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Electronic Supporting Information for

Highly covalent metal-ligand π bonding in chelated bis- and tris(iminoxolene) complexes of osmium and ruthenium

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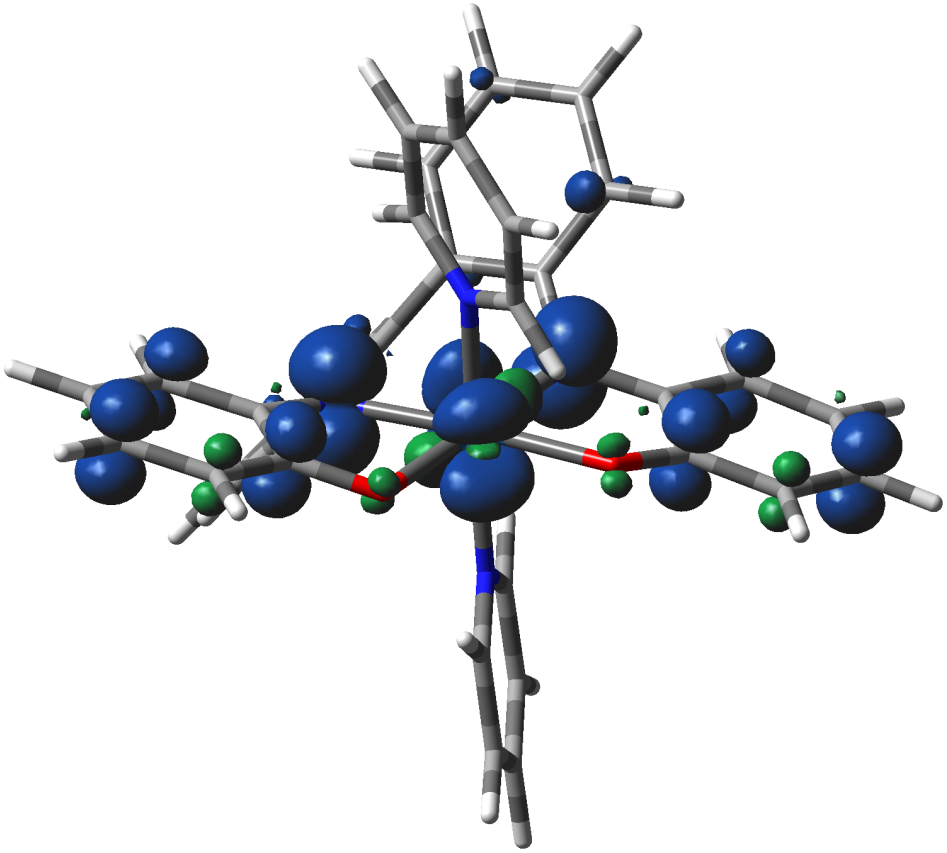

II. Metrical Oxidation State data for literature Ru and Os iminoxolenes

Table S1. Metrical oxidation state (MOS) data on ruthenium iminoxolene complexes $[Ru(RNC_6H_2{}^tBu_2O)_nL_m]^{x+}$.

CSD refcode	R	*n*	L_m	*x*	π bond order	MOS	Reference
BERYII	Ph	2	PhN=NPy	1	0.75	–0.87(6)	S1
BERYOO	3,5-$Cl_2C_6H_3$	2	PhN=NPy	0	0.50	–1.13(6) –1.45(13)	S1
BUQCIA	Ph	1	$(PhN=NPy)_2$	1	0.50	–1.04(30)[a]	S2
ETIMEA	Ph	1	Tpm, Cl	1	1.00	–0.92(12)	S3
ETIMIE	3,5-$(MeO)_2C_6H_3$	1	Tpm, Cl	1	1.00	–0.66(5)	S3
HABHUP	Ph	1	$(acac)_2$	0	1.00	–0.95(10)	S4
HABJAX	Ph	3	—	0	0.67	–1.33(19)[a] –1.15(25)[a] –1.37(18)[a]	S4
ISOKAE	2-$PhSC_6H_4$	1	$(Ph_3P)Cl_2$	0	1.00	–0.88(7)	S5
IXOPOB	3,5-$Cl_2C_6H_3$	2	bpy	0	0.50	–1.48(16)[a] –1.39(7)	S6
IXOPUH	3,5-$Cl_2C_6H_3$	2	bpy	0	0.50	–1.42(11) –1.48(11)	S6
IXOQAO	3,5-$(MeO)_2C_6H_3$	2	bpy	0	0.50	–1.47(6) –1.45(14)	S6
IXOQES	3,5-$(MeO)_2C_6H_3$	2	bpy	2	1.00	–0.51(6) –0.52(7)	S6
JIWQAH	Ph	1	$(PhNC_6H_4NH)Cl_2$	0	1.00	–0.74(9)	S7
NEFVAX	2-$CH_3SC_6H_4$	2	—	0	0.50	–1.51(10) –1.40(13)	S8
ORESEL	CMe_2-2-C_5H_4N	1	$(Ph_3P)Cl_2$	0	1.00	–0.66(9)	S9
ORESOV	CMe_2-2-C_5H_4N	1	$(Ph_3P)Cl_2$	0	1.00	–0.79(9)	S9
ORESUB	CMe_2-2-C_5H_4N	1 1 1	$(Ph_3PN)(\mu\text{-}N)$ $(Ph_3PN)(\mu\text{-}N)$ $(\mu\text{-}N)_2$	0 0 0	0.00 0.00 0.00	–1.98(10) –1.77(9) –1.81(6)	S9
SUQYUZ	Ph	1	(tpy)(NO)	2	1.00	–1.10(12)	S10
UHUWUQ	Ph	1	(μ-tppz)Cl	1	1.00	–0.63(12)	S11
UKOMIR	2-$CF_3C_6H_4$	1	cymene	0	*b*	–1.62(10)[b]	S12
UWUZIW	Ph	1	(tpy)(OAc)	1	1.00	–0.70(7)	S13
YAYLIW	2-(SOOEt)-C_6H_4	1	$(Ph_3P)Cl_2$	0	1.00	–0.69(11)	S14
ZORLOJ	2-$MeSC_6H_4$	1	cymene	0	*b*	–1.57(12)[b]	S15

ZORLUP	3-$CF_3C_6H_4$	1	cymene	0	*b*	–1.56(10)[b]	S15
ZORMAW	Ph	1	cymene	0	*b*	–1.65(10)[b] –1.60(7)[b]	S15
ZORMEA	2-EtC_6H_4	1	cymene	0	*b*	–1.51(12)[b] –1.58(11)[b]	S15
ZORMIE	2-$MeOC_6H_4$	1	cymene	0	*b*	–1.67(10)[b]	S15
ZORMOK	2-$MeSC_6H_4$	2	—	1	0.75	–1.04(4) –0.95(5)	S15
ZORMUQ	2-CH_3Se-C_6H_4	1	cymene	0	*b*	–1.63(14)[b]	S15
ZORNAX	2-CH_3Se-C_6H_4	1	cymene	1	0.50	–1.16(8)	S15
ZORNEB	2-$MeSC_6H_4$	1	cymene	1	0.50	–1.18(9) –1.23(7)	S15

[a]Not included in correlation analysis due to poor fit of structural data to MOS correlations, as indicated by the high estimated standard deviations (> 0.15). [b](Arene)Ru(iminoxolene) complex, not included in correlation due to uncertain π bond order, see text.

Table S2. Metrical oxidation state (MOS) data on osmium iminoxolene complexes $[Os(RNC_6H_2{}^tBu_2O)_nL_m]^{x+}$.

CSD refcode	R	*n*	L_m	*x*	π bond order	MOS	Reference
GEGZID	Ph	3	—	0	0.67	–1.53(11) –1.39(9) –1.35(8)	S16
GIFHOU	Ph	2	bpy	1	0.75	–1.26(7) –1.44(18)[a]	S17
IBOGIR	Ph	1	$(PhN{=}NPy)_2$	0	*b*	–1.43(13)	S18
IBOGOX	3,5-$Cl_2C_6H_3$	1	$(PhN{=}NPy)_2$	0	*b*	–1.66(16)[a]	S18
IBOGUD	3,5-$(MeO)_2C_6H_3$	1	$(PhN{=}NPy)_2$	0	*b*	–1.65(17)[a]	S18
IBOHAK	3,5-$^tBu_2C_6H_3$	1	$(PhN{=}NPy)_2$	0	*b*	–1.49(10)	S18
IBOHEO	3,5-$(MeO)_2C_6H_3$	1	$(PhN{=}NPy)_2$	2	*b*	–0.58(8)	S18
ICIHEJ	CH(CN)(5-ClC_6H_3O)	1	$(N)(CN)_2$	2–	0.00	–1.88(12)	S19
NEFVEB	2-$CH_3SC_6H_4$	2	—	0	0.50	–1.66(17)[a] –1.59(11)	S8

[a]Not included in correlation analysis due to poor fit of structural data to MOS correlations, as indicated by the high estimated standard deviations (> 0.15). [b]Not included in correlation due to uncertain π bond order, see text.

III. Energies and Cartesian coordinates of calculated structures

A. *trans*-(Clip)Os(py)$_2$

Energy of optimized structure = –1771.52918972 a.u.

Cartesian coordinates of optimized structure:

Center Number	Atomic Number	Coordinates (Å) X	Y	Z
1	76	0.000000	0.000000	0.731268
2	8	1.531183	-0.306262	2.105437
3	7	1.576174	-0.202982	-0.493774
4	6	2.606635	-0.830770	1.536456
5	6	2.696419	-0.775461	0.107083
6	6	3.839135	-1.282720	-0.541001
7	1	3.898234	-1.251654	-1.625294
8	6	4.875332	-1.831506	0.206642
9	1	5.748688	-2.234201	-0.299107
10	6	4.792026	-1.877058	1.609695
11	1	5.608104	-2.308529	2.183874
12	6	3.673993	-1.382323	2.271118
13	1	3.595831	-1.410209	3.354368
14	6	0.593721	0.455531	-2.661297
15	6	1.655795	0.493512	-1.707112
16	6	2.778039	1.313293	-1.965509
17	1	3.570089	1.338338	-1.224525
18	6	2.867704	2.098916	-3.105299
19	1	3.736824	2.734009	-3.256004
20	6	1.825996	2.084448	-4.037107
21	1	1.870075	2.702025	-4.929866
22	6	0.723221	1.269347	-3.808151
23	1	-0.084952	1.255269	-4.533754
24	7	0.259696	2.111282	0.829713
25	6	-0.125959	2.963619	-0.142944
26	1	-0.542457	2.507004	-1.031009
27	6	0.000000	4.342954	-0.017420
28	1	-0.325870	4.982788	-0.830823
29	6	0.540862	4.871863	1.153281
30	1	0.648969	5.945356	1.279174
31	6	0.940034	3.991840	2.159069
32	1	1.367730	4.351794	3.089108
33	6	0.785031	2.624247	1.965073
34	1	1.088178	1.892649	2.705158
35	8	-1.531183	0.306262	2.105437
36	7	-1.576174	0.202982	-0.493774
37	6	-2.606635	0.830770	1.536456
38	6	-2.696419	0.775461	0.107083
39	6	-3.839135	1.282720	-0.541001
40	1	-3.898234	1.251654	-1.625294
41	6	-4.875332	1.831506	0.206642
42	1	-5.748688	2.234201	-0.299107
43	6	-4.792026	1.877058	1.609695
44	1	-5.608104	2.308529	2.183874
45	6	-3.673993	1.382323	2.271118

46	1	-3.595831	1.410209	3.354368
47	6	-0.593721	-0.455531	-2.661297
48	6	-1.655795	-0.493512	-1.707112
49	6	-2.778039	-1.313293	-1.965509
50	1	-3.570089	-1.338338	-1.224525
51	6	-2.867704	-2.098916	-3.105299
52	1	-3.736824	-2.734009	-3.256004
53	6	-1.825996	-2.084448	-4.037107
54	1	-1.870075	-2.702025	-4.929866
55	6	-0.723221	-1.269347	-3.808151
56	1	0.084952	-1.255269	-4.533754
57	7	-0.259696	-2.111282	0.829713
58	6	0.125959	-2.963619	-0.142944
59	1	0.542457	-2.507004	-1.031009
60	6	0.000000	-4.342954	-0.017420
61	1	0.325870	-4.982788	-0.830823
62	6	-0.540862	-4.871863	1.153281
63	1	-0.648969	-5.945356	1.279174
64	6	-0.940034	-3.991840	2.159069
65	1	-1.367730	-4.351794	3.089108
66	6	-0.785031	-2.624247	1.965073
67	1	-1.088178	-1.892649	2.705158

B. *cis*-α-(Clip)Os(py)$_2$

Energy of optimized structure = –1771.50421986 a.u.

Cartesian coordinates of optimized structure:

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	76	-0.624801	0.000268	0.000045
2	8	-0.777880	1.152690	-1.662880
3	8	-0.778991	-1.152017	1.662910
4	7	0.870411	-1.367586	-0.327446
5	7	0.871277	1.367068	0.327727
6	6	0.768975	-2.477534	0.474523
7	6	0.326933	-4.571666	2.308092
8	1	0.161139	-5.390400	3.003037
9	6	0.330978	4.571351	-2.308187
10	1	0.166011	5.390156	-3.003246
11	6	2.029587	-1.147176	-1.122337
12	6	1.311178	4.690309	-1.304193
13	1	1.895216	5.603968	-1.229273
14	6	-0.197198	-2.344693	1.528234
15	6	0.770911	2.477035	-0.474359
16	6	1.543406	3.658801	-0.404506
17	1	2.301411	3.757038	0.366062
18	6	2.030277	1.145773	1.122655
19	6	2.114107	1.750544	2.384702
20	1	1.291997	2.383074	2.708014
21	6	-0.416594	-3.403097	2.425224
22	1	-1.150281	-3.272720	3.216368

23	6	1.540504	-3.659939	0.404740
24	1	2.298596	-3.758741	-0.365674
25	6	2.113094	-1.752063	-2.384351
26	1	1.290610	-2.384103	-2.707667
27	6	-0.413494	3.403392	-2.425365
28	1	-1.147115	3.273541	-3.216656
29	6	-0.195150	2.344890	-1.528226
30	6	3.223827	1.553584	3.205889
31	1	3.267448	2.031407	4.181125
32	6	3.085324	-0.322079	-0.671981
33	6	4.267647	-0.740455	-2.770133
34	1	5.134289	-0.570108	-3.403011
35	6	3.222952	-1.555812	-3.205525
36	1	3.266296	-2.033695	-4.180744
37	6	4.268034	0.737612	2.770476
38	1	5.134552	0.566697	3.403369
39	6	4.191197	0.131559	1.517459
40	1	4.996481	-0.516111	1.181029
41	6	4.191153	-0.134297	-1.517146
42	1	4.996832	0.512873	-1.180711
43	6	1.307239	-4.691333	1.304291
44	1	1.890548	-5.605461	1.229413
45	6	3.085505	0.320056	0.672271
46	7	-2.083134	-1.289499	-0.864509
47	6	-3.036607	-1.930575	-0.147609
48	1	-3.002070	-1.765399	0.922320
49	6	-3.986574	-2.755865	-0.736422
50	1	-4.724261	-3.247396	-0.110218
51	6	-3.970920	-2.937444	-2.120196
52	1	-4.701426	-3.577053	-2.606527
53	6	-2.991133	-2.277051	-2.861354
54	1	-2.931309	-2.383493	-3.939832
55	6	-2.066322	-1.471333	-2.206920
56	1	-1.293440	-0.931018	-2.739175
57	7	-2.082524	1.290911	0.864227
58	6	-3.035110	1.933003	0.147049
59	1	-3.000142	1.768177	-0.922921
60	6	-3.984730	2.758839	0.735656
61	1	-4.721692	3.251178	0.109234
62	6	-3.969664	2.939921	2.119500
63	1	-4.699913	3.579950	2.605664
64	6	-2.990803	2.278482	2.860944
65	1	-2.931461	2.384496	3.939492
66	6	-2.066287	1.472263	2.206714
67	1	-1.294122	0.931146	2.739181

C. *trans*-(Clip)Os(CO)$_2$

Energy of optimized structure = –1501.59695080 a.u.

Cartesian coordinates of optimized structure:

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	76	0.000000	0.000000	0.954604
2	8	-0.286035	1.566970	2.320344
3	7	-0.405187	1.557613	-0.291217
4	6	-0.179041	2.744193	1.736386
5	6	-0.261867	2.798703	0.301242
6	6	-0.204388	4.046202	-0.357849
7	1	-0.245026	4.080776	-1.442120
8	6	-0.068015	5.208701	0.383953
9	1	-0.000477	6.166072	-0.124458
10	6	0.000000	5.156617	1.792713
11	1	0.106436	6.078852	2.357434
12	6	-0.058111	3.946321	2.465371
13	1	-0.007699	3.890072	3.548317
14	6	-0.642678	0.380807	-2.448165
15	6	-1.072431	1.363329	-1.504427
16	6	-2.240305	2.115121	-1.771219
17	1	-2.558171	2.843378	-1.032298
18	6	-2.998453	1.905899	-2.912024
19	1	-3.906481	2.481031	-3.070197
20	6	-2.600498	0.933164	-3.834250
21	1	-3.190048	0.741565	-4.726065
22	6	-1.442533	0.202514	-3.597916
23	1	-1.134659	-0.549219	-4.318242
24	6	-1.924205	-0.490269	1.000107
25	8	-3.032203	-0.774232	1.060614
26	8	0.286035	-1.566970	2.320344
27	7	0.405187	-1.557613	-0.291217
28	6	0.179041	-2.744193	1.736386
29	6	0.261867	-2.798703	0.301242
30	6	0.204388	-4.046202	-0.357849
31	1	0.245026	-4.080776	-1.442120
32	6	0.068015	-5.208701	0.383953
33	1	0.000477	-6.166072	-0.124458
34	6	0.000000	-5.156617	1.792713
35	1	-0.106436	-6.078852	2.357434
36	6	0.058111	-3.946321	2.465371
37	1	0.007699	-3.890072	3.548317
38	6	0.642678	-0.380807	-2.448165
39	6	1.072431	-1.363329	-1.504427
40	6	2.240305	-2.115121	-1.771219
41	1	2.558171	-2.843378	-1.032298
42	6	2.998453	-1.905899	-2.912024
43	1	3.906481	-2.481031	-3.070197
44	6	2.600498	-0.933164	-3.834250
45	1	3.190048	-0.741565	-4.726065
46	6	1.442533	-0.202514	-3.597916
47	1	1.134659	0.549219	-4.318242
48	6	1.924205	0.490269	1.000107
49	8	3.032203	0.774232	1.060614

D. *cis*-α-(Clip)Os(CO)$_2$

Energy of optimized structure = –1501.60494051 a.u.

Cartesian coordinates of optimized structure:

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	76	0.000000	0.000000	1.519969
2	8	-0.673918	1.967415	1.419229
3	7	1.087406	0.763219	-0.157270
4	6	0.899020	2.097037	-0.342585
5	6	0.000000	2.730808	0.598562
6	6	-0.205720	4.127920	0.538949
7	1	-0.875691	4.580463	1.263089
8	6	0.416676	4.869377	-0.446871
9	1	0.254028	5.942385	-0.497069
10	6	1.258824	4.247184	-1.403150
11	1	1.741587	4.853076	-2.164476
12	6	1.484699	2.886423	-1.369727
13	1	2.145873	2.413606	-2.088023
14	6	0.700415	-0.250007	-2.369022
15	6	1.548629	-0.017239	-1.256413
16	6	2.838002	-0.555286	-1.229474
17	1	3.460188	-0.375546	-0.357899
18	6	3.319243	-1.288130	-2.315673
19	1	4.326936	-1.693011	-2.288319
20	6	2.506462	-1.494354	-3.430723
21	1	2.874596	-2.065094	-4.278603
22	6	1.206391	-0.986612	-3.447730
23	1	0.558534	-1.183024	-4.297910
24	6	-1.323388	-0.427973	2.825643
25	8	-2.179598	-0.637252	3.573338
26	8	0.673918	-1.967415	1.419229
27	7	-1.087406	-0.763219	-0.157270
28	6	-0.899020	-2.097037	-0.342585
29	6	0.000000	-2.730808	0.598562
30	6	0.205720	-4.127920	0.538949
31	1	0.875691	-4.580463	1.263089
32	6	-0.416676	-4.869377	-0.446871
33	1	-0.254028	-5.942385	-0.497069
34	6	-1.258824	-4.247184	-1.403150
35	1	-1.741587	-4.853076	-2.164476
36	6	-1.484699	-2.886423	-1.369727
37	1	-2.145873	-2.413606	-2.088023
38	6	-0.700415	0.250007	-2.369022
39	6	-1.548629	0.017239	-1.256413
40	6	-2.838002	0.555286	-1.229474

41	1	-3.460188	0.375546	-0.357899
42	6	-3.319243	1.288130	-2.315673
43	1	-4.326936	1.693011	-2.288319
44	6	-2.506462	1.494354	-3.430723
45	1	-2.874596	2.065094	-4.278603
46	6	-1.206391	0.986612	-3.447730
47	1	-0.558534	1.183024	-4.297910
48	6	1.323388	0.427973	2.825643
49	8	2.179598	0.637252	3.573338

E. *cis*-β-(Clip)$OsCl_2$

Energy of optimized structure = –2195.34617634 a.u.

Cartesian coordinates of optimized structure:

Center Number	Atomic Number	Coordinates (Å) X	Y	Z
1	76	0.013191	0.053191	-0.009511
2	17	0.376645	2.092475	-1.166675
3	17	-2.293382	0.240726	-0.548639
4	8	2.036538	0.055112	0.254512
5	7	0.599301	-1.063960	-1.511928
6	8	-0.401365	0.994999	1.783301
7	7	-0.439496	-1.496316	1.160879
8	6	2.688101	-0.348645	-0.799422
9	6	1.922149	-1.024348	-1.819222
10	6	2.579717	-1.637236	-2.915789
11	1	2.001039	-2.164553	-3.666260
12	6	3.947674	-1.512277	-3.019054
13	1	4.464859	-1.947292	-3.868912
14	6	4.699757	-0.814834	-2.032370
15	1	5.776683	-0.735897	-2.151089
16	6	4.093973	-0.247176	-0.932092
17	1	4.655310	0.274778	-0.164589
18	6	-1.098753	0.250451	2.579954
19	6	-1.151133	-1.163193	2.280179
20	6	-1.860359	-2.042809	3.140118
21	1	-1.929227	-3.096738	2.895430
22	6	-2.484725	-1.530857	4.255220
23	1	-3.056687	-2.189410	4.901654
24	6	-2.404326	-0.144812	4.567476
25	1	-2.906993	0.224189	5.457179
26	6	-1.719132	0.735097	3.760138
27	1	-1.657632	1.796025	3.977373
28	6	-0.316974	-1.944752	-2.164355

29	6	-0.754734	-3.092658	-1.477603
30	6	-1.734811	-3.883362	-2.097627
31	1	-2.093372	-4.769648	-1.581910
32	6	-2.257056	-3.548803	-3.346381
33	1	-3.024883	-4.173119	-3.794083
34	6	-1.796123	-2.413410	-4.012847
35	1	-2.201606	-2.141253	-4.982898
36	6	-0.826616	-1.606424	-3.418861
37	1	-0.485127	-0.694540	-3.898141
38	6	0.020943	-2.839228	0.993115
39	6	-0.114842	-3.568848	-0.215116
40	6	0.394648	-4.880425	-0.236302
41	1	0.298376	-5.447695	-1.156927
42	6	1.031752	-5.457400	0.859150
43	1	1.417819	-6.470248	0.789524
44	6	1.186300	-4.716802	2.029943
45	1	1.701391	-5.135249	2.889554
46	6	0.681896	-3.422664	2.090354
47	1	0.809286	-2.831459	2.990648

F. *cis*-α-(Clip)$OsCl_2$

Energy of optimized structure = –2195.34126710 a.u.

Cartesian coordinates of optimized structure:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	76	0	0.000000	0.000000	1.220643
2	8	0	-1.007900	1.782534	1.239333
3	7	0	0.934778	1.005768	-0.209878
4	6	0	0.745054	2.352303	-0.194866
5	6	0	-0.332955	2.743548	0.684907
6	6	0	-0.688433	4.111771	0.785693
7	1	0	-1.492182	4.393022	1.457589
8	6	0	0.000000	5.035452	0.030501
9	1	0	-0.254837	6.088553	0.109901
10	6	0	1.038693	4.644589	-0.861783
11	1	0	1.555304	5.405385	-1.439041
12	6	0	1.400679	3.322779	-0.995061
13	1	0	2.196088	3.019880	-1.667419
14	6	0	0.742095	-0.084333	-2.393450
15	6	0	1.558135	0.374628	-1.334261
16	6	0	2.942462	0.199565	-1.355622
17	1	0	3.528634	0.543264	-0.509134
18	6	0	3.547054	-0.416049	-2.452399

19	1	0	4.624597	-0.550818	-2.466984
20	6	0	2.764325	-0.861095	-3.518008
21	1	0	3.227869	-1.345871	-4.372307
22	6	0	1.378990	-0.698727	-3.482089
23	1	0	0.769250	-1.067007	-4.302413
24	17	0	-1.428180	-0.927275	2.875205
25	8	0	1.007900	-1.782534	1.239333
26	7	0	-0.934778	-1.005768	-0.209878
27	6	0	-0.745054	-2.352303	-0.194866
28	6	0	0.332955	-2.743548	0.684907
29	6	0	0.688433	-4.111771	0.785693
30	1	0	1.492182	-4.393022	1.457589
31	6	0	-0.000000	-5.035452	0.030501
32	1	0	0.254837	-6.088553	0.109901
33	6	0	-1.038693	-4.644589	-0.861783
34	1	0	-1.555304	-5.405385	-1.439041
35	6	0	-1.400679	-3.322779	-0.995061
36	1	0	-2.196088	-3.019880	-1.667419
37	6	0	-0.742095	0.084333	-2.393450
38	6	0	-1.558135	-0.374628	-1.334261
39	6	0	-2.942462	-0.199565	-1.355622
40	1	0	-3.528634	-0.543264	-0.509134
41	6	0	-3.547054	0.416049	-2.452399
42	1	0	-4.624597	0.550818	-2.466984
43	6	0	-2.764325	0.861095	-3.518008
44	1	0	-3.227869	1.345871	-4.372307
45	6	0	-1.378990	0.698727	-3.482089
46	1	0	-0.769250	1.067007	-4.302413
47	17	0	1.428180	0.927275	2.875205

G. *trans*-(Clip)$OsCl_2$

Energy of optimized structure = –2195.33944510 a.u.

Cartesian coordinates of optimized structure:

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	76	-0.000000	0.000000	0.922514
2	8	-0.229500	1.620481	2.273051
3	7	-0.325450	1.486852	-0.314184
4	6	-0.105436	2.749323	1.657368
5	6	-0.188989	2.746749	0.213187
6	6	-0.145958	3.964286	-0.513242
7	1	-0.189852	3.944585	-1.597061
8	6	0.000000	5.150175	0.171609
9	1	0.071998	6.086110	-0.373525

10	6	0.076718	5.158186	1.591982
11	1	0.187803	6.109259	2.106075
12	6	0.022723	3.994581	2.328066
13	1	0.082232	3.991922	3.411205
14	6	-0.641193	0.377302	-2.520787
15	6	-1.036351	1.311029	-1.537118
16	6	-2.242571	2.020988	-1.691283
17	1	-2.554551	2.695035	-0.902463
18	6	-3.050852	1.831232	-2.806148
19	1	-3.984648	2.378886	-2.891696
20	6	-2.663176	0.925037	-3.792222
21	1	-3.285353	0.759200	-4.666762
22	6	-1.472697	0.218002	-3.642621
23	1	-1.172086	-0.493897	-4.405350
24	17	-2.291389	-0.396300	1.266247
25	8	0.229500	-1.620481	2.273051
26	7	0.325450	-1.486852	-0.314184
27	6	0.105436	-2.749323	1.657368
28	6	0.188989	-2.746749	0.213187
29	6	0.145958	-3.964286	-0.513242
30	1	0.189852	-3.944585	-1.597061
31	6	-0.000000	-5.150175	0.171609
32	1	-0.071998	-6.086110	-0.373525
33	6	-0.076718	-5.158186	1.591982
34	1	-0.187803	-6.109259	2.106075
35	6	-0.022723	-3.994581	2.328066
36	1	-0.082232	-3.991922	3.411205
37	6	0.641193	-0.377302	-2.520787
38	6	1.036351	-1.311029	-1.537118
39	6	2.242571	-2.020988	-1.691283
40	1	2.554551	-2.695035	-0.902463
41	6	3.050852	-1.831232	-2.806148
42	1	3.984648	-2.378886	-2.891696
43	6	2.663176	-0.925037	-3.792222
44	1	3.285353	-0.759200	-4.666762
45	6	1.472697	-0.218002	-3.642621
46	1	1.172086	0.493897	-4.405350
47	17	2.291389	0.396300	1.266247

H. (Clamp)Os

Energy of optimized structure = –1921.72744930 a.u.

Cartesian coordinates of optimized structure:

Center Number	Atomic Number	Coordinates (Å) X	Y	Z
1	76	0.000751	0.000048	-1.000495
2	8	1.213058	-1.133042	-2.167641
3	8	-1.586092	-0.482151	-2.168146
4	8	0.376260	1.616280	-2.166413
5	7	1.759979	0.075573	0.018671
6	7	-0.814473	-1.562550	0.017638
7	7	-0.946701	1.485551	0.018102
8	7	-0.000913	-0.000444	2.266263
9	6	2.456959	-1.261386	-1.767227
10	6	2.804677	-0.627083	-0.531528
11	6	4.103491	-0.814092	-0.000196
12	1	4.365777	-0.381813	0.958782
13	6	5.028315	-1.555872	-0.714407
14	1	6.026237	-1.697078	-0.309193
15	6	4.693521	-2.135350	-1.959973
16	1	5.440349	-2.710131	-2.500535
17	6	3.422143	-1.993100	-2.488342
18	1	3.134343	-2.444931	-3.432256
19	6	-2.320111	-1.495135	-1.768601
20	6	-1.945279	-2.114898	-0.533407
21	6	-2.757623	-3.145976	-0.003170
22	1	-2.514919	-3.590424	0.955343
23	6	-3.863123	-3.573916	-0.717578
24	1	-4.485187	-4.367221	-0.312983
25	6	-4.197215	-2.992565	-1.962464
26	1	-5.069029	-3.350265	-2.503106
27	6	-3.437024	-1.963201	-2.490028
28	1	-3.683992	-1.486874	-3.433470
29	6	-0.134847	2.757683	-1.766438
30	6	-0.860008	2.741629	-0.532034
31	6	-1.348217	3.960024	-0.001733
32	1	-1.855774	3.971387	0.956114
33	6	-1.166069	5.132018	-0.715249
34	1	-1.543058	6.066909	-0.310480
35	6	-0.494232	5.131809	-1.959383
36	1	-0.367994	6.066027	-2.499399
37	6	0.018373	3.959377	-2.486978
38	1	0.555417	3.935876	-3.429849
39	6	1.043584	0.960336	2.193895
40	6	1.965088	0.944841	1.122847
41	6	3.000000	1.893379	1.100340

42	1	3.685395	1.901315	0.259309
43	6	3.108180	2.856101	2.102637
44	1	3.904953	3.592738	2.053264
45	6	2.181064	2.886628	3.145858
46	1	2.255988	3.637489	3.927193
47	6	1.161779	1.935967	3.189739
48	1	0.442315	1.930893	4.003442
49	6	0.308966	-1.385171	2.193150
50	6	-0.164738	-2.175381	1.121886
51	6	0.139623	-3.545962	1.099696
52	1	-0.195612	-4.143755	0.258603
53	6	0.919167	-4.120634	2.102433
54	1	1.159057	-5.178909	2.053264
55	6	1.408804	-3.332703	3.145554
56	1	2.021656	-3.772726	3.927018
57	6	1.094740	-1.974862	3.189080
58	1	1.449961	-1.348923	4.002617
59	6	-1.355315	0.423459	2.193095
60	6	-1.802719	1.228391	1.121586
61	6	-3.141971	1.649270	1.098532
62	1	-3.491891	2.238046	0.257064
63	6	-4.029458	1.262077	2.101419
64	1	-5.065993	1.583087	2.051723
65	6	-3.591955	0.445230	3.145458
66	1	-4.279548	0.135105	3.927066
67	6	-2.258950	0.038463	3.189451
68	1	-1.894341	-0.581411	4.003456

I. (Clamp)Ru

Energy of optimized structure = –1925.91469470 a.u.

Cartesian coordinates of optimized structure:

Center Number	Atomic Number	Coordinates (Å) X	Y	Z
1	44	0.000080	0.000360	-1.079432
2	8	1.153190	-1.198939	-2.244631
3	8	-1.616505	-0.397467	-2.243297
4	8	0.463088	1.599274	-2.243365
5	7	1.762106	0.038311	-0.063635
6	7	-0.847687	-1.545747	-0.064494
7	7	-0.914354	1.507472	-0.063698
8	7	-0.000672	-0.001071	2.167390
9	6	2.388846	-1.326150	-1.859684
10	6	2.770054	-0.686095	-0.623779
11	6	4.077807	-0.896902	-0.110501

12	1	4.357611	-0.469486	0.845701
13	6	4.979034	-1.652260	-0.833813
14	1	5.979695	-1.811190	-0.442089
15	6	4.618098	-2.229442	-2.078407
16	1	5.351331	-2.814802	-2.626389
17	6	3.345596	-2.072072	-2.590115
18	1	3.040183	-2.521902	-3.529467
19	6	-2.344366	-1.404255	-1.858924
20	6	-1.979244	-2.056197	-0.624454
21	6	-2.814910	-3.084432	-0.112028
22	1	-2.583851	-3.542314	0.843114
23	6	-3.920613	-3.485981	-0.834681
24	1	-4.558134	-4.273754	-0.443514
25	6	-4.241749	-2.882523	-2.077682
26	1	-5.116061	-3.223813	-2.625102
27	6	-3.469847	-1.858273	-2.588589
28	1	-3.707834	-1.367197	-3.526788
29	6	-0.044367	2.733095	-1.858381
30	6	-0.791029	2.742699	-0.623524
31	6	-1.263267	3.980571	-0.110696
32	1	-1.775661	4.009349	0.844292
33	6	-1.057526	5.139045	-0.832898
34	1	-1.420542	6.085043	-0.441291
35	6	-0.374493	5.115696	-2.076014
36	1	-0.232394	6.043738	-2.622918
37	6	0.125642	3.934996	-2.587614
38	1	0.669715	3.895615	-3.525930
39	6	1.058632	0.944286	2.095935
40	6	1.987101	0.906809	1.029217
41	6	3.041115	1.835360	1.011232
42	1	3.730934	1.827942	0.173743
43	6	3.159381	2.800905	2.009826
44	1	3.969300	3.523265	1.962864
45	6	2.225812	2.852851	3.046403
46	1	2.309119	3.605927	3.824786
47	6	1.189201	1.920288	3.088755
48	1	0.465934	1.931740	3.899073
49	6	0.288377	-1.391201	2.095163
50	6	-0.207300	-2.175611	1.027285
51	6	0.071419	-3.552311	1.007355
52	1	-0.278950	-4.145283	0.168916
53	6	0.848974	-4.138008	2.005272
54	1	1.070869	-5.200273	1.956782
55	6	1.359255	-3.356532	3.043366
56	1	1.969874	-3.805718	3.821383
57	6	1.068257	-1.992893	3.087682
58	1	1.438561	-1.373028	3.899155
59	6	-1.348957	0.444110	2.095168
60	6	-1.779703	1.267527	1.028388
61	6	-3.111013	1.715503	1.009196
62	1	-3.448959	2.316798	0.171616

63	6	-4.007341	1.334453	2.006617
64	1	-5.037956	1.674323	1.958585
65	6	-3.586476	0.499716	3.043316
66	1	-4.281060	0.194699	3.820779
67	6	-2.260387	0.068649	3.086915
68	1	-1.909268	-0.563731	3.897262

J. *trans*-$[(Clip)Os(py)_2]^+$

Energy of optimized structure = –1771.33785186 a.u.

Cartesian coordinates of optimized structure:

Center Number	Atomic Number	Coordinates (Å) X	Y	Z
1	76	0.000000	0.000000	0.715589
2	8	0.149475	-1.572515	2.071483
3	7	0.236226	-1.544632	-0.518882
4	6	-0.069406	-2.735049	1.489544
5	6	0.000000	-2.782685	0.053138
6	6	-0.162366	-4.012286	-0.627727
7	1	-0.126999	-4.037048	-1.712218
8	6	-0.398995	-5.163815	0.100383
9	1	-0.549431	-6.107498	-0.414055
10	6	-0.457211	-5.117928	1.512657
11	1	-0.637129	-6.035170	2.066013
12	6	-0.293826	-3.927311	2.204711
13	1	-0.332509	-3.887125	3.288563
14	6	0.607731	-0.435620	-2.706177
15	6	0.931931	-1.432876	-1.748495
16	6	2.044379	-2.272181	-1.964301
17	1	2.290827	-3.010841	-1.209707
18	6	2.842769	-2.140187	-3.093741
19	1	3.702262	-2.790527	-3.225414
20	6	2.539302	-1.160091	-4.039726
21	1	3.154765	-1.036755	-4.925606
22	6	1.435301	-0.334444	-3.841285
23	1	1.197159	0.422177	-4.582585
24	7	2.106339	0.311165	0.891359
25	6	2.868171	0.858803	-0.081030
26	1	2.365250	1.078840	-1.013804
27	6	4.220491	1.125077	0.097884
28	1	4.788328	1.565723	-0.714475
29	6	4.815866	0.821343	1.321716
30	1	5.869588	1.021865	1.489856
31	6	4.030294	0.252670	2.324412
32	1	4.447108	-0.004692	3.292156
33	6	2.684835	0.010297	2.077061
34	1	2.034456	-0.442416	2.815543
35	8	-0.149475	1.572515	2.071483
36	7	-0.236226	1.544632	-0.518882
37	6	0.069406	2.735049	1.489544

38	6	0.000000	2.782685	0.053138
39	6	0.162366	4.012286	-0.627727
40	1	0.126999	4.037048	-1.712218
41	6	0.398995	5.163815	0.100383
42	1	0.549431	6.107498	-0.414055
43	6	0.457211	5.117928	1.512657
44	1	0.637129	6.035170	2.066013
45	6	0.293826	3.927311	2.204711
46	1	0.332509	3.887125	3.288563
47	6	-0.607731	0.435620	-2.706177
48	6	-0.931931	1.432876	-1.748495
49	6	-2.044379	2.272181	-1.964301
50	1	-2.290827	3.010841	-1.209707
51	6	-2.842769	2.140187	-3.093741
52	1	-3.702262	2.790527	-3.225414
53	6	-2.539302	1.160091	-4.039726
54	1	-3.154765	1.036755	-4.925606
55	6	-1.435301	0.334444	-3.841285
56	1	-1.197159	-0.422177	-4.582585
57	7	-2.106339	-0.311165	0.891359
58	6	-2.868171	-0.858803	-0.081030
59	1	-2.365250	-1.078840	-1.013804
60	6	-4.220491	-1.125077	0.097884
61	1	-4.788328	-1.565723	-0.714475
62	6	-4.815866	-0.821343	1.321716
63	1	-5.869588	-1.021865	1.489856
64	6	-4.030294	-0.252670	2.324412
65	1	-4.447108	0.004692	3.292156
66	6	-2.684835	-0.010297	2.077061
67	1	-2.034456	0.442416	2.815543

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