Electronic Supplementary Information (ESI)

Coordination of *o*-benzosemiquinonate, *o*-iminobenzosemiquinonate, 4,4'-di-*tert*-butyl-2,2'-bipyridine and 1,10-phenanthroline anion radicals to oxidovanadium(IV)

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Table of Content

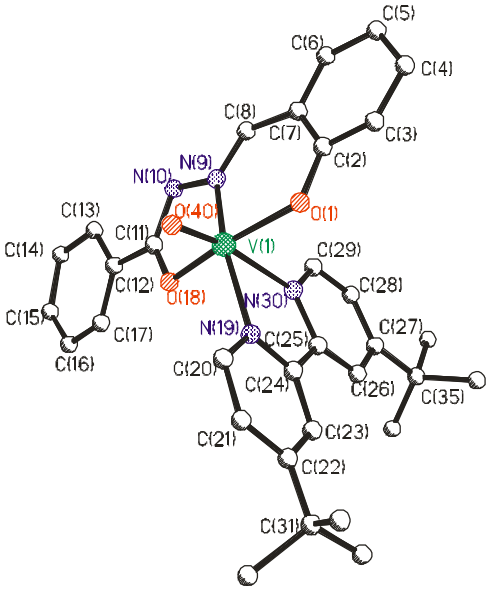

Fig. S1 Molecular geometries of **5** in crystals (H atoms are omitted for clarity).

Table S1 Gas phase optimized coordinates of **3** (CSS)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	23	5.774679	7.117826	8.838104
2	8	6.707820	5.695127	7.860360
3	6	7.866519	5.971658	7.351394
4	6	8.627309	4.889466	6.696783
5	6	8.073332	3.600303	6.626756
6	1	7.092623	3.424223	7.055897
7	6	8.780206	2.567920	6.010709
8	1	8.346181	1.573020	5.957865
9	6	10.044033	2.812415	5.462903
10	1	10.594098	2.006523	4.983546
11	6	10.600791	4.095098	5.532778
12	1	11.583453	4.285920	5.109393
13	6	9.898379	5.131649	6.145281
14	1	10.320869	6.128863	6.206196
15	7	8.388752	7.198272	7.388946
16	7	7.523047	8.008165	8.033757
17	6	7.732033	9.290167	8.159352
18	6	6.637846	9.988709	8.851200
19	6	6.592843	11.374028	9.051613
20	1	7.401472	11.995465	8.685613
21	6	5.500071	11.933825	9.712271
22	1	5.453935	13.007140	9.873626
23	6	4.470785	11.104280	10.156487
24	1	3.603918	11.497989	10.676409
25	6	4.568194	9.735181	9.906618
26	1	3.790076	9.045423	10.214011

27	7	5.615413 9.196032 9.271516
28	6	8.922022 9.998952 7.625648
29	6	9.208164 9.965190 6.251055
30	1	8.559596 9.406409 5.583877
31	6	10.318842 10.644493 5.748893
32	1	10.527836 10.618325 4.682711
33	6	11.163846 11.349598 6.612458
34	1	12.031773 11.872285 6.219033
35	6	10.892262 11.376669 7.983272
36	1	11.551161 11.913022 8.661006
37	6	9.773334 10.709454 8.487799
38	1	9.572947 10.721660 9.556409
39	8	4.985496 7.819874 6.949501
40	6	3.775228 7.430957 6.727036
41	6	3.016419 7.714855 5.560216
42	1	3.472137 8.300458 4.767724
43	6	1.724928 7.233824 5.443209
44	1	1.132500 7.431137 4.557457
45	6	1.151764 6.471040 6.485409
46	6	1.853604 6.174605 7.653342
47	1	1.385305 5.584137 8.433652
48	6	3.160662 6.654359 7.772645
49	7	4.003426 6.490025 8.844138
50	1	3.619151 5.967250 9.628980
51	7	-0.209053 5.983447 6.341201
52	8	-0.695530 5.323012 7.269837
53	8	-0.820200 6.252348 5.298516
54	8	6.094502 6.725527 10.340692

Table S2 Gas phase optimized coordinates of **5**

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	23	2.513431	3.002623	6.535059
2	8	3.221842	3.567050	4.756937
3	7	4.827752	2.347062	6.707819
4	8	2.417285	1.715747	7.989710
5	7	3.656724	4.506085	7.697903
6	7	1.990997	1.453485	5.285264
7	8	1.182681	3.860153	6.693463
8	6	2.993465	5.575048	8.168125
9	1	1.935983	5.601930	7.927193
10	6	5.638665	3.172280	7.391871
11	6	5.327180	1.231659	6.168532
12	1	4.621466	0.607661	5.627512
13	6	3.612832	6.577703	8.911865
14	1	3.032674	7.421696	9.270584
15	6	4.980649	4.383471	7.947310
16	7	2.199658	1.669623	3.932132

17	6	4.977191	6.462775	9.174529
18	6	7.521809	1.724243	6.989368
19	6	3.148214	3.257837	2.382855
20	6	1.139576	-0.067019	6.978063
21	6	6.671828	0.875281	6.280384
22	1	7.034307	-0.040129	5.823539
23	6	5.667222	5.355056	8.687082
24	1	6.728027	5.251853	8.883015
25	6	1.385528	0.351026	5.625710
26	1	1.056962	-0.299111	4.811973
27	6	7.002174	2.887740	7.554062
28	1	7.653091	3.554918	8.107610
29	6	2.836016	2.812408	3.765029
30	6	1.414204	0.116971	9.398346
31	1	1.824665	0.655398	10.247894
32	6	0.134759	-1.729761	8.464070
33	1	-0.454724	-2.630722	8.606859
34	6	0.383404	-1.245526	7.190374
35	1	-0.010200	-1.770703	6.321909
36	6	1.673720	0.639313	8.106592
37	6	3.838539	4.463965	2.185801
38	1	4.124966	5.048799	3.053652
39	6	0.660638	-1.034878	9.571175
40	1	0.475236	-1.405200	10.577142
41	6	2.764471	2.495556	1.265779
42	1	2.226451	1.566626	1.422620
43	6	3.071273	2.933511	-0.022200
44	1	2.768998	2.337855	-0.880152
45	6	3.762328	4.136372	-0.212983
46	1	3.998724	4.476347	-1.218420
47	6	4.143418	4.899871	0.894550
48	1	4.676866	5.836738	0.752839
49	1	5.500024	7.221827	9.749908
50	1	8.575933	1.486726	7.102871

Table S3 Gas phase optimized coordinates of **5**$^{+}$

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	23	2.737426	2.603657	6.744058
2	8	3.235359	3.287597	5.058530
3	7	4.981939	2.169413	6.981180
4	8	2.679846	1.125599	7.802181
5	7	3.707630	4.395902	7.506510
6	7	1.923561	1.294475	5.327725
7	8	1.352803	3.251543	7.125010

8	6	2.964474 5.477137 7.802938
9	1	1.891800 5.354883 7.704246
10	6	5.781569 3.208822 7.291471
11	6	5.520613 0.976912 6.697941
12	1	4.822819 0.176014 6.474800
13	6	3.530858 6.679990 8.216701
14	1	2.891410 7.525534 8.446440
15	6	5.058662 4.459706 7.612929
16	7	2.121157 1.610134 4.010762
17	6	4.918275 6.760218 8.325469
18	6	7.736187 1.833557 7.008317
19	6	3.177263 3.323289 2.649730
20	6	0.896662 -0.198993 6.931002
21	6	6.898791 0.762517 6.696472
22	1	7.296433 -0.218596 6.459114
23	6	5.688630 5.637463 8.022719
24	1	6.767565 5.681244 8.112674
25	6	1.143642 0.283459 5.604624
26	1	0.673952 -0.216492 4.758140
27	6	7.173348 3.072971 7.314435
28	1	7.813578 3.911353 7.563241
29	6	2.827439 2.707801 3.934920
30	6	1.506169 -0.298713 9.300096
31	1	2.136328 0.042595 10.115040
32	6	-0.286839 -1.703958 8.433109
33	1	-1.053758 -2.452355 8.604949
34	6	-0.086572 -1.189467 7.161653
35	1	-0.692812 -1.533539 6.327566
36	6	1.691295 0.242314 8.022654
37	6	3.940676 4.503001 2.620216
38	1	4.265077 4.952803 3.552813
39	6	0.513492 -1.255655 9.499010
40	1	0.360404 -1.661617 10.495012
41	6	2.748123 2.739315 1.442901
42	1	2.156137 1.830555 1.470158
43	6	3.082837 3.331144 0.227665
44	1	2.749384 2.878661 -0.701852
45	6	3.843393 4.506854 0.202442
46	1	4.100274 4.966524 -0.747963
47	6	4.270314 5.090835 1.399337
48	1	4.858293 6.004157 1.380202
49	1	5.398174 7.680224 8.645899
50	1	8.814861 1.708467 7.017962

Table S4 Gas phase optimized coordinates of **5**$^{-}$ (CSS)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	23	2.547065	3.075242	6.668721
2	8	3.165428	3.697485	4.818231
3	7	4.738811	2.298770	6.756006
4	8	2.323384	1.700604	8.125652
5	7	3.614641	4.460060	7.665583
6	7	2.093524	1.476108	5.354535
7	8	1.165467	3.869702	6.829782
8	6	2.998934	5.588049	8.151310
9	1	1.927435	5.610128	7.991012
10	6	5.602526	3.167064	7.354968
11	6	5.208672	1.133735	6.283952
12	1	4.469248	0.484782	5.822573
13	6	3.660717	6.612934	8.786467
14	1	3.093145	7.469398	9.141169
15	6	4.989343	4.376217	7.852073
16	7	2.325135	1.702741	4.007771
17	6	5.065447	6.535874	8.966969
18	6	7.448731	1.647939	6.966888
19	6	3.179002	3.338609	2.458644
20	6	1.194746	-0.101655	6.980287
21	6	6.543000	0.755056	6.359483
22	1	6.866426	-0.200248	5.956677
23	6	5.707837	5.408977	8.492666
24	1	6.782479	5.309536	8.612173
25	6	1.483996	0.364042	5.650301
26	1	1.176961	-0.267447	4.810944
27	6	6.979518	2.850164	7.464913
28	1	7.665209	3.543644	7.941229
29	6	2.873627	2.895837	3.850585
30	6	1.295997	0.029638	9.420893
31	1	1.623780	0.567019	10.307149
32	6	0.170228	-1.849825	8.363259
33	1	-0.383894	-2.781893	8.443255
34	6	0.480357	-1.315049	7.121109
35	1	0.169225	-1.834767	6.214845
36	6	1.631838	0.605402	8.158530
37	6	3.779917	4.590813	2.254432
38	1	4.005112	5.199847	3.124048
39	6	0.588292	-1.157776	9.519431
40	1	0.353022	-1.560415	10.503955
41	6	2.878697	2.537938	1.342984
42	1	2.412440	1.571989	1.507295

43	6	3.175958	2.981732	0.053659
44	1	2.937970	2.351934	-0.801501
45	6	3.775956	4.232235	-0.143485
46	1	4.006306	4.577038	-1.149653
47	6	4.075297	5.034101	0.962823
48	1	4.540417	6.007514	0.819989
49	1	5.617150	7.331086	9.461335
50	1	8.504418	1.397343	7.047231

Table S5 Gas phase optimized coordinates of **5**$^{-}$ (OSS)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	8	3.165429	3.697486	4.818231
2	7	4.738811	2.298771	6.756006
3	8	2.323384	1.700605	8.125653
4	7	3.614642	4.460060	7.665584
5	7	2.093524	1.476108	5.354536
6	8	1.165467	3.869703	6.829782
7	6	2.998935	5.588049	8.151310
8	1	1.927435	5.610129	7.991013
9	6	5.602526	3.167064	7.354969
10	6	5.208672	1.133735	6.283952
11	1	4.469248	0.484782	5.822574
12	6	3.660717	6.612934	8.786468
13	1	3.093145	7.469399	9.141170
14	6	4.989344	4.376217	7.852074
15	7	2.325135	1.702741	4.007771
16	6	5.065448	6.535874	8.966970
17	6	7.448731	1.647939	6.966888
18	6	3.179003	3.338610	2.458644
19	6	1.194746	-0.101655	6.980288
20	6	6.543000	0.755056	6.359484
21	1	6.866426	-0.200248	5.956677
22	6	5.707838	5.408978	8.492667
23	1	6.782480	5.309536	8.612174
24	6	1.483996	0.364042	5.650302
25	1	1.176961	-0.267447	4.810944
26	6	6.979518	2.850164	7.464914
27	1	7.665210	3.543644	7.941230
28	6	2.873627	2.895838	3.850585
29	6	1.295997	0.029638	9.420894
30	1	1.623780	0.567019	10.307150
31	6	0.170228	-1.849825	8.363260
32	1	-0.383894	-2.781893	8.443255
33	6	0.480357	-1.315049	7.121110

34	1	0.169225	-1.834767	6.214845
35	6	1.631838	0.605402	8.158530
36	6	3.779918	4.590813	2.254432
37	1	4.005112	5.199847	3.124048
38	6	0.588292	-1.157776	9.519431
39	1	0.353022	-1.560415	10.503956
40	6	2.878698	2.537939	1.342984
41	1	2.412440	1.571989	1.507296
42	6	3.175959	2.981732	0.053659
43	1	2.937970	2.351934	-0.801501
44	6	3.775957	4.232235	-0.143485
45	1	4.006307	4.577039	-1.149653
46	6	4.075298	5.034102	0.962823
47	1	4.540418	6.007514	0.819989
48	1	5.617150	7.331087	9.461336
49	1	8.504419	1.397343	7.047231
50	23	2.547066	3.075243	6.668721

Table S6 Gas phase optimized coordinates of **5**$^{-}$ (triplet)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	23	2.525975	3.065917	6.572924
2	8	3.177629	3.684755	4.738454
3	7	4.742297	2.328952	6.709102
4	8	2.276308	1.799064	8.072506
5	7	3.629685	4.531824	7.706342
6	7	2.048594	1.484976	5.300521
7	8	1.160417	3.891420	6.648435
8	6	3.012619	5.619901	8.195693
9	1	1.953521	5.683204	7.962811
10	6	5.588043	3.175176	7.402944
11	6	5.238066	1.202985	6.186622
12	1	4.521827	0.580239	5.654667
13	6	3.648146	6.605005	8.941120
14	1	3.091489	7.463477	9.303535
15	6	4.988526	4.352185	7.947296
16	7	2.261604	1.708192	3.951126
17	6	5.034860	6.441264	9.202064
18	6	7.453749	1.669797	6.986721
19	6	3.148651	3.306733	2.382793
20	6	1.208074	-0.072257	6.974234
21	6	6.570925	0.810661	6.284839
22	1	6.907787	-0.117883	5.834265
23	6	5.687806	5.331765	8.711902
24	1	6.746490	5.198282	8.911502
25	6	1.482948	0.360789	5.629132

26	1	1.203790	-0.306268	4.808834
27	6	6.967533	2.835912	7.538591
28	1	7.639153	3.498552	8.076068
29	6	2.845554	2.884571	3.781510
30	6	1.323177	0.119713	9.409532
31	1	1.644976	0.685293	10.279853
32	6	0.240109	-1.812806	8.404964
33	1	-0.288021	-2.756979	8.511223
34	6	0.528326	-1.301200	7.148464
35	1	0.226560	-1.851059	6.257423
36	6	1.625997	0.675717	8.132642
37	6	3.802427	4.529281	2.164333
38	1	4.068377	5.131875	3.026777
39	6	0.648950	-1.083852	9.540814
40	1	0.434655	-1.470540	10.536109
41	6	2.795516	2.514353	1.277138
42	1	2.289486	1.570769	1.452841
43	6	3.092706	2.938304	-0.018764
44	1	2.813640	2.316202	-0.866927
45	6	3.746847	4.158631	-0.230659
46	1	3.978070	4.487535	-1.241849
47	6	4.099738	4.951412	0.866200
48	1	4.608325	5.900707	0.711220
49	1	5.580097	7.181500	9.784668
50	1	8.506930	1.415217	7.090616

Table S7 Gas phase optimized coordinates of **3** (triplet)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	23	5.868228	7.150366	8.941593
2	8	6.685459	5.680819	7.871272
3	6	7.842289	5.968578	7.370389
4	6	8.602934	4.902134	6.683583
5	6	8.050302	3.613949	6.590921
6	1	7.073639	3.429257	7.025583
7	6	8.752514	2.594556	5.948141
8	1	8.318730	1.600434	5.878788
9	6	10.012268	2.850473	5.396186
10	1	10.559331	2.054795	4.896600
11	6	10.568634	4.131794	5.488844
12	1	11.548401	4.331949	5.062836
13	6	9.869849	5.155201	6.127650
14	1	10.292672	6.150926	6.206485
15	7	8.386074	7.192366	7.427490

16	7	7.540817	8.014152	8.086248
17	6	7.747515	9.299069	8.202456
18	6	6.653165	10.023674	8.878977
19	6	6.629476	11.416563	9.036448
20	1	7.450259	12.015366	8.659957
21	6	5.539475	12.014936	9.667438
22	1	5.511811	13.093559	9.795024
23	6	4.489955	11.219214	10.127244
24	1	3.626959	11.645768	10.627598
25	6	4.570310	9.841061	9.923258
26	1	3.780987	9.171095	10.250883
27	7	5.611281	9.264104	9.316496
28	6	8.939175	9.996867	7.655326
29	6	9.219285	9.952305	6.279886
30	1	8.563628	9.394452	5.618957
31	6	10.334121	10.618014	5.768355
32	1	10.538411	10.582571	4.701473
33	6	11.189530	11.320748	6.623458
34	1	12.060712	11.832604	6.222964
35	6	10.924156	11.358615	7.995245
36	1	11.590940	11.892930	8.666911
37	6	9.801288	10.704907	8.508683
38	1	9.605354	10.725662	9.577988
39	8	4.938986	7.839372	6.986878
40	6	3.759919	7.413497	6.781881
41	6	3.017390	7.660683	5.584166
42	1	3.491860	8.246512	4.803129
43	6	1.745322	7.162344	5.430604
44	1	1.174354	7.340896	4.527248
45	6	1.151069	6.390458	6.469990
46	6	1.805143	6.109797	7.653856
47	1	1.318254	5.515161	8.419145
48	6	3.120632	6.613176	7.847973
49	7	3.877608	6.437921	8.928396
50	1	3.475669	5.850250	9.655529
51	7	-0.201464	5.878501	6.273588
52	8	-0.711739	5.215105	7.183804
53	8	-0.769119	6.137036	5.205044
54	8	6.216980	6.791060	10.446239