Experimental and theoretical determination of the main types of ligands in a mixture of petroporphyrins

Yuriy A. Zhabanov, Georgiy L. Pakhomov, Vlad.V. Travkin, Dmitry A. Vyalkin, Ekaterina D. Rychikhina, Nikolay. A. Mironov, Makhmut R. Yakubov

Supporting Information

Table S1. Composition of the lowest excited states and corresponding oscillator strengths for Ni-petroporphyrins.

State	Composition, %	f	λ, nm	λ_{exp}, nm
Ni(II)-EtioP-III				
4	HOMO-1→LUMO+1 (33) HOMO→LUMO (65)	0.08	496	554 [19]
5	HOMO-1→LUMO (34) HOMO→LUMO+1 (63)	0.06	495	
Ni(II)-DPEP				
4	HOMO-1→LUMO+1 (32) HOMO→LUMO (65)	0.08	496	553 [18]
5	HOMO-1→LUMO (41) HOMO→LUMO+1 (57)	0.02	492	
Ni(II)-Rhodo				
4	HOMO-1→LUMO+1 (27) HOMO→LUMO (71)	0.14	511	566 [46]
5	HOMO-1→LUMO (31) HOMO→LUMO+1 (67)	0.13	503	
Ni(II)-diDPEP				
4	HOMO-1→LUMO+1 (32) HOMO→LUMO (66)	0.08	498	
5	HOMO-1→LUMO (50) HOMO→LUMO+1 (48)	0.001	491	
Ni(II)-DPEP-Rhodo				
4	HOMO-1→LUMO+1 (29) HOMO→LUMO (69)	0.12	509	
5	HOMO-1→LUMO (34) HOMO→LUMO+1 (63)	0.08	502	
Ni(II)-diDPEP-Rhodo				
4	HOMO-1→LUMO+1 (28) HOMO→LUMO (68)	0.13	509	
5	HOMO-1→LUMO (42) HOMO→LUMO+1 (54)	0.03	498	

Table S2. Composition of the lowest excited states and corresponding oscillator strengths for VO-petroporphyrins.

State	Composition, %	f	λ, nm	λ_{exp}, nm
VO(IV)-EtioP-III				
7	HOMO-1→LUMO+1 (35) HOMO→LUMO (62)	0.06	513	572 [47]

8	HOMO-1→LUMO (37) HOMO→ LUMO+1 (62)	0.05	512	
VO(IV)-DPEP				
7	HOMO-1→LUMO+1 (35) HOMO→LUMO (62)	0.05	514	575 [18]
8	HOMO-1→LUMO (43) HOMO→ LUMO+1 (53)	0.01	511	
14	HOMO-1→LUMO (43) HOMO→LUMO+1 (36)	1.82	347	
15	HOMO-1→LUMO+1 (49) HOMO→LUMO (28)	1.87	345	
VO(IV)-diDPEP				
6	HOMO-1→LUMO (9) HOMO-1→LUMO+1 (29) HOMO→LUMO (52) HOMO→LUMO+1 (8)	0.05	517	
7	HOMO-1→LUMO (43) HOMO-1→LUMO+1 (6) HOMO→LUMO (11) HOMO→LUMO+1 (37)	0.01	513	
VO(IV)-Rhodo				
7	HOMO-1→LUMO+1 (28) HOMO→LUMO (70)	0.11	527	
8	HOMO-1→LUMO+1 (33) HOMO→LUMO+1 (63)	0.10	518	
13	HOMO-1→ LUMO (55) HOMO→ LUMO+1 (28)	2.21	353	
15	HOMO-1→ LUMO+1 (55) HOMO→ LUMO (22)	1.56	345	
VO(IV)-DPEP-Rhodo				
6	HOMO-1→LUMO+1 (30) HOMO→LUMO (66)	0.09	529	
8	HOMO-1→LUMO (37) HOMO→LUMO+1 (60)	0.06	521	
VO(IV)-diDPEP-Rhodo				
6	HOMO-1→LUMO (4) HOMO-1→LUMO+1 (30) HOMO→LUMO (59) HOMO→LUMO+1 (5)	0.09	529	
7	HOMO-1→LUMO (40) HOMO-1→LUMO+1 (4) HOMO→LUMO (8) HOMO→LUMO+1 (47)	0.03	518	

Table S3. NICS values (in ppm) for each ring, in accordance with Figure S1.

	A	B	C	D	E	F	G	H	I	J	K
H_2											
EtioP-III	2.915	12.663	2.890	12.678	-	-	-	-	-	-	-
DPEP	3.305	13.275	2.993	11.908	-0.264	-	-	-	-	-	-
Rhodo	3.051	12.606	2.958	12.610	-	8.862	-	-	-	-	-
diDPEP	4.213	13.224	3.415	13.206	-0.332	-	-0.319	-	-	-	-

DPEP-Rhodo	3.463	13.178	1.616	11.897	-0.433	9.032	-	-	-	-	-
diDPEP-Rhodo	4.394	13.068	1.838	13.229	-0.455	9.106	-0.389	-	-	-	-
Ni(II)											
EtioP-III	6.145	6.331	6.344	6.323	-	-	-	18.171	18.128	18.127	18.155
DPEP	6.399	7.172	7.145	5.914	0.262	-	-	18.641	18.681	18.437	18.295
Rhodo	6.502	6.431	4.595	6.491	-	9.326	-	17.851	17.837	17.708	17.721
diDPEP	7.789	6.883	7.329	6.866	0.249	-	0.242	18.680	18.631	18.730	18.658
DPEP-Rhodo	6.812	7.211	4.706	5.276	0.052	9.853	-	18.497	18.557	18.198	18.048
diDPEP-Rhodo	8.161	6.958	4.762	7.047	0.056	9.822	0.173	18.483	18.522	18.486	18.294
VO(IV)											
EtioP-III	8.251	8.237	8.222	8.214	-	-	-	17.069	17.059	17.090	17.059
DPEP	8.076	9.622	8.668	7.418	-0.409	-	-	16.977	16.780	17.017	16.863
Rhodo	8.544	8.301	5.656	8.303	-	9.843	-	16.680	16.691	16.584	16.572
diDPEP	8.548	9.561	9.048	9.606	-0.447	-	-0.482	17.199	16.830	17.161	16.818
DPEP-Rhodo	8.464	9.633	5.597	7.550	-0.555	10.132	-	16.746	16.572	16.701	16.511
diDPEP-Rhodo	9.392	9.562	5.451	9.673	-0.575	10.093	-0.462	16.785	16.467	16.769	16.339

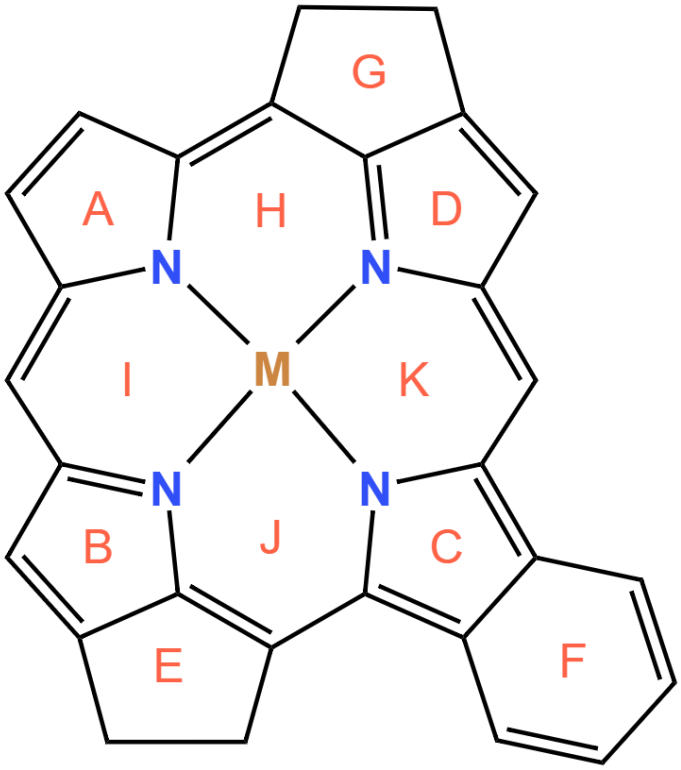

Figure S1. Structural formula of all studied compounds with letter designations of the rings used for NICS calculations.

XYZ-coordinates for H_2EtioP-III atoms (3,8,13,17- tetraethyl-2,7,12,18- tetramethylporphyrin)

N	2.165518165	0.166593486	-0.007268417
N	0.029111167	2.154997366	-0.053052861
N	-2.039174638	0.098666459	-0.041953028
N	0.097200450	-1.894249564	0.002164824
C	2.928736673	1.301559111	-0.010186716
C	-1.064321665	2.963273899	-0.076752607
C	-2.799808466	-1.038194317	-0.020553093
C	1.098308636	2.996248440	-0.045115765
C	-2.837798135	1.208513103	-0.071350999
C	-0.972227604	-2.735059396	0.016117263
C	2.961562473	-0.945790037	0.012170414
C	1.190695622	-2.702602319	0.020468787
C	4.306624317	0.886682957	0.008971770
C	-0.684682742	4.377816812	-0.082861778
C	-4.177503644	-0.627000557	-0.031349892
C	0.676903985	4.396817036	-0.058634046
C	-4.202002605	0.750338079	-0.068572861
C	-0.551038202	-4.135538069	0.045530395
C	4.325334720	-0.491136677	0.026872399
C	0.810691743	-4.117033372	0.043874244
C	2.436343471	2.599729150	-0.030470075
C	-2.388324524	2.521906739	-0.096626587
C	-2.309843289	-2.336848787	0.004788797
C	2.514440367	-2.260036486	0.018593686
H	3.181802371	3.389393473	-0.030999222
H	-3.058538996	-3.123701843	0.018079088
H	3.290058170	-3.019971074	0.030463844
C	5.471353944	1.822752357	0.063260032
C	-5.333828617	-1.569603515	0.004197159
C	1.595998324	5.572070748	-0.038353127
C	-5.395325393	1.651081727	-0.043352333
C	-1.469923865	-5.310626906	0.079599485
C	5.510218962	-1.397427650	0.067877141
C	1.757554292	-5.272031194	0.112886710
H	5.270110201	2.699847585	-0.564071455
H	-5.309129222	-2.266339127	-0.841947682
H	2.202923816	5.590570797	0.875525634
H	-5.216525889	2.519077779	-0.689937235
H	-2.145608783	-5.319105436	-0.784480852
H	5.514656032	-2.089627506	-0.782263412
H	2.622709698	-5.085838743	-0.536645869
H	6.352122277	1.337346082	-0.371977774
H	-6.284523847	-1.032811974	-0.032809814
H	2.290143420	5.555516614	-0.887547975
H	-6.258075787	1.129069259	-0.472214881

H	-0.913653327	-6.251761456	0.074968649
H	6.444320771	-0.831534584	0.042527505
H	1.271486456	-6.169667295	-0.287117934
C	5.792648368	2.276388511	1.495299453
H	6.044683131	1.416169768	2.123740965
H	4.929541117	2.774842431	1.947942275
H	6.638428702	2.971823696	1.506967645
H	1.041035837	6.512944513	-0.082129728
H	-2.096304936	-5.303282168	0.980305654
H	5.515744247	-2.004083531	0.981436787
C	-5.739268674	2.128658057	1.375610882
H	-6.606412659	2.797255813	1.366127675
H	-5.967472786	1.276332753	2.023591646
H	-4.894847506	2.665102443	1.820262098
H	-5.328697393	-2.170948322	0.921142502
C	2.241754444	-5.552645326	1.543988564
H	1.394869587	-5.797016401	2.193181752
H	2.946725497	-6.390717180	1.565386733
H	2.738038215	-4.673748922	1.968235259
C	-1.633694719	5.532743444	-0.057058761
H	-1.137686075	6.424964080	-0.456844659
H	-2.480964945	5.336245156	-0.727014168
C	-2.157586227	5.834038269	1.355785131
H	-1.329535861	6.088951132	2.024931279
H	-2.665100700	4.961082617	1.779266781
H	-2.863674766	6.671365201	1.345197393
H	-3.160871743	3.284108309	-0.124450337
H	-1.026456499	0.116196677	-0.044336287
H	1.152926097	0.151871189	-0.025847511

XYZ-coordinates for H_2DPEP atoms (7,12,18-triethyl-3,8,13,17-tetramethylcyclopenta[*at*]porphyrin)

N	2.122666031	0.086035530	0.049833025
N	0.165528664	2.023027817	0.083487348
N	-2.038652888	0.047637986	0.097606481
N	0.041535821	-2.031047309	0.062741655
C	2.962506727	1.160888911	0.046826462
C	-0.993886992	2.712501271	0.105689303
C	-2.840246646	-1.044337215	0.092092308
C	1.216054345	2.912949442	0.070710887
C	-2.879134531	1.123592450	0.107621250
C	-1.079644082	-2.820572178	0.078052604
C	2.925775724	-1.009058975	0.041859799
C	1.173951886	-2.800203953	0.052876508
C	4.361896030	0.734547849	0.035989833
C	-0.699120367	4.097093057	0.103862463
C	-4.250340169	-0.665796920	0.093366377
C	0.669902762	4.250249318	0.082211769
C	-4.278644113	0.699638096	0.104817857
C	-0.630873807	-4.186192471	0.082588163

C	4.338454169	-0.628252129	0.036544732
C	0.746734241	-4.175509544	0.062143521
C	2.542887722	2.494630551	0.050685221
C	-2.352382389	2.421606005	0.124426162
C	-2.391807857	-2.370242186	0.088062551
C	2.483930572	-2.333488062	0.038908615
H	3.303744919	3.269227114	0.041857314
H	-3.152841794	-3.145443201	0.094132725
H	3.252424343	-3.100614870	0.030679467
C	5.545828722	1.646510300	0.080249083
C	5.486588872	-1.581203263	0.043025820
C	1.672602435	-5.349083646	0.107524207
H	5.367992629	2.519303864	-0.561282594
H	5.450002302	-2.262563239	-0.815858931
H	2.552002836	-5.151736638	-0.517678342
H	6.419747755	1.136751396	-0.342211938
H	6.442953825	-1.052768892	0.007137317
H	1.179246949	-6.221625959	-0.335361369
C	-1.978183148	4.873119500	0.102063190
H	-2.045406364	5.580614535	0.936544946
H	-2.096029357	5.457464751	-0.818662064
C	-3.078249936	3.761007425	0.200655848
H	-3.618832620	3.846753059	1.151414514
H	-3.823232703	3.870779638	-0.594389618
C	-5.493325563	1.571904857	0.037250815
H	-6.339555837	1.053408695	0.503957616
H	-5.343405987	2.484905230	0.622234184
C	-5.398772618	-1.618675262	0.065838963
H	-5.361917773	-2.318609726	0.909622700
H	-6.356429483	-1.093393614	0.112375006
C	2.121876349	-5.686374077	1.537193689
H	1.258650419	-5.935369739	2.162738990
H	2.809415220	-6.538684041	1.542856866
H	2.627680102	-4.831411153	1.997055267
C	-1.542400347	-5.367270879	0.118007549
H	-2.242506918	-5.358386488	-0.725536865
H	-0.981051461	-6.303517574	0.076432154
H	-2.140385012	-5.380547758	1.037145174
C	1.477834954	5.505486129	0.067210993
H	2.153152864	5.560772602	0.929364111
H	2.096260732	5.576160762	-0.835681029
H	0.825572846	6.382431337	0.095628416
C	5.872268765	2.116645366	1.506314033
H	5.017195475	2.636096018	1.950825085
H	6.106286024	1.260441083	2.147050673
H	6.730557267	2.797155151	1.511444921
H	5.487102631	-2.201549565	0.948082988
H	-5.397782669	-2.219339620	-0.852409051
C	-5.866923068	1.935752140	-1.408130636

H	-5.029600172	2.419815987	-1.921508480
H	-6.114397465	1.032441719	-1.974960129
H	-6.728999219	2.611014435	-1.439098096
H	0.020425786	-1.020916615	0.048698814
H	0.311066959	1.020198158	0.088265225

XYZ-coordinates for H_2Rhodo atoms (8,13,18-triethyl-7,12,17-trimethylbenzo[*b*]porphyrin)

N	1.972783614	-0.003085300	0.018696279
N	-0.088085006	2.064211237	-0.095414020
N	-2.110344648	-0.073559034	-0.105071978
N	-0.012782074	-2.142190988	0.011391289
C	2.780625146	1.091323532	0.021534282
C	-1.221356599	2.826938223	-0.153650763
C	-2.895913926	-1.184637242	-0.096464974
C	1.025211946	2.861453559	-0.075854872
C	-2.932603201	1.009503037	-0.162284572
C	-1.123917297	-2.939677421	0.005809450
C	2.814631117	-1.070862096	0.072982490
C	1.123204220	-2.904418672	0.065990226
C	4.193757618	0.713904715	0.077626641
C	-0.805559056	4.204785133	-0.171796973
C	-4.308946489	-0.814635378	-0.149943690
C	0.571295327	4.224174866	-0.118701668
C	-4.332345281	0.590057999	-0.192615007
C	-0.668406183	-4.302193099	0.063930984
C	4.213168248	-0.647788672	0.113653875
C	0.709021576	-4.281627980	0.095590099
C	2.337510231	2.414545733	-0.026321598
C	-2.521883929	2.340390291	-0.188980913
C	-2.440076037	-2.500170084	-0.045166248
C	2.419334596	-2.409689102	0.089098753
H	3.097320793	3.190378431	-0.022009087
H	-3.197424773	-3.278438254	-0.044793193
H	3.209526185	-3.153478781	0.130791478
C	5.347300377	1.662989546	0.141027356
C	1.476984113	5.409908956	-0.095562592
C	-1.573854145	-5.488006616	0.092169041
C	5.388250375	-1.564348390	0.188930439
C	1.643446378	-5.443866014	0.205370727
H	5.170494760	2.512538747	-0.531252261
H	2.185154923	5.389251063	-0.932210802
H	-2.199826208	-5.536270877	-0.806848375
H	5.414681629	-2.256646182	-0.661545236
H	2.543740268	-5.250698062	-0.390711733
H	6.250664039	1.168237613	-0.234688528
H	0.911979814	6.342633170	-0.159218583
H	-1.006157907	-6.419260117	0.153555552
H	6.328617971	-1.006867148	0.191920527
H	1.176312232	-6.332187639	-0.234287671

C	5.607358292	2.180822038	1.564176910
H	5.842919508	1.349743030	2.236653465
H	4.722554172	2.686554128	1.964393570
H	6.444852441	2.886568814	1.580781110
H	2.065973121	5.442363862	0.828852760
H	-2.247189010	-5.453519347	0.956781808
H	5.364121158	-2.172908672	1.101498633
C	2.041333584	-5.740369194	1.659167012
H	1.157227553	-5.979787642	2.258640083
H	2.733983667	-6.586771294	1.712177077
H	2.523987176	-4.870143995	2.115282040
C	-1.740983132	5.371169525	-0.181463880
H	-1.241712238	6.236719264	-0.631157732
H	-2.600373648	5.151446339	-0.826894200
C	-2.234263042	5.738938595	1.226095648
H	-2.746730122	4.891619401	1.692638882
H	-1.391930411	6.011279287	1.870128613
H	-2.928350545	6.585105586	1.190397801
C	-5.539312652	1.281433485	-0.249117585
C	-6.719750714	0.545696687	-0.262744974
C	-6.696458832	-0.854305243	-0.220408199
C	-5.492117402	-1.548040276	-0.163450208
H	-5.571444907	2.367333076	-0.282261820
H	-7.674686933	1.061306092	-0.306906117
H	-7.633639746	-1.403196227	-0.232244502
H	-5.487704175	-2.634373260	-0.130740870
H	-3.306498907	3.089243742	-0.237452218
H	-0.066504945	1.052457773	-0.077509281
H	-0.019556269	-1.130666127	-0.024886580

XYZ-coordinates for H_2diDPEP atoms (7,18-diethyl-3,8,13,17-tetramethylbicyclopenta[*at*,*jk*]porphyrin)

N	2.352058787	0.252474563	0.023607538
N	0.465806007	2.268071906	0.038670137
N	-1.912238706	0.421666053	0.265021136
N	-0.027706123	-1.599737525	0.256498862
C	3.235446527	1.279600452	-0.073220684
C	-0.662298757	3.014114547	0.059393705
C	-2.790238624	-0.608879243	0.374362781
C	1.558933663	3.104212948	-0.068553030
C	-2.662001852	1.559435158	0.253562187
C	-1.119129277	-2.437765875	0.362280004
C	3.097056882	-0.886621726	0.045485396
C	1.100431247	-2.344702332	0.226570545
C	4.607078464	0.783846390	-0.118268760
C	-0.294586634	4.380770663	-0.029265850
C	-4.161256445	-0.118737392	0.440070540
C	1.076444966	4.464403335	-0.110220820
C	-4.087075708	1.244186997	0.362876309
C	-0.634462264	-3.797649872	0.400510404

C	4.523487624	-0.578725475	-0.038235387
C	0.736527272	-3.711935347	0.315490559
C	2.864446352	2.630712334	-0.122611141
C	-2.037813697	2.809697679	0.141315068
C	-2.423344910	-1.961164651	0.417742043
C	2.473856254	-2.137297118	0.139189982
H	3.651090607	3.374525014	-0.208319872
H	-3.214462052	-2.700650342	0.501942531
C	5.833613793	1.637582245	-0.173197996
C	-5.372685149	-0.979076256	0.582046170
C	1.940071742	5.677608536	-0.213375119
C	-5.231387371	2.204725851	0.460041272
C	-1.495837636	-5.011927258	0.509952286
C	5.656459813	-1.551472451	-0.023068558
H	5.659885794	2.493347861	-0.838139879
H	-5.446047658	-1.706449899	-0.235741556
H	2.548091216	5.663415767	-1.125833240
H	-5.055003654	3.080105293	-0.172585058
H	-2.194545747	-5.087054599	-0.331850040
H	5.595119264	-2.267159757	-0.851238275
H	6.660135458	1.073347206	-0.621100852
H	-6.290843231	-0.385779569	0.581691541
H	1.329020214	6.584025244	-0.231753414
H	-6.137412788	1.729334906	0.065247514
H	-0.883756296	-5.917795398	0.519445444
H	6.615711856	-1.033073840	-0.104636861
C	6.256888882	2.145568126	1.213697856
H	6.487863641	1.304825577	1.875844342
H	5.449460032	2.719443542	1.679906954
H	7.142858158	2.786297546	1.147077441
H	2.629619621	5.754251270	0.635893970
H	-2.093832721	-5.000485572	1.429073001
H	5.678907986	-2.135524161	0.904781687
C	-5.493696435	2.652273093	1.906404000
H	-6.299699253	3.392699317	1.954281818
H	-5.775926103	1.793656726	2.524271930
H	-4.594831451	3.090160951	2.352726655
C	-1.521821172	5.232895922	0.017125462
H	-1.541796349	5.865914795	0.912757463
H	-1.603431196	5.903408553	-0.846122235
C	-2.686390507	4.187754016	0.045114054
H	-3.368255159	4.379467096	0.880125829
H	-3.283100964	4.263682461	-0.872267583
H	-5.349348015	-1.548550908	1.519558580
C	1.968126814	-4.560039065	0.284726563
H	2.072983164	-5.171130585	1.188990595
H	1.971525060	-5.251983607	-0.565927707
C	3.127690839	-3.514089840	0.169655372
H	3.817754529	-3.604040741	1.016507133

H	3.722009337	-3.688937938	-0.734416858
H	-0.149670225	-0.594293413	0.211752717
H	0.585289033	1.262079486	0.071344453

XYZ-coordinates for H_2DPEP-Rhodo atoms
(13-ethyl-7,8,12,17-tetramethylbenzo[*b*]cyclopenta[*rs*]porphyrin)

N	2.008990699	0.050625580	0.050894085
N	0.042652544	1.959449631	-0.057561640
N	-2.180757776	-0.060601168	-0.087148250
N	-0.059896575	-2.096278494	0.033847408
C	2.840130881	1.133313103	0.051768549
C	-1.125021286	2.630457687	-0.114986302
C	-2.959574785	-1.167766313	-0.088817844
C	1.079624256	2.866810117	-0.050646762
C	-3.002247670	1.028866668	-0.141448897
C	-1.166230232	-2.905052700	0.014405048
C	2.819924752	-1.036800824	0.110757216
C	1.085084097	-2.846608988	0.093916337
C	4.240760602	0.719228894	0.111747054
C	-0.853526785	4.019506976	-0.144346979
C	-4.371641909	-0.796605346	-0.147093328
C	0.512821101	4.194639514	-0.105518007
C	-4.399230482	0.613936637	-0.180847460
C	-0.695340712	-4.264084978	0.065619958
C	4.227694020	-0.643672719	0.153301245
C	0.680387596	-4.228396096	0.114604664
C	2.409567427	2.463216801	-0.000521129
C	-2.477797963	2.321387303	-0.154684635
C	-2.486738242	-2.482177203	-0.042271858
C	2.387714239	-2.365579966	0.128283267
H	3.163659467	3.244466953	-0.000525088
H	-3.233491471	-3.270552066	-0.050461435
H	3.161264033	-3.126635175	0.175612248
C	5.415581574	1.641858935	0.175422436
C	1.301429814	5.462069313	-0.115545131
C	-1.596049260	-5.453700214	0.065310118
C	5.382798917	-1.584782640	0.235015256
C	1.636998408	-5.371965516	0.178745271
H	5.252419244	2.499092026	-0.490355810
H	1.981165478	5.506456809	-0.974797197
H	-2.220229471	-5.480213876	-0.835646851
H	5.392471977	-2.285276326	-0.609053860
H	2.328662596	-5.360380620	-0.671747849
H	6.306786702	1.130580029	-0.207308197
H	0.636438850	6.328134228	-0.169002027
H	-1.028195581	-6.385623480	0.101545175
H	6.334911118	-1.047558503	0.231472038
H	1.114567722	-6.330734041	0.167368030
C	5.691646189	2.144930104	1.600835046

H	5.911572002	1.304619377	2.267119679
H	4.818744181	2.666615181	2.006541848
H	6.544003699	2.832612801	1.619031952
H	1.912995927	5.563326211	0.789019466
H	-2.270716893	-5.442145872	0.929504419
H	5.346754907	-2.184419664	1.153049491
C	-5.616489620	1.292581134	-0.239672971
C	-6.791048348	0.546834229	-0.264054272
C	-6.759815439	-0.852149365	-0.230520712
C	-5.549834320	-1.536116244	-0.171673344
H	-5.665112801	2.376066473	-0.266276343
H	-7.748560339	1.057592710	-0.309914622
H	-7.692734033	-1.408041631	-0.250733684
H	-5.536306002	-2.622621540	-0.145849355
H	2.242534560	-5.334288389	1.092008568
C	-2.145478416	4.774155107	-0.210560562
H	-2.276974997	5.446431382	0.645327658
H	-2.216344145	5.392712481	-1.112929688
C	-3.231596267	3.641997143	-0.214003500
H	-3.907415854	3.746185990	0.643730866
H	-3.853368912	3.699128532	-1.115834683
H	0.214036918	0.960147887	-0.027498993
H	-0.093620331	-1.087496460	0.004006934

XYZ-coordinates for H_2diDPEP-Rhodo atoms
(13-ethyl-7,12,17-trimethylbenzo[*b*]bicyclopenta[*hi*,*rs*]porphyrin)

N	2.058950156	0.020591015	0.051761780
N	0.059424757	1.906768483	-0.067644379
N	-2.240415111	-0.113045475	-0.077943943
N	-0.208193609	-1.995226865	0.043414446
C	2.879751486	1.103380703	0.046409219
C	-1.114301535	2.573820653	-0.123690733
C	-3.043048738	-1.207964093	-0.073405426
C	1.096678913	2.819065346	-0.065729864
C	-3.029811471	0.995741460	-0.135742788
C	-1.243947191	-2.907072466	0.029656955
C	2.871314614	-1.069724492	0.121879452
C	0.968425038	-2.662188196	0.098758943
C	4.278263359	0.696097955	0.113372460
C	-0.840301507	3.964537192	-0.157968020
C	-4.443499424	-0.800578370	-0.130678288
C	0.524101413	4.143680406	-0.123368787
C	-4.437393088	0.611267550	-0.170594521
C	-0.671039680	-4.231501123	0.078180341
C	4.276154568	-0.670797893	0.166632219
C	0.693258274	-4.051942015	0.119688359
C	2.429276181	2.430434634	-0.014640932
C	-2.473227441	2.275700746	-0.156705733
C	-2.581044855	-2.527347389	-0.023341225

C	2.325763025	-2.360277729	0.140732414
H	3.172624447	3.222091625	-0.018320065
H	-3.319916721	-3.322941564	-0.027154963
C	5.448251573	1.625806136	0.173367300
C	1.306763868	5.414592815	-0.138336790
C	-1.452789051	-5.503097023	0.078230183
C	5.465232350	-1.569936279	0.260368595
H	5.274446783	2.483020676	-0.489638539
H	1.987114506	5.458134926	-0.997135950
H	-2.065658213	-5.599622340	-0.825986723
H	5.550966187	-2.229434486	-0.611709077
H	6.342348140	1.124325287	-0.215395133
H	0.637908424	6.277427350	-0.196095683
H	-0.782544220	-6.365709713	0.122136644
H	6.389182793	-0.989130151	0.326123440
C	5.726109606	2.129012258	1.598349446
H	5.955788214	1.290026331	2.263127536
H	4.849898118	2.642354752	2.007594222
H	6.572498457	2.824166372	1.614457043
H	1.917131841	5.522356617	0.766316512
H	-2.130147023	-5.559735595	0.938727537
H	5.419668918	-2.213677277	1.146280340
C	-5.639781855	1.316291390	-0.229973341
C	-6.831297876	0.597659365	-0.248330977
C	-6.832548240	-0.801456976	-0.208464107
C	-5.638593739	-1.512627167	-0.149278128
H	-5.664551724	2.400224187	-0.261488408
H	-7.776685896	1.130510051	-0.294360712
H	-7.778125988	-1.335710949	-0.223977281
H	-5.648755851	-2.599003073	-0.118492066
C	-2.126691627	4.726935306	-0.220693761
H	-2.250163212	5.400421021	0.635495149
H	-2.196142860	5.345821518	-1.122964862
C	-3.217616856	3.602414766	-0.219321483
H	-3.891933918	3.713842985	0.638651781
H	-3.839531027	3.660549347	-1.121031313
C	3.066574941	-3.690067059	0.222247063
H	3.787709244	-3.796549339	-0.595622576
H	3.641198347	-3.758283556	1.153616194
C	1.978976339	-4.814706178	0.163588281
H	2.110414572	-5.442522583	-0.725895171
H	2.042563279	-5.480111319	1.032400600
H	0.253588646	0.911373067	-0.036488730
H	-0.386621348	-0.999288319	0.017591933

XYZ-coordinates for Ni(II)-EtioP-III atoms
(3,8,13,17- tetraethyl-2,7,12,18- tetramethylporphyrinato)nickel(II)

N	2.010392000	0.166707000	0.005708000
N	0.029721000	2.078809000	-0.007235000

N	-1.881837000	0.101858000	0.033741000
N	0.097425000	-1.813273000	0.046561000
C	2.834581000	1.252991000	0.181181000
C	-1.055485000	2.897918000	-0.209487000
C	-2.700556000	-0.980455000	0.254936000
C	1.089240000	2.936749000	0.169554000
C	-2.740714000	1.154581000	-0.175784000
C	-0.958317000	-2.665763000	0.269527000
C	2.863724000	-0.894365000	-0.182582000
C	1.179661000	-2.638211000	-0.146919000
C	4.226003000	0.869248000	0.115683000
C	-0.673075000	4.289886000	-0.171329000
C	-4.091250000	-0.602472000	0.199386000
C	0.663994000	4.312798000	0.095609000
C	-4.117959000	0.727478000	-0.100454000
C	-0.532997000	-4.043386000	0.232089000
C	4.242280000	-0.471199000	-0.133898000
C	0.799076000	-4.028400000	-0.058826000
C	2.404712000	2.554748000	0.307167000
C	-2.355571000	2.465584000	-0.345557000
C	-2.270657000	-2.278022000	0.419176000
C	2.477957000	-2.209601000	-0.310181000
H	3.149473000	3.332189000	0.436583000
H	-3.016258000	-3.047497000	0.587989000
H	3.251232000	-2.955680000	-0.455344000
C	5.380738000	1.795329000	0.325972000
C	-5.235978000	-1.534082000	0.418190000
C	1.562601000	5.491433000	0.267779000
C	-5.305953000	1.624381000	-0.241205000
C	-1.425766000	-5.216725000	0.460643000
C	5.413166000	-1.382119000	-0.294047000
C	1.737176000	-5.186431000	-0.179439000
H	5.195883000	2.747032000	-0.188225000
H	-5.235954000	-2.353164000	-0.311216000
H	2.040856000	5.491066000	1.254674000
H	-5.114026000	2.383838000	-1.009158000
H	-2.243878000	-5.251607000	-0.269009000
H	5.384047000	-1.911808000	-1.253674000
H	2.492623000	-4.979237000	-0.947381000
H	6.275693000	1.370648000	-0.142473000
H	-6.190644000	-1.009703000	0.327940000
H	2.362417000	5.502916000	-0.482623000
H	-6.159245000	1.040348000	-0.605628000
H	-0.869135000	-6.153814000	0.379689000
H	6.353204000	-0.826687000	-0.249227000
H	1.184500000	-6.064566000	-0.533667000
C	5.660681000	2.059551000	1.813005000
H	5.894489000	1.123689000	2.330527000
H	4.785792000	2.497546000	2.303999000

H	6.505884000	2.744442000	1.939447000
H	1.004900000	6.426478000	0.172254000
H	-1.879715000	-5.187001000	1.458503000
H	5.441371000	-2.141433000	0.497098000
C	-5.685222000	2.309890000	1.080403000
H	-6.549701000	2.969540000	0.949816000
H	-5.932331000	1.563569000	1.842271000
H	-4.850568000	2.906028000	1.463340000
H	-5.200379000	-1.986209000	1.416665000
C	2.430242000	-5.523252000	1.149829000
H	1.689523000	-5.782401000	1.913138000
H	3.116908000	-6.368617000	1.034065000
H	2.998504000	-4.664533000	1.521731000
C	-1.612676000	5.444319000	-0.313382000
H	-1.064211000	6.311838000	-0.698815000
H	-2.377153000	5.215549000	-1.066164000
C	-2.289893000	5.818896000	1.013855000
H	-1.540249000	6.098505000	1.761004000
H	-2.854032000	4.971262000	1.416243000
H	-2.978087000	6.660726000	0.882690000
H	-3.128333000	3.209205000	-0.504038000
Ni	0.063929000	0.133886000	0.016977000

XYZ-coordinates for Ni(II)-DPEP atoms
(7,12,18-triethyl-3,8,13,17-tetramethylcyclopenta[*at*]porphyrinato)nickel(II)

N	2.029987750	0.034700926	0.052048340
N	0.104564721	1.914898729	0.074962698
N	-1.928363647	0.052598439	0.077221066
N	0.070967360	-1.930896279	0.062300076
C	2.869755972	1.127782520	-0.006862158
C	-0.992753458	2.695123730	0.151798828
C	-2.745928313	-1.046628727	0.009761872
C	1.147164801	2.823647416	0.023174444
C	-2.804233076	1.132898308	0.142819460
C	-1.019876364	-2.767746600	0.009565146
C	2.871285068	-1.051340709	0.099333127
C	1.156060500	-2.772667040	0.112356948
C	4.254919644	0.717604267	-0.001849352
C	-0.693050561	4.083266319	0.151588938
C	-4.135843788	-0.673194570	0.020792729
C	0.663666378	4.192747339	0.064684061
C	-4.175129184	0.688421213	0.113706548
C	-0.615870683	-4.153950411	0.029648277
C	4.254622513	-0.643130464	0.075749353
C	0.744834483	-4.158613925	0.097288717
C	2.468728962	2.446408179	-0.037963850
C	-2.342063408	2.434752814	0.203219259
C	-2.330808967	-2.361982594	-0.034600801
C	2.471325837	-2.367399535	0.141129899

H	3.227628057	3.219726734	-0.081006834
H	-3.095619089	-3.129488223	-0.079163197
H	3.241590208	-3.129468448	0.175286954
C	5.425233302	1.648367414	-0.009567538
C	5.415719353	-1.578361758	0.133651119
C	1.671585010	-5.328054414	0.193993418
H	5.229681874	2.493245534	-0.681578576
H	5.394773158	-2.300261989	-0.691545794
H	2.561541441	-5.152759849	-0.423665804
H	6.296392217	1.130440713	-0.427070590
H	6.361779167	-1.034393549	0.075419552
H	1.183224272	-6.213027569	-0.229530938
C	-1.963323462	4.869450304	0.210785439
H	-1.996339944	5.560054779	1.061466898
H	-2.110369637	5.473079588	-0.693125551
C	-3.070237823	3.764288376	0.325475210
H	-3.580977525	3.836167960	1.293600442
H	-3.836421654	3.893450960	-0.445766078
Ni	0.076508251	0.010685897	0.065906711
C	-5.398144258	1.551123559	0.094216147
H	-6.227938369	1.004390626	0.557911169
H	-5.250905731	2.444569017	0.707240170
C	-5.277076100	-1.631456092	-0.063337777
H	-5.249009428	-2.367017815	0.749556385
H	-6.234784660	-1.108510600	-0.003193198
C	2.097927734	-5.624833630	1.639685570
H	1.223390547	-5.852062906	2.257621134
H	2.782008705	-6.478994056	1.681733162
H	2.599740227	-4.759587359	2.084561863
C	-1.556608277	-5.311451296	-0.000815414
H	-2.196502995	-5.288529929	-0.891000555
H	-1.013496478	-6.259740989	-0.006050412
H	-2.216874544	-5.314488077	0.875009414
C	1.526594652	5.409558960	0.019285843
H	2.238768888	5.433448614	0.853166152
H	2.109774904	5.459750538	-0.908451641
H	0.914350890	6.313694985	0.077684739
C	5.770273471	2.173595639	1.392406120
H	4.917791024	2.701003813	1.832285300
H	6.024825808	1.344667546	2.060579629
H	6.621529121	2.861927904	1.357143653
H	5.422612240	-2.152217108	1.068495836
H	-5.265828046	-2.189003800	-1.007760779
C	-5.800027509	1.953784908	-1.333048415
H	-4.977865662	2.466440127	-1.842953477
H	-6.043493997	1.065442738	-1.924720472
H	-6.672488895	2.616195656	-1.328675343

XYZ-coordinates for Ni(II)-Rhodo atoms

(8,13,18-triethyl-7,12,17-trimethylbenzo[*b*]porphyrinato)nickel(II)

N	1.888749000	0.008488000	0.033110000
N	-0.076745000	1.922459000	-0.078886000
N	-2.009202000	-0.046818000	-0.049662000
N	-0.023388000	-1.961970000	0.054956000
C	2.709815000	1.090861000	0.245122000
C	-1.142290000	2.740170000	-0.362197000
C	-2.822028000	-1.127570000	0.209396000
C	0.975191000	2.780497000	0.148186000
C	-2.839631000	1.011554000	-0.342662000
C	-1.078501000	-2.806993000	0.296349000
C	2.744464000	-1.053161000	-0.142941000
C	1.058161000	-2.792689000	-0.128019000
C	4.100391000	0.703456000	0.218064000
C	-0.757504000	4.131221000	-0.329033000
C	-4.212605000	-0.749955000	0.098305000
C	0.559760000	4.155500000	0.024548000
C	-4.223000000	0.596962000	-0.286058000
C	-0.657034000	-4.185910000	0.282740000
C	4.120765000	-0.634094000	-0.051154000
C	0.673458000	-4.179393000	-0.017932000
C	2.279078000	2.394652000	0.356630000
C	-2.437357000	2.307870000	-0.550885000
C	-2.392170000	-2.413030000	0.430404000
C	2.357715000	-2.367810000	-0.282074000
H	3.020317000	3.169418000	0.518882000
H	-3.140418000	-3.175937000	0.615342000
H	3.131391000	-3.115635000	-0.415948000
C	5.251309000	1.622486000	0.474572000
C	1.448427000	5.335600000	0.233271000
C	-1.551503000	-5.352860000	0.535386000
C	5.294045000	-1.545774000	-0.188470000
C	1.606743000	-5.342638000	-0.123722000
H	5.085545000	2.581384000	-0.032722000
H	2.290548000	5.337732000	-0.469498000
H	-2.365799000	-5.405463000	-0.197586000
H	5.285925000	-2.072137000	-1.150243000
H	2.367057000	-5.145737000	-0.889470000
H	6.158320000	1.200224000	0.027721000
H	0.898064000	6.269403000	0.093838000
H	-0.994690000	-6.291661000	0.480049000
H	6.233270000	-0.991326000	-0.121009000
H	1.051506000	-6.221021000	-0.473288000
C	5.487364000	1.866949000	1.972571000
H	5.702703000	0.923985000	2.485197000
H	4.599696000	2.302115000	2.442768000
H	6.330595000	2.547131000	2.132790000
H	1.868403000	5.346937000	1.246163000
H	-2.010240000	-5.298812000	1.529962000

H	5.304259000	-2.307547000	0.600772000
C	2.291209000	-5.670752000	1.212123000
H	1.545727000	-5.921397000	1.973628000
H	2.975662000	-6.519231000	1.106939000
H	2.860293000	-4.810804000	1.579938000
C	-1.680679000	5.285065000	-0.557507000
H	-1.105133000	6.139142000	-0.933340000
H	-2.399094000	5.037914000	-1.348792000
C	-2.434531000	5.698980000	0.715694000
H	-3.028809000	4.866599000	1.106233000
H	-1.729418000	5.995268000	1.498886000
H	-3.106631000	6.541155000	0.519681000
C	-5.424697000	1.271074000	-0.505225000
C	-6.607973000	0.566920000	-0.333381000
C	-6.597588000	-0.782892000	0.054446000
C	-5.403609000	-1.455523000	0.272060000
H	-5.444802000	2.315013000	-0.805565000
H	-7.558699000	1.064726000	-0.499749000
H	-7.540505000	-1.305747000	0.184446000
H	-5.407490000	-2.499622000	0.572316000
H	-3.200389000	3.046195000	-0.770310000
Ni	-0.054710000	-0.019457000	-0.012187000

XYZ-coordinates for Ni(II)-diDPEP atoms
(7,18-diethyl-3,8,13,17-tetramethylbicyclopenta[*at*,*jk*]porphyrinato)nickel(II)

N	2.216048000	0.197950000	0.041084000
N	0.371366000	2.216518000	0.050716000
N	-1.768209000	0.476641000	0.260618000
N	0.074052000	-1.547060000	0.251284000
C	3.097482000	1.250039000	-0.060582000
C	-0.679660000	3.059130000	0.061061000
C	-2.644066000	-0.578754000	0.374145000
C	1.467743000	3.053124000	-0.057932000
C	-2.578063000	1.608148000	0.247454000
C	-1.020788000	-2.386070000	0.356978000
C	3.020506000	-0.935247000	0.057002000
C	1.124866000	-2.389380000	0.228067000
C	4.460768000	0.783550000	-0.109312000
C	-0.298128000	4.424885000	-0.031753000
C	-4.006394000	-0.118087000	0.441000000
C	1.063004000	4.449819000	-0.109410000
C	-3.968808000	1.244533000	0.358790000
C	-0.614313000	-3.782965000	0.397152000
C	4.413257000	-0.579274000	-0.029631000
C	0.746710000	-3.756135000	0.314253000
C	2.760296000	2.591353000	-0.112472000
C	-2.041624000	2.879601000	0.137915000
C	-2.311973000	-1.921281000	0.417936000
C	2.484850000	-2.207026000	0.144939000

H	3.560681000	3.317974000	-0.199730000
H	-3.117363000	-2.642941000	0.504021000
C	5.668824000	1.663847000	-0.166788000
C	-5.197125000	-1.006631000	0.588226000
C	1.996673000	5.609044000	-0.217731000
C	-5.133476000	2.179741000	0.455484000
C	-1.546391000	-4.943487000	0.505878000
C	5.567548000	-1.526736000	-0.017879000
H	5.481006000	2.517770000	-0.829149000
H	-5.268589000	-1.726824000	-0.235641000
H	2.601023000	5.559414000	-1.131778000
H	-4.973420000	3.061272000	-0.171404000
H	-2.247418000	-4.980171000	-0.336959000
H	5.522210000	-2.241163000	-0.847243000
H	6.499366000	1.112243000	-0.622106000
H	-6.123012000	-0.426435000	0.601571000
H	1.438396000	6.549087000	-0.237147000
H	-6.024470000	1.684415000	0.051778000
H	-0.987389000	-5.883250000	0.516563000
H	6.512061000	-0.983166000	-0.101099000
C	6.094161000	2.170521000	1.219433000
H	6.339028000	1.329857000	1.876679000
H	5.283572000	2.733412000	1.693142000
H	6.972521000	2.821120000	1.149867000
H	2.691850000	5.649676000	0.629853000
H	-2.144324000	-4.898805000	1.424408000
H	5.606468000	-2.109157000	0.909723000
C	-5.412650000	2.611406000	1.903026000
H	-6.241307000	3.326123000	1.951797000
H	-5.669338000	1.742216000	2.517206000
H	-4.528269000	3.075482000	2.351498000
C	-1.519537000	5.286545000	0.010385000
H	-1.538660000	5.921104000	0.904974000
H	-1.597519000	5.955679000	-0.854285000
C	-2.696814000	4.249502000	0.038803000
H	-3.378481000	4.448620000	0.872311000
H	-3.289594000	4.327840000	-0.880698000
H	-5.155959000	-1.581473000	1.521333000
C	1.972227000	-4.613965000	0.281297000
H	2.073213000	-5.230647000	1.182234000
H	1.974382000	-5.300856000	-0.573545000
C	3.145246000	-3.575917000	0.173387000
H	3.829058000	-3.673366000	1.024232000
H	3.741388000	-3.753736000	-0.728499000
Ni	0.222639000	0.335701000	0.148477000

XYZ-coordinates for Ni(II)-DPEP-Rhodo atoms
(13-ethyl-7,8,12,17-tetramethylbenzo[*b*]cyclopenta[*rs*]porphyrinato)nickel(II)

N	1.911749000	-0.004870000	0.056173000

N	-0.023168000	1.856114000	-0.050223000
N	-2.055616000	-0.035032000	-0.083651000
N	-0.028543000	-1.990093000	0.039156000
C	2.745331000	1.092708000	-0.024882000
C	-1.125661000	2.628048000	-0.027724000
C	-2.847557000	-1.150857000	-0.181491000
C	1.012727000	2.774570000	-0.114889000
C	-2.923142000	1.055026000	-0.060631000
C	-1.100280000	-2.842844000	-0.068275000
C	2.758869000	-1.078132000	0.201642000
C	1.061810000	-2.815887000	0.185025000
C	4.130235000	0.697050000	0.060282000
C	-0.844661000	4.018153000	-0.070376000
C	-4.244840000	-0.785227000	-0.227376000
C	0.513302000	4.138816000	-0.135333000
C	-4.292370000	0.613925000	-0.138310000
C	-0.681682000	-4.223633000	0.007612000
C	4.136941000	-0.657767000	0.217288000
C	0.669948000	-4.206164000	0.176329000
C	2.336464000	2.406132000	-0.128802000
C	-2.472021000	2.353084000	-0.017153000
C	-2.412971000	-2.456421000	-0.197564000
C	2.366776000	-2.395711000	0.285903000
H	3.091968000	3.182169000	-0.183069000
H	-3.164764000	-3.233732000	-0.276823000
H	3.138514000	-3.149410000	0.397886000
C	5.294072000	1.635910000	0.047280000
C	1.364765000	5.362642000	-0.203178000
C	-1.607995000	-5.389638000	-0.080164000
C	5.303612000	-1.574030000	0.377954000
C	1.619376000	-5.348264000	0.317071000
H	5.113493000	2.449075000	-0.666588000
H	2.010431000	5.359463000	-1.089592000
H	-2.135411000	-5.412286000	-1.041429000
H	5.326493000	-2.340731000	-0.405657000
H	2.363963000	-5.351514000	-0.488023000
H	6.180624000	1.107130000	-0.321621000
H	0.740473000	6.259272000	-0.247631000
H	-1.066934000	-6.333025000	0.021473000
H	6.245315000	-1.021565000	0.329425000
H	1.094629000	-6.305799000	0.284543000
C	5.594117000	2.224209000	1.434310000
H	5.834706000	1.427440000	2.145501000
H	4.725854000	2.763697000	1.826188000
H	6.441420000	2.917027000	1.393639000
H	2.016523000	5.452859000	0.674662000
H	-2.368368000	-5.358023000	0.709229000
H	5.275907000	-2.094373000	1.343066000
C	-5.519853000	1.284324000	-0.142128000

C	-6.678732000	0.527782000	-0.241702000
C	-6.627392000	-0.871979000	-0.334872000
C	-5.412651000	-1.541655000	-0.326445000
H	-5.583000000	2.364049000	-0.066839000
H	-7.643948000	1.025670000	-0.246693000
H	-7.552683000	-1.435162000	-0.412551000
H	-5.383294000	-2.625377000	-0.396926000
H	2.165596000	-5.301381000	1.266787000
C	-2.128426000	4.788285000	-0.046681000
H	-2.208248000	5.431056000	0.837983000
H	-2.241272000	5.438283000	-0.922071000
C	-3.228946000	3.667415000	-0.029872000
H	-3.878831000	3.766323000	0.847994000
H	-3.873700000	3.742472000	-0.913971000
Ni	-0.040396000	-0.050264000	-0.010250000

XYZ-coordinates for Ni(II)-diDPEP-Rhodo atoms
(13-ethyl-7,12,17-trimethylbenzo[*b*]bicyclopenta[*hi*,*rs*]porphyrinato)nickel(II)

N	1.924839000	-0.046085000	0.051389000
N	-0.032929000	1.851540000	-0.064828000
N	-2.083670000	-0.038088000	-0.079651000
N	-0.107116000	-1.934186000	0.032217000
C	2.742755000	1.061909000	0.029656000
C	-1.131970000	2.625358000	-0.109314000
C	-2.885070000	-1.157957000	-0.089898000
C	1.011213000	2.761585000	-0.075346000
C	-2.941257000	1.058262000	-0.121108000
C	-1.145034000	-2.846433000	0.006209000
C	2.797734000	-1.125011000	0.134154000
C	0.996994000	-2.704724000	0.103920000
C	4.131325000	0.684146000	0.096938000
C	-0.841470000	4.014732000	-0.147029000
C	-4.279271000	-0.779441000	-0.138338000
C	0.518059000	4.129660000	-0.127921000
C	-4.314412000	0.623205000	-0.155982000
C	-0.651096000	-4.213250000	0.060404000
C	4.165371000	-0.679899000	0.171252000
C	0.706728000	-4.094490000	0.122427000
C	2.329498000	2.381748000	-0.037894000
C	-2.479881000	2.354995000	-0.134397000
C	-2.467332000	-2.472045000	-0.055082000
C	2.341974000	-2.431058000	0.161068000
H	3.088763000	3.155796000	-0.050032000
H	-3.225769000	-3.247108000	-0.070272000
C	5.282068000	1.639316000	0.140308000
C	1.378183000	5.348879000	-0.151198000
C	-1.507678000	-5.435108000	0.047017000
C	5.373768000	-1.551615000	0.277443000
H	5.094155000	2.485705000	-0.531656000

H	2.056858000	5.349811000	-1.012781000
H	-2.103449000	-5.503205000	-0.871564000
H	5.480960000	-2.213194000	-0.589914000
H	6.178908000	1.145228000	-0.250791000
H	0.761657000	6.249998000	-0.210316000
H	-0.889588000	-6.334897000	0.111214000
H	6.280902000	-0.945753000	0.343791000
C	5.564911000	2.159137000	1.557900000
H	5.810177000	1.329934000	2.229389000
H	4.686617000	2.666750000	1.969539000
H	6.403499000	2.863685000	1.559901000
H	1.997549000	5.425682000	0.750956000
H	-2.207837000	-5.448878000	0.891226000
H	5.339283000	-2.187781000	1.168446000
C	-5.536178000	1.302513000	-0.199393000
C	-6.702801000	0.551934000	-0.225699000
C	-6.664331000	-0.851158000	-0.208963000
C	-5.455186000	-1.529583000	-0.164669000
H	-5.588471000	2.385355000	-0.211713000
H	-7.663564000	1.057285000	-0.259539000
H	-7.595122000	-1.410307000	-0.230506000
H	-5.436186000	-2.615699000	-0.151227000
C	-2.122288000	4.789129000	-0.198211000
H	-2.234514000	5.463879000	0.658520000
H	-2.196768000	5.407428000	-1.100492000
C	-3.228933000	3.673482000	-0.187252000
H	-3.892585000	3.790088000	0.678179000
H	-3.858231000	3.738602000	-1.083154000
C	3.087454000	-3.752357000	0.248909000
H	3.807269000	-3.867321000	-0.568786000
H	3.659320000	-3.823956000	1.181339000
C	1.985319000	-4.868458000	0.188985000
H	2.124200000	-5.507440000	-0.691357000
H	2.034819000	-5.523801000	1.066471000
Ni	-0.073234000	-0.041517000	-0.016303000

XYZ-coordinates for VO(IV)-EtioP-III atoms
(3,8,13,17- tetraethyl-2,7,12,18- tetramethylporphyrinato)oxovanadium(IV)

N	2.078875000	0.165526000	0.096949000
N	0.028460000	2.145421000	0.056660000
N	-1.953048000	0.096646000	0.065126000
N	0.097326000	-1.886602000	0.107296000
C	2.888314000	1.273405000	0.069655000
C	-1.079296000	2.952629000	-0.004599000
C	-2.759920000	-1.013593000	0.058214000
C	1.111372000	2.988377000	0.038859000
C	-2.796901000	1.176850000	0.001199000
C	-0.985497000	-2.730030000	0.093820000
C	2.921088000	-0.917887000	0.077891000

C	1.205900000	-2.695286000	0.086311000
C	4.279739000	0.882049000	0.030862000
C	-0.688769000	4.343715000	-0.062186000
C	-4.149979000	-0.627452000	-0.008106000
C	0.678959000	4.364688000	-0.029541000
C	-4.174362000	0.740015000	-0.049717000
C	-0.552387000	-4.107494000	0.064606000
C	4.298650000	-0.486146000	0.038752000
C	0.815612000	-4.087346000	0.054360000
C	2.437065000	2.584203000	0.057767000
C	-2.389906000	2.501664000	-0.026990000
C	-2.310971000	-2.324664000	0.088855000
C	2.516476000	-2.243580000	0.081618000
H	3.188618000	3.366762000	0.035617000
H	-3.065767000	-3.104809000	0.079450000
H	3.299206000	-2.995069000	0.063122000
C	5.439703000	1.825174000	0.040457000
C	-5.298258000	-1.579885000	-0.021912000
C	1.593624000	5.543310000	-0.054150000
C	-5.362961000	1.646496000	-0.078136000
C	-1.466397000	-5.286713000	0.051730000
C	5.476751000	-1.401415000	0.018443000
C	1.760154000	-5.246133000	0.067798000
H	5.222356000	2.692160000	-0.595985000
H	-5.236197000	-2.274152000	-0.868416000
H	2.202513000	5.594188000	0.856639000
H	-5.167528000	2.499009000	-0.740752000
H	-2.140105000	-5.264503000	-0.813157000
H	5.440959000	-2.084985000	-0.838151000
H	2.626236000	-5.029674000	-0.570185000
H	6.312596000	1.336254000	-0.406927000
H	-6.251128000	-1.050101000	-0.095146000
H	2.283980000	5.498809000	-0.904988000
H	-6.216944000	1.116585000	-0.515255000
H	-0.904821000	-6.223279000	0.012361000
H	6.413092000	-0.841303000	-0.041654000
H	1.271979000	-6.121126000	-0.376363000
C	5.792504000	2.302641000	1.457610000
H	6.065964000	1.453533000	2.091991000
H	4.937092000	2.800394000	1.925294000
H	6.633120000	3.004236000	1.438580000
H	1.033626000	6.478612000	-0.128474000
H	-2.092476000	-5.314864000	0.951702000
H	5.518473000	-2.017251000	0.925103000
C	-5.741232000	2.158028000	1.320388000
H	-6.604272000	2.830441000	1.273258000
H	-5.990629000	1.321562000	1.980930000
H	-4.906101000	2.699218000	1.776611000
V	0.058909000	0.136426000	0.611827000

O	0.047007000	0.157725000	2.200516000
H	-5.325807000	-2.183598000	0.893277000
C	2.239009000	-5.594387000	1.485506000
H	1.390649000	-5.866679000	2.121398000
H	2.941006000	-6.434711000	1.467838000
H	2.736777000	-4.737670000	1.950789000
C	-1.634797000	5.501042000	-0.089458000
H	-1.133971000	6.372306000	-0.526592000
H	-2.480709000	5.277090000	-0.751683000
C	-2.158536000	5.862245000	1.309063000
H	-1.330752000	6.138657000	1.969806000
H	-2.672465000	5.010200000	1.765545000
H	-2.858512000	6.703065000	1.261734000
H	-3.168779000	3.254762000	-0.084124000

XYZ-координаты атомов XYZ-coordinates for VO(IV)-DPEP atoms
(7,12,18-triethyl-3,8,13,17-tetramethylcyclopenta[*at*]porphyrinato)oxovanadium(IV)

N	2.090604206	0.062347913	0.169943447
N	0.118118905	1.988335762	0.145683568
N	-1.987440620	0.086199116	0.206875435
N	0.070664081	-1.958411705	0.149395490
C	2.916709910	1.161824608	0.124426461
C	-0.993664992	2.751459086	0.124934098
C	-2.787473180	-1.024437112	0.178770686
C	1.164373694	2.886417332	0.099107279
C	-2.845178947	1.173277676	0.174673298
C	-1.031583505	-2.777311269	0.132431503
C	2.913037866	-1.034514195	0.127416732
C	1.164320731	-2.784445798	0.106669282
C	4.300856413	0.743490974	0.062688754
C	-0.696659740	4.136925778	0.053618556
C	-4.177704390	-0.645410704	0.133835678
C	0.668616618	4.251930098	0.035186606
C	-4.216117054	0.724968798	0.133786648
C	-0.623320242	-4.162040250	0.069626175
C	4.297467443	-0.624662046	0.068379881
C	0.745110750	-4.167718942	0.048624437
C	2.492054903	2.484587781	0.103464229
C	-2.350562672	2.476132527	0.154925050
C	-2.345643233	-2.343798571	0.163197951
C	2.483773859	-2.353553237	0.110524482
H	3.253307023	3.257431931	0.064727188
H	-3.112507109	-3.111991908	0.144058990
H	3.253351008	-3.117862093	0.072864924
C	5.477954751	1.665381917	0.050168951
C	5.459902959	-1.558948603	0.023942952
C	1.666939084	-5.344764770	0.034260351
H	5.266271988	2.534015927	-0.585890030
H	5.406360386	-2.227893231	-0.843352470

H	2.533464514	-5.132540447	-0.604566684
H	6.334509557	1.159168287	-0.409404035
H	6.405147323	-1.013793130	-0.034112708
H	1.159742556	-6.201953157	-0.423131758
C	-1.972421966	4.916070162	0.011245023
H	-2.040130520	5.660940551	0.812466531
H	-2.088895655	5.457894494	-0.935358023
C	-3.079554471	3.812980620	0.159811893
H	-3.624226563	3.948430393	1.102338013
H	-3.818881684	3.885486470	-0.644615858
C	-5.437669223	1.582016387	0.018745702
H	-6.280749863	1.073366037	0.501112072
H	-5.300882916	2.518854628	0.566426529
C	-5.322256679	-1.601272879	0.071126070
H	-5.293932659	-2.317076557	0.900930214
H	-6.279901218	-1.076843048	0.117123275
C	2.147101462	-5.727673024	1.442616523
H	1.297245619	-5.995725348	2.078323491
H	2.833525628	-6.580180141	1.406118431
H	2.662731018	-4.888443310	1.920041894
C	-1.558189221	-5.324342729	0.042053868
H	-2.234775242	-5.276644672	-0.819627525
H	-1.013473665	-6.269970804	-0.013676694
H	-2.181257966	-5.354818430	0.944006600
C	1.519853709	5.475848541	-0.037207205
H	2.173488440	5.564706917	0.839050913
H	2.164454716	5.468092313	-0.924480258
H	0.898562325	6.374370612	-0.083052236
C	5.862429550	2.141154299	1.459574077
H	5.024237101	2.656705592	1.938888604
H	6.129975716	1.289272426	2.092764120
H	6.715865298	2.826510663	1.424204219
H	5.497437915	-2.190200053	0.920079305
H	-5.308650840	-2.180997138	-0.860075016
C	-5.801559068	1.879381622	-1.443811933
H	-4.967888423	2.359690576	-1.966491117
H	-6.026459082	0.950333291	-1.977597340
H	-6.675877722	2.535738789	-1.509887414
V	0.075334683	0.027993139	0.714977961
O	0.078984271	0.015052806	2.305159144

XYZ-coordinates for VO(IV)-Rhodo atoms
(8,13,18-triethyl-7,12,17-trimethylbenzo[*b*]porphyrinato)oxovanadium(IV)

N	1.957200000	0.001020000	0.125183000
N	-0.092981000	1.980185000	0.002266000
N	-2.102145000	-0.069774000	0.007916000
N	-0.024443000	-2.050753000	0.109472000
C	2.768089000	1.108094000	0.092905000
C	-1.196060000	2.790230000	-0.081449000

C	-2.889457000	-1.194319000	-0.017729000
C	0.993879000	2.822400000	-0.009166000
C	-2.924287000	1.025720000	-0.086602000
C	-1.103510000	-2.896553000	0.079607000
C	2.800340000	-1.082195000	0.147427000
C	1.086811000	-2.859922000	0.134214000
C	4.158434000	0.717120000	0.094186000
C	-0.802001000	4.179209000	-0.151548000
C	-4.281619000	-0.811347000	-0.128163000
C	0.565392000	4.197333000	-0.101581000
C	-4.303615000	0.593009000	-0.172227000
C	-0.669421000	-4.273337000	0.084139000
C	4.176927000	-0.651510000	0.132298000
C	0.698456000	-4.251699000	0.113495000
C	2.316872000	2.418583000	0.043016000
C	-2.509308000	2.343700000	-0.113512000
C	-2.431129000	-2.497115000	0.034743000
C	2.395171000	-2.408150000	0.161838000
H	3.069275000	3.200375000	0.022141000
H	-3.181443000	-3.280924000	0.010269000
H	3.178114000	-3.159513000	0.177458000
C	5.318598000	1.660035000	0.107177000
C	1.481890000	5.374361000	-0.128159000
C	-1.581847000	-5.453601000	0.063397000
C	5.355589000	-1.566156000	0.156686000
C	1.642053000	-5.409823000	0.173835000
H	5.114883000	2.513116000	-0.552088000
H	2.181530000	5.321332000	-0.970815000
H	-2.209930000	-5.461772000	-0.835591000
H	5.351459000	-2.251486000	-0.699328000
H	2.529319000	-5.200875000	-0.436783000
H	6.199612000	1.161154000	-0.312492000
H	0.923404000	6.309232000	-0.217666000
H	-1.018881000	-6.389872000	0.084176000
H	6.292961000	-1.005309000	0.129136000
H	1.169198000	-6.290192000	-0.276078000
C	5.644568000	2.167323000	1.520336000
H	5.903212000	1.331633000	2.178313000
H	4.781942000	2.677492000	1.960700000
H	6.487456000	2.866184000	1.502420000
H	2.080119000	5.433893000	0.789091000
H	-2.253087000	-5.452974000	0.930510000
H	5.365195000	-2.179810000	1.065572000
C	2.071531000	-5.739593000	1.611692000
H	1.201758000	-6.005051000	2.220907000
H	2.774632000	-6.578913000	1.629117000
H	2.551816000	-4.876232000	2.083007000
C	-1.743007000	5.339689000	-0.204292000
H	-1.237485000	6.199308000	-0.658797000

H	-2.588570000	5.106298000	-0.863507000
C	-2.265924000	5.731656000	1.186150000
H	-2.782097000	4.891120000	1.660811000
H	-1.437274000	6.020168000	1.840662000
H	-2.963199000	6.573505000	1.121012000
C	-5.509396000	1.285959000	-0.283420000
C	-6.683665000	0.549830000	-0.343528000
C	-6.661700000	-0.853834000	-0.299850000
C	-5.464900000	-1.547424000	-0.194664000
H	-5.539212000	2.371434000	-0.318971000
H	-7.636820000	1.063705000	-0.426016000
H	-7.598132000	-1.401566000	-0.349469000
H	-5.460223000	-2.633371000	-0.162752000
H	-3.286781000	3.096907000	-0.188361000
V	-0.074211000	-0.021227000	0.583938000
O	-0.135928000	0.020636000	2.169595000

XYZ-coordinates for VO(IV)-diDPEP atoms
(7,18-diethyl-3,8,13,17-tetramethylbicyclopenta[*at*,*jk*]porphyrinato)oxovanadium(IV)

N	2.284886000	0.201280000	0.179078000
N	0.387281000	2.257135000	0.105519000
N	-1.823571000	0.485491000	0.402421000
N	0.061608000	-1.583830000	0.305535000
C	3.148444000	1.260251000	0.046533000
C	-0.681247000	3.078485000	0.083270000
C	-2.685754000	-0.580168000	0.479825000
C	1.483214000	3.084593000	-0.029235000
C	-2.617216000	1.618636000	0.346527000
C	-1.035813000	-2.416237000	0.383163000
C	3.068004000	-0.938020000	0.149498000
C	1.126187000	-2.408112000	0.247727000
C	4.509904000	0.785485000	-0.046285000
C	-0.307836000	4.437817000	-0.079330000
C	-4.051554000	-0.115776000	0.505800000
C	1.060113000	4.471604000	-0.155464000
C	-4.012346000	1.251891000	0.419438000
C	-0.619560000	-3.810972000	0.348739000
C	4.460191000	-0.583174000	0.022897000
C	0.748189000	-3.775381000	0.263795000
C	2.782533000	2.604083000	-0.037655000
C	-2.049488000	2.883646000	0.189868000
C	-2.328532000	-1.928670000	0.485868000
C	2.495529000	-2.208393000	0.192575000
H	3.581815000	3.330580000	-0.146976000
H	-3.135017000	-2.653197000	0.547359000
C	5.722082000	1.656076000	-0.145131000
C	-5.249118000	-1.000954000	0.609408000
C	1.975040000	5.639090000	-0.321817000
C	-5.181507000	2.184680000	0.469880000

C	-1.539483000	-4.985125000	0.401707000
C	5.611641000	-1.532907000	-0.023525000
H	5.516732000	2.511156000	-0.800854000
H	-5.290967000	-1.720174000	-0.217231000
H	2.584572000	5.548553000	-1.229049000
H	-5.009913000	3.050867000	-0.175695000
H	-2.246150000	-4.982331000	-0.437000000
H	5.555642000	-2.202879000	-0.889104000
H	6.535256000	1.100323000	-0.625881000
H	-6.175417000	-0.421651000	0.591947000
H	1.404317000	6.568920000	-0.393431000
H	-6.066016000	1.679469000	0.064608000
H	-0.974202000	-5.920091000	0.360089000
H	6.559486000	-0.992404000	-0.084363000
C	6.190728000	2.161409000	1.227774000
H	6.447608000	1.320309000	1.879697000
H	5.398354000	2.731185000	1.723496000
H	7.071711000	2.804805000	1.131214000
H	2.665005000	5.733292000	0.525562000
H	-2.131250000	-4.991424000	1.325136000
H	5.650479000	-2.163748000	0.871616000
C	-5.482430000	2.654930000	1.901206000
H	-6.310895000	3.371191000	1.916807000
H	-5.749740000	1.803235000	2.534889000
H	-4.604646000	3.130384000	2.350529000
C	-1.536049000	5.291434000	-0.072592000
H	-1.548156000	5.978032000	0.782625000
H	-1.631502000	5.907559000	-0.974192000
C	-2.706344000	4.249284000	0.031480000
H	-3.373929000	4.487116000	0.866625000
H	-3.316630000	4.280178000	-0.879318000
V	0.258895000	0.365668000	0.809874000
O	0.352311000	0.440450000	2.396756000
H	-5.238470000	-1.577158000	1.542491000
C	1.977170000	-4.627648000	0.202048000
H	2.066331000	-5.287194000	1.073182000
H	1.993994000	-5.271033000	-0.685683000
C	3.149932000	-3.582360000	0.162363000
H	3.821647000	-3.721304000	1.017301000
H	3.758775000	-3.716945000	-0.738681000

XYZ-coordinates for VO(IV)-DPEP-Rhodo atoms
(13-ethyl-7,8,12,17-tetramethylbenzo[*b*]cyclopenta[*rs*]porphyrinato)oxovanadium(IV)

N	1.967990000	0.008572000	0.185663000
N	-0.020316000	1.907633000	0.018495000
N	-2.133479000	-0.027485000	0.046010000
N	-0.030486000	-2.036717000	0.117746000
C	2.784010000	1.117179000	0.146647000
C	-1.136246000	2.655921000	-0.075301000

C	-2.905340000	-1.156149000	0.010973000
C	1.017528000	2.819594000	-0.010245000
C	-2.976882000	1.066931000	-0.048343000
C	-1.116315000	-2.873063000	0.063424000
C	2.804588000	-1.078644000	0.212896000
C	1.077600000	-2.848030000	0.142638000
C	4.172087000	0.714647000	0.160926000
C	-0.857173000	4.042121000	-0.177215000
C	-4.302960000	-0.788735000	-0.089736000
C	0.506836000	4.175129000	-0.138749000
C	-4.347184000	0.619083000	-0.125945000
C	-0.685443000	-4.253284000	0.037612000
C	4.183701000	-0.653939000	0.207346000
C	0.681789000	-4.237104000	0.087481000
C	2.346259000	2.434366000	0.066154000
C	-2.489116000	2.363205000	-0.097152000
C	-2.439659000	-2.463147000	0.033409000
C	2.388585000	-2.403558000	0.207696000
H	3.100868000	3.214210000	0.037987000
H	-3.191990000	-3.244479000	-0.004896000
H	3.164750000	-3.162247000	0.227419000
C	5.339282000	1.649160000	0.172255000
C	1.345282000	5.407881000	-0.209157000
C	-1.607572000	-5.423864000	-0.030294000
C	5.358254000	-1.573541000	0.242191000
C	1.633313000	-5.385969000	0.086183000
H	5.144505000	2.499503000	-0.493112000
H	2.028140000	5.383690000	-1.066983000
H	-2.244877000	-5.379877000	-0.921405000
H	5.354918000	-2.263860000	-0.609824000
H	2.322545000	-5.333906000	-0.765006000
H	6.218239000	1.141204000	-0.240856000
H	0.715786000	6.296316000	-0.307511000
H	-1.055140000	-6.365543000	-0.065336000
H	6.298376000	-1.017207000	0.215825000
H	1.105912000	-6.340692000	0.027271000
C	5.663864000	2.163064000	1.583329000
H	5.914017000	1.329656000	2.247467000
H	4.803377000	2.682301000	2.017168000
H	6.512008000	2.855563000	1.564073000
H	1.958834000	5.529571000	0.691728000
H	-2.269488000	-5.460507000	0.843333000
H	5.360577000	-2.182108000	1.154517000
C	-5.571972000	1.286314000	-0.222031000
C	-6.731637000	0.526801000	-0.279461000
C	-6.684195000	-0.875536000	-0.246073000
C	-5.472846000	-1.545083000	-0.153044000
H	-5.630950000	2.368912000	-0.246652000
H	-7.694392000	1.024428000	-0.349964000

H	-7.610200000	-1.441009000	-0.292138000
H	-5.446602000	-2.630882000	-0.126656000
V	-0.066334000	-0.038880000	0.632572000
O	-0.148795000	-0.008538000	2.218880000
H	2.242111000	-5.400072000	0.998186000
C	-2.143976000	4.800798000	-0.282837000
H	-2.269668000	5.519639000	0.535165000
H	-2.216054000	5.368587000	-1.217971000
C	-3.241231000	3.676961000	-0.222127000
H	-3.911482000	3.831684000	0.632278000
H	-3.865734000	3.691877000	-1.123699000

XYZ-coordinates for VO(IV)-diDPEP-Rhodo atoms
(13-ethyl-7,12,17-trimethylbenzo[*b*]bicyclopenta[*hi*,*rs*]porphyrinato)oxovanadium(IV)

N	1.982310000	-0.042298000	0.199181000
N	-0.026837000	1.888122000	-0.010551000
N	-2.162529000	-0.036776000	0.070832000
N	-0.124412000	-1.970036000	0.093228000
C	2.784424000	1.072106000	0.153377000
C	-1.139430000	2.640770000	-0.099553000
C	-2.943534000	-1.164685000	0.035414000
C	1.020087000	2.790064000	-0.039260000
C	-2.995590000	1.063945000	-0.029984000
C	-1.164075000	-2.875099000	0.053381000
C	2.838333000	-1.128642000	0.224943000
C	0.996030000	-2.722739000	0.118307000
C	4.174919000	0.686777000	0.173072000
C	-0.849827000	4.024642000	-0.208170000
C	-4.338229000	-0.781386000	-0.059700000
C	0.515275000	4.149072000	-0.173070000
C	-4.370547000	0.626957000	-0.100056000
C	-0.654115000	-4.237446000	0.029175000
C	4.208518000	-0.684241000	0.224057000
C	0.710542000	-4.110700000	0.071558000
C	2.342201000	2.392807000	0.054601000
C	-2.495283000	2.356151000	-0.100042000
C	-2.494013000	-2.480353000	0.043878000
C	2.347006000	-2.433931000	0.196757000
H	3.100701000	3.168879000	0.025904000
H	-3.250005000	-3.258817000	0.011728000
C	5.332765000	1.633856000	0.185403000
C	1.360553000	5.376849000	-0.245074000
C	-1.493712000	-5.470075000	-0.026326000
C	5.420600000	-1.556463000	0.259932000
H	5.129186000	2.482891000	-0.478757000
H	2.047429000	5.344456000	-1.099411000
H	-2.124056000	-5.489897000	-0.923582000
H	5.522780000	-2.151771000	-0.655367000
H	6.217615000	1.137867000	-0.229460000

H	0.736755000	6.268513000	-0.350260000
H	-0.864281000	-6.363969000	-0.039943000
H	6.328360000	-0.957601000	0.366809000
C	5.650678000	2.149523000	1.597293000
H	5.907264000	1.318240000	2.261778000
H	4.784118000	2.659781000	2.029754000
H	6.492211000	2.850182000	1.580539000
H	1.970691000	5.498565000	0.658176000
H	-2.160273000	-5.542523000	0.841662000
H	5.388850000	-2.258017000	1.100131000
C	-5.589322000	1.304802000	-0.195360000
C	-6.756540000	0.556174000	-0.246134000
C	-6.721378000	-0.846138000	-0.208325000
C	-5.515586000	-1.526422000	-0.117784000
H	-5.637813000	2.387840000	-0.223806000
H	-7.714911000	1.062457000	-0.314832000
H	-7.652515000	-1.403606000	-0.249134000
H	-5.499563000	-2.612336000	-0.088808000
V	-0.091808000	-0.024370000	0.648344000
O	-0.155931000	0.021341000	2.236500000
C	-2.132856000	4.792001000	-0.300451000
H	-2.244697000	5.508958000	0.521297000
H	-2.210877000	5.364007000	-1.232484000
C	-3.238145000	3.675585000	-0.229279000
H	-3.903771000	3.841178000	0.626655000
H	-3.865900000	3.690513000	-1.128668000
C	3.090234000	-3.761536000	0.223621000
H	3.825505000	-3.832449000	-0.585312000
H	3.646223000	-3.878353000	1.161484000
C	1.994338000	-4.879429000	0.090246000
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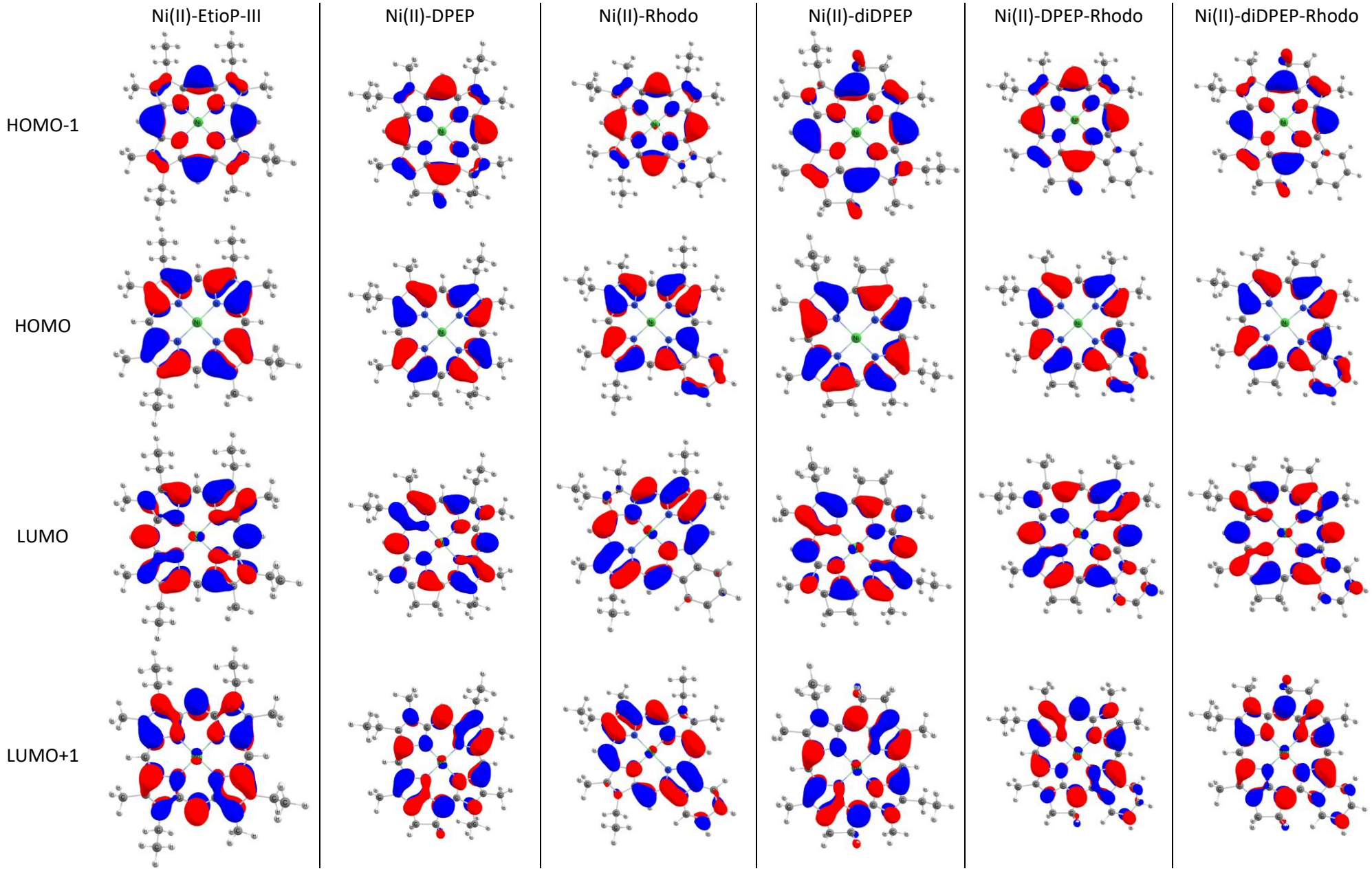

Figure S2. Shapes of molecular orbitals involved in the most intense transitions for Ni-petroporphyrins.

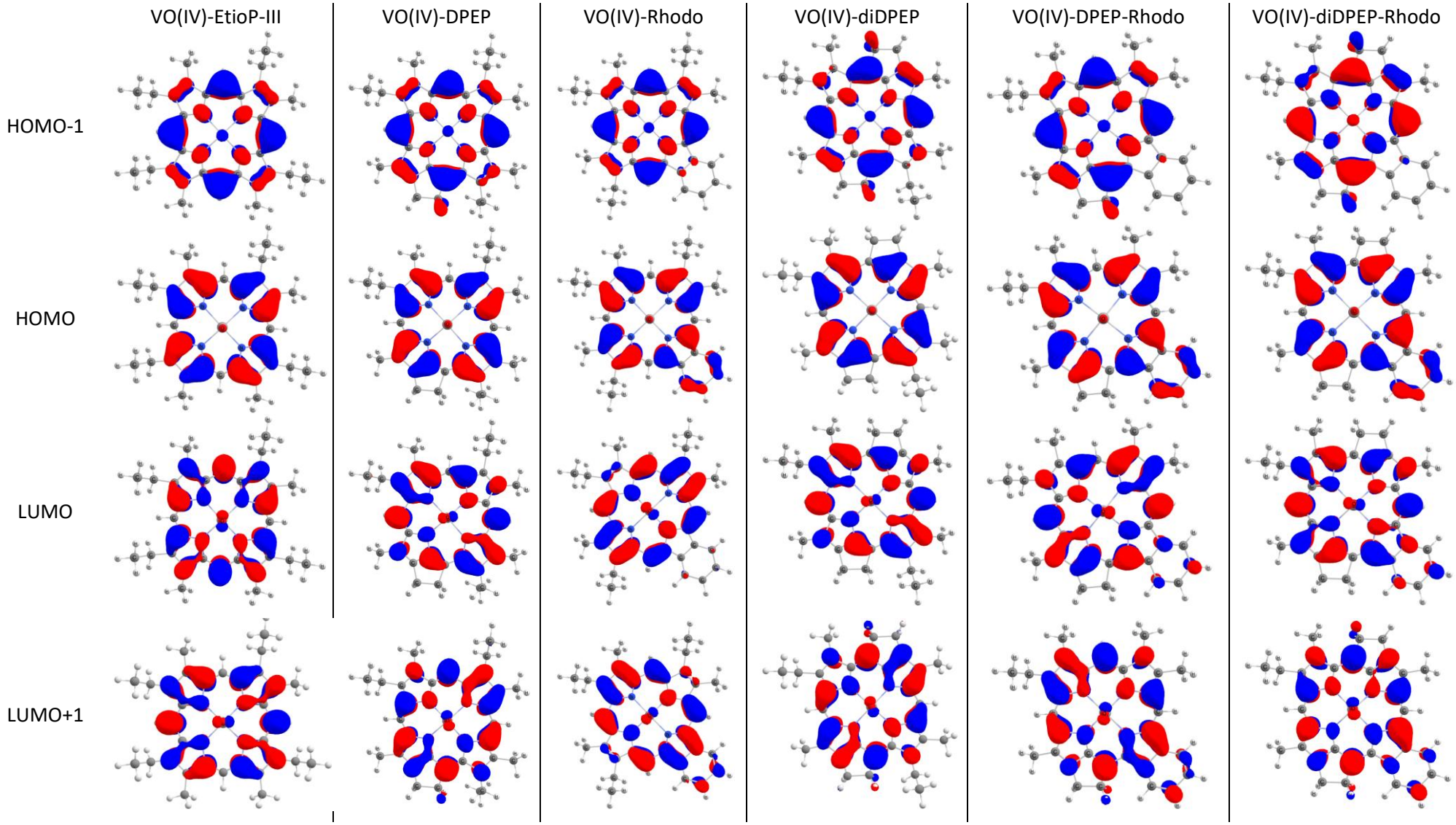

Figure S3. Shapes of molecular orbitals involved in the most intense transitions for VO-petroporphyrins.

Table S4. Bond lengths of the macrocyclic ring of petroporphyrins, Å.

	Ni						V					
	EtioP-III	DPEP	Rhodo	diDPEP	DPEP-Rhodo	diDPEP-Rhodo	EtioP-III	DPEP	Rhodo	diDPEP	DPEP-Rhodo	diDPEP-Rhodo
	Distances, Å											
M-O	-	-	-	-	-	-	1.589	1.590	1.587	1.591	1.589	1.590
M-N	1.947	1.952	1.947	1.945	1.954	1.950	2.085	2.079	2.090	2.075	2.084	2.080
N-C_α	1.375	1.375	1.375	1.374	1.375	1.375	1.372	1.372	1.373	1.371	1.373	1.371
C_α-C_β	1.443	1.441	1.443	1.439	1.441	1.439	1.445	1.443	1.445	1.440	1.443	1.441
C_β-C_β	1.363	1.364	1.373	1.365	1.373	1.375	1.368	1.369	1.378	1.371	1.379	1.381
C_α-C_m	1.377	1.377	1.376	1.379	1.376	1.378	1.386	1.388	1.385	1.390	1.387	1.389
N…N	3.893	3.903	3.893	3.890	3.909	3.899	4.033	4.012	4.047	3.992	4.025	4.004