Supplementary material

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Electron Paramagnetic Resonance and DFT Analysis of a Vanadyl Perfluoroalkyl Perfluorinated Phthalocyanine

1. DFT results

Below are the coordinates (in Å) for the different DFT-computed models discussed in the main text.

Model A (no ligation, in vacuum)

F	-3.420083	8.185560	-1.677822
F	-2.408845	6.283824	-1.952300
F	3.645320	6.832582	-1.774861
F	5.192609	8.270945	-1.204633
F	5.717041	6.475476	-2.322224
F	3.292381	7.584249	0.822109
F	4.086396	6.054397	2.174149
F	5.231596	7.847325	1.739582
F	7.960488	4.597376	1.469166
F	8.082819	2.446575	1.189507
F	7.540948	-3.619592	-1.972998
F	7.165025	-5.712841	-2.415702
F	8.996772	-5.142687	-1.382556
F	7.187427	-6.359742	0.252079
F	8.671533	-5.042405	1.572335
F	6.891309	-3.879954	2.013725
F	8.372959	-3.147667	0.576045
F	3.264581	-7.924385	1.332922
F	4.546682	-9.411695	0.367081
F	5.423885	-7.791782	1.530877
F	2.400742	-8.362693	-1.213623
F	5.731269	-7.506884	-1.182125
C	8.242309	3.633587	0.577692
C	4.515838	-7.230192	-0.615550
F	6.758620	2.411424	-2.633589
F	8.409867	1.671370	-1.398910
F	8.675818	3.430902	-2.625281
F	7.561820	4.998872	-1.218841
C	5.166856	6.200537	-0.005232
F	-2.300936	-8.132325	-1.153429
F	-2.891220	-6.455385	-2.433658
F	-4.085786	-8.267198	-2.364494
F	-3.025501	-7.653098	1.431209
F	-7.703033	-2.413258	0.898921
F	-8.153758	-4.286874	1.877032
F	-6.262389	-3.303024	2.289183

F	-6.979917	-2.919359	-1.673208
F	-6.808497	-5.030057	-2.157570
F	-8.556074	-4.313176	-1.071460
F	-6.829583	-5.716006	0.505258
F	-5.532923	-6.973399	-0.983565
F	-3.640033	8.702192	1.239720
F	-4.433638	6.999150	2.342792
F	-2.293671	7.154035	2.001178
F	-1.166241	5.466276	0.290888
F	2.557451	5.297057	0.087987
F	6.207985	1.266151	-0.262169
F	6.060463	-2.449542	-0.114492
F	2.030156	-6.117141	-0.154676
F	-1.683814	-5.944023	-0.087938
F	-5.352701	-1.923190	0.171223
N	1.778678	-1.797026	0.206147
N	0.595762	3.057326	0.289134
C	1.735228	2.379671	0.224986
C	3.048134	3.009199	0.076362
C	3.993880	1.970226	0.010797
C	3.478523	4.337239	0.002145
C	4.848859	4.685097	-0.119479
C	5.806619	3.612313	-0.313651
C	5.344495	2.278030	-0.176537
C	-0.854207	-3.041495	0.199387
C	4.371765	-5.715294	-0.308139
C	5.448239	-4.748717	-0.195883
C	5.101001	-3.374836	-0.124704
C	-2.609621	-4.987015	-0.024981
N	-2.943214	-0.177282	0.323291
C	-2.372930	-1.374620	0.276612
N	-1.019689	-1.669794	0.303019
C	-3.121706	-2.626890	0.165530
C	-2.175243	-3.666127	0.119115
C	-4.484504	-2.932754	0.109597
C	-4.960001	-4.267075	0.027645
C	-3.982509	-5.326272	-0.141279
C	1.484144	-3.148744	0.132628
C	2.737158	-3.892243	-0.003175
C	3.775443	-2.943585	-0.019852
C	3.149284	-1.626332	0.099796
C	3.041841	-5.249242	-0.143708
C	-3.513264	5.064812	0.290810
C	-4.226735	2.714112	0.380242
C	-2.897320	2.283293	0.357794
C	-1.860026	3.233044	0.350642
C	-2.174531	4.594931	0.321141
C	-2.265907	0.963426	0.356506
N	-0.891079	1.131691	0.367970
C	-0.601056	2.486428	0.345290
N	3.823978	-0.483999	0.073240
C	3.253679	0.713350	0.124644
N	0.285713	-3.718743	0.141858
N	1.905985	1.005039	0.258753
V	0.463602	-0.345423	0.835767
C	-3.680770	6.596941	0.102213
C	-3.501607	7.381952	1.455235

C	-6.498825	-4.436956	0.145325
C	-7.228489	-4.162280	-1.222542
C	-7.168156	-3.567445	1.324336
C	-4.276926	-6.816872	-0.461350
C	-4.225117	-7.720319	0.827089
C	-3.345652	-7.433732	-1.621720
C	6.967365	-5.059717	-0.117599
C	7.744061	-4.241281	1.031867
C	7.685129	-4.872681	-1.506297
C	7.307082	3.765243	-0.682041
C	7.798852	2.775330	-1.853632
C	3.488045	-7.772022	-1.730928
C	4.429348	-8.110628	0.686894
F	9.528553	3.763114	0.206884
F	-5.154536	-7.321698	1.710699
F	3.096896	-6.766004	-2.541966
F	4.118562	-8.681345	-2.485774
F	-4.475566	-9.000022	0.498038
C	4.404167	6.939285	1.205848
C	4.917885	6.963625	-1.359628
F	6.483014	6.407689	0.310820
F	-4.934108	6.905682	-0.354994
F	-5.182196	1.784987	0.403127
C	-2.737118	7.224808	-1.041594
F	-1.614033	7.779906	-0.562827
C	-4.578438	4.087962	0.421768
F	-8.196743	4.538973	-0.498509
F	-6.782192	3.062510	-1.277750
F	-5.870021	3.070825	2.665331
F	-7.677140	4.249227	2.418689
F	-7.443757	2.424271	1.285035
C	-6.089054	4.384459	0.624066
C	-6.786631	3.489513	1.767440
F	-6.286293	5.656386	1.090937
C	-6.896051	4.282970	-0.723905
F	-6.435870	5.181308	-1.609944
O	0.521128	-0.381988	2.417629

Model B (no ligation, in ethanol surrounding)

F	-3.405258	8.161122	-1.753591
F	-2.387305	6.260105	-2.004932
F	3.657940	6.834938	-1.740222
F	5.204571	8.268624	-1.157209
F	5.733671	6.472431	-2.271349
F	3.286249	7.590360	0.848219
F	4.068470	6.068634	2.215687
F	5.219900	7.855960	1.776260
F	7.945917	4.597780	1.538963
F	8.073821	2.446292	1.262019
F	7.490937	-3.608685	-2.075319
F	7.105033	-5.702860	-2.508852
F	8.961605	-5.131458	-1.522184
F	7.199490	-6.350499	0.156346
F	8.722954	-5.033342	1.427510

F	6.958046	-3.872918	1.929890
F	8.390678	-3.136978	0.445597
F	3.291647	-7.921384	1.319189
F	4.562696	-9.404516	0.332963
F	5.454404	-7.779032	1.477787
F	2.384828	-8.370695	-1.206704
F	5.712535	-7.504552	-1.239506
C	8.233719	3.632800	0.651083
C	4.505164	-7.223651	-0.652487
F	6.798073	2.409560	-2.579751
F	8.430380	1.671763	-1.319392
F	8.712293	3.433477	-2.538809
F	7.574456	4.998003	-1.151115
C	5.163622	6.196969	0.041195
F	-2.302225	-8.144544	-1.104692
F	-2.886584	-6.477119	-2.399403
F	-4.087369	-8.283744	-2.314627
F	-3.026446	-7.656961	1.470421
F	-7.708159	-2.412078	0.928097
F	-8.164181	-4.287366	1.900148
F	-6.277147	-3.302348	2.327567
F	-6.981239	-2.916153	-1.638480
F	-6.805635	-5.027050	-2.123754
F	-8.554212	-4.313416	-1.037086
F	-6.832837	-5.714551	0.537248
F	-5.531573	-6.976981	-0.946375
F	-3.648424	8.711084	1.142993
F	-4.445697	7.023989	2.267633
F	-2.303124	7.179984	1.939596
F	-1.164943	5.462799	0.258474
F	2.558531	5.296208	0.127698
F	6.209909	1.265245	-0.224919
F	6.056199	-2.445067	-0.155955
F	2.028345	-6.116532	-0.165636
F	-1.683717	-5.945832	-0.064166
F	-5.352336	-1.925222	0.218982
N	1.779474	-1.798877	0.234232
N	0.596064	3.054745	0.310954
C	1.735282	2.376087	0.254604
C	3.048421	3.006255	0.110852
C	3.993149	1.968480	0.043821
C	3.480370	4.332970	0.042783
C	4.849043	4.682833	-0.072555
C	5.807913	3.610401	-0.265949
C	5.342995	2.277915	-0.138116
C	-0.852777	-3.041662	0.229938
C	4.366076	-5.709900	-0.347110
C	5.443672	-4.742751	-0.245078
C	5.094408	-3.372126	-0.156688
C	-2.609799	-4.985329	0.004267
N	-2.941844	-0.179761	0.357316
C	-2.370099	-1.376589	0.314788
N	-1.018721	-1.672239	0.339659
C	-3.119292	-2.628609	0.204914
C	-2.173840	-3.666467	0.152121
C	-4.480846	-2.935621	0.152052
C	-4.958326	-4.267121	0.066107

C	-3.980816	-5.326178	-0.108228
C	1.483743	-3.147888	0.148703
C	2.735143	-3.890072	-0.008010
C	3.771690	-2.941905	-0.028915
C	3.146668	-1.626320	0.111580
C	3.040302	-5.244241	-0.163150
C	-3.510318	5.059169	0.248593
C	-4.223149	2.712175	0.371411
C	-2.895122	2.279880	0.363535
C	-1.858890	3.228538	0.349260
C	-2.174233	4.588379	0.295192
C	-2.263249	0.960396	0.383147
N	-0.890340	1.129568	0.403716
C	-0.600099	2.482029	0.363842
N	3.823218	-0.484958	0.090136
C	3.252334	0.711557	0.152001
N	0.286194	-3.719722	0.162937
N	1.906769	1.003334	0.289348
V	0.465260	-0.347396	0.857612
C	-3.674473	6.586886	0.039276
C	-3.507163	7.392301	1.381125
C	-6.495863	-4.433904	0.179410
C	-7.224282	-4.159403	-1.188640
C	-7.171672	-3.566443	1.355618
C	-4.273988	-6.816036	-0.423105
C	-4.226145	-7.715991	0.867226
C	-3.344066	-7.442623	-1.578878
C	6.963367	-5.048746	-0.206335
C	7.773993	-4.231450	0.919718
C	7.644544	-4.861193	-1.612773
C	7.310571	3.762414	-0.617077
C	7.820523	2.774794	-1.782214
C	3.460865	-7.775842	-1.746508
C	4.445209	-8.100877	0.652915
F	9.525494	3.764476	0.290778
F	-5.154006	-7.313126	1.750355
F	3.051930	-6.782740	-2.559736
F	4.082363	-8.692853	-2.504380
F	-4.484508	-8.997288	0.540444
C	4.393931	6.942256	1.243195
C	4.926779	6.959453	-1.315166
F	6.479355	6.408589	0.366549
F	-4.926258	6.893049	-0.431034
F	-5.182657	1.783100	0.403846
C	-2.724179	7.203893	-1.104579
F	-1.605805	7.769655	-0.623099
C	-4.576680	4.084302	0.387989
F	-8.188745	4.529438	-0.564936
F	-6.774286	3.040147	-1.319004
F	-5.900679	3.095522	2.634226
F	-7.700654	4.275133	2.346950
F	-7.456702	2.434289	1.241624
C	-6.087274	4.382251	0.571530
C	-6.799815	3.504242	1.718101
F	-6.291271	5.662117	1.020720
C	-6.884841	4.266634	-0.780349
F	-6.420087	5.154716	-1.673590

O	0.526666	-0.384734	2.444616

Model C (one ethanol molecule ligated, in vacuum)

F	-3.416888	8.230228	-1.765716
F	-2.411516	6.326177	-2.044033
F	3.773526	6.917408	-1.628702
F	5.301560	8.332644	-0.957957
F	5.865068	6.560340	-2.093524
F	3.303514	7.602679	0.963873
F	4.034474	6.040408	2.314701
F	5.199249	7.841052	1.973868
F	7.938126	4.590369	1.748856
F	8.067435	2.446631	1.421580
F	7.552922	-3.606728	-2.077133
F	7.165660	-5.695003	-2.532982
F	9.006179	-5.140021	-1.507333
F	7.203053	-6.362188	0.129554
F	8.698973	-5.060727	1.451058
F	6.926583	-3.894194	1.911830
F	8.402745	-3.157634	0.470425
F	3.273812	-7.916459	1.216451
F	4.550289	-9.402561	0.241577
F	5.433857	-7.789821	1.410690
F	2.402241	-8.339072	-1.329678
F	5.735922	-7.496409	-1.302588
C	8.256817	3.647749	0.847389
C	4.523106	-7.216340	-0.731299
F	6.921226	2.515961	-2.461589
F	8.509969	1.735675	-1.170627
F	8.838668	3.526864	-2.333798
F	7.660530	5.060545	-0.941979
C	5.212562	6.234821	0.190666
F	-2.323488	-8.141403	-1.063573
F	-2.955377	-6.497814	-2.367354
F	-4.142128	-8.309734	-2.218367
F	-2.973512	-7.601007	1.527829
F	-7.682304	-2.389174	1.014410
F	-8.101898	-4.242920	2.042654
F	-6.202794	-3.247420	2.383809
F	-7.028892	-2.948550	-1.566537
F	-6.865950	-5.068995	-2.009332
F	-8.584304	-4.331698	-0.891016
F	-6.811417	-5.697568	0.665982
F	-5.552320	-6.986077	-0.828628
F	-3.613448	8.755369	1.152351
F	-4.396471	7.055297	2.267767
F	-2.259880	7.209547	1.905401
F	-1.152531	5.511194	0.188781
F	2.600996	5.335017	0.143225
F	6.259781	1.307139	-0.147889
F	6.088142	-2.445563	-0.196627
F	2.043377	-6.096129	-0.264032
F	-1.682994	-5.925870	-0.072298
F	-5.353867	-1.909246	0.215162

N	1.814788	-1.785228	0.133464
N	0.617053	3.090497	0.202284
C	1.764280	2.419050	0.157121
C	3.087031	3.047464	0.084194
C	4.035329	2.006532	0.034798
C	3.524317	4.375211	0.071350
C	4.898836	4.723843	0.023257
C	5.863581	3.654605	-0.155115
C	5.393274	2.318484	-0.076713
C	-0.847871	-3.017005	0.132738
C	4.386576	-5.702653	-0.416076
C	5.466364	-4.741959	-0.297344
C	5.123671	-3.366861	-0.213198
C	-2.609254	-4.968911	-0.002431
N	-2.934175	-0.141949	0.261494
C	-2.372191	-1.346845	0.222127
N	-1.025189	-1.650807	0.215722
C	-3.122045	-2.606151	0.155419
C	-2.173112	-3.645470	0.100055
C	-4.484017	-2.918143	0.147481
C	-4.958966	-4.255039	0.106060
C	-3.984114	-5.314743	-0.070328
C	1.504274	-3.126387	0.046378
C	2.757813	-3.875060	-0.098601
C	3.801345	-2.929658	-0.105302
C	3.178564	-1.607664	0.029699
C	3.058356	-5.231046	-0.247746
C	-3.500455	5.115069	0.212186
C	-4.217127	2.766499	0.315770
C	-2.890246	2.330712	0.279114
C	-1.849404	3.279545	0.258576
C	-2.162694	4.641088	0.230893
C	-2.260869	1.005907	0.276341
N	-0.892210	1.182781	0.271865
C	-0.588771	2.529119	0.247627
N	3.851359	-0.459770	0.023250
C	3.289886	0.745052	0.080415
N	0.298495	-3.687343	0.060215
N	1.942756	1.047361	0.155635
V	0.471365	-0.310833	0.597454
C	-3.665309	6.646833	0.021308
C	-3.472828	7.435385	1.370337
C	-6.493272	-4.425517	0.270704
C	-7.261580	-4.181874	-1.081418
C	-7.132771	-3.533195	1.449143
C	-4.282246	-6.813003	-0.346531
C	-4.190330	-7.684244	0.961634
C	-3.383226	-7.456411	-1.517589
C	6.984505	-5.058492	-0.228715
C	7.771218	-4.251687	0.922134
C	7.694677	-4.863893	-1.619976
C	7.379567	3.813810	-0.449382
C	7.924243	2.854177	-1.622353
C	3.490632	-7.749786	-1.846125
C	4.436718	-8.102253	0.567277
F	9.559118	3.781819	0.537936
F	-5.093841	-7.264855	1.862426

F	3.101351	-6.739355	-2.653021
F	4.115888	-8.658521	-2.606765
F	-4.448231	-8.972280	0.672150
C	4.396100	6.946490	1.382601
C	5.027431	7.030869	-1.154656
F	6.513074	6.431143	0.572382
F	-4.921817	6.958490	-0.426056
F	-5.175649	1.839695	0.352306
C	-2.730403	7.269959	-1.131958
F	-1.601998	7.824593	-0.665585
C	-4.566221	4.141415	0.356038
F	-8.191554	4.597952	-0.533834
F	-6.788621	3.114375	-1.320062
F	-5.840292	3.133951	2.614672
F	-7.645998	4.316915	2.380741
F	-7.428512	2.487653	1.250871
C	-6.074006	4.441478	0.571061
C	-6.763345	3.552348	1.723885
F	-6.265172	5.715822	1.034520
C	-6.893463	4.337133	-0.768886
F	-6.438579	5.230679	-1.663039
O	0.522000	-0.340736	2.185337
O	0.460177	-0.289570	-1.960278
C	-0.597909	-0.207552	-2.931296
C	-0.138656	-0.625137	-4.322501
H	-1.033178	0.818665	-2.949017
H	-1.389133	-0.889165	-2.560360
H	0.277205	-1.652313	-4.311034
H	0.640847	0.061158	-4.716514
H	-0.988050	-0.601520	-5.035290
H	1.183785	0.301035	-2.247008

Model D (one ethanol molecule ligated, in ethanol surrounding)

F	-3.405158	8.245633	-1.781467
F	-2.395905	6.344447	-2.063870
F	3.788090	6.925707	-1.620505
F	5.308559	8.339809	-0.930793
F	5.885609	6.570139	-2.063498
F	3.293922	7.614075	0.964328
F	4.012249	6.059030	2.329570
F	5.181994	7.855835	1.987427
F	7.918158	4.597116	1.797587
F	8.051711	2.452750	1.471986
F	7.542382	-3.599151	-2.128389
F	7.154376	-5.688975	-2.580636
F	8.998619	-5.131399	-1.563465
F	7.205744	-6.354325	0.080130
F	8.717337	-5.055337	1.382590
F	6.952395	-3.887956	1.867948
F	8.410698	-3.150109	0.409640
F	3.278013	-7.910731	1.184662
F	4.550412	-9.395634	0.202919
F	5.439621	-7.784006	1.368882
F	2.398690	-8.340325	-1.354960

F	5.731111	-7.492157	-1.342970
C	8.243964	3.653699	0.899783
C	4.518350	-7.207599	-0.768422
F	6.965450	2.524368	-2.430283
F	8.530084	1.744011	-1.110762
F	8.878189	3.538040	-2.263762
F	7.672404	5.068034	-0.894423
C	5.207515	6.238869	0.212451
F	-2.338694	-8.146941	-1.051047
F	-2.977957	-6.514784	-2.364852
F	-4.168178	-8.321751	-2.187589
F	-2.965983	-7.594500	1.536550
F	-7.682583	-2.380330	1.048559
F	-8.096852	-4.233698	2.079408
F	-6.197996	-3.235935	2.413515
F	-7.053589	-2.945742	-1.533741
F	-6.893342	-5.068151	-1.972152
F	-8.598745	-4.329014	-0.835580
F	-6.811745	-5.689488	0.701894
F	-5.563657	-6.983119	-0.799918
F	-3.612796	8.765449	1.123681
F	-4.405987	7.069931	2.238346
F	-2.266226	7.220091	1.889777
F	-1.152351	5.518254	0.168737
F	2.601026	5.341069	0.154915
F	6.261683	1.314182	-0.135240
F	6.087549	-2.440224	-0.222885
F	2.041574	-6.090162	-0.306824
F	-1.688806	-5.920630	-0.090912
F	-5.357293	-1.904052	0.240989
N	1.815793	-1.782272	0.119956
N	0.616535	3.095086	0.202107
C	1.763916	2.423130	0.158085
C	3.087112	3.052110	0.090656
C	4.034720	2.012479	0.039716
C	3.525298	4.378163	0.084482
C	4.898098	4.729038	0.044339
C	5.864106	3.660643	-0.132611
C	5.391466	2.326148	-0.064784
C	-0.850946	-3.010790	0.116320
C	4.383987	-5.695069	-0.455790
C	5.464168	-4.734565	-0.334093
C	5.119799	-3.362064	-0.241955
C	-2.615168	-4.960535	-0.009320
N	-2.937161	-0.135374	0.261824
C	-2.375064	-1.340913	0.219609
N	-1.029749	-1.646388	0.203197
C	-3.124404	-2.600393	0.158374
C	-2.176470	-3.638799	0.092453
C	-4.485067	-2.913981	0.163108
C	-4.961969	-4.248330	0.124997
C	-3.988352	-5.308234	-0.061901
C	1.502691	-3.120751	0.023146
C	2.756218	-3.868564	-0.128939
C	3.799190	-2.923895	-0.130088
C	3.177273	-1.602434	0.014952
C	3.058074	-5.222223	-0.286410

C	-3.499378	5.122652	0.188066
C	-4.216676	2.776987	0.298774
C	-2.891786	2.338627	0.266975
C	-1.850779	3.285694	0.245213
C	-2.164193	4.645898	0.210795
C	-2.263531	1.012965	0.271348
N	-0.896724	1.190784	0.271176
C	-0.590325	2.534292	0.241930
N	3.850985	-0.454340	0.017479
C	3.289096	0.750542	0.078923
N	0.296004	-3.681332	0.036782
N	1.944698	1.053986	0.155725
V	0.469064	-0.305633	0.557850
C	-3.659985	6.653015	-0.002412
C	-3.475002	7.443337	1.345989
C	-6.493407	-4.416553	0.301183
C	-7.275944	-4.177502	-1.043237
C	-7.127141	-3.523685	1.481696
C	-4.287618	-6.805949	-0.328679
C	-4.187399	-7.673106	0.980861
C	-3.400303	-7.459762	-1.502597
C	6.981377	-5.048566	-0.276424
C	7.780401	-4.244155	0.866843
C	7.683913	-4.855141	-1.671286
C	7.382080	3.818979	-0.406678
C	7.947297	2.862308	-1.571871
C	3.484308	-7.747640	-1.878018
C	4.437865	-8.093151	0.530200
F	9.551998	3.788746	0.604447
F	-5.083009	-7.251826	1.888350
F	3.090012	-6.747776	-2.690259
F	4.109915	-8.663476	-2.634181
F	-4.451840	-8.963403	0.696554
C	4.382175	6.955481	1.394550
C	5.036094	7.035684	-1.133780
F	6.506398	6.439725	0.605904
F	-4.915847	6.969528	-0.455260
F	-5.179501	1.850407	0.336724
C	-2.720252	7.279363	-1.149712
F	-1.594941	7.836806	-0.674526
C	-4.566521	4.150309	0.332244
F	-8.188598	4.611476	-0.574040
F	-6.786421	3.125441	-1.356782
F	-5.867167	3.146461	2.586603
F	-7.666668	4.333685	2.329886
F	-7.441559	2.501150	1.207103
C	-6.073808	4.450345	0.536466
C	-6.775432	3.565206	1.684200
F	-6.269455	5.727205	0.998301
C	-6.887710	4.347720	-0.806573
F	-6.431744	5.242073	-1.698197
O	0.517016	-0.342471	2.154320
O	0.457104	-0.270316	-1.881183
C	-0.595486	-0.298693	-2.868612
C	-0.090283	-0.770651	-4.224518
H	-1.069605	0.705120	-2.950185
H	-1.358647	-0.996005	-2.470731

H	0.360120	-1.780985	-4.152087
H	0.671818	-0.074167	-4.632929
H	-0.928885	-0.812668	-4.949142
H	1.163438	0.319989	-2.212676

2. UV-visible absorption spectra

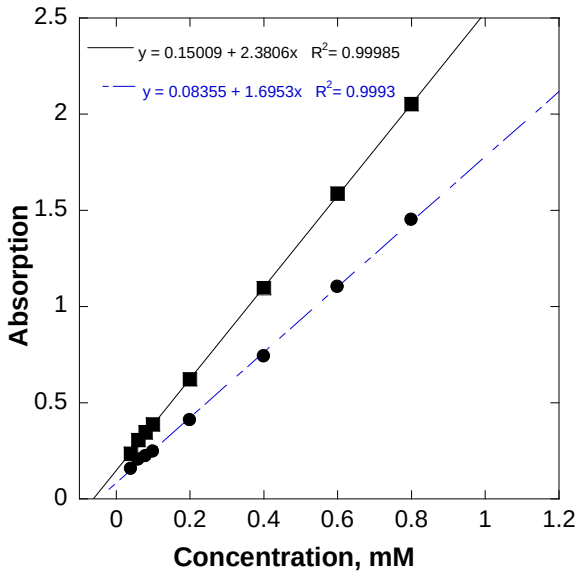

Figure S1. Absorption vs. concentration plot for F_{64}PcVO in ethanol: comparative plots at 396 and 324 nm. The three lowest and the single highest values have been excluded from the fits.

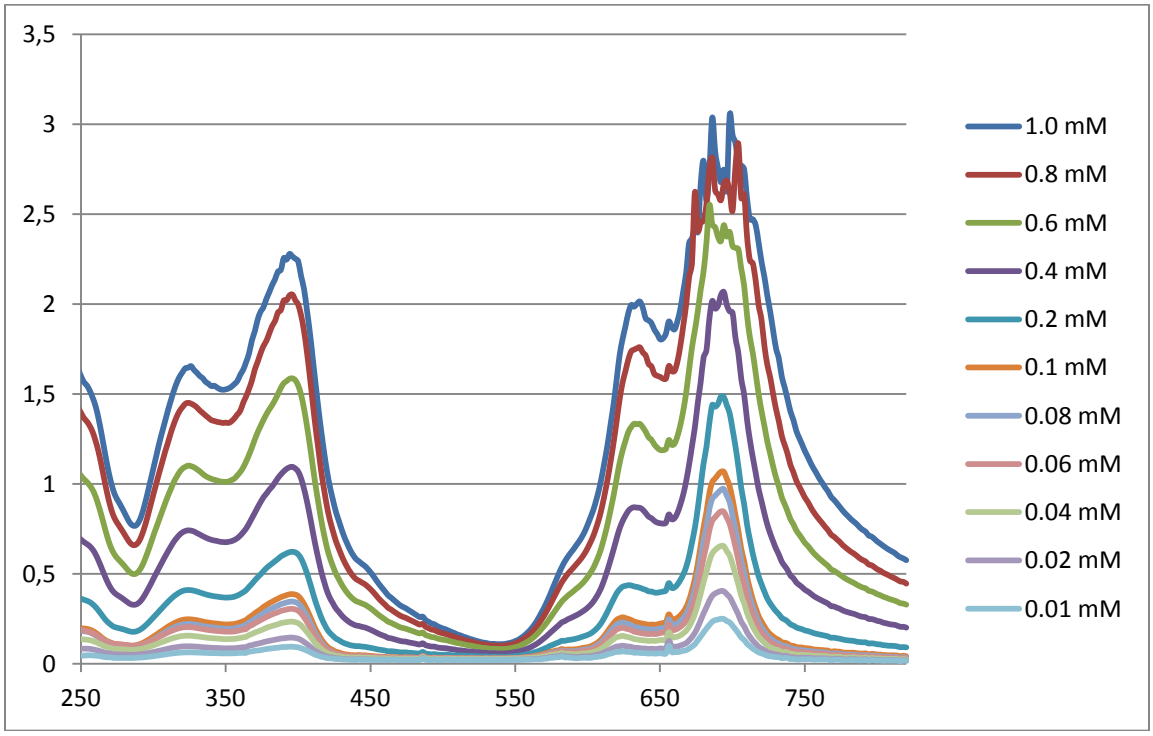

Figure S2. Absorption vs. concentration spectra of F_{64}PcVO in ethanol, 1 mm cell. The onset of saturation is observed above absorptions of 1.