Supporting Information

for

Supramolecular dimeric structures of pyrazole-containing *meso*-oxo carbaphlorin analogues

Masatoshi Ishida^a, Hiroyuki Fujimoto^a, Tatsuki Morimoto^{a,b}, Shigeki Mori^c, Motoki Toganoh^a, Soji Shimizu^a and Hiroyuki Furuta^{a,*}

^a*Department of Chemistry and Biochemistry, Graduate School of Engineering, Education Center for Global Leaders in Molecular Systems for Devices and Center, Center for Molecular Systems, Kyushu University, Fukuoka 819-0395, Japan*

^b*Department of Applied Chemistry, School of Engineering, Tokyo University of Technology, Tokyo 192-0982, Japan*

^c*Integrated Center for Sciences, Ehime University, Matsuyama 790-8577, Japan*

*Correspondence to: Hiroyuki Furuta, email: hfuruta@cstf.kyushu-u.ac.jp, fax: +81-92-802-2865

Table S1. Crystal data and structure analysis results.

	5	6•CHCl₃	13•2CHCl₃
formula	C ₃₆ H ₃₉ N ₅ O	C ₃₀ H ₃₄ Cl ₃ N ₅ O	C ₄₇ H ₂₈ Cl ₈ N ₆ O ₂
cryst syst	monoclinic	triclinic	monoclinic
space group	<i>P</i> 2 ₁ / <i>c</i>	<i>P</i> -1	<i>P</i> 2 ₁ / <i>n</i>
<i>R</i>	0.0419	0.0604	0.0621
<i>wR</i> ₂ (all data)	0.1236	0.1803	0.1847
GOF	0.991	1.062	1.049
<i>a</i> (Å)	9.6920(19)	9.3214(7)	17.6407(10)
<i>b</i> (Å)	14.928(3)	11.9048(8)	13.2173(9)
<i>c</i> (Å)	21.266(4)	13.2244(9)	19.1359(13)
<i>α</i> (deg)		92.431(1)	
<i>β</i> (deg)	98.28(3)	92.001(2)	100.131(2)
<i>γ</i> (deg)		95.310(2)	
<i>V</i> (Å ³)	3044.7(11)	1458.78(18)	4392.2(5)
<i>Z</i>	4	2	4
<i>D</i> _{calcd} (g cm ⁻³)	1.217	1.336	1.501
2 θ _{max} (deg)	20.812	25.498	49.4
No. of rflns measd (unique)	3193	5401	24651
No. of rflns measd (<i>I</i> > 2 σ (<i>I</i>))	1884	4043	7482
No. of params	385	386	596
CCDC reference No.	1408461	1408459	1408460

Figure S1. ^1H NMR spectra of *N*-benzyl oxophlorins **5** in CDCl_3 . Asterisks indicate the peaks of residual solvent and impurities.

Figure S2. Partial FTIR spectra of (a) **5** and (b) **6**.

Figure S3. UV-vis absorption (solid line) and emission ($\lambda_{\text{ex}} = 380$ nm, broken line) spectra of **5** in CH_2Cl_2 .

Figure S4. UV-vis-NIR absorption spectrum of **13** in CH_2Cl_2 .

Figure S5. (a) ^1H and (b) ^{13}C NMR spectra of **13** recorded in CDCl_3 . Asterisk indicates the peaks of residual solvent and impurities.

Figure S6. Conformations of the optimized structures of **13** and its isomeric form **13'** obtained by B3LYP/6-31G(d,p) level calculations

Scheme S1. Prausible reaction mechanism for macrocycle **13**.

Figure S7. ^{13}C NMR spectrum of **6** recorded in CDCl_3 . Asterisk shows the residual solvent peak.

Figure S8. (a) Concentration-dependent ^1H NMR spectral change of **6** in CDCl_3 . (b) Plots for the $\Delta\delta$ (of the signal of C_{21}H) versus concentration of the sample solution with a nonlinear fitting curves; $K = 92.9 \pm 13.1 \text{ M}^{-1}$; $R^2 = 0.9814$.

Figure S9. Temperature-variable ^1H NMR spectral change of **6** (CDCl_3) recorded at (a) 20 $^\circ\text{C}$, (b) 0 $^\circ\text{C}$, (c) -20 $^\circ\text{C}$ and (d) -40 $^\circ\text{C}$.

Figure S10. Temperature-dependent UV-vis absorption and emission spectral changes of **6** in CH_2Cl_2 . The black line indicates the spectrum recorded at 298 K and the red one is at 238 K. $\lambda_{\text{ex}} = 640 \text{ nm}$.

Figure S11. Configurations of the assembled dimer $[6]_2$ obtained by B3LYP/6-31G(d,p) level calculation.