Synthesis of Tetrabenzotriazacorrole μ-Oxo Dimer and Investigation of Its Stacking Effect

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Supporting information

Table of Contents

General Comments

Unless otherwise noted, solvents and reagents were purchased from Tokyo Kasei Co. and Wako Chemicals Co. and were used after appropriate purification (distillation or recrystallization).

Electronic absorption spectra were recorded on a JASCO V-570 spectrophotometer. Magnetic circular dichroism (MCD) spectra were obtained on a JASCO J-725 spectrodichrometer equipped with a JASCO electromagnet capable of producing magnetic fields of up to 1.03 T (1 T = 1 tesla) with both parallel and antiparallel fields. The magnitudes were expressed in terms of molar ellipticity per tesla ($[\theta]_M$ / deg $dm^3mol^{-1}cm^{-1}T^{-1}$). NMR spectra were obtained on a Bruker AVANCE III 500 spectrometer. Unless otherwise noted, samples were recorded in $CDCl_3$. Chemical shifts are expressed in δ (ppm) values, and coupling constants are expressed in hertz (Hz). ^{1}H-NMR spectra were referenced to the residual solvent as an internal standard. ^{31}P-NMR spectra were referenced to external 85% H_3PO_4 solution (0.0 ppm). The following abbreviations are used: s = singlet, d = doublet, t = triplet, and m = multiplet. High-resolution mass spectra (HRMS) were recorded on a Bruker Daltonics Apex-III spectrometer. Cyclic voltammetry (CV) measurements were recorded with a Hokuto Denko HZ5000 potentiostat under a nitrogen atmosphere in solutions with 0.1 M of tetrabutylammonium perchlorate (TBAP) as supporting electrolyte. Measurements were made with a glassy carbon (GC) electrode (area = 0.07 cm^2), an Ag/AgCl reference electrode, and a Pt wire counter electrode. The concentration of the solution was fixed at 1.0 mM and the sweep rates were set to 100 mV/s. Singlet oxygen quantum yields (ΦΔ) were determined in $CHCl_3$ using a steady-state method[i] with ZnPc[ii] (**Std-ZnPc**) as reference. 1,3-diphenylisobenzofuran (DPBF) was used as the chemical quencher for single oxygen in $CHCl_3$. Equation (1) was employed for the calculations:

$$\Phi_\Delta = \Phi_\Delta^{Std} \frac{R \bullet I_{abs}^{Std}}{R^{Std} \bullet I_{abs}} \qquad (1)$$

where $\Phi^{Std}\Delta$ is the singlet oxygen quantum yield for the standard ZnPc (**Std-ZnPc**) ($\Phi^{Std}\Delta$ = 0.73 in $CHCl_3$). R and R_{Std} are the DPBF photobleaching rates in the presence of the samples and standard, respectively. I_{abs} and I^{Std}_{abs} are the rates of light absorption (>600 nm) by the samples and standard, respectively.

Crystallographic Data Collection

A prism shaped and dark green single crystal of **3** 0.20 × 0.15 × 0.10 mm, was selected for measurements. The diffraction data were collected using a RIGAKU R-AXIS RAPID with Cu*K*α radiation (λ = 1.54178 Å) at –183°C. The structures were solved by a direct method (SIR2004)[iii] and refined using a full-matrix least square technique (SHELXL-97).[iv] All non-hydrogen atoms were refined anisotropically. Positions of all hydrogen atoms were calculated geometrically, and refined by applying riding models. The peripheral phenoxy substituents were severely disordered despite the low measurement temperature. Therefore, the structure was refined under thermally and positionally restrained conditions, using DFIX, FLAT, SIMU, ISOR, and DELU commands. After the above-mentioned refinement, one electron density with 1.01 was still observed, which is not an essential problem in the structural analysis. CCDC-985980 contains the supplementary crystallographic data for **3**. Its data can be obtained free of charge from Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif.

Additional Experimental and Computational Results

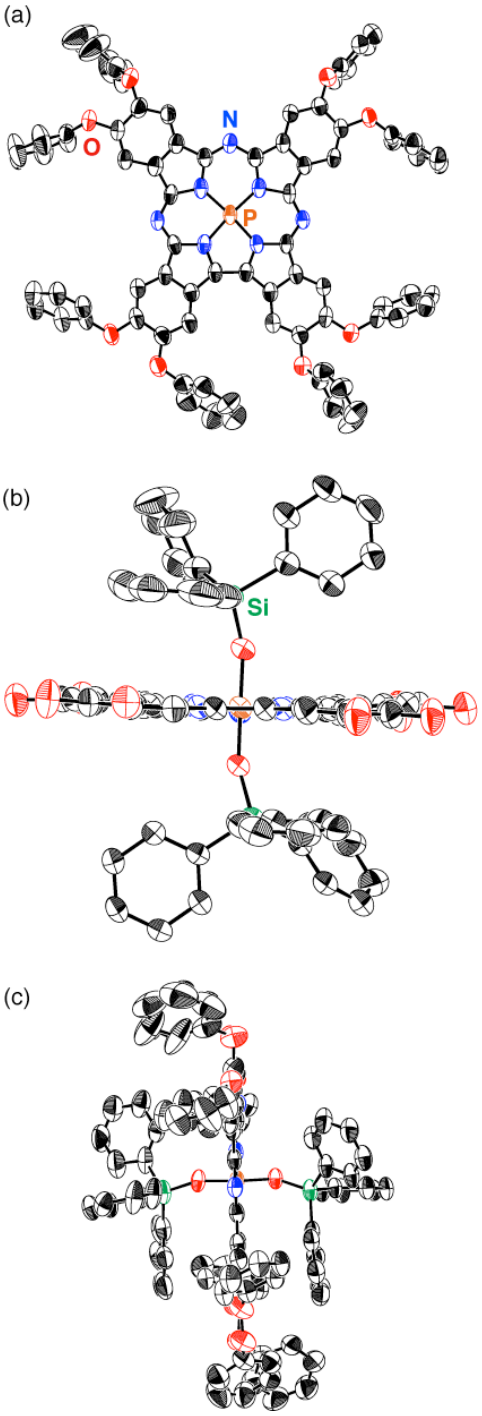


Figure S1. X-ray crystal structure of **3**. The thermal ellipsoids were scaled to the 50% probability level. H atoms have been omitted for clarity. (a) Top view (axial ligands have been omitted); (b) front view (peripheral phenyl groups have been omitted); (c) side view.

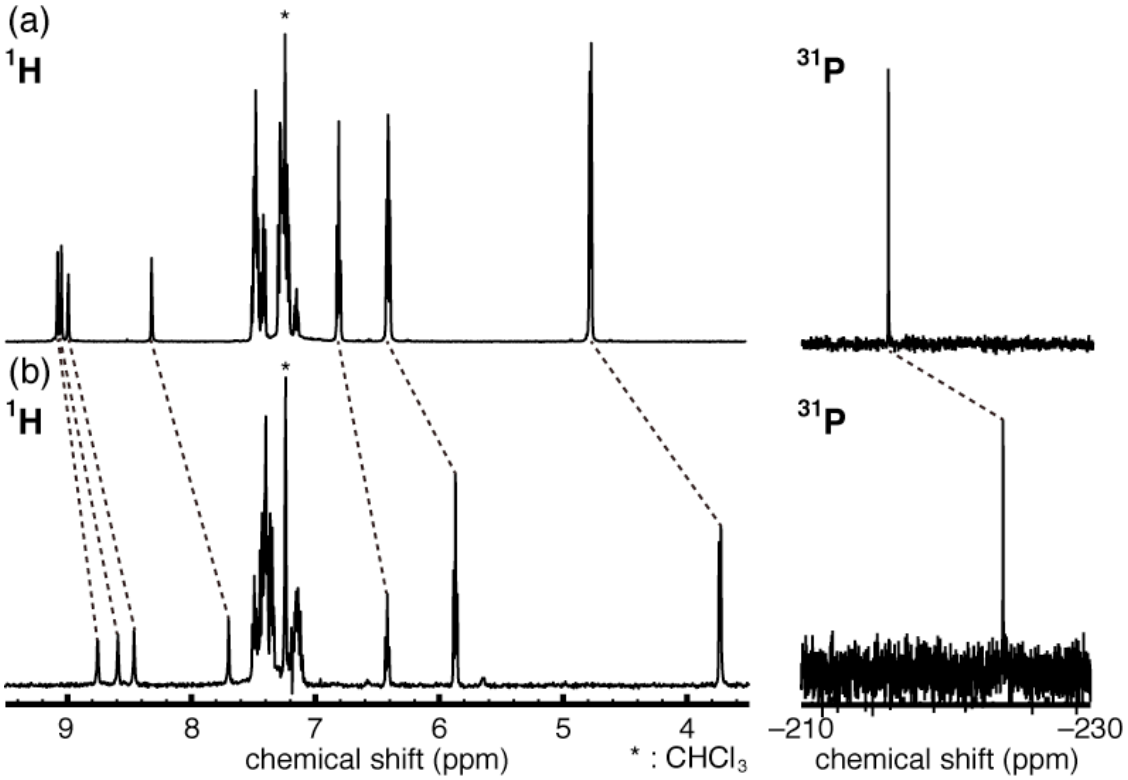


Figure S2. ^{1}H and ^{31}P NMR spectra of (a) monomer **3** and (b) dimer **4** in $CDCl_3$.

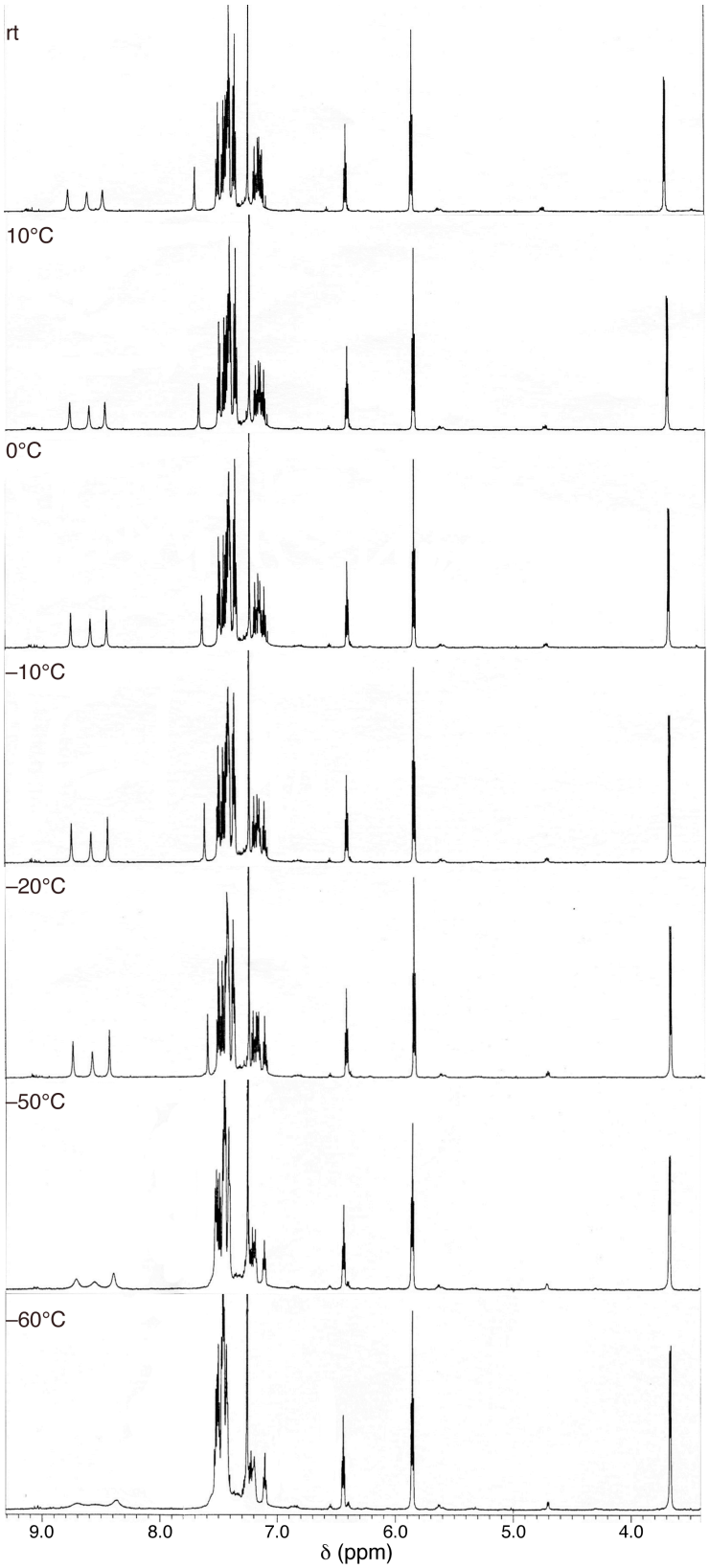


Figure S3. ^{1}H VT-NMR of **4** in $CHCl_3$.

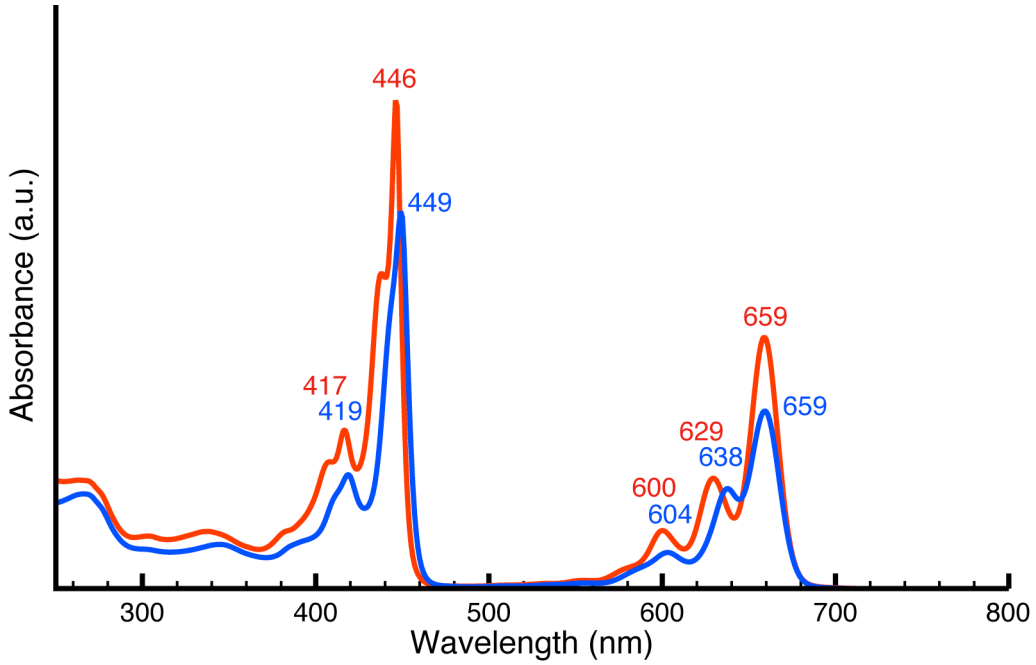


Figure S4. UV-vis spectra of **2** (red) and **3** (blue) in THF. Concentration ~ 1 x 10^{-5} M and concentration of each sample is different for clarity.

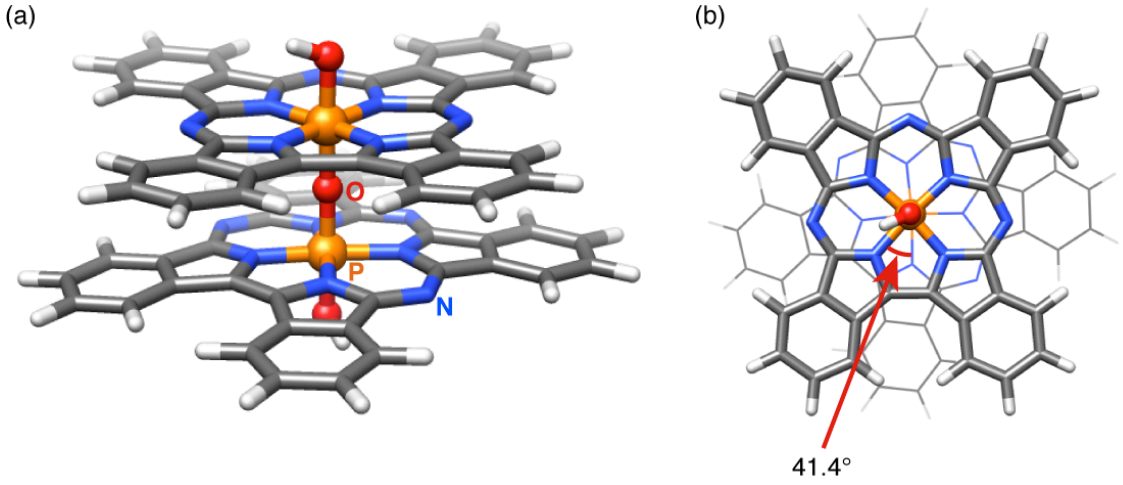


Figure S5. Optimized structure of μ-oxo dimer **4'**. (a) side view; (b) top view.

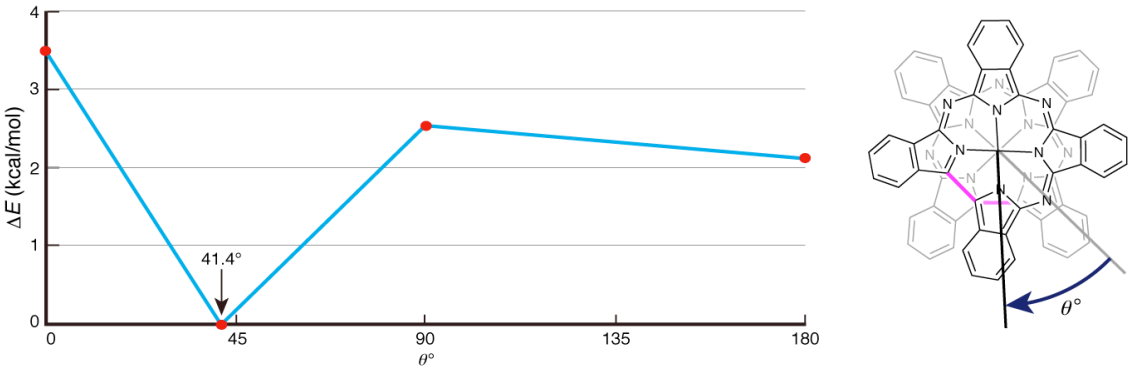


Figure S6. Plot of relative all-electron energies versus torsion angle (θ) of TBC dimer.

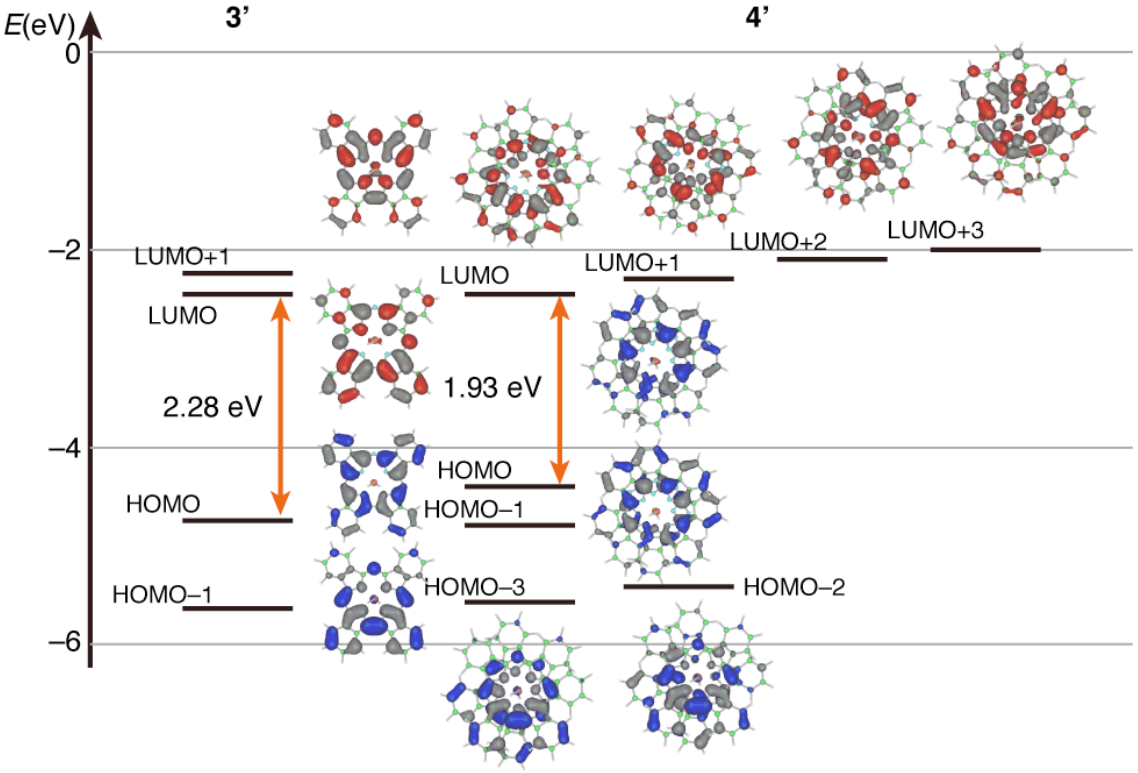


Figure S7. Partial molecular energy diagrams and orbitals of monomer **3'** (left) and **4'** (right). Blue and red plots indicate occupied and unoccupied MOs, respectively.

Table S1. Calculated excited wavelength (λ) and oscillator strengths (*f*) for components of selected transition energies.

Compound	λ (nm)	*f*	Composition (%)[a]
3'	594.5	0.29	H–>L (88%), H-1–>L+1 (12%)
	563.5	0.12	H–>L+1 (82%), H-1–>L (17%)
	398.6	0.76	H-1–>L (80%), H–>L+1 (17%)
	390.4	0.65	H-1–>L+1 (86%), H–>L (12%)
4'	808.6	0.01	H–>L (97%)
	582.8	0.31	H-1–>L (46%), H–>L+2 (33%), H-3–>L+1 (7%), H-2–>L+3 (6%), H–>L+1 (5%)
	564.7	0.15	H-1–>L+1 (58%), H–>L+3 (20%), H-3–>L (12%), H-2–>L+2 (6%)
	383.5	0.86	H-2–>L+3 (44%), H-3–>L+1 (24%), H-1–>L (7%), H-3–>L+2 (6%), H–>L+2 (6%)
	382.9	0.73	H–>L+5 (29%), H-2–>L+2 (28%), H-3–>L (12%), H-3–>L+3 (9%), H-1–>L+1 (7%), H–>L+3 (5%)

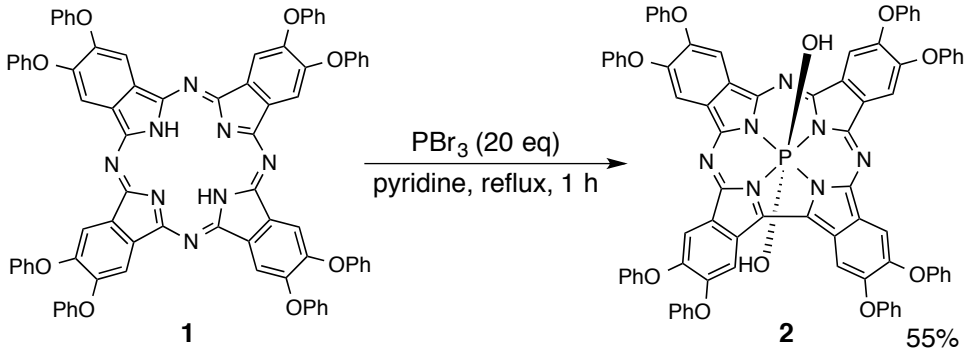
[a]H-m, H, L, and L+n denote HOMO-m, HOMO, LUMO, and LUMO+n, respectively.

Full Experimental Procedures

Materials

Free-base Pc **1**[v] was synthesized according to published procedures.

α-(PhO)$_8$TBCP(OH)$_2$ (2)



1 (200 mg, 0.16 mmol) was dissolved in 3 ml of pyridine. PBr_3 (0.30 mL, 3.2 mmol) was added to the solution and the mixture was stirred under reflux for 2 h. After the mixture was cooled to room temperature, poured into water (150 mL) and extracted with $CHCl_3$ (150 mL). The organic layer was washed with a 2% solution of hydrochloric acid (150 mL), water (150 mL) and brine (150 mL), dried over $MgSO_4$, filetered and concentrated *in vacuo*. The product was purified by alumina gel chromatography (THF), followed by recrystallization from THF/n-hexane. The title compound was obtained (129 mg, 62%) as green powder. (202 mg, 74%)

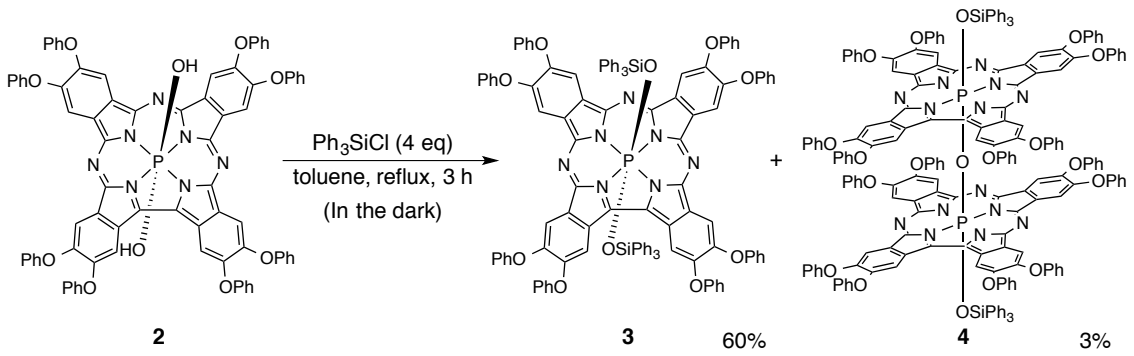
500 MHz ^{1}H NMR (pyridine-d_5) δ (ppm): 9.57 (s, 2H), 9.52 (s, 2H), 9.48 (s, 2H), 9.17 (s, 2H), 7.44-7.40 (m, 16H), 7.37-7.33 (m, 16H), 7.17-7.11 (m, 8H). 200 MHz ^{31}P NMR (pyridine-d_5) δ (ppm): –200 (s).

HRMS-MALDI (*m/z*) Calcd for $C_{80}H_{50}N_7O_{10}P$ $[M]^+$: 1299.3352. Found: 1299.3351.

UV-vis (THF) λ_{max} nm (ε x 10^{-4}): 659 (12), 629 (5.3), 600 (2.8), 446 (22), 438 (15), 417 (7.6).

Φ_{FL} = 0.22, $\lambda_{FL,\,max}$ ($CHCl_3$): 671 nm.

α-(PhO)$_8$TBCP(OH)$_2$ (3) and TBC μ–oxo dimer (4)



2 (30 mg, 23 μmol) and triphenylsilyl chloride (25 mg, 84 μmol) were dissolved in 1 mL of dehydrated toluene and the mixture was stirred under reflux for 3 h in the dark. After the solvent was removed, the residue was purified by alumina gel chromatography ($CHCl_3$), followed by size exclusion chromatography (Bio-Beads S-X1 with toluene). **3** (25 mg, 60%) and **4** (2.4 mg, 3.4%) were obtained as green powder.

3: 500 MHz ^{1}H NMR ($CDCl_3$) δ (ppm): 9.11 (s, 2H), 9.08 (s, 2H), 9.02 (s, 2H), 8.34 (s, 2H), 7.53-7.42 (m, 16H), 7.31-7.17 (m, 24H), 6.82 (tt, 6H, *J* =1.25, 7.45 Hz), 6.42(m, 12H), 4.78(dd, 12H, 1.25, 7.80 Hz). 200 MHz ^{31}P NMR (pyridine-d_5) δ (ppm): –216 (s).

HRMS-MALDI (*m/z*) Calcd for $C_{116}H_{78}N_7O_{10}PSi_2$ $[M]^+$: 1815.5081. Found: 1815.5080.

UV-vis ($CHCl_3$) λ_{max} nm (ε x 10^{-4}): 662 (10), 639 (5.4), 605 (2.1), 451 (21), 420 (6.5).

Φ_{FL} = 0.21, $\lambda_{FL,\,max}$ ($CHCl_3$): 671 nm.

4: 500 MHz ^{1}H NMR ($CDCl_3$) δ (ppm): 8.76 (s, 4H), 8.59 (s, 4H), 8.46 (s, 4H), 7.70 (s, 4H), 7.51-7.28 (m, 64H), 7.22-7.10 (m, 16H), 6.42 (t, 12H, *J* = 7.45 Hz), 5.87(m, 24H), 3.73(d, 24H, 6.65 Hz). 200 MHz ^{31}P NMR (pyridine-d_5) δ (ppm): –224 (s).

HRMS-MALDI (*m/z*) Calcd for $C_{196}H_{126}N_{14}O_{19}P_2Si_2$ $[M]^+$: 3096.8332. Found: 3096.8363.

UV-vis ($CHCl_3$) λ_{max} nm (ε x 10^{-4}): 635 (9.9), 425 (14).

Full Computational Details

Computational Details

Geometry optimization for all molecules was performed at the DFT level, by means of the hybrid Becke3LYP[vi] (B3LYP) functional as implemented in Gaussian 2009.[vii] The 6-31G* basis set was used for the all atoms. After the geometry optimization, the time-dependent (TD) DFT calculations[viii] were performed to evaluate the stick absorption spectrum employing with the same theory and basis set. All stationary points were optimized without any symmetry assumptions and characterized by normal coordinate analysis at the same level of the theory (the number of imaginary frequency, Nimag, 0).

Cartesian Coordinates and Total Electron Energies

TBC Monomer (3')

SCF Done: E(RB3LYP) = -2105.38080364 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.325132	3.422888	0.016179
2	6	0	3.350992	2.454183	0.012864
3	6	0	2.719354	1.157436	0.012709
4	7	0	1.343280	1.354475	0.024767
5	6	0	1.061256	2.723142	0.019875
6	7	0	-0.126697	3.311376	0.027847
7	6	0	-1.225336	2.569006	0.039113
8	6	0	-2.606832	2.994477	0.010810
9	6	0	-3.425875	1.824618	0.007180
10	6	0	-2.529382	0.697102	0.035848
11	7	0	-1.240470	1.201520	0.086271
12	6	0	-2.529297	-0.697393	-0.035888
13	6	0	-3.425618	-1.825030	-0.007215
14	6	0	-2.606437	-2.994766	-0.010628
15	6	0	-1.224984	-2.569149	-0.038690
16	7	0	-1.240263	-1.201638	-0.086052
17	7	0	-0.126264	-3.311401	-0.027351
18	6	0	1.061634	-2.723034	-0.019566
19	6	0	2.325608	-3.422639	-0.016116
20	6	0	3.351356	-2.453785	-0.013112
21	6	0	2.719497	-1.157122	-0.012933
22	7	0	1.343489	-1.354358	-0.024524
23	7	0	3.356329	0.000205	-0.000205
24	6	0	4.700225	-2.830722	-0.009627
25	6	0	4.993249	-4.188895	-0.009473
26	6	0	3.966102	-5.159434	-0.012657
27	6	0	2.626323	-4.790524	-0.016528
28	6	0	2.625667	4.790825	0.016780
29	6	0	3.965387	5.159912	0.012681
30	6	0	4.992670	4.189503	0.009143
31	6	0	4.699826	2.831299	0.009206
32	6	0	-4.823286	1.952803	-0.032305
33	6	0	-5.373199	3.228067	-0.062484
34	6	0	-4.557768	4.379919	-0.055719
35	6	0	-3.173511	4.274058	-0.020094
36	6	0	-3.172947	-4.274427	0.020220
37	6	0	-4.557198	-4.380467	0.055552

38	6	0	-5.372782	-3.228719	0.062017
39	6	0	-4.823028	-1.953386	0.031863
40	15	0	0.124049	-0.000008	0.000061
41	8	0	0.184682	0.139725	-1.690047
42	8	0	0.184626	-0.139670	1.690231
43	1	0	5.482117	-2.078046	-0.006852
44	1	0	6.029718	-4.515034	-0.006619
45	1	0	4.233145	-6.212701	-0.011523
46	1	0	1.831179	-5.529240	-0.018070
47	1	0	1.830414	5.529422	0.018584
48	1	0	4.232294	6.213214	0.011651
49	1	0	6.029093	4.515785	0.006090
50	1	0	5.481801	2.078711	0.006173
51	1	0	-5.467932	1.079940	-0.041545
52	1	0	-6.453191	3.342209	-0.092908
53	1	0	-5.023526	5.361012	-0.080337
54	1	0	-2.535805	5.152535	-0.018795
55	1	0	-2.535121	-5.152814	0.019173
56	1	0	-5.022827	-5.361620	0.080196
57	1	0	-6.452768	-3.342995	0.092150
58	1	0	-5.467785	-1.080603	0.040865
59	1	0	-0.256326	-0.613805	-2.114433
60	1	0	-0.256274	0.613983	2.114519

TD–DFT output

HOMO**: 145**, LUMO**: 146**

Excited State 1: Singlet-A 2.0855 eV 594.50 nm f=0.2880 <S**2>=0.000
144 ->147 -0.24334
145 ->146 0.66432
This state for optimization and/or second-order correction.
Total Energy, E(TD-HF/TD-KS) = -2105.30416182
Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: Singlet-A 2.2004 eV 563.47 nm f=0.1228 <S**2>=0.000
144 ->146 0.29300
145 ->147 0.63912

Excited State 3: Singlet-A 3.1106 eV 398.58 nm f=0.7619 <S**2>=0.000
144 ->146 0.63097
145 ->147 -0.28919

Excited State 4: Singlet-A 3.1755 eV 390.44 nm f=0.6465 <S**2>=0.000
144 ->147 0.65451
145 ->146 0.24176

Excited State 5: Singlet-A 3.3659 eV 368.35 nm f=0.0027 <S**2>=0.000
145 ->149 0.69588

Excited State 6: Singlet-A 3.4131 eV 363.26 nm f=0.0274 <S**2>=0.000
143 ->146 -0.12498
145 ->148 0.68126

Excited State 7: Singlet-A 3.6261 eV 341.92 nm f=0.0334 <S**2>=0.000
140 ->146 0.10863
142 ->146 0.19284
143 ->147 -0.10144
145 ->150 0.65605

Excited State 8: Singlet-A 3.6568 eV 339.05 nm f=0.0005 <S**2>=0.000
141 ->146 -0.12269
142 ->147 -0.19487
143 ->146 0.60134
145 ->148 0.10156
145 ->151 -0.25282

Excited State 9: Singlet-A 3.7251 eV 332.84 nm f=0.0097 <S**2>=0.000

143 ->146 0.27925
145 ->151 0.63276

Excited State 10: Singlet-A 3.7415 eV 331.38 nm f=0.0393 <S**2>=0.000
140 ->146 -0.19863
142 ->146 0.53788
143 ->147 -0.34607
145 ->150 -0.17883

TBC Monomer (4')

SCF Done: E(RB3LYP) = -4134.32580432 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.388093	-2.468527	1.788254
2	6	0	4.002151	-1.200261	1.824011
3	6	0	2.952627	-0.211854	1.784957
4	7	0	1.736608	-0.883930	1.707144
5	6	0	1.959402	-2.263773	1.727497
6	7	0	1.061909	-3.236612	1.718995
7	6	0	-0.228455	-2.935424	1.689392
8	6	0	-1.364820	-3.829039	1.744725
9	6	0	-2.547186	-3.031080	1.742893
10	6	0	-2.110359	-1.658293	1.684590
11	7	0	-0.730571	-1.669196	1.625338
12	6	0	-2.606376	-0.354574	1.736128
13	6	0	-3.842476	0.376858	1.838746
14	6	0	-3.493768	1.760913	1.879271
15	6	0	-2.054307	1.859588	1.806675
16	7	0	-1.580783	0.576575	1.721537
17	7	0	-1.294294	2.944111	1.849780
18	6	0	0.025645	2.820117	1.824658
19	6	0	0.954444	3.921185	1.912289
20	6	0	2.258229	3.382729	1.912343
21	6	0	2.131660	1.949281	1.825390
22	7	0	0.777105	1.641551	1.757618
23	7	0	3.138615	1.093612	1.830655
24	6	0	3.382283	4.214560	1.996139
25	6	0	3.168652	5.584632	2.082290
26	6	0	1.862044	6.123939	2.085118
27	6	0	0.744172	5.303209	2.000387
28	6	0	4.152437	-3.641317	1.819083
29	6	0	5.534494	-3.511251	1.887226
30	6	0	6.149788	-2.239652	1.923662
31	6	0	5.395032	-1.073349	1.892600
32	6	0	-3.805208	-3.649731	1.796617
33	6	0	-3.860472	-5.037372	1.855775
34	6	0	-2.686809	-5.819659	1.860254
35	6	0	-1.432411	-5.224480	1.804170
36	6	0	-4.476308	2.752883	1.985747
37	6	0	-5.805601	2.356796	2.054908
38	6	0	-6.157743	0.990290	2.014810
39	6	0	-5.192739	-0.002615	1.905408
40	15	0	0.115340	-0.066440	1.679203
41	8	0	0.175062	-0.163290	3.382794
42	1	0	4.381468	3.791477	1.991111
43	1	0	4.019160	6.257662	2.149773
44	1	0	1.734107	7.200852	2.154824
45	1	0	-0.263114	5.707267	1.999575
46	1	0	3.670797	-4.613162	1.787914
47	1	0	6.157035	-4.401563	1.913678
48	1	0	7.233375	-2.177168	1.977261
49	1	0	5.857556	-0.091943	1.918510
50	1	0	-4.720158	-3.066791	1.786793
51	1	0	-4.827711	-5.530558	1.899300
52	1	0	-2.769228	-6.901937	1.907606

53	1	0	-0.521262	-5.814375	1.804945
54	1	0	-4.191413	3.799870	2.012855
55	1	0	-6.588198	3.105406	2.142197
56	1	0	-7.206020	0.709959	2.070633
57	1	0	-5.485227	-1.046635	1.870700
58	1	0	-0.449679	0.456534	3.791595
59	8	0	0.174506	0.000117	0.000005
60	15	0	0.115361	0.066446	-1.679206
61	7	0	0.777150	-1.641540	-1.757472
62	7	0	-1.580754	-0.576587	-1.721510
63	7	0	-0.730570	1.669197	-1.625468
64	7	0	1.736621	0.883952	-1.707198
65	8	0	0.175105	0.163160	-3.382804
66	6	0	2.131709	-1.949259	-1.825234
67	6	0	0.025703	-2.820117	-1.824509
68	6	0	-2.054262	-1.859610	-1.806625
69	6	0	-2.606358	0.354548	-1.736149
70	6	0	-2.110358	1.658276	-1.684678
71	6	0	-0.228469	2.935428	-1.689534
72	6	0	1.959396	2.263798	-1.727620
73	6	0	2.952648	0.211889	-1.784955
74	1	0	-0.449675	-0.456652	-3.791565
75	6	0	2.258294	-3.382708	-1.912136
76	7	0	3.138654	-1.093578	-1.830556
77	6	0	0.954515	-3.921177	-1.912089
78	7	0	-1.294234	-2.944124	-1.849671
79	6	0	-3.493722	-1.760953	-1.879249
80	6	0	-3.842448	-0.376904	-1.838763
81	6	0	-2.547203	3.031058	-1.742994
82	6	0	-1.364846	3.829030	-1.744860
83	7	0	1.061892	3.236627	-1.719154
84	6	0	3.388084	2.468567	-1.788387
85	6	0	4.002159	1.200308	-1.824066
86	6	0	3.382360	-4.214529	-1.995896
87	6	0	0.744260	-5.303205	-2.000161
88	6	0	-4.476249	-2.752939	-1.985715
89	6	0	-5.192714	0.002552	-1.905458
90	6	0	-3.805232	3.649692	-1.796692
91	6	0	-1.432456	5.224469	-1.804313
92	6	0	4.152412	3.641366	-1.819281
93	6	0	5.395043	1.073412	-1.892641
94	6	0	3.168744	-5.584605	-2.082018
95	1	0	4.381538	-3.791436	-1.990867
96	6	0	1.862142	-6.123926	-2.084856
97	1	0	-0.263022	-5.707273	-1.999364
98	6	0	-5.805545	-2.356870	-2.054906
99	1	0	-4.191342	-3.799924	-2.012790
100	6	0	-6.157704	-0.990367	-2.014850
101	1	0	-5.485214	1.046570	-1.870783
102	6	0	-3.860516	5.037333	-1.855862
103	1	0	-4.720176	3.066742	-1.786836
104	6	0	-2.686862	5.819635	-1.860375
105	1	0	-0.521313	5.814375	-1.805107
106	6	0	5.534471	3.511317	-1.887411
107	1	0	3.670757	4.613206	-1.788173
108	6	0	6.149783	2.239724	-1.923769
109	1	0	5.857581	0.092011	-1.918491
110	1	0	4.019260	-6.257628	-2.149474
111	1	0	1.734216	-7.200841	-2.154541
112	1	0	-6.588132	-3.105492	-2.142189
113	1	0	-7.205984	-0.710050	-2.070696
114	1	0	-4.827761	5.530507	-1.899367
115	1	0	-2.769294	6.901911	-1.907733
116	1	0	6.156998	4.401635	-1.913913
117	1	0	7.233370	2.177252	-1.977360

TD–DFT output

HOMO**: 285**, LUMO**: 286**

Excited State 1:	Singlet-A	1.5334 eV	808.56 nm	f=0.0057	<S**2>=0.000
285 -> 286	0.69496				

This state for optimization and/or second-order correction.

Total Energy, E(TD-HF/TD-KS) = -4134.26945333

Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2:	Singlet-A	1.6954 eV	731.29 nm	f=0.0019	<S**2>=0.000
284 -> 286	-0.21487				
285 -> 287	0.66560				
Excited State 3:	Singlet-A	1.8404 eV	673.70 nm	f=0.0000	<S**2>=0.000
284 -> 286	0.42912				
285 -> 287	0.13018				
285 -> 288	0.53592				
Excited State 4:	Singlet-A	1.9470 eV	636.81 nm	f=0.0075	<S**2>=0.000
284 -> 287	0.38214				
285 -> 289	0.58488				
Excited State 5:	Singlet-A	2.1272 eV	582.84 nm	f=0.3128	<S**2>=0.000
282 -> 287	-0.18627				
283 -> 289	0.17634				
284 -> 286	0.47983				
285 -> 287	0.15156				
285 -> 288	-0.40918				
Excited State 6:	Singlet-A	2.1954 eV	564.74 nm	f=0.1547	<S**2>=0.000
282 -> 286	0.24691				
283 -> 288	-0.17428				
284 -> 287	0.53955				
285 -> 289	-0.31920				
Excited State 7:	Singlet-A	2.2871 eV	542.10 nm	f=0.0027	<S**2>=0.000
282 -> 286	0.10213				
283 -> 287	0.21074				
284 -> 288	0.65346				
Excited State 8:	Singlet-A	2.3238 eV	533.54 nm	f=0.0032	<S**2>=0.000
283 -> 286	-0.36512				
284 -> 289	0.59532				
Excited State 9:	Singlet-A	2.5718 eV	482.09 nm	f=0.0076	<S**2>=0.000
282 -> 287	-0.23834				
282 -> 288	0.16016				
283 -> 286	0.56121				
284 -> 289	0.30064				
Excited State 10:	Singlet-A	2.6562 eV	466.78 nm	f=0.0314	<S**2>=0.000
282 -> 286	0.48925				
283 -> 287	-0.39996				
283 -> 288	0.28194				
Excited State 11:	Singlet-A	2.7761 eV	446.61 nm	f=0.0109	<S**2>=0.000
282 -> 286	0.23971				
282 -> 289	0.15837				
283 -> 287	0.49887				
283 -> 288	0.36054				
284 -> 288	-0.17034				
Excited State 12:	Singlet-A	2.8591 eV	433.65 nm	f=0.0186	<S**2>=0.000
282 -> 287	0.48032				
282 -> 288	0.15831				
283 -> 289	0.46977				
Excited State 13:	Singlet-A	3.1023 eV	399.66 nm	f=0.0163	<S**2>=0.000

282 -> 287	-0.18035				
282 -> 288	0.62323				
283 -> 286	-0.15479				
284 -> 289	-0.15696				
Excited State 14:	Singlet-A	3.1264 eV	396.57 nm	f=0.1164	<S**2>=0.000
282 -> 286	-0.16615				
282 -> 289	0.58992				
283 -> 287	-0.17683				
283 -> 288	0.19604				
284 -> 288	0.13196				
285 -> 291	-0.10783				
Excited State 15:	Singlet-A	3.1356 eV	395.41 nm	f=0.0101	<S**2>=0.000
282 -> 288	-0.10333				
285 -> 290	0.68915				
Excited State 16:	Singlet-A	3.1626 eV	392.03 nm	f=0.1332	<S**2>=0.000
282 -> 286	0.15411				
282 -> 289	0.24735				
283 -> 288	-0.23947				
285 -> 291	0.57283				
Excited State 17:	Singlet-A	3.2089 eV	386.38 nm	f=0.0448	<S**2>=0.000
285 -> 292	0.68745				
Excited State 18:	Singlet-A	3.2328 eV	383.52 nm	f=0.8607	<S**2>=0.000
282 -> 287	-0.34550				
282 -> 288	-0.16916				
283 -> 289	0.46842				
284 -> 286	-0.18138				
285 -> 288	0.16773				
285 -> 293	0.12693				
285 -> 294	0.14125				
Excited State 19:	Singlet-A	3.2377 eV	382.93 nm	f=0.7255	<S**2>=0.000
282 -> 286	-0.24499				
282 -> 289	-0.20975				
283 -> 288	0.37674				
284 -> 287	0.18086				
285 -> 289	-0.15707				
285 -> 291	0.37956				
285 -> 292	-0.12852				
Excited State 20:	Singlet-A	3.2498 eV	381.52 nm	f=0.0215	<S**2>=0.000
285 -> 293	0.68155				

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