Journal Name

ARTICLE TYPE

Cite this: DOI: 10.1039/xxxxxxxxxx

Supporting Information: New Insights on Aromatic Pathways of Carbachlorins and Carbaporphyrins Based on Calculations of Magnetically Induced Current Densities

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Contents

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† Electronic Supplementary Information (ESI) available: See DOI: 10.1039/b000000x/

1 Equilibrium geometries of carbaporphyrinoids

The Cartesian coordinates (in Å) of the electronic ground state of the investigated molecules that have been optimized at the B3LYP/def2-TZVP level of theory.

1.1 carbaporphyrinoid (1)

Atom X Y Z
Energy = -1086.572806785

H	1.1171401	-0.4897571	-0.0575302
N	2.1195059	-0.4227286	0.0200028
C	2.8702295	-1.5667544	0.0193230
C	2.9202613	0.6985675	0.0640082
C	4.2389512	-1.1583899	0.0755794
C	4.2673356	0.2066739	0.1016028
H	5.0782940	-1.8349736	0.0930098
H	5.1348505	0.8456968	0.1456466
C	2.3402383	-2.8500726	-0.0294028
H	3.0557078	-3.6622531	-0.0334927
H	-1.1491048	-0.4210364	-0.0586489
N	-0.0725671	-2.3470654	-0.0486614
N	-2.1461892	-0.2934613	0.0163875
C	0.0644921	2.0605325	0.0956345
C	-1.1865988	-3.1382023	-0.0636715
C	-2.8770734	0.8714717	0.0618869
C	1.3117255	2.6789535	0.0243434
C	0.9882508	-3.2016264	-0.0619636
C	-2.9658947	-1.3904860	0.0162531
C	-1.1499013	2.7608274	0.0288863
C	-0.8150769	-4.5445764	-0.0972895
C	-4.2472683	0.4664164	0.0995664
C	0.5345265	-4.5842595	-0.0961361
C	-4.3027533	-0.9020218	0.0726063
C	-1.0783385	4.2069376	-0.0817274
H	-1.5091586	-5.3711944	-0.1147311
H	-5.0763419	1.1546665	0.1449161
H	1.1788330	-5.4502367	-0.1124535
H	-5.1826482	-1.5247908	0.0899644
H	-2.0149729	4.7529753	-0.1215477
C	-2.5104709	-2.7062535	-0.0324972
C	-2.4336055	2.1912752	0.0566160
C	2.5628425	2.0358883	0.0578914
H	-3.2742388	-3.4733652	-0.0374385
H	-3.2514618	2.9034713	0.0537251
H	3.4025024	2.7213291	0.0521861
C	0.0893636	4.8714721	-0.1394008
C	1.3724552	4.1742324	-0.0951042
H	0.1317907	5.9501556	-0.2206633
O	2.4350798	4.7841396	-0.1513055
H	0.0292886	0.9978228	0.2636299

1.2 carbaporphyrinoid (2)

Energy = -1126.849866673

Atom	X	Y	Z
C	-0.4236255	-4.1086092	0.1235368
C	-1.5144727	-3.2571493	-0.0087997
C	-2.9060035	-3.5611317	-0.0982760
C	-3.5907273	-2.3778338	-0.2023963
H	-3.3182277	-4.5574490	-0.0829641
C	-2.6482675	-1.3028495	-0.1859061
H	-4.6573867	-2.2455441	-0.2916860
N	-1.4133631	-1.8934081	-0.0744473
H	-0.5184046	-1.4480153	0.0513205
C	-2.9158034	0.0658855	-0.2357559
C	-1.9877245	1.1059229	-0.2473640
H	-3.9678414	0.3247769	-0.2148373
C	-0.5939768	1.0176877	-0.4014783
C	-2.2937999	2.5341334	-0.0408792
C	0.0177447	2.2738796	-0.2533131
H	-0.0818459	0.1368711	-0.7407049
C	-1.0724901	3.2454355	-0.0448466
C	-3.4940386	3.2012944	0.1569933
C	-3.4751725	4.5846752	0.3319928
H	-4.4364384	2.6666488	0.1751835
C	-2.2711738	5.2859355	0.3281127
H	-4.4059342	5.1193744	0.4760771
C	-1.0595214	4.6191406	0.1491377
H	-2.2763111	6.3597517	0.4691765
H	-0.1292790	5.1748013	0.1615277
C	1.3802931	2.5676805	-0.2485932
C	2.4390248	1.6596478	-0.2020035
H	1.6744400	3.6104687	-0.2315801
C	3.8388673	1.9489169	-0.2273960
C	4.5308842	0.7697160	-0.1252868
H	4.2495290	2.9417355	-0.3212152
C	3.5804950	-0.2903839	-0.0277518
H	5.6009368	0.6367663	-0.1163760
N	2.3440534	0.2943918	-0.0870711
H	1.5159008	-0.2639558	0.0453273
C	3.7835559	-1.6590404	0.1062113
C	2.8124767	-2.6640799	0.1735464
H	4.8154891	-1.9831945	0.1550787
N	1.4578613	-2.5023083	0.1127132
C	3.1542056	-4.0711321	0.2963869
C	1.9859033	-4.7512831	0.3017392
H	4.1573210	-4.4647142	0.3628386
C	0.9302295	-3.7598958	0.1815962
H	1.8333595	-5.8176739	0.3736802
H	-0.6507414	-5.1658861	0.1787516

1.3 carbaporphyrinoid (3)

Atom X Y Z
Energy = -1164.886589682

C	-3.1445447	-4.0943295	0.0063011
C	-1.8286127	-4.6034895	-0.0240664
N	-3.4535669	-2.7915524	0.0291633
C	-4.3499426	-4.9217755	0.0152716
C	-5.3933798	-4.0635632	0.0426639
H	-4.3740093	-6.0012929	0.0001895
C	-4.8243081	-2.7190383	0.0518246
H	-6.4476939	-4.2975066	0.0564495
C	-5.5763206	-1.5592377	0.0719037
C	-5.0861940	-0.2294068	0.0799878
H	-6.6505833	-1.7030654	0.0735340

C	-3.7395537	0.1590610	0.1188769
C	-5.8702785	0.9747221	0.0327577
C	-3.6040436	1.5540459	0.0826983
H	-2.9187306	-0.5234980	0.1816729
C	-4.9312443	2.1046734	0.0344764
C	-5.2407779	3.4561414	-0.0059465
C	-6.4887915	4.0756038	-0.0484254
H	-4.3930201	4.1321851	-0.0034844
C	-7.7522946	3.4942242	-0.0680503
H	-6.4706377	5.1596175	-0.0703931
C	-8.0927551	2.1456006	-0.0515279
H	-8.5861431	4.1872928	-0.1025475
C	-7.2555362	1.0318945	-0.0099496
H	-9.1551206	1.9295376	-0.0752652
H	-7.7651111	0.0747774	-0.0108769
C	-2.3863118	2.2791988	0.0771308
C	-1.1085507	1.7519880	0.0572959
H	-2.4413114	3.3616435	0.0802733
C	0.1091912	2.5574478	0.0501230
C	1.1438068	1.6886657	0.0217610
H	0.1461856	3.6367446	0.0658422
C	0.5508243	0.3522282	0.0108627
H	2.2007007	1.9098287	0.0070923
N	-0.7865234	0.4176738	0.0329338
C	1.2922116	-0.8482468	-0.0207685
C	0.7922345	-2.1350465	-0.0329482
H	2.3714312	-0.7606699	-0.0315530
C	1.5551335	-3.3577439	-0.0480366
C	0.6866304	-4.4027569	-0.0489700
H	2.6330143	-3.3969040	-0.0535642
N	-0.5291127	-2.5090036	-0.0261535
C	-0.6550424	-3.8764413	-0.0343939
H	0.9222709	-5.4552824	-0.0556385
H	-1.3068525	-1.8622450	-0.0365572
H	-1.7171662	-5.6805047	-0.0357696

1.4 carbaporphyrinoid (4) (C_1)

Atom X Y Z

Energy = -1050.606203420

C	-1.3016890	-3.1343166	0.0447214
C	-0.1638690	-3.9213419	0.0134815
C	1.1630134	-3.4819337	-0.0350111
H	-0.3253361	-4.9918648	0.0335960
C	2.3035614	-4.3724148	-0.0694990
C	3.4054369	-3.5820768	-0.1000470
H	2.2548082	-5.4509458	-0.0685919
C	2.9284767	-2.2157441	-0.0802943
H	4.4422008	-3.8819208	-0.1274759
N	1.5662491	-2.1801565	-0.0458437
N	-1.3055773	-1.7541261	0.0113573
C	-2.6644382	-3.5412378	0.1090060
C	-3.4393586	-2.4160105	0.1036819
H	-2.9934700	-4.5671597	0.1552073
C	-2.5866566	-1.2643394	0.0385453
H	-4.5154739	-2.3601308	0.1465516
H	-0.4310298	-1.2639517	-0.0945602
C	-3.0848757	0.0367781	0.0084021
C	-2.5498144	1.3446953	-0.0172914
H	-4.1678418	0.0155268	0.0010361
C	-1.1709323	1.6272388	0.0550311
C	-3.6004964	2.3632332	-0.1236081
C	-3.5405126	3.7054809	-0.1309690
H	-4.5973386	1.9450426	-0.2061297
C	-0.4593551	2.8445788	0.0601733
H	-0.5462564	0.7514243	0.1589330
C	-2.3753855	4.5442178	-0.0337864
H	-4.4867806	4.2286647	-0.2164773
C	-1.0871560	4.1705568	0.0454765
H	-2.5674817	5.6116970	-0.0290837
H	-0.3735640	4.9845477	0.1065032
C	0.9505713	2.9294356	0.0946508
C	2.0247370	2.0412681	0.0660321
H	1.3183708	3.9477224	0.1280892
C	3.3892994	2.4840073	0.0691543
C	4.2095649	1.3928395	0.0114880
H	3.6794618	3.5219652	0.1064135
C	3.3884273	0.2305339	-0.0236886
H	5.2877390	1.3794620	-0.0051896
N	2.0809729	0.6721233	0.0100716
H	1.3356528	-0.0068789	0.0006006
C	3.7700821	-1.0989665	-0.0732111
H	4.8360637	-1.2875234	-0.0974459

1.5 carbaporphyrinoid (4) (C_s)

Atom X Y Z

Energy = -1050.6059979280

C	-1.3024755	-3.1379799	0.0000000
C	-0.1640419	-3.9250950	0.0000000
C	1.1634641	-3.4849283	0.0000000
H	-0.3259337	-4.9957228	0.0000000
C	2.3051185	-4.3744996	0.0000000
C	3.4068646	-3.5834166	0.0000000
H	2.2570356	-5.4530412	0.0000000
C	2.9288648	-2.2172839	0.0000000
H	4.4441885	-3.8826258	0.0000000
N	1.5663051	-2.1827005	0.0000000
N	-1.3032575	-1.7575633	0.0000000
C	-2.6670688	-3.5435308	0.0000000
C	-3.4393699	-2.4164889	0.0000000
H	-2.9993516	-4.5694406	0.0000000
C	-2.5833455	-1.2651648	0.0000000
H	-4.5162318	-2.3589393	0.0000000
H	-0.4209950	-1.2697917	0.0000000
C	-3.0820816	0.0366836	0.0000000
C	-2.5509237	1.3463566	0.0000000
H	-4.1650224	0.0134357	0.0000000
C	-1.1704789	1.6310642	0.0000000
C	-3.6064044	2.3653373	0.0000000
C	-3.5469393	3.7077062	0.0000000
H	-4.6068552	1.9476355	0.0000000
C	-0.4592277	2.8479125	0.0000000
H	-0.5405160	0.7535777	0.0000000
C	-2.3779880	4.5469030	0.0000000
H	-4.4970888	4.2309070	0.0000000
C	-1.0871247	4.1739110	0.0000000
H	-2.5698516	5.6144711	0.0000000
H	-0.3713333	4.9881463	0.0000000
C	0.9515271	2.9322206	0.0000000

C	2.0252349	2.0431243	0.0000000
H	1.3199355	3.9507835	0.0000000
C	3.3900690	2.4855055	0.0000000
C	4.2104948	1.3930713	0.0000000
H	3.6800639	3.5241638	0.0000000
C	3.3894390	0.2300286	0.0000000
H	5.2888017	1.3791137	0.0000000
N	2.0819352	0.6727580	0.0000000
H	1.3369727	-0.0063651	0.0000000
C	3.7707431	-1.1004005	0.0000000
H	4.8368486	-1.2898387	0.0000000

1.6 carbaporphyrinoid (6b-cis)

Atom X Y Z
Energy = -1089.919437064

C	-0.9303332	-4.9248814	-0.1697211
C	-2.0531893	-4.1468577	0.0682581
C	0.3985636	-4.4967614	-0.2977598
H	-1.1009348	-5.9908203	-0.2556624
C	1.4957988	-5.4157236	-0.5247586
C	2.6240762	-4.6667659	-0.5619561
H	1.4005637	-6.4857350	-0.6331624
C	2.2131919	-3.2922009	-0.3579799
H	3.6412743	-4.9982902	-0.7072583
N	0.8574461	-3.2132536	-0.2070232
C	3.1274724	-2.2310223	-0.3068074
C	2.8567679	-0.8861014	-0.1033860
H	4.1711117	-2.4910802	-0.4328548
C	3.7437404	0.2262700	-0.0187374
C	2.9892544	1.3551458	0.1779246
H	4.8173125	0.1620552	-0.0982646
C	1.6103752	0.9809337	0.2248207
H	3.3445531	2.3673461	0.2892381
N	1.5898885	-0.3790231	0.0569660
H	0.7956479	-0.9904965	-0.0417702
C	0.5068399	1.8302972	0.3770058
C	-0.8349313	1.4792986	0.4565113
H	0.7520361	2.8866451	0.3899140
C	-1.9787644	2.4854288	0.3847120
C	-1.3865303	0.2043928	0.5704495
C	-2.7812608	0.1927776	0.5510173
H	-0.7968986	-0.6747589	0.7557084
C	-3.2825293	1.6298448	0.5179706
C	-3.2987656	2.8966933	-1.5340542
C	-2.1344509	3.1655324	-0.9550154
H	-3.6077649	3.2736384	-2.5016412
H	-1.3571465	3.7889274	-1.3791677
C	-3.6212492	-0.9151299	0.5538020
C	-3.2713398	-2.2639624	0.4136580
H	-4.6880060	-0.7362533	0.6317419
C	-4.1518822	-3.3903360	0.4456864
C	-3.4159792	-4.5290982	0.2378611
H	-5.2149070	-3.3205589	0.6142558
H	-3.7765830	-5.5449272	0.2047026
N	-2.0210886	-2.7784280	0.1885768
H	-1.1539530	-2.2892602	0.0358603
C	-4.1764779	2.0037728	-0.6988479
H	-5.0850105	2.5283201	-0.3846139
H	-4.5066496	1.1193511	-1.2510894
H	-1.8720732	3.2253936	1.1860621
H	-3.8083961	1.8451333	1.4510490

1.7 carbaporphyrinoid (6b-trans)

Atom X Y Z
Energy = -1089.885958171

C	-0.8360406	-5.0661789	0.0691320
C	-1.9823444	-4.2941693	0.1736253
C	0.4892461	-4.6211727	-0.0525894
H	-0.9829884	-6.1390506	0.0749750
C	1.6094278	-5.5335890	-0.1724543
C	2.7223972	-4.7669925	-0.2609041
H	1.5375720	-6.6107991	-0.1843252
C	2.2800398	-3.3885021	-0.1888125
H	3.7486869	-5.0879243	-0.3583462
N	0.9192535	-3.3260715	-0.0690675
C	3.1728832	-2.3100930	-0.2090365
C	2.8808252	-0.9566278	-0.1035232
H	4.2228754	-2.5606840	-0.2979510
C	3.7540772	0.1675949	-0.0644500
C	2.9842934	1.2966821	0.0727623
H	4.8290914	0.1120366	-0.1299235
C	1.6116013	0.9085422	0.1219785
H	3.3270379	2.3169225	0.1413920
N	1.6064718	-0.4564846	0.0104446
H	0.8176942	-1.0803472	-0.0414352
C	0.4939462	1.7500440	0.2444849
C	-0.8386096	1.3801182	0.2884288
H	0.7259241	2.8086332	0.2623457
C	-2.0442544	2.2969938	0.3578698
C	-1.3875103	0.0801659	0.3684102
C	-2.7744535	0.0383099	0.1519587
H	-0.8111716	-0.7746741	0.6736433
C	-3.1317624	1.4408547	-0.2993343
C	-4.3735118	2.3288123	-0.1798020
H	-2.8930445	1.4494012	-1.3730788
C	-3.7115998	3.6880582	-0.4183185
H	-4.8199666	2.2896235	0.8227780
H	-5.1607925	2.1039221	-0.9016258
C	-2.3945448	3.6627733	-0.1807178
H	-4.2727313	4.5666464	-0.7114418
H	-1.7317733	4.5159633	-0.2384240
H	-2.2773420	2.3383221	1.4373766
C	-3.6196704	-1.0669589	0.1617787
C	-3.2535322	-2.4157098	0.2205516
H	-4.6839272	-0.8866609	0.0647551
C	-4.1175798	-3.5530842	0.2998043
C	-3.3496831	-4.6886968	0.2777579
H	-5.1918395	-3.4919924	0.3732987
H	-3.6908977	-5.7106869	0.3241212
N	-1.9803151	-2.9207421	0.1610007
H	-1.1185682	-2.4274659	-0.0113524

1.8 carbaporphyrinoid (9)

Atom X Y Z
Energy = -1088.703545280

C	-0.7635196	-3.3973146	0.0313129
C	0.5032300	-3.9571057	-0.1046833
C	1.7289497	-3.2880364	-0.1734270
H	0.5408971	-5.0380176	-0.1557276
C	-2.0366794	-4.0366847	0.1254338
C	-2.9929735	-3.0594798	0.2292020
H	-2.1892029	-5.1040881	0.1118310
C	-2.3450553	-1.7856236	0.2099475
H	-4.0589522	-3.1953621	0.3216037
N	-1.0022369	-2.0524790	0.0947188
H	-0.2516623	-1.3923293	-0.0363589
C	-2.9352453	-0.5231101	0.2618078
C	-2.2812253	0.7099832	0.2748883
H	-4.0191475	-0.5218394	0.2393543
C	-0.8942036	0.9535630	0.4360380
C	-2.8906875	2.0173739	0.0572941
C	-1.9172275	2.9716107	0.0580558
C	-0.6150052	2.3283947	0.2813100
H	-0.1970882	0.2350134	0.8272303
C	-4.2107278	2.6470687	-0.2613966
C	-3.8306618	4.1046021	-0.4223831
H	-4.9583750	2.5133781	0.5299636
H	-4.6620899	2.2508780	-1.1788834
C	-2.5031016	4.2685875	-0.2433774
H	-4.5472834	4.8842272	-0.6380576
H	-1.9726530	5.2089070	-0.3060829
C	0.6277548	2.9600300	0.2637014
C	1.8781556	2.3443270	0.2011161
H	0.6466912	4.0435634	0.2437514
C	3.1659146	2.9627065	0.2098950
C	4.1198316	1.9840631	0.0947188
H	3.3272541	4.0249890	0.3034109
C	3.4502147	0.7263961	0.0045880
H	5.1903464	2.1116776	0.0714769
N	2.1123813	0.9960761	0.0794461
H	1.4320042	0.2624823	-0.0420882
C	3.9802326	-0.5534262	-0.1337081
C	3.2846233	-1.7645638	-0.1877975
H	5.0596167	-0.6149484	-0.1941527
N	1.9328736	-1.9399762	-0.1124097
C	2.9957343	-3.9921493	-0.3020098
C	3.9607813	-3.0470141	-0.3115957
H	3.1083691	-5.0637768	-0.3695942
H	5.0291484	-3.1825737	-0.3883628

1.9 carbaporphyrinoid (14) (C_1)

Atom X Y Z
Energy = -1086.553336621

C	-1.3721186	-3.0754652	0.0147344
C	-0.1455372	-3.7258970	-0.0897222
C	1.1240929	-3.1438517	-0.1335218
H	-0.1833632	-4.8067882	-0.1361848
C	2.3425528	-3.9367983	-0.2272591
C	3.3704549	-3.0625805	-0.2177718
H	2.3807388	-5.0140456	-0.2861605
C	-2.6912554	-3.6234792	0.0740709
C	-3.5773565	-2.5819704	0.1466644
H	-2.9181377	-4.6774406	0.0577361
C	-2.8398400	-1.3559449	0.1422356
H	-4.6525855	-2.6412000	0.2061662
C	2.7825740	-1.7334085	-0.1192940
H	4.4281732	-3.2726849	-0.2675900
C	3.5598294	-0.5749269	-0.0581133
C	3.1145631	0.7410664	0.0468883
H	4.6333629	-0.7117860	-0.0870427
C	3.8657640	1.9521779	0.1400126
C	2.9777544	2.9942029	0.2051389
H	4.9425333	2.0067535	0.1519111
C	1.6508682	2.4640354	0.1620264
H	3.2077698	4.0447689	0.2861704
C	0.4483835	3.1677920	0.1715284
C	-0.8395376	2.6219581	0.1681831
H	0.5540061	4.2447400	0.1317891
C	-1.1959528	1.2800255	0.3706202
C	-2.5825473	1.1245097	0.1724530
H	-0.5491040	0.5315761	0.7901326
C	-3.1156611	2.4439775	-0.1141366
C	-2.0926525	3.3500055	-0.1238173
H	-4.1496611	2.6707785	-0.3293420
C	-2.2293540	4.7726371	-0.4156216
O	-3.2815275	5.3374754	-0.6389925
H	-1.2854938	5.3550115	-0.4225411
C	-3.3348337	-0.0572555	0.1606474
H	-4.4137294	0.0321059	0.1076378
N	-1.5140894	-1.7192976	0.0711648
H	-0.7134482	-1.1168303	-0.0392504
N	1.7975749	1.0996635	0.0730443
H	1.0766623	0.4096117	-0.0683638
N	1.4201280	-1.8132216	-0.0762307

1.10 carbaporphyrinoid (14) (C_s)

Atom X Y Z
Energy = -1086.5504467380

C	-1.3803030	-3.0976845	0.0000000
C	-0.1436210	-3.7390475	0.0000000
C	1.1251291	-3.1483877	0.0000000
H	-0.1682940	-4.8212130	0.0000000
C	2.3452059	-3.9433486	0.0000000
C	3.3742443	-3.0704359	0.0000000
H	2.3831474	-5.0221723	0.0000000
C	-2.7049744	-3.6354545	0.0000000
C	-3.5838358	-2.5843275	0.0000000
H	-2.9422104	-4.6871733	0.0000000
C	-2.8389209	-1.3611252	0.0000000
H	-4.6612000	-2.6352245	0.0000000
C	2.7891648	-1.7371961	0.0000000
H	4.4323956	-3.2839219	0.0000000
C	3.5771390	-0.5821320	0.0000000
C	3.1432095	0.7427159	0.0000000
H	4.6489828	-0.7327911	0.0000000
C	3.8831871	1.9638738	0.0000000
C	2.9824280	2.9981210	0.0000000
H	4.9590845	2.0323118	0.0000000
C	1.6584497	2.4556118	0.0000000
H	3.2020570	4.0540692	0.0000000
C	0.4525977	3.1590607	0.0000000
C	-0.8418010	2.6275957	0.0000000
H	0.5649034	4.2360885	0.0000000
C	-1.1953484	1.2751840	0.0000000

C	−2.5914494	1.1289046	0.0000000
H	−0.5027863	0.4681116	0.0000000
C	−3.1412738	2.4756543	0.0000000
C	−2.1169573	3.3812455	0.0000000
H	−4.1918271	2.7272571	0.0000000
C	−2.2731566	4.8312989	0.0000000
O	−3.3380381	5.4161619	0.0000000
H	−1.3301015	5.4153269	0.0000000
C	−3.3339902	−0.0598743	0.0000000
H	−4.4146684	0.0232137	0.0000000
N	−1.5162471	−1.7412694	0.0000000
H	−0.6896871	−1.1685623	0.0000000
N	1.8249344	1.0910618	0.0000000
H	1.1310188	0.3631936	0.0000000
N	1.4234128	−1.8147207	0.0000000

1.11 carbaporphyrinoid (19)

Atom X Y Z
Energy = −975.1149316034

C	−0.9380359	−3.1488440	−0.0269737
C	0.3690964	−3.6279382	0.0366651
C	1.5600475	−2.8785416	0.0755801
H	0.4814284	−4.7130422	0.0500435
C	−2.1805359	−3.8544464	−0.0885947
C	−3.1960077	−2.9208587	−0.1236962
H	−2.2766928	−4.9361818	−0.1036368
C	−2.6153825	−1.6090959	−0.0882778
H	−4.2642891	−3.1104671	−0.1767447
N	−1.2527745	−1.8052644	−0.0368705
H	−0.5042283	−1.1222944	0.0683757
N	1.6727764	−1.5067404	0.0515320
C	−3.2989353	−0.3800753	−0.0753947
C	−2.7532255	0.9045101	−0.0654195
H	−4.3865032	−0.4685610	−0.0204800
C	−3.5694728	2.1705155	0.1590700
C	−1.4100566	1.2705156	−0.2258238
C	−1.1857446	2.6436948	−0.0598443
H	−0.6397542	0.5775403	−0.5462919
C	−2.5292968	3.3225575	0.1716205
H	−4.1312632	2.1170746	1.1037772
H	−4.3160466	2.2961528	−0.6406126
H	−2.5357562	3.8663027	1.1284683
H	−2.7277761	4.0697076	−0.6124214
C	0.0351204	3.3203535	−0.0680206
C	1.3286149	2.7685991	−0.0841430
H	0.0098325	4.4110737	−0.0095673
C	2.5728389	3.4825460	−0.1214688
C	3.6070496	2.5695796	−0.0904263
H	2.6504477	4.5648416	−0.1732732
C	3.0346338	1.2603188	−0.0289861
H	4.6728510	2.7779305	−0.1080659
N	1.6655816	1.4336258	−0.0357037
H	1.0644025	0.6181424	0.0715370
C	3.6471343	0.0100498	0.0329979
C	3.0254741	−1.2522771	0.0734811
H	4.7380616	0.0111072	0.0444008
C	3.7831989	−2.4908172	0.1224358
C	2.8705677	−3.5035897	0.1238838
H	3.0544111	−4.5752717	0.1498150
H	4.8682087	−2.5624323	0.1470535

1.12 carbaporphyrinoid (19′)

Atom X Y Z
Energy = −974.4433241197

C	−0.9332892	−3.0416556	0.0076629
C	0.3643238	−3.5342702	0.0542220
C	1.5837265	−2.8534799	0.0805612
H	0.4489466	−4.6134804	0.0447607
C	−2.1466431	−3.7646598	−0.1732112
C	−3.1885950	−2.8691793	−0.2005559
H	−2.2034064	−4.8346165	−0.2968461
C	−2.6629595	−1.5556400	−0.0393399
H	−4.2332796	−3.0907995	−0.3509017
N	−1.2978932	−1.7103158	0.0764294
H	−0.7142398	−0.9917776	0.4636745
N	1.8122581	−1.4945090	0.0240546
C	−3.3410980	−0.3338154	−0.0165822
C	−2.7743010	0.9390573	0.0018091
H	−4.4227702	−0.4079024	−0.0067473
C	−3.5793908	2.2196333	0.1675005
C	−1.4299048	1.2814567	−0.1294619
C	−1.1965040	2.6504679	−0.0322923
H	−0.6152143	0.6188238	−0.3492769
C	−2.5279965	3.3598137	0.1447210
H	−4.1445098	2.2085562	1.1028205
H	−4.3122548	2.3224674	−0.6373218
H	−2.5446449	3.9430299	1.0687679
H	−2.7071534	4.0645504	−0.6714799
C	0.0433306	3.2731937	−0.0736261
C	1.3174465	2.6738540	−0.1116214
H	0.0530120	4.3579991	−0.0346157
C	2.5452709	3.4598632	−0.1306127
C	3.5724772	2.5794786	−0.1197362
H	2.5930756	4.5385749	−0.1466987
C	2.9714740	1.2567423	−0.0876777
H	4.6319756	2.7875486	−0.1214197
N	1.6083125	1.3492794	−0.0937490
C	3.6922375	0.0664244	−0.0227376
C	3.1590037	−1.2214060	0.0435409
H	4.7725539	0.1386146	−0.0112235
C	3.8262943	−2.4738490	0.1329766
C	2.8727014	−3.4605504	0.1551341
H	3.0341849	−4.5248542	0.2222339
H	4.8967965	−2.5966252	0.1762982
H	1.1766462	−0.7160431	−0.1094326

1.13 carbaporphyrinoid ($19H^+$)

Atom X Y Z
Energy = −974.8506575665

C	−0.3531500	−3.6060562	−0.0206576
C	0.9609558	−3.1527634	−0.1611150
C	2.1084073	−3.9166594	−0.4844215
C	3.2049216	−3.0858514	−0.4770102
H	2.0934465	−4.9687954	−0.7205517
C	2.7772114	−1.7766495	−0.1487799

H	4.2237666	-3.3545380	-0.7065819
C	3.5677548	-0.6349165	0.0049336
C	3.1571398	0.6807645	0.1563899
H	4.6370059	-0.8017436	-0.0000830
C	3.9431510	1.8325033	0.4519081
C	3.1182434	2.9263804	0.4737104
H	5.0036879	1.8133050	0.6467701
C	1.7863147	2.4983544	0.1945068
H	3.3964750	3.9457365	0.6888901
C	0.6334738	3.2753146	0.0772657
C	-0.6808373	2.8268397	-0.0557123
H	0.8003502	4.3462751	0.0754684
C	-1.1570590	1.5258615	0.1176456
C	-2.5378497	1.4203446	-0.0614583
H	-0.5507311	0.7235048	0.5003038
C	-1.8546909	3.7307890	-0.3785109
C	-3.0899061	2.7976852	-0.3738759
H	-1.7158362	4.2156208	-1.3471857
H	-1.9383271	4.5315209	0.3598824
H	-3.6075897	2.8020233	-1.3352647
H	-3.8267574	3.0933766	0.3766861
C	-3.3254132	0.2754704	0.0606977
C	-2.8895594	-1.0453723	0.1710858
H	-4.4016191	0.4042056	0.0551785
C	-3.6632929	-2.2138980	0.4373198
C	-2.8329672	-3.3036968	0.4123455
H	-4.7211764	-2.2077167	0.6463070
C	-1.5099535	-2.8561890	0.1280845
H	-3.1023332	-4.3313034	0.5982145
H	-0.4815616	-4.6805434	-0.0341893
N	-1.5851489	-1.4750576	0.0224011
H	-0.9213738	-0.9528196	-0.5236393
N	1.3918269	-1.8361619	-0.0031030
H	0.9229124	-1.2229646	0.6473061
N	1.8487381	1.1268740	0.0413396
H	1.1713507	0.6309464	-0.5125006

1.14 carbaporphyrinoid (20) (C_1)

Energy = -973.2344352621

C	0.2826332	4.2251223	0.1792579
C	-1.0631947	4.0989093	0.1831701
C	0.8765768	2.9159533	-0.1249038
C	-1.4050633	2.7018685	-0.1182354
C	-0.1913158	2.0252047	-0.3325565
N	0.1880029	-1.9993715	0.0581912
C	1.0675134	-4.1418621	0.1685259
C	-0.2768021	-4.2681274	0.1719026
C	-2.6961023	2.1730134	-0.0960696
C	-3.0412874	0.8223176	-0.0915657
C	-2.1930998	-2.6669661	0.0688025
C	-2.8273998	-1.4301923	-0.0052319
C	-4.2203993	-1.1202832	-0.0447749
C	-4.3476199	0.2442086	-0.0919322
C	3.0445348	-0.8791339	-0.0198921
C	4.3551893	-0.3149504	-0.0663958
C	4.2253593	1.0492528	-0.1140756
N	2.1715959	0.1709429	-0.0564083
N	-2.1657198	-0.2358364	-0.0451838
C	-0.8191101	-2.9198038	0.1004422
H	0.8516204	5.1146632	0.4067295
H	-1.7863334	4.8671682	0.4145444
H	-5.2620806	0.8140241	-0.1314651
H	-3.5272751	2.8644032	-0.0184556
H	-5.0121551	-1.8516859	-0.0326502
H	-2.8430295	-3.5318217	0.1025975
H	-0.8631604	-5.1732141	0.2146450
H	1.8122835	-4.9219849	0.2079460
C	1.3490671	-2.7162210	0.0950998
C	2.6518605	-2.2123076	0.0571351
H	3.4514536	-2.9411751	0.0876832
H	5.2694064	-0.8859153	-0.0580700
H	5.0173340	1.7795152	-0.1583814
C	2.8341866	1.3736748	-0.1072767
C	2.2435659	2.6364956	-0.1103743
H	2.9320219	3.4705145	-0.0373679
H	-1.1640437	-0.2018490	0.0602819
H	1.1816093	0.0173421	0.0532470
H	-0.1006227	1.0481075	-0.7689350

1.15 carbaporphyrinoid (20) (C_s)

Atom X Y Z

Energy = -973.2314372692

C	0.3015715	-3.4519536	0.0000000
C	-1.0247536	-3.0245736	0.0000000
C	1.4558684	-2.6602605	0.0000000
H	0.4568008	-4.5234011	0.0000000
C	2.7893551	-3.2422671	0.0000000
C	3.6609207	-2.2108602	0.0000000
H	3.0053203	-4.3000268	0.0000000
C	2.8647006	-0.9931322	0.0000000
H	4.7399161	-2.2472295	0.0000000
C	3.4532113	0.2768899	0.0000000
C	2.8113593	1.5136255	0.0000000
H	4.5355507	0.3021548	0.0000000
C	-2.2433074	-3.7686992	0.0000000
C	-3.2820395	-2.8718642	0.0000000
H	-2.3078619	-4.8449985	0.0000000
C	-2.7451174	-1.5463104	0.0000000
H	-4.3369362	-3.0967356	0.0000000
C	-3.4446107	-0.3370317	0.0000000
C	-2.9047946	0.9507708	0.0000000
H	-4.5245945	-0.4324321	0.0000000
C	-1.5513716	1.3117520	0.0000000
C	-3.6646738	2.2126236	0.0000000
C	-2.7914746	3.2455572	0.0000000
H	-4.7432562	2.2768896	0.0000000
C	-1.4206968	2.7062951	0.0000000
H	-0.7395918	0.6253457	0.0000000
H	-3.0342493	4.2983974	0.0000000
C	-0.2408189	3.4532185	0.0000000
C	1.0679195	2.9647371	0.0000000
H	-0.3266651	4.5339409	0.0000000
N	-1.3803841	-1.7072113	0.0000000
H	-0.6577315	-1.0080629	0.0000000
N	1.5307976	-1.2946108	0.0000000
N	1.4533228	1.6456658	0.0000000
H	0.8834549	0.8173601	0.0000000
C	2.2859931	3.7142906	0.0000000
C	3.3427637	2.8389457	0.0000000

H	2.3327277	4.7918474	0.0000000
H	4.3933755	3.0813535	0.0000000

1.16 carbaporphyrinoid ($20H^{+}$)

Atom X Y Z
Energy = -973.6280875879

C	0.2669452	-3.4422795	-0.0102524
C	-1.0397894	-2.9692251	0.1302164
C	1.4397086	-2.7097740	-0.1347942
H	0.3809075	-4.5180641	-0.0341199
C	2.7378013	-3.2083592	-0.4445260
C	3.6209095	-2.1636146	-0.4424982
H	2.9527989	-4.2408469	-0.6700921
C	2.9125116	-0.9673383	-0.1317112
H	4.6752004	-2.2031911	-0.6662004
C	3.4389366	0.3110264	-0.0048868
C	2.7541611	1.5205612	0.1337908
H	4.5187171	0.3781226	-0.0263702
C	-2.2291915	-3.7083389	0.3922923
C	-3.2869890	-2.8328851	0.4003062
H	-2.2623899	-4.7718688	0.5668087
C	-2.7881555	-1.5228861	0.1528180
H	-4.3227391	-3.0671338	0.5880260
C	-3.4772561	-0.3159870	0.0311371
C	-2.9024099	0.9511720	-0.0806097
H	-4.5578009	-0.3911903	-0.0059991
C	-1.5603422	1.3184880	0.1460734
C	-3.6217870	2.1766110	-0.4622856
C	-2.7508126	3.2070730	-0.4640955
H	-4.6677770	2.2113179	-0.7283008
C	-1.4220855	2.7026967	-0.0833570
H	-0.8447455	0.7149013	0.6743706
H	-2.9597763	4.2321237	-0.7317717
C	-0.2685807	3.4809978	0.0265680
C	1.0363508	3.0031810	0.1503307
H	-0.3746030	4.5588818	-0.0127551
N	-1.4194571	-1.6514521	0.0218375
H	-0.8766035	-0.9558161	-0.4628320
N	1.5723588	-1.3285068	0.0117056
N	1.3917515	1.6749422	0.0217386
H	0.7980630	1.0229312	-0.4639976
C	2.2441228	3.7138615	0.3998473
C	3.2837827	2.8168190	0.3959572
H	2.3019946	4.7743709	0.5865975
H	4.3263437	3.0274096	0.5730964
H	0.9799261	-0.8287312	0.6579372

1.17 carbaporphyrinoid ($20H_2^{2+}$)

Atom X Y Z
Energy = -973.9030872914

C	0.3086321	-3.4712612	0.0229028
C	-1.0010430	-3.0117665	0.1082685
C	1.4860969	-2.7264093	-0.0905879
H	0.4361655	-4.5466205	0.0340964
C	2.7830901	-3.2245816	-0.3857429
C	3.6646003	-2.1721790	-0.3820662
H	3.0068404	-4.2571578	-0.6049468
C	2.9456483	-0.9838693	-0.0848916
H	4.7210954	-2.2105986	-0.5978745
C	3.4715348	0.3057241	0.0346274
C	2.7886802	1.5139921	0.1196301
C	-2.1952467	-3.7501317	0.3734607
C	-3.2514127	-2.8780346	0.3476887
C	-2.7520128	-1.5708312	0.0587145
C	-3.4727757	-0.3704229	-0.0429196
C	-2.9321646	0.9006910	-0.1503533
C	-1.4640591	1.2261693	-0.1821801
C	-3.6256629	2.1297403	-0.1740232
C	-2.7328977	3.1956958	-0.1737887
C	-1.4012429	2.7285319	-0.1497096
C	-0.2449616	3.4838617	-0.0400235
C	1.0631013	2.9850028	0.0647840
N	-1.3843430	-1.6951946	-0.0534678
N	1.6050538	-1.3439744	0.0513205
N	1.4261123	1.6606279	-0.0489895
C	2.2609271	3.7054222	0.3610134
C	3.3045527	2.8185367	0.3905825
H	2.3047838	4.7665012	0.5509012
H	4.3377687	3.0365961	0.6112656
H	-4.2885832	-3.1082727	0.5351305
H	-4.5509103	-0.4631558	0.0164852
H	-4.7028062	2.2275944	-0.1684823
H	-3.0181507	4.2389852	-0.1679441
H	-1.0204876	0.8550195	-1.1164734
H	-0.9422646	0.7891444	0.6721368
H	-0.3433449	4.5614731	0.0202684
H	4.5524099	0.3690150	0.0510105
H	1.0148068	-0.8516236	0.7073938
H	-0.8121658	-1.0389925	-0.5520641
H	0.8835400	0.9836924	-0.5529912
H	-2.2289044	-4.8069392	0.5878389

1.18 carbaporphyrinoid (1) with Dispersion Correction

Atom X Y Z
Energy = -1086.615681033

H	1.1135500	-0.4843719	-0.0586318
N	2.1156629	-0.4213067	0.0202047
C	2.8662481	-1.5654629	0.0195255
C	2.9179153	0.6980066	0.0642888
C	4.2351333	-1.1587534	0.0756580
C	4.2646605	0.2061785	0.1017699
H	5.0727672	-1.8372887	0.0926162
H	5.1312690	0.8461971	0.1453430
C	2.3394964	-2.8490625	-0.0293500
H	3.0564239	-3.6598746	-0.0332849
H	-1.1451539	-0.4156720	-0.0595367
N	-0.0725735	-2.3449502	-0.0487698
N	-2.1422983	-0.2918074	0.0165578
C	0.0646367	2.0571942	0.0952061
C	-1.1863209	-3.1364716	-0.0637456
C	-2.8748669	0.8712352	0.0621900
C	1.3115897	2.6763475	0.0239460
C	0.9881192	-3.1998177	-0.0620081
C	-2.9616893	-1.3891867	0.0163952
C	-1.1494942	2.7581659	0.0284337

C	-0.8150998	-4.5431343	-0.0972536
C	-4.2447602	0.4659957	0.0997477
C	0.5347081	-4.5827246	-0.0960791
C	-4.2988674	-0.9023818	0.0727464
C	-1.0788004	4.2045809	-0.0819444
H	-1.5102003	-5.3689136	-0.1144633
H	-5.0733509	1.1546648	0.1446460
H	1.1803606	-5.4476577	-0.1122198
H	-5.1770331	-1.5273605	0.0897284
H	-2.0147820	4.7520073	-0.1215538
C	-2.5095808	-2.7050922	-0.0324265
C	-2.4330678	2.1902968	0.0566861
C	2.5625854	2.0346156	0.0581332
H	-3.2747962	-3.4706515	-0.0372193
H	-3.2522012	2.9010861	0.0541712
H	3.4051780	2.7165678	0.0532207
C	0.0884970	4.8689239	-0.1395324
C	1.3716073	4.1723151	-0.0954274
H	0.1329421	5.9473936	-0.2202250
O	2.4325656	4.7851835	-0.1515818
H	0.0290209	0.9949868	0.2640386

2 Nuclear magnetic shieldings of the investigated carbaporphyrinoids

Nuclear magnetic resonance shieldings (in ppm) calculated at the B3LYP/def2-TZVP level.

2.1 Carbaporphyrinoid (1)

NO.	TYPE	MULT.	ISOTROPIC
1	h	1	37.07575867
2	n	1	106.01638102
3	c	1	36.20314117
4	c	1	42.28835352
5	c	1	54.05663063
6	c	1	44.25621826
7	h	1	22.28895290
8	h	1	21.94164124
9	c	1	79.05083227
10	h	1	21.69240784
11	h	1	36.85026235
12	n	1	-3.51756013
13	n	1	103.81555497
14	c	1	64.24287144
15	c	1	20.25561677
16	c	1	44.37612747
17	c	1	48.32571296
18	c	1	18.95007817
19	c	1	37.98272938
20	c	1	52.25354857
21	c	1	42.04932756
22	c	1	47.99297929
23	c	1	42.66198245
24	c	1	55.34251033
25	c	1	30.37519302
26	h	1	22.30677178
27	h	1	22.14109865
28	h	1	22.33375903
29	h	1	22.29769645
30	h	1	22.72273617
31	c	1	77.47927705
32	c	1	65.66176258
33	c	1	67.97305500
34	h	1	21.63038617
35	h	1	21.78742121
36	h	1	20.22847282
37	c	1	45.71787745
38	c	1	-9.30371777
39	h	1	24.16360160
40	o	1	-242.22549793
41	h	1	40.57181563

2.2 Carbaporphyrinoid (2)

NO.	TYPE	MULT.	ISOTROPIC
1	c	1	77.00042080
2	c	1	40.49874169
3	c	1	53.81693163
4	c	1	51.38734570
5	h	1	22.11938109
6	c	1	40.91228627
7	h	1	22.01376936
8	n	1	102.31300299
9	h	1	37.99156928
10	c	1	77.98513485
11	c	1	39.43973697
12	h	1	20.98503533
13	c	1	67.81796583
14	c	1	33.09538545
15	c	1	39.39284128
16	h	1	40.68421436
17	c	1	33.11378871
18	c	1	58.16938104
19	c	1	51.84822736
20	h	1	22.68659900
21	c	1	51.83148110
22	h	1	23.84908389
23	c	1	58.05961281
24	h	1	23.84116328
25	h	1	22.68286190
26	c	1	77.91648496
27	c	1	40.79521212
28	h	1	20.94269205
29	c	1	51.33572936
30	c	1	53.84631626
31	h	1	22.00397098
32	c	1	40.46355251
33	h	1	22.10738326
34	n	1	102.23051409
35	h	1	38.00029427
36	c	1	77.08687220
37	c	1	21.77766429
38	h	1	21.41914193
39	n	1	-7.52365150
40	c	1	43.19161881
41	c	1	43.20160576
42	h	1	22.16216601
43	c	1	21.78812170
44	h	1	22.16488499
45	h	1	21.43292763

2.3 Carbaporphyrinoid (3)

NO.	TYPE	MULT.	ISOTROPIC
1	c	1	13.74956778
2	c	1	78.61704352
3	n	1	-39.48138240
4	c	1	46.96200447
5	c	1	40.74258511
6	h	1	23.44967269
7	c	1	19.08076559
8	h	1	23.14157436
9	c	1	69.42642703
10	c	1	51.38980045
11	h	1	22.53743686
12	c	1	34.95340737
13	c	1	22.74653593
14	c	1	51.38925626
15	h	1	29.28466337
16	c	1	22.86423839
17	c	1	42.07424507
18	c	1	45.59599181
19	h	1	22.42240477
20	c	1	38.63712668
21	h	1	24.14476159
22	c	1	46.09466616
23	h	1	24.11939945
24	c	1	42.53190156
25	h	1	24.13941794
26	h	1	22.40679491
27	c	1	68.86450549
28	c	1	19.32833110
29	h	1	22.60396203
30	c	1	40.50776617
31	c	1	46.74898923
32	h	1	23.14259940
33	c	1	14.13383408
34	h	1	23.43716136
35	n	1	-38.98032100
36	c	1	78.31938721
37	c	1	33.73745366
38	h	1	23.30345753
39	c	1	49.11333519
40	c	1	49.20332929
41	h	1	23.28653102
42	n	1	98.31152737
43	c	1	33.56494478
44	h	1	23.28933098
45	h	1	30.09516310
46	h	1	23.33290689

2.4 Carbaporphyrinoid (4) (C_1)

NO.	TYPE	MULT.	ISOTROPIC
1	c	1	40.61591088
2	c	1	75.72828371
3	c	1	23.85420704
4	h	1	22.11801424
5	c	1	46.23069278
6	c	1	46.15192610
7	h	1	22.70349318
8	c	1	23.85466932
9	h	1	22.70268819
10	n	1	-8.56084147
11	n	1	109.74759406
12	c	1	54.25394915
13	c	1	50.79024478
14	h	1	22.65353517
15	c	1	42.49752510
16	h	1	22.90923013
17	h	1	35.96945923
18	c	1	73.17932974
19	c	1	34.24499721
20	h	1	23.37439991
21	c	1	48.15986846
22	c	1	25.84789160
23	c	1	45.55234586
24	h	1	24.93370095
25	c	1	34.54075070
26	h	1	41.53291364
27	c	1	45.61763531
28	h	1	26.47347759
29	c	1	26.24505788
30	h	1	26.47874900
31	h	1	24.90789291
32	c	1	73.06723165
33	c	1	42.65675946
34	h	1	23.36121852
35	c	1	50.66678762
36	c	1	54.28112191
37	h	1	22.91140683
38	c	1	40.41849639
39	h	1	22.64040797
40	n	1	109.31417409
41	h	1	35.87194615
42	c	1	75.59039766
43	h	1	22.09691378

2.5 Carbaporphyrinoid (4) (C_s)

NO.	TYPE	MULT.	ISOTROPIC
1	c	1	40.40244964
2	c	1	75.76124308
3	c	1	23.95026898
4	h	1	22.10359650
5	c	1	46.18438370
6	c	1	46.19574884
7	h	1	22.69796675
8	c	1	23.96629185
9	h	1	22.70028028
10	n	1	-7.34134003
11	n	1	109.65497640
12	c	1	54.34349905
13	c	1	50.65270179
14	h	1	22.63789271
15	c	1	42.63656385
16	h	1	22.91055758
17	h	1	35.97351932
18	c	1	73.26146828
19	c	1	34.36605054
20	h	1	23.34185019
21	c	1	48.89975485
22	c	1	25.97450050
23	c	1	45.53973508
24	h	1	24.90569367

25	c	1	34.37935842
26	h	1	41.70245255
27	c	1	45.51449623
28	h	1	26.46447971
29	c	1	25.99816077
30	h	1	26.46162897
31	h	1	24.90684133
32	c	1	73.28655055
33	c	1	42.65214331
34	h	1	23.34574072
35	c	1	50.66920731
36	c	1	54.35469988
37	h	1	22.90965437
38	c	1	40.39048562
39	h	1	22.64082546
40	n	1	109.66074712
41	h	1	35.98487921
42	c	1	75.75028572
43	h	1	22.10810564

2.6 Carbaporphyrinoid (6b-cis)

NO.	TYPE	MULT.	ISOTROPIC
1	c	1	76.17725016
2	c	1	43.02975307
3	c	1	23.85592204
4	h	1	21.39163460
5	c	1	44.82599191
6	c	1	44.71772981
7	h	1	22.21743895
8	c	1	23.93082620
9	h	1	22.21074497
10	n	1	-8.91664500
11	c	1	75.90348944
12	c	1	43.24932578
13	h	1	21.35768137
14	c	1	53.77471072
15	c	1	54.83866230
16	h	1	22.13981684
17	c	1	40.21901766
18	h	1	22.29980454
19	n	1	105.68410549
20	h	1	38.26121401
21	c	1	80.46705056
22	c	1	24.16933932
23	h	1	21.91273004
24	c	1	113.67212080
25	c	1	58.19212503
26	c	1	22.54149817
27	h	1	41.28713920
28	c	1	124.65861575
29	c	1	46.26284415
30	c	1	40.43895155
31	h	1	25.99998073
32	h	1	25.18091097
33	c	1	80.20003703
34	c	1	39.98605713
35	h	1	21.99008769
36	c	1	54.89335737
37	c	1	53.95812955
38	h	1	22.31458277
39	h	1	22.15891043
40	n	1	105.87415941
41	h	1	38.19386267
42	c	1	136.95190729
43	h	1	28.00503331
44	h	1	28.67183243
45	h	1	24.97238921
46	h	1	25.22989649

2.7 Carbaporphyrinoid (6b-trans)

NO.	TYPE	MULT.	ISOTROPIC
1	c	1	76.49281236
2	c	1	42.43039788
3	c	1	23.12569459
4	h	1	21.45796531
5	c	1	44.95208420
6	c	1	44.12319097
7	h	1	22.25706287
8	c	1	24.10084009
9	h	1	22.21941073
10	n	1	-9.55680802
11	c	1	74.89725235
12	c	1	43.52035932
13	h	1	21.37804901
14	c	1	53.76322881
15	c	1	55.06951773
16	h	1	22.15582968
17	c	1	40.62735345
18	h	1	22.31677651
19	n	1	104.04234393
20	h	1	37.97436618
21	c	1	80.31392480
22	c	1	30.11750733
23	h	1	21.81318596
24	c	1	107.35886659
25	c	1	56.22362114
26	c	1	30.16128909
27	h	1	40.84685238
28	c	1	117.17250077
29	c	1	146.46147450
30	h	1	27.35653747
31	c	1	38.74787193
32	h	1	28.31219761
33	h	1	28.49949990
34	c	1	41.42707650
35	h	1	24.90645621
36	h	1	24.01080070
37	h	1	24.47864265
38	c	1	81.50752719
39	c	1	40.08121218
40	h	1	22.04304755
41	c	1	54.10209703
42	c	1	53.50164979
43	h	1	22.30889829
44	h	1	22.19310993
45	n	1	105.52239597
46	h	1	38.04484534

2.8 Carbaporphyrinoid (9)

NO.	TYPE	MULT.	ISOTROPIC

1	c	1	39.60076648
2	c	1	77.83953437
3	c	1	20.90669985
4	h	1	21.52533322
5	c	1	54.18174564
6	c	1	50.94958494
7	h	1	22.22967426
8	c	1	41.15207105
9	h	1	22.13298738
10	n	1	100.29736746
11	h	1	37.80676322
12	c	1	73.41321879
13	c	1	39.30799339
14	h	1	21.40926943
15	c	1	74.70468041
16	c	1	26.62214222
17	c	1	23.52504485
18	c	1	42.24638510
19	h	1	40.89801872
20	c	1	142.92479270
21	c	1	41.89154234
22	h	1	27.11224086
23	h	1	27.67377883
24	c	1	48.34502178
25	h	1	24.62356594
26	h	1	23.70565460
27	c	1	72.57120585
28	c	1	41.31725805
29	h	1	21.30944170
30	c	1	50.84208912
31	c	1	54.30432330
32	h	1	22.10634775
33	c	1	39.81269516
34	h	1	22.24740402
35	n	1	99.57875749
36	h	1	37.84638632
37	c	1	77.68463717
38	c	1	21.07765571
39	h	1	21.58276221
40	n	1	-7.33065541
41	c	1	42.75157287
42	c	1	42.74080436
43	h	1	22.23960084
44	h	1	22.24282563

2.9 Carbaporphyrinoid (14) (C_1)

NO.	TYPE	MULT.	ISOTROPIC
1	c	1	37.71359167
2	c	1	78.01029587
3	c	1	19.17766459
4	h	1	21.57747813
5	c	1	41.78225185
6	c	1	41.55163809
7	h	1	22.25548202
8	c	1	53.38677915
9	c	1	48.74735399
10	h	1	22.23152226
11	c	1	40.93297902
12	h	1	22.04683876
13	c	1	19.56905267
14	h	1	22.23897021
15	c	1	77.40424250
16	c	1	38.19529407
17	h	1	21.54552522
18	c	1	53.71589773
19	c	1	48.95606034
20	h	1	22.21749197
21	c	1	41.43338910
22	h	1	22.00546341
23	c	1	70.96361807
24	c	1	38.26661724
25	h	1	20.87405360
26	c	1	76.41796643
27	c	1	40.29755586
28	h	1	40.26545302
29	c	1	41.94781797
30	c	1	40.06146588
31	h	1	22.33582717
32	c	1	-3.92395216
33	o	1	-295.81650400
34	h	1	19.71844392
35	c	1	67.51316963
36	h	1	21.26514514
37	n	1	99.58205107
38	h	1	37.47714490
39	n	1	99.20375950
40	h	1	37.45840533
41	n	1	-6.42579983

2.10 Carbaporphyrinoid (14) (C_s)

NO.	TYPE	MULT.	ISOTROPIC
1	c	1	37.91184638
2	c	1	78.26482716
3	c	1	19.16510578
4	h	1	21.52858759
5	c	1	41.69103889
6	c	1	41.59410072
7	h	1	22.20755862
8	c	1	54.48023183
9	c	1	47.87995120
10	h	1	22.25013617
11	c	1	41.78047493
12	h	1	22.04154901
13	c	1	19.69033826
14	h	1	22.20634897
15	c	1	77.50926879
16	c	1	38.42778498
17	h	1	21.58397223
18	c	1	55.10819446
19	c	1	47.79718412
20	h	1	22.25092225
21	c	1	42.46281808
22	h	1	21.99440466
23	c	1	71.95561018
24	c	1	40.51084028
25	h	1	20.81598863
26	c	1	76.69438656
27	c	1	42.23533707
28	h	1	41.23248567
29	c	1	37.14237541
30	c	1	36.19971199

31	h	1	21.94314873	
32	c	1	-4.47380377	
33	o	1	-299.48001655	1
34	h	1	19.61976763	
35	c	1	69.00275332	
36	h	1	21.25577327	
37	n	1	99.97279905	
38	h	1	37.32564937	
39	n	1	99.66053716	
40	h	1	37.21634188	
41	n	1	-2.99939148	

2.11 Carbaporphyrinoid (19)

NO.	TYPE	MULT.	ISOTROPIC
1	c	1	44.65781081
2	c	1	77.18592472
3	c	1	25.94407869
4	h	1	21.18970335
5	c	1	56.14880086
6	c	1	56.43124765
7	h	1	22.02732080
8	c	1	43.33585452
9	h	1	22.19692864
10	n	1	102.33615267
11	h	1	36.67274052
12	n	1	-3.62034188
13	c	1	80.24515718
14	c	1	28.68129144
15	h	1	21.77665294
16	c	1	141.34833886
17	c	1	57.23470516
18	c	1	28.67347973
19	h	1	39.81225984
20	c	1	141.46881593
21	h	1	26.59585286
22	h	1	26.10826336
23	h	1	26.61262198
24	h	1	26.12807002
25	c	1	80.21480461
26	c	1	43.34986228
27	h	1	21.76579932
28	c	1	56.39090036
29	c	1	56.19475231
30	h	1	22.19999297
31	c	1	44.68594908
32	h	1	22.04382569
33	n	1	102.37468613
34	h	1	36.66680624
35	c	1	77.12215396
36	c	1	26.00163740
37	h	1	21.22810351
38	c	1	46.27443091
39	c	1	46.22706090
40	h	1	22.02728702
41	h	1	22.03213244

2.12 Carbaporphyrinoid (19′)

NO.	TYPE	MULT.	ISOTROPIC
1	c	1	46.82779785
2	c	1	85.89197122
3	c	1	46.93666358
4	h	1	21.37196874
5	c	1	54.83564060
6	c	1	57.37941844
7	h	1	22.18408787
8	c	1	39.52024363
9	h	1	22.37864502
10	n	1	117.33958271
11	h	1	40.52095557
12	n	1	106.16905614
13	c	1	79.77924266
14	c	1	27.08075367
15	h	1	21.85539714
16	c	1	142.73266643
17	c	1	49.68370131
18	c	1	22.84089742
19	h	1	40.04556652
20	c	1	143.82952648
21	h	1	26.81375165
22	h	1	26.43051753
23	h	1	26.84682978
24	h	1	26.46104198
25	c	1	68.79869676
26	c	1	19.50689210
27	h	1	21.74938130
28	c	1	43.30460651
29	c	1	44.84409810
30	h	1	22.38777006
31	c	1	22.25842799
32	h	1	22.28220934
33	n	1	-6.97458504
34	c	1	78.14336890
35	c	1	40.17341902
36	h	1	21.58241555
37	c	1	55.66100963
38	c	1	52.75359305
39	h	1	22.09274407
40	h	1	22.18439362
41	h	1	37.19165410

2.13 Carbaporphyrinoid ($19H^+$)

NO.	TYPE	MULT.	ISOTROPIC
1	c	1	78.42131423
2	c	1	39.23760156
3	c	1	48.30310036
4	c	1	48.35693774
5	h	1	21.61321702
6	c	1	39.32846437
7	h	1	21.61808839
8	c	1	78.39815575
9	c	1	42.06317323
10	h	1	20.79243669
11	c	1	47.05725596
12	c	1	49.09251830
13	h	1	21.73255905
14	c	1	34.44607596
15	h	1	21.91990216
16	c	1	72.01723532
17	c	1	15.81830786
18	h	1	21.37630362

19	c	1	50.07569693
20	c	1	15.81824966
21	h	1	40.61346653
22	c	1	141.76531013
23	c	1	141.61851170
24	h	1	26.83887261
25	h	1	26.22276345
26	h	1	26.80764413
27	h	1	26.19905812
28	c	1	71.94717798
29	c	1	34.29333775
30	h	1	21.34896267
31	c	1	49.11114015
32	c	1	47.02176260
33	h	1	21.90529838
34	c	1	42.00796955
35	h	1	21.70794793
36	h	1	20.74525922
37	n	1	119.62541782
38	h	1	40.83077161
39	n	1	124.59543872
40	h	1	40.55630095
41	n	1	119.73720728
42	h	1	40.81760087

2.14 Carbaporphyrinoid (20) (C_1)

NO.	TYPE	MULT.	ISOTROPIC
1	c	1	48.14543823
2	c	1	48.20212803
3	c	1	35.23857650
4	c	1	35.19526104
5	c	1	76.83505714
6	n	1	-6.03214982
7	c	1	42.46539370
8	c	1	42.43358204
9	c	1	70.15909293
10	c	1	41.55493576
11	c	1	78.10652926
12	c	1	39.60808432
13	c	1	54.24139343
14	c	1	50.50292770
15	c	1	39.57221967
16	c	1	54.19019436
17	c	1	50.60341120
18	n	1	99.82861656
19	n	1	99.79355907
20	c	1	20.77435525
21	h	1	23.39266626
22	h	1	23.39802443
23	h	1	22.08471806
24	h	1	21.45395403
25	h	1	22.19655667
26	h	1	21.46135817
27	h	1	22.21215196
28	h	1	22.21460834
29	c	1	20.78474119
30	c	1	78.05812998
31	h	1	21.45796810
32	h	1	22.19632140
33	h	1	22.08636030
34	c	1	41.57985405
35	c	1	70.17887741
36	h	1	21.45715384
37	h	1	37.96631604
38	h	1	37.96412508
39	h	1	40.67653060

2.15 Carbaporphyrinoid (20) (C_s)

NO.	TYPE	MULT.	ISOTROPIC
1	c	1	78.22938766
2	c	1	39.79381600
3	c	1	20.68705198
4	h	1	21.48063295
5	c	1	42.36934869
6	c	1	42.31937350
7	h	1	22.16770387
8	c	1	20.62453968
9	h	1	22.16594244
10	c	1	78.25027876
11	c	1	39.70738046
12	h	1	21.44548420
13	c	1	55.52563355
14	c	1	49.59005499
15	h	1	22.22979650
16	c	1	42.57135240
17	h	1	22.07805013
18	c	1	71.36643887
19	c	1	37.52801879
20	h	1	21.43605066
21	c	1	78.58990518
22	c	1	43.89938993
23	c	1	43.75841125
24	h	1	23.06782841
25	c	1	37.56509844
26	h	1	41.76130796
27	h	1	23.05485817
28	c	1	71.30906622
29	c	1	42.40310477
30	h	1	21.36854767
31	n	1	100.40546893
32	h	1	37.71271211
33	n	1	-2.93070108
34	n	1	100.34994131
35	h	1	37.74091099
36	c	1	49.54402218
37	c	1	55.46867956
38	h	1	22.06187544
39	h	1	22.21989509

2.16 Carbaporphyrinoid ($20H^+$)

NO.	TYPE	MULT.	ISOTROPIC
1	c	1	78.93497294
2	c	1	39.03167953
3	c	1	36.62859542
4	h	1	20.83558622
5	c	1	45.60318841
6	c	1	45.58241322
7	h	1	21.60469087
8	c	1	36.64564659
9	h	1	21.60164515

10	c	1	78.93421379
11	c	1	38.99657463
12	h	1	20.83173040
13	c	1	48.43889270
14	c	1	45.64846137
15	h	1	21.78417564
16	c	1	36.24023791
17	h	1	21.64380026
18	c	1	61.73266316
19	c	1	29.81055378
20	h	1	20.84250038
21	c	1	74.58865024
22	c	1	42.64364072
23	c	1	42.67791233
24	h	1	23.12359468
25	c	1	29.75160005
26	h	1	40.94891402
27	h	1	23.12535796
28	c	1	61.74487279
29	c	1	36.24755610
30	h	1	20.83605971
31	n	1	108.16599129
32	h	1	40.10408026
33	n	1	125.91244687
34	n	1	108.16570025
35	h	1	40.10647629
36	c	1	45.64018935
37	c	1	48.46270576
38	h	1	21.63949262
39	h	1	21.78381843
40	h	1	40.58668295

2.17 Carbaporphyrinoid ($20H_2^{2+}$)

NO.	TYPE	MULT.	ISOTROPIC
1	c	1	66.59534848
2	c	1	36.07080276
3	c	1	32.75099139
4	h	1	19.49211298
5	c	1	38.22307020
6	c	1	38.21949536
7	h	1	20.63009826
8	c	1	32.76643914
9	h	1	20.62825992
10	c	1	66.61087749
11	c	1	36.02393436
12	c	1	38.20808095
13	c	1	39.36893226
14	c	1	30.81484044
15	c	1	58.94644818
16	c	1	26.17233455
17	c	1	152.71317424
18	c	1	19.80687846
19	c	1	19.76836132
20	c	1	26.14933714
21	c	1	58.94079324
22	c	1	30.80123685
23	n	1	110.94943031
24	n	1	122.85409566
25	n	1	110.93026164
26	c	1	39.37965835
27	c	1	38.25118484
28	h	1	20.79140297
29	h	1	20.75033428
30	h	1	20.79333821
31	h	1	19.14985225
32	h	1	19.46011142
33	h	1	19.45683082
34	h	1	42.54880578
35	h	1	43.52826226
36	h	1	19.14000751
37	h	1	19.48997580
38	h	1	41.68341865
39	h	1	41.20422243
40	h	1	41.20602940
41	h	1	20.74601840

2.18 Carbaporphyrinoid (1) with Dispersion correction (D3)

NO.	TYPE	MULT.	ISOTROPIC
1	h	1	37.09446246
2	n	1	106.35600622
3	c	1	36.29772132
4	c	1	42.20355047
5	c	1	54.12320632
6	c	1	44.24066594
7	h	1	22.29594605
8	h	1	21.93883689
9	c	1	79.14467334
10	h	1	21.71854242
11	h	1	36.86173738
12	n	1	-3.35647655
13	n	1	104.19011910
14	c	1	64.27548513
15	c	1	20.32205878
16	c	1	44.43748728
17	c	1	48.31969137
18	c	1	18.98605679
19	c	1	38.06403066
20	c	1	52.29832866
21	c	1	42.15757155
22	c	1	48.13266267
23	c	1	42.68779083
24	c	1	55.27583855
25	c	1	30.39373140
26	h	1	22.31542282
27	h	1	22.14994541
28	h	1	22.34051738
29	h	1	22.30372819
30	h	1	22.72233402
31	c	1	77.56127233
32	c	1	65.85330732
33	c	1	68.34755247
34	h	1	21.65522416
35	h	1	21.78602103
36	h	1	20.23336894
37	c	1	45.61579474
38	c	1	-9.34072929
39	h	1	24.15520068
40	o	1	-242.11700821
41	h	1	40.59007833

3 Summary of calculated current strength susceptibilities

Integrated current strength suceptibilities for the investigated molecules are given in nA/T below. Current strengths for the lower in energy structures are reported when different structures have been investigated. All results have been obtained on B3LYP/def2-TZVP level.

		meso bond			C=C			CNC		
	ring	tot	dia	para	tot	dia	para	tot	dia	para
Molecule 1	A	24.3	28.6	-4.2	0.7	6.7	-6.0	23.4	27.6	-4.2
	B	24.4	29.2	-4.8	18.0	21.6	-3.6	6.5	14.0	-7.5
	C	24.0	27.5	-3.5	12.4	16.8	-4.4	12.0	19.1	-8.9
	D	24.5	28.2	-3.7	18.7	22.3	-3.5	5.8	13.0	-7.2
Molecule 2	A	26.4	30.4	-4.0	3.8	10.7	-6.9	22.5	27.0	-4.6
	B	26.1	30.15	-4.1	19.1	22.6	-3.5	6.9	14.0	-7.1
	C	26.5	30.0	-3.5	13.9	17.9	-4.0	12.6	19.5	-6.9
	D	26.1	30.2	-4.1	19.1	22.6	-3.5	6.9	14.0	7.1
Molecule 3	A	15.4	23.4	-8.1	18.7	26.3	-7.6	-3.2	0.6	-4.2
	B	15.0	24.2	-9.2	8.9	15.2	-6.3	5.9	12.9	-7.0
	C	15.2	22.3	-7.1	12.0	17.6	-5.6	3.2	9.4	-6.2
	D	15.0	24.2	-9.2	8.9	15.2	-6.3	5.9	12.9	-7.0
Molecule 4(C_1)	A	21.9	26.6	-4.7	-16.3	36.3	-20.0	37.9	41.1	-3.2
	B	21.8	25.9	-4.1	17.8	21.5	-3.7	4.1	11.3	-7.2
	C	21.9	25.8	-3.9	13.1	17.2	-4.1	8.8	15.9	-7.1
	D	21.8	25.9	-4.1	17.8	21.5	-3.7	4.1	11.3	-7.2
Molecule 6b (cis)	A	26.0	30.2	-4.2	1.4	8.0	-6.7	24.5	28.5	-4.0
	B	25.8	29.2	-3.4	19.0	23.4	-4.4	6.5	13.3	-6.8
	C	25.4	29.8	-4.4	13.7	17.8	-4.1	11.5	17.4	-5.9
	D	25.8	29.2	-3.4	19.0	23.4	-4.4	6.5	13.3	-6.8
Molecule 6b(trans)	A	25.4	29.2	-3.8	1.3	7.9	-6.6	24.3	28.4	4.1
	B	26.3	30.4	-4.1	19.5	23.4	-3.9	6.3	13.2	-6.9
	C	25.6	29.6	-4.0	14.1	17.6	-3.5	11.3	17.3	-6.3
	D	26.3	30.4	-4.1	19.5	23.4	-3.9	6.3	13.2	-6.9
Molecule 9	A	26.5	30.9	-4.4	3.8	8.3	-4.6	23.0	28.1	-5.1
	B	25.9	29.7	-3.8	18.4	22.2	-3.8	7.2	13.7	-6.5
	C	25.9	30.2	-4.3	13.1	17.3	-4.2	12.8	19.4	-6.3
	D	25.9	29.7	-3.8	18.4	22.2	-3.8	7.2	13.7	-6.5
Molecule 14 (C_1)	A	24.0	28.6	-4.6	3.8	10.7	-6.9	20.3	25.7	-5.4
	B	24.6	28.6	-4.0	17.8	21.5	-3.7	6.8	14.0	-7.2
	C	24.9	28.9	-4.0	12.8	16.9	-4.1	12.3	19.1	-6.8
	D	24.6	28.6	-4.0	17.8	21.5	-3.7	6.8	14.0	-7.2
Molecule 19	A	24.8	28.6	-3.8	1.5	8.0	-6.5	23.8	27.5	-3.7
	B	24.4	28.1	-3.7	18.5	22.1	-3.6	5.9	12.7	-6.8
	C	24.3	28.1	-3.7	13.5	17.6	-4.1	10.8	17.2	-6.4
	D	24.4	28.1	-3.1	18.5	22.1	-3.6	5.9	12.7	-6.8
Molecule 19′	A	26.0	29.6	-3.6	1.6	8.2	-6.6	24.3	28.4	-4.1
	B	26.3	30.0	-3.6	13.6	17.7	-4.1	12.7	19.1	-6.4
	C	26.0	29.7	-3.4	20.0	23.3	-3.3	6.2	13.1	-6.9
	D	26.0	29.4	-3.4	20.4	23.7	-3.3	5.6	12.6	-7.0

		meso bond			C=C			CNC		
	ring	tot	dia	para	tot	dia	para	tot	dia	para
Molecule $19H^+$	A	26.1	29.6	-3.52	1.4	7.9	-6.5	24.7	28.6	-3.9
	B	26.7	30.0	-3.2	20.3	23.5	-3.2	6.4	13.0	-6.6
	C	27.0	30.6	-3.6	20.9	24.2	-3.3	5.6	11.6	-6.0
	D	26.7	29.9	-3.2	20.3	23.5	-3.2	6.4	13.0	-6.6
Molecule 20(C_s)	A	26.2	30.4	-4.2	4.2	7.7	-3.5	22.1	27.3	-5.2
	B	26.1	30.0	-4.0	19.0	22.5	-3.5	7.0	13.1	-6.1
	C	25.8	29.5	-3.6	13.3	17.5	-4.2	12.8	18.9	-6.1
	D	26.1	30.0	-4.0	19.0	22.5	-3.5	7.0	13.1	-6.1
Molecule $20H^+$	A	25.8	29.2	-3.4	1.8	6.1	-4.3	23.9	28.7	-4.8
	B	26.7	29.8	-3.1	19.2	22.4	-3.2	6.5	13.1	-6.6
	C	27.7	31.0	-3.3	21.1	24.4	-3.3	6.0	12.6	-6.6
	D	26.7	29.8	-3.1	19.2	23.4	-3.2	6.5	13.1	-6.6
Molecule $20H_2^{2+}$	A	27.9	31.4	-3.5	27.0	29.9	-2.9	0.9	7.0	-6.0
	B	27.9	31.2	-3.3	19.6	23.1	-3.5	8.1	14.4	-6.3
	C	27.7	31.0	-3.3	21.1	24.4	-3.3	6.4	13.0	-6.6
	D	27.9	31.2	-3.3	19.7	21.2	-3.5	8.2	14.4	-6.2

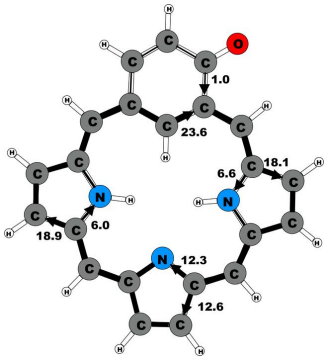

Fig. 1 Calculated B3LYP/def2-TZVP/D3 integrated current strength susceptibilities for oxybenziporphyrin **1**.