A Structure-Property Study Toward π -Extended Phosphole Chromophores with Ambipolar Redox Properties

Supporting Information

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Figure S1. Frontier Orbitals for **3** (B3LYP/6-31+G(d) level of theory).

Figure S2. Frontier Orbitals for **4** (B3LYP/6-31+G(d) level of theory).

Figure S3. Frontier Orbitals for **5** (B3LYP/6-31+G(d) level of theory).

Figure S4. Frontier Orbitals for **6** (B3LYP/6-31+G(d) level of theory; PCM, CH₂Cl₂).

Figure S5. Frontier Orbitals for **3-ox** (B3LYP/6-31+G(d) level of theory; PCM, CH₂Cl₂).

Figure S6. Frontier Orbitals for **4-ox** (B3LYP/6-31+G(d) level of theory; PCM, CH₂Cl₂).

Figure S7. Frontier Orbitals for **5-ox** (B3LYP/6-31+G(d) level of theory; PCM, CH₂Cl₂).

Figure S8. Frontier Orbitals for **5-ox2** (B3LYP/6-31+G(d) level of theory; PCM, CH₂Cl₂).

Figure S9. Frontier Orbitals for **3-red** (B3LYP/6-31+G(d) level of theory; PCM, CH₂Cl₂).

Figure S10. Frontier Orbitals for **4-red** (B3LYP/6-31+G(d) level of theory; PCM, CH₂Cl₂).

Figure S11. Frontier Orbitals for **5-red** (B3LYP/6-31+G(d) level of theory; PCM, CH₂Cl₂).

Table S1. Cartesian coordinates for minimized structure of compound **3**.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	15	0	0.000077	1.560695	-1.173516
2	6	0	-1.304254	0.371059	-0.677799
3	6	0	-0.724506	-0.789900	-0.192950
4	6	0	0.724919	-0.789691	-0.192751
5	6	0	1.304565	0.371475	-0.677335
6	6	0	-2.718373	0.331508	-0.664119
7	6	0	-3.226514	-0.855434	-0.172053
8	16	0	-1.915280	-1.952840	0.277546
9	16	0	1.915927	-1.952611	0.277448
10	6	0	3.226985	-0.854937	-0.171864
11	6	0	2.718653	0.332015	-0.663815
12	6	0	-4.629307	-1.252198	-0.016089
13	6	0	4.629869	-1.251488	-0.015903
14	6	0	-5.616053	-0.698624	-0.854278
15	6	0	-6.955377	-1.048591	-0.705368
16	6	0	-7.340415	-1.970152	0.271198
17	6	0	-6.370894	-2.535562	1.101507
18	6	0	-5.031589	-2.178104	0.964006
19	6	0	5.032189	-2.178011	0.963563
20	6	0	6.371564	-2.535318	1.101064
21	6	0	7.341101	-1.969033	0.271507
22	6	0	6.956005	-1.046891	-0.704474
23	6	0	5.616736	-0.697077	-0.853430
24	8	0	0.000489	2.075585	-2.582043
25	6	0	-0.000648	2.906339	0.061660
26	6	0	-0.001076	2.668763	1.443963
27	6	0	-0.001578	3.739754	2.335392
28	6	0	-0.001781	5.052071	1.852892
29	6	0	-0.001373	5.291979	0.478374
30	6	0	-0.000830	4.221640	-0.418581
31	1	0	-3.352259	1.151846	-0.981060
32	1	0	3.352343	1.152607	-0.980573
33	1	0	-5.324091	-0.008408	-1.640007
34	1	0	-7.699469	-0.609917	-1.364616
35	1	0	-8.385081	-2.247016	0.381460
36	1	0	-6.658215	-3.251081	1.867198
37	1	0	-4.292709	-2.604544	1.637457
38	1	0	4.293252	-2.605112	1.636608
39	1	0	6.658836	-3.251269	1.866349
40	1	0	8.385801	-2.245784	0.381731
41	1	0	7.700292	-0.607476	-1.363233
42	1	0	5.324896	-0.006416	-1.638847
43	1	0	-0.000953	1.650367	1.823666
44	1	0	-0.001891	3.552779	3.405773
45	1	0	-0.002232	5.885634	2.550301
46	1	0	-0.001545	6.311553	0.102382
47	1	0	-0.000496	4.390803	-1.491309

Table S2. Cartesian coordinates for minimized structure of compound **4**.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	15	0	-3.373315	0.473506	1.133977
2	6	0	-1.698185	-0.109764	0.668030
3	6	0	-1.780827	-1.361435	0.082364
4	6	0	-3.126892	-1.895487	-0.019585
5	6	0	-4.118040	-1.069543	0.482919
6	6	0	-0.371965	0.376168	0.752701
7	6	0	0.563812	-0.499319	0.235380
8	16	0	-0.223068	-1.964951	-0.364365
9	16	0	-3.776163	-3.379709	-0.630867
10	6	0	-5.393471	-2.877894	-0.204310
11	6	0	-5.416918	-1.635844	0.375921
12	6	0	2.017272	-0.339176	0.159298
13	6	0	2.690876	0.487701	1.078434
14	6	0	4.066870	0.665160	1.007695
15	6	0	4.839951	0.017399	0.027874
16	6	0	4.166830	-0.815608	-0.881962
17	6	0	2.788798	-0.987901	-0.821866
18	6	0	6.309951	0.203686	-0.040076
19	6	0	7.157955	-0.860892	-0.391443
20	6	0	8.539267	-0.686299	-0.455202
21	6	0	9.105207	0.557230	-0.167849
22	6	0	8.276153	1.624439	0.182763
23	6	0	6.894768	1.449740	0.245463
24	8	0	-3.629671	0.843601	2.564465
25	6	0	-3.814373	1.815823	-0.023969
26	6	0	-3.650106	1.706585	-1.412661
27	6	0	-4.004120	2.768818	-2.242241
28	6	0	-4.523448	3.944336	-1.691501
29	6	0	-4.688283	4.056366	-0.310560
30	6	0	-4.334717	2.994388	0.524629
31	1	0	-0.104464	1.345586	1.157688
32	1	0	-6.224829	-3.539770	-0.406476
33	1	0	-6.327517	-1.155164	0.715558
34	1	0	2.131903	0.968975	1.875333
35	1	0	4.558125	1.286292	1.751206
36	1	0	4.727098	-1.307495	-1.671980
37	1	0	2.300643	-1.610940	-1.566871
38	1	0	6.731502	-1.840458	-0.588813
39	1	0	9.175561	-1.526499	-0.720716
40	1	0	10.182090	0.693474	-0.216772
41	1	0	8.704994	2.599239	0.399958
42	1	0	6.258078	2.294874	0.492159
43	1	0	-3.245878	0.794999	-1.845222
44	1	0	-3.875121	2.681509	-3.317671
45	1	0	-4.798302	4.771359	-2.340785
46	1	0	-5.091623	4.969591	0.118719
47	1	0	-4.455657	3.065532	1.601532

Table S3. Cartesian coordinates for minimized structure of compound **5**.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	15	0	0.000450	2.358359	-1.166522
2	6	0	-1.303326	1.139911	-0.745424
3	6	0	-0.722822	-0.048792	-0.332926
4	6	0	0.725888	-0.046496	-0.327892
5	6	0	1.305489	1.144276	-0.735701
6	6	0	-2.716754	1.098047	-0.737774
7	6	0	-3.225415	-0.118696	-0.322624
8	16	0	-1.913034	-1.240640	0.060720
9	16	0	1.917220	-1.235815	0.070381
10	6	0	3.228250	-0.118584	-0.330127
11	6	0	2.718989	1.100853	-0.736426
12	6	0	-4.625575	-0.525845	-0.195775
13	6	0	4.628624	-0.525548	-0.204827
14	6	0	-5.623802	0.106846	-0.961377
15	6	0	-6.959099	-0.255919	-0.838546
16	6	0	-7.363824	-1.275544	0.041269
17	6	0	-6.364911	-1.912484	0.797076
18	6	0	-5.028980	-1.545251	0.685945
19	6	0	5.026531	-1.871219	-0.305075
20	6	0	6.362657	-2.235680	-0.186507
21	6	0	7.366461	-1.276119	0.029263
22	6	0	6.967052	0.068628	0.127068
23	6	0	5.631864	0.436543	0.019856
24	6	0	-8.789601	-1.665481	0.163645
25	6	0	8.792059	-1.666339	0.152833
26	6	0	-9.158082	-3.007865	0.358986
27	6	0	-10.498057	-3.374208	0.473148
28	6	0	-11.501164	-2.406383	0.393829
29	6	0	-11.151144	-1.068848	0.199721
30	6	0	-9.811026	-0.702822	0.086382
31	6	0	9.812435	-0.850789	-0.366567
32	6	0	11.152287	-1.216402	-0.249001
33	6	0	11.503190	-2.407248	0.389734
34	6	0	10.501221	-3.228511	0.909973
35	6	0	9.161562	-2.861919	0.793365
36	8	0	0.003400	2.956127	-2.541843
37	6	0	-0.004994	3.628752	0.146267
38	6	0	-0.009303	3.310836	1.512319
39	6	0	-0.013159	4.327703	2.465131
40	6	0	-0.012719	5.666080	2.060653
41	6	0	-0.008407	5.985962	0.702560
42	6	0	-0.004538	4.970078	-0.255688
43	1	0	-3.350365	1.936045	-1.005078
44	1	0	3.351646	1.920634	-1.057275
45	1	0	-5.343843	0.868486	-1.682993
46	1	0	-7.698812	0.233068	-1.465997
47	1	0	-6.643279	-2.683093	1.510209
48	1	0	-4.292044	-2.036894	1.315686

49	1	0	4.285128	-2.638870	-0.510599
50	1	0	6.637422	-3.280324	-0.300460
51	1	0	7.710853	0.833672	0.330342
52	1	0	5.355576	1.479566	0.142561
53	1	0	-8.388049	-3.773526	0.393265
54	1	0	-10.759151	-4.419656	0.615028
55	1	0	-12.545865	-2.691805	0.482175
56	1	0	-11.923150	-0.305777	0.144915
57	1	0	-9.549481	0.344448	-0.036994
58	1	0	9.550297	0.063886	-0.891017
59	1	0	11.923251	-0.573722	-0.665927
60	1	0	12.547652	-2.692623	0.481006
61	1	0	10.763097	-4.153588	1.416859
62	1	0	8.392831	-3.495050	1.227690
63	1	0	-0.009746	2.272016	1.832308
64	1	0	-0.016727	4.077852	3.522681
65	1	0	-0.015895	6.457263	2.805785
66	1	0	-0.008196	7.025774	0.386799
67	1	0	-0.001237	5.201967	-1.316597

Table S4. Cartesian coordinates for minimized structure of compound **6**.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	15	0	-0.074675	-0.942890	2.162865
2	6	0	-1.393987	-0.876705	0.935579
3	6	0	-0.806831	-0.840288	-0.324386
4	6	0	0.638955	-0.889823	-0.327862
5	6	0	1.230732	-0.974363	0.929369
6	6	0	-2.809156	-0.866104	0.910583
7	6	0	-3.316503	-0.809767	-0.375531
8	16	0	-2.004439	-0.763596	-1.561974
9	16	0	1.831919	-0.858045	-1.570048
10	6	0	3.147505	-0.937296	-0.390831
11	6	0	2.646722	-0.996586	0.897019
12	6	0	-4.714537	-0.784663	-0.805108
13	6	0	4.542815	-0.943738	-0.829632
14	6	0	-5.719511	-0.321200	0.065544
15	6	0	-7.051767	-0.306049	-0.325265
16	6	0	-7.445622	-0.741571	-1.604138
17	6	0	-6.437802	-1.196923	-2.473015
18	6	0	-5.104524	-1.221979	-2.084099
19	6	0	4.942394	-0.328583	-2.029859
20	6	0	6.272791	-0.340403	-2.428999
21	6	0	7.265811	-0.957513	-1.647494
22	6	0	6.861438	-1.570342	-0.447175
23	6	0	5.531405	-1.570605	-0.047989
24	6	0	-8.867908	-0.719606	-2.019653
25	6	0	8.685496	-0.963899	-2.073623
26	6	0	-9.227523	-0.403128	-3.341119
27	6	0	-10.565128	-0.382305	-3.731168
28	6	0	-11.570400	-0.680559	-2.809244
29	6	0	-11.227901	-0.998008	-1.493440
30	6	0	-9.890686	-1.015703	-1.101934
31	6	0	9.504809	-2.080577	-1.833541
32	6	0	10.838897	-2.086759	-2.235990
33	6	0	11.382555	-0.975557	-2.883298
34	6	0	10.581042	0.141413	-3.126824
35	6	0	9.245916	0.146888	-2.727855
36	6	0	-0.102292	-2.418509	3.207775
37	6	0	0.673667	-3.537488	2.863845
38	6	0	0.626966	-4.680840	3.660318
39	6	0	-0.187442	-4.713706	4.793742
40	6	0	-0.960786	-3.601886	5.137435
41	6	0	-0.921710	-2.453628	4.349627
42	1	0	-3.444073	-0.938541	1.785654
43	1	0	3.286177	-1.022763	1.771324
44	1	0	-5.451211	0.059986	1.046873
45	1	0	-7.799398	0.084504	0.358469
46	1	0	-6.708294	-1.571307	-3.455418
47	1	0	-4.363230	-1.619511	-2.772691
48	1	0	4.209186	0.179284	-2.651204
49	1	0	6.546268	0.123505	-3.371556
50	1	0	7.604998	-2.042354	0.187751

51	1	0	5.252406	-2.075208	0.872669
52	1	0	-8.456134	-0.142337	-4.060323
53	1	0	-10.822870	-0.125360	-4.754785
54	1	0	-12.612906	-0.666025	-3.113961
55	1	0	-12.003016	-1.240754	-0.771912
56	1	0	-9.634649	-1.292229	-0.082865
57	1	0	9.085449	-2.961893	-1.356244
58	1	0	11.452412	-2.964127	-2.051147
59	1	0	12.422809	-0.980171	-3.195985
60	1	0	10.997896	1.013936	-3.622076
61	1	0	8.640000	1.032466	-2.898214
62	1	0	1.309190	-3.514086	1.984301
63	1	0	1.228847	-5.544554	3.394966
64	1	0	-0.219577	-5.605895	5.411898
65	1	0	-1.592575	-3.627608	6.019948
66	1	0	-1.527877	-1.596780	4.630237
67	6	0	-0.032323	0.572308	3.230765
68	1	0	-0.965657	0.570869	3.806249
69	1	0	0.785944	0.409646	3.941283
70	6	0	0.147215	1.854897	2.453358
71	6	0	-0.965733	2.516570	1.912122
72	6	0	1.421458	2.377677	2.273739
73	6	0	-0.780004	3.692940	1.184117
74	1	0	-1.960054	2.109203	2.049535
75	6	0	1.620815	3.570576	1.556839
76	1	0	2.299883	1.895947	2.691184
77	6	0	0.515161	4.241409	1.003072
78	8	0	2.922438	3.930772	1.428936
79	8	0	0.703212	5.339830	0.207780
80	8	0	-1.785770	4.382194	0.581298
81	6	0	3.320038	5.289173	1.212270
82	1	0	4.393952	5.301256	1.409656
83	1	0	3.122775	5.608464	0.188080
84	1	0	2.818012	5.964762	1.914120
85	6	0	0.156305	6.585916	0.666925
86	1	0	0.454002	7.329133	-0.074974
87	1	0	-0.932743	6.541962	0.730400
88	1	0	0.575536	6.857194	1.644212
89	6	0	-3.110154	3.871071	0.660895
90	1	0	-3.728043	4.560968	0.084799
91	1	0	-3.177878	2.867755	0.221690
92	1	0	-3.468211	3.842824	1.698117

Table S5. Cartesian coordinates for minimized structure of compound **3-ox**.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	15	0	-0.000001	1.592541	-1.123858
2	6	0	-1.295552	0.385462	-0.598946
3	6	0	-0.705660	-0.806018	-0.112813
4	6	0	0.705652	-0.806021	-0.112818
5	6	0	1.295548	0.385455	-0.598957
6	6	0	-2.681396	0.333536	-0.617293
7	6	0	-3.201856	-0.885342	-0.140597
8	16	0	-1.896593	-1.984509	0.327102
9	16	0	1.896582	-1.984519	0.327089
10	6	0	3.201848	-0.885352	-0.140602
11	6	0	2.681391	0.333523	-0.617307
12	6	0	-4.589075	-1.273882	-0.017406
13	6	0	4.589066	-1.273894	-0.017409
14	6	0	-5.602633	-0.488247	-0.619284
15	6	0	-6.936797	-0.852936	-0.508307
16	6	0	-7.295525	-2.003760	0.202606
17	6	0	-6.307177	-2.792735	0.802883
18	6	0	-4.971094	-2.435417	0.695078
19	6	0	4.971085	-2.435414	0.695101
20	6	0	6.307167	-2.792733	0.802907
21	6	0	7.295515	-2.003775	0.202607
22	6	0	6.936787	-0.852966	-0.508331
23	6	0	5.602622	-0.488276	-0.619310
24	8	0	-0.000009	1.987652	-2.564027
25	6	0	0.000010	2.969139	0.048524
26	6	0	0.000019	2.780423	1.440203
27	6	0	0.000028	3.885813	2.287210
28	6	0	0.000028	5.177370	1.750400
29	6	0	0.000020	5.366239	0.367457
30	6	0	0.000011	4.264403	-0.489089
31	1	0	-3.312881	1.149254	-0.946903
32	1	0	3.312879	1.149239	-0.946917
33	1	0	-5.340104	0.394548	-1.191991
34	1	0	-7.701249	-0.244215	-0.980824
35	1	0	-8.340603	-2.285632	0.287646
36	1	0	-6.583592	-3.683673	1.357808
37	1	0	-4.218515	-3.049700	1.181751
38	1	0	4.218507	-3.049682	1.181792
39	1	0	6.583583	-3.683659	1.357852
40	1	0	8.340592	-2.285647	0.287648
41	1	0	7.701237	-0.244259	-0.980867
42	1	0	5.340092	0.394505	-1.192038
43	1	0	0.000018	1.779160	1.864334
44	1	0	0.000034	3.743127	3.363763
45	1	0	0.000036	6.037107	2.414193
46	1	0	0.000021	6.370092	-0.046495
47	1	0	0.000005	4.396968	-1.566770

Table S6. Cartesian coordinates for minimized structure of compound **4-ox**.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	15	0	-3.356230	0.460275	1.114326
2	6	0	-1.674701	-0.096140	0.580480
3	6	0	-1.740687	-1.382682	-0.005698
4	6	0	-3.048616	-1.929822	-0.083216
5	6	0	-4.059892	-1.105125	0.442799
6	6	0	-0.380791	0.385196	0.677094
7	6	0	0.591449	-0.502916	0.162995
8	16	0	-0.181372	-1.979451	-0.449174
9	16	0	-3.679787	-3.437862	-0.668209
10	6	0	-5.281681	-2.955860	-0.203076
11	6	0	-5.331450	-1.699246	0.373326
12	6	0	2.010588	-0.325097	0.107021
13	6	0	2.617022	0.854690	0.621750
14	6	0	3.982387	1.033276	0.571570
15	6	0	4.840125	0.051434	0.014443
16	6	0	4.234977	-1.125539	-0.495291
17	6	0	2.869993	-1.307929	-0.454898
18	6	0	6.293017	0.244094	-0.032767
19	6	0	7.171540	-0.862066	-0.014633
20	6	0	8.548233	-0.677265	-0.051675
21	6	0	9.081840	0.613584	-0.123190
22	6	0	8.227399	1.720571	-0.149541
23	6	0	6.850587	1.540454	-0.097339
24	8	0	-3.529272	0.715495	2.575697
25	6	0	-3.872836	1.817601	0.035926
26	6	0	-3.805714	1.743271	-1.364879
27	6	0	-4.222366	2.826170	-2.135092
28	6	0	-4.706795	3.981205	-1.512655
29	6	0	-4.775806	4.055657	-0.120549
30	6	0	-4.359573	2.975690	0.659238
31	1	0	-0.126440	1.345710	1.107960
32	1	0	-6.108108	-3.633143	-0.379384
33	1	0	-6.250325	-1.247204	0.727998
34	1	0	2.006043	1.626029	1.076950
35	1	0	4.408398	1.931695	1.004251
36	1	0	4.852329	-1.886190	-0.960111
37	1	0	2.453346	-2.219379	-0.874151
38	1	0	6.774343	-1.868429	0.071796
39	1	0	9.208613	-1.538423	-0.018775
40	1	0	10.157798	0.756085	-0.157879
41	1	0	8.637485	2.723618	-0.216551
42	1	0	6.200535	2.408028	-0.149351
43	1	0	-3.435052	0.846631	-1.855790
44	1	0	-4.173176	2.770758	-3.218555
45	1	0	-5.032917	4.822947	-2.116730
46	1	0	-5.155125	4.952390	0.360173
47	1	0	-4.411096	3.018546	1.742948

Table S7. Cartesian coordinates for minimized structure of compound **5-ox**.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	15	0	0.000450	2.358359	-1.166522
2	6	0	-1.303326	1.139911	-0.745424
3	6	0	-0.722822	-0.048792	-0.332926
4	6	0	0.725888	-0.046496	-0.327892
5	6	0	1.305489	1.144276	-0.735701
6	6	0	-2.716754	1.098047	-0.737774
7	6	0	-3.225416	-0.118696	-0.322624
8	16	0	-1.913035	-1.240640	0.060720
9	16	0	1.917221	-1.235815	0.070381
10	6	0	3.228250	-0.118584	-0.330127
11	6	0	2.718990	1.100854	-0.736426
12	6	0	-4.625575	-0.525845	-0.195775
13	6	0	4.628625	-0.525548	-0.204828
14	6	0	-5.623802	0.106846	-0.961377
15	6	0	-6.959099	-0.255919	-0.838546
16	6	0	-7.363824	-1.275544	0.041269
17	6	0	-6.364911	-1.912484	0.797076
18	6	0	-5.028980	-1.545251	0.685945
19	6	0	5.026532	-1.871219	-0.305075
20	6	0	6.362658	-2.235681	-0.186507
21	6	0	7.366462	-1.276119	0.029263
22	6	0	6.967052	0.068628	0.127068
23	6	0	5.631865	0.436543	0.019856
24	6	0	-8.789602	-1.665481	0.163645
25	6	0	8.792060	-1.666339	0.152833
26	6	0	-9.158082	-3.007865	0.358986
27	6	0	-10.498057	-3.374208	0.473148
28	6	0	-11.501165	-2.406383	0.393829
29	6	0	-11.151145	-1.068848	0.199721
30	6	0	-9.811027	-0.702822	0.086382
31	6	0	9.812436	-0.850789	-0.366567
32	6	0	11.152287	-1.216402	-0.249001
33	6	0	11.503191	-2.407248	0.389734
34	6	0	10.501222	-3.228511	0.909973
35	6	0	9.161562	-2.861919	0.793365
36	8	0	0.003400	2.956127	-2.541843
37	6	0	-0.004994	3.628753	0.146267
38	6	0	-0.009303	3.310836	1.512319
39	6	0	-0.013159	4.327704	2.465131
40	6	0	-0.012719	5.666080	2.060653
41	6	0	-0.008407	5.985962	0.702560
42	6	0	-0.004538	4.970079	-0.255688
43	1	0	-3.350365	1.936046	-1.005078
44	1	0	3.351646	1.920634	-1.057275
45	1	0	-5.343843	0.868486	-1.682993
46	1	0	-7.698812	0.233068	-1.465997
47	1	0	-6.643279	-2.683093	1.510209
48	1	0	-4.292044	-2.036894	1.315686

49	1	0	4.285128	-2.638870	-0.510599
50	1	0	6.637423	-3.280325	-0.300460
51	1	0	7.710853	0.833672	0.330342
52	1	0	5.355576	1.479566	0.142561
53	1	0	-8.388050	-3.773527	0.393265
54	1	0	-10.759152	-4.419656	0.615028
55	1	0	-12.545866	-2.691806	0.482175
56	1	0	-11.923151	-0.305777	0.144915
57	1	0	-9.549482	0.344448	-0.036994
58	1	0	9.550298	0.063886	-0.891017
59	1	0	11.923251	-0.573722	-0.665927
60	1	0	12.547653	-2.692623	0.481006
61	1	0	10.763097	-4.153588	1.416859
62	1	0	8.392832	-3.495050	1.227690
63	1	0	-0.009746	2.272017	1.832308
64	1	0	-0.016727	4.077852	3.522681
65	1	0	-0.015895	6.457263	2.805785
66	1	0	-0.008196	7.025775	0.386799
67	1	0	-0.001237	5.201967	-1.316597

Table S8. Cartesian coordinates for minimized structure of compound **5-ox2**.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	15	0	-0.000698	2.375082	-1.070335
2	6	0	-1.293374	1.145477	-0.568259
3	6	0	-0.696147	-0.076853	-0.119018
4	6	0	0.696592	-0.075908	-0.118001
5	6	0	1.292844	1.147469	-0.565671
6	6	0	-2.663046	1.088654	-0.609448
7	6	0	-3.195145	-0.167209	-0.185387
8	16	0	-1.888291	-1.278903	0.266841
9	16	0	1.889870	-1.275492	0.271932
10	6	0	3.195868	-0.162179	-0.178817
11	6	0	2.662733	1.093134	-0.603117
12	6	0	-4.558143	-0.550780	-0.115539
13	6	0	4.559263	-0.544331	-0.108037
14	6	0	-5.594763	0.353040	-0.505881
15	6	0	-6.916632	-0.012699	-0.443732
16	6	0	-7.315196	-1.306324	0.000513
17	6	0	-6.279368	-2.207600	0.386792
18	6	0	-4.956900	-1.845329	0.336678
19	6	0	4.959868	-1.831731	0.362512
20	6	0	6.283380	-2.188231	0.425666
21	6	0	7.316684	-1.296952	0.010745
22	6	0	6.915646	-0.015053	-0.464047
23	6	0	5.594093	0.353488	-0.516483
24	6	0	-8.716574	-1.692416	0.057174
25	6	0	8.718298	-1.682008	0.068480
26	6	0	-9.098486	-3.059040	0.022080
27	6	0	-10.435410	-3.422970	0.062078
28	6	0	-11.428087	-2.438739	0.159786
29	6	0	-11.073898	-1.083681	0.207088
30	6	0	-9.739753	-0.712746	0.146351
31	6	0	9.682910	-1.048702	-0.757911
32	6	0	11.016185	-1.424566	-0.707863
33	6	0	11.430196	-2.425928	0.180805
34	6	0	10.496948	-3.057862	1.013498
35	6	0	9.158876	-2.701158	0.952686
36	8	0	0.000237	2.755099	-2.512184
37	6	0	-0.002445	3.732580	0.111602
38	6	0	-0.003101	3.527010	1.502401
39	6	0	-0.004197	4.623600	2.359866
40	6	0	-0.004631	5.920743	1.835058
41	6	0	-0.004010	6.125397	0.453831
42	6	0	-0.002908	5.033771	-0.415167
43	1	0	-3.291492	1.907481	-0.936815
44	1	0	3.290658	1.913486	-0.927663
45	1	0	-5.345521	1.341613	-0.873698
46	1	0	-7.666776	0.692129	-0.782185
47	1	0	-6.537079	-3.189161	0.766310
48	1	0	-4.208155	-2.562514	0.660675

49	1	0	4.210645	-2.555200	0.671044
50	1	0	6.539243	-3.186336	0.760769
51	1	0	7.668370	0.707025	-0.757531
52	1	0	5.344853	1.346806	-0.871289
53	1	0	-8.346538	-3.833188	-0.085362
54	1	0	-10.712324	-4.471128	0.012398
55	1	0	-12.474283	-2.726799	0.198969
56	1	0	-11.843204	-0.323383	0.295767
57	1	0	-9.483169	0.338739	0.215177
58	1	0	9.376250	-0.294310	-1.474240
59	1	0	11.737842	-0.945563	-1.361729
60	1	0	12.476487	-2.713025	0.223990
61	1	0	10.821247	-3.824056	1.710319
62	1	0	8.456676	-3.179584	1.626734
63	1	0	-0.002705	2.521864	1.917933
64	1	0	-0.004641	4.471117	3.434861
65	1	0	-0.005404	6.773403	2.507604
66	1	0	-0.004330	7.133600	0.051261
67	1	0	-0.002366	5.180072	-1.491065

Table S9. Cartesian coordinates for minimized structure of compound **3-red**.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	15	0	0.000000	1.507585	-1.199766
2	6	0	-1.296349	0.348497	-0.684781
3	6	0	-0.702311	-0.839709	-0.180347
4	6	0	0.702311	-0.839709	-0.180347
5	6	0	1.296349	0.348497	-0.684782
6	6	0	-2.693885	0.317138	-0.667954
7	6	0	-3.246063	-0.861956	-0.167488
8	16	0	-1.929677	-1.992546	0.303240
9	16	0	1.929676	-1.992547	0.303239
10	6	0	3.246063	-0.861957	-0.167489
11	6	0	2.693885	0.317136	-0.667956
12	6	0	-4.635009	-1.224559	-0.008090
13	6	0	4.635008	-1.224559	-0.008090
14	6	0	-5.679188	-0.342050	-0.391874
15	6	0	-7.015644	-0.685472	-0.237285
16	6	0	-7.384713	-1.922949	0.305527
17	6	0	-6.373736	-2.808148	0.689169
18	6	0	-5.032327	-2.471563	0.537978
19	6	0	5.032327	-2.471564	0.537977
20	6	0	6.373735	-2.808149	0.689169
21	6	0	7.384713	-1.922950	0.305528
22	6	0	7.015643	-0.685473	-0.237284
23	6	0	5.679187	-0.342050	-0.391874
24	8	0	0.000000	2.076400	-2.597302
25	6	0	0.000000	2.894401	0.016278
26	6	0	0.000001	2.677284	1.401624
27	6	0	0.000001	3.756791	2.284163
28	6	0	0.000002	5.065446	1.791364
29	6	0	0.000001	5.288813	0.413817
30	6	0	0.000000	4.206854	-0.470356
31	1	0	-3.309054	1.139673	-1.018846
32	1	0	3.309054	1.139672	-1.018849
33	1	0	-5.429589	0.625217	-0.817964
34	1	0	-7.782846	0.022584	-0.545641
35	1	0	-8.432190	-2.187987	0.424518
36	1	0	-6.631582	-3.776887	1.113460
37	1	0	-4.272098	-3.183750	0.847892
38	1	0	4.272097	-3.183751	0.847890
39	1	0	6.631581	-3.776888	1.113460
40	1	0	8.432189	-2.187988	0.424518
41	1	0	7.782845	0.022583	-0.545639
42	1	0	5.429589	0.625217	-0.817963
43	1	0	0.000000	1.660637	1.785916
44	1	0	0.000002	3.578938	3.357139
45	1	0	0.000002	5.906774	2.481118
46	1	0	0.000001	6.305604	0.026616
47	1	0	0.000000	4.358626	-1.545965

Table S10. Cartesian coordinates for minimized structure of compound **4-red**.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	15	0	-3.371701	0.426678	1.147296
2	6	0	-1.714536	-0.149922	0.673014
3	6	0	-1.812437	-1.418405	0.043090
4	6	0	-3.130885	-1.904959	-0.073976
5	6	0	-4.135015	-1.056197	0.451296
6	6	0	-0.405860	0.320448	0.775559
7	6	0	0.567106	-0.537545	0.246425
8	16	0	-0.227004	-2.017352	-0.405079
9	16	0	-3.834573	-3.369765	-0.734847
10	6	0	-5.460303	-2.820556	-0.303239
11	6	0	-5.438039	-1.593172	0.309719
12	6	0	1.988477	-0.364138	0.180074
13	6	0	2.632961	0.773902	0.743649
14	6	0	4.001628	0.950500	0.671582
15	6	0	4.851802	0.009205	0.043655
16	6	0	4.218756	-1.125199	-0.509186
17	6	0	2.847658	-1.306906	-0.449502
18	6	0	6.308469	0.203210	-0.030319
19	6	0	7.199541	-0.891145	-0.100277
20	6	0	8.577343	-0.706534	-0.176858
21	6	0	9.125224	0.579537	-0.177110
22	6	0	8.262968	1.677156	-0.103342
23	6	0	6.884466	1.493443	-0.035721
24	8	0	-3.663543	0.831649	2.571741
25	6	0	-3.783831	1.835004	0.027557
26	6	0	-3.550425	1.787235	-1.354389
27	6	0	-3.881903	2.873292	-2.163750
28	6	0	-4.451359	4.019701	-1.600720
29	6	0	-4.685853	4.074580	-0.226076
30	6	0	-4.352380	2.986476	0.584703
31	1	0	-0.149096	1.273585	1.226416
32	1	0	-6.311233	-3.449413	-0.527152
33	1	0	-6.339588	-1.094875	0.654364
34	1	0	2.037314	1.520954	1.260298
35	1	0	4.436318	1.824990	1.150311
36	1	0	4.816756	-1.866340	-1.034807
37	1	0	2.417398	-2.190149	-0.914789
38	1	0	6.800900	-1.901006	-0.064179
39	1	0	9.230660	-1.575732	-0.222707
40	1	0	10.201464	0.723146	-0.233009
41	1	0	8.666994	2.687643	-0.111895
42	1	0	6.233987	2.363241	-0.016594
43	1	0	-3.105057	0.897919	-1.792675
44	1	0	-3.694374	2.827965	-3.234206
45	1	0	-4.708202	4.866898	-2.233137
46	1	0	-5.125907	4.965882	0.216462
47	1	0	-4.520668	3.011742	1.657587

Table S11. Cartesian coordinates for minimized structure of compound **5-red**.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	15	0	0.000644	2.308721	-1.180884
2	6	0	-1.297392	1.106805	-0.765534
3	6	0	-0.702646	-0.112278	-0.352246
4	6	0	0.704601	-0.110586	-0.347880
5	6	0	1.299028	1.109556	-0.758497
6	6	0	-2.693137	1.073204	-0.758218
7	6	0	-3.243213	-0.145207	-0.351039
8	16	0	-1.925164	-1.301774	0.036473
9	16	0	1.927501	-1.296950	0.049160
10	6	0	3.245214	-0.139601	-0.337149
11	6	0	2.694776	1.077936	-0.746539
12	6	0	-4.627069	-0.520396	-0.226016
13	6	0	4.629134	-0.513698	-0.209583
14	6	0	-5.675864	0.371491	-0.576910
15	6	0	-7.007647	0.018119	-0.449875
16	6	0	-7.403673	-1.250821	0.027083
17	6	0	-6.367309	-2.141697	0.370627
18	6	0	-5.030944	-1.793328	0.253286
19	6	0	5.033202	-1.812115	0.195425
20	6	0	6.369576	-2.157811	0.320208
21	6	0	7.405864	-1.243097	0.046197
22	6	0	7.009622	0.049754	-0.361316
23	6	0	5.677850	0.405222	-0.482253
24	6	0	-8.825368	-1.622174	0.159633
25	6	0	8.827624	-1.614955	0.176541
26	6	0	-9.255072	-2.956751	0.005916
27	6	0	-10.596730	-3.307628	0.136527
28	6	0	-11.560494	-2.335798	0.417193
29	6	0	-11.156640	-1.007008	0.568721
30	6	0	-9.813762	-0.657579	0.446141
31	6	0	9.819003	-1.027192	-0.636674
32	6	0	11.162165	-1.374262	-0.510955
33	6	0	11.563755	-2.328489	0.427102
34	6	0	10.597029	-2.926001	1.239775
35	6	0	9.254993	-2.572783	1.119668
36	8	0	0.003337	2.979021	-2.530756
37	6	0	-0.003986	3.585126	0.146673
38	6	0	-0.006718	3.253511	1.509141
39	6	0	-0.010278	4.256535	2.477532
40	6	0	-0.011165	5.601249	2.094297
41	6	0	-0.008475	5.937773	0.740028
42	6	0	-0.004889	4.932971	-0.230757
43	1	0	-3.309595	1.918978	-1.044557
44	1	0	3.310956	1.921971	-1.038586
45	1	0	-5.431943	1.354187	-0.969416
46	1	0	-7.767012	0.730954	-0.762584
47	1	0	-6.616259	-3.120405	0.773944
48	1	0	-4.275348	-2.515035	0.552419

49	1	0	4.277719	-2.565667	0.402026
50	1	0	6.618757	-3.177447	0.604243
51	1	0	7.768795	0.804301	-0.553087
52	1	0	5.433819	1.420079	-0.781821
53	1	0	-8.526861	-3.721923	-0.247601
54	1	0	-10.893421	-4.346034	0.005051
55	1	0	-12.608035	-2.609335	0.515592
56	1	0	-11.891099	-0.237515	0.796846
57	1	0	-9.515834	0.375379	0.602250
58	1	0	9.523689	-0.308927	-1.396347
59	1	0	11.898834	-0.905083	-1.159649
60	1	0	12.611594	-2.601645	0.523255
61	1	0	10.891420	-3.664061	1.982885
62	1	0	8.524448	-3.023479	1.785545
63	1	0	-0.006023	2.209135	1.809960
64	1	0	-0.012347	3.990458	3.531926
65	1	0	-0.013921	6.382562	2.851063
66	1	0	-0.009142	6.982805	0.437998
67	1	0	-0.002720	5.174376	-1.289805

Figure S12. ^1H NMR spectrum of **4** in CDCl_3 .

Figure S13. $^{13}\text{C}\{^1\text{H}\}$ APT NMR spectrum of **4** in CDCl_3 .

Figure S14. $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum of **4** in CDCl_3 .

Figure S15. ^1H NMR spectrum of **5** in CDCl_3 .

Figure S16. $^{13}\text{C}\{^1\text{H}\}$ APT NMR spectrum of **5** in CDCl_3 .

Figure S17. $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum of **5** in CDCl_3 .

Figure S18. ^1H NMR spectrum of **6** in CDCl_3 .

Figure S19. $^{13}\text{C}\{^1\text{H}\}$ APT NMR spectrum of **6** in CDCl_3 .

Figure S20. $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum of **6** in CDCl_3 .