Electronic Supplementary Information

9,10-Phenanthrenesemiquinone radical complexes of ruthenium(III), osmium(III) and rhodium(III) and redox series

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Table S1 X band EPR spectral parameters of **3** and **1**$^{-}$ complexes

complexes	conditions	g_{iso}/g_{av}	g_1	g_2	g_3	[a]Δg	[b]linewidth/G
3	Solid (83 K)	1.999	2.005	2.005	1.987	0.018	6.5, 6.0
	CH_2Cl_2 solution (298 K)	1.998					1.5 A(^{31}P)-9.5 A(^{103}Rh)-1.7 A(^{35,37}Cl)-1.4
	CH_2Cl_2frozen glass (83 K)	1.999	2.005	2.005	1.987	0.018	6.4, 5.8 A_{11}(^{31}P)-10.0 A_{22}(^{31}P)-10.0 A_{33}(^{31}P)-11.57
1^{-}	CH_2Cl_2frozen glass (83 K) *trans*-[$Ru^{III}(PQ^{2-})(PPh_3)_2X_2$]$^{-}$component *trans*-[$Ru^{II}(PQ^{\bullet-})(PPh_3)_2X_2$]$^{-}$component	2.298 1.999	2.456 2.004	2.456 2.004	1.983 1.991		65.0, 9.0 20.0, 7.0

[a]$\Delta g=g_{max}-g_{min,}$ [b]linewidth = linewidth is the peak-to-peak width of the spectrum. Line width values were obtained from the simulation of the spectra using the WINEPR SimFonia program.

Table S2 Redox potentials of **1**-**3** complexes in CH_2Cl_2 solution (0.20 M [N(*n*-Bu)$_4$]PF_6) at 298 K

complexes	$E^1_{1/2}$/V(ΔE^a/mV)	$E^2_{1/2}$/V(ΔE^a/mV)	$E^3_{1/2}$/V(ΔE^a/mV)
1	+0.22 (69)	-0.72 (89),	-1.0(120)
2	+0.22 (134)	-0.92 (142)	-
3	+0.16 (81), +0.16 (87)[c]	-0.92[b], -0.89 (88)[c]	-

[a]peak-to-peak separation, [b]cathodic peak potential, [c]redox potentials in presence of 0.025 mM PPh_3 at 298 K

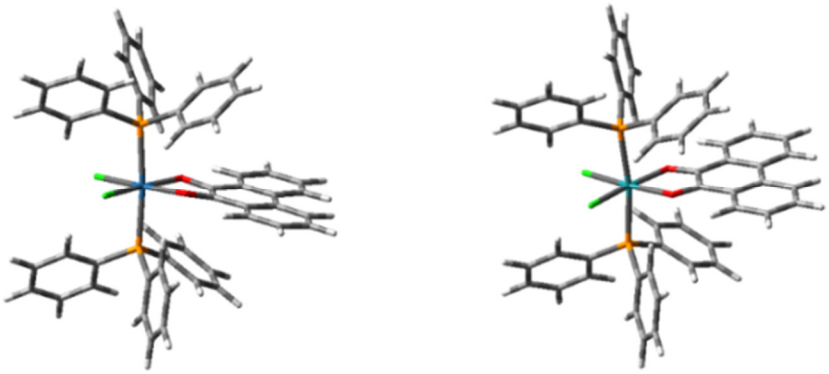

Fig. S1 Gas phase optimized geometries of **1** and **2** (at the RB3LYP level of the theory).

OPTIMIZED COORDINATES

Table S3 Optimized coordinates of **1**

S. No.	Symbol	X	Y	Z	S. No.	Symbol	X	Y	Z
1	Ru	-6.4E-05	-0.80723	-0.00019	49	C	-4.81601	-0.37902	-3.92215
2	P	2.461624	-0.99449	-0.05651	50	C	-5.48697	-0.7793	-2.76137
3	P	-2.46181	-0.99416	0.056528	51	C	-4.77829	-0.96758	-1.57386
4	Cl	-0.04213	-2.43756	-1.81004	52	C	-3.19258	-2.5608	0.703233
5	Cl	0.041846	-2.43833	1.808976	53	C	-4.26149	-2.57374	1.612397
6	O	0.095515	0.827325	1.27945	54	C	-4.82653	-3.78572	2.022108
7	O	-0.09544	0.827247	-1.27951	55	C	-4.3324	-4.99365	1.524734
8	C	0.061041	1.972765	0.723842	56	C	-3.26745	-4.98474	0.618669
9	C	-0.06072	1.97274	-0.72398	57	C	-2.69516	-3.77879	0.211219
10	C	-0.14325	3.222671	-1.45469	58	H	-0.3299	2.256804	-3.36473
11	C	-0.28853	3.213902	-2.85539	59	H	-0.48847	4.3942	-4.64213
12	C	-0.37458	4.404666	-3.56176	60	H	-0.37978	6.561666	-3.40868
13	C	-0.31291	5.621811	-2.86695	61	H	-0.12383	6.602016	-0.98433
14	C	-0.16669	5.640101	-1.48262	62	H	0.124706	6.602073	0.983799
15	C	-0.07796	4.449399	-0.73539	63	H	0.380575	6.561893	3.408159
16	C	0.078575	4.449443	0.735031	64	H	0.488932	4.394516	4.641796
17	C	0.167433	5.640193	1.482171	65	H	0.330137	2.257034	3.364565
18	C	0.313607	5.621999	2.866509	66	H	2.171215	-0.57257	-2.90828
19	C	0.375092	4.404907	3.561418	67	H	2.927606	1.186778	-4.47386
20	C	0.288921	3.214095	2.855143	68	H	4.246153	3.128838	-3.63603
21	C	0.143693	3.222765	1.454446	69	H	4.815405	3.278615	-1.21607
22	C	3.111092	0.320719	-1.17689	70	H	4.107787	1.497465	0.339546
23	C	2.770678	0.25677	-2.54169	71	H	1.648079	-0.22739	2.683941
24	C	3.186567	1.256889	-3.42011	72	H	2.902545	0.115924	4.788731
25	C	3.927386	2.348379	-2.94957	73	H	5.364742	-0.24437	4.851015
26	C	4.247371	2.431939	-1.59377	74	H	6.55872	-0.95822	2.78283
27	C	3.842453	1.423328	-0.71053	75	H	5.309035	-1.29854	0.686222
28	C	3.389171	-0.74952	1.526199	76	H	4.65763	-1.64448	-2.01152
29	C	2.722493	-0.35879	2.69607	77	H	5.651841	-3.77934	-2.73133
30	C	3.434805	-0.17486	3.886315	78	H	4.769984	-5.93539	-1.84773
31	C	4.814874	-0.38208	3.923141	79	H	2.868768	-5.92053	-0.23692
32	C	5.485893	-0.78287	2.762577	80	H	1.856197	-3.78131	0.476219
33	C	4.777483	-0.97041	1.574791	81	H	-4.10741	1.498588	-0.3373
34	C	3.19228	-2.56079	-0.70417	82	H	-4.81399	3.278833	1.219771
35	C	4.261283	-2.57327	-1.61323	83	H	-4.24415	3.127133	3.639481
36	C	4.826185	-3.78506	-2.0237	84	H	-2.9261	1.18398	4.475567
37	C	4.331829	-4.99325	-1.52718	85	H	-2.17076	-0.57451	2.908549
38	C	3.266778	-4.9848	-0.62123	86	H	-1.64862	-0.22727	-2.6841
39	C	2.694629	-3.77903	-0.21303	87	H	-2.90356	0.117334	-4.7884
40	C	-3.11074	0.320356	1.178027	88	H	-5.3661	-0.24075	-4.84981
41	C	-3.84183	1.42357	0.712656	89	H	-6.55997	-0.95366	-2.78123
42	C	-4.24616	2.431688	1.59672	90	H	-5.3098	-1.29529	-0.68511
43	C	-3.92585	2.34705	2.952382	91	H	-4.65764	-1.64516	2.011371
44	C	-3.18531	1.254947	3.421939	92	H	-5.6521	-3.78035	2.729843
45	C	-2.77002	0.255301	2.542698	93	H	-4.77066	-5.93594	1.84469
46	C	-3.38976	-0.74794	-1.52577	94	H	-2.86962	-5.92028	0.233693
47	C	-2.72316	-0.3577	-2.69584	95	H	-1.8568	-3.78073	-0.47811
48	C	-3.43575	-0.17305	-3.88581					

Table S4 Optimized coordinates of close shell singlet solutions of $\mathbf{1}_{Me}$

S. No.	Symbol	X	Y	Z	S. No.	Symbol	X	Y	Z
1	Ru	0.007308	4.853641	4.363339	28	H	-1.26477	12.17469	7.59537
2	P	2.261207	4.457531	5.142078	29	C	2.731486	2.690517	5.299703
3	Cl	0.63333	3.265539	2.59056	30	H	3.766385	2.603272	5.650982
4	P	-2.24234	4.437117	3.582916	31	H	2.050435	2.20666	6.004212
5	O	0.443965	6.463705	3.167349	32	H	2.620669	2.208063	4.325565
6	C	0.244483	7.614303	3.699615	33	C	2.629083	5.159453	6.808647
7	C	0.503086	8.864622	3.014392	34	H	2.521455	6.248746	6.793398
8	C	1.004947	8.859796	1.697346	35	H	1.907999	4.750647	7.522881
9	C	1.256232	10.05341	1.037304	36	H	3.64682	4.905614	7.129106
10	C	1.006692	11.26966	1.692964	37	C	3.562598	5.166813	4.043685
11	C	0.510192	11.2839	2.992532	38	H	4.567156	4.903052	4.3955
12	C	0.242754	10.09002	3.693011	39	H	3.410382	4.771891	3.034735
13	O	-0.44798	6.450053	5.571747	40	H	3.47139	6.257074	4.005967
14	C	-0.2609	7.606607	5.047951	41	C	-2.6928	2.665916	3.414901
15	C	-0.53259	8.849211	5.742143	42	H	-3.72589	2.569257	3.060768
16	C	-1.0339	8.82966	7.05928	43	H	-2.00487	2.193548	2.709261
17	C	-1.29735	10.0158	7.72799	44	H	-2.57875	2.179318	4.386583
18	C	-1.06076	11.23927	7.08103	45	C	-3.55073	5.1256	4.686243
19	C	-0.5649	11.26809	5.781465	46	H	-4.55257	4.851555	4.334583
20	C	-0.2852	10.08216	5.072337	47	H	-3.39241	4.72798	5.693191
21	H	1.187674	7.903198	1.217449	48	H	-3.4725	6.216697	4.728768
22	H	1.642844	10.04692	0.022023	49	C	-2.61937	5.144392	1.920644
23	H	1.201041	12.21084	1.185458	50	H	-2.52494	6.234789	1.942132
24	H	0.331661	12.24413	3.463469	51	H	-1.89384	4.74838	1.20371
25	H	-1.68346	9.998004	8.743328	52	H	-3.63415	4.880094	1.599287
26	H	-0.39656	12.23348	5.317402	53	Cl	-0.60011	3.245034	6.124068
27	H	-1.2063	7.867774	7.53238					

Table S5 Optimized coordinates of open shell solutions of $\mathbf{1}_{Me}^{+}$

S. No.	Symbol	X	Y	Z	S. No.	Symbol	X	Y	Z
1	Ru	-1.52843	0	0	28	H	5.87353	0.616802	3.374068
2	P	-1.75314	-2.41242	0.427145	29	C	-3.49631	-2.97964	0.51127
3	Cl	-3.0134	-0.31197	-1.78196	30	H	-3.52992	-4.05875	0.697969
4	P	-1.75314	2.412424	-0.42715	31	H	-4.01421	-2.45226	1.316597
5	O	0.152197	-0.2229	-1.24477	32	H	-3.99964	-2.75415	-0.43233
6	C	1.300551	-0.13123	-0.72969	33	C	-1.01359	-2.97627	2.017075
7	C	2.541461	-0.26288	-1.44958	34	H	0.069174	-2.81575	2.015711
8	C	2.527989	-0.51577	-2.83704	35	H	-1.44964	-2.40042	2.838907
9	C	3.720809	-0.64404	-3.53398	36	H	-1.21201	-4.04181	2.179486
10	C	4.932368	-0.51852	-2.84065	37	C	-0.98581	-3.48032	-0.86257
11	C	4.953119	-0.26782	-1.46671	38	H	-1.18373	-4.53866	-0.65836
12	C	3.766276	-0.13278	-0.7302	39	H	-1.40379	-3.21804	-1.83913
13	O	0.152197	0.222895	1.24477	40	H	0.097247	-3.32483	-0.89478
14	C	1.300551	0.13123	0.729685	41	C	-3.49631	2.979641	-0.51127
15	C	2.541461	0.262878	1.449575	42	H	-3.52992	4.058749	-0.69797
16	C	2.527989	0.515771	2.837041	43	H	-4.01421	2.452261	-1.3166
17	C	3.720809	0.644036	3.533981	44	H	-3.99964	2.754156	0.43233
18	C	4.932368	0.518521	2.840647	45	C	-0.98581	3.480324	0.86257
19	C	4.95312	0.267814	1.466713	46	H	-1.18372	4.538657	0.658362
20	C	3.766276	0.132774	0.7302	47	H	-1.40379	3.218041	1.839127
21	H	1.571989	-0.60761	-3.3432	48	H	0.097248	3.324831	0.894781
22	H	3.715841	-0.83941	-4.60171	49	C	-1.01359	2.976268	-2.01708
23	H	5.87353	-0.6168	-3.37407	50	H	0.069178	2.815749	-2.01571
24	H	5.916748	-0.17943	-0.9794	51	H	-1.44964	2.400415	-2.83891
25	H	3.715842	0.839411	4.601708	52	H	-1.21201	4.041808	-2.17949
26	H	5.916748	0.179425	0.979404	53	Cl	-3.0134	0.311972	1.781958
27	H	1.57199	0.607605	3.343199					

Table S6 Optimized coordinates of open shell solutions of $\mathbf{1}_{Me}^{-}$

S. No.	Symbol	X	Y	Z	S. No.	Symbol	X	Y	Z
1	Ru	1.514092	0.002255	-0.08666	28	H	-5.81657	3.443908	0.309434
2	P	1.777976	0.079861	-2.45495	29	C	3.516788	0.069728	-3.06671
3	Cl	3.182876	-1.85392	-0.07512	30	H	3.555345	0.114511	-4.16306
4	P	1.553129	-0.07964	2.312373	31	H	4.04015	0.926766	-2.63292
5	O	-0.08838	-1.32386	-0.19069	32	H	4.005018	-0.84031	-2.70614
6	C	-1.23554	-0.70329	-0.05422	33	C	1.065153	1.57501	-3.27785
7	C	-2.48345	-1.43198	0.000134	34	H	-0.01191	1.620432	-3.08792
8	C	-2.4756	-2.84754	-0.04251	35	H	1.522829	2.461483	-2.82739
9	C	-3.65613	-3.56861	0.011424	36	H	1.246961	1.572493	-4.36058
10	C	-4.88652	-2.88816	0.112424	37	C	1.009411	-1.3182	-3.39192
11	C	-4.91115	-1.50063	0.154375	38	H	1.180764	-1.23013	-4.47283
12	C	-3.72592	-0.73059	0.098379	39	H	1.440566	-2.25517	-3.02496
13	O	-0.08585	1.333799	-0.121	40	H	-0.06687	-1.34427	-3.1938
14	C	-1.23452	0.709048	-0.0183	41	C	3.23723	-0.06483	3.060754
15	C	-2.48172	1.435708	0.068981	42	H	3.189575	-0.10801	4.156741
16	C	-2.47266	2.851693	0.092747	43	H	3.794951	-0.92148	2.670948
17	C	-3.65281	3.570607	0.176017	44	H	3.750214	0.845783	2.737811
18	C	-4.88409	2.887434	0.241643	45	C	0.708013	1.314043	3.188827
19	C	-4.90989	1.499478	0.220188	46	H	0.802515	1.227778	4.279321
20	C	-3.72515	0.731729	0.132075	47	H	1.159549	2.253027	2.852827
21	H	-1.51339	-3.34491	-0.11855	48	H	-0.35229	1.333865	2.917261
22	H	-3.63424	-4.65598	-0.02224	49	C	0.785642	-1.58386	3.066133
23	H	-5.81927	-3.44644	0.158057	50	H	-0.27534	-1.62934	2.801013
24	H	-5.87351	-1.00349	0.231074	51	H	1.27799	-2.46346	2.63936
25	H	-3.62997	4.658352	0.19193	52	H	0.889645	-1.5932	4.159078
26	H	-5.87291	1.000243	0.27074	53	Cl	3.187575	1.851016	0.027887
27	H	-1.50984	3.351212	0.043006					

Table S7 Optimized coordinates of **2**

S. No.	Symbol	X	Y	Z	S. No.	Symbol	X	Y	Z
1	P	2.3587	-0.8753	-0.0979	33	C	4.7768	-3.6253	-2.0653
2	P	-2.5535	-1.0112	0.0503	34	C	4.3368	-4.8426	-1.5412
3	O	-0.0732	0.7293	1.3366	35	C	3.2909	-4.8567	-0.6138
4	O	-0.256	0.8255	-1.1937	36	C	2.6847	-3.665	-0.2131
5	C	0.1571	1.8956	0.803	37	C	-3.3002	0.3488	1.0521
6	C	0.0418	1.9528	-0.6114	38	C	-4.1701	1.3041	0.5062
7	C	0.0666	3.2161	-1.3076	39	C	-4.6757	2.3386	1.3018
8	C	-0.1113	3.2695	-2.706	40	C	-4.3236	2.425	2.6499
9	C	-0.093	4.4838	-3.3734	41	C	-3.4537	1.4773	3.2011
10	C	0.1173	5.6688	-2.6485	42	C	-2.9367	0.453	2.4075
11	C	0.299	5.6278	-1.2711	43	C	-3.4412	-0.9118	-1.5706
12	C	0.2758	4.4107	-0.5578	44	C	-2.8491	-0.2775	-2.6733
13	C	0.4379	4.3476	0.9038	45	C	-3.5418	-0.1713	-3.883
14	C	0.6619	5.496	1.6923	46	C	-4.8282	-0.7005	-4.0098
15	C	0.7837	5.4186	3.0747	47	C	-5.4227	-1.34	-2.918
16	C	0.684	4.1793	3.7291	48	C	-4.7337	-1.4469	-1.7078
17	C	0.4732	3.0296	2.9849	49	C	-3.2467	-2.5582	0.784
18	C	0.3532	3.0949	1.5807	50	C	-4.2758	-2.5466	1.7369
19	C	2.9765	0.4182	-1.2595	51	C	-4.8089	-3.7475	2.2179
20	C	2.5884	0.3239	-2.6091	52	C	-4.3233	-4.9692	1.7477
21	C	3.0185	1.2747	-3.5341	53	C	-3.2987	-4.9857	0.7957
22	C	3.8228	2.3449	-3.1243	54	C	-2.7584	-3.7909	0.3191
23	C	4.1897	2.4594	-1.7827	55	H	-0.2565	2.3397	-3.2457
24	C	3.7695	1.5008	-0.853	56	H	-0.2361	4.5185	-4.4501
25	C	3.3006	-0.6038	1.4715	57	H	0.137	6.6259	-3.1633
26	C	2.6381	-0.2954	2.6677	58	H	0.4521	6.5633	-0.7444
27	C	3.364	-0.1152	3.8502	59	H	0.7416	6.4703	1.2227
28	C	4.7539	-0.2415	3.8521	60	H	0.9565	6.3253	3.6487
29	C	5.4223	-0.5586	2.6643	61	H	0.7756	4.122	4.8104
30	C	4.7006	-0.7438	1.4847	62	H	0.3999	2.0604	3.467
31	C	3.1245	-2.4371	-0.7336	63	H	1.9475	-0.4937	-2.9298
32	C	4.1763	-2.4281	-1.6629	64	H	2.7209	1.1829	-4.5758

S. No.	Symbol	X	Y	Z	S. No.	Symbol	X	Y	Z
65	H	4.1517	3.0882	-3.8461	81	H	-3.1708	1.54	4.2489
66	H	4.803	3.2938	-1.452	82	H	-2.2476	-0.2677	2.8389
67	H	4.0677	1.6011	0.1858	83	H	-1.8469	0.1237	-2.5907
68	H	1.5582	-0.2198	2.6803	84	H	-3.0668	0.3167	-4.7306
69	H	2.8356	0.113	4.7724	85	H	-5.3617	-0.6225	-4.954
70	H	5.3146	-0.1048	4.7735	86	H	-6.4207	-1.762	-3.007
71	H	6.5038	-0.6699	2.657	87	H	-5.2046	-1.9549	-0.872
72	H	5.2306	-1.0077	0.5741	88	H	-4.6697	-1.607	2.1102
73	H	4.5323	-1.4937	-2.0845	89	H	-5.6045	-3.7219	2.9586
74	H	5.5877	-3.6007	-2.7893	90	H	-4.7371	-5.9023	2.1222
75	H	4.8028	-5.7734	-1.8552	91	H	-2.9082	-5.9318	0.4295
76	H	2.9357	-5.7989	-0.2043	92	H	-1.9524	-3.8139	-0.4072
77	H	1.8657	-3.6908	0.498	93	Os	-0.1156	-0.8175	0.0048
78	H	-4.4593	1.2452	-0.5382	94	Br	-0.0096	-2.579	1.8924
79	H	-5.3466	3.073	0.8632	95	Br	-0.1503	-2.5314	-1.9281
80	H	-4.7193	3.2271	3.2679					

Table S8 Optimized coordinates of close shell singlet solutions of $\mathbf{2}_{Me}$

S. No.	Symbol	X	Y	Z	S. No.	Symbol	X	Y	Z
1	P	-1.82682	2.518306	-0.1436	28	H	-3.60684	4.190741	-0.26695
2	P	-1.46628	-2.29275	0.067075	29	H	-4.07716	2.646344	-1.0458
3	O	0.04069	0.301416	1.308464	30	H	-4.0827	2.773246	0.721511
4	C	1.214778	0.043534	0.797901	31	C	-1.07724	3.30661	-1.63295
5	C	2.416994	-0.02063	1.592514	32	H	0.002315	3.128206	-1.64756
6	C	2.346503	0.049176	3.000728	33	H	-1.50979	2.84826	-2.52742
7	C	3.500087	-0.01819	3.765738	34	H	-1.26637	4.386243	-1.64738
8	C	4.745452	-0.16411	3.130607	35	C	-1.10073	3.459837	1.266936
9	C	4.82582	-0.23434	1.744794	36	H	-1.27852	4.53608	1.158234
10	C	3.67414	-0.16155	0.932508	37	H	-1.55439	3.108674	2.198866
11	O	0.147301	0.222465	-1.24061	38	H	-0.02327	3.276261	1.322727
12	C	1.274115	-0.00121	-0.61879	39	C	-3.12175	-3.0918	0.019886
13	C	2.536862	-0.11548	-1.30607	40	H	-3.02215	-4.18231	0.06505
14	C	2.581711	-0.14135	-2.71683	41	H	-3.71478	-2.73613	0.866832
15	C	3.793653	-0.25867	-3.37856	42	H	-3.63147	-2.80145	-0.90276
16	C	4.982049	-0.36146	-2.63503	43	C	-0.56348	-3.11371	-1.31744
17	C	4.948555	-0.33876	-1.24568	44	H	-0.62902	-4.20517	-1.23781
18	C	3.734794	-0.21115	-0.53718	45	H	-1.0078	-2.78964	-2.26366
19	H	1.371333	0.155834	3.465791	46	H	0.490511	-2.81991	-1.31383
20	H	3.441639	0.038312	4.849301	47	C	-0.70369	-2.99012	1.5953
21	H	5.654757	-0.22222	3.723035	48	H	0.348106	-2.69698	1.66445
22	H	5.804828	-0.34241	1.290813	49	H	-1.23246	-2.58228	2.462256
23	H	3.824362	-0.27503	-4.46462	50	H	-0.77065	-4.08428	1.606506
24	H	5.886424	-0.41804	-0.70694	51	Os	-1.49058	0.138322	-0.02925
25	H	1.647967	-0.06852	-3.26588	52	Br	-3.24369	0.10711	1.839175
26	H	5.936342	-0.4596	-3.1458	53	Br	-3.09545	-0.03142	-2.02016
27	C	-3.57142	3.098003	-0.18836					

Table S9 Optimized coordinates of open shell solutions of $\mathbf{2}_{Me}$

S. No.	Symbol	X	Y	Z	S. No.	Symbol	X	Y	Z
1	P	-1.82682	2.518306	-0.1436	28	H	-3.60684	4.190741	-0.26695
2	P	-1.46628	-2.29275	0.067075	29	H	-4.07716	2.646344	-1.0458
3	O	0.04069	0.301416	1.308464	30	H	-4.0827	2.773247	0.721511
4	C	1.214778	0.043534	0.797901	31	C	-1.07724	3.30661	-1.63295
5	C	2.416994	-0.02063	1.592514	32	H	0.002315	3.128207	-1.64756
6	C	2.346503	0.049176	3.000728	33	H	-1.50979	2.848261	-2.52742
7	C	3.500088	-0.01819	3.765738	34	H	-1.26637	4.386244	-1.64738
8	C	4.745453	-0.16411	3.130608	35	C	-1.10073	3.459837	1.266936
9	C	4.82582	-0.23434	1.744794	36	H	-1.27852	4.53608	1.158234
10	C	3.67414	-0.16155	0.932508	37	H	-1.55439	3.108674	2.198866
11	O	0.147301	0.222465	-1.24061	38	H	-0.02327	3.276261	1.322727
12	C	1.274115	-0.00121	-0.61879	39	C	-3.12175	-3.0918	0.019886
13	C	2.536862	-0.11548	-1.30607	40	H	-3.02215	-4.18232	0.06505
14	C	2.581711	-0.14135	-2.71683	41	H	-3.71478	-2.73614	0.866832
15	C	3.793653	-0.25867	-3.37856	42	H	-3.63147	-2.80145	-0.90276
16	C	4.98205	-0.36146	-2.63503	43	C	-0.56348	-3.11371	-1.31744
17	C	4.948555	-0.33876	-1.24568	44	H	-0.62902	-4.20517	-1.23781
18	C	3.734794	-0.21115	-0.53718	45	H	-1.0078	-2.78964	-2.26366
19	H	1.371333	0.155834	3.465791	46	H	0.490511	-2.81991	-1.31383
20	H	3.44164	0.038312	4.849301	47	C	-0.70369	-2.99012	1.5953
21	H	5.654757	-0.22222	3.723036	48	H	0.348106	-2.69698	1.66445
22	H	5.804829	-0.34241	1.290813	49	H	-1.23246	-2.58228	2.462256
23	H	3.824362	-0.27503	-4.46462	50	H	-0.77065	-4.08428	1.606506
24	H	5.886425	-0.41804	-0.70694	51	Os	-1.49058	0.138322	-0.02925
25	H	1.647967	-0.06852	-3.26588	52	Br	-3.24369	0.10711	1.839176
26	H	5.936342	-0.4596	-3.1458	53	Br	-3.09545	-0.03142	-2.02016
27	C	-3.57142	3.098003	-0.18836					

Table S10 Optimized coordinates of $\mathbf{3}_{Me}$

S. No.	Symbol	X	Y	Z	S. No.	Symbol	X	Y	Z
1	Cl	0.375581	3.029006	2.715632	28	H	-4.16464	3.025497	2.720084
2	P	-2.38061	4.583777	3.331539	29	H	-2.57146	2.223635	2.821924
3	O	0.039489	6.429267	2.975572	30	H	-3.47902	2.607685	4.306806
4	C	-0.0221	7.519486	3.657637	31	C	-3.63768	5.727797	4.046476
5	C	0.311476	8.800383	3.056828	32	H	-4.59332	5.628219	3.518495
6	C	0.778985	8.837869	1.726638	33	H	-3.78742	5.515164	5.108914
7	C	1.10105	10.04515	1.125452	34	H	-3.28765	6.760263	3.956948
8	C	0.961337	11.23841	1.853041	35	C	-2.326	5.041361	1.55319
9	C	0.508884	11.21223	3.167762	36	H	-1.90063	6.04186	1.447336
10	C	0.173964	10.00127	3.808065	37	H	-1.67083	4.337502	1.032932
11	O	-0.76273	6.313188	5.544123	38	H	-3.3332	5.010676	1.121493
12	C	-0.45758	7.465646	5.027327	39	Rh	-0.23514	4.73882	4.28339
13	C	-0.59504	8.684264	5.798462	40	Cl	2.078334	5.09038	4.950634
14	C	-1.02657	8.620191	7.141516	41	P	-0.48162	3.192294	5.986484
15	C	-1.17302	9.773411	7.89624	42	C	0.841748	3.219608	7.259454
16	C	-0.88679	11.02002	7.31539	43	H	0.573717	2.530868	8.070126
17	C	-0.45481	11.09675	5.995842	44	H	1.791868	2.926526	6.809045
18	C	-0.29375	9.943271	5.201414	45	H	0.9608	4.233324	7.648809
19	H	0.89145	7.897917	1.19617	46	C	-0.59724	1.410235	5.547848
20	H	1.466014	10.06685	0.102138	47	H	0.310128	1.119377	5.012601
21	H	1.21376	12.19023	1.392757	48	H	-0.70066	0.812269	6.460886
22	H	0.422683	12.15254	3.701346	49	H	-1.4481	1.219753	4.889766
23	H	-1.5025	9.713684	8.930181	50	C	-1.99276	3.528085	6.992493
24	H	-0.23838	12.07532	5.581523	51	H	-2.90267	3.342566	6.414574
25	H	-1.23319	7.644878	7.569262	52	H	-2.00904	2.89068	7.884032
26	H	-0.9971	11.93135	7.897372	53	H	-1.98299	4.578359	7.298539
27	C	-3.2357	2.950933	3.297148					

Table S11 Optimized coordinates of $\mathbf{3}_{Me}^{+}$

S. No.	Symbol	X	Y	Z	S. No.	Symbol	X	Y	Z
1	Cl	0.356184	3.209539	2.739346	28	H	-4.1399	2.597943	2.680346
2	P	-2.59116	4.366591	3.309104	29	H	-2.46914	1.991327	2.812522
3	O	-0.33027	6.610798	2.886688	30	H	-3.44548	2.273407	4.279843
4	C	-0.17423	7.638841	3.571759	31	C	-3.96084	5.340426	4.063715
5	C	0.340466	8.887211	3.046539	32	H	-4.89966	5.150232	3.531319
6	C	0.842475	8.911769	1.731145	33	H	-4.09029	5.074943	5.116994
7	C	1.356864	10.0882	1.20031	34	H	-3.73338	6.408823	4.006263
8	C	1.370948	11.2414	1.992417	35	C	-2.59574	4.856542	1.539811
9	C	0.87728	11.22235	3.300643	36	H	-2.34317	5.914873	1.442009
10	C	0.351	10.0515	3.86293	37	H	-1.84274	4.271186	1.005488
11	O	-1.09276	6.484223	5.434115	38	H	-3.5852	4.674151	1.105892
12	C	-0.64552	7.580837	5.020972	39	Rh	-0.4598	4.827824	4.23595
13	C	-0.66184	8.791853	5.810372	40	Cl	1.77091	5.566439	4.86761
14	C	-1.14869	8.744111	7.133325	41	P	-0.49506	3.280751	5.948799
15	C	-1.17029	9.887873	7.917547	42	C	0.873924	3.4734	7.151478
16	C	-0.69712	11.08995	7.376005	43	H	0.725597	2.75287	7.964723
17	C	-0.20833	11.14631	6.068817	44	H	1.831293	3.289804	6.659683
18	C	-0.1742	10.00804	5.250405	45	H	0.89055	4.489566	7.550944
19	H	0.832236	7.993402	1.153225	46	C	-0.43861	1.503846	5.502318
20	H	1.749864	10.10952	0.188749	47	H	0.496836	1.29325	4.978927
21	H	1.774515	12.16791	1.593851	48	H	-0.49135	0.908568	6.421136
22	H	0.918081	12.14108	3.873299	49	H	-1.26517	1.22966	4.844626
23	H	-1.54471	9.852207	8.935762	50	C	-2.00674	3.484584	6.979603
24	H	0.146362	12.10065	5.698929	51	H	-2.9065	3.213841	6.421053
25	H	-1.50136	7.795713	7.524322	52	H	-1.93897	2.840452	7.863574
26	H	-0.70544	11.99504	7.976766	53	H	-2.09269	4.525745	7.303658
27	C	-3.2197	2.638754	3.274051					

Table S12 Optimized coordinates of $\mathbf{3}_{Me}^{-}$

S. No.	Symbol	X	Y	Z	S. No.	Symbol	X	Y	Z
1	Cl	0.371797	2.920289	2.646794	28	H	-4.19628	3.273628	2.776385
2	P	-2.26343	4.693778	3.314812	29	H	-2.67334	2.341776	2.88952
3	O	0.139799	6.341617	2.971748	30	H	-3.52201	2.854283	4.370094
4	C	0.003855	7.460464	3.685927	31	C	-3.41414	5.96517	3.989236
5	C	0.271304	8.738929	3.076867	32	H	-4.37394	5.946439	3.457793
6	C	0.730149	8.795208	1.734711	33	H	-3.5773	5.794674	5.057298
7	C	0.987518	10.00511	1.116905	34	H	-2.95181	6.950756	3.880694
8	C	0.796062	11.21101	1.827218	35	C	-2.20022	5.067591	1.51708
9	C	0.35742	11.17596	3.142118	36	H	-1.65204	6.002681	1.381569
10	C	0.084826	9.956531	3.809817	37	H	-1.63972	4.27107	1.020114
11	O	-0.66977	6.20236	5.575028	38	H	-3.21294	5.142468	1.101217
12	C	-0.41186	7.400414	5.013841	39	Rh	-0.14533	4.714709	4.265494
13	C	-0.60122	8.598484	5.778554	40	Cl	2.216519	4.93946	4.951182
14	C	-1.02821	8.524608	7.132681	41	P	-0.4562	3.182333	5.991662
15	C	-1.23158	9.666162	7.885555	42	C	0.867402	3.136053	7.270313
16	C	-1.01282	10.93723	7.309663	43	H	0.567274	2.472752	8.092466
17	C	-0.58778	11.03115	5.992363	44	H	1.799788	2.792301	6.817846
18	C	-0.3661	9.886776	5.189519	45	H	1.041696	4.149455	7.640225
19	H	0.886751	7.853356	1.218045	46	C	-0.68101	1.391768	5.601163
20	H	1.345956	10.02848	0.089265	47	H	0.181507	1.051527	5.021622
21	H	0.999691	12.16746	1.349338	48	H	-0.77167	0.804635	6.523776
22	H	0.227915	12.11695	3.669479	49	H	-1.57164	1.240744	4.985088
23	H	-1.55501	9.586123	8.922236	50	C	-1.93438	3.593854	7.026569
24	H	-0.4209	12.01925	5.572755	51	H	-2.8609	3.437029	6.465163
25	H	-1.18162	7.539262	7.561403	52	H	-1.96606	2.981943	7.936662
26	H	-1.16997	11.84058	7.895805	53	H	-1.86937	4.653396	7.292235
27	C	-3.26732	3.140107	3.344761					

Table S13 Optimized coordinates of $\mathbf{4}_{Me}^{+}$

S. No.	Symbol	X	Y	Z	S. No.	Symbol	X	Y	Z
1	P	-1.72409	2.432193	-0.06983	28	H	5.864214	-0.16858	-3.39362
2	P	-1.7304	-2.43326	0.184704	29	C	-3.3881	3.085998	-0.48353
3	O	-3.49613	-0.1311	-2.45885	30	H	-3.40939	4.178811	-0.38514
4	C	-2.77981	-0.08321	-1.54618	31	H	-3.65211	2.812671	-1.51256
5	O	0.098606	0.046943	1.263092	32	H	-4.12279	2.640856	0.197091
6	C	1.250951	0.029375	0.731107	33	C	-0.58552	3.294561	-1.23623
7	C	2.488039	0.073546	1.46944	34	H	0.457088	3.032538	-1.01811
8	C	2.462248	0.148253	2.877096	35	H	-0.81237	2.988515	-2.26469
9	C	3.646358	0.195851	3.594842	36	H	-0.69794	4.383304	-1.15288
10	C	4.864795	0.169037	2.902946	37	C	-1.32846	3.137308	1.580315
11	C	4.899583	0.095304	1.511453	38	H	-1.43968	4.229233	1.571375
12	C	3.719983	0.045537	0.751956	39	H	-2.00867	2.702023	2.320993
13	O	0.120142	-0.06585	-1.28844	40	H	-0.29986	2.880419	1.860193
14	C	1.270956	-0.03801	-0.732	41	C	-3.38932	-3.13178	-0.17304
15	C	2.512534	-0.07214	-1.46071	42	H	-3.41281	-4.20573	0.05223
16	C	2.512858	-0.14574	-2.86815	43	H	-4.1326	-2.61115	0.441579
17	C	3.710304	-0.18025	-3.56549	44	H	-3.64002	-2.98079	-1.23025
18	C	4.917647	-0.14151	-2.85612	45	C	-0.57449	-3.41094	-0.86803
19	C	4.926579	-0.06878	-1.46438	46	H	-0.6777	-4.48453	-0.66327
20	C	3.733281	-0.03206	-0.7259	47	H	-0.79122	-3.22466	-1.92687
21	H	1.49757	0.16865	3.380723	48	H	0.462667	-3.11406	-0.66876
22	H	3.631355	0.254111	4.68135	49	C	-1.34795	-2.96134	1.902616
23	H	5.802375	0.20672	3.45566	50	H	-0.32369	-2.66896	2.162473
24	H	5.869641	0.078052	1.022502	51	H	-2.03739	-2.45932	2.590461
25	H	3.712341	-0.23741	-4.65224	52	H	-1.45152	-4.04942	2.002377
26	H	5.887359	-0.04152	-0.95778	53	Os	-1.57579	-0.01159	-0.13707
27	H	1.559468	-0.17547	-3.39206	54	Br	-3.39356	0.08614	1.671973