Electronic Supporting Information for

Optically active bis(aminophenols) and their metal complexes

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I. Additional crystallographic information

Figure S1. Thermal ellipsoid plot of (*R*)-BiniqH_4 • CH_3OH • $PhCH_3$ showing hydrogen bonding interactions. The toluene of solvation is not shown.

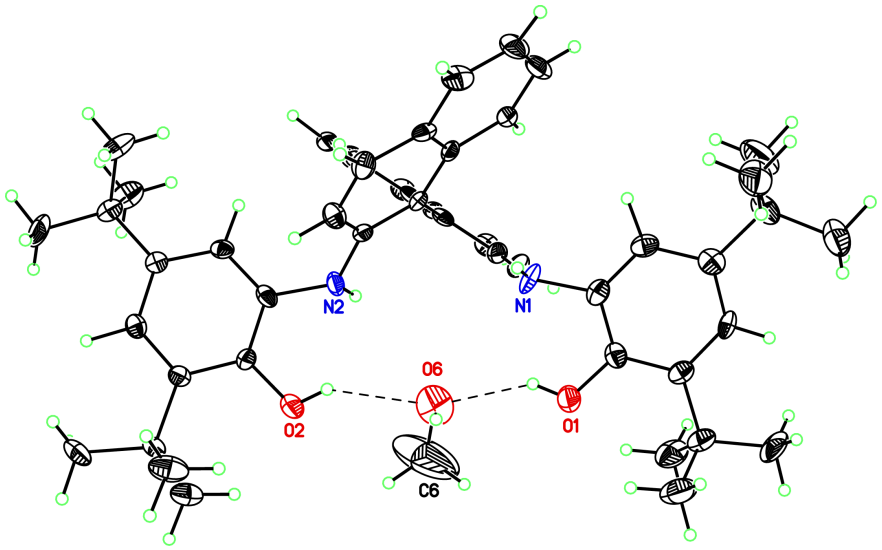


Figure S2. Thermal ellipsoid plot of (*R*,*R*)-2,3-$C_4H_8(O_2CC_6H_4$-2-$NH_2)_2$.

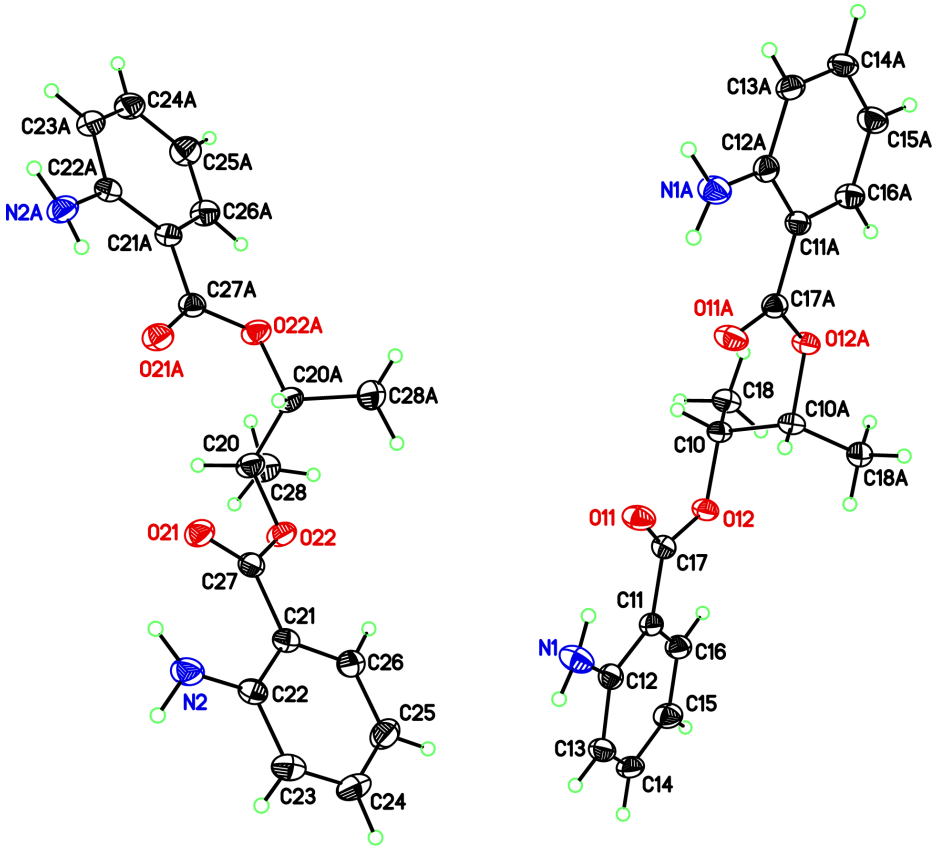


Figure S3. Thermal ellipsoid plot of second crystallograpically unique palladium complex in (*C*,*R*,*R*)-(Bdan)Pd • 0.25 CH_3OH. Hydrogen atoms are omitted for clarity.

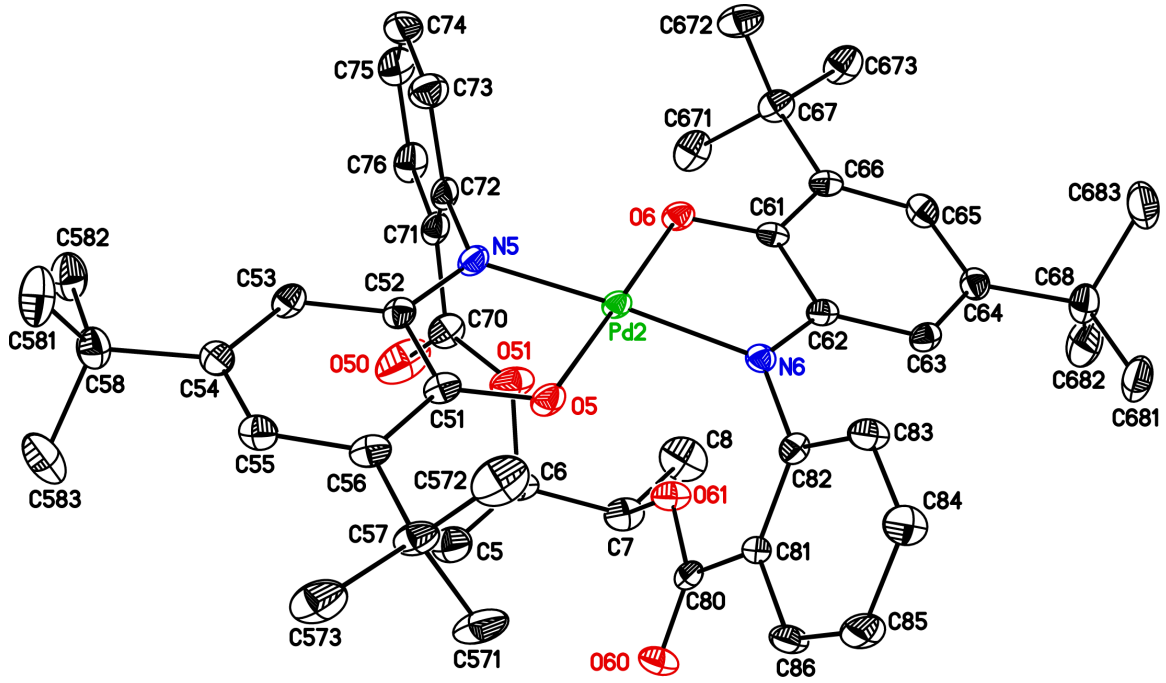


Figure S4. Thermal ellipsoid plot of second crystallograpically unique osmium complex in (*C*,*R*,*R*)-(Bdan)OsO • CH_3OH. Hydrogen atoms are omitted for clarity.

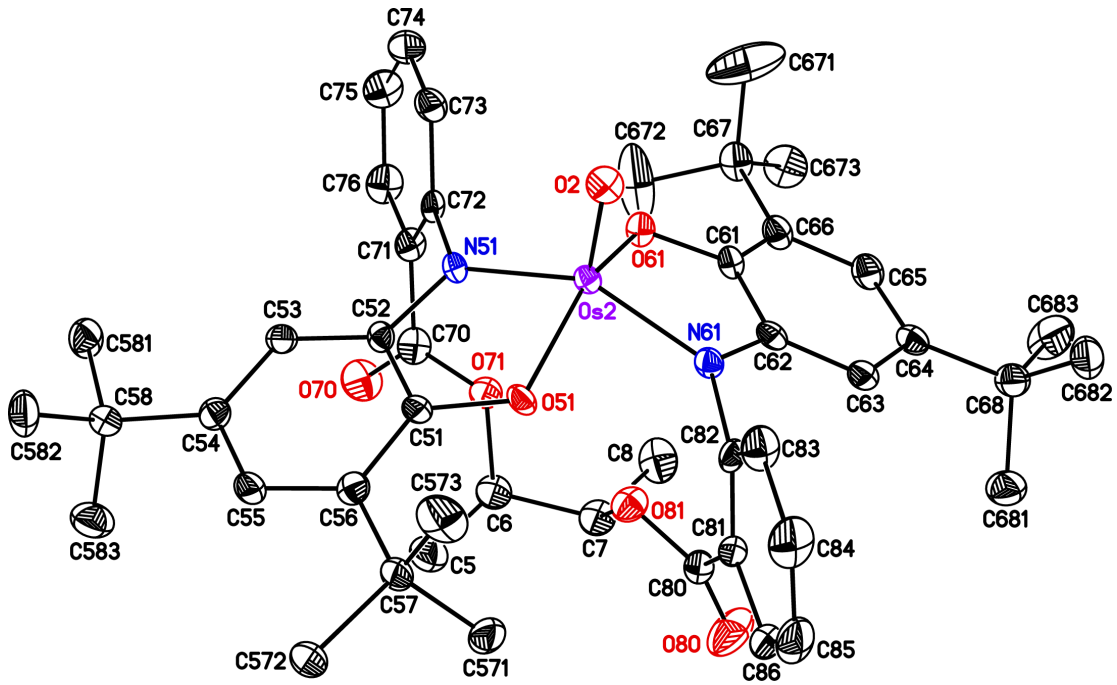
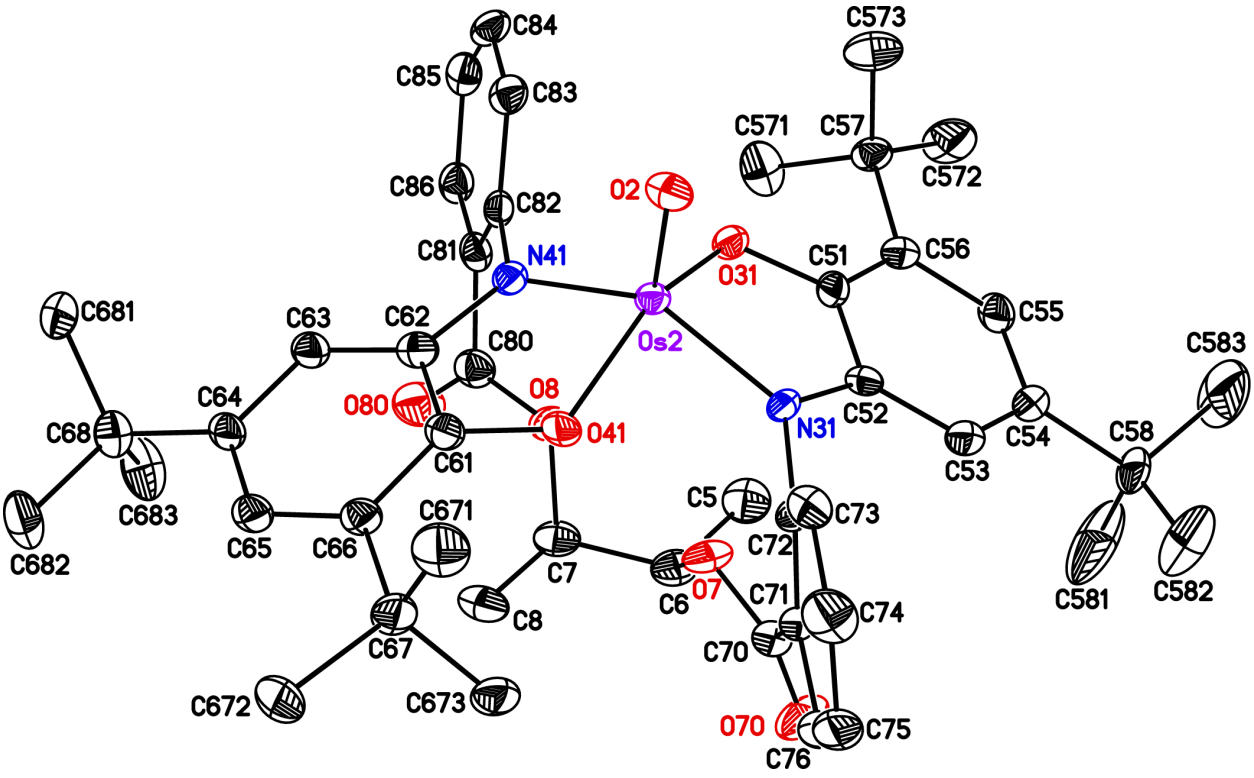


Figure S5. Thermal ellipsoid plot of molecule of (*C*,*R*,*R*)-(Bdan)OsO in (*C*,*R*,*R*)-(Bdan)OsO • (*A*,*R*,*R*)-(Bdan)OsO. Hydrogen atoms omitted for clarity.



II. ^{1}H NMR spectra

Figure S6. ^{1}H NMR spectrum of (*R*)-BiniqH$_4$ (C_6D_6, 500 MHz).

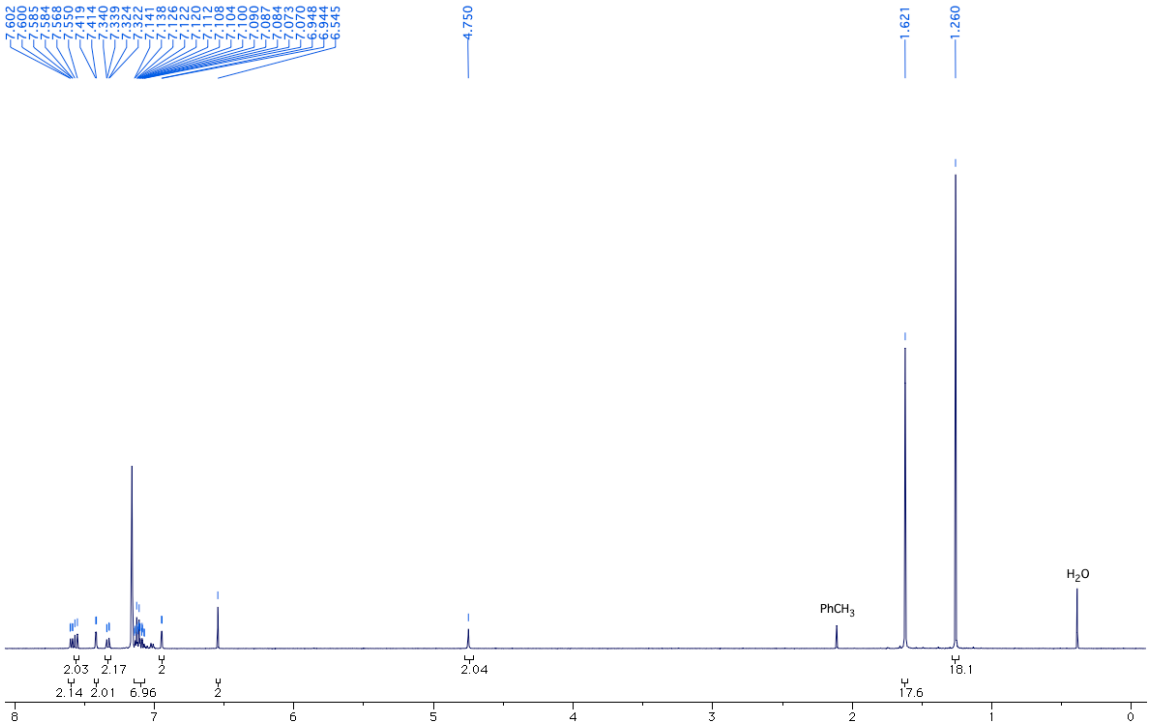


Figure S7. ^{1}H NMR spectrum of (*R*,*R*)-2,3-$C_4H_8(O_2CC_6H_4$-2-$NH_2)_2$ ($CDCl_3$, 400 MHz)

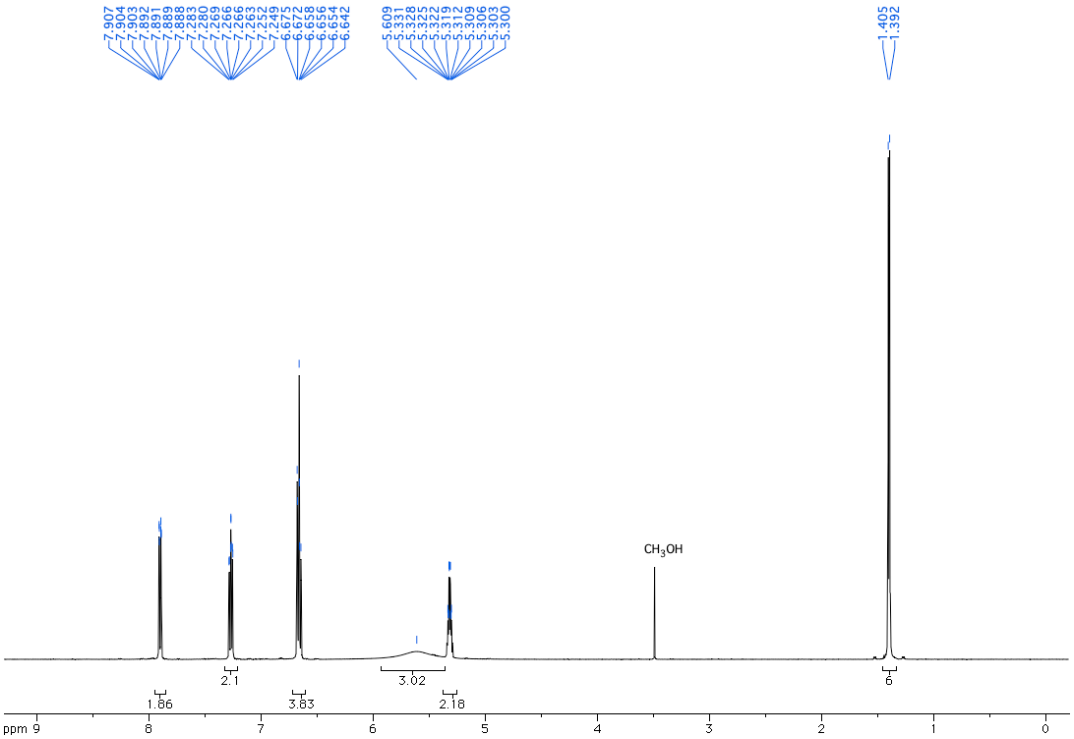


Figure S8. Experimental (**black**, bottom) and simulated (red, top) aliphatic ^{1}H NMR signals for (*R*,*R*)-2,3-$C_4H_8(O_2CC_6H_4$-2-$NH_2)_2$. Simulation parameters for the $A_3BB'A'_3$ spin system: linewidth = 1.0 Hz, δ_A = 1.4010 ppm, δ_B = 5.3177 ppm, J_{AB} = 6.5 Hz, $J_{BB'}$ = 4.6 Hz.

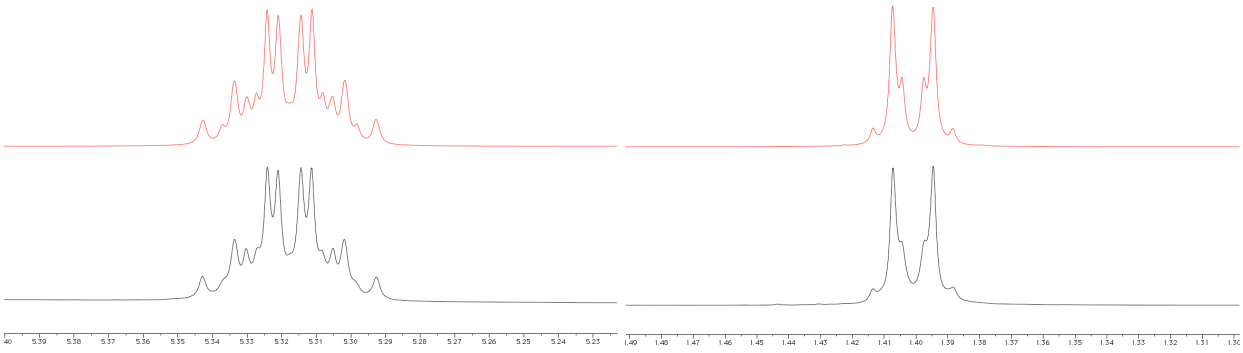


Figure S9. ^{1}H NMR spectrum of (*R*,*R*)-BdanH$_4$ ($CDCl_3$, 400 MHz)

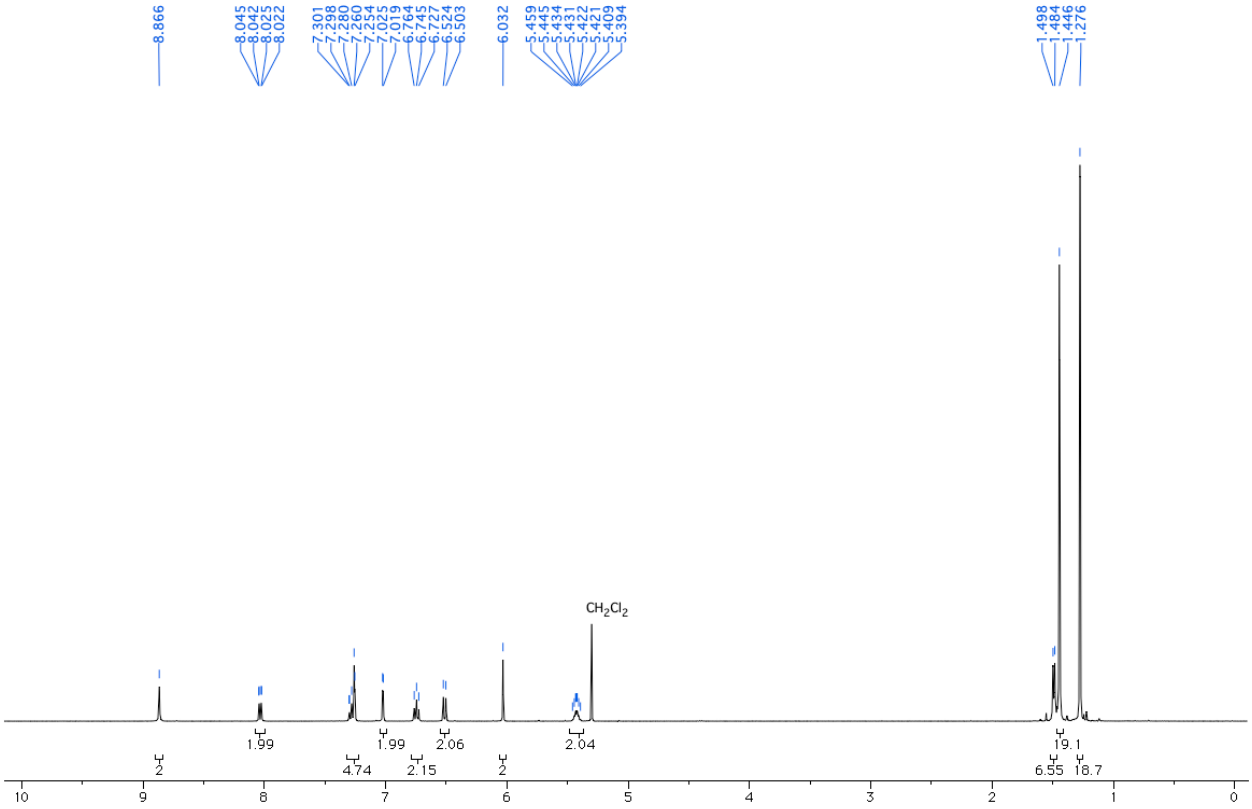


Figure S10. Experimental (**black**, bottom) and simulated (red, top) aliphatic ^{1}H NMR signals for (*R*,*R*)-BdanH$_4$. Simulation parameters for the $A_3BB'A'_3$ spin system: linewidth = 2.0 Hz, δ_A = 1.4910 ppm, δ_B = 5.4267 ppm, J_{AB} = 6.4 Hz, $J_{BB'}$ = 5.2 Hz.

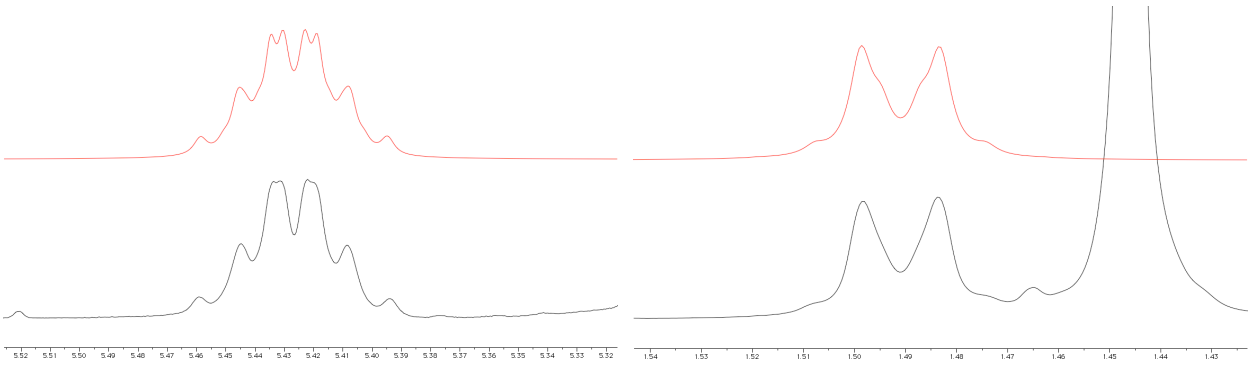


Figure S11. ^{1}H NMR spectrum of (*R*)-(Biniq)Pd ($CDCl_3$, 500 MHz). The peak at δ 1.6 ppm is due to H_2O.

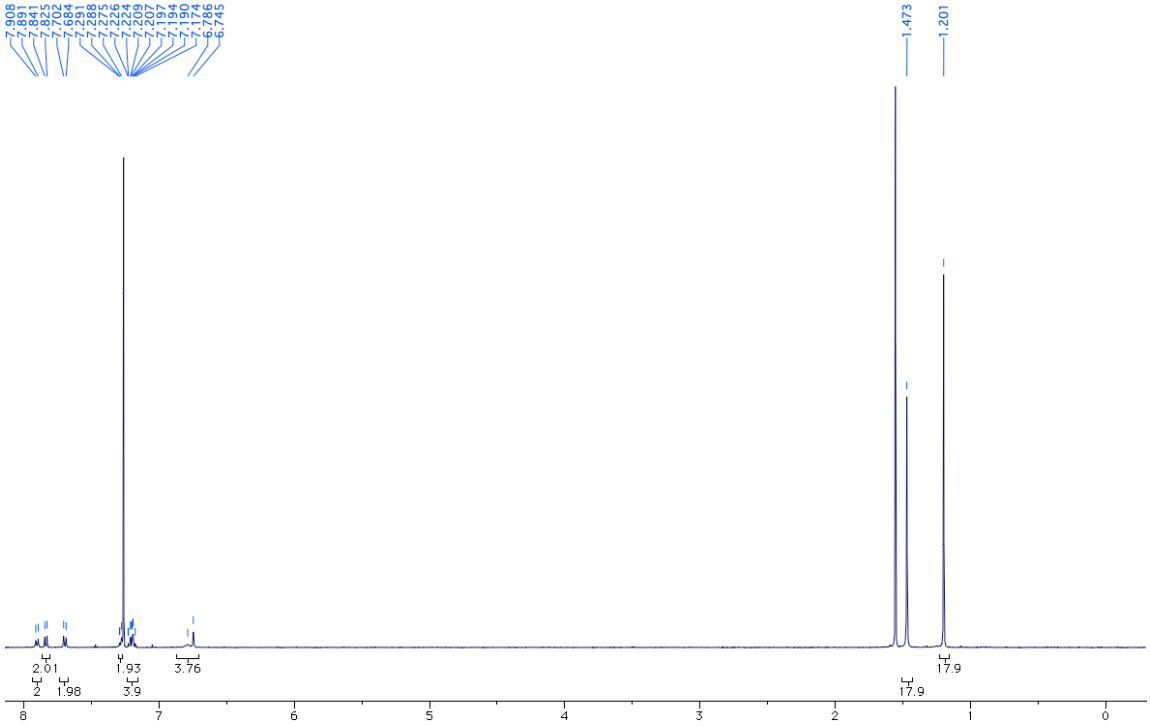


Figure S12. ^{1}H NMR spectrum of (*R*)-(Biniq)Pt (C_6D_6, 500 MHz). The peak at δ 0.4 ppm is due to H_2O.

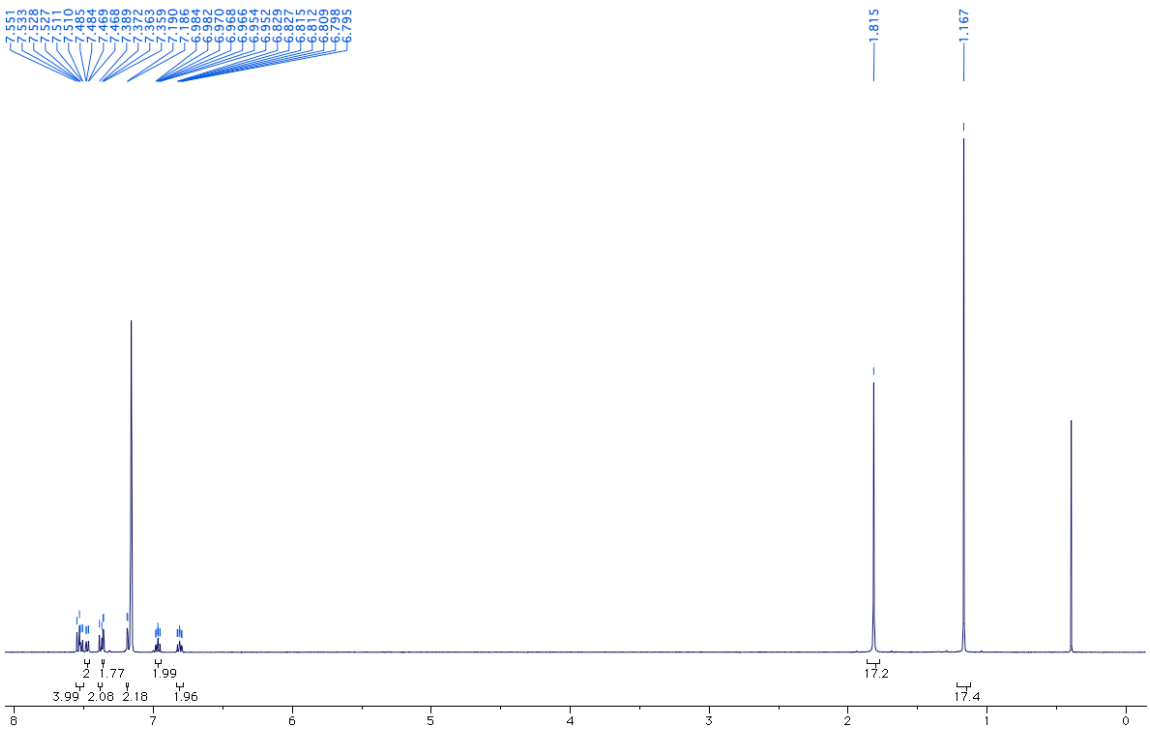


Figure S13. ^{1}H NMR spectrum of (*C*,*R*,*R*)-(Bdan)Pd ($CDCl_3$, 500 MHz)

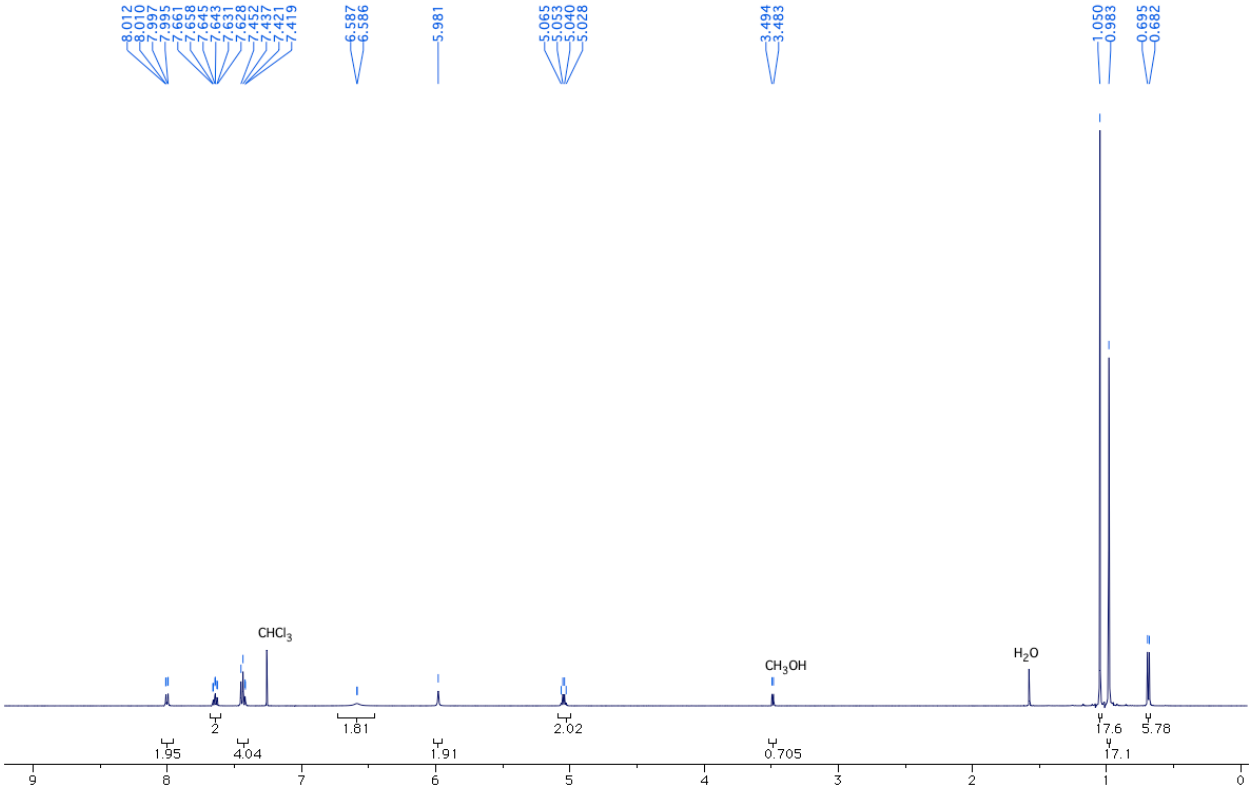


Figure S14. Experimental (**black**, bottom) and simulated (red, top) aliphatic ^{1}H NMR signals for (*C*,*R*,*R*)-(Bdan)Pd. Simulation parameters for the $A_3BB'A'_3$ spin system: linewidth = 1.2 Hz, δ_A = 0.6883 ppm, δ_B = 5.0463 ppm, J_{AB} = 6.5 Hz, $J_{BB'}$ = 1.2 Hz.

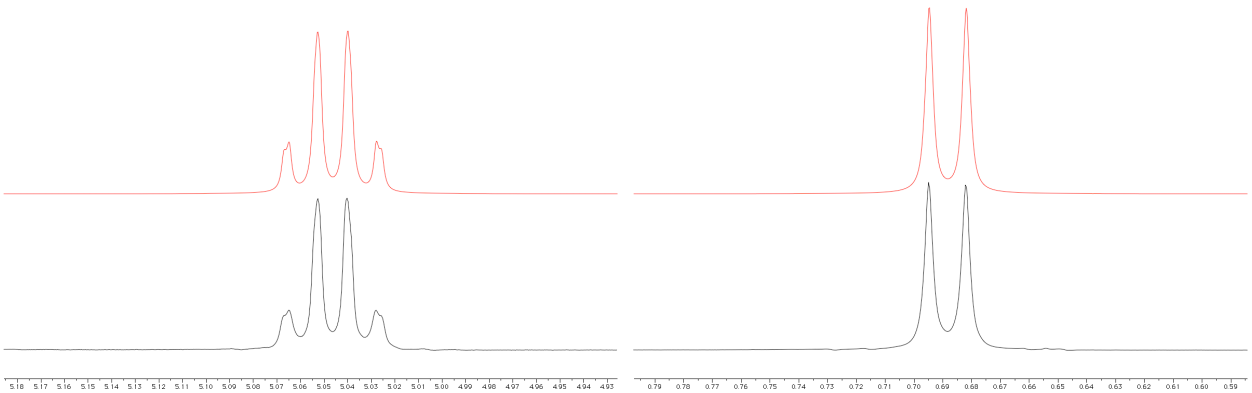


Figure S15. ^{1}H NMR spectrum of (*C*,*R*,*R*)-(Bdan)OsO (CD_2Cl_2, 500 MHz)

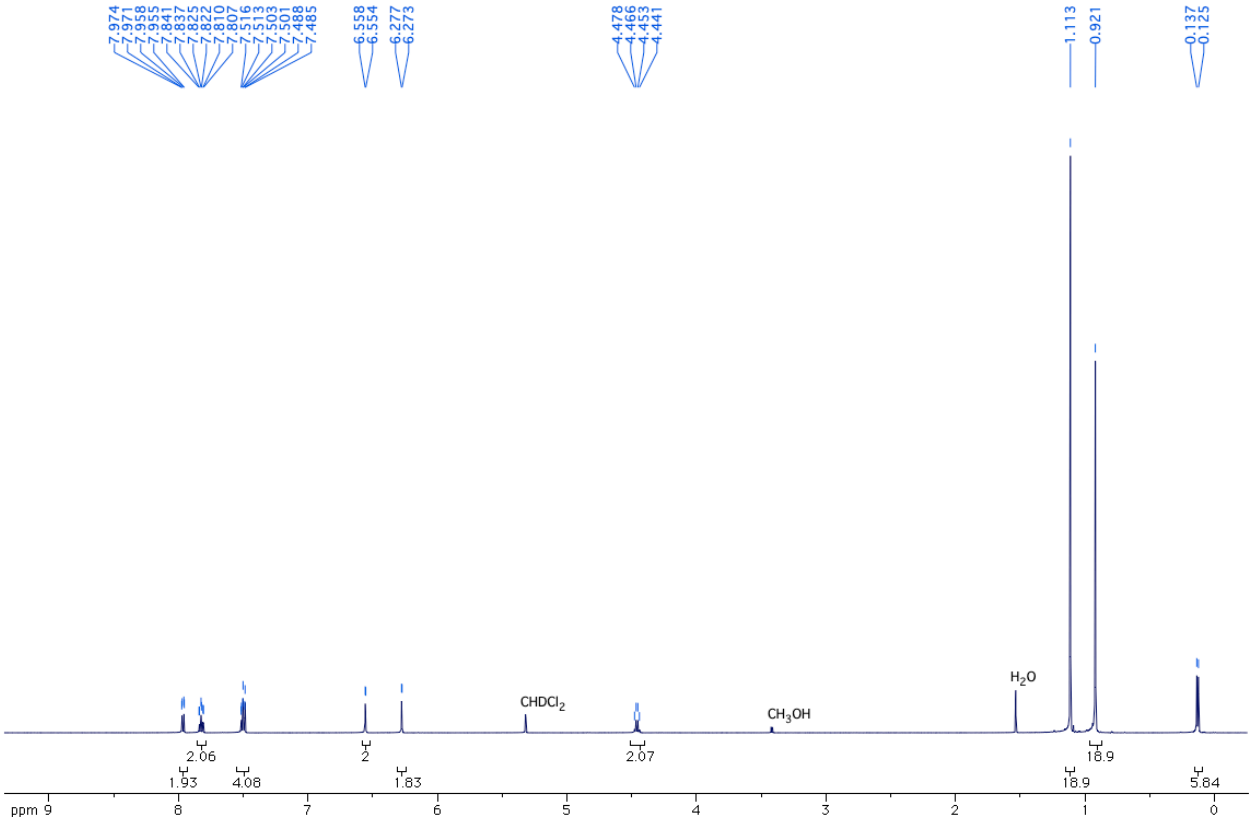


Figure S16. Experimental (**black**, bottom) and simulated (red, top) aliphatic ^{1}H NMR signals for (*C*,*R*,*R*)-(Bdan)OsO. Simulation parameters for the $A_3BB'A'_3$ spin system: linewidth = 1.26 Hz, δ_A = 0.1310 ppm, δ_B = 4.4595 ppm, J_{AB} = 6.5 Hz, $J_{BB'}$ = 1.2 Hz.

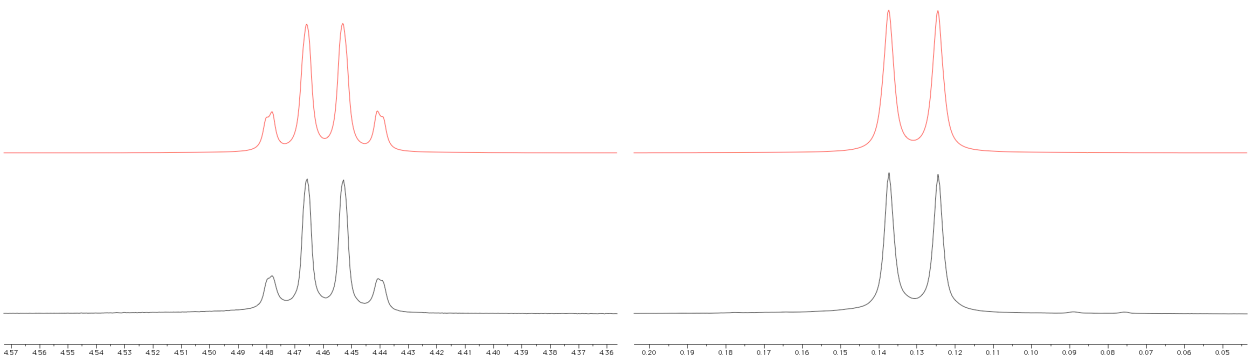
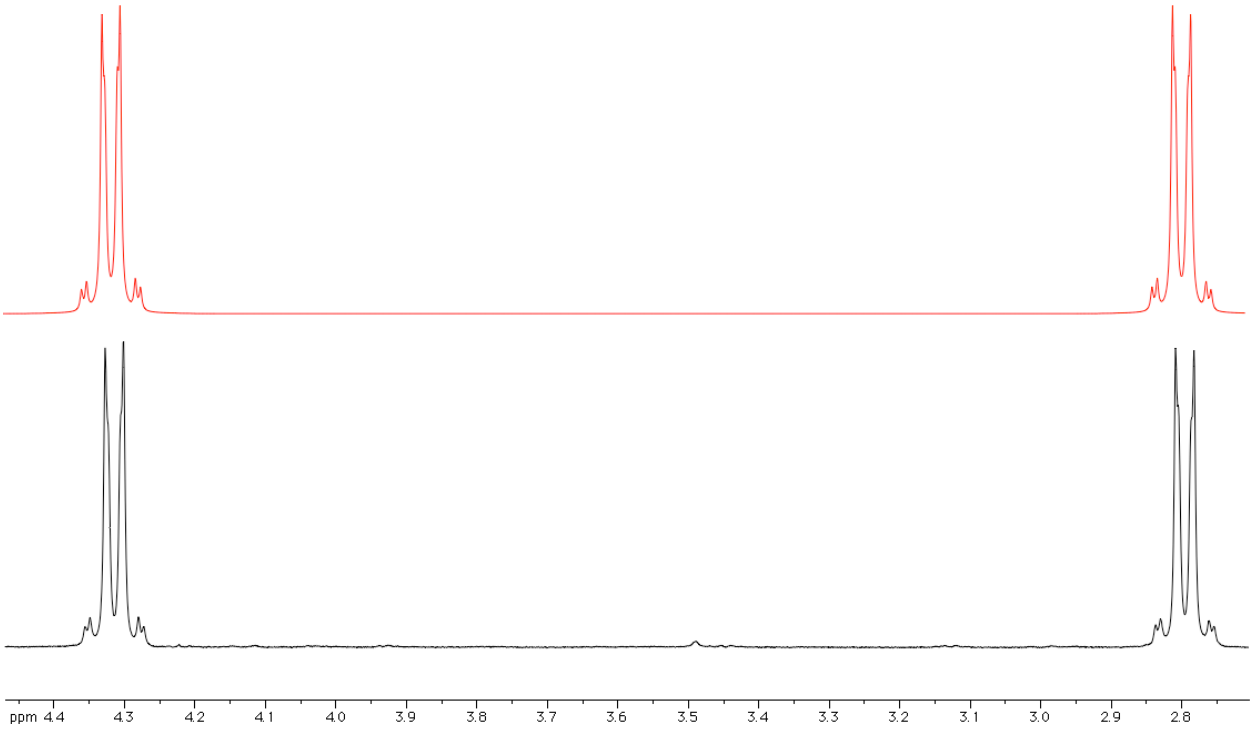


Figure S17. Experimental (**black**, bottom) and simulated (red, top) aliphatic ^{1}H NMR signals for (Egan)OsO ($CDCl_3$, 400 MHz). Simulation parameters for the *AA'BB'* spin system: δ_A = 2.796 ppm, δ_B = 4.314 ppm, J_{AB} = –12.5 Hz, $J_{AB'}$ = 2.1 Hz, $J_{AA'}$ = 11.8 Hz, $J_{BB'}$ = 1.8 Hz.



III. $^{13}C\{^1H\}$ NMR spectra

Figure S18. $^{13}C\{^1H\}$ NMR spectrum of (*R*)-BiniqH_4 (C_6D_6, 125.7 MHz)

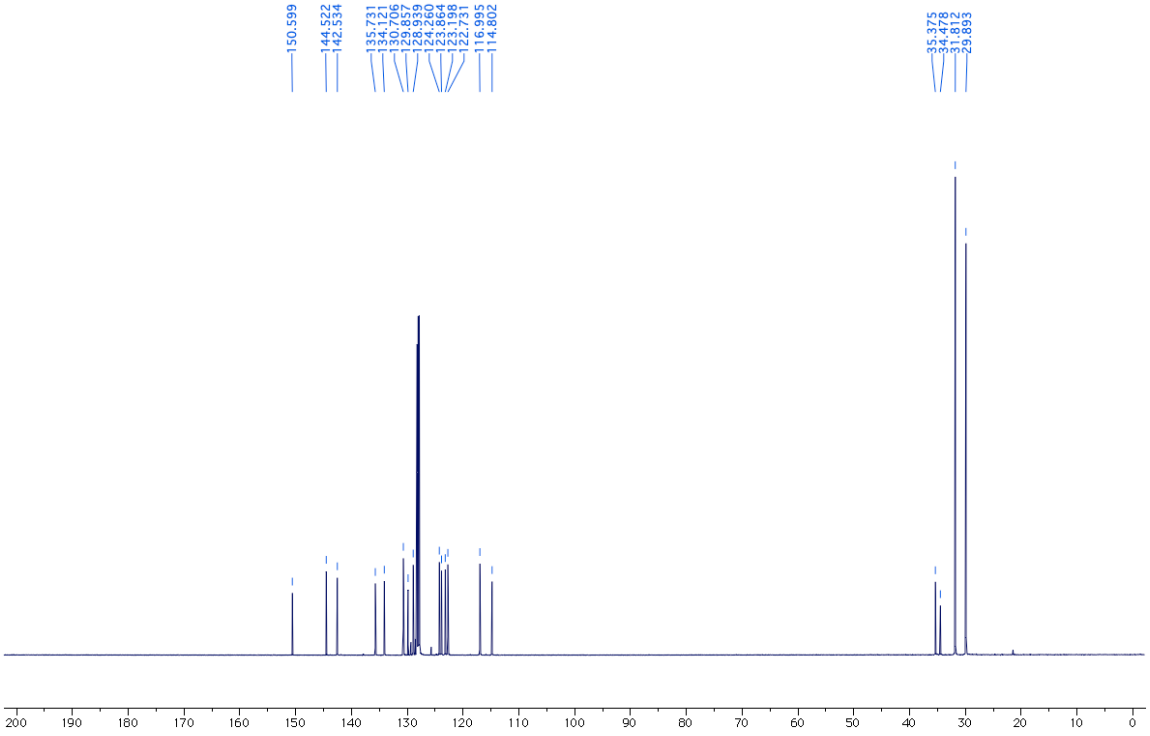


Figure S19. $^{13}C\{^1H\}$ NMR spectrum of (*R*,*R*)-2,3-$C_4H_8(O_2CC_6H_4$-2-$NH_2)_2$ ($CDCl_3$, 100.6 MHz)

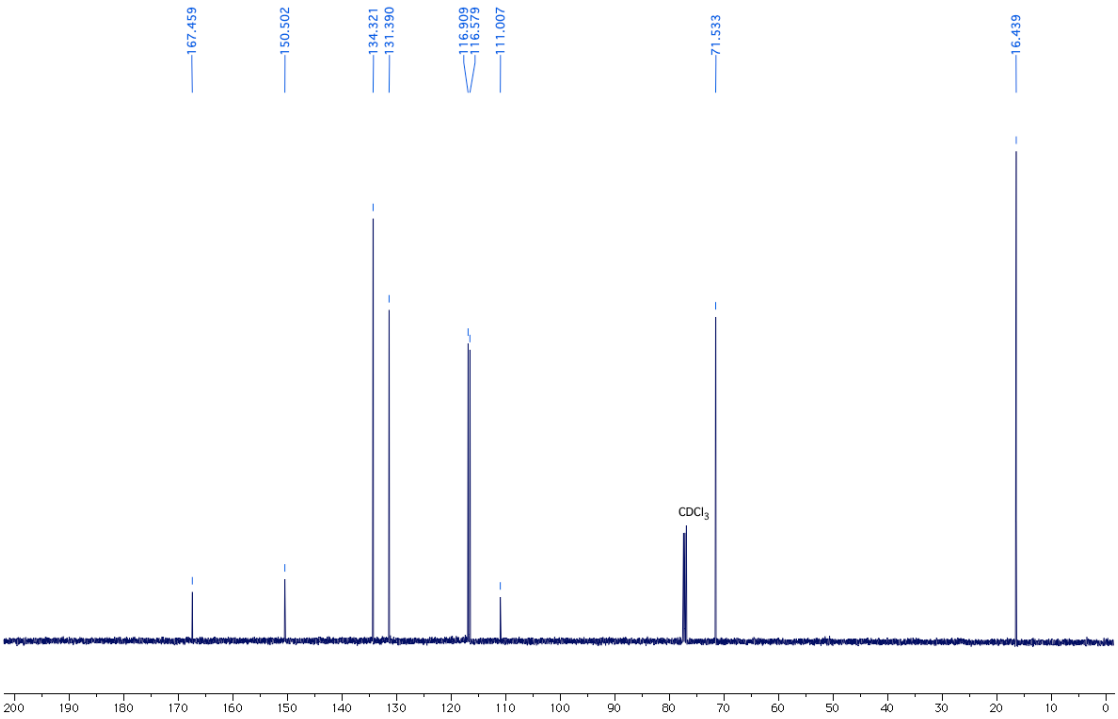


Figure S20. $^{13}C\{^{1}H\}$ NMR spectrum of (*R*,*R*)-BdanH_4 ($CDCl_3$, 100.6 MHz)

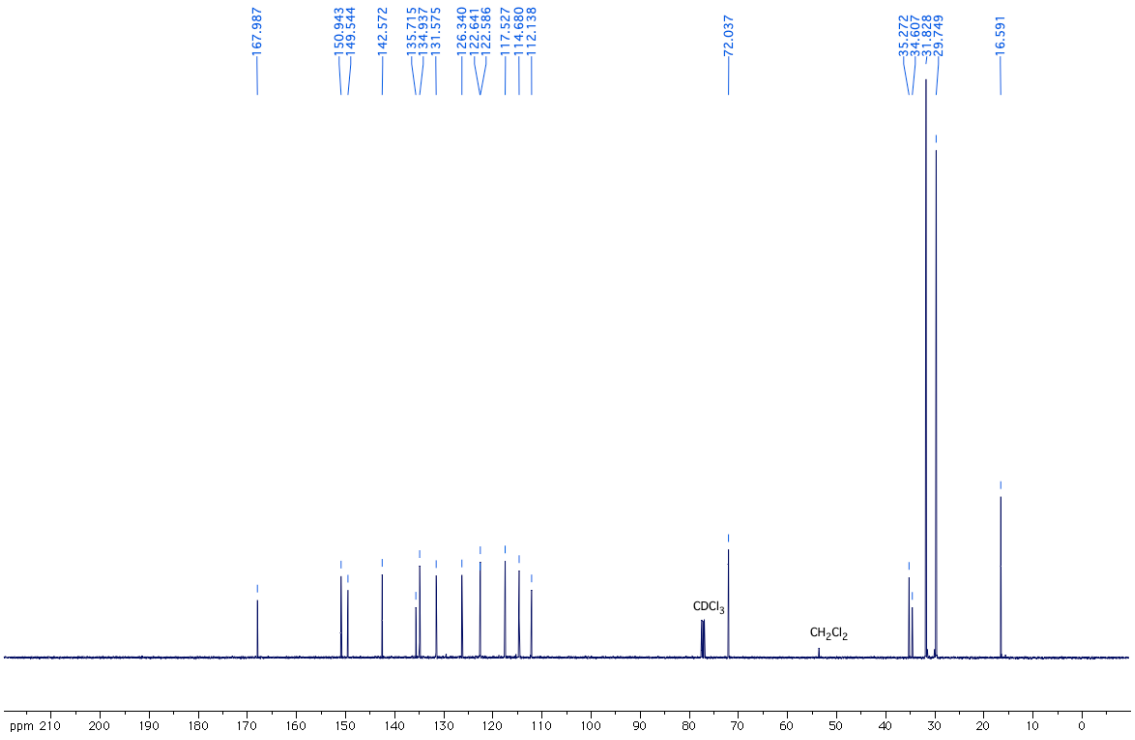


Figure S21. $^{13}C\{^{1}H\}$ NMR spectrum of (*R*,*R*)-(Biniq)Pd (CD_2Cl_2, 125.7 MHz)

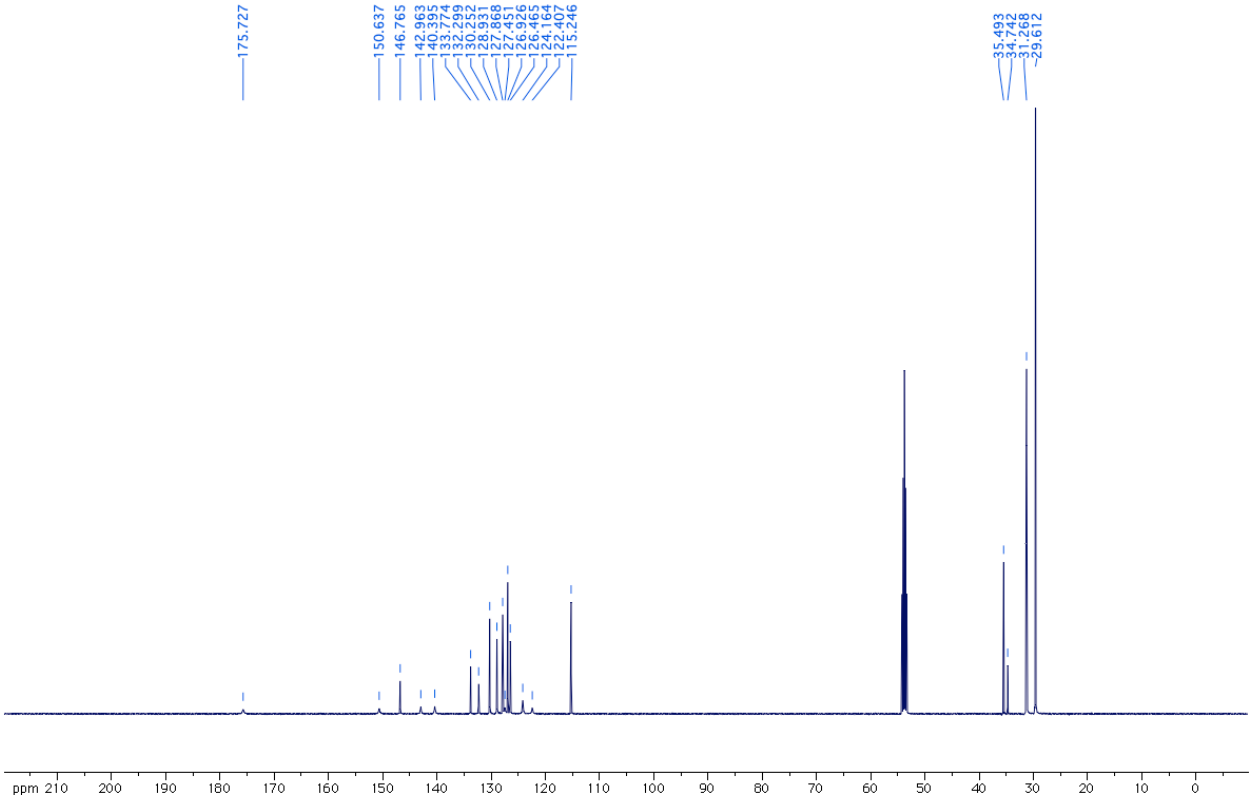


Figure S22. $^{13}C\{^{1}H\}$ NMR spectrum of (*R*,*R*)-(Biniq)Pt (C_6D_6, 125.7 MHz)

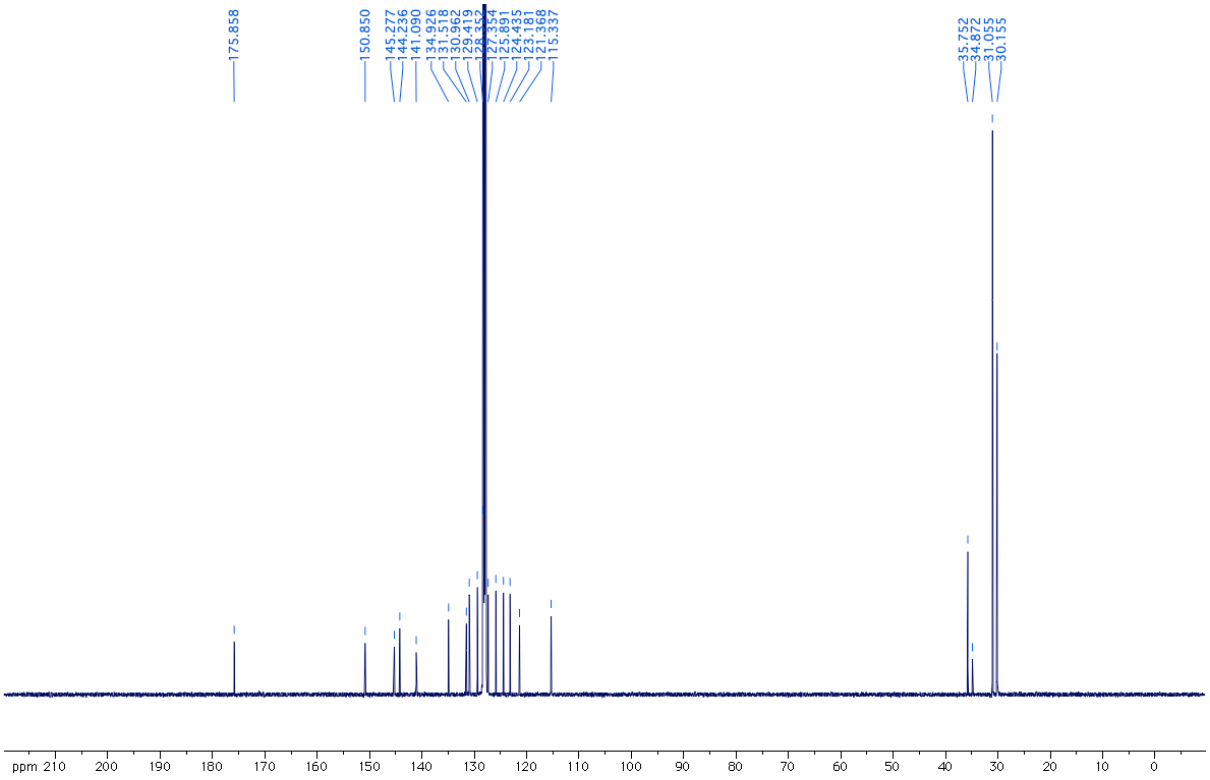


Figure S23. $^{13}C\{^{1}H\}$ NMR spectrum of (*C*,*R*,*R*)-(Bdan)Pd ($CDCl_3$, 125.7 MHz)

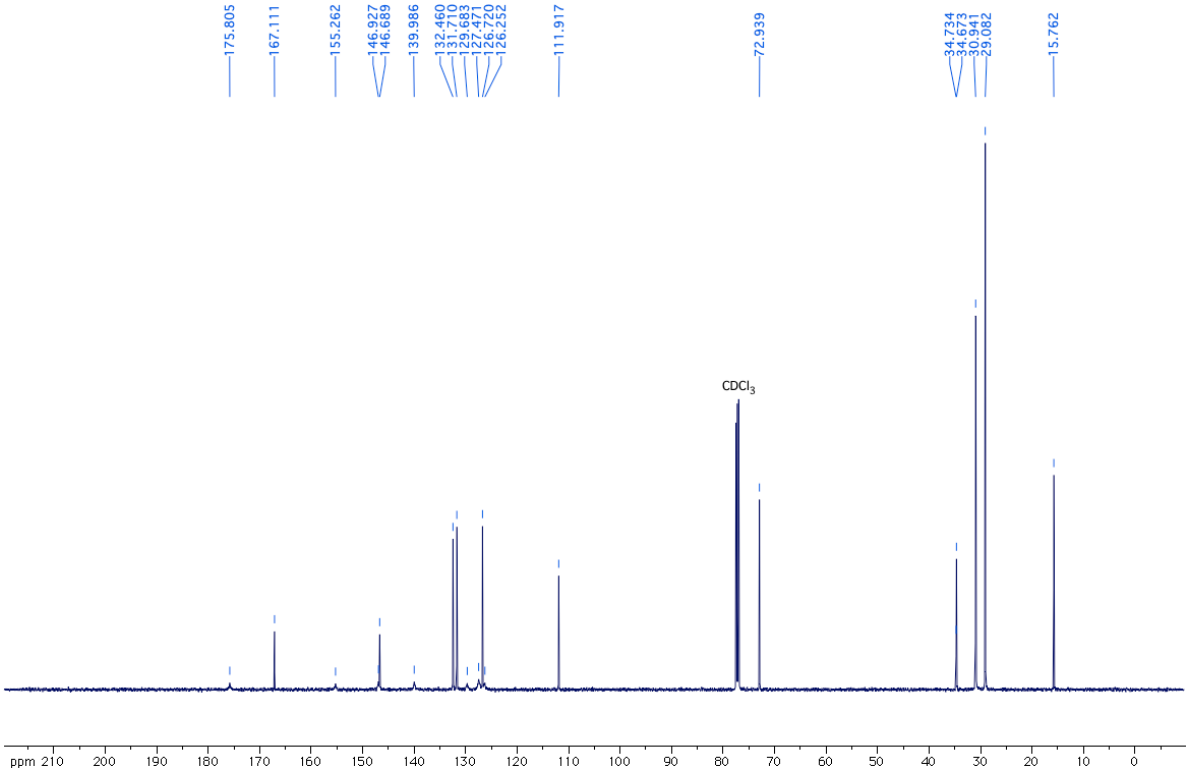
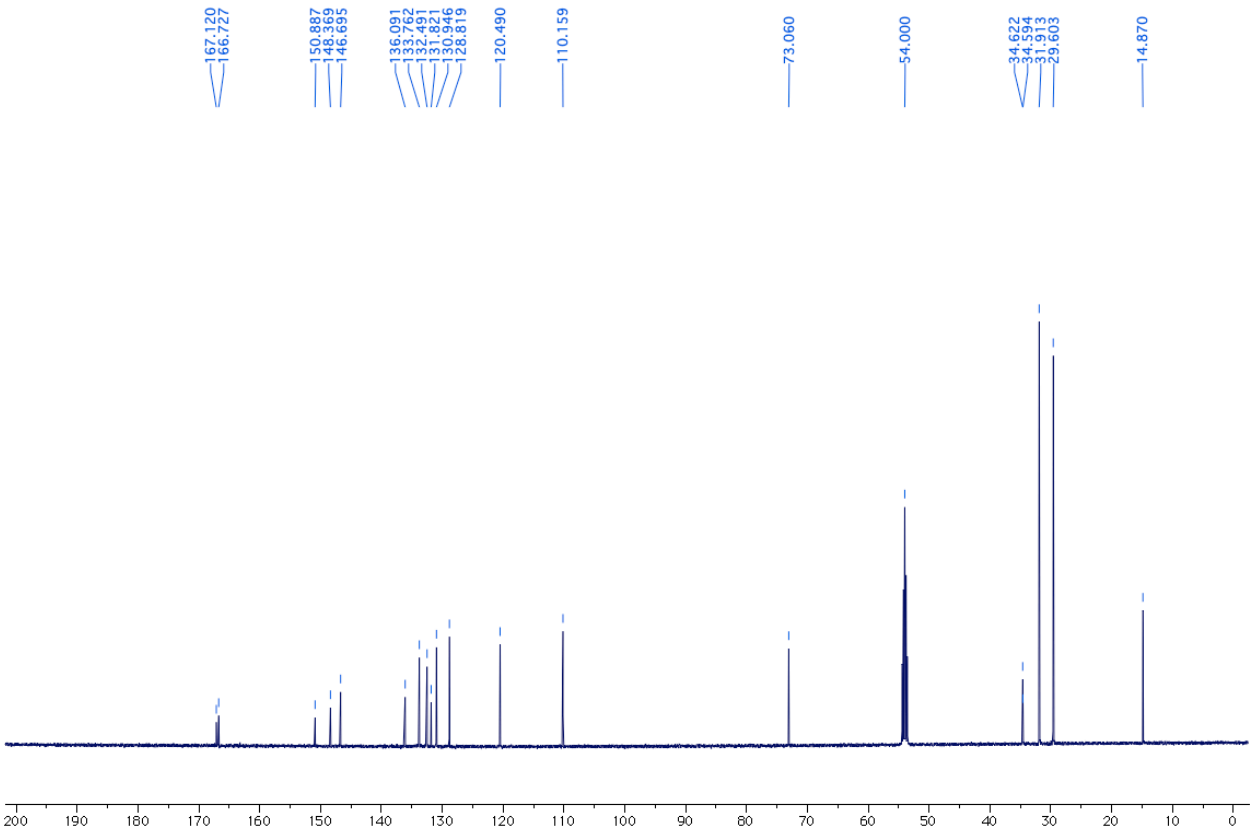


Figure S24. $^{13}C\{^{1}H\}$ NMR spectrum of (*C*,*R*,*R*)-(Bdan)OsO (CD_2Cl_2, 125.7 MHz)



IV. IR spectra

Figure S25. IR spectrum of (*R*)-BiniqH_4 (evapd film)

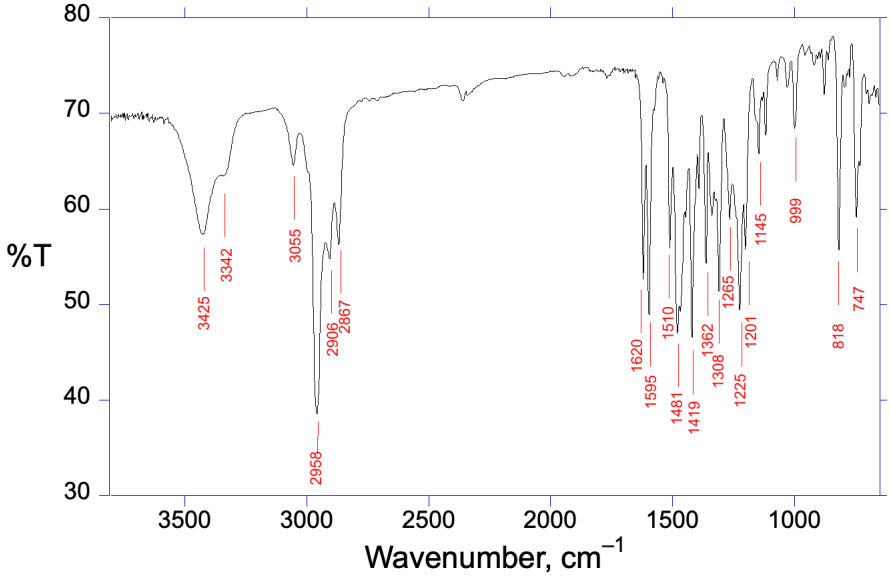


Figure S26. IR spectrum of (*R*,*R*)-2,3-$C_4H_8(O_2CC_6H_4$-2-$NH_2)_2$ (ATR)

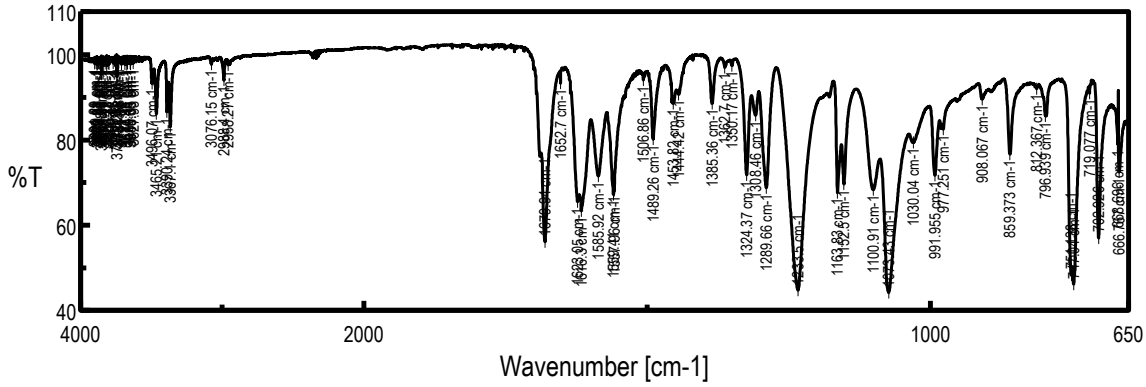


Figure S27. IR spectrum of (*R*,*R*)-BdanH_4 (ATR)

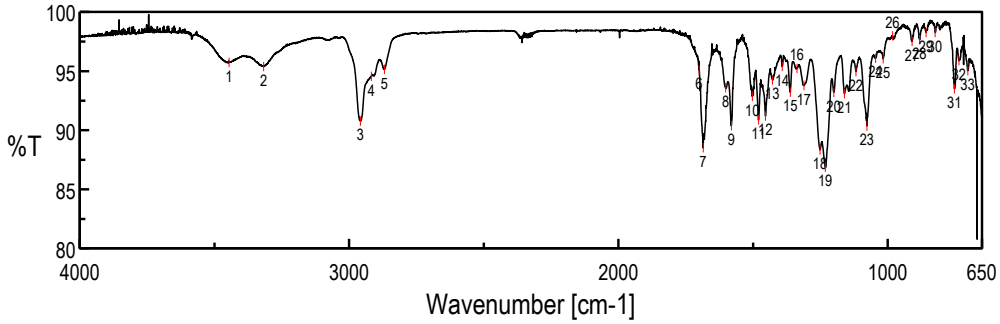


Figure S28. IR spectrum of (*R*)-(Biniq)Pd (evapd film)

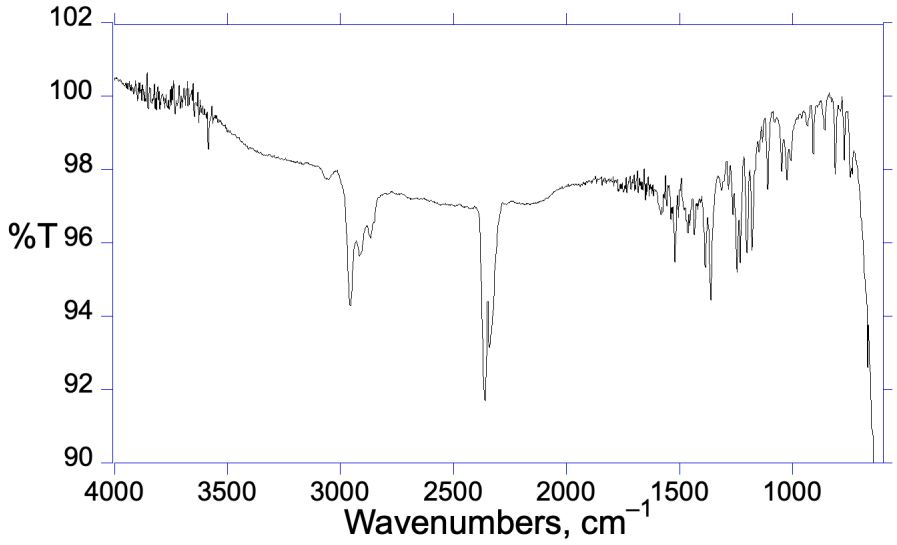


Figure S29. IR spectrum of (*R*)-(Biniq)Pt (evapd film)

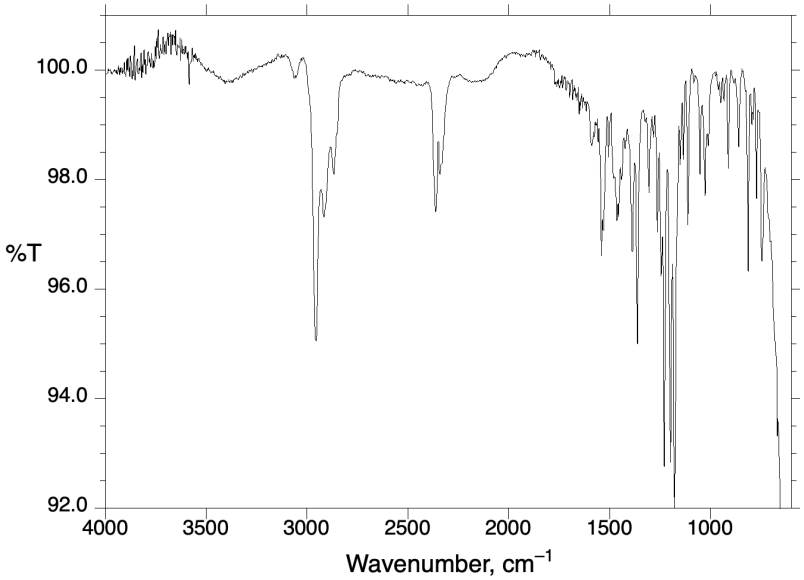


Figure S30. IR spectrum of (*C*,*R*,*R*)-(Bdan)Pd (evapd film)

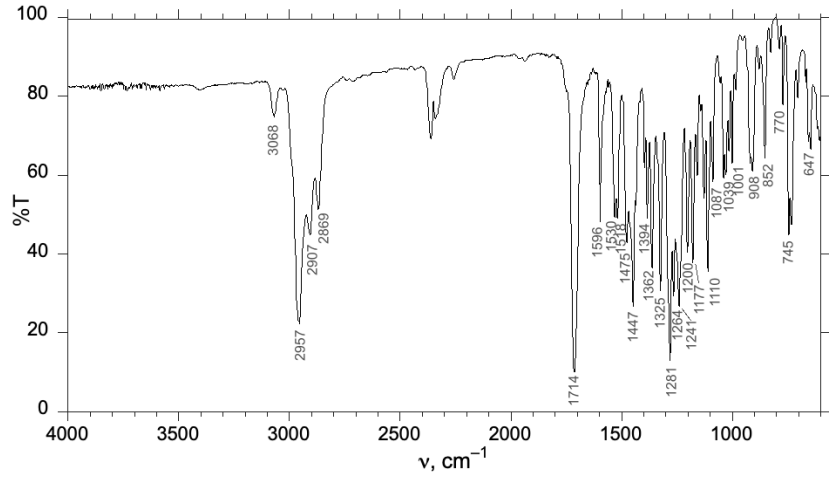
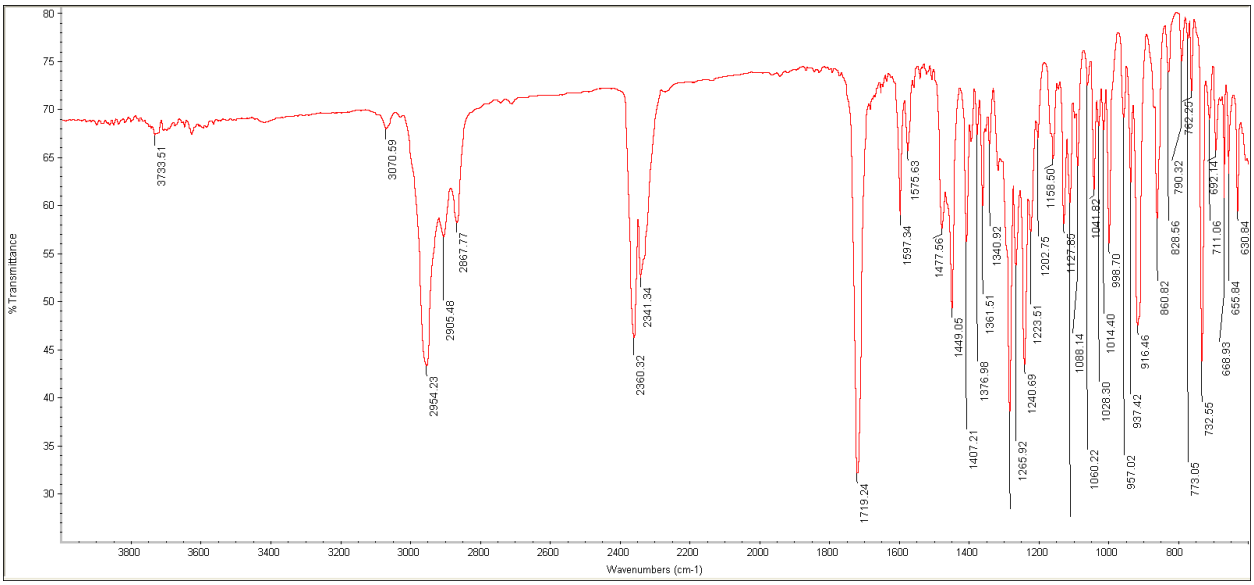


Figure S31. IR spectrum of (*C*,*R*,*R*)-(Bdan)OsO (evapd film)



V. Electrochemistry

Figure S32. CV of (*C*,*R*,*R*)-(Bdan)Pd (CH_2Cl_2, 50 mV s^{-1}, 0.1 M Bu_4NPF_6).

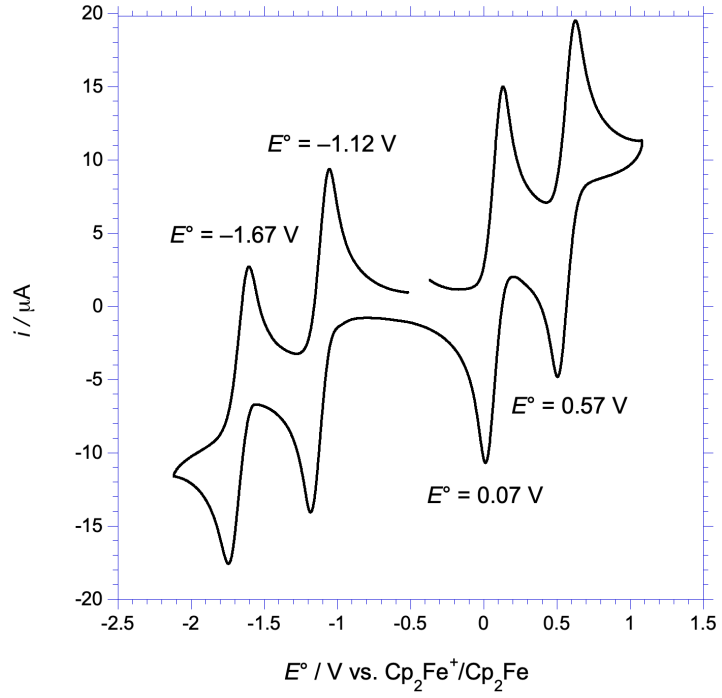
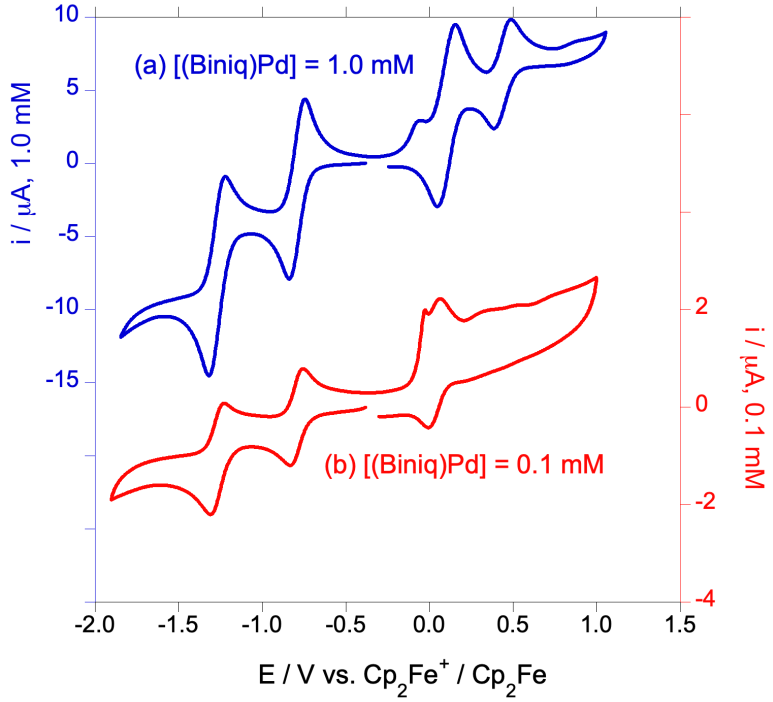


Figure S33. CV of (*R*)-(Biniq)Pd (CH_2Cl_2, 20 mV s^{-1}, 0.1 M Bu_4NPF_6) at (a) 1.0 mM (Biniq)Pd (top, left) and (b) 0.1 mM (Biniq)Pd (bottom, right).



VI. Variable-temperature NMR spectroscopy

Figure S34. Variable-temperature ^{1}H NMR spectra (downfield region) of (*C*,*R*,*R*)-(Bdan)Pd ($CDCl_2CDCl_2$). The signal at δ 6.0 is due to the solvent residual.

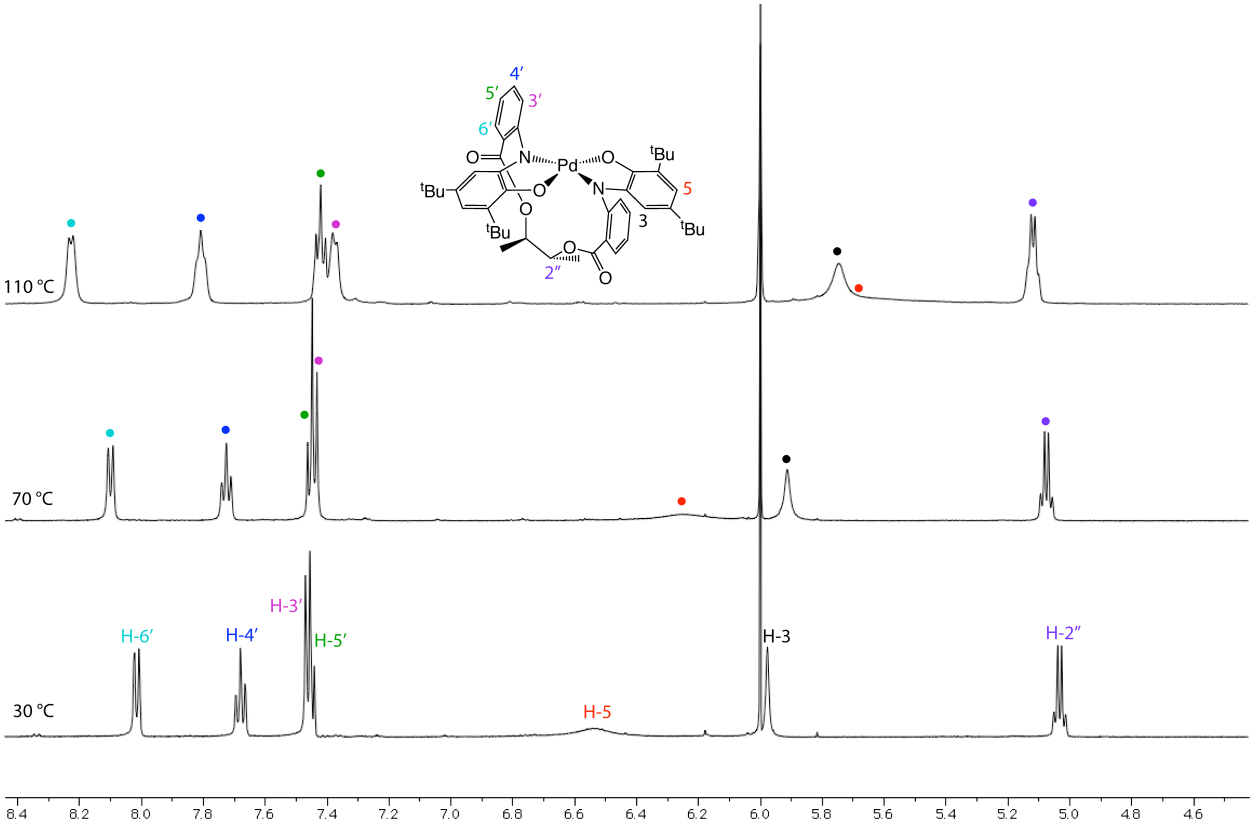


Figure S35. Temperature-dependence of ^{1}H chemical shifts of (*R*)-(Biniq)Pd ($CDCl_2CDCl_2$). Solid lines are fit to eq 1 with (a) a model with $A_{H\text{-}5}$ constrained to be –4.26 MHz; (b) an unconstrained model.

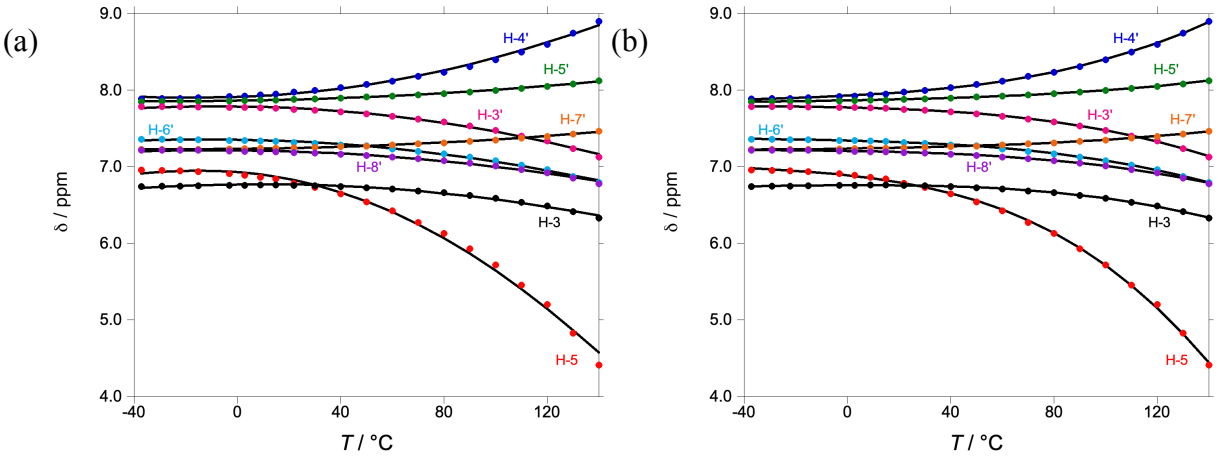


Figure S36. Temperature-dependence of ^{1}H chemical shifts of (*C*,*R*,*R*)-(Bdan)Pd ($CDCl_2CDCl_2$). Solid lines are fit to eq 1 with (a) a model with $A_{H\text{-}5}$ constrained to be –5.90 MHz; (b) an unconstrained model.

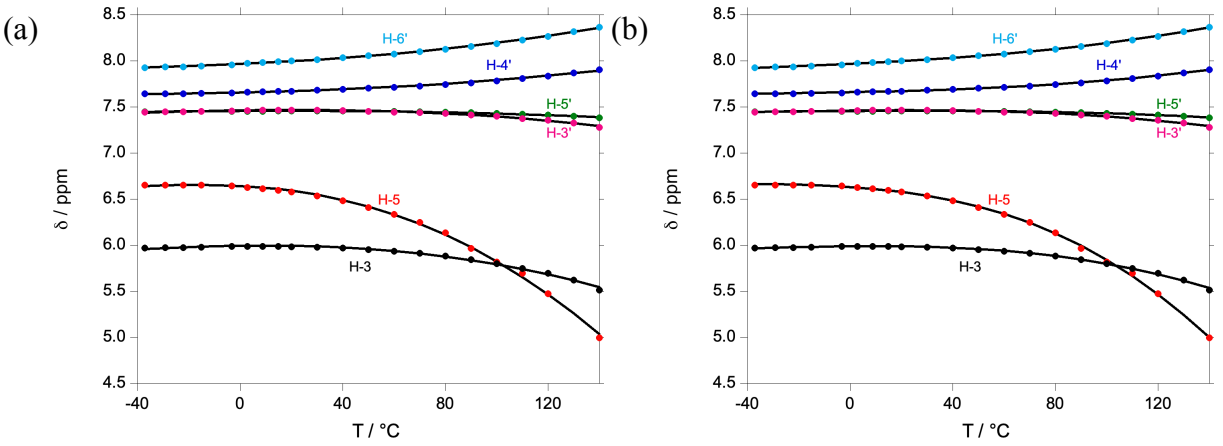


Table S1. Parameters describing temperature-dependent chemical shifts of (*R*)-(Biniq)Pd and (*C*,*R*,*R*)-(Bdan)Pd. *n. d.* = Not determined. *n. a.* = Not applicable.

	(*R*)-(Biniq)Pd			(*C*,*R*,*R*)-(Bdan)Pd		
	Unconstrained model	Constrained model	DFT	Unconstrained model	Constrained model	DFT
ΔE, cm^{-1}	2230(30)	1458(9)	*n. d.*	2050(30)	1729(4)	*n. d.*
A, H-3, MHz	–8.3(7)	–1.01(9)	–1.68	–5.3(5)	–2.12(7)	–3.25
A, H-5, MHz	–37(3)	*–4.26*	–4.26	–15.0(14)	*–5.90*	–5.90
A, H-3', MHz	–10.0(8)	–1.22(9)	–1.59	–2.3(2)	–0.96(7)	–0.73
A, H-4', MHz	13.6(11)	1.66(9)	2.26	1.8(2)	0.63(6)	0.96
A, H-5', MHz	3.3(3)	0.40(9)	0.77	–1.02(14)	–0.37(6)	–0.19
A, H-6', MHz	–8.2(7)	–1.00(9)	–1.36	2.2(2)	0.91(6)	0.88
A, H-7', MHz	3.0(3)	0.37(9)	0.69	*n. a.*		
A, H-8', MHz	–6.4(6)	–0.77(9)	–1.18	*n. a.*		

VII. Details of assignments of optical and chiroptical spectra

Table S2. Optical and chiroptical assignments for (*C*,*R*,*R*)-(Bdan)Pd (CH_2Cl_2).

λ_{exptl}, nm	ε_{exptl}, $M^{-1}\,cm^{-1}$	$\Delta\varepsilon_{exptl}$, $M^{-1}\,cm^{-1}$	λ_{calc}, nm	f_{calc}	R_{vel}, calc (10^{-40} erg esu cm G^{-1})	Assignment
876	34600	+18.6	840	0.324	+51.4	HOMO→LUMO
677	5100	–4.5	653	0.003	–18.3	HOMO–3→LUMO
574	4000	–4.3	542	0.031	–32.0	HOMO–2→LUMO
430	2400	+3.7	433	0.005	+6.6	HOMO–1→LUMO+1

Table S3. Optical and chiroptical assignments for (*R*)-(Biniq)Pd (CH_2Cl_2).

λ_{exptl}, nm	ε_{exptl}, $M^{-1}\,cm^{-1}$	$\Delta\varepsilon_{exptl}$, $M^{-1}\,cm^{-1}$	λ_{calc}, nm	f_{calc}	R_{vel}, calc (10^{-40} erg esu cm G^{-1})	Assignment
1031	27400	–13.2	1027	0.150	–88.4	HOMO→LUMO
822	11100	+5.6	759	0.059	+119.2	HOMO–1→LUMO
600	5000	+8.3	612	0.021	+51.9	HOMO→LUMO+1
530	3400	–8.6	590	0.031	–90.3	HOMO–3→LUMO
422	13700	–44.7	397	0.041	–168.1	HOMO→LUMO+2

Table S4. Optical and chiroptical assignments for (*R*)-(Biniq)Pt (CH_2Cl_2).

λ_{exptl}, nm	ε_{exptl}, $M^{-1}\,cm^{-1}$	$\Delta\varepsilon_{exptl}$, $M^{-1}\,cm^{-1}$	λ_{calc}, nm	f_{calc}	R_{vel}, calc (10^{-40} erg esu cm G^{-1})	Assignment
924	37000	–7.9	866	0.164	–115.4	HOMO→LUMO
704	7300	+20.3	683	0.072	+165.7	HOMO–2→LUMO
537	2300	–15.3	557	0.046	–105.7	HOMO–3→LUMO
426	11500	+19.9	457	0.028	+80.5	HOMO→LUMO+1

Table S5. Optical and chiroptical assignments for (*C*,*R*,*R*)-(Bdan)OsO (CH_2Cl_2).

λ_{exptl}, nm	ε_{exptl}, $M^{-1}\,cm^{-1}$	$\Delta\varepsilon_{exptl}$, $M^{-1}\,cm^{-1}$	λ_{calc}, nm	f_{calc}	R_{vel}, calc (10^{-40} erg esu cm G^{-1})	Assignment
579	2400	+3.0	518	0.004	–1.1	HOMO–1→LUMO
444	13100	+15.4	491	0.065	+68.8	HOMO–1→LUMO+1
410		+12.7	431	0.062	+73.9	HOMO–2→LUMO
358	18800	–0.3	360	0.158	+13.8	HOMO→LUMO+2
333	17000	+2.4	339	0.162	+0.8	HOMO→LUMO+3

VIII. Structural comparison between (Clip)M and (Biniq)M (M = Pd, Pt)

Figure S37. Overlay of calculated structures of (Clip)Pd (pink solid lines) and (Biniq)Pd (green dashed lines). Structures have been oriented to align the nonhydrogen atoms of the Pd(iminoxolene)$_2$ core (rmsd = 0.017 Å for 17 atoms). Structures are viewed down the molecular twofold axis.

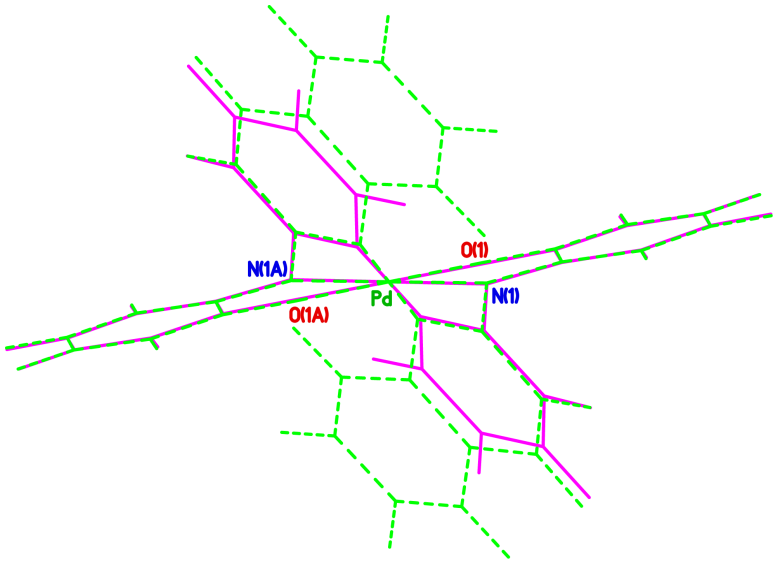


Figure S38. Overlay of calculated structures of (Clip)Pt (pink solid lines) and (Biniq)Pt (green dashed lines). Structures have been oriented to align the nonhydrogen atoms of the Pt(iminoxolene)$_2$ core (rmsd = 0.015 Å for 17 atoms). Structures are viewed down the molecular twofold axis.

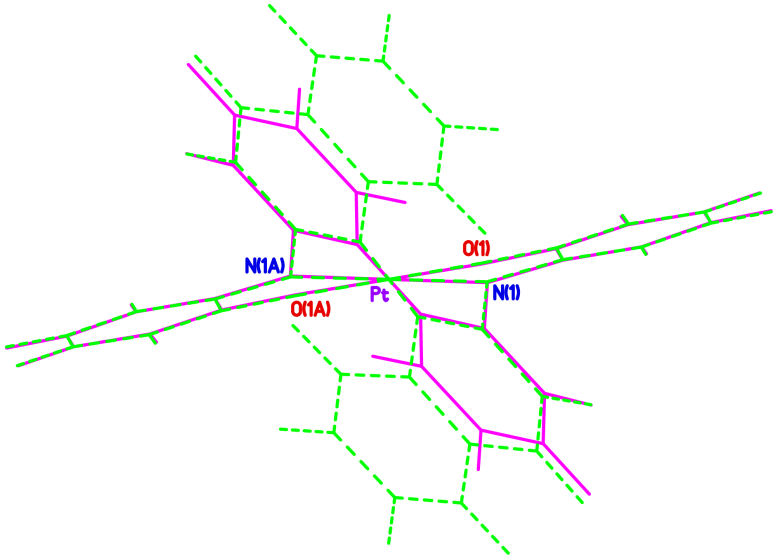


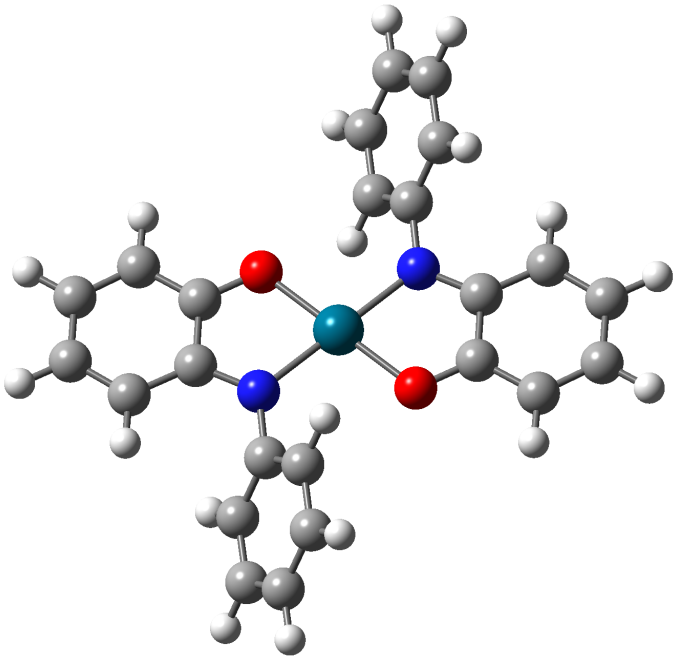
Table S6. Selected metrical data on calculated structures of (Clip)M and (Biniq)M (M = Pd, Pt).

	(Clip)Pd	(Biniq)Pd	(Clip)Pt	(Biniq)Pt
M–O, Å	2.007	2.009	2.017	2.019
M–N, Å	1.986	1.988	1.978	1.980
Metrical oxidation state (MOS)[1]	–1.23(8)	–1.23(7)	–1.34(7)	–1.34(7)
C11–N1–M–N1A, °	163.3	164.1	161.8	162.5
M–N1–C22–C21, °	57.4	57.8	55.6	55.8
C22–C21–C21A–C22A, °	–61.5	–71.0	–62.0	–71.7

IX. Energies and Cartesian coordinates of calculated structures

All structures were optimized as singlets unless otherwise stated.

A. $(^{H}ap)_2Pd$



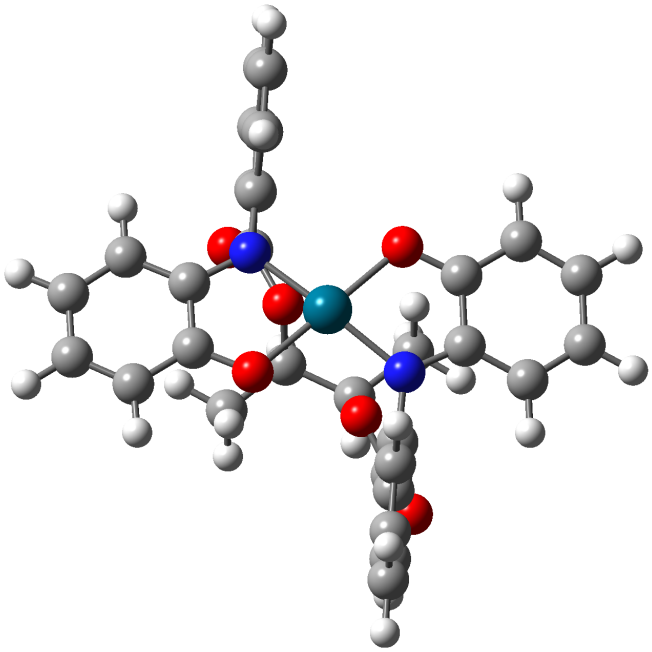
Energy of optimized structure = –1313.27725613 a.u.

Cartesian coordinates of optimized structure:

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	46	0.000000	0.000000	0.000000
2	7	-2.000157	0.057382	0.080777
3	8	-0.252980	1.979773	-0.153151
4	6	-1.510005	2.344153	-0.136318
5	6	-2.514696	1.318980	-0.000088
6	6	-3.881950	1.697270	0.088566
7	1	-4.641791	0.938599	0.235456
8	6	-4.227220	3.031131	0.001454
9	1	-5.271945	3.319471	0.073384
10	6	-3.237766	4.031581	-0.169291
11	1	-3.538377	5.073508	-0.236428
12	6	-1.897605	3.699746	-0.234156
13	1	-1.122521	4.451370	-0.345241
14	6	-2.827418	-1.087511	0.113071
15	6	-3.807868	-1.304666	-0.872817
16	1	-3.929988	-0.578366	-1.670457
17	6	-4.590768	-2.456156	-0.838916
18	1	-5.337987	-2.617660	-1.611260
19	6	-4.411100	-3.403165	0.173321

20	1	-5.024732	-4.299311	0.197642
21	6	-3.433062	-3.193779	1.148232
22	1	-3.284037	-3.926540	1.936624
23	6	-2.639423	-2.048838	1.119451
24	1	-1.873285	-1.882100	1.868173
25	7	2.000157	-0.057382	-0.080777
26	8	0.252980	-1.979773	0.153151
27	6	1.510005	-2.344153	0.136318
28	6	2.514696	-1.318980	0.000088
29	6	3.881950	-1.697270	-0.088566
30	1	4.641791	-0.938599	-0.235456
31	6	4.227220	-3.031131	-0.001454
32	1	5.271945	-3.319471	-0.073384
33	6	3.237766	-4.031581	0.169291
34	1	3.538377	-5.073508	0.236428
35	6	1.897605	-3.699746	0.234156
36	1	1.122521	-4.451370	0.345241
37	6	2.827418	1.087511	-0.113071
38	6	3.807868	1.304666	0.872817
39	1	3.929988	0.578366	1.670457
40	6	4.590768	2.456156	0.838916
41	1	5.337987	2.617660	1.611260
42	6	4.411100	3.403165	-0.173321
43	1	5.024732	4.299311	-0.197642
44	6	3.433062	3.193779	-1.148232
45	1	3.284037	3.926540	-1.936624
46	6	2.639423	2.048838	-1.119451
47	1	1.873285	1.882100	-1.868173

B. (*C*,*R*,*R*)-(Bdan)Pd



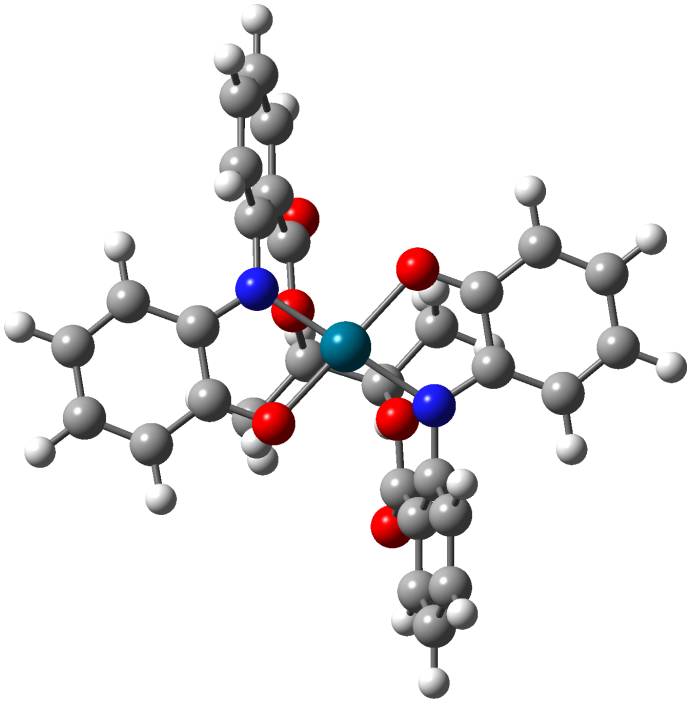
Energy of optimized structure = –1846.44593057 a.u.

Cartesian coordinates of optimized structure:

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	46	-0.000165	0.000489	-1.132751
2	8	-0.006754	2.009604	-1.144357
3	8	0.006464	-2.008658	-1.145858
4	8	-1.394179	-0.219355	1.742151
5	8	-3.306344	-0.534996	2.913348
6	8	1.395021	0.216875	1.741921
7	8	3.307270	0.532302	2.913056
8	7	-1.959144	0.297086	-0.972366
9	7	1.958890	-0.296023	-0.973099
10	6	-0.774903	1.804783	2.929483
11	1	-1.817087	2.134370	2.971154
12	1	-0.307429	2.218330	2.031991
13	1	-0.256087	2.199221	3.810780
14	6	-0.710389	0.281511	2.922201
15	1	-1.228063	-0.118591	3.798935
16	6	0.711639	-0.285446	2.921576
17	1	1.229642	0.113536	3.798631
18	6	0.776127	-1.808730	2.926884
19	1	1.818321	-2.138394	2.967649
20	1	0.308229	-2.221144	2.029088
21	1	0.257717	-2.204274	3.807925
22	6	-1.204024	2.517892	-1.001494
23	6	-2.312269	1.605115	-0.855755
24	6	-3.617515	2.116637	-0.629754
25	1	-4.450630	1.432238	-0.511070
26	6	-3.809873	3.483486	-0.585329
27	1	-4.808102	3.879754	-0.423854
28	6	-2.723383	4.378750	-0.754411
29	1	-2.905392	5.449178	-0.715798
30	6	-1.438500	3.910742	-0.962406
31	1	-0.594170	4.582024	-1.083732
32	6	1.203807	-2.516911	-1.003426
33	6	2.312079	-1.604105	-0.857257
34	6	3.617373	-2.115698	-0.631672
35	1	4.450473	-1.431338	-0.512665
36	6	3.809788	-3.482559	-0.588043
37	1	4.808048	-3.878874	-0.426879
38	6	2.723332	-4.377797	-0.757547
39	1	2.905426	-5.448233	-0.719560
40	6	1.438397	-3.909777	-0.965164
41	1	0.594108	-4.581056	-1.086792
42	6	-2.689679	-0.578008	1.866250
43	6	-3.275294	-1.117474	0.594763
44	6	-2.900052	-0.734355	-0.714434
45	6	-3.481725	-1.380779	-1.812536
46	1	-3.172062	-1.079620	-2.808280
47	6	-4.440373	-2.375536	-1.630831
48	1	-4.878061	-2.864188	-2.496896
49	6	-4.840232	-2.732458	-0.341768
50	1	-5.592860	-3.500900	-0.191802
51	6	-4.261936	-2.101514	0.756017
52	1	-4.555224	-2.364873	1.766817

53	6	2.690372	0.576051	1.866126
54	6	3.275440	1.117019	0.595033
55	6	2.899671	0.735353	-0.714441
56	6	3.480667	1.383199	-1.812053
57	1	3.170586	1.083157	-2.808002
58	6	4.439212	2.377926	-1.629623
59	1	4.876389	2.867690	-2.495318
60	6	4.839621	2.733402	-0.340332
61	1	5.592176	3.501809	-0.189821
62	6	4.261953	2.101070	0.756986
63	1	4.555626	2.363329	1.767966

C. (*C*,*R*,*R*)-(Bdan)Pd triplet



Energy of optimized structure = –1846.44952027 a.u.

Cartesian coordinates of optimized structure:

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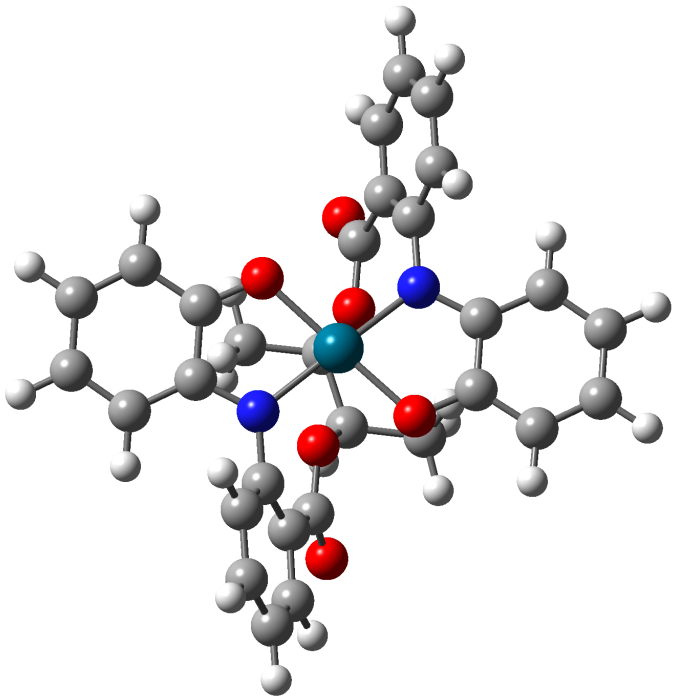
1	46	0.000000	-0.000000	-0.929707
2	8	-1.497966	1.373242	-1.003967
3	8	1.497966	-1.373242	-1.003967
4	8	-0.911383	-1.127790	1.749612
5	8	-0.656008	-3.032732	2.941043
6	8	0.911383	1.127790	1.749612
7	8	0.656008	3.032732	2.941043
8	7	-1.597500	-1.261436	-0.855603

9	7	1.597500	1.261436	-0.855603
10	6	-1.821633	0.744253	2.925841
11	1	-2.794965	0.251577	3.013243
12	1	-1.812996	1.327562	2.001002
13	1	-1.697150	1.430826	3.768941
14	6	-0.709120	-0.297146	2.925585
15	1	-0.783289	-0.943351	3.804550
16	6	0.709120	0.297146	2.925585
17	1	0.783289	0.943351	3.804550
18	6	1.821633	-0.744253	2.925841
19	1	2.794965	-0.251577	3.013243
20	1	1.812996	-1.327562	2.001002
21	1	1.697150	-1.430826	3.768941
22	6	-2.680879	0.822271	-1.016515
23	6	-2.785518	-0.622514	-0.914689
24	6	-4.073628	-1.228269	-0.848487
25	1	-4.150337	-2.305642	-0.748636
26	6	-5.201798	-0.441313	-0.924093
27	1	-6.184269	-0.902573	-0.882921
28	6	-5.097404	0.969427	-1.054749
29	1	-6.003786	1.565718	-1.114524
30	6	-3.865163	1.593191	-1.097222
31	1	-3.770568	2.671249	-1.181300
32	6	2.680879	-0.822271	-1.016515
33	6	2.785518	0.622514	-0.914689
34	6	4.073628	1.228269	-0.848487
35	1	4.150337	2.305642	-0.748636
36	6	5.201798	0.441313	-0.924093
37	1	6.184269	0.902573	-0.882921
38	6	5.097404	-0.969427	-1.054749
39	1	6.003786	-1.565718	-1.114524
40	6	3.865163	-1.593191	-1.097222
41	1	3.770568	-2.671249	-1.181300
42	6	-0.878776	-2.470239	1.884359
43	6	-1.141974	-3.218260	0.609521
44	6	-1.497966	-2.656661	-0.642081
45	6	-1.720869	-3.505829	-1.736692
46	1	-1.977827	-3.055699	-2.690673
47	6	-1.601534	-4.887294	-1.611456
48	1	-1.776345	-5.522480	-2.475560
49	6	-1.253664	-5.446936	-0.380322
50	1	-1.155281	-6.523039	-0.272251
51	6	-1.030395	-4.614836	0.710715
52	1	-0.763943	-5.025018	1.678524
53	6	0.878776	2.470239	1.884359
54	6	1.141974	3.218260	0.609521
55	6	1.497966	2.656661	-0.642081
56	6	1.720869	3.505829	-1.736692
57	1	1.977827	3.055699	-2.690673
58	6	1.601534	4.887294	-1.611456
59	1	1.776345	5.522480	-2.475560
60	6	1.253664	5.446936	-0.380322
61	1	1.155281	6.523039	-0.272251
62	6	1.030395	4.614836	0.710715
63	1	0.763943	5.025018	1.678524

D. (*A*,*R*,*R*)-(Bdan)Pd



Energy of optimized structure = –1846.44487448 a.u.

Cartesian coordinates of optimized structure:

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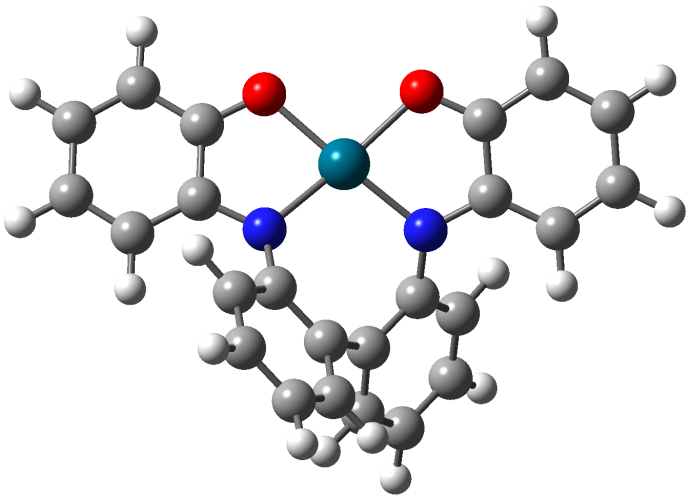
1	46	-0.000017	0.000090	-0.875697
2	8	-0.237402	1.993294	-0.959059
3	8	0.237618	-1.993028	-0.958983
4	8	1.303977	-0.515823	1.750147
5	8	2.833458	-1.847323	2.730218
6	8	-1.304052	0.515864	1.750026
7	8	-2.833753	1.847032	2.730202
8	7	1.913670	0.538133	-0.760161
9	7	-1.913692	-0.538063	-0.760394
10	6	-0.290764	-1.941237	2.949886
11	1	0.417661	-2.771393	2.989887
12	1	-0.922367	-2.047458	2.064803
13	1	-0.927692	-1.991383	3.840695
14	6	0.458235	-0.612082	2.931120
15	1	1.108284	-0.543854	3.809397
16	6	-0.458397	0.612167	2.931055
17	1	-1.108513	0.543987	3.809289
18	6	0.290546	1.941352	2.949782
19	1	-0.417916	2.771443	2.989723
20	1	0.922159	2.047574	2.064706
21	1	0.927454	1.991582	3.840607
22	6	0.894868	2.646282	-0.918019

23	6	2.115048	1.883693	-0.789933
24	6	3.355439	2.567238	-0.673167
25	1	4.271591	2.001105	-0.546787
26	6	3.378005	3.946882	-0.725233
27	1	4.325488	4.470925	-0.639300
28	6	2.181752	4.691067	-0.884662
29	1	2.230433	5.775714	-0.923657
30	6	0.956542	4.057234	-0.978493
31	1	0.028985	4.610576	-1.086379
32	6	-0.894625	-2.646130	-0.918064
33	6	-2.114887	-1.883691	-0.790115
34	6	-3.355195	-2.567389	-0.673385
35	1	-4.271415	-2.001376	-0.547057
36	6	-3.377601	-3.947040	-0.725405
37	1	-4.325028	-4.471187	-0.639497
38	6	-2.181254	-4.691082	-0.884748
39	1	-2.229793	-5.775737	-0.923724
40	6	-0.956120	-4.057088	-0.978506
41	1	-0.028486	-4.610311	-1.086305
42	6	2.453530	-1.218753	1.758359
43	6	3.232389	-1.185656	0.472285
44	6	2.997935	-0.366648	-0.660808
45	6	3.862111	-0.463132	-1.765665
46	1	3.658189	0.162836	-2.628893
47	6	4.933941	-1.349035	-1.771407
48	1	5.577157	-1.410043	-2.645017
49	6	5.170811	-2.157392	-0.657327
50	1	6.003648	-2.854281	-0.648065
51	6	4.329217	-2.065234	0.444140
52	1	4.499361	-2.674867	1.324250
53	6	-2.453733	1.218589	1.758298
54	6	-3.232594	1.185478	0.472232
55	6	-2.998037	0.366586	-0.660934
56	6	-3.862179	0.463155	-1.765813
57	1	-3.658182	-0.162685	-2.629111
58	6	-4.934076	1.348975	-1.771492
59	1	-5.577251	1.410041	-2.645121
60	6	-5.171065	2.157177	-0.657327
61	1	-6.003961	2.853995	-0.648015
62	6	-4.329495	2.064968	0.444149
63	1	-4.499707	2.674499	1.324313

E. (Clip)Pd



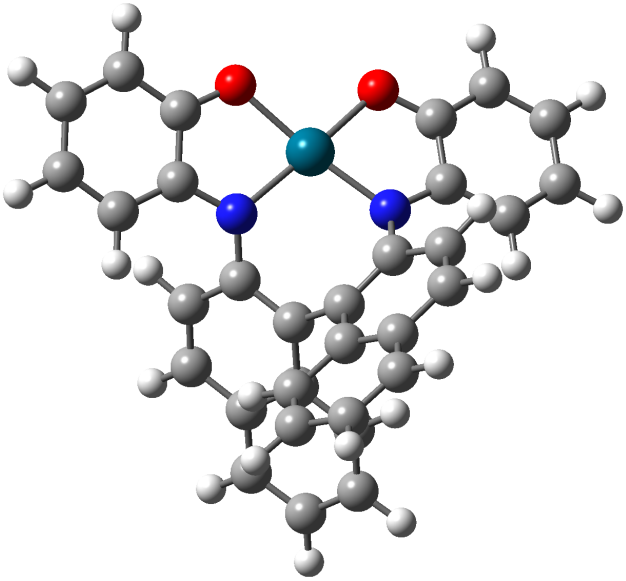
Energy of optimized structure = –1312.07123373 a.u.

Cartesian coordinates of optimized structure:

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	46	0.044222	0.000000	0.000000
2	8	1.395339	-1.479992	0.101589
3	7	-1.199614	-1.532225	-0.219529
4	6	0.833094	-2.658308	0.184393
5	6	1.578445	-3.836146	0.426871
6	1	2.649181	-3.745563	0.579185
7	6	0.931917	-5.056922	0.466579
8	1	1.502109	-5.961383	0.660011
9	6	-0.467785	-5.146845	0.269991
10	1	-0.957442	-6.114175	0.333566
11	6	-1.221524	-4.015483	0.019241
12	1	-2.296675	-4.083131	-0.108310
13	6	-0.587860	-2.748991	-0.024906
14	6	-2.389111	-1.399518	-0.941994
15	6	-2.591936	-2.218665	-2.078036
16	1	-1.809779	-2.919967	-2.347907
17	6	-3.724726	-2.106283	-2.867516
18	1	-3.831888	-2.732605	-3.748706
19	6	-4.704568	-1.164444	-2.539152
20	1	-5.593041	-1.051931	-3.153498
21	6	-4.522665	-0.353558	-1.425202
22	1	-5.276858	0.387256	-1.177432
23	6	-3.380790	-0.431619	-0.603256
24	8	1.395339	1.479992	-0.101589
25	7	-1.199614	1.532225	0.219529
26	6	0.833094	2.658308	-0.184393
27	6	1.578445	3.836146	-0.426871
28	1	2.649181	3.745563	-0.579185
29	6	0.931917	5.056922	-0.466579

30	1	1.502109	5.961383	-0.660011
31	6	-0.467785	5.146845	-0.269991
32	1	-0.957442	6.114175	-0.333566
33	6	-1.221524	4.015483	-0.019241
34	1	-2.296675	4.083131	0.108310
35	6	-0.587860	2.748991	0.024906
36	6	-2.389111	1.399518	0.941994
37	6	-2.591936	2.218665	2.078036
38	1	-1.809779	2.919967	2.347907
39	6	-3.724726	2.106283	2.867516
40	1	-3.831888	2.732605	3.748706
41	6	-4.704568	1.164444	2.539152
42	1	-5.593041	1.051931	3.153498
43	6	-4.522665	0.353558	1.425202
44	1	-5.276858	-0.387256	1.177432
45	6	-3.380790	0.431619	0.603256

F. (Biniq)Pd



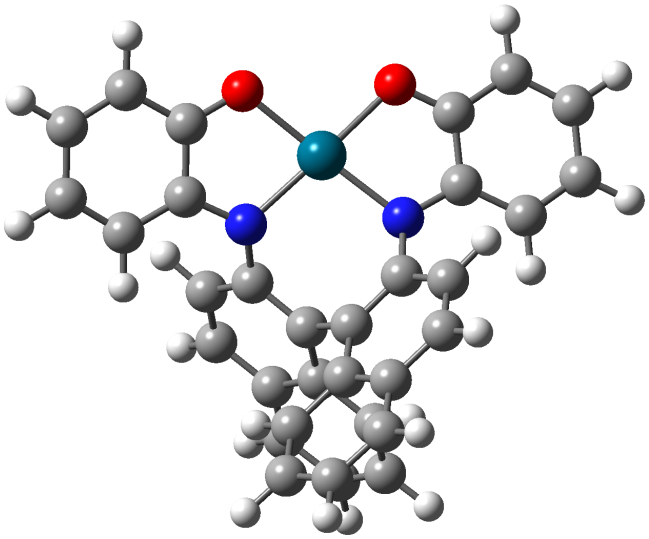
Energy of optimized structure = –1619.34523591 a.u.

Cartesian coordinates of optimized structure:

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	46	0.000000	0.000000	2.046777
2	7	-0.708661	1.372411	0.794771
3	8	-0.952467	1.152578	3.388794
4	6	-1.689561	2.072257	2.820242
5	6	-1.560036	2.265641	1.400072
6	6	-2.304729	3.285493	0.759928
7	1	-2.228241	3.412118	-0.315085
8	6	-3.158426	4.076642	1.506914

9	1	-3.752954	4.839674	1.013121
10	6	-3.283181	3.888160	2.904791
11	1	-3.960260	4.523214	3.469457
12	6	-2.564938	2.903786	3.557605
13	1	-2.649060	2.742974	4.627630
14	6	0.497653	2.996623	-0.541367
15	1	0.256191	3.730273	0.219707
16	6	1.303265	3.331022	-1.591477
17	1	1.688496	4.343609	-1.683028
18	6	1.698154	2.353963	-2.545121
19	6	2.583333	2.676162	-3.604485
20	1	2.937268	3.700773	-3.690181
21	6	2.997525	1.714729	-4.499664
22	1	3.679382	1.971395	-5.305499
23	6	1.208134	1.014644	-2.405245
24	6	1.675212	0.044552	-3.338636
25	1	1.349509	-0.984069	-3.238806
26	6	2.542753	0.384477	-4.353999
27	1	2.885627	-0.380700	-5.045046
28	6	0.305634	0.677177	-1.331195
29	6	-0.000000	1.663940	-0.372009
30	7	0.708661	-1.372411	0.794771
31	8	0.952467	-1.152578	3.388794
32	6	1.689561	-2.072257	2.820242
33	6	1.560036	-2.265641	1.400072
34	6	2.304729	-3.285493	0.759928
35	1	2.228241	-3.412118	-0.315085
36	6	3.158426	-4.076642	1.506914
37	1	3.752954	-4.839674	1.013121
38	6	3.283181	-3.888160	2.904791
39	1	3.960260	-4.523214	3.469457
40	6	2.564938	-2.903786	3.557605
41	1	2.649060	-2.742974	4.627630
42	6	-0.497653	-2.996623	-0.541367
43	1	-0.256191	-3.730273	0.219707
44	6	-1.303265	-3.331022	-1.591477
45	1	-1.688496	-4.343609	-1.683028
46	6	-1.698154	-2.353963	-2.545121
47	6	-2.583333	-2.676162	-3.604485
48	1	-2.937268	-3.700773	-3.690181
49	6	-2.997525	-1.714729	-4.499664
50	1	-3.679382	-1.971395	-5.305499
51	6	-1.208134	-1.014644	-2.405245
52	6	-1.675212	-0.044552	-3.338636
53	1	-1.349509	0.984069	-3.238806
54	6	-2.542753	-0.384477	-4.353999
55	1	-2.885627	0.380700	-5.045046
56	6	-0.305634	-0.677177	-1.331195
57	6	0.000000	-1.663940	-0.372009

G. (Biniq)Pd triplet



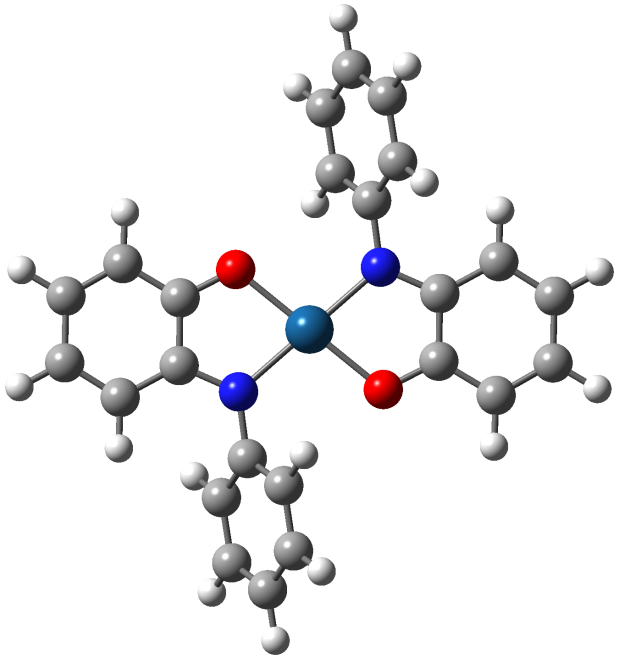
Energy of optimized structure = –1619.34600456 a.u.

Cartesian coordinates of optimized structure:

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	46	0.000000	-0.000000	2.038683
2	7	-0.750932	1.357898	0.740462
3	8	-0.999371	1.177464	3.374936
4	6	-1.722861	2.077382	2.774155
5	6	-1.600272	2.241027	1.339492
6	6	-2.344267	3.255074	0.680099
7	1	-2.263108	3.357026	-0.397446
8	6	-3.188788	4.066695	1.408167
9	1	-3.778512	4.825205	0.901947
10	6	-3.310444	3.907361	2.814321
11	1	-3.983776	4.558524	3.365215
12	6	-2.595751	2.938558	3.488524
13	1	-2.677355	2.806695	4.562665
14	6	0.549541	2.979020	-0.535511
15	1	0.282962	3.726656	0.203359
16	6	1.434806	3.276992	-1.535567
17	1	1.858409	4.275688	-1.608865
18	6	1.846014	2.285007	-2.464938
19	6	2.791930	2.570250	-3.482591
20	1	3.197740	3.577137	-3.546062
21	6	3.195862	1.595815	-4.367921
22	1	3.923058	1.825080	-5.141813
23	6	1.293135	0.964955	-2.358507
24	6	1.735114	-0.016274	-3.293007
25	1	1.336553	-1.022332	-3.229285
26	6	2.662572	0.289759	-4.264588
27	1	2.987278	-0.480122	-4.959264
28	6	0.332236	0.671441	-1.332990

29	6	-0.000000	1.665400	-0.406289
30	7	0.750932	-1.357898	0.740462
31	8	0.999371	-1.177464	3.374936
32	6	1.722861	-2.077382	2.774155
33	6	1.600272	-2.241027	1.339492
34	6	2.344267	-3.255074	0.680099
35	1	2.263108	-3.357026	-0.397446
36	6	3.188788	-4.066695	1.408167
37	1	3.778512	-4.825205	0.901947
38	6	3.310444	-3.907361	2.814321
39	1	3.983776	-4.558524	3.365215
40	6	2.595751	-2.938558	3.488524
41	1	2.677355	-2.806695	4.562665
42	6	-0.549541	-2.979020	-0.535511
43	1	-0.282962	-3.726656	0.203359
44	6	-1.434806	-3.276992	-1.535567
45	1	-1.858409	-4.275688	-1.608865
46	6	-1.846014	-2.285007	-2.464938
47	6	-2.791930	-2.570250	-3.482591
48	1	-3.197740	-3.577137	-3.546062
49	6	-3.195862	-1.595815	-4.367921
50	1	-3.923058	-1.825080	-5.141813
51	6	-1.293135	-0.964955	-2.358507
52	6	-1.735114	0.016274	-3.293007
53	1	-1.336553	1.022332	-3.229285
54	6	-2.662572	-0.289759	-4.264588
55	1	-2.987278	0.480122	-4.959264
56	6	-0.332236	-0.671441	-1.332990
57	6	0.000000	-1.665400	-0.406289

H. $(^{H}ap)_2Pt$

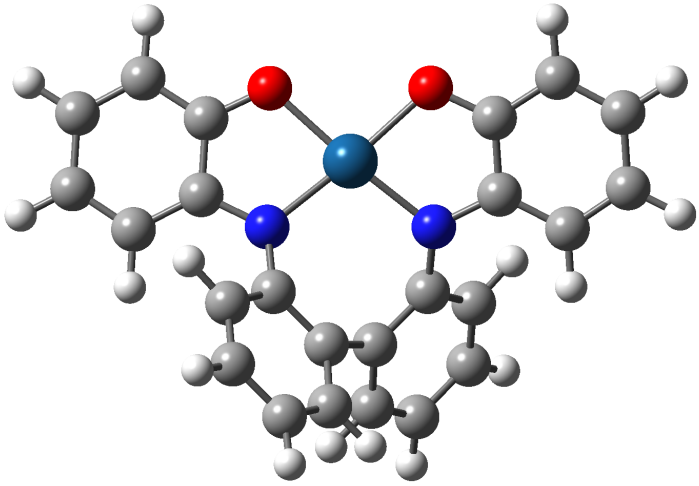


Energy of optimized structure = –1304.75826641 a.u.

Cartesian coordinates of optimized structure:

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	78	-0.000047	0.000015	-0.000011
2	7	-1.544700	-1.259425	-0.036654
3	8	-1.493024	1.314117	-0.309318
4	6	-2.683829	0.759285	-0.373729
5	6	-2.766852	-0.664683	-0.221494
6	6	-4.038936	-1.290829	-0.225184
7	1	-4.115540	-2.360864	-0.071186
8	6	-5.172750	-0.522832	-0.413038
9	1	-6.148316	-1.000176	-0.412993
10	6	-5.081316	0.877723	-0.594912
11	1	-5.988208	1.457724	-0.741678
12	6	-3.855084	1.518479	-0.572560
13	1	-3.764091	2.593385	-0.691946
14	6	-1.415392	-2.670476	0.047999
15	6	-1.907371	-3.501920	-0.972377
16	1	-2.392996	-3.056447	-1.835138
17	6	-1.744473	-4.883048	-0.885605
18	1	-2.119013	-5.516950	-1.684758
19	6	-1.095446	-5.449595	0.214733
20	1	-0.971705	-6.526904	0.280001
21	6	-0.601107	-4.622865	1.225876
22	1	-0.092316	-5.054794	2.083264
23	6	-0.752538	-3.239525	1.145288
24	1	-0.365929	-2.589120	1.921922
25	7	1.544628	1.259420	0.036632
26	8	1.492898	-1.314113	0.309375
27	6	2.683704	-0.759283	0.373881
28	6	2.766740	0.664676	0.221606
29	6	4.038824	1.290819	0.225388
30	1	4.115448	2.360844	0.071344
31	6	5.172621	0.522834	0.413373
32	1	6.148184	1.000183	0.413401
33	6	5.081174	-0.877720	0.595287
34	1	5.988057	-1.457717	0.742151
35	6	3.854943	-1.518476	0.572846
36	1	3.763932	-2.593378	0.692251
37	6	1.415393	2.670470	-0.048126
38	6	1.907289	3.501934	0.972262
39	1	2.392743	3.056484	1.835116
40	6	1.744506	4.883070	0.885386
41	1	2.118975	5.516989	1.684559
42	6	1.095682	5.449598	-0.215081
43	1	0.972031	6.526917	-0.280436
44	6	0.601431	4.622840	-1.226248
45	1	0.092804	5.054751	-2.083742
46	6	0.752740	3.239492	-1.145545
47	1	0.366230	2.589091	-1.922182

I. (Clip)Pt



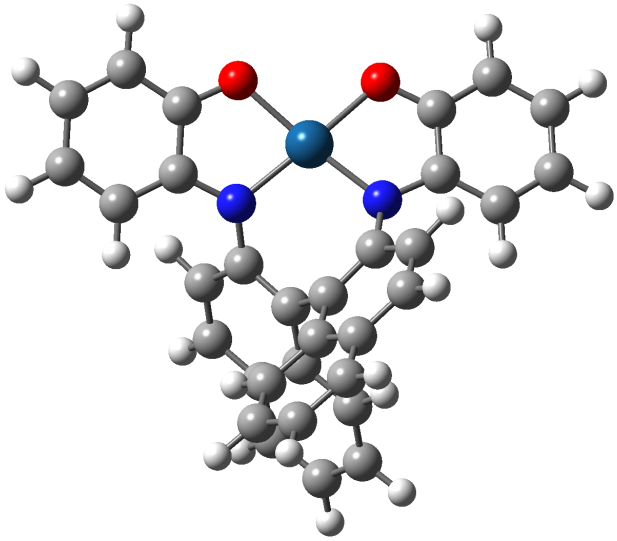
Energy of optimized structure = –1303.55180173 a.u.

Cartesian coordinates of optimized structure:

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	78	0.036602	0.000000	0.000000
2	8	1.391646	-1.492901	0.066987
3	7	-1.182651	-1.539415	-0.236826
4	6	0.833373	-2.679651	0.165733
5	6	1.580493	-3.852119	0.406858
6	1	2.653169	-3.764210	0.546362
7	6	0.929473	-5.071793	0.462797
8	1	1.499417	-5.976405	0.655797
9	6	-0.470744	-5.158226	0.283069
10	1	-0.962984	-6.123528	0.356233
11	6	-1.224613	-4.024774	0.033674
12	1	-2.300986	-4.089069	-0.085160
13	6	-0.584004	-2.765943	-0.026969
14	6	-2.385399	-1.404664	-0.948324
15	6	-2.596418	-2.227654	-2.077623
16	1	-1.820209	-2.935303	-2.347807
17	6	-3.732647	-2.111630	-2.862456
18	1	-3.848318	-2.741816	-3.739713
19	6	-4.703904	-1.161690	-2.533600
20	1	-5.594359	-1.045323	-3.144359
21	6	-4.512602	-0.349256	-1.422807
22	1	-5.261461	0.396376	-1.173676
23	6	-3.367684	-0.432384	-0.604072
24	8	1.391646	1.492901	-0.066987
25	7	-1.182651	1.539415	0.236826
26	6	0.833373	2.679651	-0.165733
27	6	1.580493	3.852119	-0.406858
28	1	2.653169	3.764210	-0.546362
29	6	0.929473	5.071793	-0.462797

30	1	1.499417	5.976405	-0.655797
31	6	-0.470744	5.158226	-0.283069
32	1	-0.962984	6.123528	-0.356233
33	6	-1.224613	4.024774	-0.033674
34	1	-2.300986	4.089069	0.085160
35	6	-0.584004	2.765943	0.026969
36	6	-2.385399	1.404664	0.948324
37	6	-2.596418	2.227654	2.077623
38	1	-1.820209	2.935303	2.347807
39	6	-3.732647	2.111630	2.862456
40	1	-3.848318	2.741816	3.739713
41	6	-4.703904	1.161690	2.533600
42	1	-5.594359	1.045323	3.144359
43	6	-4.512602	0.349256	1.422807
44	1	-5.261461	-0.396376	1.173676
45	6	-3.367684	0.432384	0.604072

J. (Biniq)Pt



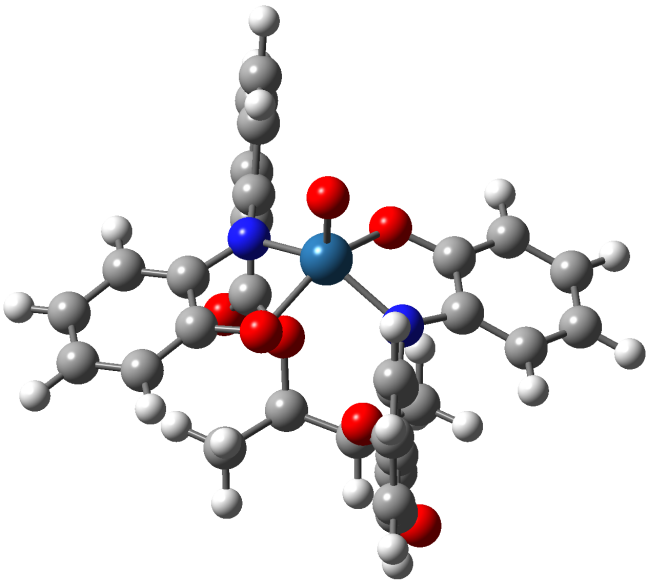
Energy of optimized structure = –1610.82544563 a.u.

Cartesian coordinates of optimized structure:

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	78	0.000000	0.000000	1.836636
2	7	-0.697432	1.387630	0.607930
3	8	-0.926827	1.185913	3.182295
4	6	-1.683997	2.101184	2.616836
5	6	-1.568715	2.278452	1.199408
6	6	-2.327358	3.278792	0.551329
7	1	-2.259976	3.394322	-0.525601
8	6	-3.180554	4.072939	1.298348
9	1	-3.784977	4.825953	0.801299

10	6	-3.288913	3.900969	2.697776
11	1	-3.965310	4.536794	3.262302
12	6	-2.554517	2.929806	3.355949
13	1	-2.626661	2.781233	4.428572
14	6	0.486325	3.005829	-0.754362
15	1	0.240856	3.744445	0.000425
16	6	1.287692	3.336140	-1.809596
17	1	1.664910	4.350653	-1.911940
18	6	1.688213	2.352402	-2.753402
19	6	2.571335	2.670145	-3.816346
20	1	2.919471	3.695921	-3.911229
21	6	2.990612	1.703131	-4.702674
22	1	3.670987	1.956181	-5.510830
23	6	1.205695	1.011857	-2.601672
24	6	1.677297	0.036360	-3.526682
25	1	1.357049	-0.993109	-3.418276
26	6	2.543092	0.371933	-4.545027
27	1	2.889922	-0.397507	-5.229240
28	6	0.304883	0.678743	-1.523057
29	6	-0.000000	1.672325	-0.574851
30	7	0.697432	-1.387630	0.607930
31	8	0.926827	-1.185913	3.182295
32	6	1.683997	-2.101184	2.616836
33	6	1.568715	-2.278452	1.199408
34	6	2.327358	-3.278792	0.551329
35	1	2.259976	-3.394322	-0.525601
36	6	3.180554	-4.072939	1.298348
37	1	3.784977	-4.825953	0.801299
38	6	3.288913	-3.900969	2.697776
39	1	3.965310	-4.536794	3.262302
40	6	2.554517	-2.929806	3.355949
41	1	2.626661	-2.781233	4.428572
42	6	-0.486325	-3.005829	-0.754362
43	1	-0.240856	-3.744445	0.000425
44	6	-1.287692	-3.336140	-1.809596
45	1	-1.664910	-4.350653	-1.911940
46	6	-1.688213	-2.352402	-2.753402
47	6	-2.571335	-2.670145	-3.816346
48	1	-2.919471	-3.695921	-3.911229
49	6	-2.990612	-1.703131	-4.702674
50	1	-3.670987	-1.956181	-5.510830
51	6	-1.205695	-1.011857	-2.601672
52	6	-1.677297	-0.036360	-3.526682
53	1	-1.357049	0.993109	-3.418276
54	6	-2.543092	-0.371933	-4.545027
55	1	-2.889922	0.397507	-5.229240
56	6	-0.304883	-0.678743	-1.523057
57	6	-0.000000	-1.672325	-0.574851

K. (*C*,*R*,*R*)-(Bdan)OsO



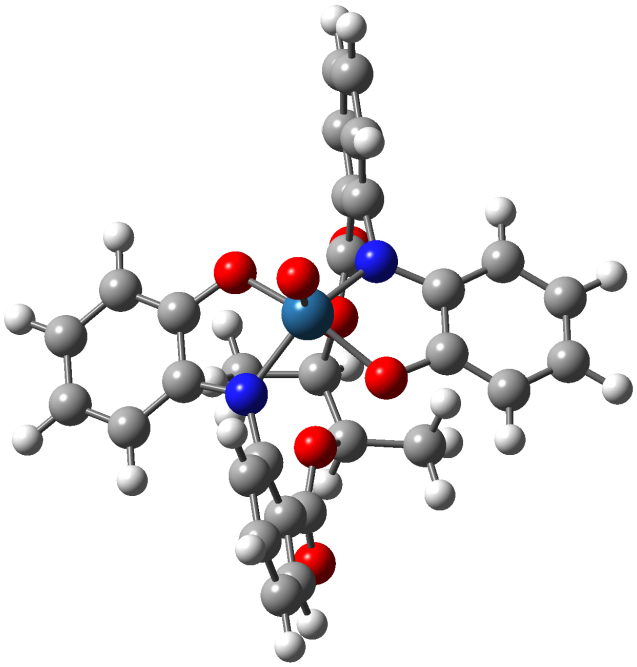
Energy of optimized structure = –1884.51453544 a.u.

Cartesian coordinates of optimized structure:

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	76	0.000162	-0.000646	-1.468348
2	8	0.000312	-0.001307	-3.185913
3	8	-0.305042	-1.850236	-0.887207
4	8	0.305224	1.849404	-0.888558
5	8	1.369830	0.124367	1.934979
6	8	3.335972	0.280011	3.045536
7	8	-1.370493	-0.121951	1.934899
8	8	-3.336783	-0.277240	3.045262
9	7	1.806637	-0.436835	-0.815571
10	7	-1.806447	0.435996	-0.816279
11	6	0.698718	-1.834177	3.217089
12	1	1.725943	-2.208773	3.223349
13	1	0.172179	-2.267382	2.363234
14	1	0.207737	-2.164860	4.139688
15	6	0.696968	-0.311462	3.148334
16	1	1.250450	0.097819	3.998321
17	6	-0.697815	0.314998	3.147943
18	1	-1.251423	-0.093496	3.998251
19	6	-0.699557	1.837777	3.215300
20	1	-1.726766	2.212387	3.221054
21	1	-0.172886	2.270195	2.361122
22	1	-0.208695	2.169285	4.137661
23	6	0.812733	-2.536621	-0.527815
24	6	1.996960	-1.783618	-0.455018
25	6	3.190062	-2.401812	-0.065089
26	1	4.111975	-1.832789	-0.010179

27	6	3.174677	-3.764849	0.243176
28	1	4.099143	-4.250813	0.541065
29	6	1.989775	-4.505232	0.170303
30	1	1.995584	-5.563707	0.413433
31	6	0.793200	-3.892398	-0.212057
32	1	-0.140612	-4.442545	-0.271931
33	6	-0.812643	2.536028	-0.529925
34	6	-1.996859	1.783042	-0.456753
35	6	-3.190043	2.401462	-0.067454
36	1	-4.111928	1.832429	-0.012257
37	6	-3.174774	3.764731	0.239788
38	1	-4.099303	4.250877	0.537173
39	6	-1.989894	4.505112	0.166522
40	1	-1.995786	5.563773	0.408837
41	6	-0.793232	3.892049	-0.215207
42	1	0.140558	4.442209	-0.275364
43	6	2.693511	0.373685	2.017557
44	6	3.284942	0.858748	0.728288
45	6	2.836799	0.517407	-0.567943
46	6	3.449342	1.101902	-1.682766
47	1	3.090132	0.826503	-2.669617
48	6	4.501587	2.003216	-1.532163
49	1	4.960049	2.447034	-2.411328
50	6	4.968715	2.318978	-0.255544
51	1	5.795380	3.011586	-0.127437
52	6	4.365850	1.742455	0.859586
53	1	4.712989	1.973978	1.860980
54	6	-2.694108	-0.371595	2.017478
55	6	-3.285135	-0.857996	0.728528
56	6	-2.836548	-0.518106	-0.567934
57	6	-3.448593	-1.103976	-1.682309
58	1	-3.089019	-0.829699	-2.669339
59	6	-4.500827	-2.005194	-1.531058
60	1	-4.958911	-2.450078	-2.409883
61	6	-4.968440	-2.319480	-0.254253
62	1	-5.795106	-3.011988	-0.125655
63	6	-4.366031	-1.741626	0.860436
64	1	-4.713508	-1.972037	1.861988

L. (*A*,*R*,*R*)-(Bdan)OsO



Energy of optimized structure = –1884.51052501 a.u.

Cartesian coordinates of optimized structure:

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	76	0.000043	0.000146	-1.416406
2	8	0.000077	0.000269	-3.133766
3	8	0.500212	-1.817040	-0.862132
4	8	-0.500102	1.817268	-0.861898
5	8	-1.331895	0.352080	1.889722
6	8	-3.187867	0.997518	3.000896
7	8	1.331768	-0.352092	1.889745
8	8	3.187320	-0.998809	3.000810
9	7	-1.734810	-0.624593	-0.736346
10	7	1.734864	0.624693	-0.736179
11	6	-0.064645	1.959085	3.214233
12	1	-0.913812	2.647801	3.222657
13	1	0.592473	2.213764	2.379656
14	1	0.489263	2.093224	4.150478
15	6	-0.558057	0.519725	3.112674
16	1	-1.218730	0.298464	3.955223
17	6	0.557825	-0.519974	3.112606
18	1	1.218437	-0.298932	3.955258
19	6	0.064258	-1.959307	3.213824
20	1	0.913338	-2.648137	3.222178
21	1	-0.592829	-2.213701	2.379135
22	1	-0.489751	-2.093566	4.149993
23	6	-0.530042	-2.610408	-0.468604

24	6	-1.782384	-1.979042	-0.366263
25	6	-2.896027	-2.705736	0.068304
26	1	-3.866003	-2.226938	0.151050
27	6	-2.736672	-4.057788	0.383956
28	1	-3.597956	-4.629491	0.717102
29	6	-1.487232	-4.678893	0.276421
30	1	-1.381377	-5.730611	0.525816
31	6	-0.368336	-3.955105	-0.145426
32	1	0.613016	-4.411397	-0.228513
33	6	0.530177	2.610534	-0.468222
34	6	1.782486	1.979095	-0.365918
35	6	2.896153	2.705676	0.068776
36	1	3.866101	2.226823	0.151488
37	6	2.736857	4.057696	0.384596
38	1	3.598159	4.629313	0.717840
39	6	1.487449	4.678875	0.277103
40	1	1.381638	5.730566	0.526629
41	6	0.368533	3.955200	-0.144872
42	1	-0.612793	4.411555	-0.227934
43	6	-2.635838	0.691964	1.959873
44	6	-3.343822	0.735592	0.637254
45	6	-2.900121	0.189159	-0.588337
46	6	-3.653689	0.401555	-1.749960
47	1	-3.289657	-0.023832	-2.680333
48	6	-4.842296	1.127431	-1.716980
49	1	-5.407369	1.279024	-2.632349
50	6	-5.299326	1.648384	-0.506094
51	1	-6.226273	2.212719	-0.463221
52	6	-4.553458	1.450083	0.651445
53	1	-4.884606	1.854879	1.601204
54	6	2.635551	-0.692565	1.959854
55	6	3.343725	-0.735817	0.637315
56	6	2.900151	-0.189106	-0.588201
57	6	3.653812	-0.401270	-1.749801
58	1	3.289852	0.024297	-2.680117
59	6	4.842423	-1.127144	-1.716867
60	1	5.407575	-1.278550	-2.632218
61	6	5.299343	-1.648344	-0.506050
62	1	6.226294	-2.212675	-0.463208
63	6	4.553353	-1.450320	0.651458
64	1	4.884390	-1.855361	1.601149

References

S1 S. N. Brown, *Inorg. Chem.*, 2012, **51**, 1251-1260.