Supporting information

Water-soluble Sulfonated Phosphorus(v) Corrolazines and Porphyrazines: Effect of Macrocycle Contraction and Pyrazine Ring Fusion on Spectral, Acid-base and Photophysical Properties

Svetlana Ivanova,[a] Denis S. Salnikov,[a] Gleb Knorr,[a] Olesja Ledovich,[a] Valerij Sliznev,[a] Pavel Kubat,[b] Veronika Novakova,[c] and Pavel A. Stuzhin*[a]*

[a.] *Institute of Macroheterocycles, Ivanovo State University of Chemistry and Technology, 153000 Ivanovo, Russia, e-mail: stuzhin@isuct.ru*
[b.] *J. Heyrovsky Institute of Physical Chemistry, Czech Academy of Sciences, 182 23 Prague, Czech Republic.*
[c.] *Faculty of Pharmacy in Hradec Kralove, Charles University, Hradec Kralove, 500 05 Czech Republic.*

Content

I. Spectral characterization

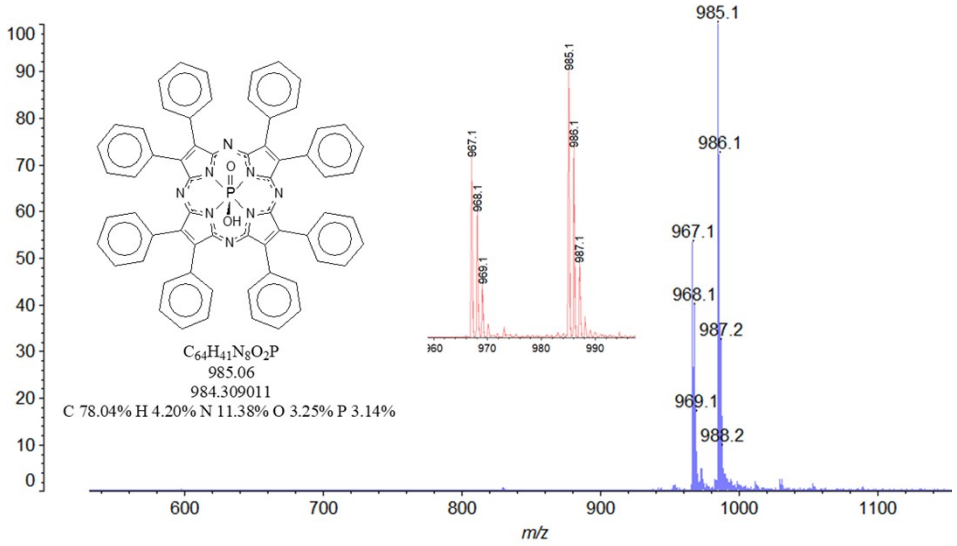


Figure S1-A. MALDI mass-spectra of P(V) porphyrazine complexes **3a**

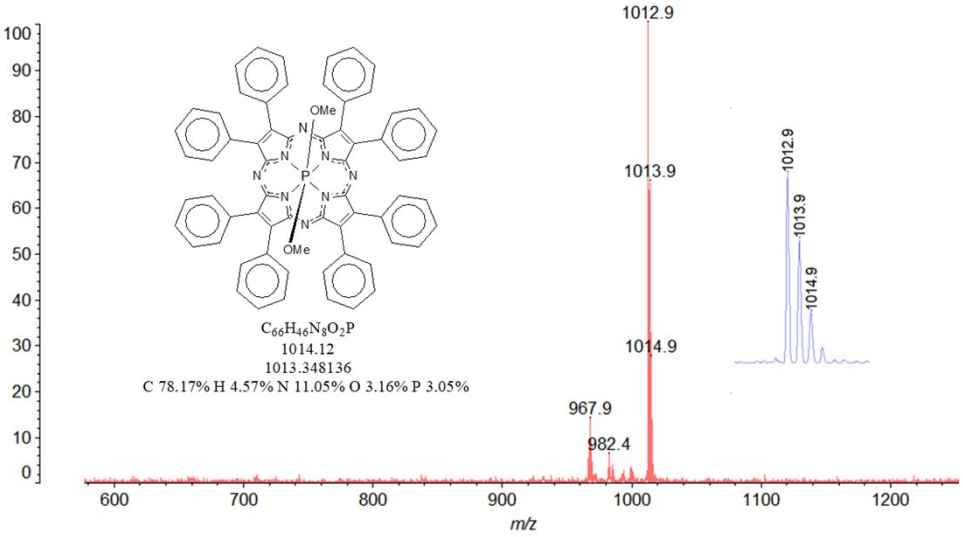


Figure S1-B. MALDI mass-spectra of P(V) porphyrazine complexes **3b**

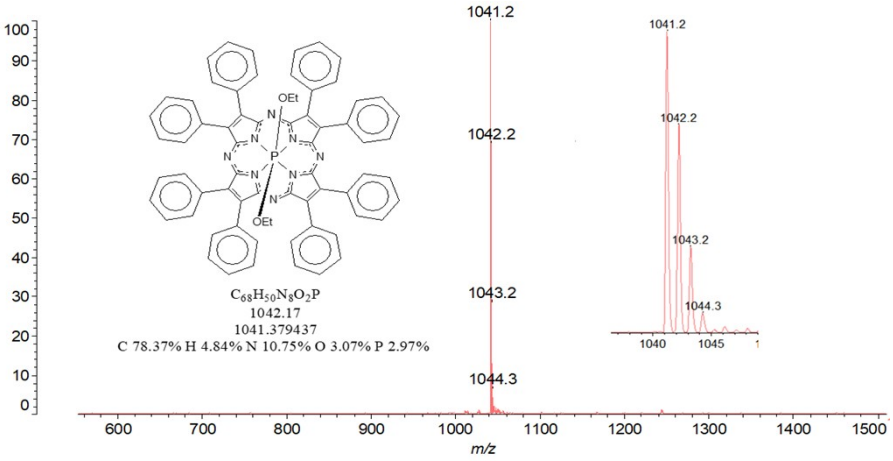


Figure S1-C. MALDI mass-spectra of P(V) porphyrazine complexes **3c**

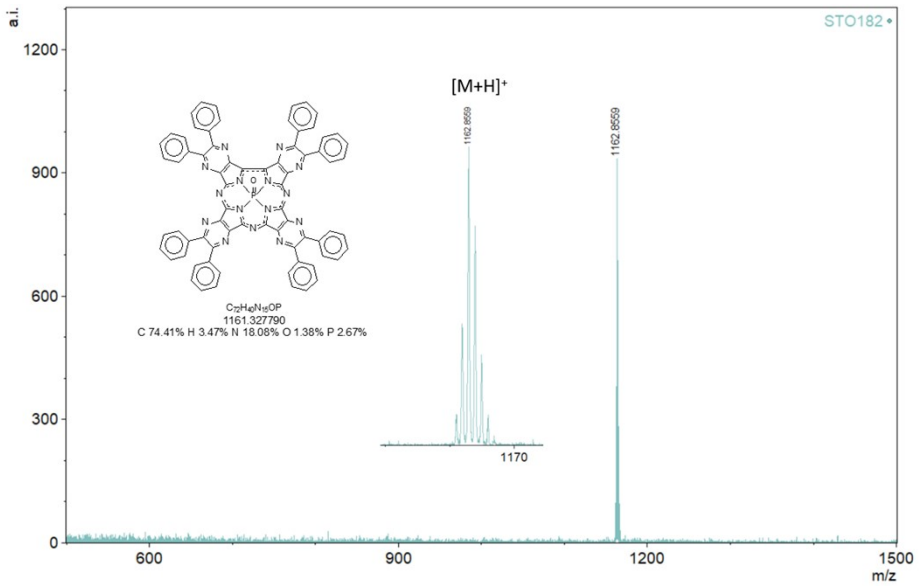


Figure S2-A. MALDI mass-spectra of P(V) tetrapyrazinocorrolazine complexes **5a**

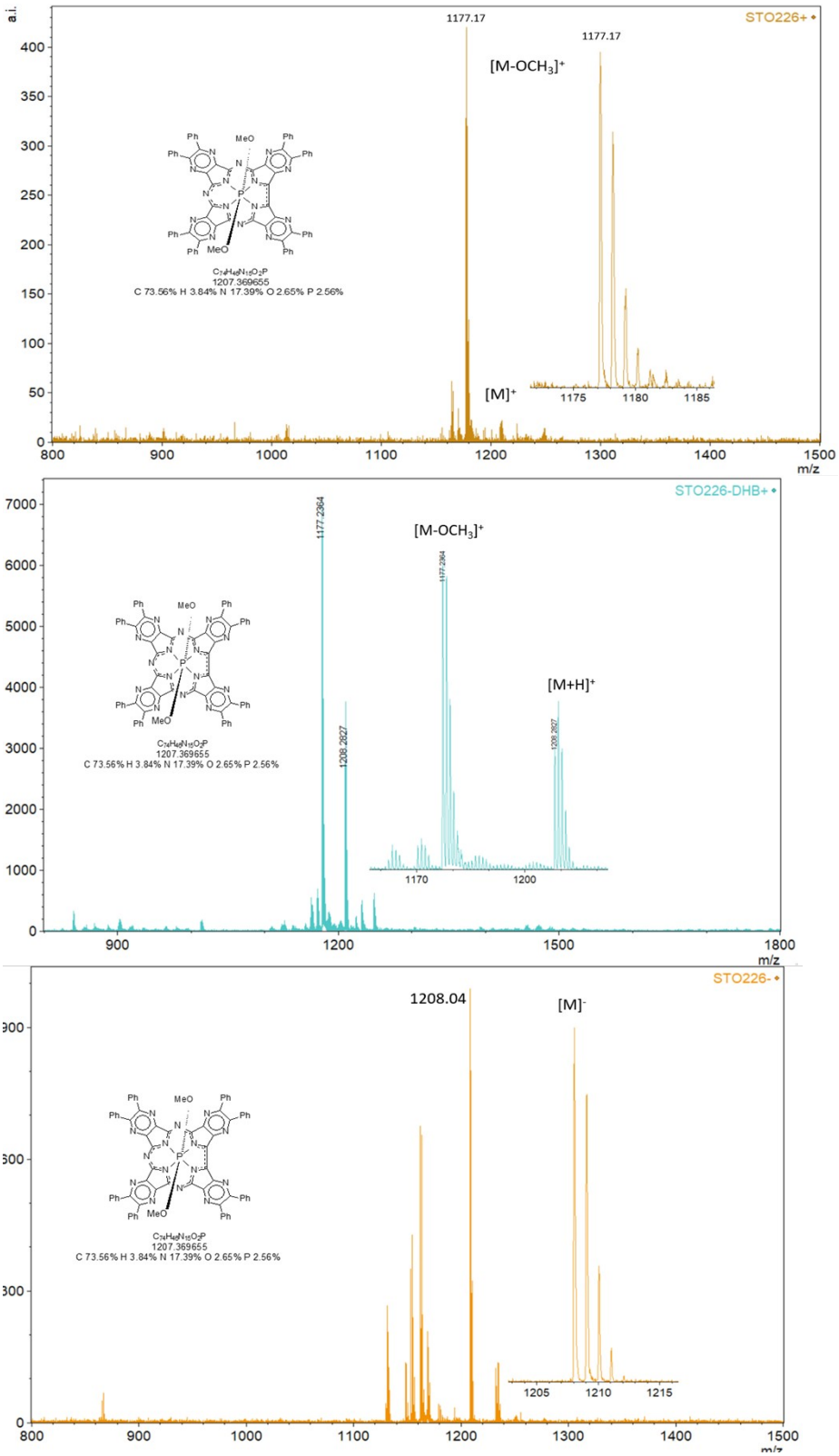


Figure S2-B. MALDI mass-spectra of P(V) tetrapyrazinocorrolazine complexes **5b**

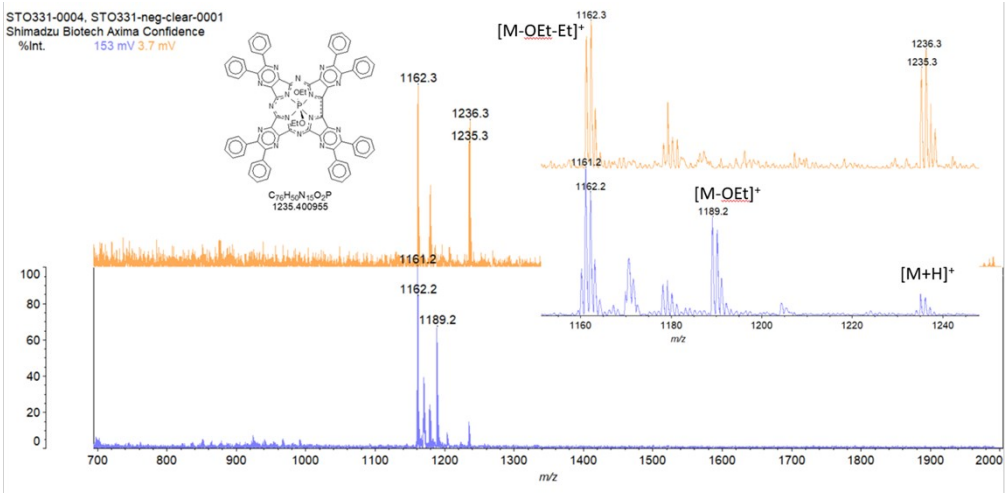


Figure S2-C. MALDI mass-spectra of P(V) tetrapyrazinocorrolazine complexes **5c.**

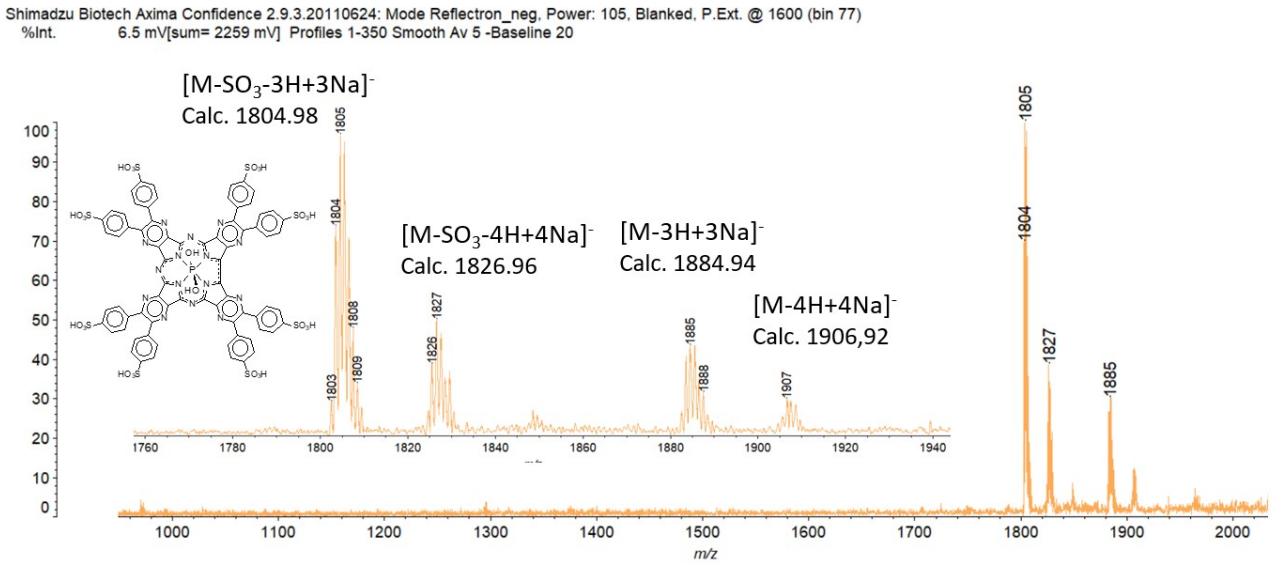


Figure S3. MALDI mass-spectrum of sulfonated P(V) tetrapyrazinoporphyrazine complex **8**.

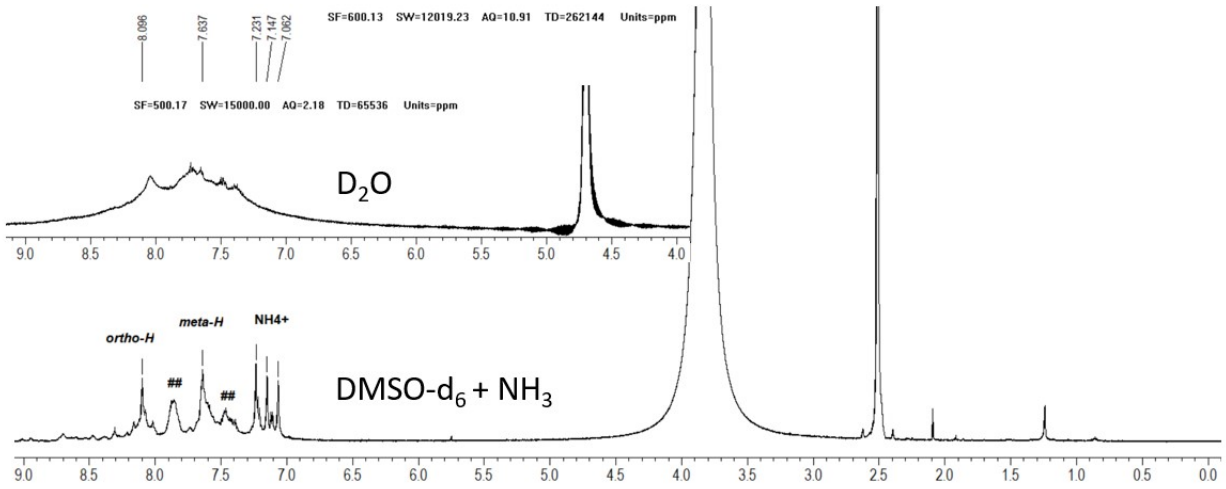


Figure S4. ^{1}H NMR spectrum of sulfonated P(V) tetrapyrazinoporphyrazine complex **8** in D_2O (~3 mM) and in DMSO-d_6 with addition of NH_3. Resonance signals of associates are marked by ##.

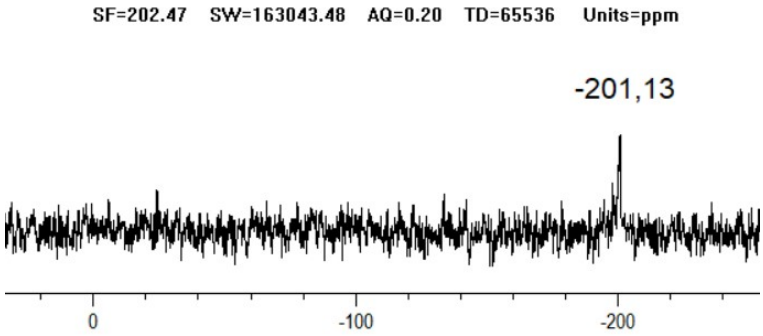


Figure S5. ^{31}P NMR spectrum of sulfonated P(V) tetrapyrazinoporphyrazine complex **8** in D_2O

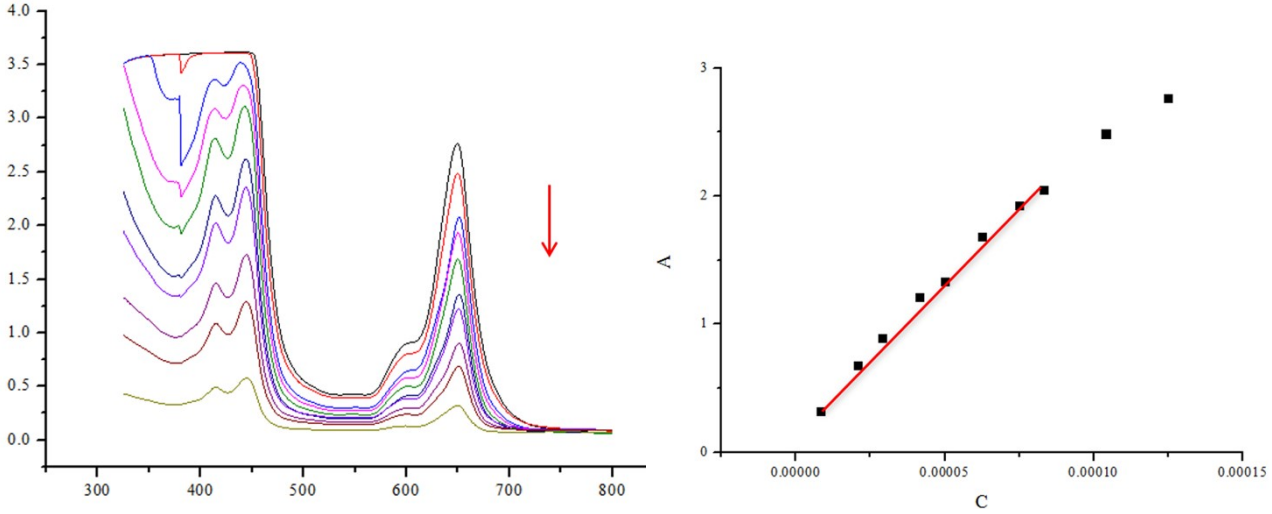


Figure S6. Concentration dependence of the UV-VIS spectra for sulfonated P(V) tetrapyrazinoporphyrazine complex **8**.

II. Photophysical measurements in water solutions

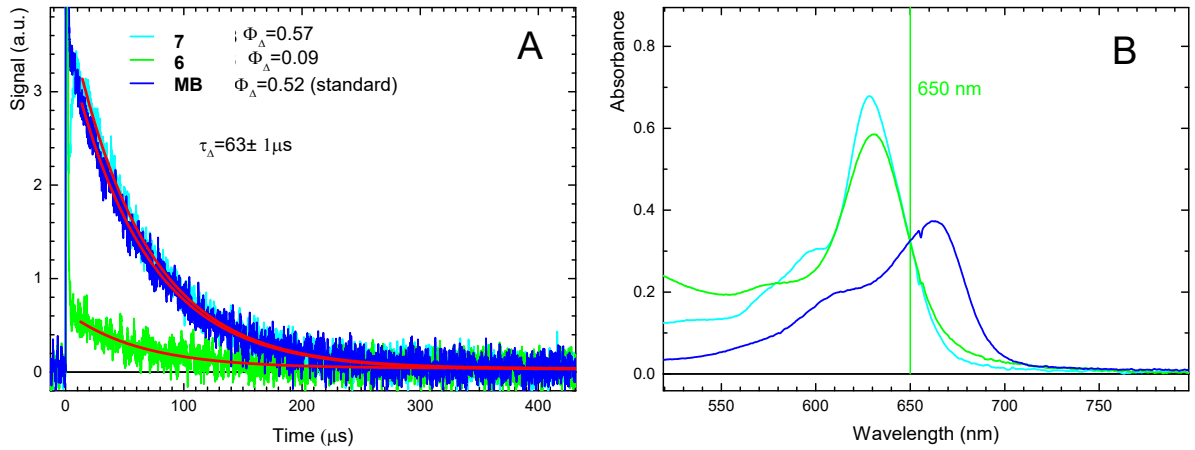


Figure S7. Panel A: Comparison of singlet oxygen phosphorescence generated from of **6, 7** and methylene blue (**MB)** (absorbance at 650 nm is 0.324) in D_2O.Excited by 650 nm. Panel B: Visible spectra of **6, 7** (with background correction) and **MB** (standard) in D_2O used for calculation of Φ_Δ.

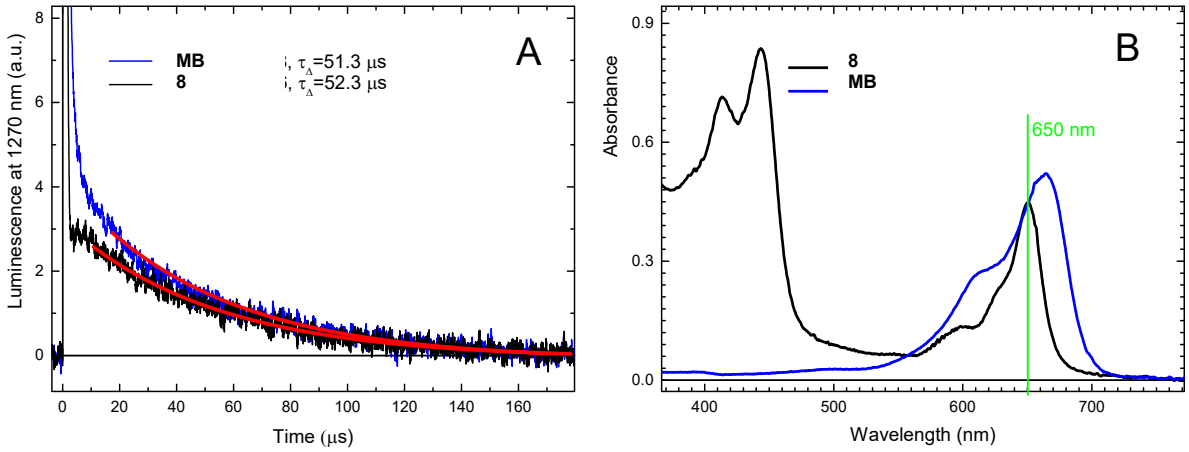


Figure S8. Panel A: Comparison of singlet oxygen phosphorescence generated from **8** (absorbance at 650 nm 0.448) and **MB** (absorbance at 650 nm 0.444) in D_2O.Excited by 650 nm. Panel B: Visible spectra of **8** and **MB** (standard) in D_2O used for calculation of Φ_Δ.

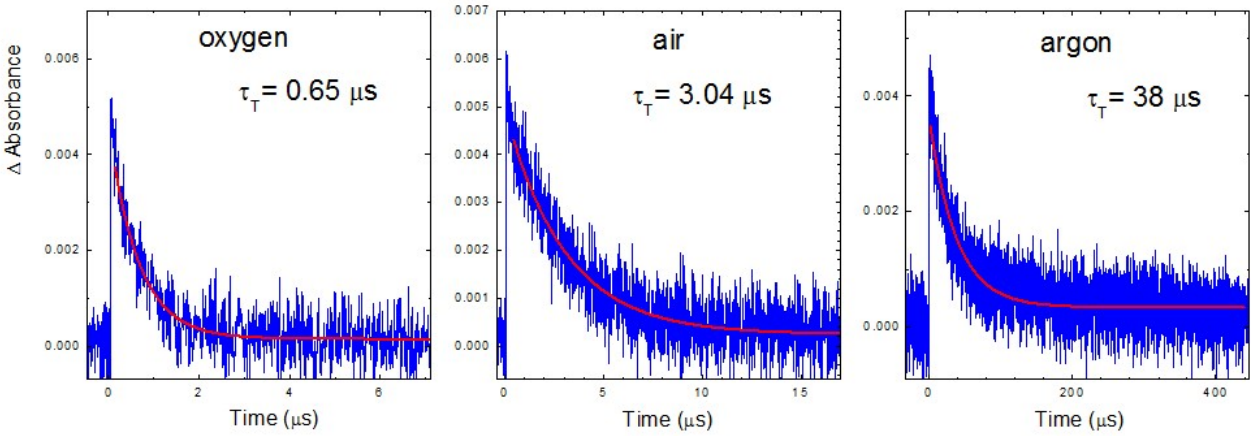


Figure S9. Kinetics of the triplet states of **6** in oxygen-, air-, and argon saturated D_2O measured by transient absorption at 500 nm after excitation by dye laser at 650 nm.

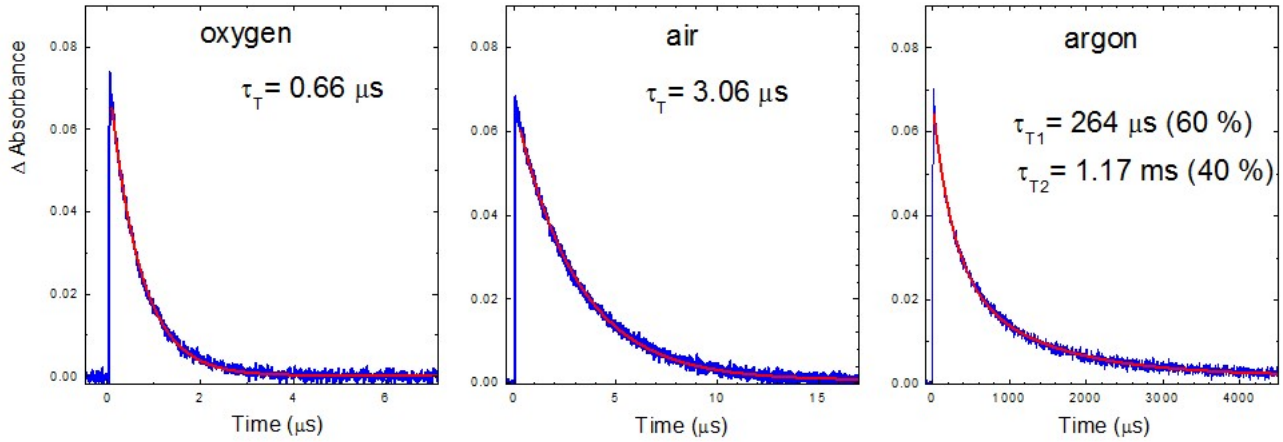


Figure S10. Kinetics of the triplet states of **7** in oxygen-, air-, and argon saturated D_2O measured by transient absorption at 500 nm after excitation by dye laser at 650 nm.

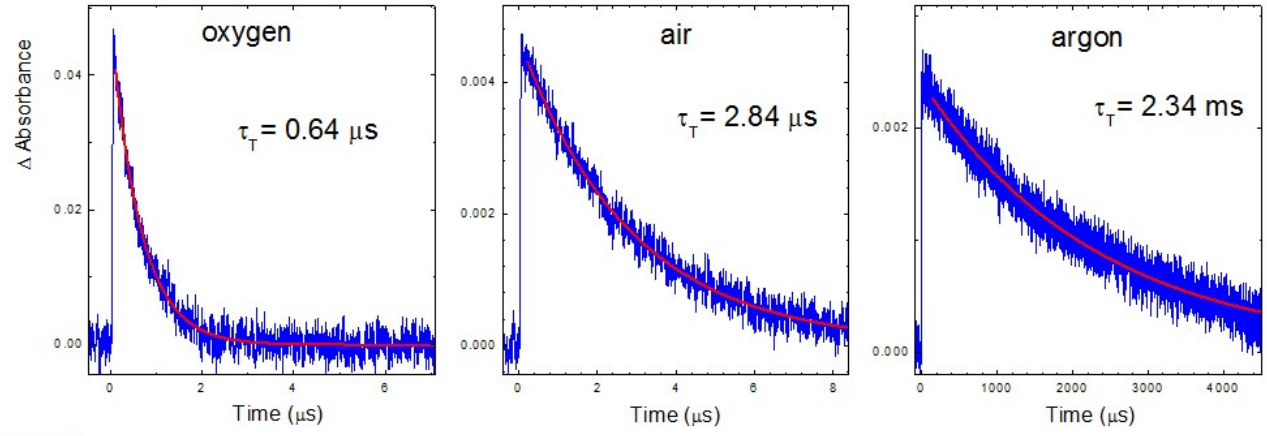


Figure S11. Kinetics of the triplet states of **8** in oxygen-, air-, and argon saturated D_2O measured by transient absorption at 500 nm after excitation by dye laser at 650 nm.

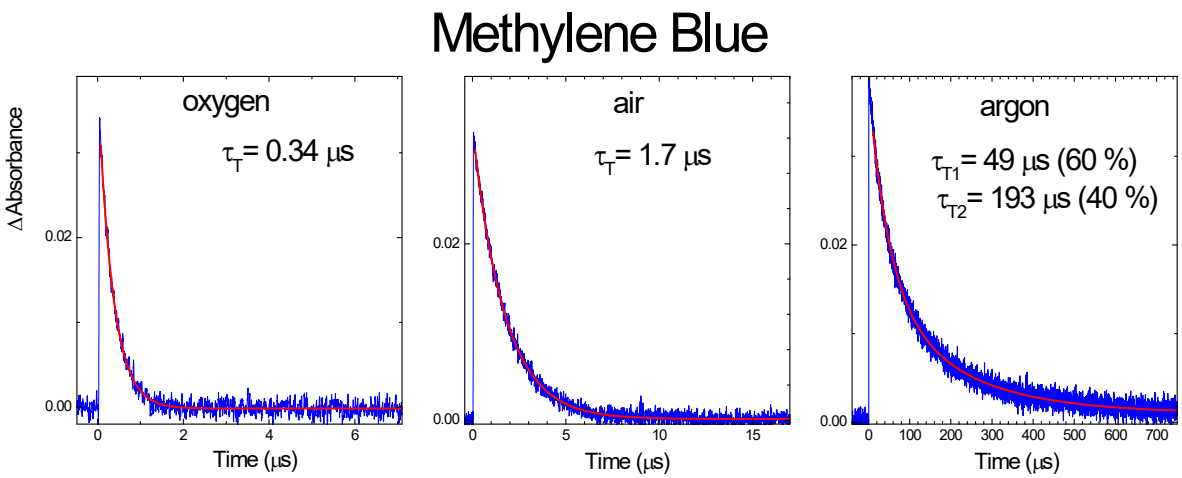


Figure S12. Kinetics of the triplet states of **MB** in oxygen-, air-, and argon saturated D_2O measured by transient absorption at 420 nm after excitation by dye laser at 650 nm.

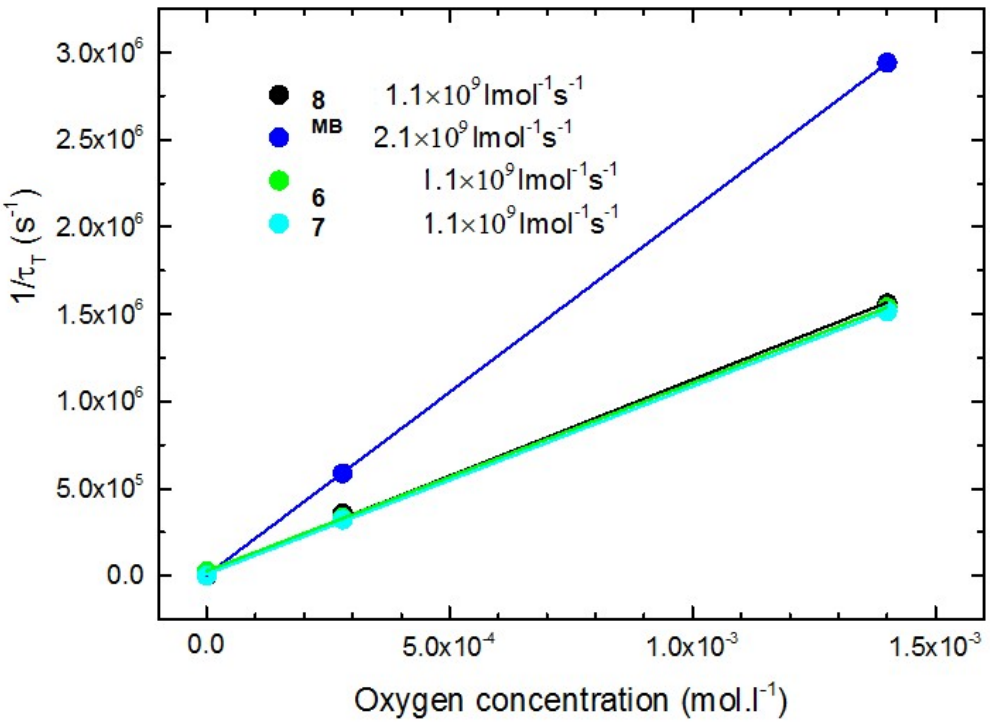


Figure S13. Quenching of the triplet states of **6, 7, 8** and **MB** (standard) by oxygen

III. DFT calculations results

Computational procedure

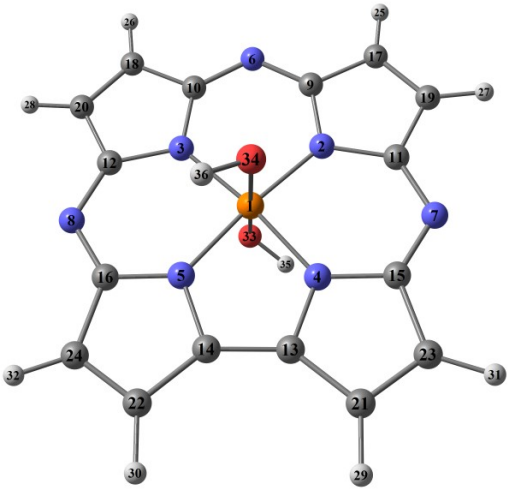
Calculations of the molecular and electronic structures were accomplished by the electron density functional method with DFT/B3LYP {1,2,3] using the Firefly 8 program [4] which is partly based on the initial code of the GAMESS (US) program [5]. For all atoms, correlation-consistent triple-zeta (cc-pvtz) basis sets[6] were used. The exponents and contracting ratios were taken from the database [7]. Geometric parameters of all considered configurations were optimized using a gradient method. For the optimized structures, force field constants were obtained and normal mode frequencies and band intensities in the IR spectra were calculated in harmonic approximation using the numerical method implemented in the Firefly 8 program [4,5]. The energies of the vertical electronic transitions and oscillator strengths were calculated for the **optimized** geometries by the TD DFT method [8] without consideration of the excitations from the molecular orbitals corresponding to the 1s-orbitals of C and N and 1s-, 2s-, 2p orbitals of S (frozen core approximation).

1. A. D. Becke, *J. Chem. Phys*., 1993, **98**, 5648-5642.
2. P. J. Stephens, F. J. Devlin, C. F. Chablowski and M. J. Frisch, *J. Phys. Chem.*, 1994, **98**, 11623-11627.
3. R. H. Hertwig and W. Koch, *Chem. Phys. Lett*., 1997, **268**, 345-351.
4. A. A. Granovsky, Firefly version 8, www http://classic.chem.msu.su/gran/firefly/index.html.
5. M. W. Schmidt, K. K. Baldridge, J. A. Boatz, S. T. Elbert, M. S. Gordon, J. H. Jensen, S. Koseki, N. Matsunaga, K. A. Nguyen, S. J. Su, T. L. Windus, M. Dupuis and J. A. Montgomery, *J. Comput. Chem*., 1993, **14**, 1347-1363.
6. T. H. Dunning, *J. Chem. Phys.*, 1989, **90**, 1007–1023. DOI: 10.1063/1.456153.
7. The Extensible Computational Chemistry Environment Basis Set Database, Version 6/19/03 (by the Molecular Science Computing Facility, Environmental and Molecular Sciences Laboratory).
8. Y. Towada, T. Tsuneda, S. Yanagisawa, Y. Yanai and K. Hirao, *J. Chem. Phys.*, 2004, **120**, 8425-8433.

For the optimized structures the following data are presented:

- Calculated (TDDFT) wavelengths (λ, in nm) and oscillator strengths (in parentheses) corresponding to the energies of the transition from the ground state [*)] to the nearest excited electronic states. [**)] the weight (%) of the Slater determinant in the wave function of the excited electronic state is indicated in parentheses.
- Cartesian coordinates (Å):
- TOTAL ENERGY
- Frequencies (ω_i – cm^{-1}) and IR intensities (A_i – D^2*amu/$Å^2$)
- The electronic absorption spectrum (TDDFT calculation): ΔE – excitation energy (eV), λ - wave length (nm), *f* – oscillator strength

1. [*CAP* $(OH)_2$]



State	Composition[**)]	λ
…(41b)²(44a)²(42b)²(45a)²(43b)²(46a)²(47a)²(44b)²(45b)²(48a)²(49a)⁰(46b)⁰(47b)⁰(50a)⁰…		
1^1A	*48a→49a*(80); *45b→46b*(19)	512(0.122)
3^1B	*48a→46b*(38);*45b→49a*(33); *44b→49a*(20)	364(0.420)
4^1B	*44b→49a*(77);*45b→49a*(11)	360(0.115)
5^1A	*47a→49a*(64); *45b→46b*(27)	350(0.129)
6^1A	*45b→46b*(48);*47a→49a*(29); *48a→49a*(15)	340(0.448)
11^1B	*43b→49a*(45); *47a→46b*(39)	307(0.171)
16^1A	*43b→46b*(91)	272(0.106)
19^1B	*48a→47b*(79); *41b→48a*(17)	260(0.113)

Cartesian coordinates (Å):

Atom	X	Y	Z
P1	0.000000000000	0.000000000000	0.050091267132
N2	1.330116452063	0.104849107382	1.257133256439
N3	-1.330116452063	-0.104849107382	1.257133256439
N4	1.183242990790	0.152584345531	-1.297436728456
N5	-1.183242990790	-0.152584345531	-1.297436728456
N6	0.000000000000	0.000000000000	3.268188356051
N7	3.286442672342	0.224026824449	-0.193176199992
N8	-3.286442672342	-0.224026824449	-0.193176199992
C9	1.150761119465	0.080227378793	2.622318077250
C10	-1.150761119465	-0.080227378793	2.622318077250
C11	2.695215605322	0.180961038091	0.985910948021
C12	-2.695215605322	-0.180961038091	0.985910948021
C13	0.701071355163	0.073201385987	-2.576237780199
C14	-0.701071355163	-0.073201385987	-2.576237780199
C15	2.547834272323	0.191960585023	-1.299471900234
C16	-2.547834272323	-0.191960585023	-1.299471900234
C17	2.445214862910	0.154991684123	3.239637334143
C18	-2.445214862910	-0.154991684123	3.239637334143
C19	3.376539536189	0.214386727731	2.251104296131
C20	-3.376539536189	-0.214386727731	2.251104296131
C21	1.816452260246	0.109057073007	-3.454543413307
C22	-1.816452260246	-0.109057073007	-3.454543413307
C23	2.951711182897	0.183132825178	-2.671374871018
C24	-2.951711182897	-0.183132825178	-2.671374871018
H25	2.591912106624	0.156918713079	4.306049160397
H26	-2.591912106624	-0.156918713079	4.306049160397
H27	4.447925523277	0.277497272498	2.337666432699
H28	-4.447925523277	-0.277497272498	2.337666432699
H29	1.772128059856	0.072205168011	-4.529861228737
H30	-1.772128059856	-0.072205168011	-4.529861228737
H31	3.975783394793	0.220143451069	-3.002447055600
H32	-3.975783394793	-0.220143451069	-3.002447055600
O33	-0.237819360117	1.679929294504	0.112384903358
O34	0.237819360117	-1.679929294504	0.112384903358
H35	0.451208106283	2.160628565081	-0.355872482764
H36	-0.451208106283	-2.160628565081	-0.355872482764

TOTAL ENERGY = -1490.5624756650 Hartree

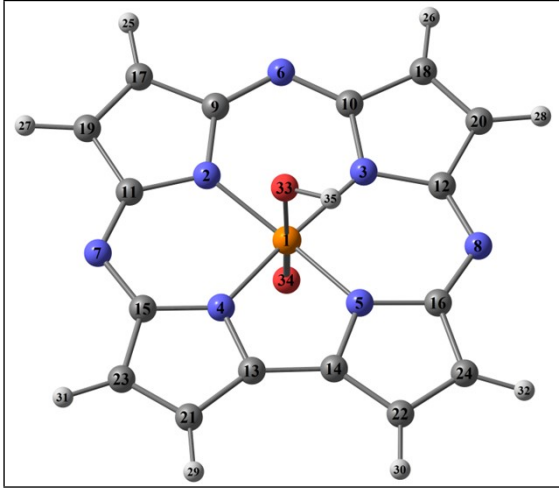
Frequencies (ω_i – cm^{-1}) and IR intensities (A_i – D^2*amu/$Å^2$)

ω_i	A_i	ω_i	A_i	ω_i	A_i	ω_i	A_i
73.36	0.02044	515.34	0.00421	913.02	0.00775	1380.92	0.01152
81.38	0.00018	552.33	0.36998	938.71	0.00033	1408.6	0.19148
90.85	0.03119	574.41	0.58105	939.84	0.00061	1409.23	0.09352
124.97	1E-5	577.49	0.25392	1017.19	1.58149	1450.86	1.37958
126.26	0.02105	608.59	0.00577	1034.85	0.1886	1467.89	0.04982
209.82	0	656.65	0.00384	1041.06	0.51894	1488.45	0.00674
224.74	0.06671	673.22	0.00067	1046.87	6.28352	1489.39	0.87795
224.89	0.48838	681.6	0.00488	1056.38	0.8305	1519.18	0.88033
245.52	0.27455	697.45	0.0032	1064.02	0.08446	1536.97	0.73974
276.09	0.26731	721.35	0.0007	1065.07	0.66993	1544.28	0.3949
288.07	0.12278	723.92	0.38515	1074.66	3.09943	1558.17	0.38613
309.21	0.11749	731.92	0.6346	1077.28	0.70593	1570.8	1.65485
329.57	0.09961	731.93	7E-5	1078.42	0.21909	1574.23	0.52927
345.76	0.00579	741.05	0.08317	1097.33	3.13544	1596.49	0.29443
354.87	0.01776	750.91	0.32211	1109.29	0.421	3238.25	0.00014
367.79	0.32015	786.52	1.29567	1110.61	3.41128	3238.84	0.01443
370.91	0.07719	795.97	0.34862	1184.95	0.0178	3243.63	0.00258
402.35	0.10446	800.84	4.74819	1209.67	0.02024	3243.66	0.00075
418.63	0.20641	803.76	0.03035	1215.75	0.29712	3253.9	0.07286
425.12	0.0035	808.56	0.01724	1281.99	0.12383	3253.9	0.01811
431.36	0.00584	813.59	0.07905	1293.59	0.70549	3260.47	0.01027
450.24	0.00393	816.56	0.12522	1299.8	0.31197	3260.53	0.00906
477.9	0.10249	822.94	0.00538	1324.81	0.01358	3828.26	0.02945
490.78	0.09021	827.43	4.3352	1327.17	0.09406	3828.43	1.19499
495.82	0.00049	904.4	0.07703	1352.73	0.04873		
501.39	0.03809	912.79	0.0017	1366.37	0.07172		

The electronic absorption spectrum (TDDFT calculation): ΔE – excitation energy (eV), λ - wave length (nm), *f* – oscillator strength

State	ΔE	λ	*f*	State	ΔE	λ	*f*
^{1}A	2.4203	512.27	0.1218058	^{1}A	4.5580	272.02	0.1064608
^{1}B	2.5998	476.90	0.0001180	^{1}A	4.6792	264.97	0.0000512
^{1}B	3.4021	364.44	0.4200273	^{1}A	4.7197	262.69	0.0018008
^{1}B	3.4443	359.96	0.1147690	^{1}B	4.7733	259.75	0.1132297
^{1}A	3.5428	349.96	0.1290496	^{1}B	4.9902	248.46	0.0027869
^{1}A	3.6495	339.73	0.4484154	^{1}B	5.0215	246.91	0.0009863
^{1}A	3.7804	327.97	0.0051768	^{1}A	5.1492	240.79	0.0012156
^{1}A	3.8338	323.40	0.0095464	^{1}B	5.2148	237.75	0.0040579
^{1}A	4.0122	309.02	0.0096833	^{1}B	5.2537	235.99	0.0152583
^{1}B	4.0142	308.86	0.0026584	^{1}A	5.2609	235.67	0.0046016
^{1}B	4.0389	306.97	0.1712068	^{1}A	5.4229	228.63	0.0036165
^{1}B	4.0944	302.82	0.0164471	^{1}A	5.6583	219.12	0.0000006
^{1}B	4.2384	292.52	0.0003305	^{1}A	5.7546	215.45	0.0048657
^{1}B	4.3524	284.86	0.0206353	^{1}B	5.8050	213.58	0.0150244
^{1}A	4.4671	277.55	0.0000876	^{1}B	5.8808	210.83	0.0000395

2. Anion [*CAP*(O-)(OH)$_2$]



State	Composition **)	λ
…(91a)²(92a)²(93a)²(94a)⁰(95a)⁰(96a)⁰…		
4^1A	91*a*→94*a*(62); 90*a*→95*a*(20); 93*a*→94*a*(15)	501(0.089)
8^1A	91*a*→95*a*(38); 90*a*→94*a*(24); 93*a*→96*a*(21)	377(0.428)
9^1A	90*a*→95*a*(66); 91*a*→94*a*(11)	362(0.464)
10^1A	88*a*→94*a*(48); 89*a*→95*a*(46)	332(0.075)
14^1A	87*a*→94*a*(64); 86*a*→94*a*(23)	311(0.107)
21^1A	93*a*→96*a*(80); 91*a*→96*a*(15)	274(0.085)
23^1A	92*a*→96*a*(91)	260(0.085)
27^1A	80*a*→94*a*(43); 82*a*→94*a*(26); 91*a*→96*a*(22)	252(0.089)

Cartesian coordinates (Å):

Atom	X	Y	Z
P1	-0.001409003	-0.119794665	0.004306589
N2	1.355515755	-0.167854856	1.229070401
N3	-1.337335520	0.219837920	1.236117896
N4	1.199245008	-0.142040158	-1.364512731
N5	-1.170299733	0.249148079	-1.356572511
N6	0.010316202	0.019149118	3.225483860
N7	3.270971477	-0.456069857	-0.240564127
N8	-3.263183656	0.436357007	-0.230962289
C9	1.160577760	-0.146977813	2.578405882
C10	-1.144047143	0.176376473	2.584790831
C11	2.689347951	-0.376520517	0.948078972
C12	-2.680753434	0.360150774	0.958411804
C13	0.718808092	-0.042822033	-2.626510616
C14	-0.687511253	0.171993630	-2.625388675
C15	2.539760018	-0.338235507	-1.353776790
C16	-2.525560703	0.365608159	-1.345611192
C17	2.447290846	-0.352485614	3.206118820
C18	-2.439087474	0.314524688	3.216315837
C19	3.371200148	-0.492151236	2.217783720
C20	-3.368939382	0.423227191	2.229842885
C21	1.828230180	-0.192514262	-3.513636437
C22	-1.802929149	0.274393730	-3.505814248
C23	2.952287035	-0.374265200	-2.730966258
C24	-2.935922126	0.397091769	-2.719845004
H25	2.591207078	-0.384164288	4.273355675
H26	-2.585164157	0.317202662	4.283842446
H27	4.431823764	-0.660660985	2.306968271
H28	-4.436774380	0.537331918	2.320891827
H29	1.786396156	-0.161605456	-4.590366435
H30	-1.762585854	0.254878702	-4.582923511
H31	3.967158365	-0.520353054	-3.062903779
H32	-3.956827621	0.492757025	-3.051752784
O33	0.321398173	1.619671952	0.098714299
O34	-0.243591074	-1.630230948	0.029185181
H35	-0.391509137	2.100146418	-0.330796568

TOTAL ENERGY = -1490.0036282760 Hartree

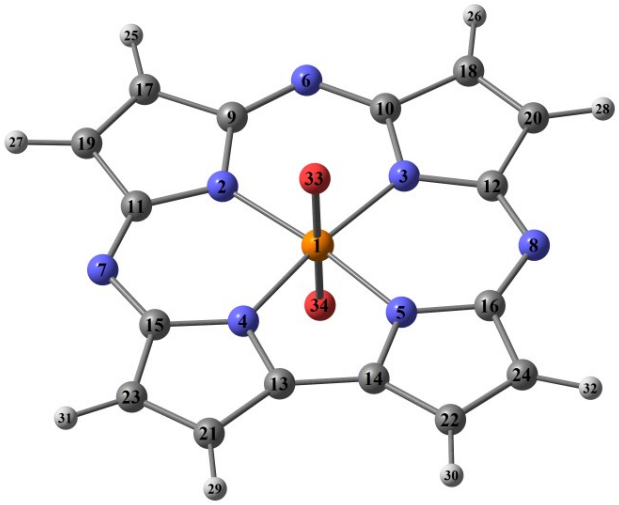
Frequencies (ω_i – cm^{-1}) and IR intensities (A_i – D^2*amu/$Å^2$)

ω_i	A_i	ω_i	A_i	ω_i	A_i	ω_i	A_i
67.55	0.04894	506.78	0.00273	897.72	0.00112	1363.44	0.10428
83.90	0.00098	524.18	0.74244	900.34	0.00484	1372.03	0.03549
101.39	0.02250	555.97	0.45770	904.82	0.08711	1406.67	0.11604
119.23	0.02250	561.44	0.71983	1010.36	1.94447	1414.65	0.21103
124.87	0.00508	568.48	0.80901	1020.07	0.55624	1441.48	1.99514
199.00	0.25208	656.44	0.00803	1030.02	5.37862	1464.77	0.06998
219.99	0.00239	668.48	0.00132	1035.57	0.05182	1473.28	1.17087
238.25	0.04715	680.43	0.00854	1044.42	3.66242	1482.57	0.09675
261.24	0.13380	692.40	0.00455	1052.51	0.17328	1503.03	1.64252
281.96	0.07251	714.40	0.04616	1060.78	3.46075	1518.37	1.05451
292.07	0.07052	719.77	1.33737	1063.87	1.29168	1521.86	0.82026
320.13	0.20065	721.17	0.22878	1066.63	0.22271	1536.63	0.01656
344.69	0.00970	725.58	0.58399	1082.64	0.30801	1549.79	2.84864
352.99	0.04260	735.17	0.00531	1084.30	1.73753	1561.95	1.44686
364.56	0.01459	748.40	0.39169	1094.45	2.65593	1568.21	0.13028
369.97	0.17065	771.96	1.07441	1097.00	1.18775	3216.33	0.05481
396.89	0.02014	782.32	0.00836	1173.97	0.09658	3217.21	0.18709
406.44	0.04707	792.21	0.42830	1208.43	0.01529	3222.33	0.08013
424.58	0.05725	799.05	0.04160	1230.04	0.41120	3223.96	0.06919
435.16	0.01180	803.63	0.17215	1276.41	0.20235	3234.99	0.59433
440.19	0.01906	806.12	1.84557	1295.51	0.74853	3235.53	0.89788
463.44	0.00741	810.28	0.09285	1298.44	1.31891	3242.32	0.50289
472.21	0.01630	812.93	0.31182	1323.59	0.06952	3243.73	0.49382
492.56	0.09202	857.81	0.00521	1337.00	0.11867	3824.99	0.14965
501.87	0.00872	861.39	0.01124	1358.42	0.14381		

The electronic absorption spectrum (TDDFT calculation): ΔE – excitation energy (eV), λ - wave length (nm), *f* – oscillator strength

State	ΔE	λ	*f*	State	ΔE	λ	*f*
^{1}A	1.9832	625.17	0.0107286	^{1}A	4.2945	288.70	0.0004626
^{1}A	2.0337	609.65	0.0154338	^{1}A	4.3105	287.63	0.0005505
^{1}A	2.3803	520.88	0.0015078	^{1}A	4.3373	285.85	0.0081840
^{1}A	2.4748	500.98	0.0885925	^{1}A	4.4249	280.19	0.0263229
^{1}A	2.5960	477.60	0.0102613	^{1}A	4.4973	275.69	0.0583415
^{1}A	2.6984	459.46	0.0086870	^{1}A	4.5250	274.00	0.0848372
^{1}A	3.2005	387.39	0.0136831	^{1}A	4.5956	269.79	0.0000707
^{1}A	3.2848	377.45	0.4277041	^{1}A	4.7657	260.16	0.0851732
^{1}A	3.4239	362.11	0.4641804	^{1}A	4.8132	257.59	0.0027712
^{1}A	3.7336	332.08	0.0750207	^{1}A	4.8510	255.58	0.0012026
^{1}A	3.7754	328.40	0.0095733	^{1}A	4.8938	253.35	0.0202608
^{1}A	3.8560	321.53	0.0014972	^{1}A	4.9253	251.73	0.0885692
^{1}A	3.9511	313.80	0.0181680	^{1}A	5.0317	246.41	0.0001495
^{1}A	3.9846	311.16	0.1071032	^{1}A	5.0955	243.32	0.0105531
^{1}A	4.0675	304.82	0.0008902	^{1}A	5.1887	238.95	0.0000713

3. Dinion [*CAP*(O-)$_2$]



State	Composition **)	λ
9^1A_1	$6a_2 \rightarrow 8a_2$(70); $11b_1 \rightarrow 13b_1$ (28)	509(0.067)
10^1B_2	$11b_1 \rightarrow 8a_2$(80); $6a_2 \rightarrow 13b_1$ (15)	501(0.027)
11^1B_2	$6a_2 \rightarrow 13b_1$(77); $11b_1 \rightarrow 8a_2$(13)	390(0.388)
12^1A_1	$11b_1 \rightarrow 13b_1$ (66); $6a_2 \rightarrow 8a_2$(23)	389(0.417)
14^1A_1	$5a_2 \rightarrow 8a_2$(95)	333(0.064)
16^1B_2	$10b_1 \rightarrow 8a_2$(96)	320(0.042)
25^1B_2	$7a_2 \rightarrow 14b_1$(90)	292(0.103)
26^1A_1	$10b_1 \rightarrow 13b_1$ (84); $4a_2 \rightarrow 8a_2$(10)	288(0.044)
30^1A_1	$33b_2 \rightarrow 34b_2$(85); $12b_1 \rightarrow 14b_1$ (10)	281(0.042)

Cartesian coordinates (Å):

Atom	X	Y	Z
P1	0.000000000	0.000000000	0.015116288
N2	0.000000000	-1.394480206	-1.238747660
N3	0.000000000	1.394480206	-1.238747660
N4	0.000000000	-1.211186971	1.405771152
N5	0.000000000	1.211186971	1.405771152
N6	0.000000000	0.000000000	-3.213184142
N7	0.000000000	-3.307065536	0.251770831
N8	0.000000000	3.307065536	0.251770831
C9	0.000000000	-1.177390512	-2.574201547
C10	0.000000000	1.177390512	-2.574201547
C11	0.000000000	-2.730582949	-0.950161410
C12	0.000000000	2.730582949	-0.950161410
C13	0.000000000	-0.721040257	2.661150035
C14	0.000000000	0.721040257	2.661150035
C15	0.000000000	-2.566029273	1.376354206
C16	0.000000000	2.566029273	1.376354206
C17	0.000000000	-2.487993295	-3.215096205
C18	0.000000000	2.487993295	-3.215096205
C19	0.000000000	-3.428648441	-2.228639395
C20	0.000000000	3.428648441	-2.228639395
C21	0.000000000	-1.846594177	3.544380879
C22	0.000000000	1.846594177	3.544380879
C23	0.000000000	-2.989596800	2.754516940
C24	0.000000000	2.989596800	2.754516940
H25	0.000000000	-2.638964791	-4.284269013
H26	0.000000000	2.638964791	-4.284269013
H27	0.000000000	-4.503853480	-2.328956151
H28	0.000000000	4.503853480	-2.328956151
H29	0.000000000	-1.809561911	4.624294087
H30	0.000000000	1.809561911	4.624294087
H31	0.000000000	-4.016430429	3.088794063
H32	0.000000000	4.016430429	3.088794063
O33	-1.568608754	0.000000000	-0.050406546
O34	1.568608754	0.000000000	-0.050406546

TOTAL ENERGY = -1489.2961306327 Hartree

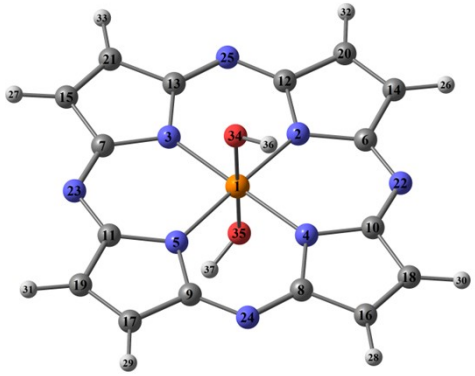
Frequencies (ω_i – cm^{-1}) and IR intensities (A_i – D^2*amu/Å^2)

ω_i	A_i	ω_i	A_i	ω_i	A_i	ω_i	A_i
49.03	0.08543	509.38	0.00024	840.93	0.00000	1377.90	0.03470
84.65	0.00000	546.93	0.49418	900.38	0.14776	1408.32	0.08930
108.02	0.00000	561.23	0.73311	998.89	0.45914	1418.10	1.95124
114.63	0.02330	641.11	0.05181	999.10	1.02170	1439.42	2.58696
123.57	0.00038	646.45	0.00000	1010.43	6.08927	1444.78	0.30602
231.47	0.00000	666.29	0.30931	1020.93	0.10097	1467.42	0.15966
234.15	0.04519	674.00	0.00000	1027.78	5.32180	1474.91	1.68920
249.14	0.04080	685.65	0.00000	1033.22	2.56331	1491.53	1.44150
268.57	0.02824	691.11	2.42401	1035.82	0.15740	1493.65	1.49679
275.98	0.02015	697.03	0.00000	1045.96	0.13786	1500.33	0.23071
304.58	0.17487	714.12	0.04460	1049.84	0.68125	1527.63	3.95926
328.09	0.00000	719.82	0.76634	1065.54	0.65169	1532.14	0.68601
347.60	0.05271	742.07	0.46099	1075.00	2.38392	1544.56	1.82890
349.38	0.00002	752.53	0.23396	1078.18	0.73021	3178.13	0.10171
365.82	0.00000	754.09	0.00000	1158.85	0.13352	3179.61	1.05544
387.07	0.00348	773.21	0.00000	1200.79	0.00773	3186.35	0.38993
396.21	0.02689	780.12	0.25946	1239.80	0.65123	3186.71	0.23408
423.19	0.07023	780.63	0.00000	1265.89	0.06676	3202.53	2.03265
428.03	0.00801	784.68	0.48101	1287.11	0.78104	3203.43	3.04330
438.12	0.00000	786.63	0.91487	1288.98	2.49235	3209.52	2.30810
442.14	0.41303	791.38	0.69382	1316.57	0.14965	3210.18	1.73055
443.60	0.14526	803.98	0.10725	1338.53	0.95741	3241.87	0.49016
463.93	0.45761	806.46	0.18014	1348.99	0.13306	3242.60	0.50222
502.79	0.00000	810.11	0.21023	1354.30	0.05041	3843.23	0.18693
504.59	0.78653	839.27	0.00000	1358.39	0.44971		

The electronic absorption spectrum (TDDFT calculation): ΔE – excitation energy (eV), λ - wave length (nm), *f* – oscillator strength

State	ΔE	λ	*f*	State	ΔE	λ	*f*
$^1A_2$	1.1119	1115.03	0.0000000	$^1B_2$	3.8721	320.20	0.0415318
$^1B_1$	1.2535	989.10	0.0014702	$^1A_2$	3.8765	319.84	0.0000000
$^1A_2$	1.5623	793.60	0.0000000	$^1B_1$	3.9090	317.17	0.0005386
$^1B_2$	1.6207	764.99	0.0038926	$^1B_1$	3.9497	313.91	0.0047865
$^1A_1$	1.6514	750.80	0.0155144	$^1B_2$	4.0167	308.67	0.0032645
$^1B_1$	1.8338	676.09	0.0059916	$^1A_1$	4.0630	305.15	0.0086739
$^1B_2$	1.9496	635.94	0.0000449	$^1B_1$	4.0684	304.75	0.0007448
$^1A_1$	2.2954	540.13	0.0025540	$^1B_2$	4.2063	294.76	0.0007137
$^1A_1$	2.4344	509.29	0.0674682	$^1A_2$	4.2205	293.77	0.0000000
$^1B_2$	2.4736	501.24	0.0269982	$^1B_2$	4.2423	292.25	0.1028789
$^1B_2$	3.1829	389.53	0.3878363	$^1A_1$	4.2977	288.49	0.0439717
$^1A_1$	3.1913	388.51	0.4165013	$^1B_1$	4.2978	288.48	0.0000613
$^1A_2$	3.4211	362.41	0.0000000	$^1B_2$	4.3402	285.67	0.0145182
$^1A_1$	3.7181	333.46	0.0644630	$^1A_1$	4.3982	281.90	0.0181687
$^1A_2$	3.8334	323.43	0.0000000	$^1A_1$	4.4146	280.85	0.0421009

4. Cation [*PAP* $(OH)_2$]$^+$



State	Composition **)	λ
…$(4a_2)^2(32b_2)^2(9b_1)^2(39a_1)^2(10b_1)^2(5a_2)^2(40a_1)^2(11b_1)^2(6a_2)^2(12b_1)^2(7a_2)^2(41a_1)^2(33b_2)^2(8a_2)^0(13b_1)^0(42a_1)^0(14b_1)^0(43a_1)^0(34b_2)^0$…		
1^1A	*50a→51a*(83); *46b→47b*(15)	503(0.135)
2^1B	*50a→47b*(83); *46b→51a*(15)	503(0.134)
17^1B	*46b→51a*(76); *50a→47b*(16)	313(0.757)
18^1A	*46b→47b*(77); *50a→51a*(16)	313(0.756)

Cartesian coordinates (Å):

Atom	X	Y	Z
P1	0.000000000	0.000000000	0.013887590
N2	-1.302710523	0.257478467	1.322320077
N3	1.302710523	-0.257478467	1.322320077
N4	-1.291967890	0.323950711	-1.333691237
N5	1.291967890	-0.323950711	-1.333691237
C6	-2.649292474	0.515708796	1.133355741
C7	2.649292474	-0.515708796	1.133355741
C8	-1.113696949	0.252329424	-2.708608699
C9	1.113696949	-0.252329424	-2.708608699
C10	-2.647733796	0.546574692	-1.147502928
C11	2.647733796	-0.546574692	-1.147502928
C12	-1.117706914	0.222431511	2.692378208
C13	1.117706914	-0.222431511	2.692378208
C14	-3.305608677	0.643495093	2.407989147
C15	3.305608677	-0.643495093	2.407989147
C16	-2.366048985	0.477944982	-3.375385456
C17	2.366048985	-0.477944982	-3.375385456
C18	-3.305671200	0.654182172	-2.419929039
C19	3.305671200	-0.654182172	-2.419929039
C20	-2.367738417	0.467995660	3.361930297
C21	2.367738417	-0.467995660	3.361930297
N22	-3.283983286	0.648232151	-0.005150722
N23	3.283983286	-0.648232151	-0.005150722
N24	0.000000000	0.000000000	-3.352926002
N25	0.000000000	0.000000000	3.339185256
H26	-4.358158039	0.847461225	2.505236744
H27	4.358158039	-0.847461225	2.505236744
H28	-2.465991184	0.481570763	-4.447361326
H29	2.465991184	-0.481570763	-4.447361326
H30	-4.361751762	0.838646588	-2.519631785
H31	4.361751762	-0.838646588	-2.519631785
H32	-2.462112277	0.491039334	4.434072638
H33	2.462112277	-0.491039334	4.434072638
O34	0.426794743	1.601877789	0.057206235
O35	-0.426794743	-1.601877789	0.057206235
H36	-0.101680496	2.159536715	-0.524451543
H37	0.101680496	-2.159536715	-0.524451543

TOTAL ENERGY = -1545.0643754173 Hartree

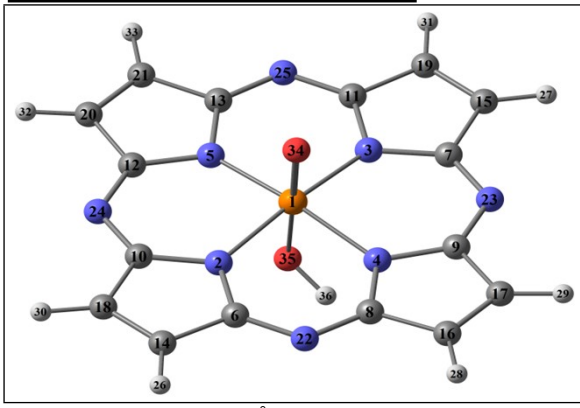
Frequencies (ω_i – cm^{-1}) and IR intensities (A_i – D^2*amu/$Å^2$)

ω_i	A_i	ω_i	A_i	ω_i	A_i	ω_i	A_i
13.68	0.00660	485.45	0.00057	973.67	0.00033	1375.32	0.00143
54.07	0.00221	498.78	1.33922	974.02	0.00000	1421.28	0.00175
109.61	0.07631	500.07	1.21640	974.91	0.00002	1498.09	0.02128
140.71	0.00357	501.96	0.00601	1009.63	0.00992	1499.02	0.01853
140.77	0.01038	654.63	0.00264	1016.36	4.85042	1523.51	0.00105
165.20	0.01395	669.60	0.00223	1017.55	4.68171	1544.03	0.00015
165.84	0.00849	687.16	0.01018	1026.65	0.03066	1550.36	0.28418
233.11	0.40263	687.63	0.00427	1039.65	0.26444	1558.70	0.77293
249.71	0.21087	706.49	0.00222	1042.94	0.36323	1558.80	1.11294
260.27	0.31495	707.73	0.00000	1044.02	0.58395	1573.23	0.09912
275.71	0.02332	737.19	0.35885	1056.45	0.10991	1595.67	0.29601
279.97	0.14060	745.45	0.25971	1061.97	3.18551	1596.39	0.28781
287.61	0.07614	745.72	0.18191	1077.98	0.01326	1606.27	0.02538
292.01	0.23518	748.02	0.36687	1090.23	1.81999	1642.85	0.02328
313.17	0.45799	748.07	0.34091	1090.34	1.99587	3251.36	0.05043
343.89	0.00420	752.64	0.00213	1093.14	0.29696	3251.55	0.08664
354.00	0.00336	763.92	0.00946	1093.83	0.40598	3252.74	0.12094
354.46	0.08711	802.93	0.03081	1187.00	0.03413	3252.87	0.11762
393.07	0.01888	803.42	0.02874	1187.75	0.03527	3266.87	0.29105
396.16	0.06770	808.52	0.00158	1191.84	0.00634	3266.91	0.26481
398.57	0.00006	809.81	0.00000	1213.72	0.00041	3268.49	0.19563
438.75	0.01726	846.74	0.01118	1301.45	0.07807	3268.52	0.22895
439.13	0.00159	849.43	0.27465	1303.13	0.05634	3811.18	0.23901
461.40	0.00110	849.48	0.00003	1324.39	0.00149	3811.37	2.21576
462.95	0.27323	850.99	1.73293	1330.26	0.00028		
470.62	0.00309	884.16	9.27286	1359.61	0.47723		
473.91	0.02678	972.85	0.00028	1360.40	0.49912		

The electronic absorption spectrum (TDDFT calculation): ΔE – excitation energy (eV), λ - wave length (nm), *f* – oscillator strength

State	ΔE	λ	*f*	State	ΔE	λ	*f*
^{1}A	2.4640	503.18	0.1352778	^{1}A	3.8222	324.38	0.0032042
^{1}B	2.4655	502.87	0.1339845	^{1}B	3.9621	312.93	0.7569650
^{1}B	3.2468	381.87	0.0000397	^{1}A	3.9622	312.92	0.7564006
^{1}A	3.2567	380.71	0.0000263	^{1}B	4.2145	294.18	0.0000774
^{1}B	3.3935	365.36	0.0006653	^{1}A	4.5016	275.42	0.0009070
^{1}A	3.4683	357.48	0.0006906	^{1}B	4.5073	275.07	0.0010407
^{1}B	3.4768	356.60	0.0003992	^{1}B	4.7989	258.36	0.0006425
^{1}A	3.4842	355.85	0.0012972	^{1}A	4.8046	258.05	0.0000039
^{1}B	3.5442	349.82	0.0058864	^{1}A	4.9058	252.73	0.0013363
^{1}A	3.5517	349.08	0.0048219	^{1}B	4.9583	250.05	0.0047760
^{1}B	3.7739	328.53	0.0017313	^{1}B	5.1463	240.92	0.0003522
^{1}A	3.7850	327.56	0.0014183	^{1}A	5.2955	234.13	0.0017756
^{1}B	3.7868	327.41	0.0038340	^{1}A	5.3076	233.60	0.0298025
^{1}B	3.7934	326.84	0.0076493	^{1}A	5.3164	233.21	0.0035445
^{1}A	3.8162	324.89	0.0015930	^{1}B	5.3337	232.45	0.0327787

5. Porphyrazine [*PA*P(=O)(OH)]



State	Composition **)	λ
…(53a′)²(54a′)²(36a″)²(55a′)²(37a″)²(56a′)²(57a′)²(38a″)²(39a″)²(58a′)⁰(40a″)⁰(41a″)⁰(59a′)⁰…		
4^1A′	*39a″→40a″*(82); *56a′→58a′*(16)	497(0.150)
5^1A″	*39a″→58a′*(83); *56a′→40a″*(15)	495(0.155)
9^1A′	*56a′→58a′*(41); *55a′→58a′*(36); *54a′→58a′*(11)	358(0.092)
12^1A″	*55a′→40a″*(28); *56a′→40a″*(25); *54a′→40a″*(21); *36a″→58a′*(17)	349(0.082)
19^1A′	*38a″→41a″*(54); *54a′→58a′*(35)	310(0.084)
21^1A″	*54a′→40a″*(46); *57a′→41a″*(34); *56a′→40a″*(10)	308(0.173)
24^1A′	*38a″→41a″*(40); *54a′→58a′*(26); *56a′→58a′*(20)	300(0.490)
25^1A″	*57a′→41a″*(61); *56a′→40a″*(16); *54a′→40a″*(14)	298(0.400)

Cartesian coordinates (Å):

Atom	X	Y	Z
P1	-0.020126825	0.069133058	0.000000000
N2	0.000906918	-0.048414833	1.920495241
N3	0.000906918	-0.048414833	-1.920495241
N4	1.914671128	-0.117484230	0.000000000
N5	-1.900866823	-0.043025752	0.000000000
C6	1.103649785	-0.017740971	2.732522608
C7	1.103649785	-0.017740971	-2.732522608
C8	2.731507893	-0.042272078	1.103441424
C9	2.731507893	-0.042272078	-1.103441424
C10	-1.096712089	-0.016763141	2.736295680
C11	-1.096712089	-0.016763141	-2.736295680
C12	-2.716403374	-0.017600193	1.103457576
C13	-2.716403374	-0.017600193	-1.103457576
C14	0.679337097	0.025109199	4.117673358
C15	0.679337097	0.025109199	-4.117673358
C16	4.109462561	0.035769999	0.675613045
C17	4.109462561	0.035769999	-0.675613045
C18	-0.669523549	0.024277995	4.120204083
C19	-0.669523549	0.024277995	-4.120204083
C20	-4.097510109	0.015134606	0.674593405
C21	-4.097510109	0.015134606	-0.674593405
N22	2.370409754	-0.022472869	2.370749755
N23	2.370409754	-0.022472869	-2.370749755
N24	-2.362641821	-0.014035763	2.371857582
N25	-2.362641821	-0.014035763	-2.371857582
H26	1.367732975	0.053690274	4.944865233
H27	1.367732975	0.053690274	-4.944865233
H28	4.937598885	0.093915313	1.361017992
H29	4.937598885	0.093915313	-1.361017992
H30	-1.354864190	0.053374673	4.949880776
H31	-1.354864190	0.053374673	-4.949880776
H32	-4.925629145	0.039019886	1.361834732
H33	-4.925629145	0.039019886	-1.361834732
O34	0.036372784	1.581329450	0.000000000
O35	-0.113043158	-1.627493931	0.000000000
H36	0.767545790	-2.015034238	0.000000000

TOTAL ENERGY = -1544.6565990413 Hartree

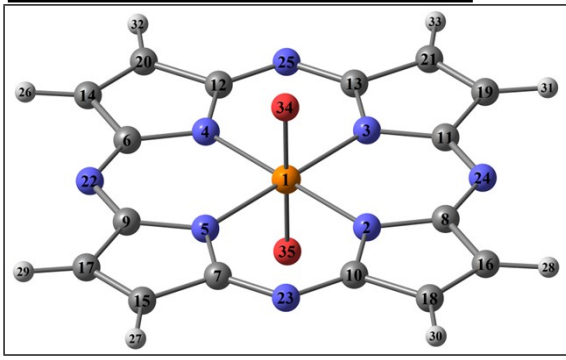
Frequencies (ω_i – cm^{-1}) and IR intensities (A_i – D^2*amu/$Å^2$)

ω_i	A_i	ω_i	A_i	ω_i	A_i	ω_i	A_i
55.02	0.00488	483.14	1.43827	946.48	0.00117	1361.00	0.00017
59.25	0.00001	486.69	1.50975	948.33	0.00025	1362.68	0.24870
99.47	0.10519	494.73	0.04426	948.85	0.00001	1364.42	0.28961
133.11	0.00730	496.95	0.00166	1005.67	4.66315	1418.91	0.13533
134.55	0.02162	653.24	0.64709	1006.73	4.59634	1487.79	0.10265
179.89	0.00149	674.07	0.02204	1014.59	0.02592	1494.69	0.05383
181.39	0.00448	690.41	0.04074	1017.74	0.21854	1507.96	0.00669
216.20	0.18192	690.80	0.00446	1025.24	0.37757	1523.02	0.00294
236.88	0.00530	709.61	0.00040	1042.89	0.00016	1537.97	0.16477
267.96	0.00922	709.94	0.01343	1044.47	0.03541	1546.31	1.27918
269.13	0.05512	735.10	0.81974	1075.77	0.06782	1549.21	0.21571
269.26	0.09598	745.91	0.03485	1076.77	1.80440	1552.70	1.28909
301.92	0.00078	746.50	0.12551	1081.37	1.18220	1586.43	1.07925
315.47	0.07241	748.19	0.73062	1081.41	2.06422	1589.54	1.21025
320.97	0.37410	751.51	0.85003	1082.39	1.25277	1599.69	0.03806
321.97	0.37810	754.36	0.00906	1085.74	1.70372	1617.36	0.00536
343.86	0.00842	763.71	0.00347	1130.77	1.59312	3243.67	0.00052
372.86	0.01330	800.90	0.22312	1190.03	0.03149	3243.91	0.00217
403.13	0.02379	803.16	0.16677	1192.38	0.02466	3244.17	0.00712
404.87	0.00049	806.35	0.01219	1206.83	0.00042	3245.71	0.00431
420.88	0.21469	816.24	0.00016	1214.14	0.00027	3261.45	0.00911
424.62	0.13582	826.06	0.00690	1298.95	0.39419	3261.84	0.02016
446.24	0.01008	831.09	0.00109	1303.94	0.36755	3262.08	0.00001
452.30	0.00086	831.83	0.04056	1335.46	0.00105	3263.50	0.00552
479.56	0.01794	837.99	3.87184	1340.85	0.01298	3827.83	0.55913
480.32	0.01954	946.12	0.00000				

The electronic absorption spectrum (TDDFT calculation): ΔE – excitation energy (eV), λ - wave length (nm), *f* – oscillator strength

State	ΔE	λ	*f*	State	ΔE	λ	*f*
^{1}A"	2.1541	575.56	0.0000087	^{1}A'	3.8240	324.23	0.0033791
^{1}A"	2.2301	555.96	0.0000033	^{1}A"	3.9356	315.03	0.0038712
^{1}A'	2.2494	551.19	0.0000562	^{1}A'	3.9555	313.45	0.0001123
^{1}A'	2.4963	496.68	0.1503304	^{1}A'	3.9944	310.39	0.0837578
^{1}A"	2.5043	495.08	0.1553198	^{1}A"	3.9956	310.30	0.0048147
^{1}A'	2.6718	464.04	0.0058752	^{1}A"	4.0204	308.39	0.1732007
^{1}A"	3.2759	378.47	0.0000018	^{1}A'	4.0245	308.07	0.0013928
^{1}A'	3.4221	362.31	0.0023060	^{1}A'	4.0892	303.20	0.0065186
^{1}A'	3.4648	357.84	0.0917941	^{1}A'	4.1282	300.34	0.4904777
^{1}A"	3.5297	351.26	0.0158092	^{1}A"	4.1544	298.44	0.4002973
^{1}A'	3.5341	350.83	0.0002237	^{1}A'	4.4813	276.67	0.0010200
^{1}A"	3.5476	349.48	0.0819127	^{1}A"	4.4828	276.58	0.0044398
^{1}A"	3.6858	336.38	0.0336791	^{1}A"	4.8406	256.13	0.0000012
^{1}A"	3.7436	331.19	0.0002482	^{1}A"	4.8742	254.37	0.0012547
^{1}A'	3.7496	330.66	0.0373690	^{1}A'	4.8752	254.31	0.0015215

6. Porphyrazine anion [*PA*P(O)(O-)]



State	Composition **)	λ
…$(18e_u)^4(16a_{1g})^2(6a_{2u})^2(8b_{2g})^2(2b_{2u})^2(7a_{2u})^2(4e_g)^4(1a_{1u})^2(19e_u)^4(5e_g)^0(2b_{1u})^0(3b_{2u})^0(17a_{1g})^0(6e_g)^0$…		
8^1E_u	$1a_{1u}\rightarrow 5e_g$(77); $7a_{2u}\rightarrow 5e_g$(19)	494(0.280)
11^1E_u	$7a_{2u}\rightarrow 5e_g$(52); $4e_g\rightarrow 2b_{1u}$(18); $1a_{1u}\rightarrow 5e_g$(11); $2b_{2u}\rightarrow 5e_g$(11)	374(0.244)
13^1E_u	$4e_g\rightarrow 2b_{1u}$(65); $2b_{2u}\rightarrow 5e_g$(24)	333(0.138)
14^1E_u	$2b_{2u}\rightarrow 5e_g$(61); $7a_{2u}\rightarrow 5e_g$(15); $4e_g\rightarrow 2b_{1u}$(11)	330(0.220)
21^1E_u	$6a_{2u}\rightarrow 5e_g$(74)	293(0.822)

Cartesian coordinates (Å):

Atom	X	Y	Z
P1	0.000000000	0.000000000	0.000000000
N2	-1.952326463	0.000000000	0.000000000
N3	0.000000000	-1.952326463	0.000000000
N4	1.952326463	0.000000000	0.000000000
N5	0.000000000	1.952326463	0.000000000
C6	2.747640173	1.103297665	0.000000000
C7	-1.103297665	2.747640173	0.000000000
C8	-2.747640173	-1.103297665	0.000000000
C9	1.103297665	2.747640173	0.000000000
C10	-2.747640173	1.103297665	0.000000000
C11	-1.103297665	-2.747640173	0.000000000
C12	2.747640173	-1.103297665	0.000000000
C13	1.103297665	-2.747640173	0.000000000
C14	4.140528278	0.675643897	0.000000000
C15	-0.675643897	4.140528278	0.000000000
C16	-4.140528278	-0.675643897	0.000000000
C17	0.675643897	4.140528278	0.000000000
C18	-4.140528278	0.675643897	0.000000000
C19	-0.675643897	-4.140528278	0.000000000
C20	4.140528278	-0.675643897	0.000000000
C21	0.675643897	-4.140528278	0.000000000
N22	2.374882032	2.374882032	0.000000000
N23	-2.374882032	2.374882032	0.000000000
N24	-2.374882032	-2.374882032	0.000000000
N25	2.374882032	-2.374882032	0.000000000
H26	4.974134669	1.358406283	0.000000000
H27	-1.358406283	4.974134669	0.000000000
H28	-4.974134669	-1.358406283	0.000000000
H29	1.358406283	4.974134669	0.000000000
H30	-4.974134669	1.358406283	0.000000000
H31	-1.358406283	-4.974134669	0.000000000
H32	4.974134669	-1.358406283	0.000000000
H33	1.358406283	-4.974134669	0.000000000
O34	0.000000000	0.000000000	1.538055922
O35	0.000000000	0.000000000	-1.538055922

TOTAL ENERGY = -1544.1058420340 Hartree

Frequencies (ω_i – cm^{-1}) and IR intensities (A_i – D^2*amu/Å^2)

ω_i	A_i	ω_i	A_i	ω_i	A_i	ω_i	A_i
61.57	0.00000	483.99	0.00000	906.47	0.00000	1344.34	0.00000
78.20	0.17204	488.27	0.00000	908.44	0.00000	1359.29	0.11215
80.52	0.00000	488.27	0.00000	908.44	0.00000	1359.29	0.11215
125.20	0.00000	505.64	0.00000	909.04	0.00000	1394.03	0.00000
125.20	0.00000	672.06	0.00000	993.39	4.63143	1469.67	0.18031
196.46	0.00000	686.46	0.00000	993.39	4.63143	1469.67	0.18031
196.46	0.00000	686.46	0.00000	998.74	0.00000	1482.16	0.00000
221.67	0.00000	704.38	0.00000	1008.40	0.00000	1499.59	0.00000
223.54	0.00000	704.64	0.00000	1010.04	0.00000	1504.62	0.00000
237.66	0.06518	724.36	1.75537	1035.23	0.24829	1517.51	0.00000
237.66	0.06518	738.04	0.00000	1035.23	0.24829	1535.31	1.72703
287.54	0.36991	738.04	0.00000	1066.71	2.00340	1535.31	1.72703
287.54	0.36991	746.45	1.38762	1066.71	2.00340	1572.61	2.97161
314.34	0.00000	746.45	1.38762	1066.97	0.00000	1572.61	2.97161
321.07	0.06544	750.47	0.00000	1068.52	0.00000	1585.48	0.00000
336.02	0.00000	757.79	0.00000	1068.83	0.00000	1586.59	0.00000
349.58	0.00000	799.06	0.28031	1136.00	2.12067	3223.22	0.00000
406.33	0.41296	799.06	0.28031	1196.76	0.21671	3223.36	0.00000
406.33	0.41296	800.77	0.00000	1196.76	0.21671	3223.47	0.10441
408.93	0.16924	801.64	0.00000	1205.91	0.00000	3223.47	0.10441
410.22	0.00000	812.15	0.00000	1224.84	0.00000	3243.94	1.07993
410.22	0.00000	812.15	0.00000	1288.39	0.57259	3243.94	1.07993
441.81	0.00000	817.37	0.00000	1288.39	0.57259	3244.02	0.00000
483.80	1.46469	821.82	2.68502	1339.95	0.00000	3244.40	0.00000
483.80	1.46469	851.24	0.00000	1343.99	0.00000		

The electronic absorption spectrum (TDDFT calculation): ΔE – excitation energy (eV), λ - wave length (nm), *f* – oscillator strength

State	ΔE	λ	*f*	State	ΔE	λ	*f*
$^1A_{1u}$	1.4385	861.92	0.0000000	^1E_g	3.5849	345.85	0.0000000
$^1A_{1u}$	1.4862	834.22	0.0000000	^1E_u	3.7263	332.73	0.0691578
$^1A_{2u}$	1.5006	826.23	0.0000000	^1E_u	3.7544	330.23	0.1095530
$^1A_{2u}$	1.9403	639.01	0.0096253	$^1B_{1g}$	3.9366	314.95	0.0000000
$^1A_{2g}$	1.9884	623.53	0.0000000	^1E_g	3.9462	314.19	0.0000000
$^1A_{2g}$	2.0561	603.00	0.0000000	$^1A_{2u}$	3.9639	312.78	0.0012813
$^1A_{1g}$	2.1048	589.05	0.0000000	$^1B_{1u}$	3.9863	311.03	0.0000000
^1E_u	2.5096	494.04	0.1401842	$^1A_{2u}$	4.0746	304.29	0.0000000
$^1A_{1g}$	2.5508	486.06	0.0000000	$^1A_{1u}$	4.0769	304.12	0.0000000
^1E_g	3.0834	402.10	0.0000000	^1E_u	4.2382	292.54	0.4114700
^1E_u	3.3130	374.23	0.1224442	$^1B_{2g}$	4.2458	292.02	0.0000000