6-Azahemiporphycene: A New Member of the Porphyrinoid Family

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SUPPORTING INFORMATION

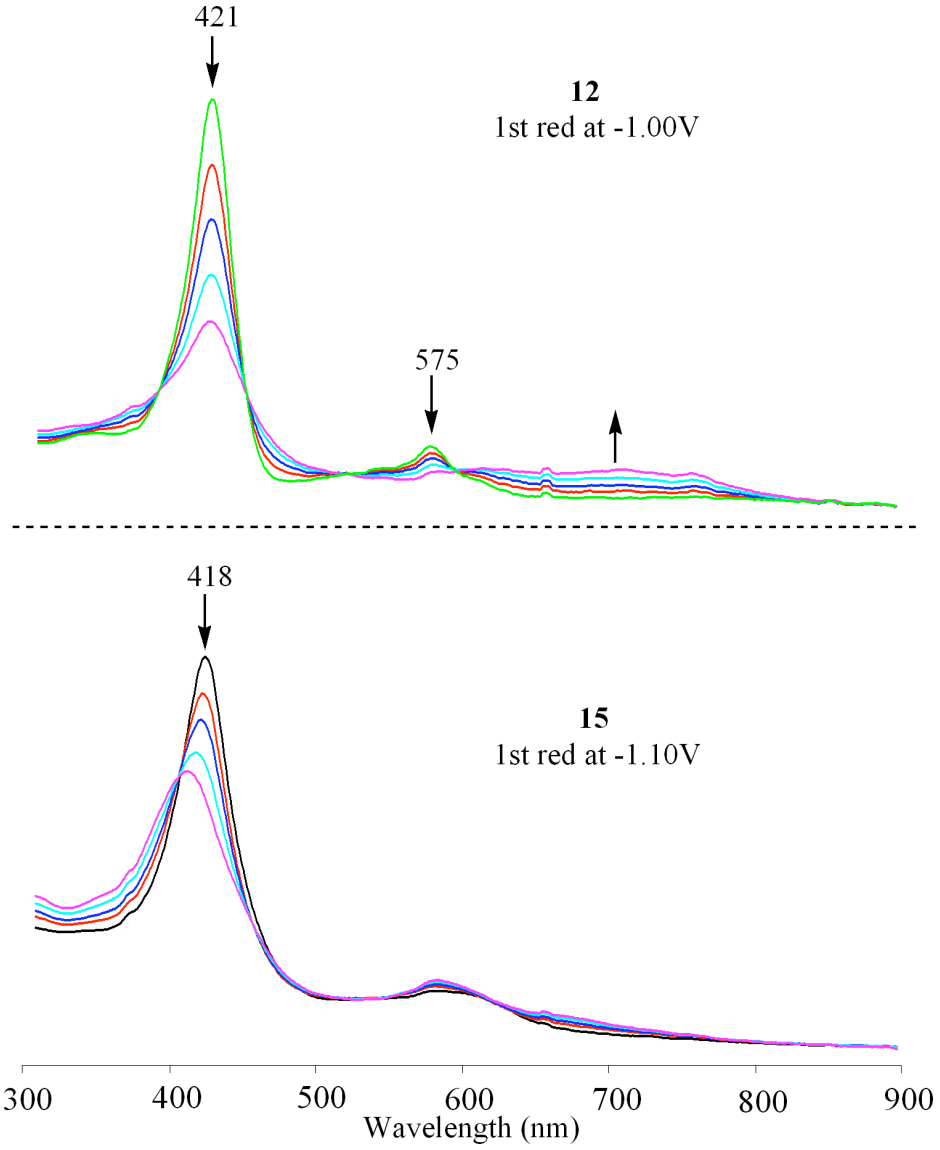


Figure S1. UV-visible spectral changes during the first reduction of free-base and Co^{II} azahemiporphycenes in PhCN, 0.1 M TBAP.

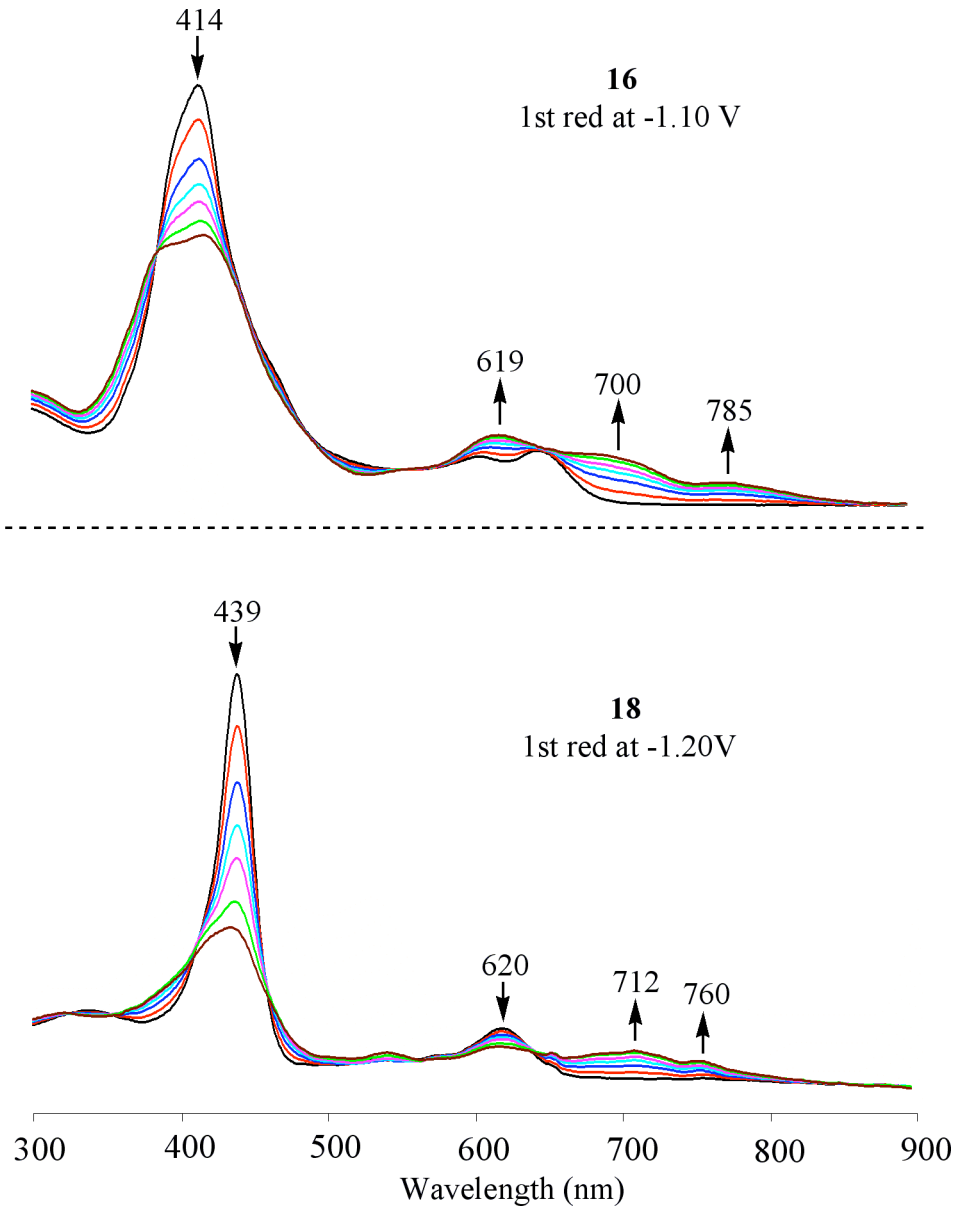


Figure S2. UV-visible spectral changes during the first reduction of the Ni^{II} and Zn^{II} azahemiporphycenes in PhCN, 0.1 M TBAP.

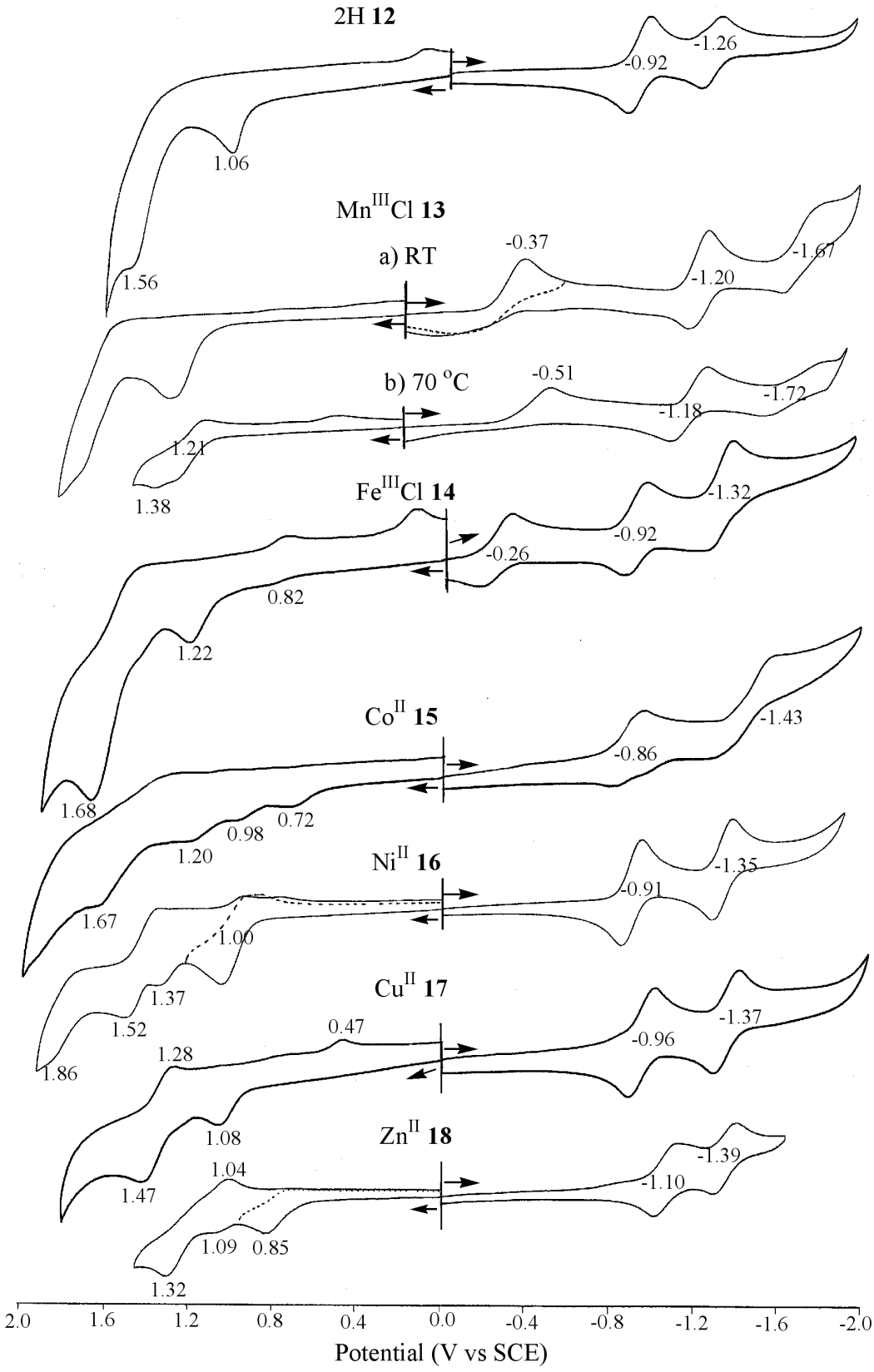


Figure S3. Cyclic voltammograms of M-6-aza-5,11,16-tris-(4-tert-butylphenyl) hemiporphycene in CH_2Cl_2 containing 0.1 M TBAP. M is indicated in the figure.

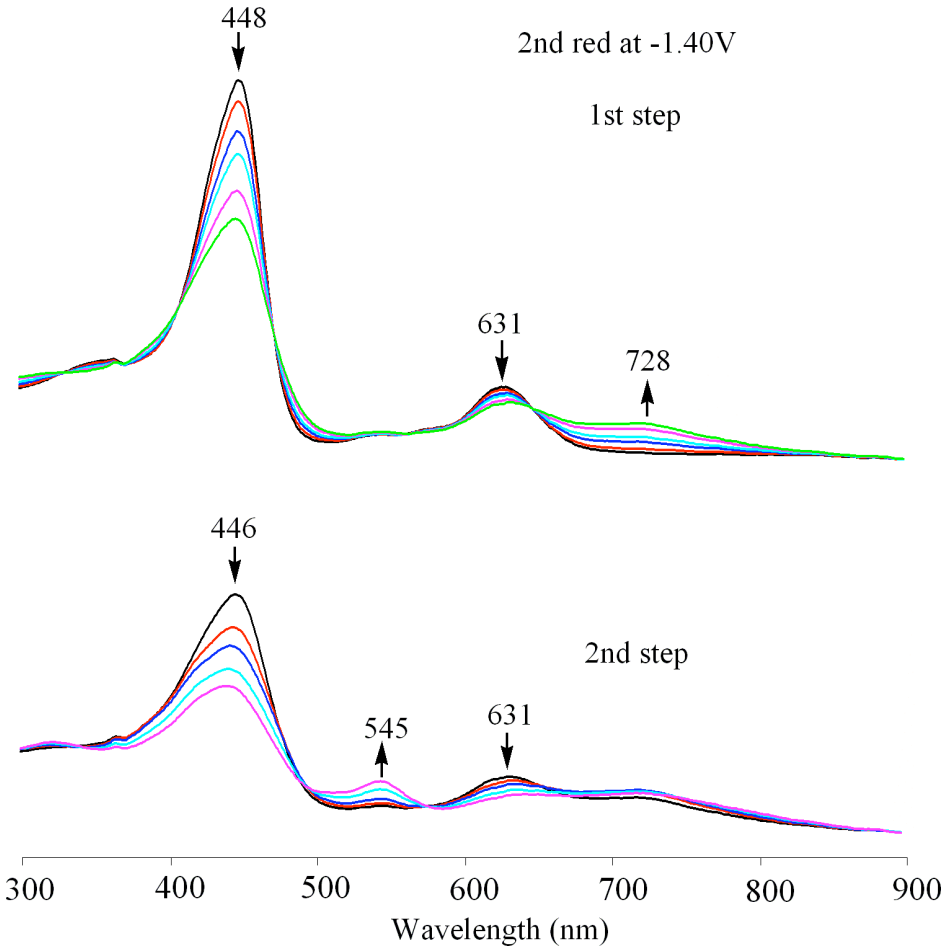
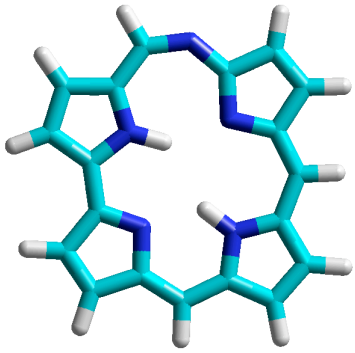


Figure S4. UV-visible spectral changes during the second reduction of the $Mn^{III}Cl$ azahemiporphycene **13** in PhCN, 0.1 M TBAP.

Computational results

6-Azahemiporphycene AC optimized at the B3LYP/6-311+G(d) level

EE (hartrees) = -1005.8020657

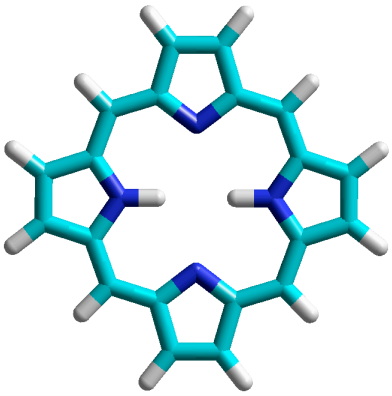


37

C	4.936171	-2.968358	1.244869
C	4.610979	-2.055379	0.193472
N	5.766801	-1.813270	-0.477271
C	6.817558	-2.507377	0.066508
C	6.286491	-3.244380	1.166285
C	3.356684	-1.499316	-0.116992
C	8.127516	-2.432462	-0.448382
C	8.463911	-1.651518	-1.549358
N	7.511597	-0.905666	-2.189532
C	8.107003	-0.271521	-3.195522
C	9.524012	-0.595346	-3.245613
C	9.745897	-1.460864	-2.212296
C	7.296674	0.568596	-4.009448
N	5.966136	0.684115	-3.729166
C	5.361895	1.526736	-4.615619
C	6.368808	1.974831	-5.513857
C	7.563219	1.382353	-5.138707
C	3.991226	1.877784	-4.627352
N	2.962059	1.552746	-3.884967
C	2.818159	0.745392	-2.809001
N	3.699721	-0.016641	-2.113769
C	2.955855	-0.617615	-1.113340
C	1.556323	-0.204560	-1.200230
C	1.471066	0.638481	-2.249085
H	8.895506	-3.017437	0.046015
H	3.743467	2.570553	-5.433952
H	5.450149	0.222586	-2.973189
H	5.914052	-1.211137	-1.286984
H	8.528892	1.504949	-5.606919
H	6.206086	2.656671	-6.336206
H	0.613535	1.161000	-2.646855
H	0.771283	-0.534621	-0.532834
H	4.229355	-3.360012	1.962350

H	6.858461	-3.897620	1.809677
H	10.683806	-1.921543	-1.932139
H	10.246655	-0.223547	-3.958814
H	2.557886	-1.821726	0.544556

Porphyrin optimized at the B3LYP/6-311+G(d) level
EE (hartrees) = -989.771521



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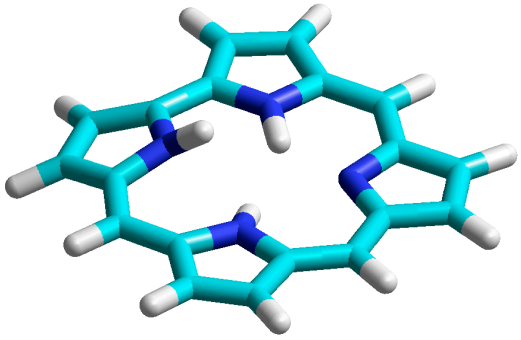
N	2.169081	-2.687098	1.769407
C	1.319849	-3.205879	2.698538
C	2.026989	-4.103647	3.605572
C	3.319836	-4.111227	3.199694
C	3.391203	-3.218532	2.047868
C	-0.048085	-2.930706	2.792014
C	-0.794919	-2.090079	1.970861
C	-2.195980	-1.797691	2.053586
C	-2.507334	-0.921634	1.046507
C	-1.308049	-0.646001	0.310881
N	-0.309515	-1.372904	0.907290
C	-1.156029	0.188234	-0.793512
C	0.022581	0.447363	-1.500246
C	0.094022	1.340236	-2.651929
C	1.387032	1.333217	-3.057298
C	2.094079	0.435173	-2.150461
N	1.244882	-0.083541	-1.221333
C	3.462208	0.160589	-2.243481
C	4.209068	-0.679795	-1.422190
C	5.610185	-0.972088	-1.504806
C	5.921582	-1.847920	-0.497600
C	4.722236	-2.123779	0.237893
N	3.723582	-1.397193	-0.358769
C	4.569944	-2.959048	1.341401
H	2.757611	-1.391150	-0.054799
H	0.656347	-1.379391	0.602974
H	5.469413	-3.459830	1.684370
H	6.888662	-2.273751	-0.271065
H	6.278193	-0.556326	-2.245630
H	1.832694	1.872765	-3.882550
H	-0.737424	1.887727	-3.075902
H	-2.055647	0.688587	-1.136716
H	-3.474314	-0.495453	0.820212
H	-2.863942	-2.213378	2.794491
H	-0.595409	-3.422504	3.589531

H	1.581358	-4.643219	4.430840
H	4.151361	-4.658444	3.623833
H	4.009292	0.651798	-3.041525

Corrole optimized at the B3LYP/6-311+G(d) level
EE (hartrees) = -951.6431401



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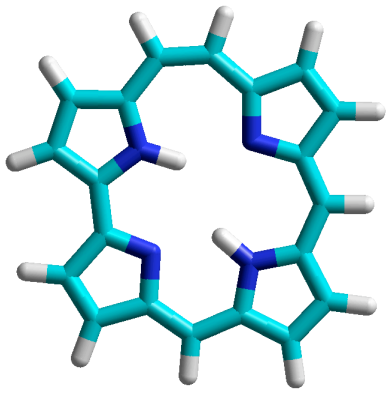
N	2.326160	-2.379036	2.084855
C	1.404993	-3.202959	2.711104
C	2.136951	-4.303270	3.194397
C	3.478982	-4.129174	2.834813
C	3.599537	-2.920035	2.110681
C	0.041339	-2.870710	2.481408
C	-1.240700	-3.267759	2.944908
C	-2.196077	-2.547787	2.229938
C	-1.514218	-1.700874	1.309134
N	-0.183734	-1.920233	1.526741
C	-1.887556	-0.821408	0.274066
C	-0.971270	-0.167411	-0.562027
C	-1.307767	0.783746	-1.605773
C	-0.133050	1.209538	-2.145636
C	0.932027	0.514925	-1.438585
N	0.401412	-0.311676	-0.499902
C	2.310137	0.701868	-1.686150
C	3.373543	0.084510	-1.034786
N	3.227266	-0.874825	-0.053516
C	4.457666	-1.336197	0.405347
C	5.435578	-0.578121	-0.322130
C	4.787676	0.273481	-1.183021
C	4.644482	-2.316714	1.378211
H	2.183591	-1.382926	2.006612
H	5.658136	-2.658805	1.551519
H	4.278500	-4.837638	2.998568
H	1.714128	-5.173481	3.675344
H	-1.430436	-3.988470	3.726961
H	-3.268546	-2.620467	2.341718
H	-2.943866	-0.642887	0.106309
H	-2.309846	1.090274	-1.875910
H	0.006865	1.926128	-2.944329
H	2.572869	1.417609	-2.458067
H	5.243103	0.987052	-1.855185
H	6.503112	-0.664262	-0.175128

H	2.348767	-1.360251	0.035732
H	0.472568	-1.489822	0.872580

Hemiporphycene optimized at the B3LYP/6-311+G(d) level
EE (hartrees) = -989.7622354



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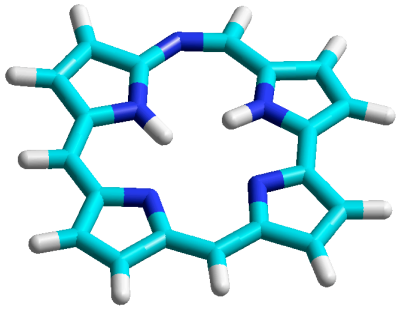
C	0.026937	0.010829	-0.063884
C	-0.002084	0.001762	1.395002
N	1.253933	-0.000882	1.905480
C	2.099374	0.005346	0.813680
C	1.330602	0.013202	-0.423043
C	-1.268112	-0.002688	2.050133
C	-1.700109	-0.010887	3.360293
C	-0.999598	-0.018213	4.582601
N	0.358378	-0.019014	4.719366
C	0.707640	-0.026861	6.043676
C	-0.493097	-0.031329	6.795120
C	-1.545984	-0.026160	5.896472
C	2.076431	-0.029104	6.411382
N	2.986225	-0.023315	5.437741
C	4.219421	-0.026841	6.028219
C	4.059734	-0.035577	7.476453
C	2.716751	-0.036939	7.718671
C	5.378882	-0.022275	5.259280
C	5.361946	-0.013752	3.850821
N	4.202506	-0.009073	3.120029
C	4.458695	-0.001058	1.783327
C	5.883065	-0.000412	1.644375
C	6.434221	-0.008106	2.908148
C	3.492981	0.005281	0.767942
H	6.345749	-0.025328	5.750504
H	-2.779507	-0.011955	3.486634
H	1.001465	-0.014361	3.922559
H	3.296690	-0.011729	3.588691
H	-0.554069	-0.037702	7.873554
H	-2.602098	-0.027621	6.125477
H	-0.844320	0.014688	-0.705095
H	1.752476	0.019363	-1.419353
H	6.409823	0.005224	0.700727
H	7.484111	-0.009784	3.164311
H	4.858964	-0.039982	8.205716

H	2.220888	-0.042644	8.679605
H	3.909281	0.011266	-0.235176
H	-2.085194	0.001454	1.333205

6-Azahemiporphycene AB optimized at the B3LYP/6-311++G(d,p) level
EE (hartrees) = -1005.79603437



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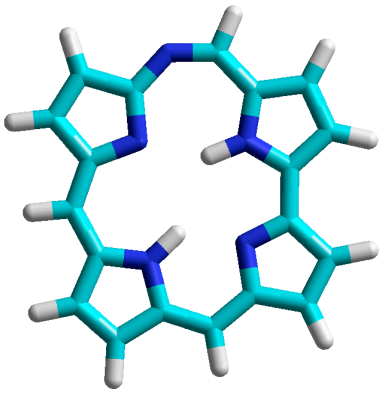
C	4.913985	-3.084684	1.235508
C	4.505514	-2.156666	0.189593
N	5.559352	-1.800204	-0.587646
C	6.637251	-2.444496	-0.081963
C	6.248933	-3.270302	1.060079
C	3.218393	-1.644722	-0.005094
C	7.967486	-2.339197	-0.551989
C	8.413306	-1.515198	-1.578017
N	7.574368	-0.669755	-2.228087
C	8.265347	-0.105159	-3.216001
C	9.646573	-0.562682	-3.226041
C	9.742248	-1.443966	-2.187160
C	7.482342	0.738175	-4.064184
N	6.173965	0.858216	-3.694178
C	5.447962	1.536589	-4.626870
C	6.375326	1.917479	-5.637927
C	7.627359	1.423385	-5.292158
C	4.052258	1.760865	-4.630252
N	3.054614	1.420156	-3.849387
C	2.825118	0.677047	-2.764752
N	3.583165	-0.201277	-1.992466
C	2.802997	-0.735894	-0.978072
C	1.502582	-0.168008	-1.105319
C	1.517116	0.680863	-2.179121
H	8.700555	-2.973169	-0.062365
H	3.739508	2.363631	-5.484085
H	5.895967	0.435321	-2.819118
H	8.541142	1.513217	-5.858371
H	6.118462	2.474144	-6.526583
H	0.714299	1.282484	-2.574076
H	0.676324	-0.388950	-0.446499
H	4.271247	-3.521476	1.986582
H	6.916397	-3.887854	1.644770
H	10.615401	-2.001917	-1.879072
H	10.424723	-0.265326	-3.913751
H	2.446047	-1.961895	0.687798

H 4.534511 -0.549051 -2.089577

6-Azahemiporphycene AC optimized at the B3LYP/6-311++G(d,p) level
EE (hartrees) = -1005.82824421



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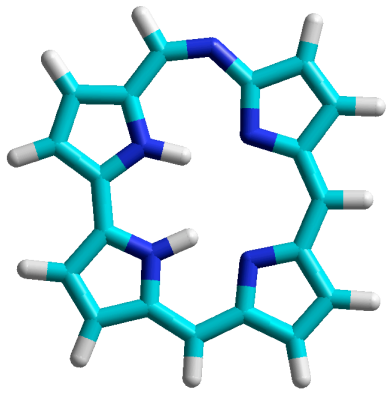
C	4.937840	-2.962536	1.246801
C	4.617278	-2.053062	0.190098
N	5.774836	-1.814320	-0.478039
C	6.821777	-2.508162	0.071858
C	6.287973	-3.240539	1.173661
C	3.363455	-1.498954	-0.124492
C	8.131463	-2.434978	-0.443917
C	8.462378	-1.655668	-1.547955
N	7.506544	-0.911895	-2.185492
C	8.098095	-0.277347	-3.193587
C	9.515348	-0.599549	-3.248566
C	9.741854	-1.463958	-2.215313
C	7.287606	0.564320	-4.005269
N	5.957435	0.684202	-3.725525
C	5.359564	1.531009	-4.612231
C	6.368897	1.976640	-5.509100
C	7.559922	1.378289	-5.133292
C	3.990564	1.887579	-4.625775
N	2.960070	1.560912	-3.885400
C	2.817900	0.749045	-2.812819
N	3.702957	-0.011915	-2.120144
C	2.961664	-0.617891	-1.121338
C	1.560158	-0.210507	-1.207395
C	1.471228	0.635203	-2.253692
H	8.900835	-3.017006	0.049509
H	3.748105	2.583690	-5.430300
H	5.431420	0.225595	-2.970001
H	5.937705	-1.216018	-1.292466
H	8.526221	1.496286	-5.598577
H	6.208989	2.659810	-6.329382
H	0.613380	1.155418	-2.650743
H	0.778586	-0.546636	-0.540926
H	4.228268	-3.349108	1.962572
H	6.857681	-3.890585	1.820288
H	10.679562	-1.923371	-1.937048
H	10.233223	-0.227048	-3.964316

H 2.564112 -1.822065 0.534647

6-Azahemiporphycene AD optimized at the B3LYP/6-311++G(d,p) level
EE (hartrees) = -1005.82135586



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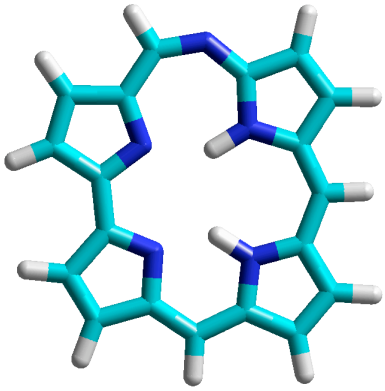
C	2.944573	-3.096949	0.000074
C	1.638553	-2.444681	-0.000142
N	1.792011	-1.115062	-0.000130
C	3.136465	-0.852808	0.000098
C	3.876652	-2.102714	-0.000059
C	0.396864	-3.118591	-0.000199
C	3.628667	0.458711	0.000202
C	2.776692	1.574796	0.000165
N	1.419600	1.387272	0.000304
C	0.757468	2.562486	0.000146
C	1.739667	3.596905	0.000070
C	2.983928	2.987199	0.000085
C	-0.660776	2.559133	0.000165
N	-1.365232	1.385716	0.000250
C	-2.707882	1.649956	0.000110
C	-2.860736	3.061457	0.000119
C	-1.596069	3.622746	0.000098
C	-3.749204	0.690443	0.000024
N	-3.777347	-0.619399	-0.000096
C	-2.779820	-1.533422	-0.000208
N	-1.433183	-1.386536	-0.000026
C	-0.918779	-2.669915	-0.000188
C	-2.009985	-3.646641	-0.000070
C	-3.161029	-2.943823	0.000059
H	4.699792	0.621331	0.000187
H	-4.738286	1.150846	-0.000004
H	-1.037255	0.396393	0.000352
H	-1.345392	4.672164	0.000041
H	-3.807147	3.580393	0.000069
H	-4.182884	-3.290378	0.000206
H	-1.874003	-4.718852	-0.000023
H	3.115901	-4.164036	0.000160
H	4.952691	-2.202094	-0.000054
H	3.944912	3.478957	0.000031
H	1.536520	4.656390	0.000005
H	0.483426	-4.201523	-0.000160

H	1.083626	0.397529	0.000539

6-Azahemiporphycene BC optimized at the B3LYP/6-311++G(d,p) level
EE (hartrees) = -1005.82128754



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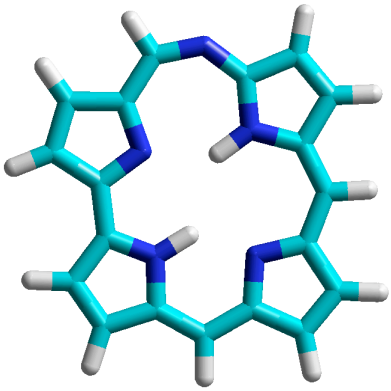
C	4.946743	-2.971475	1.245730
C	4.647040	-2.060925	0.179379
N	5.817709	-1.837772	-0.475879
C	6.848243	-2.539269	0.092441
C	6.293168	-3.263482	1.191725
C	3.400828	-1.502546	-0.138145
C	8.163723	-2.465736	-0.417855
C	8.475765	-1.676593	-1.523033
N	7.494489	-0.952755	-2.135427
C	8.035162	-0.289189	-3.152849
C	9.465220	-0.579431	-3.235153
C	9.738999	-1.445717	-2.217616
C	7.195092	0.541130	-3.945760
N	5.879455	0.639766	-3.654976
C	5.348064	1.490033	-4.571116
C	6.374563	1.953589	-5.487400
C	7.536138	1.355518	-5.091966
C	3.998899	1.884022	-4.646452
N	2.921577	1.591679	-3.932537
C	2.755062	0.803984	-2.875240
N	3.643419	0.021307	-2.158312
C	2.971809	-0.620992	-1.126558
C	1.593617	-0.208744	-1.215958
C	1.462475	0.646654	-2.265332
H	8.936521	-3.043524	0.074245
H	3.788209	2.575710	-5.461903
H	8.516897	1.457919	-5.532822
H	6.225209	2.636641	-6.311317
H	0.579464	1.149020	-2.626442
H	0.825207	-0.549573	-0.538020
H	4.224193	-3.347653	1.954264
H	6.846768	-3.916535	1.849229
H	10.694680	-1.881915	-1.964076
H	10.158555	-0.181737	-3.961593
H	2.599622	-1.820170	0.520592
H	6.067794	-1.252693	-1.301214

H 4.640186 0.007830 -2.456686

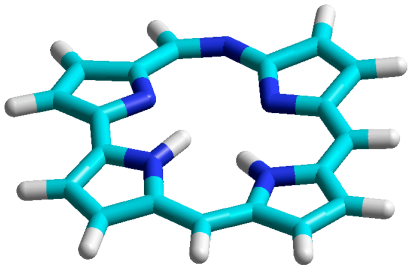
6-Azahemiporphycene BD optimized at the B3LYP/6-311++G(d,p) level
EE (hartrees) = -1005.82774939



37

C	4.948567	-2.986391	1.241745
C	4.656154	-2.059803	0.156284
N	5.775129	-1.789551	-0.542495
C	6.790367	-2.498576	0.036945
C	6.280977	-3.258916	1.165427
C	3.387097	-1.522961	-0.123596
C	8.116564	-2.461159	-0.431475
C	8.504337	-1.692659	-1.531728
N	7.575761	-0.940728	-2.193219
C	8.111344	-0.262420	-3.225671
C	9.505698	-0.589901	-3.251765
C	9.746951	-1.467776	-2.211974
C	7.252119	0.559693	-3.998403
N	5.941644	0.626629	-3.667610
C	5.371578	1.474152	-4.564448
C	6.366671	1.962220	-5.500968
C	7.551580	1.384862	-5.142753
C	4.016594	1.858978	-4.623807
N	2.938905	1.569073	-3.913175
C	2.758059	0.783146	-2.856468
N	3.628781	-0.005264	-2.130466
C	2.947499	-0.641772	-1.104654
C	1.574022	-0.220245	-1.204716
C	1.458963	0.635877	-2.256806
H	8.865635	-3.051899	0.082008
H	3.804440	2.552193	-5.438006
H	8.518450	1.509230	-5.607756
H	6.183235	2.648361	-6.315331
H	0.583240	1.145013	-2.626192
H	0.796969	-0.554243	-0.533320
H	4.232922	-3.369026	1.955427
H	6.863583	-3.906938	1.804562
H	10.693644	-1.913292	-1.945864
H	10.224928	-0.211449	-3.961259
H	2.594487	-1.848996	0.542609
H	6.599191	-0.945311	-1.877534
H	4.622669	-0.056481	-2.380991

6-Azahemiporphycene CD optimized at the B3LYP/6-311++G(d,p) level
EE (hartrees) = -1005.79476173

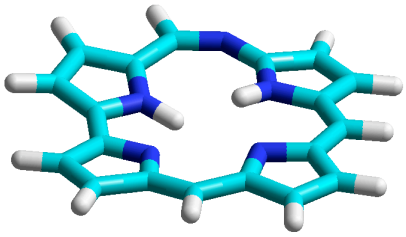


37

C	3.649915	-2.291508	-0.022135
C	2.938299	-1.058041	-0.067884
N	1.604378	-1.365634	-0.105759
C	1.416381	-2.738734	-0.074465
C	2.725329	-3.310469	-0.034293
C	3.426765	0.256176	-0.035276
C	0.203852	-3.435916	-0.034502
C	-1.068952	-2.881245	0.073758
N	-1.294378	-1.544376	0.255404
C	-2.612521	-1.227968	0.160076
C	-3.311625	-2.454121	-0.031900
C	-2.369122	-3.465854	-0.077258
C	-2.881168	0.165529	0.149540
N	-1.781035	0.949645	0.184058
C	-2.204160	2.209953	-0.008233
C	-3.657516	2.241918	-0.130082
C	-4.083144	0.945906	-0.033502
C	-1.379636	3.349632	-0.153362
N	-0.085659	3.578499	-0.099070
C	1.037269	2.850016	-0.010765
N	1.313129	1.522948	-0.101025
C	2.681115	1.429752	-0.018641
C	3.300974	2.748870	0.133679
C	2.283561	3.628626	0.147249
H	0.272075	-4.514878	-0.102488
H	-1.954793	4.261024	-0.334468
H	-5.095055	0.573168	-0.095025
H	-4.262165	3.124083	-0.286470
H	2.301551	4.703897	0.238556
H	4.362414	2.933226	0.219911
H	4.724333	-2.380475	0.025443
H	2.919653	-4.371530	0.009377
H	-2.553978	-4.517212	-0.239088
H	-4.379268	-2.556403	-0.146386
H	4.504404	0.359281	0.022538
H	-0.657863	-0.775786	0.425600

H 0.950481 -0.599283 -0.254351

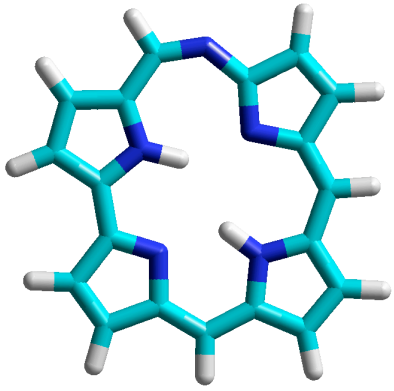
6-Azahemiporphycene AB optimized at the M05-2X/6-311++G(d,p) level
EE (hartrees) = -1005.68442539



37

C	4.911870	-3.096767	1.200724
C	4.513324	-2.173777	0.154485
N	5.570527	-1.818234	-0.617413
C	6.630311	-2.454145	-0.104409
C	6.244765	-3.280232	1.032085
C	3.242706	-1.649924	-0.036719
C	7.972814	-2.342542	-0.558942
C	8.409296	-1.496529	-1.549134
N	7.562492	-0.640195	-2.183061
C	8.239854	-0.080215	-3.159952
C	9.623936	-0.533881	-3.193127
C	9.732359	-1.417604	-2.167666
C	7.455298	0.758956	-4.018261
N	6.156442	0.894445	-3.647226
C	5.439476	1.529177	-4.609473
C	6.351685	1.860688	-5.633834
C	7.604940	1.379025	-5.267952
C	4.038866	1.746227	-4.639668
N	3.044337	1.412454	-3.875505
C	2.839552	0.672594	-2.771814
N	3.600833	-0.213877	-2.036643
C	2.838295	-0.732647	-1.005937
C	1.555522	-0.140894	-1.088043
C	1.557183	0.711248	-2.159906
H	8.699282	-2.989985	-0.083083
H	3.741378	2.329777	-5.508568
H	5.873839	0.544930	-2.744696
H	8.515660	1.430230	-5.838890
H	6.089028	2.370335	-6.545815
H	0.763716	1.333187	-2.534916
H	0.749381	-0.345833	-0.403668
H	4.264865	-3.529551	1.946557
H	6.912010	-3.892560	1.617755
H	10.603986	-1.979180	-1.871774
H	10.386807	-0.227897	-3.889658
H	2.467478	-1.950946	0.656956
H	4.528036	-0.596132	-2.188662

6-Azahemiporphycene AC optimized at the M05-2X/6-311++G(d,p) level
EE (hartrees) = -1005.71853131

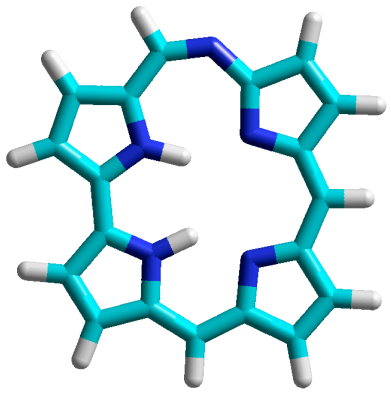


37

C	4.936195	-2.954661	1.231730
C	4.614611	-2.053475	0.185185
N	5.755641	-1.807986	-0.492239
C	6.803181	-2.494503	0.048856
C	6.289238	-3.226830	1.146863
C	3.354797	-1.495408	-0.124712
C	8.118988	-2.422899	-0.462743
C	8.451786	-1.651187	-1.553133
N	7.499958	-0.906311	-2.198865
C	8.097323	-0.280002	-3.188154
C	9.515740	-0.596279	-3.237881
C	9.735349	-1.458153	-2.209237
C	7.288412	0.565404	-4.007509
N	5.968701	0.671907	-3.721562
C	5.366682	1.512373	-4.600327
C	6.357976	1.966930	-5.496363
C	7.557103	1.375585	-5.125993
C	3.994589	1.866647	-4.613782
N	2.973194	1.546004	-3.879701
C	2.843934	0.730062	-2.799032
N	3.715474	-0.022211	-2.117692
C	2.969192	-0.623350	-1.113759
C	1.572171	-0.206161	-1.200802
C	1.493530	0.632821	-2.245335
H	8.881083	-3.005342	0.036556
H	3.757686	2.558830	-5.419697
H	5.459549	0.207307	-2.966650
H	5.885632	-1.206162	-1.300992
H	8.520064	1.499020	-5.590949
H	6.186911	2.649556	-6.311571
H	0.648095	1.161781	-2.650483
H	0.792923	-0.535782	-0.532544
H	4.232690	-3.341459	1.949627
H	6.868878	-3.872313	1.785011
H	10.667841	-1.916494	-1.922774
H	10.232405	-0.218717	-3.948190

H 2.557371 -1.813665 0.535178

6-Azahemiporphycene AD optimized at the M05-2X/6-311++G(d,p) level
EE (hartrees) = -1005.71039844

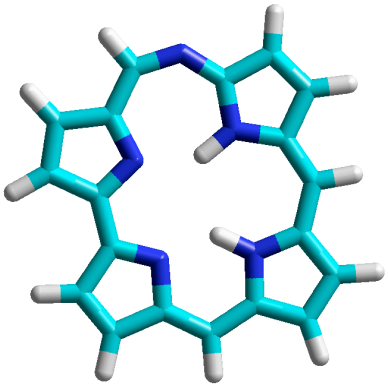


37

C	2.930947	-3.084450	-0.004630
C	1.630377	-2.431069	-0.001798
N	1.770751	-1.114490	-0.001416
C	3.114931	-0.847819	-0.003145
C	3.858291	-2.091028	-0.005637
C	0.387097	-3.116713	0.001641
C	3.608217	0.451090	-0.001151
C	2.760535	1.570509	0.001873
N	1.408085	1.391025	0.001684
C	0.762348	2.565086	0.003759
C	1.739795	3.590870	0.005876
C	2.980016	2.972132	0.004719
C	-0.660924	2.560539	0.002072
N	-1.345361	1.387541	-0.000809
C	-2.684430	1.638334	-0.004356
C	-2.854676	3.038460	-0.003684
C	-1.594572	3.613328	0.000617
C	-3.727060	0.679744	-0.007506
N	-3.763277	-0.619705	-0.005081
C	-2.752943	-1.526808	-0.000323
N	-1.425696	-1.379176	-0.001572
C	-0.910502	-2.665198	0.002715
C	-2.003721	-3.640578	0.007627
C	-3.145374	-2.936273	0.005710
H	4.677645	0.609987	-0.001858
H	-4.709456	1.147934	-0.012217
H	-1.006473	0.410351	-0.001208
H	-1.350443	4.661742	0.002135
H	-3.805712	3.543799	-0.006098
H	-4.169109	-3.269322	0.007872
H	-1.865399	-4.709886	0.011878
H	3.099673	-4.149148	-0.005748
H	4.932184	-2.184426	-0.007752
H	3.943187	3.453625	0.005745
H	1.539730	4.648305	0.007994
H	0.475829	-4.196975	0.004047

H	1.058490	0.412063	0.000227

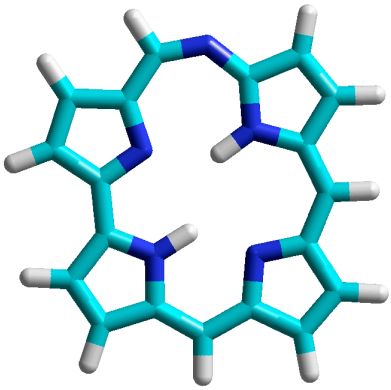
6-Azahemiporphycene BC optimized at the M05-2X/6-311++G(d,p) level
EE (hartrees) = -1005.70918643



37

C	4.944957	-2.962877	1.229023
C	4.648969	-2.056089	0.172370
N	5.808690	-1.827371	-0.485244
C	6.834606	-2.525645	0.076244
C	6.292297	-3.252011	1.169229
C	3.400778	-1.495866	-0.143182
C	8.155158	-2.454942	-0.430368
C	8.464574	-1.671504	-1.523412
N	7.485320	-0.945740	-2.137469
C	8.026335	-0.291234	-3.142084
C	9.456848	-0.578407	-3.227570
C	9.728750	-1.441225	-2.215033
C	7.185498	0.539892	-3.938206
N	5.882759	0.630472	-3.644388
C	5.348307	1.476472	-4.558044
C	6.364699	1.942176	-5.473784
C	7.527434	1.348769	-5.080193
C	4.006566	1.867948	-4.636107
N	2.931455	1.578313	-3.924254
C	2.781086	0.791131	-2.867865
N	3.661193	0.016826	-2.158100
C	2.987853	-0.621372	-1.126950
C	1.609892	-0.206925	-1.215697
C	1.483504	0.641479	-2.260920
H	8.922333	-3.034334	0.063223
H	3.799271	2.555386	-5.452017
H	8.506584	1.450879	-5.518581
H	6.209043	2.622530	-6.295322
H	0.609456	1.148640	-2.629894
H	0.845864	-0.546799	-0.535903
H	4.224582	-3.340205	1.935289
H	6.850504	-3.904245	1.819477
H	10.680267	-1.878094	-1.959335
H	10.145229	-0.178709	-3.953755
H	2.599195	-1.810008	0.513020
H	6.045253	-1.239352	-1.305869
H	4.655457	-0.001586	-2.452356

6-Azahemiporphycene BD optimized at the M05-2X/6-311++G(d,p) level
EE (hartrees) = -1005.71597528

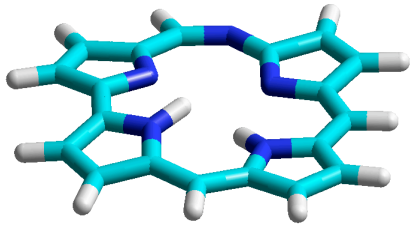


37

C	4.950167	-2.973295	1.228947
C	4.658321	-2.051378	0.146741
N	5.760987	-1.775605	-0.554880
C	6.777196	-2.480444	0.019755
C	6.279900	-3.241096	1.147392
C	3.383844	-1.519280	-0.127326
C	8.098286	-2.449274	-0.441184
C	8.490084	-1.685816	-1.538044
N	7.570342	-0.933689	-2.201047
C	8.111610	-0.265274	-3.223699
C	9.499807	-0.593637	-3.249839
C	9.732919	-1.469705	-2.210260
C	7.247599	0.557817	-3.993847
N	5.951065	0.615551	-3.655505
C	5.374720	1.460654	-4.545479
C	6.357127	1.954494	-5.483818
C	7.543754	1.381815	-5.133711
C	4.028050	1.844556	-4.606628
N	2.950754	1.555946	-3.900009
C	2.783115	0.768544	-2.847237
N	3.644091	-0.012629	-2.126224
C	2.959145	-0.645831	-1.104753
C	1.584980	-0.224049	-1.207957
C	1.477286	0.626193	-2.254913
H	8.841077	-3.041120	0.075413
H	3.820551	2.536315	-5.419053
H	8.507906	1.506771	-5.598243
H	6.163318	2.640352	-6.292618
H	0.611769	1.139821	-2.635342
H	0.810023	-0.558935	-0.538232
H	4.237093	-3.354637	1.941786
H	6.868888	-3.884811	1.780562
H	10.673196	-1.919430	-1.939068
H	10.217846	-0.217447	-3.957929
H	2.592195	-1.844131	0.536616
H	6.594425	-0.922575	-1.903565

H 4.635318 -0.071075 -2.364244

6-Azahemiporphycene CD optimized at the M05-2X/6-311++G(d,p) level
EE (hartrees) = -1005.68292367

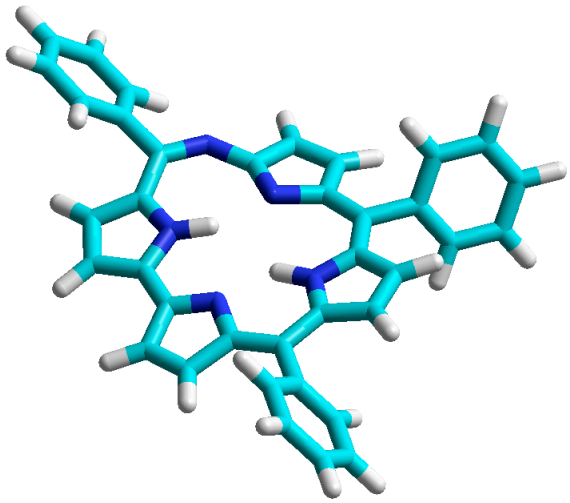


37

C	3.572993	-2.348709	0.014253
C	2.875834	-1.115996	-0.060203
N	1.547184	-1.398503	-0.109379
C	1.345339	-2.764692	-0.060508
C	2.636305	-3.354675	0.005674
C	3.396006	0.189732	-0.045979
C	0.127061	-3.447428	-0.027249
C	-1.122580	-2.862892	0.077540
N	-1.306609	-1.524397	0.277295
C	-2.600659	-1.170398	0.145915
C	-3.337043	-2.365968	-0.088939
C	-2.432015	-3.403255	-0.122648
C	-2.837436	0.225915	0.142424
N	-1.727615	0.981955	0.182869
C	-2.132877	2.245526	0.017826
C	-3.578268	2.308311	-0.102763
C	-4.024910	1.020706	-0.028669
C	-1.302703	3.379109	-0.106615
N	-0.011772	3.592145	-0.077991
C	1.084316	2.817582	-0.017134
N	1.313308	1.497004	-0.093587
C	2.678759	1.365424	-0.035958
C	3.341310	2.668605	0.080044
C	2.352918	3.570163	0.099029
H	0.177011	-4.524604	-0.102638
H	-1.872437	4.296731	-0.250098
H	-5.039098	0.662795	-0.092761
H	-4.162520	3.203775	-0.241950
H	2.390460	4.643808	0.172312
H	4.407197	2.818864	0.139951
H	4.643362	-2.446123	0.077846
H	2.812042	-4.415558	0.069453
H	-2.641438	-4.442350	-0.315435
H	-4.400379	-2.423423	-0.244016
H	4.473572	0.269396	0.001911
H	-0.649381	-0.797057	0.518094

H 0.905007 -0.635573 -0.300119

6-aza-5,11,16-triphenylhemiporphycene AC optimized at the M05-2X/6-31G(d) level
EE (hartrees) = -1698.59224561 at the same level
-1698.9885953 at the M05-2X/6-311++G(d,p) level

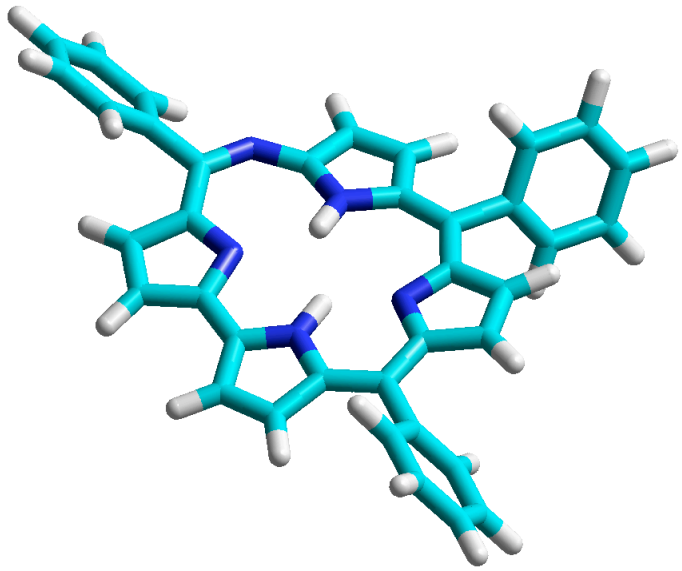


67

C	4.876166	-3.185084	1.064181
C	4.576542	-2.145456	0.177070
C	5.600873	-1.609261	-0.611745
C	6.895278	-2.107057	-0.517811
C	7.184793	-3.141483	0.368318
C	6.172939	-3.678377	1.159174
C	3.190504	-1.632881	0.069519
C	2.141423	-2.506138	-0.165770
N	0.844280	-2.058105	-0.194994
C	0.086547	-3.097207	-0.474414
C	0.871929	-4.305105	-0.652351
C	2.166866	-3.932404	-0.459602
C	-1.328414	-2.889724	-0.534843
N	-1.816621	-1.652528	-0.269775
C	-3.176137	-1.666135	-0.308743
C	-3.571168	-2.978268	-0.645416
C	-2.416089	-3.739623	-0.787577
C	-3.982096	-0.500422	-0.082274
C	-5.431050	-0.736056	0.192289
C	-6.378621	0.131514	-0.359176
C	-7.730765	-0.050228	-0.103213
C	-8.152712	-1.087388	0.726758
C	-7.214424	-1.939693	1.299606
C	-5.859550	-1.768976	1.031286
H	-9.207048	-1.224504	0.931336
H	8.193946	-3.526124	0.442682
N	-3.641307	0.752479	-0.130401
C	-2.497306	1.465834	-0.279917
N	-1.209958	1.174963	-0.059366
C	-0.537496	2.389587	-0.188658
C	-1.477208	3.450530	-0.563379

C	-2.689375	2.875644	-0.620495
C	0.805855	2.660228	0.005828
C	1.239263	4.089274	0.021079
C	2.152537	4.567315	-0.923756
C	2.559494	5.896792	-0.900660
C	2.067464	6.761354	0.074000
C	1.164060	6.291960	1.023000
C	0.751036	4.963749	0.996108
H	2.387752	7.795415	0.093989
C	1.869056	1.722894	0.196140
N	1.769050	0.386245	0.006055
C	2.974037	-0.227672	0.209620
C	3.892699	0.786006	0.569162
C	3.213097	1.991555	0.557337
H	-1.257486	-0.825956	-0.049926
H	0.926210	-0.142438	-0.199477
H	-2.348367	-4.784621	-1.043185
H	-4.587834	-3.302427	-0.790343
H	-3.650602	3.307610	-0.847221
H	-1.209999	4.474763	-0.762613
H	3.607044	2.965540	0.792956
H	4.927077	0.622950	0.822114
H	3.049214	-4.548213	-0.531288
H	0.492657	-5.285487	-0.894543
H	-6.033129	0.941209	-0.987315
H	-8.457403	0.617942	-0.548017
H	-7.534206	-2.733941	1.962142
H	-5.128899	-2.419696	1.493841
H	2.532597	3.891557	-1.680002
H	3.258298	6.258081	-1.644518
H	0.782641	6.957806	1.786654
H	0.050521	4.590539	1.732803
H	5.369314	-0.814973	-1.310164
H	7.676733	-1.690717	-1.140674
H	6.393513	-4.476965	1.856049
H	4.089095	-3.586313	1.690045

6-aza-5,11,16-triphenylhemiporphycene BD optimized at the M05-2X/6-31G(d) level
EE (hartrees) = -1698.5879212 at the same level
-1698.9840477 at the M05-2X/6-311++G(d,p) level

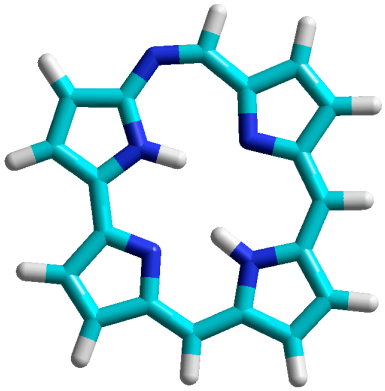


67

C	3.276977	1.950178	0.468886
C	1.892622	1.645533	0.155335
N	1.719792	0.327351	-0.012612
C	2.948266	-0.249682	0.152177
C	3.935972	0.760615	0.467431
C	0.863358	2.621174	0.018732
C	1.317368	4.045116	0.050263
C	2.166712	4.536842	-0.945004
C	2.599583	5.858145	-0.912045
C	2.194405	6.700843	0.120021
C	1.353784	6.217221	1.118442
C	0.916287	4.896932	1.083068
C	3.188962	-1.638837	0.051484
C	2.138025	-2.551130	-0.118408
N	0.843650	-2.124412	-0.132026
C	-0.012603	-3.131022	-0.342579
C	0.762023	-4.320624	-0.470592
C	2.088469	-3.963318	-0.337103
C	-1.400516	-2.830408	-0.388502
N	-1.800473	-1.563062	-0.190263
C	-3.156613	-1.597541	-0.241941
C	-3.620784	-2.942052	-0.513504
C	-2.503213	-3.720117	-0.607211
C	-3.991185	-0.461298	-0.105604
N	-3.691237	0.824625	-0.198228
C	-2.581575	1.539246	-0.274579
N	-1.255285	1.251465	-0.091530
C	-0.499931	2.415875	-0.153490
C	-1.432186	3.484266	-0.437367
C	-2.676970	2.958387	-0.509331

C	4.572628	-2.163123	0.121761
C	4.900107	-3.182917	1.022428
C	6.195504	-3.685407	1.077652
C	7.178687	-3.178756	0.232270
C	6.861306	-2.165525	-0.668427
C	5.567869	-1.659231	-0.723614
C	-5.448061	-0.693217	0.120854
C	-6.386477	0.114417	-0.529706
C	-7.745170	-0.071021	-0.313773
C	-8.185808	-1.049309	0.575979
C	-7.258886	-1.838021	1.249375
C	-5.897024	-1.662781	1.023240
H	-9.245499	-1.188075	0.749769
H	8.186662	-3.571150	0.275368
H	2.533987	7.728496	0.146857
H	-2.442451	-4.777060	-0.815226
H	-4.646120	-3.241142	-0.654822
H	-3.617204	3.451168	-0.691675
H	-1.142249	4.512114	-0.572184
H	3.677485	2.927166	0.683733
H	4.975842	0.581459	0.687723
H	2.946954	-4.611872	-0.399436
H	0.366291	-5.307959	-0.644277
H	-6.030077	0.881421	-1.203655
H	-8.462607	0.549105	-0.836306
H	-7.593230	-2.584153	1.959132
H	-5.175255	-2.259792	1.565414
H	2.479774	3.876504	-1.744287
H	3.250927	6.229777	-1.692885
H	1.040325	6.865596	1.926749
H	0.265208	4.513582	1.859168
H	5.312403	-0.882984	-1.433822
H	7.619771	-1.772844	-1.333647
H	6.438126	-4.467046	1.786386
H	4.138039	-3.560223	1.692762
H	-0.941014	0.292858	0.038260
H	0.617329	-1.133439	-0.076198

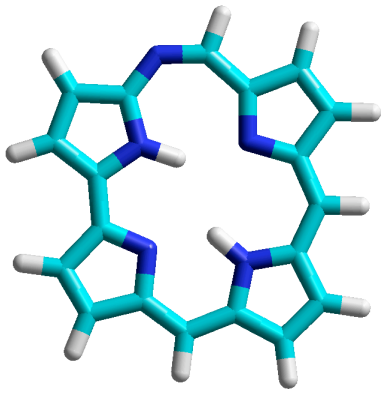
5-Azahemiporphycene optimized at the B3LYP/6-311++G(d,p) level
EE (hartrees) = -1005.8279741



37

C	4.927040	-2.952142	1.225420
C	4.596131	-2.025319	0.152813
N	5.696632	-1.722201	-0.583752
C	6.731104	-2.429326	-0.014687
C	6.254123	-3.202399	1.120500
C	3.234811	-1.596016	0.041372
N	2.534802	-0.803622	-0.742696
C	2.952888	-0.087354	-1.786743
N	4.216859	0.003359	-2.305365
C	4.225349	0.849236	-3.383503
C	2.896787	1.324852	-3.564266
C	2.114264	0.751335	-2.585268
C	5.431530	1.090682	-4.075346
N	6.536079	0.475261	-3.645326
C	7.562998	0.855943	-4.457105
C	7.059861	1.779122	-5.470708
C	5.726151	1.927290	-5.232804
C	8.852997	0.370690	-4.251689
C	9.163447	-0.525779	-3.210875
N	8.224816	-0.984504	-2.328219
C	8.772534	-1.837405	-1.418492
C	10.166886	-1.932465	-1.742434
C	10.404978	-1.131864	-2.836355
C	8.079901	-2.474839	-0.387084
H	9.656043	0.684700	-4.907235
H	5.021433	-0.505504	-1.915153
H	7.252765	-0.673382	-2.413758
H	2.584222	2.010671	-4.336472
H	1.057703	0.879843	-2.411415
H	4.226522	-3.344735	1.947990
H	6.866823	-3.842586	1.739108
H	10.882714	-2.535336	-1.204268
H	11.347004	-0.972961	-3.338942
H	7.644355	2.245764	-6.250828
H	5.022659	2.535715	-5.781689
H	8.696250	-3.117353	0.233239
H	2.618917	-2.051140	0.816547

5-Azahemiporphycene optimized at the M05-2X/6-311++G(d,p) level
EE (hartrees) = -1005.7164416

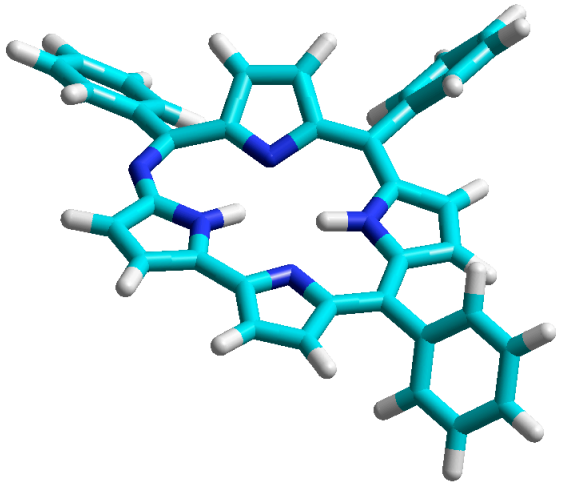


37

C	4.927040	-2.952142	1.225420
C	4.596131	-2.025319	0.152813
N	5.696632	-1.722201	-0.583752
C	6.731104	-2.429326	-0.014687
C	6.254123	-3.202399	1.120500
C	3.234811	-1.596016	0.041372
N	2.534802	-0.803622	-0.742696
C	2.952888	-0.087354	-1.786743
N	4.216859	0.003359	-2.305365
C	4.225349	0.849236	-3.383503
C	2.896787	1.324852	-3.564266
C	2.114264	0.751335	-2.585268
C	5.431530	1.090682	-4.075346
N	6.536079	0.475261	-3.645326
C	7.562998	0.855943	-4.457105
C	7.059861	1.779122	-5.470708
C	5.726151	1.927290	-5.232804
C	8.852997	0.370690	-4.251689
C	9.163447	-0.525779	-3.210875
N	8.224816	-0.984504	-2.328219
C	8.772534	-1.837405	-1.418492
C	10.166886	-1.932465	-1.742434
C	10.404978	-1.131864	-2.836355
C	8.079901	-2.474839	-0.387084
H	9.656043	0.684700	-4.907235
H	5.021433	-0.505504	-1.915153
H	7.252765	-0.673382	-2.413758
H	2.584222	2.010671	-4.336472
H	1.057703	0.879843	-2.411415
H	4.226522	-3.344735	1.947990
H	6.866823	-3.842586	1.739108
H	10.882714	-2.535336	-1.204268
H	11.347004	-0.972961	-3.338942
H	7.644355	2.245764	-6.250828
H	5.022659	2.535715	-5.781689
H	8.696250	-3.117353	0.233239

H 2.618917 -2.051140 0.816547

5-aza-6,11,16-triphenylhemiporphycene optimized at the M05-2X/6-31G(d) level
EE (hartrees) = -1698.5849916 at the same level
-1698.9811507 at the M05-2X/6-311++G(d,p) level



67

N	3.314889	-2.580183	-0.175452
C	2.134220	-3.181308	-0.388239
C	1.975574	-4.562133	-0.663503
C	0.617286	-4.822457	-0.735296
C	-0.052416	-3.606897	-0.489876
C	-1.418441	-3.247172	-0.376108
C	-2.629148	-4.054295	-0.470270
C	-3.660596	-3.196494	-0.263944
C	-3.062323	-1.878392	-0.048110
C	-3.675923	-0.653955	0.156903
C	-2.905162	0.551300	0.214969
C	-3.329735	1.873004	0.510247
C	-2.225811	2.695827	0.420557
C	-1.107129	1.886703	0.076595
C	0.226683	2.301302	-0.161827
C	1.367787	1.512747	-0.334646
C	2.625479	2.092492	-0.768718
C	3.540984	1.099245	-0.722090
C	2.834418	-0.087129	-0.264797
C	3.611189	-1.318147	-0.057082
N	0.891645	-2.639648	-0.301316
N	-1.701772	-1.980410	-0.131726
N	-1.565814	0.610788	-0.022676
N	1.529789	0.156917	-0.081799
C	-5.146646	-0.564468	0.310696
C	-5.806526	-1.358255	1.255302
C	-7.188740	-1.289799	1.393185
C	-7.929388	-0.426286	0.591285
C	-7.281517	0.368379	-0.350971
C	-5.900266	0.301297	-0.490780
C	0.405621	3.781927	-0.228047

C	1.245817	4.433256	0.679979
C	1.402242	5.814173	0.629431
C	0.726889	6.558933	-0.333629
C	-0.109408	5.917935	-1.243701
C	-0.274901	4.538203	-1.187420
H	0.711948	-1.660461	-0.079777
H	-1.027190	-0.234050	-0.199713
H	2.797567	-5.248013	-0.782657
H	0.137274	-5.768355	-0.928055
H	-2.676098	-5.113415	-0.669775
H	-4.716361	-3.415888	-0.277237
H	-5.223782	-2.012151	1.892089
H	-7.685192	-1.904343	2.133385
H	-9.005119	-0.371931	0.700279
H	-7.853182	1.035794	-0.983372
H	-5.397172	0.904118	-1.236396
H	-4.335588	2.155515	0.772726
H	-2.189017	3.757340	0.597817
H	1.767300	3.848166	1.426915
H	2.049577	6.307668	1.343128
H	0.852235	7.633469	-0.375253
H	-0.631552	6.490993	-1.999330
H	-0.922775	4.035295	-1.894584
H	2.768944	3.110153	-1.091052
H	4.582353	1.142571	-0.993616
C	5.050876	-1.098344	0.294385
C	5.429705	-0.123661	1.222570
C	6.765219	0.027484	1.582491
C	7.738299	-0.787915	1.013552
C	7.367673	-1.766440	0.093276
C	6.033169	-1.927842	-0.254980
H	4.672789	0.506933	1.671916
H	7.043025	0.778980	2.310866
H	8.778382	-0.666310	1.288890
H	8.120411	-2.405266	-0.351475
H	5.729719	-2.695972	-0.953283