

Supplementary information

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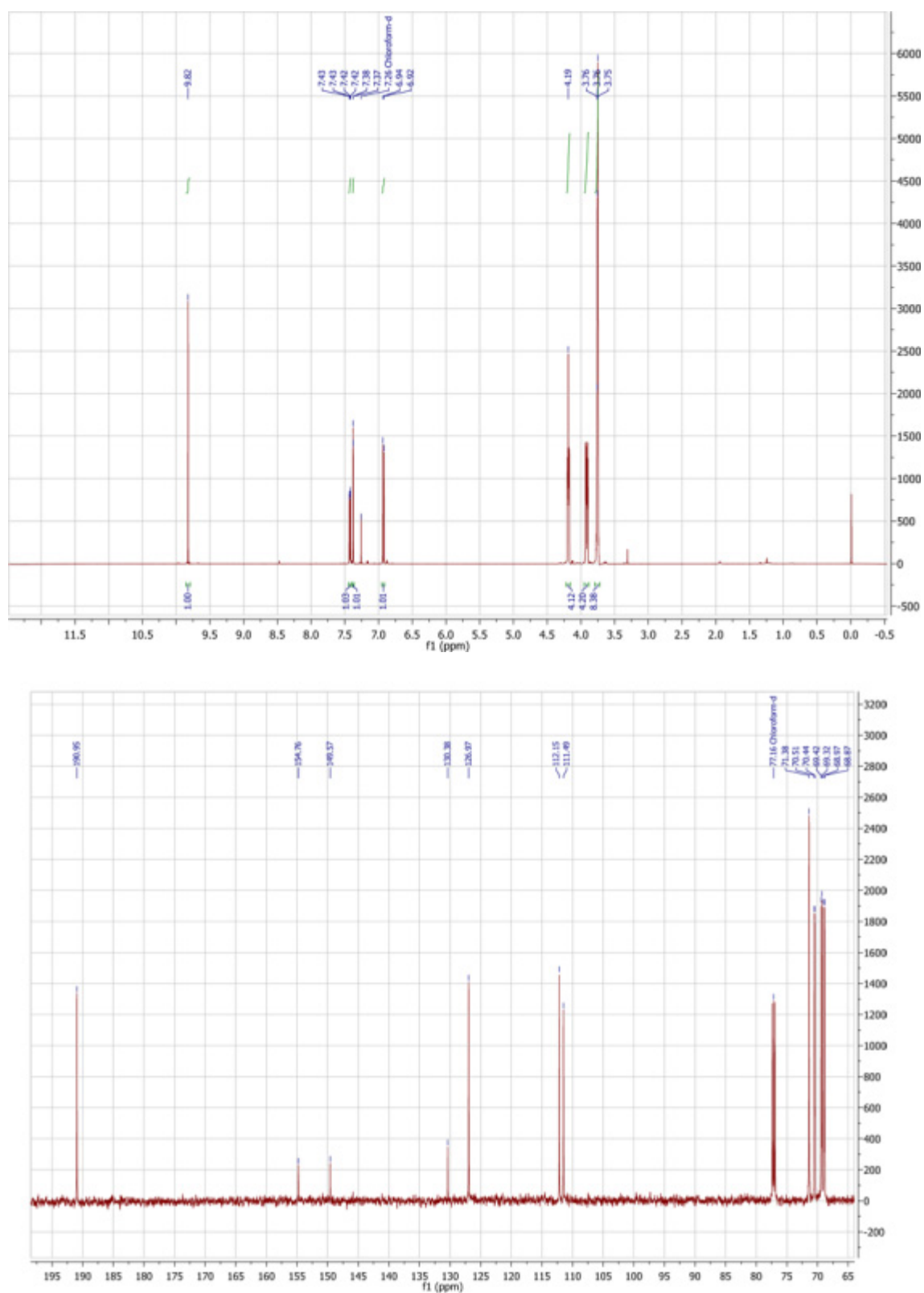
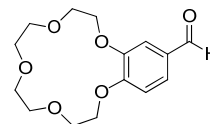
Figure S1. ^1H and ^{13}C -NMR spectra of aldehyde **2**

Figure S2. ^1H and ^{13}C -NMR spectra of phenol **3**

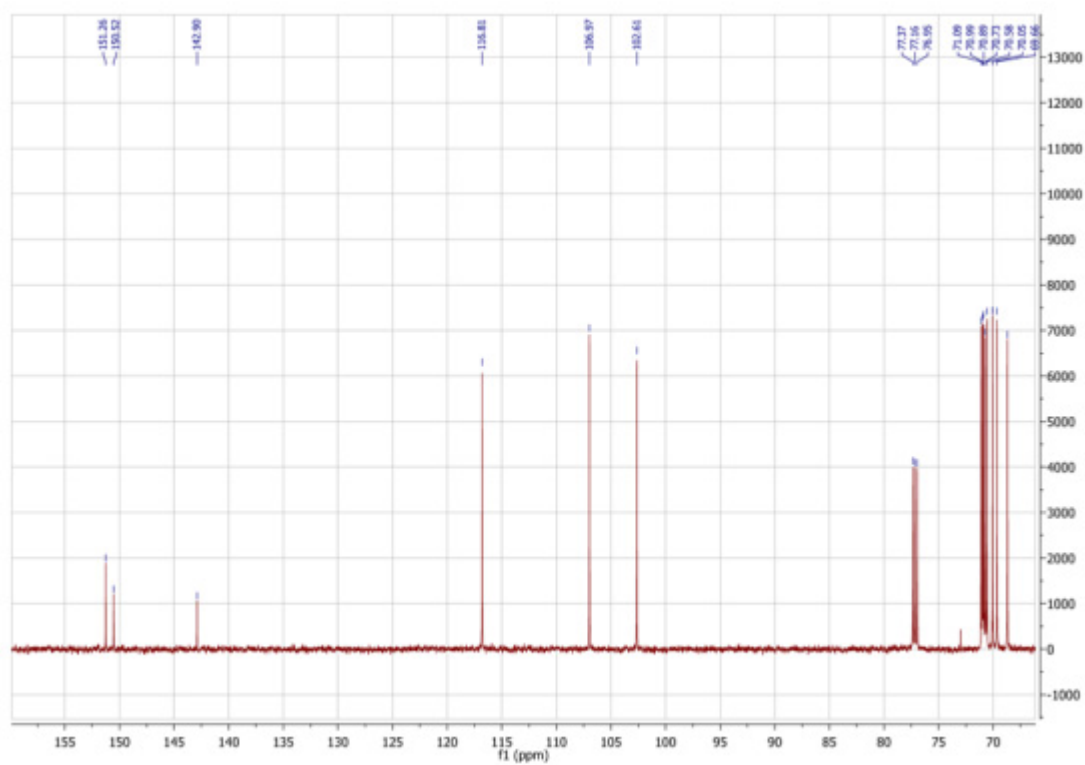
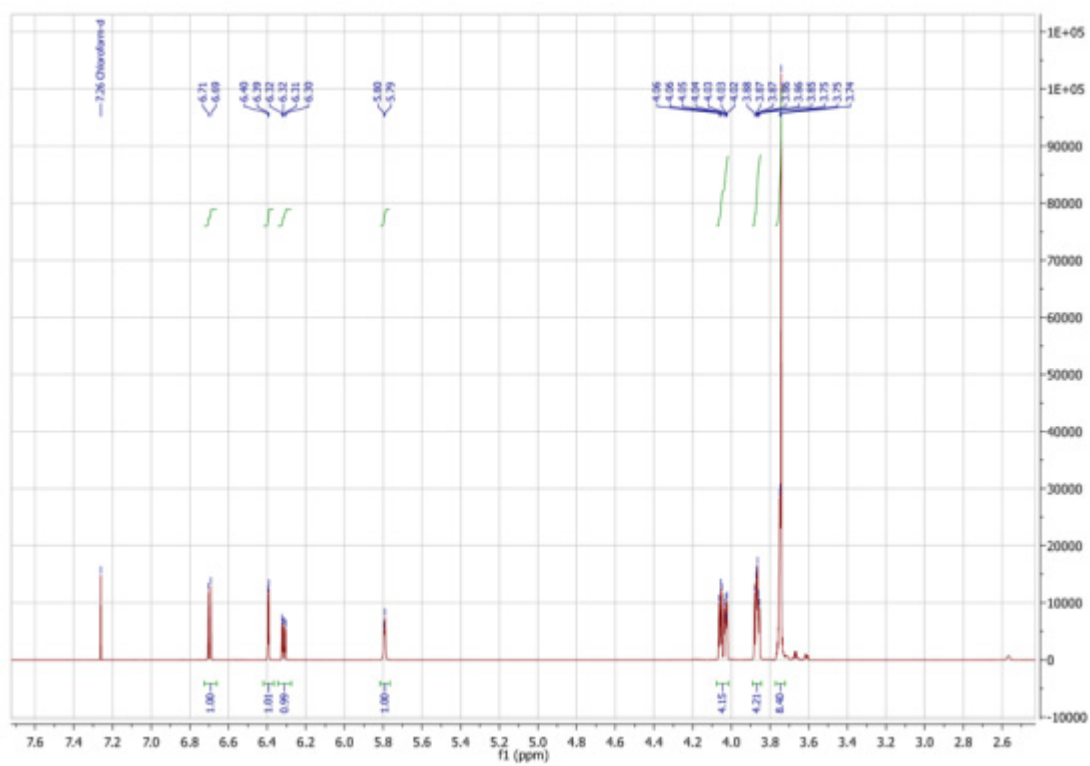
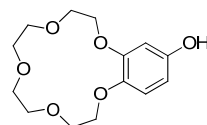


Figure S3. ^1H and ^{13}C -NMR spectra of quinone **4**

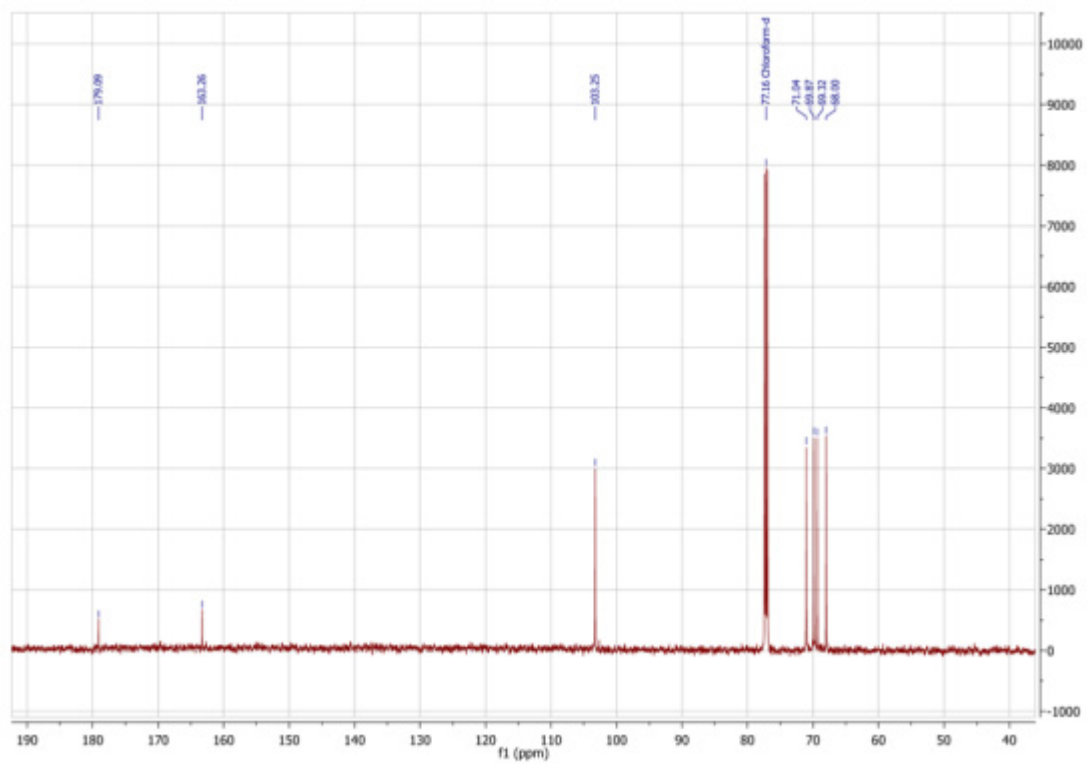
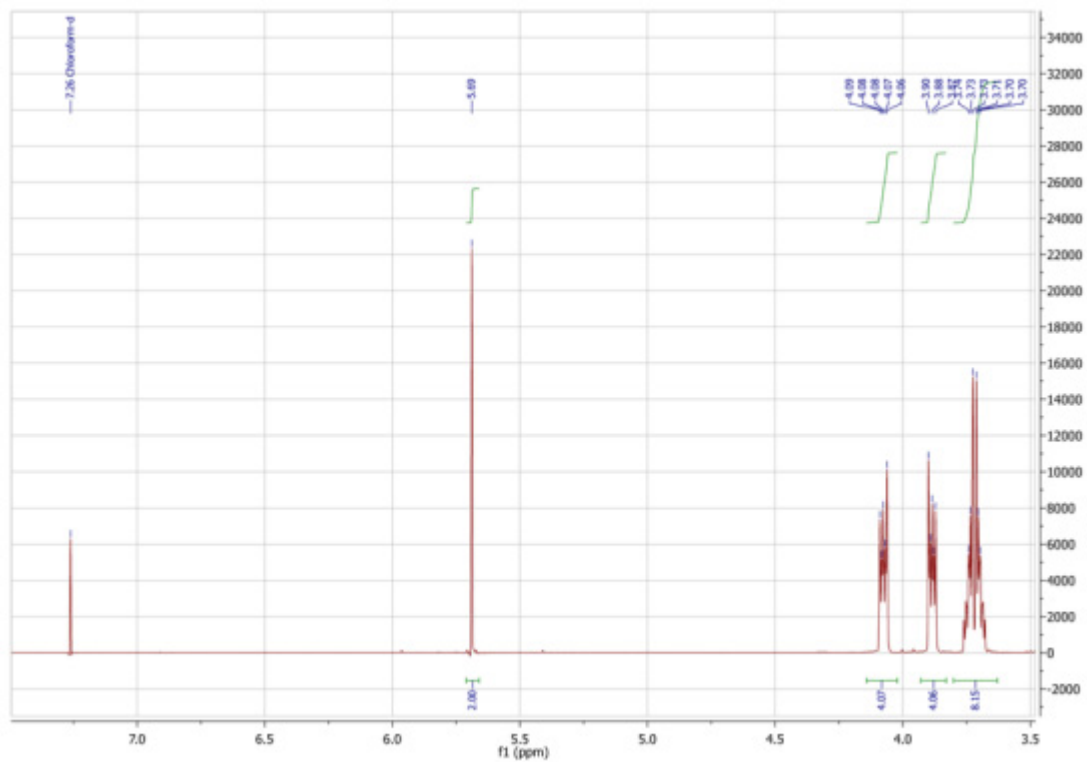
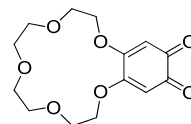


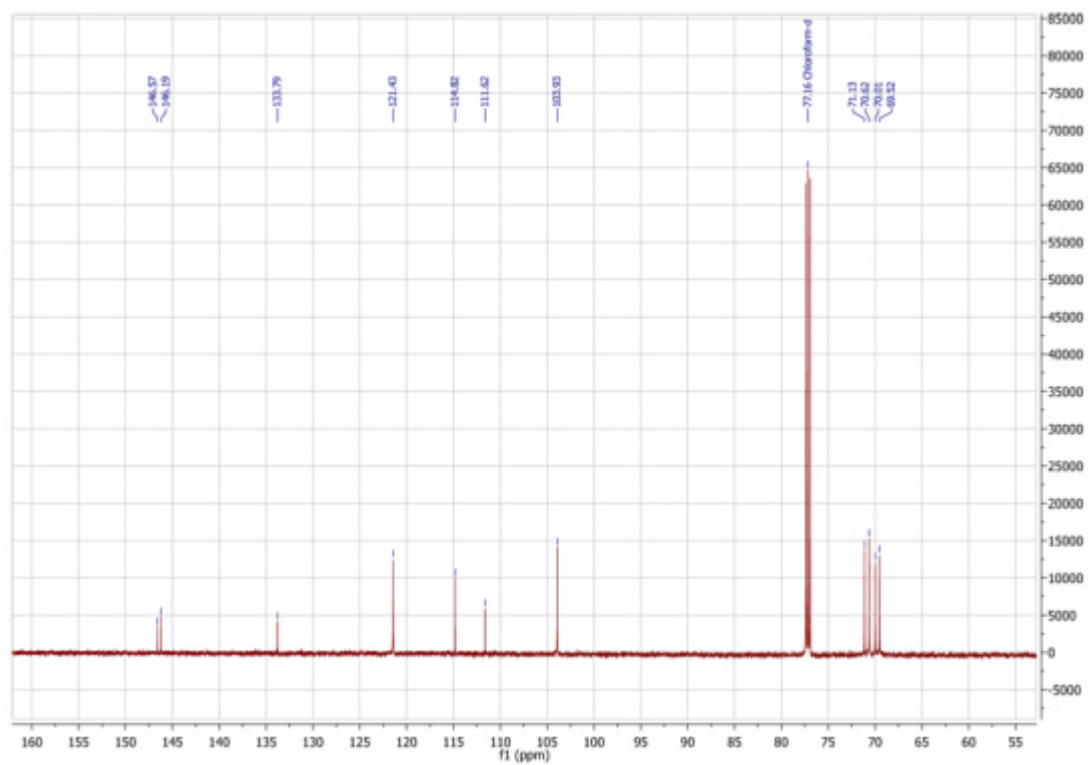
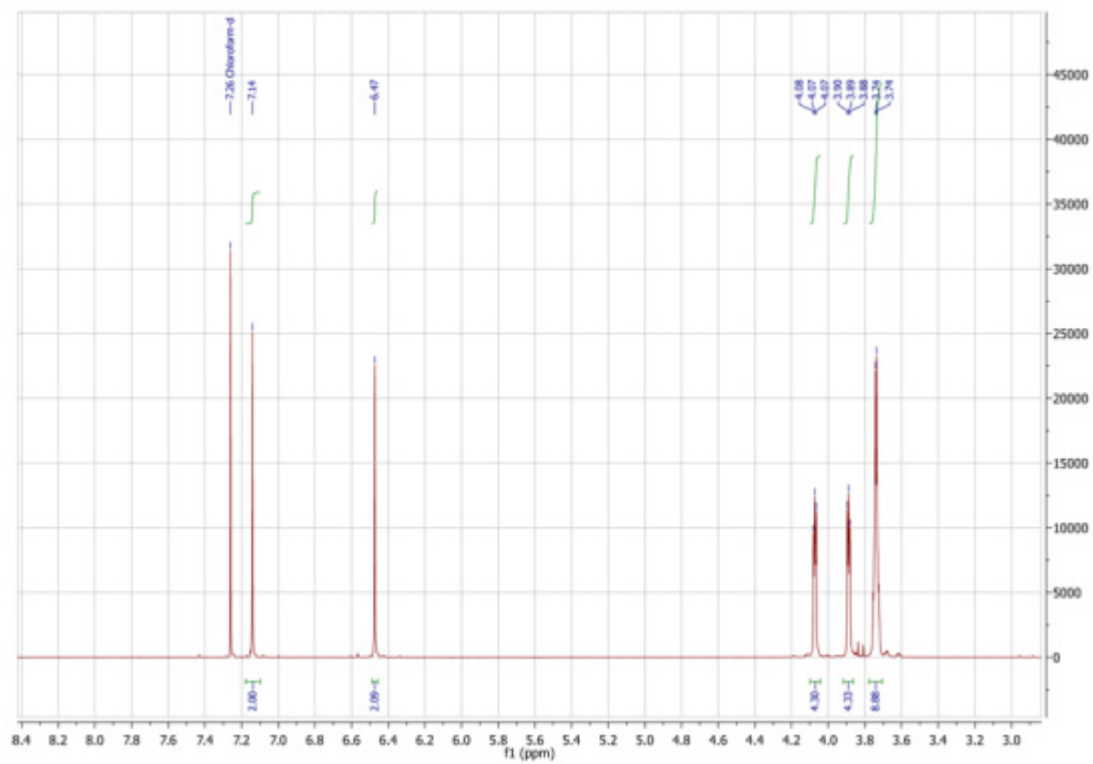
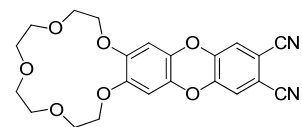
Figure S4. ^1H and ^{13}C -NMR spectra of phthalonitrile **7**

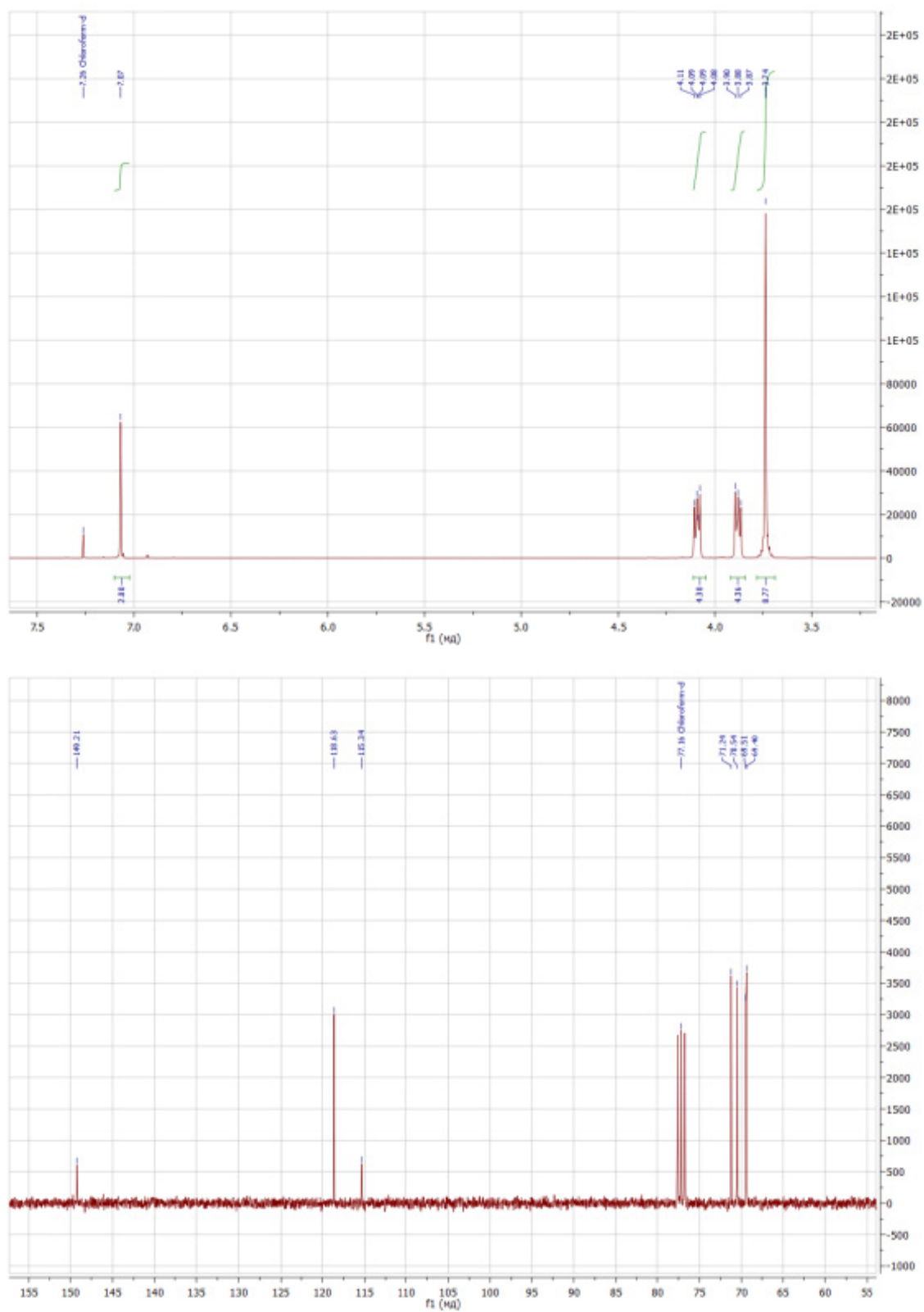
Figure S5. ^1H and ^{13}C -NMR spectra of dibromide **9**

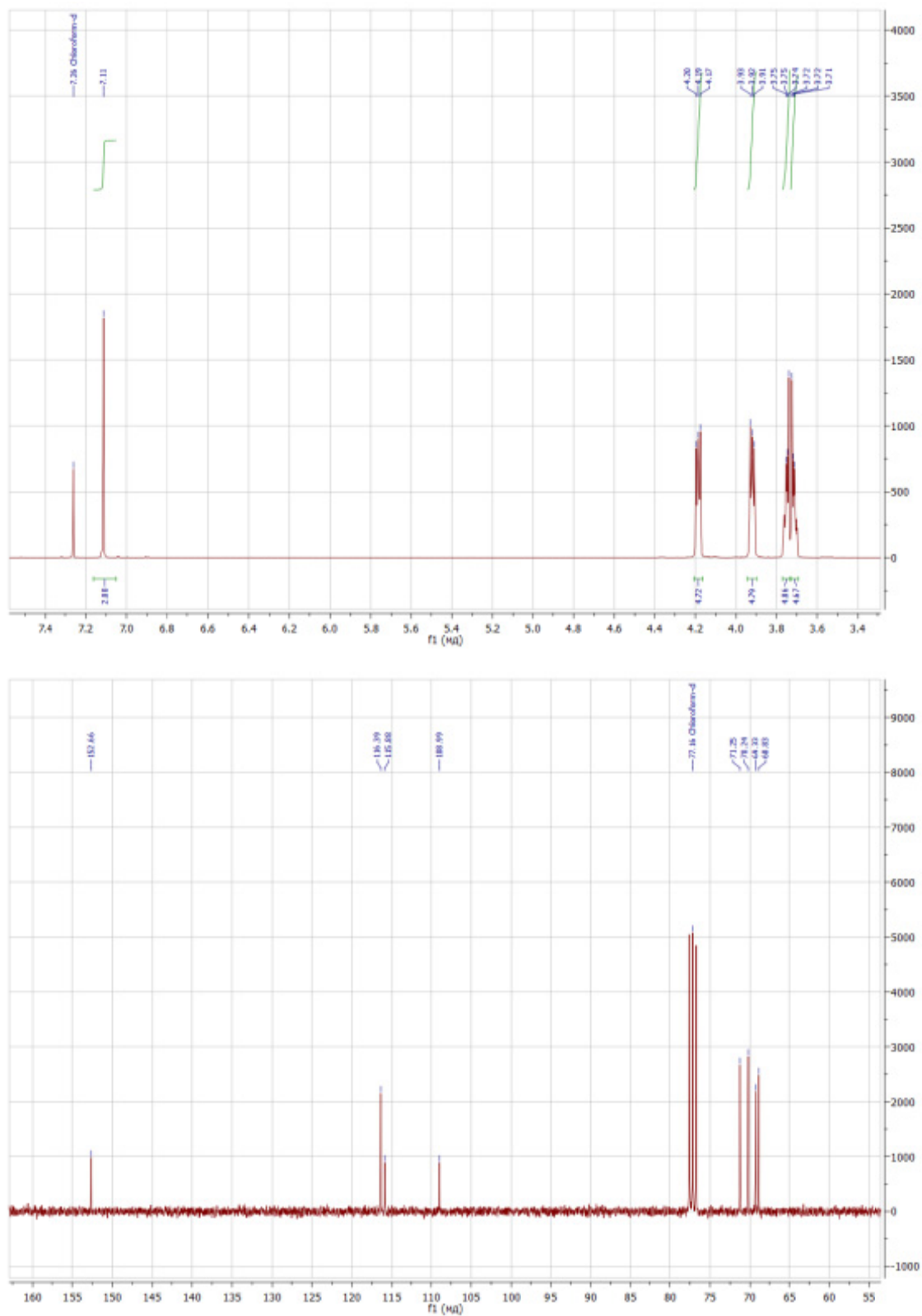
Figure S6. ^1H and ^{13}C -NMR spectra of phthalonitrile **10**

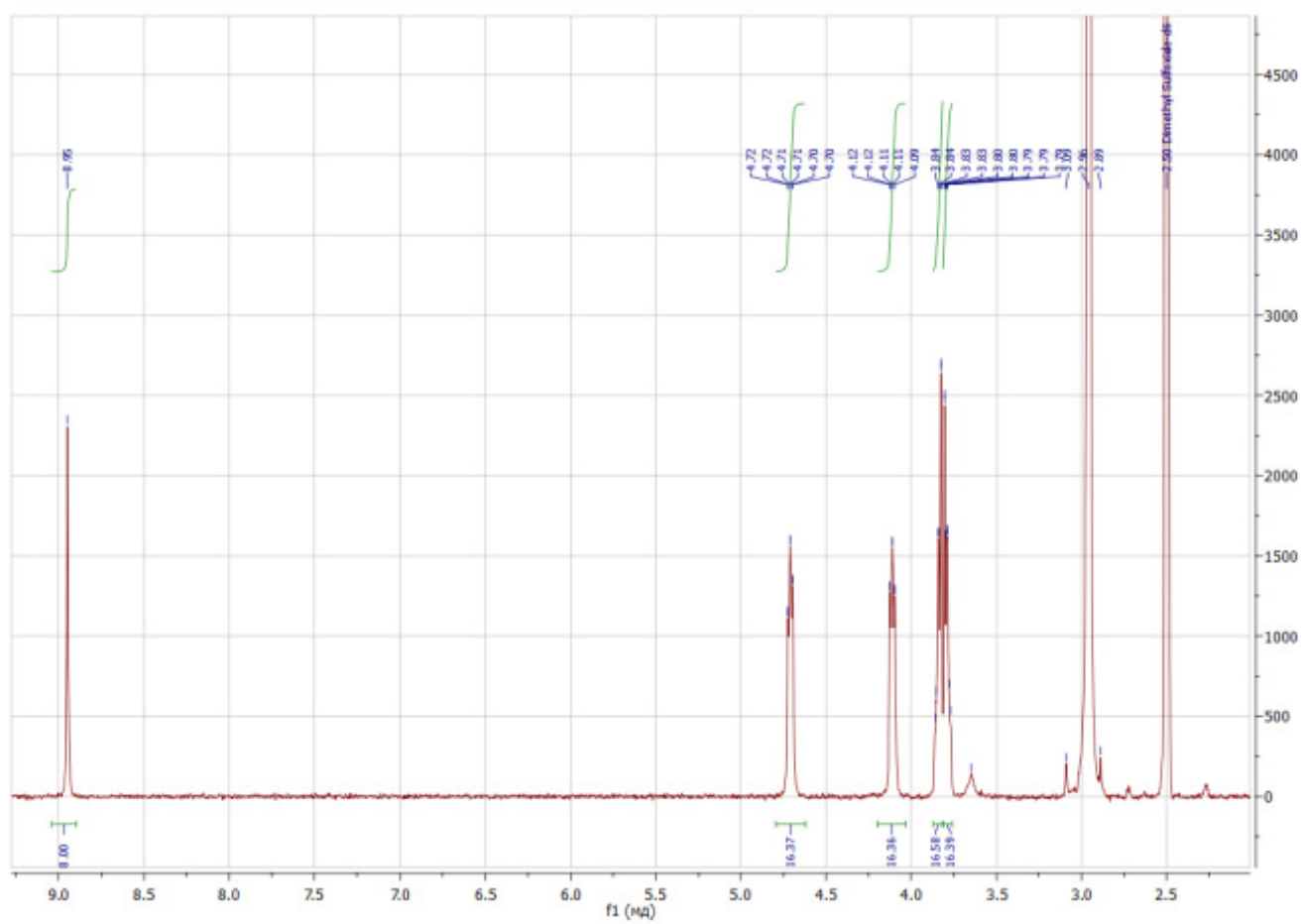
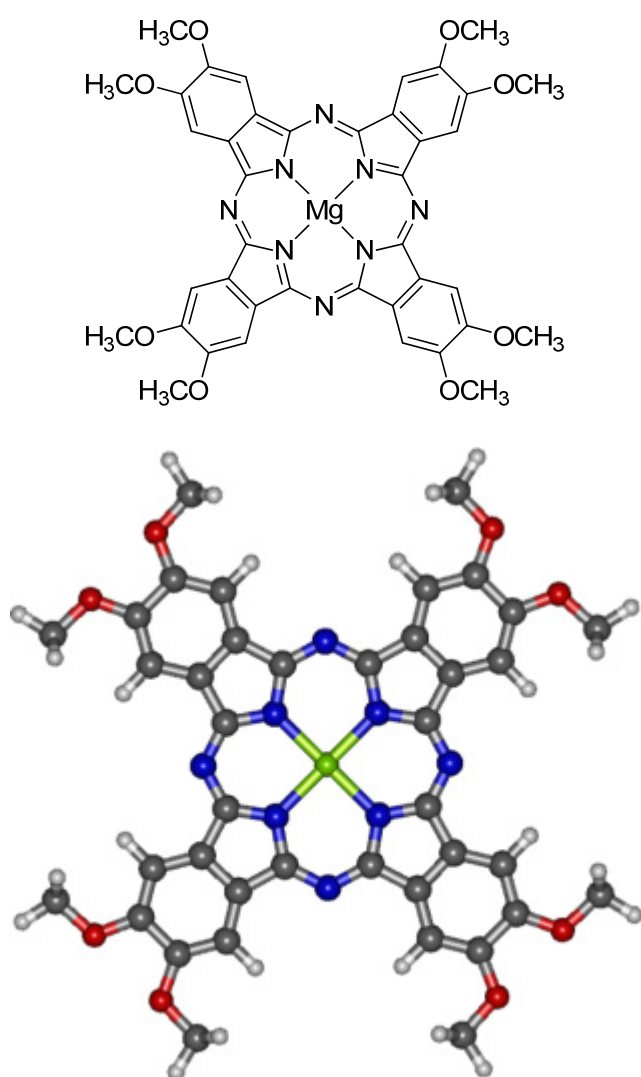
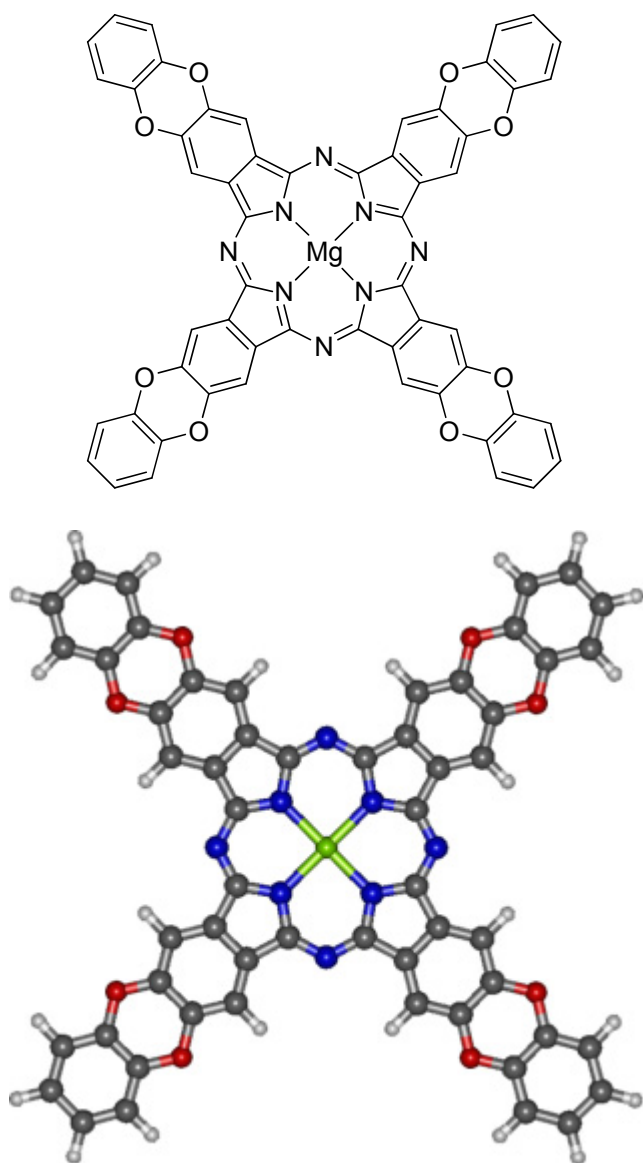
Figure S7. ^1H spectrum of complex **11**

Table S1. DFT-optimized (BP/TZV) structure of Mg[(MeO)₈Pc]-----
CARTESIAN COORDINATES (ANGSTROM)

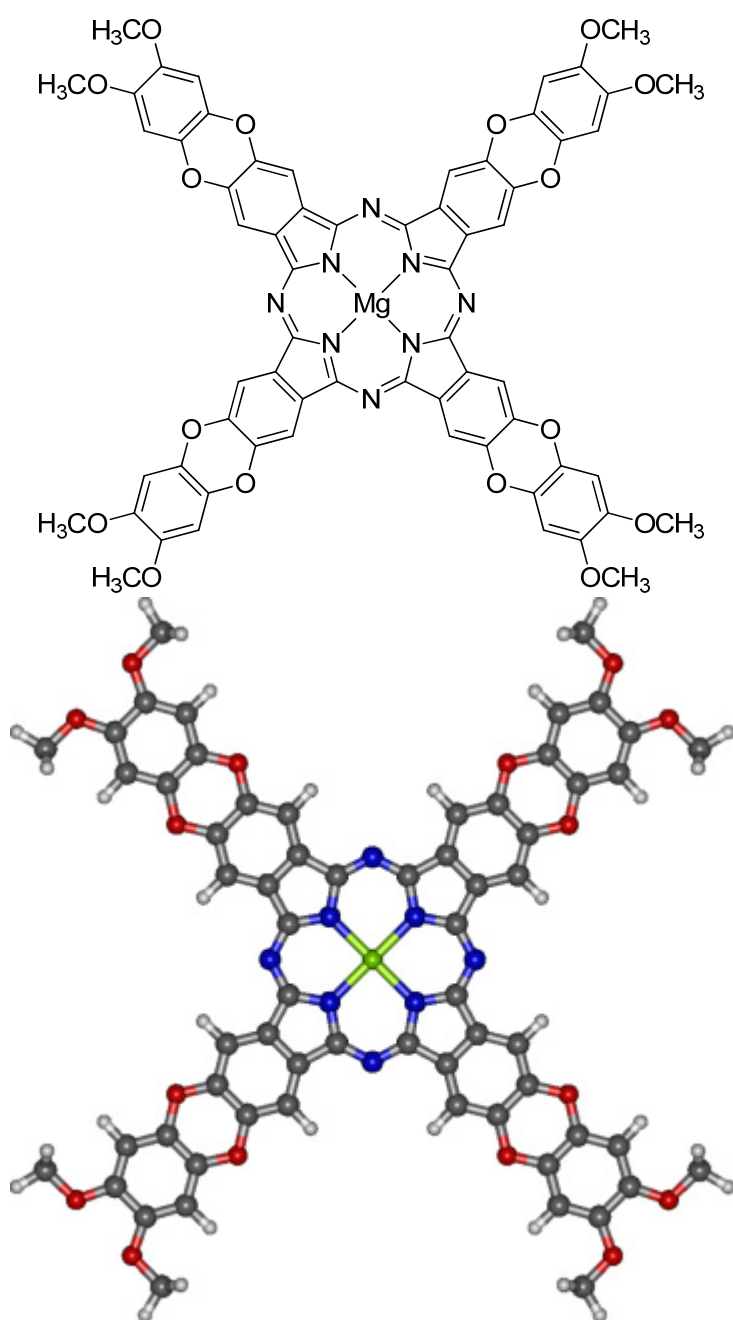
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N	0.293989	-1.986833	-0.001008
C	1.524526	-2.608265	-0.000965
C	4.053443	1.311740	-0.000772
C	4.259534	-0.081894	-0.000770
C	2.937884	-0.703949	-0.000945
N	1.986813	0.294022	-0.001020
C	2.608228	1.524571	-0.000925
N	2.730503	-2.026702	-0.000937
C	-1.311745	4.053473	-0.000798
C	0.081866	4.259568	-0.000804
C	0.703933	2.937935	-0.000920
N	-0.294046	1.986868	-0.000992
C	-1.524616	2.608261	-0.000910
N	2.026675	2.730536	-0.000901
C	-4.053463	-1.311803	-0.000761
C	-4.259607	0.081829	-0.000735
C	-2.937967	0.703958	-0.000896
N	-1.986878	-0.293967	-0.000979
C	-2.608257	-1.524526	-0.000914
N	-2.026690	-2.730486	-0.000918
N	-2.730596	2.026709	-0.000878
C	-2.201196	5.135014	-0.000666
C	-1.676531	6.426749	-0.000542
C	-0.255699	6.636790	-0.000557
C	0.620279	5.552174	-0.000679
C	5.134959	2.201190	-0.000592
C	6.426687	1.676549	-0.000430
C	6.636738	0.255726	-0.000419
C	5.552132	-0.620284	-0.000599
C	-5.134945	-2.201308	-0.000604
C	-6.426715	-1.676697	-0.000432
C	-6.636797	-0.255873	-0.000391
C	-5.552226	0.620186	-0.000556
C	2.201101	-5.135056	-0.000713
C	1.676335	-6.426746	-0.000633
C	0.255481	-6.636724	-0.000682
C	-0.620444	-5.552060	-0.000795
O	7.570707	2.422389	-0.000262
O	7.947604	-0.127223	-0.000259
O	-2.422354	7.570787	-0.000400
O	0.127268	7.947657	-0.000416
O	-7.570720	-2.422578	-0.000280
O	-7.947671	0.127049	-0.000201
O	2.422085	-7.570824	-0.000514
O	-0.127548	-7.947571	-0.000592
Mg	-0.000005	-0.000044	-0.001173
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H	1.699893	5.690803	-0.000669
H	4.955231	3.274718	-0.000587
H	5.690788	-1.699894	-0.000608
H	-4.955169	-3.274825	-0.000616
H	-5.690920	1.699789	-0.000537

H	3.274642	-4.955408	-0.000684
H	-1.700064	-5.690625	-0.000811
C	8.214061	-1.530865	-0.000189
H	7.802274	-2.017581	0.899134
H	9.305601	-1.624113	-0.000002
H	7.802601	-2.017609	-0.899639
C	7.419660	3.843105	-0.000188
H	6.884680	4.189860	0.899119
H	6.884949	4.189983	-0.899610
H	8.437560	4.248131	-0.000001
C	1.530914	8.214085	-0.000412
H	2.017658	7.802354	0.898915
H	1.624175	9.305629	-0.000281
H	2.017622	7.802558	-0.899850
C	-3.843065	7.419768	-0.000367
H	-4.189871	6.884853	0.898958
H	-4.189931	6.885010	-0.899769
H	-4.248087	8.437671	-0.000258
C	-8.214167	1.530683	-0.000115
H	-7.802406	2.017407	0.899209
H	-9.305714	1.623891	0.000068
H	-7.802699	2.017466	-0.899544
C	-7.419630	-3.843280	-0.000241
H	-6.884635	-4.190046	0.899055
H	-6.884924	-4.190130	-0.899677
H	-8.437510	-4.248357	-0.000062
C	-1.531206	-8.213927	-0.000606
H	-2.017935	-7.802186	0.898728
H	-1.624525	-9.305466	-0.000508
H	-2.017889	-7.802347	-0.900037
C	3.842805	-7.419886	-0.000472
H	4.189638	-6.885004	0.898868
H	4.189704	-6.885125	-0.899859
H	4.247768	-8.437812	-0.000388

Table S2. DFT-optimized (BP/TZV) structure of Mg[(Ox)₄Pc]-----
CARTESIAN COORDINATES (ANGSTROM)

C	-1.607886	-3.946806	-0.020236
C	-2.811171	-3.202789	-0.020253
C	-2.432661	-1.791683	-0.016317
N	-1.056941	-1.710424	-0.013636
C	-0.514741	-2.977353	-0.016308
C	3.946790	-1.607992	-0.019527
C	3.202787	-2.811280	-0.019414
C	1.791638	-2.432756	-0.016081
N	1.710393	-1.057023	-0.013477
C	2.977328	-0.514820	-0.016193
N	0.781098	-3.309223	-0.016748
C	1.607880	3.946649	-0.020156
C	2.811157	3.202642	-0.020233
C	2.432700	1.791535	-0.016299
N	1.056970	1.710234	-0.013641
C	0.514743	2.977156	-0.016287
N	3.309200	0.781022	-0.016838
C	-3.946762	1.607888	-0.019460
C	-3.202688	2.811135	-0.019285
C	-1.791599	2.432522	-0.016056
N	-1.710377	1.056814	-0.013509
C	-2.977329	0.514666	-0.016172
N	-3.309174	-0.781176	-0.016835
N	-0.781080	3.309005	-0.016707
C	1.626450	5.342772	-0.024837
C	2.863747	5.978703	-0.029657
C	4.068096	5.233947	-0.029630
C	4.051918	3.842900	-0.024921
C	5.342939	-1.626634	-0.023632
C	5.978919	-2.863980	-0.027359
C	5.234127	-4.068328	-0.027092
C	3.843053	-4.052064	-0.023278
C	-5.342921	1.626634	-0.023536
C	-5.978772	2.864050	-0.027121
C	-5.233895	4.068343	-0.026776
C	-3.842824	4.051962	-0.023040
C	-1.626492	-5.342942	-0.024998
C	-2.863853	-5.978820	-0.029793
C	-4.068171	-5.234006	-0.029707
C	-4.051939	-3.842977	-0.024928
O	7.362291	-2.868878	-0.031431
C	7.978957	-4.110518	-0.033187
C	7.242637	-5.301077	-0.032802
O	5.856306	-5.303848	-0.030667
O	2.868545	7.362010	-0.034962
C	4.110085	7.978613	-0.038583
C	5.300659	7.242333	-0.038442
O	5.303552	5.856095	-0.034697
O	-7.362151	2.869081	-0.031080
C	-7.978709	4.110776	-0.033097
C	-7.242302	5.301269	-0.032626
O	-5.855975	5.303923	-0.030156
O	-2.868736	-7.362123	-0.035170
C	-4.110313	-7.978660	-0.038741
C	-5.300840	-7.242323	-0.038574

O	-5.303659	-5.856092	-0.034822
C	9.370934	-4.150332	-0.035697
C	10.031901	-5.382339	-0.037792
C	9.297396	-6.569950	-0.037386
C	7.899877	-6.528757	-0.034880
C	-4.150046	-9.370536	-0.043030
C	-5.381994	-10.031385	-0.047228
C	-6.569584	-9.296839	-0.047049
C	-6.528460	-7.899422	-0.042679
C	-9.370685	4.150699	-0.035916
C	-10.031548	5.382766	-0.038209
C	-9.296943	6.570319	-0.037689
C	-7.899430	6.529014	-0.034909
C	4.149765	9.370489	-0.042878
C	5.381666	10.031403	-0.047086
C	6.569301	9.296932	-0.046922
C	6.528237	7.899519	-0.042561
Mg	0.000014	-0.000106	-0.011810
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H	4.989718	3.287548	-0.025279
H	5.933951	-0.710895	-0.024005
H	3.287679	-4.989853	-0.023348
H	-5.934012	0.710950	-0.023942
H	-3.287373	4.989704	-0.023063
H	-0.710760	-5.933958	-0.025405
H	-4.989707	-3.287579	-0.025250
H	9.919259	-3.207724	-0.035969
H	7.301336	-7.440306	-0.034529
H	-3.207443	-9.918867	-0.043118
H	-7.439998	-7.300864	-0.042501
H	-9.919088	3.208135	-0.036255
H	-7.300809	7.440510	-0.034475
H	3.207135	9.918777	-0.042950
H	7.439812	7.301014	-0.042396
H	-11.121419	5.408350	-0.040420
H	-9.806427	7.534123	-0.039477
H	5.407065	11.121186	-0.050557
H	7.532968	9.806439	-0.050251
H	11.121778	-5.407833	-0.039774
H	9.806961	-7.533706	-0.039037
H	-5.407459	-11.121165	-0.050707
H	-7.533269	-9.806298	-0.050377

Table S3. DFT-optimized (BP/TZV) structure of Mg[(MeO₂Ox)₄Pc]

 CARTESIAN COORDINATES (ANGSTROM)

C	3.323557	2.667982	0.020493
C	2.266815	3.608738	0.020433
C	1.022644	2.843148	0.018695
N	1.337443	1.501194	0.017290
C	2.706765	1.343497	0.018650
C	2.668125	-3.323677	0.020053
C	3.608905	-2.266949	0.020181
C	2.843349	-1.022672	0.018449
N	1.501411	-1.337500	0.017070
C	1.343702	-2.706807	0.018248
N	3.395026	0.196209	0.018896
C	-3.323488	-2.668134	0.019449
C	-2.266765	-3.608913	0.019414
C	-1.022524	-2.843352	0.017849
N	-1.337316	-1.501406	0.016560
C	-2.706637	-1.343684	0.017805
N	0.196371	-3.395031	0.018339
C	-2.667947	3.323455	0.020182
C	-3.608798	2.266798	0.019864
C	-2.843215	1.022493	0.018064
N	-1.501263	1.337301	0.017046
C	-1.343555	2.706598	0.018565
N	-0.196251	3.394829	0.019030
N	-3.394889	-0.196394	0.018161
C	-4.655741	-3.085801	0.021624
C	-4.914662	-4.453329	0.023290
C	-3.855347	-5.396216	0.023162
C	-2.527082	-4.980541	0.021447
C	3.085775	-4.655958	0.022335
C	4.453327	-4.914836	0.024300
C	5.396182	-3.855508	0.024257
C	4.980510	-2.527267	0.022446
C	-3.085536	4.655729	0.022648
C	-4.453054	4.914722	0.024406
C	-5.396008	3.855454	0.023915
C	-4.980393	2.527186	0.021869
C	4.655794	3.085698	0.022759
C	4.914684	4.453237	0.024588
C	3.855348	5.396092	0.024436
C	2.527104	4.980384	0.022565
O	4.848708	-6.239315	0.025381
C	6.221024	-6.466986	0.035977
C	7.143048	-5.430795	0.035757
O	6.757525	-4.094317	0.025033
O	-6.239143	-4.848641	0.024090
C	-6.466875	-6.220917	0.034770
C	-5.430725	-7.143008	0.034588
O	-4.094225	-6.757552	0.023719
O	-4.848299	6.239209	0.025740
C	-6.220595	6.466991	0.036507
C	-7.142729	5.430898	0.035818
O	-6.757335	4.094406	0.024477
O	6.239158	4.848573	0.025670
C	6.466848	6.220889	0.035521
C	5.430678	7.142947	0.035301

O	4.094169	6.757442	0.025245
C	6.657434	-7.794510	0.046467
C	8.021749	-8.091444	0.056245
C	8.966024	-7.030089	0.055919
C	8.512298	-5.709647	0.045915
C	7.794385	6.657294	0.045328
C	8.091396	8.021604	0.054479
C	7.030079	8.965926	0.054183
C	5.709630	8.512181	0.044815
C	-6.656834	7.794532	0.047657
C	-8.021130	8.091638	0.057596
C	-8.965539	7.030406	0.056773
C	-8.511957	5.709942	0.046116
C	-7.794422	-6.657239	0.045290
C	-8.091469	-8.021505	0.055142
C	-7.030191	-8.965866	0.054897
C	-5.709731	-8.512217	0.044861
O	8.543339	-9.355743	0.066528
C	7.615512	-10.440558	0.066553
O	10.282423	-7.400815	0.065828
C	11.251761	-6.352936	0.065447
O	9.355730	8.543175	0.064101
C	10.440500	7.615307	0.064123
O	7.400844	10.282330	0.063474
C	6.352998	11.251700	0.063060
O	-8.542567	9.355971	0.068479
C	-7.614564	10.440628	0.069663
O	-10.281910	7.401267	0.066899
C	-11.251375	6.353529	0.065999
O	-9.355817	-8.542973	0.065448
C	-10.440550	-7.615070	0.065282
O	-7.401002	-10.282226	0.064914
C	-6.353196	-11.251641	0.064603
Mg	0.000039	-0.000146	0.015342
H	-5.483283	-2.376461	0.021843
H	-1.726530	-5.720190	0.021527
H	2.376441	-5.483504	0.022481
H	5.720159	-1.726713	0.022605
H	-2.376126	5.483208	0.023144
H	-5.720100	1.726686	0.021686
H	5.483358	2.376383	0.022972
H	1.726536	5.720016	0.022626
H	5.904579	-8.580391	0.046468
H	9.205111	-4.870339	0.045493
H	8.580241	5.904413	0.045324
H	4.870348	9.205030	0.044412
H	-5.903832	8.580268	0.048009
H	-9.204904	4.870747	0.045332
H	-8.580245	-5.904327	0.045266
H	-4.870478	-9.205102	0.044467
H	8.224711	-11.351083	0.075123
H	6.972641	-10.421051	0.962451
H	6.983732	-10.430660	-0.837390
H	12.227021	-6.851947	0.073879
H	11.168104	-5.726788	-0.838578
H	11.157715	-5.716525	0.961241
H	11.351057	8.224497	0.072195
H	10.421249	6.972762	0.960282
H	10.430276	6.983213	-0.839601
H	6.852044	12.226965	0.070974
H	5.726559	11.167726	-0.840755
H	5.716870	11.158005	0.959101

H	-8.223683	11.351169	0.079004
H	-6.971813	10.420187	0.965617
H	-6.982598	10.431531	-0.834151
H	-12.226596	6.852620	0.074722
H	-11.167822	5.727864	-0.838360
H	-11.157384	5.716652	0.961454
H	-11.351134	-8.224184	0.073826
H	-10.421098	-6.972118	0.961120
H	-10.430522	-6.983412	-0.838724
H	-6.852277	-12.226858	0.073127
H	-5.727043	-11.168129	-0.839432
H	-5.716768	-11.157560	0.960370