Redox bifunctionality in Pt(II) dithiolene complex of a tetrathiafulvalene diphosphine ligand

Kyong-Soon Shin, YounJung Jung, Su-Kyung Lee, Marc Fourmigué, Frédéric Barrière, Jean-François Bergamini and Dong-Youn Noh

Supplementary Information

Atomic coordinates of the optimized structure of (**P2**)Pt(dmit) (B3LYP/LanL2DZ)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	78	0	-1.663365	-0.000796	0.031578
2	15	0	0.056329	-1.642688	0.126084
3	15	0	0.057271	1.642879	0.119308
4	16	0	6.570997	-1.539109	0.156399
5	16	0	6.577175	1.527002	0.129539
6	16	0	3.237435	-1.535743	0.657460
7	16	0	3.238588	1.540494	0.635893
8	16	0	-3.370435	-1.715679	-0.055493
9	16	0	-3.378429	1.705724	-0.072400
10	16	0	-6.483657	-1.523875	-0.292544
11	16	0	-6.491564	1.498003	-0.297540
12	16	0	-9.181160	-0.020222	-0.486873
13	6	0	9.264816	-1.630102	-0.675423
14	1	0	10.177185	-1.081011	-0.924984
15	1	0	9.010147	-2.269121	-1.531164
16	1	0	9.490001	-2.287104	0.175413
17	6	0	9.271742	1.591770	-0.703314
18	1	0	10.181916	1.034247	-0.941976
19	1	0	9.499110	2.263234	0.135544
20	1	0	9.020483	2.216123	-1.570801
21	6	0	8.133005	-0.688953	-0.345936
22	6	0	8.135800	0.661517	-0.357606
23	6	0	5.578815	-0.002797	0.283675
24	6	0	4.245130	0.000881	0.483978
25	6	0	1.646106	-0.676438	0.378359
26	6	0	1.648126	0.677659	0.358842
27	6	0	-4.858351	-0.686009	-0.178117
28	6	0	-4.862189	0.668633	-0.180254
29	6	0	-7.499537	-0.015721	-0.366482
30	6	0	0.318652	-2.637903	-1.437307
31	6	0	1.244803	-3.702040	-1.497681
32	1	0	1.818028	-3.990246	-0.620424
33	6	0	1.425121	-4.402706	-2.702709
34	1	0	2.138599	-5.221521	-2.747808
35	6	0	0.682553	-4.046512	-3.846766
36	1	0	0.821914	-4.593016	-4.776436
37	6	0	-0.243780	-2.989022	-3.782820
38	1	0	-0.826800	-2.717342	-4.658718
39	6	0	-0.428098	-2.282585	-2.579287
40	1	0	-1.156192	-1.477883	-2.520434
41	6	0	0.026914	-2.863410	1.541875
42	6	0	-0.583989	-4.122816	1.368435
43	1	0	-0.985460	-4.414745	0.401835
44	6	0	-0.690661	-5.004526	2.458903

45	1	0	-1.167841	-5.971277	2.321824
46	6	0	-0.193870	-4.632818	3.722360
47	1	0	-0.279659	-5.315369	4.564185
48	6	0	0.406570	-3.370695	3.895586
49	1	0	0.786111	-3.075719	4.870480
50	6	0	0.512112	-2.483014	2.810779
51	1	0	0.966756	-1.507108	2.959968
52	6	0	0.004278	2.857016	1.543389
53	6	0	-0.880242	2.600245	2.610445
54	1	0	-1.545575	1.742200	2.569303
55	6	0	-0.919466	3.477574	3.710487
56	1	0	-1.609311	3.283060	4.527297
57	6	0	-0.079566	4.606365	3.745122
58	1	0	-0.113885	5.284539	4.594372
59	6	0	0.799257	4.864046	2.673819
60	1	0	1.444535	5.738496	2.694826
61	6	0	0.842470	3.992824	1.571807
62	1	0	1.512864	4.207392	0.743045
63	6	0	0.343484	2.663437	-1.422937
64	6	0	-0.449492	3.811668	-1.635618
65	1	0	-1.178117	4.126717	-0.893183
66	6	0	-0.312002	4.546474	-2.826071
67	1	0	-0.929375	5.426213	-2.987094
68	6	0	0.610848	4.138335	-3.808573
69	1	0	0.713794	4.706991	-4.729477
70	6	0	1.394889	2.988433	-3.597705
71	1	0	2.106501	2.666119	-4.353602
72	6	0	1.260650	2.247717	-2.409196
73	1	0	1.870213	1.360677	-2.261369

Orbitals energies for the optimized structure of (**P2**)Pt(dmit) (B3LYP/LanL2DZ)

Alpha occ. eigenvalues -- -10.27708 -10.27542 -10.27457 -10.27383 -10.27163
Alpha occ. eigenvalues -- -10.25949 -10.25875 -10.23521 -10.23503 -10.23485
Alpha occ. eigenvalues -- -10.23467 -10.22910 -10.22839 -10.22658 -10.22601
Alpha occ. eigenvalues -- -10.22379 -10.22353 -10.22283 -10.22227 -10.22212
Alpha occ. eigenvalues -- -10.22157 -10.22111 -10.22088 -10.22070 -10.22052
Alpha occ. eigenvalues -- -10.22045 -10.22040 -10.21985 -10.21974 -10.21885
Alpha occ. eigenvalues -- -10.21882 -10.21825 -10.21796 -10.21789 -10.21762
Alpha occ. eigenvalues -- -3.94268 -2.17165 -2.16903 -2.12796 -0.91787
Alpha occ. eigenvalues -- -0.89727 -0.88442 -0.88240 -0.87743 -0.87704
Alpha occ. eigenvalues -- -0.87503 -0.83631 -0.80860 -0.79968 -0.79870
Alpha occ. eigenvalues -- -0.78994 -0.78197 -0.77391 -0.77200 -0.77170
Alpha occ. eigenvalues -- -0.77131 -0.76981 -0.76867 -0.76845 -0.76258
Alpha occ. eigenvalues -- -0.73361 -0.71774 -0.71035 -0.69799 -0.69130
Alpha occ. eigenvalues -- -0.68190 -0.66229 -0.63448 -0.63283 -0.63159
Alpha occ. eigenvalues -- -0.63155 -0.62999 -0.62241 -0.62209 -0.60709
Alpha occ. eigenvalues -- -0.59846 -0.56246 -0.55175 -0.54330 -0.54205
Alpha occ. eigenvalues -- -0.54031 -0.53499 -0.52414 -0.51823 -0.50404
Alpha occ. eigenvalues -- -0.50096 -0.48835 -0.48191 -0.48085 -0.47898
Alpha occ. eigenvalues -- -0.47654 -0.47404 -0.47306 -0.46900 -0.46852
Alpha occ. eigenvalues -- -0.46379 -0.45943 -0.45051 -0.44810 -0.44723
Alpha occ. eigenvalues -- -0.44616 -0.44372 -0.44144 -0.44141 -0.43701
Alpha occ. eigenvalues -- -0.43631 -0.43033 -0.42516 -0.41987 -0.41350
Alpha occ. eigenvalues -- -0.41044 -0.40320 -0.39317 -0.39222 -0.39030
Alpha occ. eigenvalues -- -0.38781 -0.38719 -0.38304 -0.38205 -0.38104
Alpha occ. eigenvalues -- -0.37838 -0.37308 -0.37201 -0.37117 -0.36947
Alpha occ. eigenvalues -- -0.36756 -0.36408 -0.36242 -0.35974 -0.35825
Alpha occ. eigenvalues -- -0.35743 -0.35555 -0.33780 -0.32052 -0.31876

Alpha occ. eigenvalues -- -0.31535 -0.30944 -0.30833 -0.30043 -0.29090
Alpha occ. eigenvalues -- -0.28788 -0.28525 -0.28374 -0.28189 -0.28106
Alpha occ. eigenvalues -- -0.27780 -0.27651 -0.27352 -0.27340 -0.27221
Alpha occ. eigenvalues -- -0.26252 -0.26081 -0.25677 -0.24749 -0.22140
Alpha occ. eigenvalues -- -0.21488 -0.20575 -0.20452 -0.17344
Alpha virt. eigenvalues -- -0.07462 -0.07189 -0.06363 -0.05162 -0.04779
Alpha virt. eigenvalues -- -0.04554 -0.04136 -0.03748 -0.03515 -0.03493
Alpha virt. eigenvalues -- -0.03011 -0.02439 -0.02111 -0.01476 -0.01078
Alpha virt. eigenvalues -- -0.00788 -0.00375 0.00020 0.01049 0.01831
Alpha virt. eigenvalues -- 0.03302 0.03860 0.03987 0.04132 0.04314
Alpha virt. eigenvalues -- 0.05501 0.05849 0.06503 0.06624 0.07004
Alpha virt. eigenvalues -- 0.07695 0.07740 0.08597 0.09238 0.09572
Alpha virt. eigenvalues -- 0.09872 0.11062 0.11467 0.11532 0.11814
Alpha virt. eigenvalues -- 0.12177 0.12725 0.13152 0.13471 0.13762
Alpha virt. eigenvalues -- 0.13964 0.14383 0.14429 0.14674 0.14697
Alpha virt. eigenvalues -- 0.14830 0.15116 0.15186 0.15358 0.15499
Alpha virt. eigenvalues -- 0.15717 0.16191 0.16265 0.16596 0.17012
Alpha virt. eigenvalues -- 0.17120 0.17335 0.17522 0.17653 0.18027
Alpha virt. eigenvalues -- 0.18733 0.19564 0.19594 0.20619 0.21490
Alpha virt. eigenvalues -- 0.21901 0.22009 0.22393 0.22769 0.23257
Alpha virt. eigenvalues -- 0.23682 0.23868 0.24033 0.24370 0.24447
Alpha virt. eigenvalues -- 0.24718 0.24818 0.25566 0.26025 0.26479
Alpha virt. eigenvalues -- 0.26617 0.26982 0.27190 0.27337 0.27815
Alpha virt. eigenvalues -- 0.27951 0.28628 0.28833 0.29124 0.29738
Alpha virt. eigenvalues -- 0.30006 0.30371 0.30758 0.30827 0.31172
Alpha virt. eigenvalues -- 0.31355 0.31491 0.32144 0.32638 0.32930
Alpha virt. eigenvalues -- 0.33380 0.33676 0.33837 0.34578 0.34787
Alpha virt. eigenvalues -- 0.34927 0.35330 0.35463 0.35606 0.35825
Alpha virt. eigenvalues -- 0.36043 0.36453 0.36656 0.37136 0.37193
Alpha virt. eigenvalues -- 0.37679 0.38103 0.38299 0.38433 0.38565
Alpha virt. eigenvalues -- 0.38627 0.38668 0.38778 0.39238 0.39380
Alpha virt. eigenvalues -- 0.40071 0.40180 0.40363 0.40654 0.41184
Alpha virt. eigenvalues -- 0.41239 0.41353 0.41587 0.42090 0.42145
Alpha virt. eigenvalues -- 0.42333 0.42371 0.42467 0.42595 0.42895
Alpha virt. eigenvalues -- 0.43571 0.43646 0.43914 0.44414 0.44551
Alpha virt. eigenvalues -- 0.44779 0.44890 0.45247 0.45414 0.45897
Alpha virt. eigenvalues -- 0.46205 0.46418 0.46573 0.46689 0.46996
Alpha virt. eigenvalues -- 0.47244 0.47686 0.48124 0.48201 0.48477
Alpha virt. eigenvalues -- 0.49137 0.49366 0.49520 0.49725 0.50192
Alpha virt. eigenvalues -- 0.50603 0.51433 0.51738 0.52083 0.52257
Alpha virt. eigenvalues -- 0.52535 0.52686 0.52933 0.53598 0.54189
Alpha virt. eigenvalues -- 0.54252 0.54682 0.55367 0.55945 0.56102
Alpha virt. eigenvalues -- 0.56589 0.57045 0.57122 0.57656 0.58110
Alpha virt. eigenvalues -- 0.58294 0.58544 0.58655 0.59690 0.59975
Alpha virt. eigenvalues -- 0.60099 0.60518 0.61077 0.61301 0.61905
Alpha virt. eigenvalues -- 0.62582 0.63121 0.64078 0.64098 0.64418
Alpha virt. eigenvalues -- 0.65047 0.65345 0.65693 0.66355 0.66482
Alpha virt. eigenvalues -- 0.66735 0.67092 0.67553 0.67710 0.67855
Alpha virt. eigenvalues -- 0.68702 0.69202 0.70007 0.70683 0.71044
Alpha virt. eigenvalues -- 0.71853 0.72501 0.72827 0.73047 0.73804
Alpha virt. eigenvalues -- 0.74354 0.74794 0.75470 0.75835 0.75945
Alpha virt. eigenvalues -- 0.76275 0.76990 0.77670 0.78876 0.80715
Alpha virt. eigenvalues -- 0.81068 0.82465 0.84340 0.85755 0.86381
Alpha virt. eigenvalues -- 0.87873 0.89170 0.91442 0.92019 0.93378
Alpha virt. eigenvalues -- 0.94181 0.94303 0.96954 0.98719 0.99449
Alpha virt. eigenvalues -- 1.01136 1.01834 1.02427 1.05083 1.05357
Alpha virt. eigenvalues -- 1.05744 1.05901 1.05952 1.06091 1.06234
Alpha virt. eigenvalues -- 1.06547 1.07199 1.08888 1.10485 1.10917
Alpha virt. eigenvalues -- 1.11421 1.12031 1.12819 1.12900 1.14650
Alpha virt. eigenvalues -- 1.15580 1.15684 1.15883 1.15950 1.16541

Alpha virt. eigenvalues -- 1.20948 1.21092 1.21926 1.22370 1.22950
Alpha virt. eigenvalues -- 1.23568 1.24280 1.24923 1.25620 1.26753
Alpha virt. eigenvalues -- 1.28096 1.28465 1.28916 1.34086 1.35727
Alpha virt. eigenvalues -- 1.36616 1.38293 1.39076 1.40113 1.40402
Alpha virt. eigenvalues -- 1.41315 1.43910 1.45832 1.46744 1.52040
Alpha virt. eigenvalues -- 1.53469 1.54877 1.64905 1.65722 1.68695
Alpha virt. eigenvalues -- 1.69016 6.85901 9.38571 11.19113 12.56916
Alpha virt. eigenvalues -- 12.69467 13.91879 14.33089 14.49895 16.33915
Alpha virt. eigenvalues -- 17.31650 19.40343 19.64519