 4978
R_{int}	0.090
$(\sin \theta/\lambda)_{max}$ (Å^{-1})	0.626
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.054, 0.154, 1.18
No. of reflections	7555
No. of parameters	489
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.91, −0.89

Table S4. Crystallographic details for complex **16**.

Chemical formula	$C_{30}H_{24}N_6BrRu^+ \cdot PF_6^- \cdot C_3H_6O$
M_r	852.58
Crystal system, space group	Triclinic, *P-1*
Temperature (K)	295
a, *b*, *c* (Å)	9.1654 (2), 13.4071 (3), 15.9969 (15)
α, β, γ (°)	111.791 (5), 93.342 (12), 106.886 (9)
V (Å^3)	1715.8 (2)
Z	2
F(000)	852
D_x (Mg m^{-3})	1.650
Radiation type	Mo Kα
μ (mm^{-1})	1.74
Crystal size (mm)	0.18 × 0.06 × 0.01
Diffractometer	Rigaku Saturn724+ CCD (2x2 bin mode) diffractometer
Absorption correction	Multi-scan R.H. Blessing, Acta Cryst. (1995), A51, 33-38
T_{min}, T_{max}	0.651, 1.000
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	20146, 5967, 4621
R_{int}	0.048
$(\sin \theta/\lambda)_{max}$ (Å^{-1})	0.595
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, *S*	0.055, 0.125, 1.06
No. of reflections	5967
No. of parameters	445
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.72, −0.38

Table S5. Crystallographic details for complex **17**.

Chemical formula	$C_{30}H_{24}N_7O_2Ru^+ \cdot PF_6^- \cdot CH_2Cl_2$
M_r	845.53
Crystal system, space group	Monoclinic, C_c
Temperature (K)	295
a, b, c (Å)	11.0190 (5), 21.7448 (9), 14.3951 (7)
β (°)	92.226 (3)
V (Å^3)	3446.5 (3)
Z	4
F(000)	1696
D_x (Mg m^{-3})	1.629
Radiation type	Mo Kα
μ (mm^{-1})	0.73
Crystal size (mm)	2.12 × 0.13 × 0.05
Diffractometer	Rigaku Saturn724+ (2x2 bin mode) diffractometer
Absorption correction	Multi-scan R.H. Blessing, Acta Cryst. (1995), A51, 33-38
T_{min}, T_{max}	0.9, 1
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	37893, 6317, 6178
R_{int}	0.037
$(\sin \theta/\lambda)_{max}$ (Å^{-1})	0.676
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.038, 0.103, 1.05
No. of reflections	6317
No. of parameters	463
No. of restraints	6
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	1.23, −0.43
Absolute structure	Refined as an inversion twin.
Absolute structure parameter	0.27 (4)

Figure S21. Normalized emission spectra of selected complexes recorded in deaerated acetonitrile solution at room temperature.

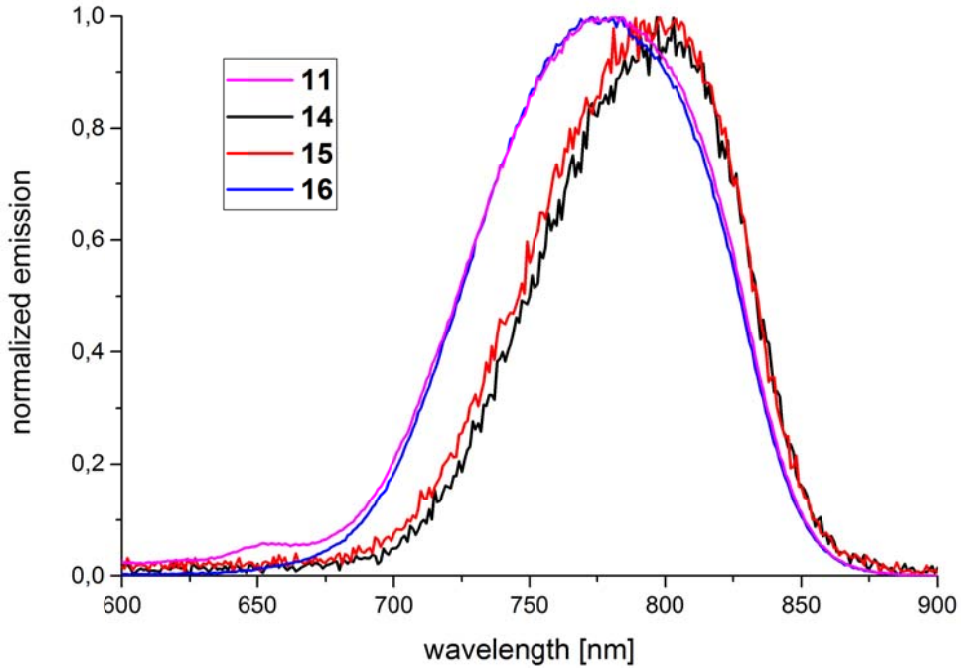


Figure S22. TD-DFT calculated absorption spectrum of **14_dcbp** (see experimental section for details).

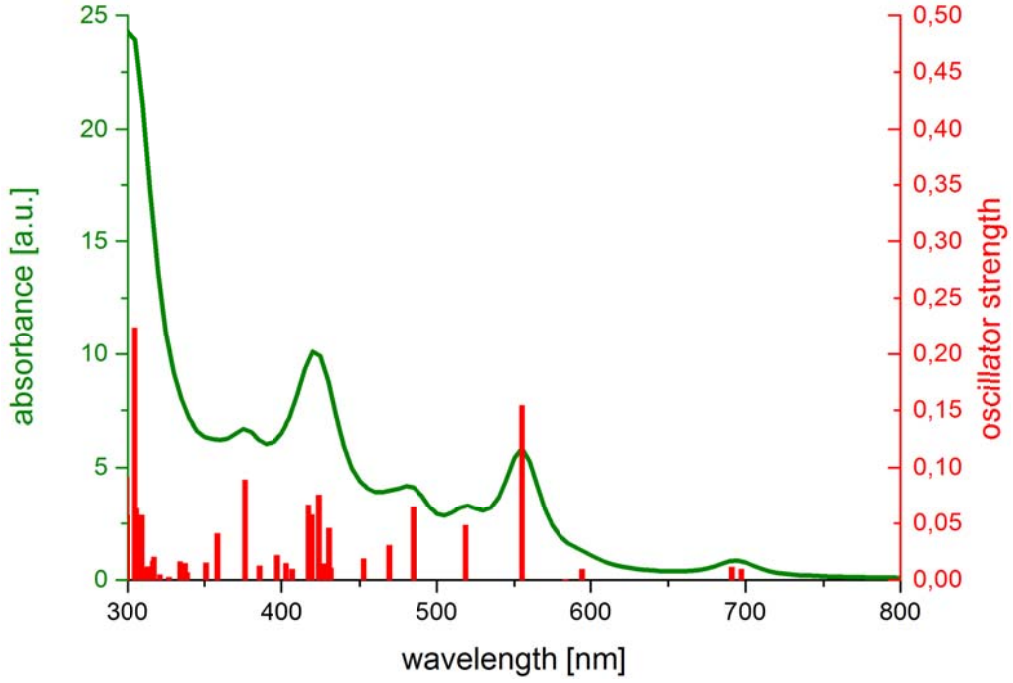
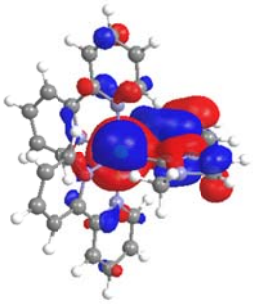
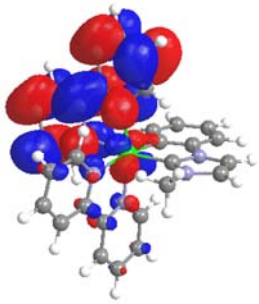
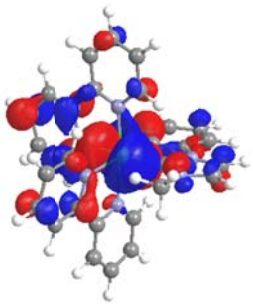
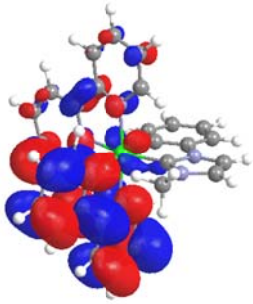
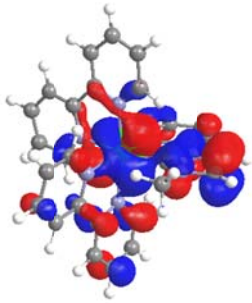
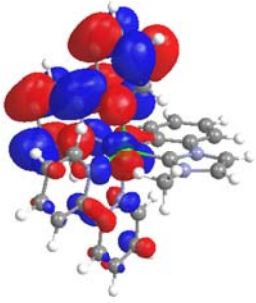
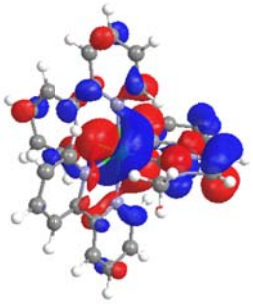
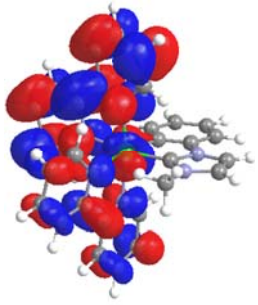
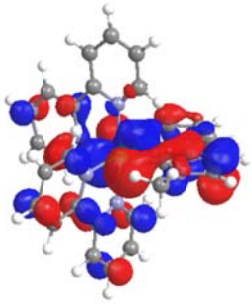
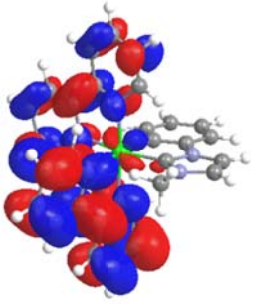


Table S6. NTOs of selected electron transitions (singlet, 6 lowest transitions with $f \geq 0.01$) for complex **14** as calculated *via* TD-DFT and visualized by Chemissian (isovalue 0.02).

	λ [nm], osc. Strength *f*, Eigenvalue [%]	NTO "hole"	NTO "particle"
S2	603, 0.010, 98		
S3	531, 0.015, 77		
S3	531, 0.015, 22		
S5	504, 0.106, 64		
S5	504, 0.106, 33		

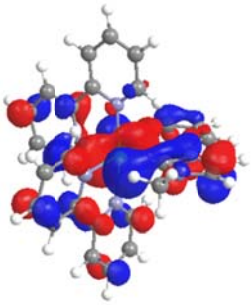
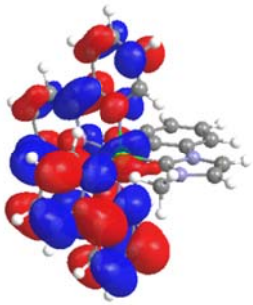
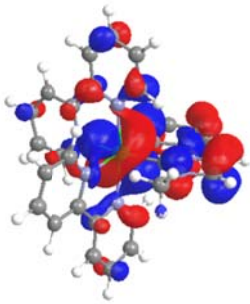
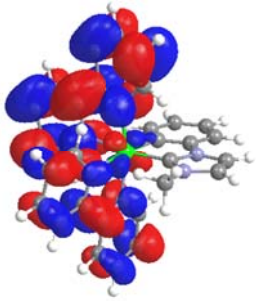
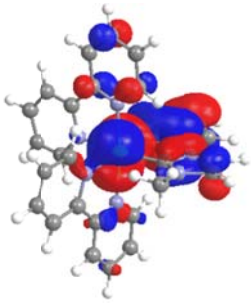
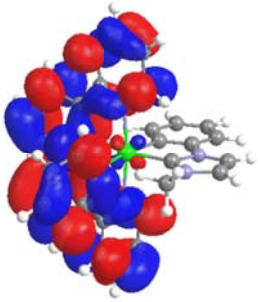
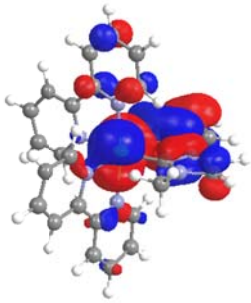
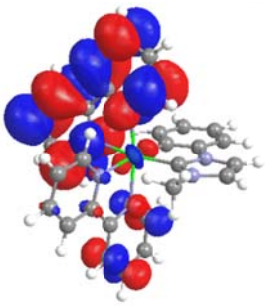
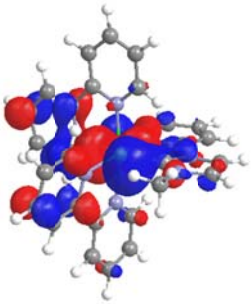
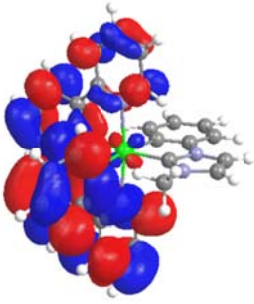
S6	474, 0.060, 74		
S6	474, 0.060, 19		
S7	420, 0.012, 97		
S11	380, 0.054, 54		
S11	380, 0.054, 41		

Figure S23. CV spectrum of complex **11** before (blue line) and after (orange line) addition of ferrocene. Arrow indicating starting potential and initial scanning direction.

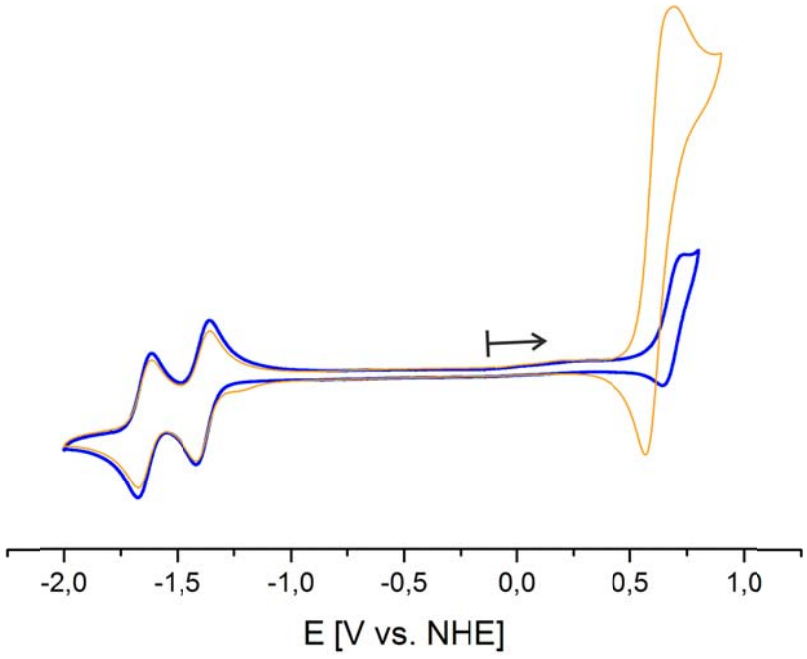


Figure S24. CV spectrum of complex **12** before (blue line) and after (orange line) addition of ferrocene. Arrow indicating starting potential and initial scanning direction.

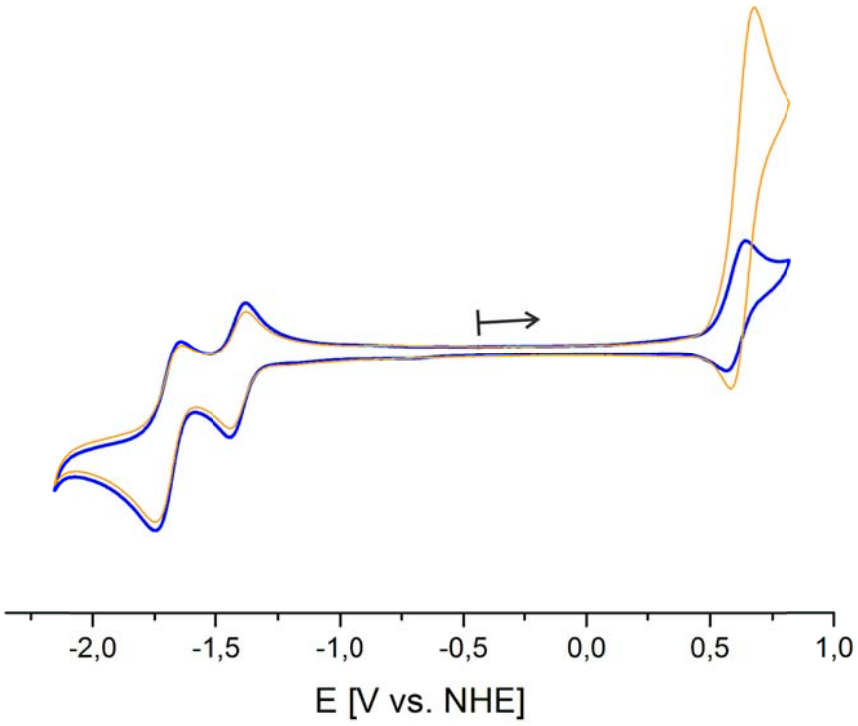


Figure S25. CV spectrum of complex **13** before (blue line) and after (orange line) addition of ferrocene. Arrow indicating starting potential and initial scanning direction.

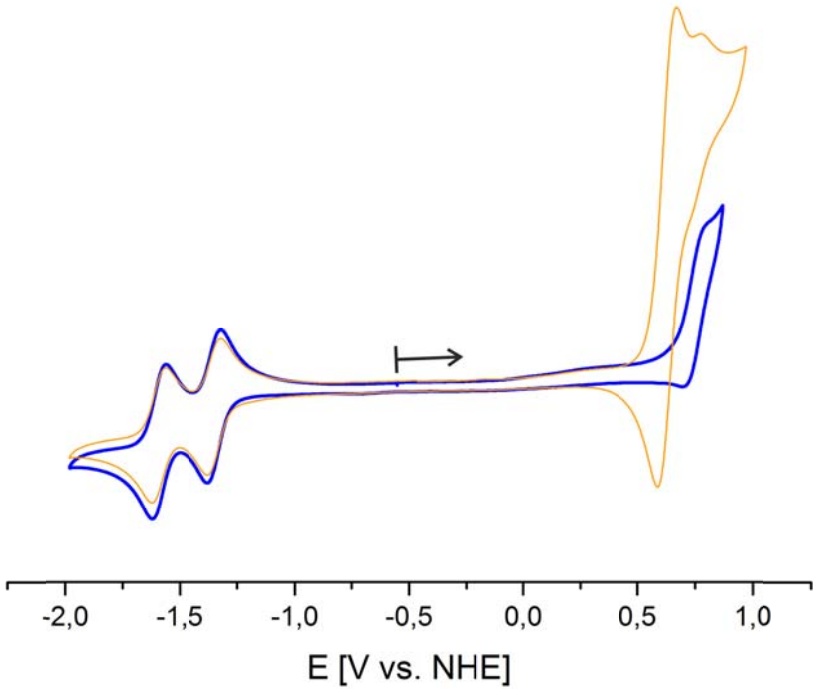


Figure S26. CV spectrum of complex **14** before (blue line) and after (orange line) addition of ferrocene. Arrow indicating starting potential and initial scanning direction.

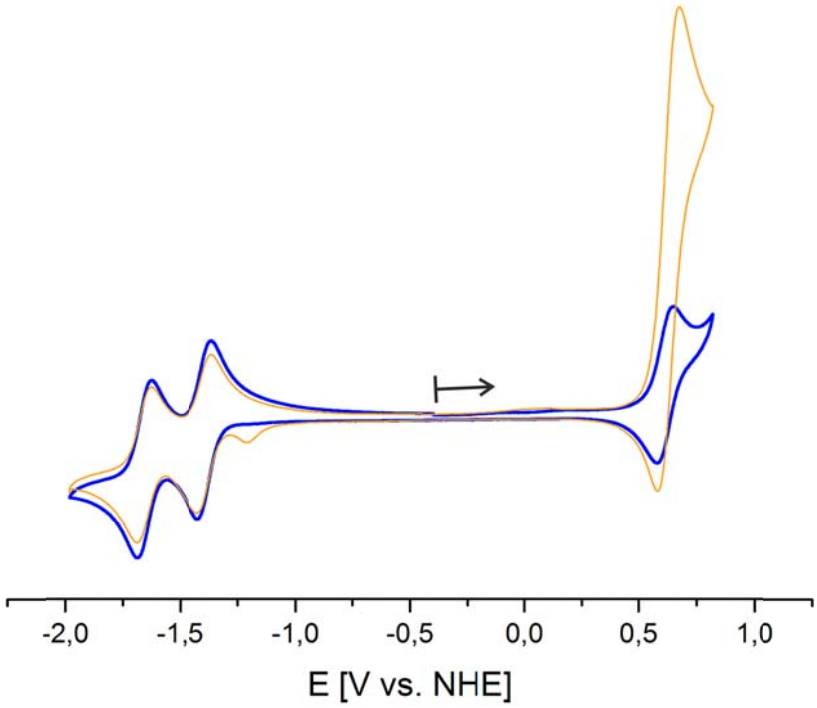


Figure S27. CV spectrum of complex **15** before (blue line) and after (orange line) addition of ferrocene. Arrow indicating starting potential and initial scanning direction.

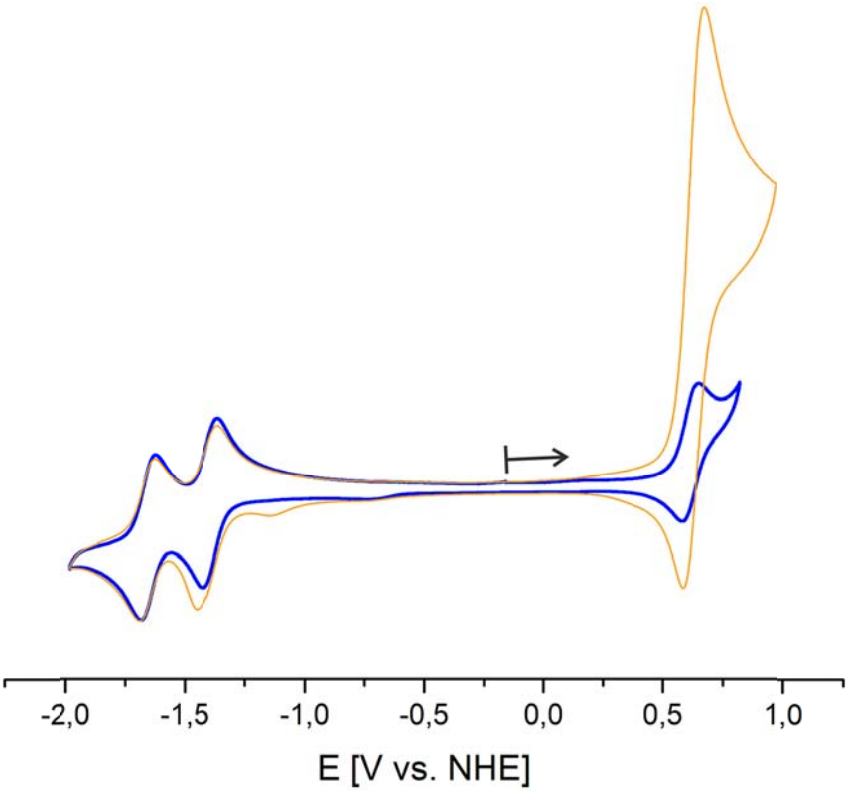


Figure S28. CV spectrum of complex **16** before (blue line) and after (orange line) addition of ferrocene. Arrow indicating starting potential and initial scanning direction.

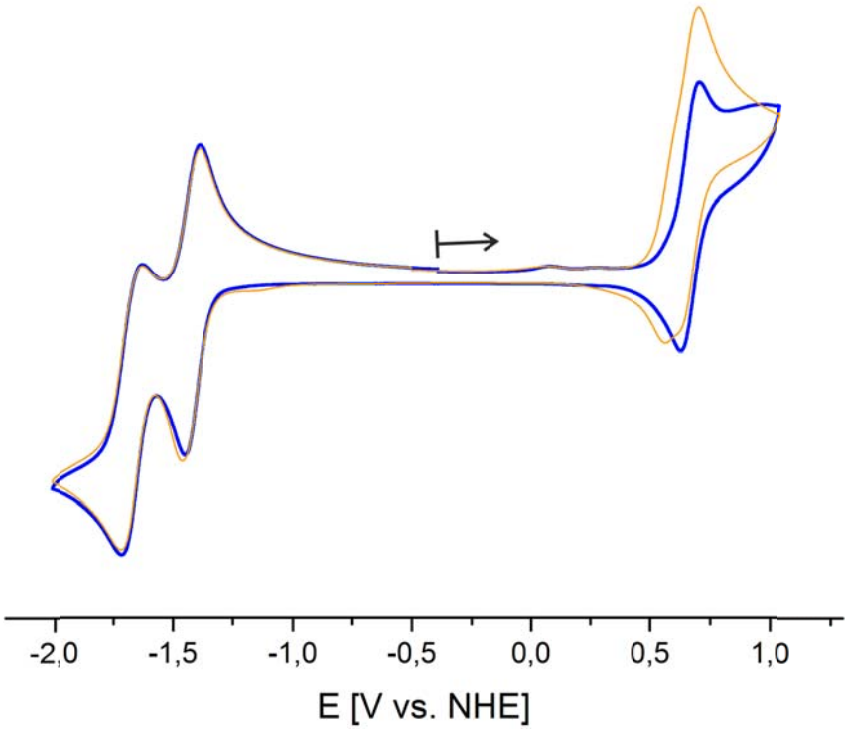


Figure S29. CV spectrum of complex **17** before (blue line) and after (orange line) addition of ferrocene. Arrow indicating starting potential and initial scanning direction.

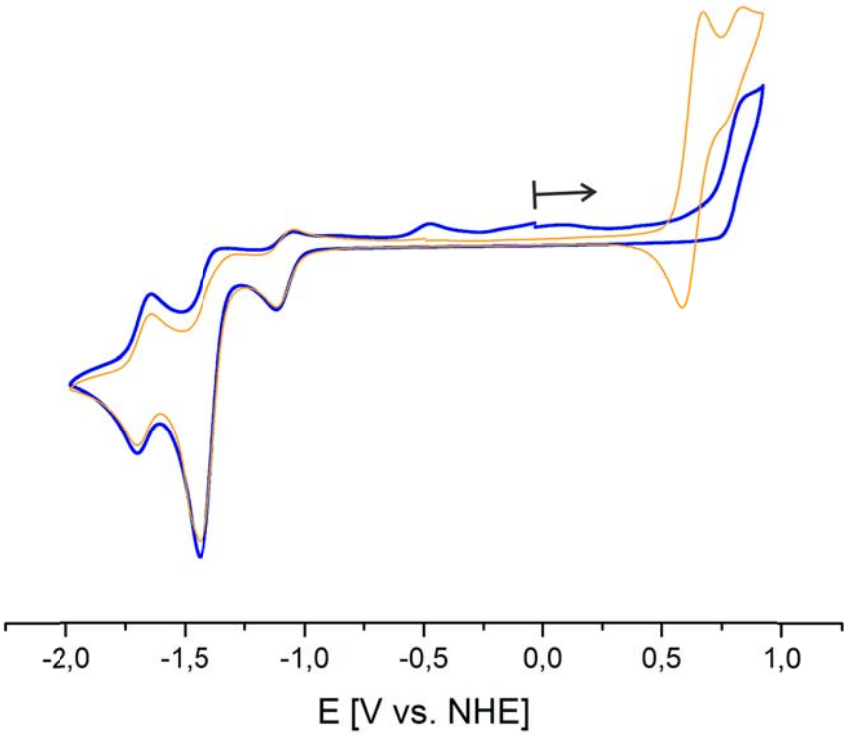
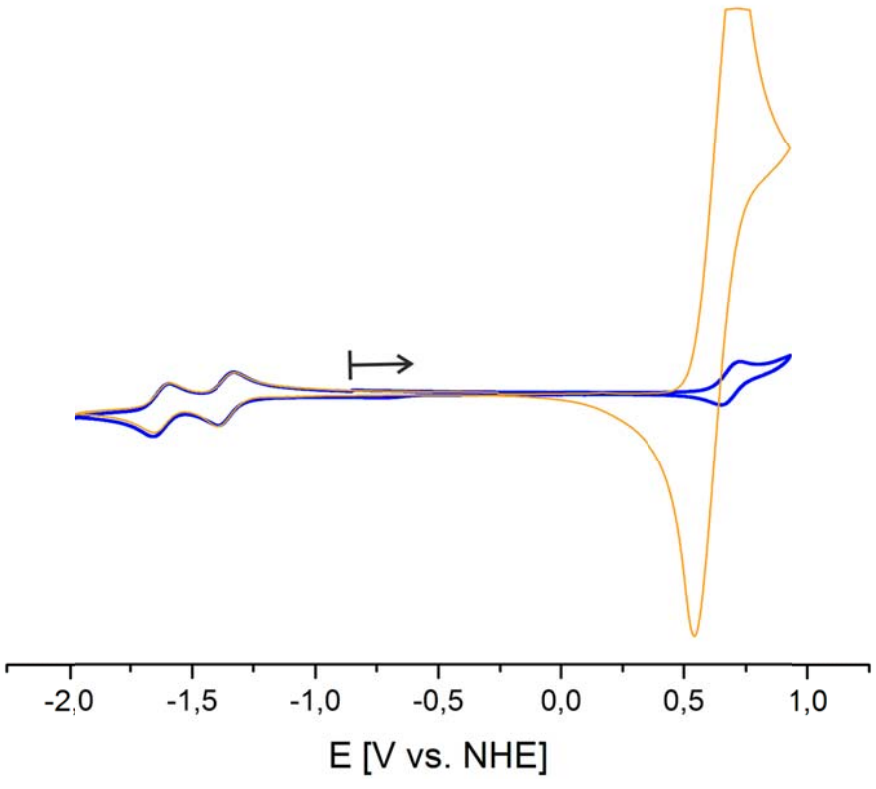


Figure S30. CV spectrum of complex **B2P** before (blue line) and after (orange line) addition of ferrocene. Arrow indicating starting potential and initial scanning direction.



The following tables list the xyz coordinates of the DFT optimized complexes **11**-**17**, **14_dcbp** and **B2P**:

xyz-coordinates of complex **11**.

Ru	-0.47903	0.06291	0.14516
N	0.11192	1.25557	1.77064
C	0.05642	0.88386	3.06747
C	0.46239	1.70347	4.11258
C	0.95760	2.97384	3.81710
C	1.02565	3.36594	2.48536
C	0.60257	2.49533	1.47353
H	-0.32685	-0.11164	3.25200
H	0.39281	1.34471	5.13399
H	1.28667	3.64369	4.60504
H	1.40925	4.34721	2.23359
N	0.17555	1.88673	-0.80482
C	0.20423	2.12162	-2.12872
C	0.69707	3.29917	-2.67954
C	1.18396	4.28425	-1.82040
C	1.15867	4.05028	-0.44961
C	0.65119	2.84007	0.03966
H	-0.17189	1.32330	-2.75826
H	0.70509	3.43073	-3.75609
H	1.58290	5.21548	-2.20973
H	1.54152	4.80211	0.22989
N	-1.18853	-0.88241	-1.61317
C	-2.46764	-0.60766	-2.00387
C	-0.45396	-1.73296	-2.36102
C	-3.01539	-1.20480	-3.14632
C	-3.21558	0.34835	-1.15879
C	-0.94206	-2.34700	-3.50865
H	0.55637	-1.90587	-2.01203
C	-2.25148	-2.08240	-3.90839
H	-4.03550	-0.98844	-3.43980
C	-4.50279	0.80855	-1.47057
N	-2.56864	0.77815	-0.04412
H	-0.30115	-3.01876	-4.06958
H	-2.67099	-2.54766	-4.79472
C	-5.13305	1.71932	-0.62932
H	-5.00838	0.46868	-2.36645
C	-3.18446	1.66380	0.75984
C	-4.45994	2.15884	0.51174
H	-6.12875	2.08257	-0.86358
H	-2.62053	1.97687	1.63283
H	-4.90841	2.87179	1.19557
C	1.42740	-0.75419	0.07272
C	2.57040	-0.27763	-0.57900
C	1.58387	-1.99819	0.72581
C	3.79410	-0.97370	-0.57399
H	2.53962	0.65213	-1.13839
C	2.77079	-2.72824	0.73999
N	0.38998	-2.45958	1.34516
C	3.88760	-2.20526	0.08633
H	2.83898	-3.69385	1.23349
C	0.13964	-3.59766	2.09634
C	-0.73357	-1.67745	1.21736
H	4.80889	-2.77731	0.06601
C	-1.16754	-3.53771	2.45291
H	0.89316	-4.33574	2.31885
N	-1.68824	-2.36076	1.91571
H	-1.76806	-4.21587	3.03954
C	-3.09325	-1.97105	2.05614
H	-3.15022	-0.90623	1.83101
H	-3.37371	-2.10733	3.10659
C	-4.02541	-2.77257	1.14556
H	-3.97374	-3.84433	1.36375
H	-5.06074	-2.44794	1.29463
H	-3.76317	-2.62564	0.09301
C	4.90137	-0.40617	-1.41216
O	6.19437	-0.56290	-1.02634
O	4.67392	0.16620	-2.45623
C	6.58606	-0.74311	0.33943
H	7.46707	-0.11443	0.49022
H	5.79833	-0.44357	1.03547
H	6.85908	-1.78708	0.52342

xyz-coordinates of complex **12**.

C	0.100950	-1.658120	4.102650
C	-1.027472	-1.020377	4.617870
C	-1.677200	-0.077126	3.829176
C	-1.197559	0.215272	2.546157
N	-0.099962	-0.423343	2.045982
C	0.526726	-1.335190	2.819648
C	-1.826620	1.218188	1.660303
N	-1.310418	1.299382	0.407428
C	-1.822053	2.203230	-0.443999
C	-2.856716	3.068351	-0.104501
C	-3.391676	2.992810	1.181482
C	-2.870936	2.058125	2.070128
Ru	0.495044	0.053399	0.070737
N	1.675035	1.787413	0.564964
C	2.189091	2.461682	-0.498139
C	2.975836	3.606449	-0.315608
C	3.244793	4.061668	0.970479
C	2.718025	3.360019	2.055739
C	1.941896	2.234348	1.805459
C	1.865826	1.893666	-1.820167
N	1.077848	0.777702	-1.809077
C	0.774565	0.200341	-2.991452
C	1.208063	0.694562	-4.214534
C	2.002869	1.841218	-4.233689
C	2.332172	2.438652	-3.022906
C	-0.355021	-1.701375	-0.583352
N	0.505858	-2.760028	-0.709403
C	-0.149136	-3.913997	-1.110171
C	-1.457569	-3.584724	-1.246451
N	-1.574096	-2.228461	-0.927537
C	1.879107	-2.532433	-0.396682
C	2.147275	-1.210624	0.023438
C	3.484298	-0.948266	0.352868
C	4.500881	-1.920282	0.275786
C	4.165005	-3.209934	-0.148324
C	2.847339	-3.526777	-0.488573
C	-2.606548	-1.234249	-0.844247
C	-3.154088	-0.910718	0.398341
C	-4.202099	0.006940	0.474350
C	-4.725037	0.610518	-0.677584
C	-4.158128	0.271761	-1.915196
C	-3.112614	-0.645755	-2.004602
C	5.924977	-1.569394	0.644181
C	-5.887711	1.571302	-0.594704
H	-2.311392	-4.170450	-1.548284
H	0.355715	-4.854034	-1.263859
H	2.601470	-4.533328	-0.817328
H	3.766648	0.049235	0.687617
H	4.933509	-3.975249	-0.216903
H	5.999057	-1.228232	1.684675
H	6.314195	-0.759782	0.013875
H	6.592906	-2.428691	0.529082
H	-2.761138	-1.377933	1.296722
H	-2.693363	-0.913268	-2.969730
H	-4.624660	0.251911	1.445489
H	-4.550018	0.722154	-2.823904
H	-5.806835	2.366574	-1.343344

H	-6.838464	1.053259	-0.775332
H	-5.954384	2.037912	0.393106
H	0.167958	-0.693854	-2.930443
H	2.957474	3.323285	-3.012991
H	0.930629	0.181262	-5.129127
H	2.364817	2.256372	-5.168800
H	3.379833	4.138317	-1.168621
H	3.855907	4.945864	1.121863
H	1.516378	1.653709	2.616208
H	2.903461	3.673332	3.077646
H	-1.374434	2.225432	-1.432181
H	-3.266654	1.996838	3.076952
H	-3.227695	3.782719	-0.831973
H	-4.196444	3.652719	1.490310
H	-2.559333	0.424568	4.208211
H	-1.396076	-1.252246	5.612183
H	1.394752	-1.804913	2.372943
H	0.646017	-2.399735	4.676940

xyz-coordinates of complex **13**.

Ru	0.41691	0.24624	0.04266
N	0.93345	-0.43634	1.96364
C	0.05686	-0.87145	2.89316
C	0.44297	-1.34173	4.14182
C	1.80135	-1.37402	4.45720
C	2.71411	-0.93087	3.50705
C	2.26500	-0.46658	2.26492
H	-0.98580	-0.83813	2.60362
H	-0.31095	-1.67984	4.84469
H	2.14397	-1.73930	5.41997
H	3.77376	-0.95062	3.73079
N	2.56709	0.44534	0.06831
C	3.33112	0.89532	-0.94300
C	4.71926	0.94429	-0.88124
C	5.35030	0.50708	0.28360
C	4.56830	0.04243	1.33581
C	3.17368	0.01861	1.20789
H	2.79777	1.21417	-1.83152
H	5.28637	1.31047	-1.73029
H	6.43200	0.52264	0.37084
H	5.04428	-0.30599	2.24433
N	0.09904	1.13225	-1.85357
C	0.00970	2.49366	-1.90619
C	-0.03278	0.43223	-3.00023
C	-0.22487	3.15342	-3.11906
C	0.17626	3.20631	-0.62143
C	-0.25860	1.03357	-4.23278
H	0.05338	-0.64267	-2.90111
C	-0.36085	2.42307	-4.29477
H	-0.30729	4.23328	-3.14606
C	0.22097	4.60350	-0.51579
N	0.29896	2.41596	0.47707
H	-0.35389	0.41676	-5.12003
H	-0.54363	2.92922	-5.23734
C	0.39149	5.19662	0.73078
H	0.13417	5.22653	-1.39788
C	0.46983	2.99929	1.67735
C	0.51974	4.37772	1.85372
H	0.42864	6.27757	0.82222
H	0.56628	2.32148	2.51958
H	0.65824	4.79355	2.84615
C	0.52738	-1.71602	-0.62821
C	1.64648	-2.45200	-1.03285
C	-0.70410	-2.40874	-0.68997
C	1.54505	-3.79105	-1.46810
H	2.63446	-2.00118	-1.02360
C	-0.84063	-3.73036	-1.11386
N	-1.81064	-1.61805	-0.28350
C	0.29739	-4.43139	-1.50722
H	-1.80924	-4.22086	-1.14274
C	-3.15918	-1.92083	-0.20884
C	-1.56513	-0.33235	0.11416
H	0.22322	-5.46088	-1.84028
C	-3.81033	-0.81505	0.24899
H	-3.54754	-2.88771	-0.47944
N	-2.79925	0.15498	0.44827
C	-2.99157	1.53768	0.87303
H	-2.02766	1.92339	1.19692
H	-3.69610	1.59245	1.70291
C	2.73007	-4.49048	-1.87020
N	3.70536	-5.03765	-2.19242
C	-5.29990	-0.66044	0.52396
C	-5.57095	-0.52111	2.04292
H	-5.13045	0.38330	2.47408
H	-6.65063	-0.47268	2.22323
H	-5.17497	-1.38364	2.58976
C	-5.90384	0.54227	-0.24033
H	-6.99132	0.54990	-0.10860
H	-5.52975	1.50498	0.11780
H	-5.69610	0.47075	-1.31374
C	-6.02040	-1.93694	0.03440
H	-5.87827	-2.09292	-1.04045
H	-5.67152	-2.82894	0.56595
H	-7.09504	-1.84320	0.21961
H	-3.36350	2.15420	0.04916

xyz-coordinates of complex **14**.

Ru	-0.02516	-0.05216	-0.05212
N	-1.48876	1.02985	-1.09686
C	-2.09194	0.62053	-2.23333
C	-3.07715	1.35562	-2.87960
C	-3.47409	2.57602	-2.33246
C	-2.86483	3.00591	-1.15953
C	-1.87645	2.22141	-0.55289
H	-1.76225	-0.33585	-2.61851
H	-3.52413	0.96953	-3.78951
H	-4.24373	3.17773	-2.80507
H	-3.16185	3.94783	-0.71443
N	-0.25967	1.72636	1.14496
C	0.40267	2.00762	2.28149
C	0.18401	3.16441	3.02066
C	-0.76672	4.07792	2.56358
C	-1.45696	3.79567	1.38981
C	-1.18951	2.60983	0.69340
H	1.12506	1.26516	2.60171
H	0.74518	3.33827	3.93261
H	-0.96947	4.99261	3.11163
H	-2.20066	4.49316	1.02374
N	1.57003	-0.90062	1.05157
C	2.83786	-0.50064	0.74092
C	1.40343	-1.82131	2.02484
C	3.94618	-1.03813	1.40747
C	2.95550	0.51782	-0.32465
C	2.46529	-2.38339	2.72368
H	0.37645	-2.09655	2.23153
C	3.76467	-1.98746	2.40739
H	4.94826	-0.72223	1.14344
C	4.17218	1.10654	-0.69724
N	1.79189	0.86918	-0.93190
H	2.26799	-3.11925	3.49595
H	4.62007	-2.40894	2.92581
C	4.19543	2.06527	-1.70467
H	5.09444	0.82836	-0.20136
C	1.82418	1.80205	-1.90082
C	2.99522	2.42319	-2.32102
H	5.13249	2.52723	-1.99922
H	0.86611	2.04693	-2.34850
H	2.96238	3.16841	-3.10883
C	-1.54807	-1.05286	0.95117
C	-2.27239	-0.66487	2.09053
C	-1.89881	-2.31275	0.41877

C	-3.26931	-1.47516	2.65119
H	-2.06157	0.29146	2.56431
C	-2.88395	-3.14246	0.95027
N	-1.12928	-2.67372	-0.72694
C	-3.57758	-2.71202	2.08387
H	-3.11719	-4.10535	0.50328
C	-1.16752	-3.80669	-1.52314
C	-0.17975	-1.78317	-1.15816
H	-4.35063	-3.34092	2.51526
C	-0.22343	-3.63178	-2.48237
H	-1.84927	-4.62416	-1.35309
N	0.36878	-2.39178	-2.25221
H	-3.80677	-1.13728	3.53392
H	0.07754	-4.26850	-3.30008
C	1.46361	-1.87061	-3.05875
H	1.58135	-0.81011	-2.84641
H	2.39884	-2.39169	-2.82762
H	1.23703	-2.00486	-4.12040

xyz-coordinates of complex **15**.

Ru	-0.302691	-0.009099	0.161826
N	0.367734	1.481507	1.478158
C	0.527950	1.325158	2.809593
C	1.003983	2.329679	3.642013
C	1.341180	3.562878	3.083510
C	1.185620	3.734703	1.713108
C	0.700146	2.684888	0.924059
H	0.264847	0.350294	3.199812
H	1.111509	2.139504	4.704607
H	1.720693	4.371653	3.699668
H	1.445946	4.682596	1.257873
N	0.027020	1.675900	-1.142299
C	-0.165573	1.694982	-2.473361
C	0.104625	2.806535	-3.263124
C	0.599107	3.957212	-2.647953
C	0.801697	3.947063	-1.272254
C	0.510180	2.792254	-0.534791
H	-0.542133	0.775876	-2.908145
H	-0.065873	2.764254	-4.333578
H	0.826075	4.845879	-3.228345
H	1.189320	4.830986	-0.780356
N	-1.109687	-1.314227	-1.295633
C	-2.451340	-1.241116	-1.537227
C	-0.377942	-2.218283	-1.981052
C	-3.062799	-2.091067	-2.467425
C	-3.195079	-0.221672	-0.766746
C	-0.929982	-3.082000	-2.919700
H	0.680798	-2.226112	-1.752692
C	-2.301351	-3.021241	-3.166670
H	-4.130248	-2.031467	-2.642602
C	-4.558620	0.044544	-0.955923
N	-2.466534	0.468730	0.149087
H	-0.290279	-3.787487	-3.439220
H	-2.770195	-3.683737	-3.887374
C	-5.181550	1.030043	-0.197548
H	-5.130706	-0.504702	-1.694112
C	-3.076762	1.424948	0.872475
C	-4.424724	1.738541	0.737271
H	-6.236478	1.243878	-0.337740
H	-2.446726	1.948437	1.584749
H	-4.864786	2.519289	1.348725
C	1.664408	-0.657779	-0.024679
C	2.675223	-0.179317	-0.861200
C	2.021775	-1.747174	0.805380
C	3.967264	-0.741869	-0.875564
H	2.502258	0.652223	-1.539271
C	3.285313	-2.322967	0.813294
N	0.950268	-2.208189	1.626142
C	4.276384	-1.817828	-0.036076
H	3.524713	-3.159669	1.464699
C	0.896640	-3.233952	2.554791

C	-0.251487	-1.558521	1.520218
H	5.262609	-2.265624	-0.028376
C	-0.366992	-3.234687	3.052241
H	1.741328	-3.861410	2.789098
N	-1.056040	-2.204049	2.418278
H	-0.832692	-3.865928	3.793336
C	-2.466350	-1.924140	2.649604
H	-2.672325	-0.888743	2.384167
H	-3.101171	-2.582947	2.047288
H	-2.698857	-2.078527	3.706557
O	4.845786	-0.165615	-1.746791
C	6.169214	-0.676179	-1.808342
H	6.181489	-1.728965	-2.120027
H	6.689130	-0.073759	-2.555228
H	6.683606	-0.580033	-0.843149

xyz-coordinates of complex **16**.

Ru	-0.61994	-0.02406	0.19351
N	-0.11305	1.40081	1.65408
C	-0.16731	1.19697	2.98726
C	0.20823	2.15557	3.91961
C	0.67022	3.39069	3.46487
C	0.73383	3.61156	2.09398
C	0.34036	2.60691	1.20179
H	-0.52168	0.22203	3.29687
H	0.14339	1.92864	4.97840
H	0.97835	4.16402	4.16112
H	1.09398	4.56214	1.71976
N	-0.03749	1.69126	-0.98119
C	-0.02100	1.76065	-2.32433
C	0.40574	2.88582	-3.02057
C	0.83693	3.99567	-2.29340
C	0.82266	3.93362	-0.90408
C	0.38174	2.76803	-0.26452
H	-0.35576	0.87143	-2.84663
H	0.40290	2.88450	-4.10529
H	1.18187	4.89268	-2.79776
H	1.15901	4.78556	-0.32574
N	-1.24013	-1.24451	-1.42124
C	-2.52118	-1.09512	-1.86885
C	-0.45082	-2.16346	-2.01671
C	-3.01404	-1.88302	-2.91652
C	-3.33211	-0.06425	-1.18606
C	-0.88387	-2.96771	-3.06439
H	0.55610	-2.23493	-1.62447
C	-2.19362	-2.82837	-3.52275
H	-4.03614	-1.76398	-3.25528
C	-4.63157	0.28160	-1.58251
N	-2.73262	0.55325	-0.13442
H	-0.20194	-3.68812	-3.50340
H	-2.57082	-3.44269	-4.33416
C	-5.32378	1.27117	-0.89232
H	-5.09924	-0.20853	-2.42801
C	-3.40800	1.51368	0.52251
C	-4.69927	1.90336	0.18404
H	-6.32985	1.54639	-1.19278
H	-2.88015	1.97617	1.35049
H	-5.19710	2.68350	0.75020
C	1.32879	-0.74057	0.29080
C	2.47679	-0.26655	-0.36355
C	1.52242	-1.86410	1.12462
C	3.71759	-0.88657	-0.18014
H	2.41915	0.59035	-1.02694
C	2.75134	-2.48994	1.31647
N	0.32408	-2.31230	1.75051
C	3.87508	-1.99235	0.65177
H	2.85746	-3.35302	1.96812
C	0.09646	-3.36541	2.62192
C	-0.82886	-1.61771	1.48153
H	4.84464	-2.45846	0.78301
C	-1.22820	-3.33837	2.91472

H	0.87463	-4.03003	2.96075
N	-1.78034	-2.26559	2.21755
H	-1.82277	-3.97680	3.54997
C	-3.20020	-1.94186	2.25021
H	-3.34109	-0.94204	1.84522
H	-3.77547	-2.65829	1.65425
H	-3.56134	-1.96926	3.28224
Br	5.25515	-0.19151	-1.10640

xyz-coordinates of complex **17**.

Ru	-0.406166	-0.038784	0.183439
N	0.240566	1.329088	1.646098
C	0.285934	1.082422	2.972210
C	0.743405	2.006416	3.903007
C	1.183675	3.251054	3.452876
C	1.144611	3.515854	2.088777
C	0.672414	2.544447	1.197935
H	-0.056168	0.101562	3.277228
H	0.756927	1.746182	4.956003
H	1.552915	3.998773	4.147370
H	1.484600	4.475292	1.718494
N	0.099855	1.712253	-0.976497
C	0.015753	1.825065	-2.313852
C	0.421972	2.960338	-3.006184
C	0.940899	4.032867	-2.281048
C	1.029768	3.926180	-0.897098
C	0.603678	2.753156	-0.261723
H	-0.382854	0.962685	-2.836192
H	0.338776	2.993837	-4.087117
H	1.276448	4.934616	-2.783123
H	1.437933	4.747866	-0.321310
N	-1.187530	-1.182064	-1.419379
C	-2.500667	-0.995848	-1.743106
C	-0.469809	-2.081034	-2.125370
C	-3.097169	-1.726816	-2.778062
C	-3.231344	0.011303	-0.943981
C	-1.006798	-2.829373	-3.166323
H	0.567036	-2.183356	-1.830188
C	-2.349539	-2.652165	-3.498575
H	-4.142943	-1.578847	-3.018853
C	-4.556183	0.388235	-1.204530
N	-2.530355	0.573699	0.075242
H	-0.378346	-3.535876	-3.697934
H	-2.807229	-3.221981	-4.300969
C	-5.168798	1.351987	-0.410282
H	-5.105707	-0.057549	-2.024904
C	-3.129487	1.509763	0.833427
C	-4.440509	1.927516	0.631969
H	-6.193864	1.651005	-0.605223
H	-2.522156	1.929023	1.629245
H	-4.873748	2.685911	1.275482
C	1.535091	-0.765503	0.077496
C	2.626160	-0.271732	-0.648552
C	1.798200	-1.923287	0.847721
C	3.872973	-0.903078	-0.590991
H	2.539099	0.607681	-1.274943
C	3.037855	-2.561786	0.913376
N	0.660040	-2.391629	1.555605
C	4.101176	-2.041498	0.178756
H	3.190514	-3.448776	1.521173
C	0.501868	-3.480316	2.400660
C	-0.509986	-1.679861	1.417849
H	5.083086	-2.496691	0.195193
C	-0.790809	-3.459144	2.808808
H	1.300990	-4.162330	2.642015
N	-1.394990	-2.355268	2.207359
H	-1.332303	-4.121073	3.467115
C	-2.803873	-2.027057	2.382852
H	-2.975253	-1.015746	2.020400
H	-3.436194	-2.724869	1.824013
H	-3.066324	-2.082215	3.443164
N	4.987461	-0.344602	-1.372715
O	6.075256	-0.915418	-1.308681
O	4.765744	0.663218	-2.047027

xyz-coordinates of complex **14_dcbp**.

Ru	-0.04808	-0.69019	-0.11227
N	-2.01811	-0.42808	-0.76243
C	-2.59668	-1.09062	-1.78563
C	-3.92228	-0.90953	-2.15795
C	-4.71054	0.00467	-1.45087
C	-4.11366	0.70479	-0.40304
C	-2.78131	0.46853	-0.06462
H	-1.96033	-1.78822	-2.31443
H	-4.30127	-1.46342	-3.01169
H	-4.71449	1.43135	0.13015
N	-0.80695	0.78939	1.25579
C	-0.12848	1.36963	2.26046
C	-0.68920	2.31946	3.10700
C	-2.01972	2.70260	2.90500
C	-2.72061	2.11596	1.85124
C	-2.10274	1.15459	1.04938
H	0.90117	1.05367	2.38344
H	-0.06751	2.76373	3.87864
H	-3.74104	2.43585	1.67913
N	1.94135	-0.70291	0.59308
C	2.79935	0.22982	0.07847
C	2.41390	-1.57324	1.50921
C	4.13381	0.27926	0.48267
C	2.22470	1.16838	-0.90805
C	3.73441	-1.57366	1.94330
H	1.69059	-2.27939	1.89810
C	4.62579	-0.63417	1.41516
H	4.81962	1.02183	0.09414
C	2.95071	2.22694	-1.46787
N	0.92532	0.94928	-1.23822
H	4.02458	-2.28988	2.70650
C	2.32944	3.07751	-2.38121
H	3.98464	2.40205	-1.20040
C	0.33232	1.78170	-2.11532
C	0.98908	2.85046	-2.70958
H	-0.70756	1.56869	-2.34039
H	0.48483	3.50319	-3.41337
C	-0.69082	-2.28420	1.06251
C	-1.25311	-2.27079	2.34905
C	-0.52347	-3.56391	0.49111
C	-1.62007	-3.45019	3.01194
H	-1.41421	-1.32333	2.85880
C	-0.87706	-4.75478	1.12213
N	0.06234	-3.52938	-0.80960
C	-1.43390	-4.69100	2.40171
H	-0.72870	-5.71803	0.64139
C	0.38005	-4.55259	-1.68803
C	0.37452	-2.30186	-1.33111
H	-1.71917	-5.60572	2.91235
C	0.90273	-3.95923	-2.79146
H	0.20675	-5.59373	-1.46903
N	0.88796	-2.58493	-2.56410
H	-2.05441	-3.39780	4.00707
H	1.27793	-4.38447	-3.70962
C	1.42130	-1.61354	-3.51175
H	0.94602	-0.64915	-3.34184
H	2.50494	-1.50817	-3.39523
H	1.20572	-1.94598	-4.53015
C	3.03621	4.23042	-3.02512
C	6.07467	-0.49438	1.81340
C	-6.14646	0.33126	-1.77521
C	-2.74008	3.75545	3.71237
O	-6.84319	-0.57993	-2.48901
H	-6.37038	-1.42579	-2.55295
O	-2.24605	4.04588	4.93522
H	-1.56965	3.40708	5.21340

O	6.65398	-1.54002	2.43945
H	6.08855	-2.32935	2.42897
O	4.31463	4.34303	-2.61275
H	4.69955	5.11324	-3.07384
O	-6.65216	1.36807	-1.42414
O	-3.71141	4.32417	3.28067
O	2.51144	4.97154	-3.82514
O	6.69389	0.51651	1.58862

xyz-coordinates of complex **B2P**.

Ru	0.03276	-0.02141	-0.01536
N	-1.74533	0.29303	1.10398
C	-1.82011	1.11048	2.17514
C	-3.00139	1.33982	2.87141
C	-4.16648	0.70336	2.44571
C	-4.09931	-0.14141	1.34279
C	-2.87981	-0.33855	0.68336
H	-0.88990	1.58451	2.46343
H	-2.99865	2.00843	3.72563
H	-5.10975	0.86079	2.95913
H	-4.99556	-0.64101	0.99572
N	-1.49856	-1.27677	-1.04588
C	-1.29410	-2.07236	-2.10993
C	-2.29372	-2.85657	-2.67625
C	-3.56850	-2.81631	-2.11027
C	-3.78926	-1.99793	-1.00692
C	-2.73606	-1.23182	-0.48854
H	-0.28638	-2.06873	-2.51344
H	-2.07400	-3.48063	-3.53602
H	-4.37801	-3.41320	-2.51860
H	-4.77326	-1.96339	-0.55512
N	1.72420	-0.54893	-1.11907
C	2.42503	-1.62788	-0.66299
C	2.18527	0.10890	-2.20264
C	3.59159	-2.05601	-1.30705
C	1.86142	-2.27966	0.53039
C	3.33568	-0.26947	-2.88297
H	1.60130	0.96594	-2.51426
C	4.05492	-1.37539	-2.42741
H	4.13871	-2.91290	-0.93238
C	2.42415	-3.40627	1.14202
N	0.72689	-1.70370	1.02327
H	3.65914	0.29969	-3.74793
H	4.96065	-1.69832	-2.93053
C	1.82725	-3.95244	2.27252
H	3.32545	-3.85304	0.73953
C	0.15612	-2.24113	2.12038
C	0.66831	-3.35567	2.77196
H	2.25839	-4.82410	2.75429
H	-0.73678	-1.74207	2.47734
H	0.16673	-3.74155	3.65303
C	-1.21362	1.88049	-2.13970
C	0.23993	2.89410	-0.60225
C	-1.46199	3.08016	-2.79203
H	-1.68011	0.95737	-2.46565
C	0.02130	4.13499	-1.22439
C	-0.82741	4.23234	-2.31851
H	0.52016	5.01919	-0.84549
H	-0.99394	5.19270	-2.79745
H	-2.13357	3.10713	-3.64330
C	1.11257	2.66373	0.55284
C	1.83601	3.69668	1.17745
C	1.18208	1.32116	1.02316
C	2.64020	3.42317	2.27816
H	1.77590	4.71829	0.81156
C	2.00598	1.08436	2.13838
C	2.72299	2.11155	2.75803
H	3.19819	4.22173	2.75805
H	2.09458	0.07788	2.54155
H	3.35047	1.89067	3.61860
N	-0.38943	1.77609	-1.07844