Electronic Supplementary Information

Magnetic Investigations over Reversibly Switched Chiral (Phthalocyaninato)(porphyrinato) Dysprosium Double-decker Compounds

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Experimental section

General remarks. All the reagents and solvents were used as received. The compounds of metal free phthalocyanine (*R*)- and (*S*)-$H_2Pc(OBNP)_2$ and reduced protonated (*R*)/(*S*)-{DyH[$Pc(OBNP)_2$](TClPP)} (**1a, 1b**) were prepared according to the published procedure.[1,2] The ultraviolet-visible spectra were recorded on a Hitachi U-4100 spectrophotometer. MALDI-TOF mass spectra were taken on a Bruker BIFLEX III ultrahighresolution Fourier transform ion cyclotron resonance (FT-ICR) mass spectrometer with alpha-cyano-4-hydroxycinnamic acid as matrix. Elemental analysis was performed on an Elementar Vavio El Ш. Crystal data for **1a**, **1b**, and **2b** were determined by X-ray diffraction analysis at 120 K using Oxford Diffraction Gemini E system, and details of the structure refinement are given in Table S2 (Electronic Supplementary Information). The important structural parameters together with selected bond lengths and angles have been listed in Tables S3 and S4 (Electronic Supplementary Information). CCDC number of 1862109-1862111 for **1a**, **1b**, and **2b** containing the supplementary crystallographic data for this paper can be obtained free of charge from the Cambridge Crystallographic Data Centre *via* www.ccdc.cam.ac.uk/data_request/cif. Magnetic measurements were performed on a Quantum Design MPMS XL-5 SQUID magnetometer on multicrystalline samples. Data were corrected for the diamagnetism of the samples using Pascal constants and the sample holder by measurement.

Chiral reduced protonated (*R*)/(*S*)-{DyH[$Pc(OBNP)_2$](TClPP)} (1) and neutral unprotonated (*R*)/(*S*)-{Dy[$Pc(OBNP)_2$](TClPP)} (2): A mixture of $Dy(acac)_3{\cdot}6H_2O$ (57 mg, 0.1 mmol), H_2TClPP (75 mg, 0.1 mmol), and optically active

(*R*)/(*S*)-$H_2Pc(OBNP)_2$ (107 mg, 0.1 mmol) in *n*-octanol (6 mL) was heated to reflux under nitrogen for approximately 6 h. After being cooled to room temperature, the volatile compounds were removed under reduced pressure. The residue was chromatographed on a silica gel column by using $CHCl_3$/petroleum ether (1/1, v/v) as the eluent. A small amount of unreacted H_2TClPP was eluted first, then a green band containing a mixture of the reduced protonated double-decker **1** and neutral unprotonated species **2** were eluted followed by a small blue band that contains the unreacted metal-free phthalocyanine. The mixture was further chromatographed on a silica gel column with $CHCl_3$/petroleum ether (2/3, v/v) as the eluent. A brown band containing a trace amount of neutral unprotonated double-decker **2** was separated first. Then a light green band containing the main product of **2** was eluted. Repeated chromatography followed by recrystallization from chloroform and methanol gave **1** in the yield of 28-36% and **2** in a trace amount.

Large amount of **2** could be isolated from the oxidation reaction of reduced protonated (*R*)/(*S*)-{DyH[Pc(OBNP)$_2$](TClPP)} (**1**) (40 mg, 0.02 mmol) in the presence of excess amount of 2,3-dichloro-5,6-dicyano-1,4-benzoquinone (DDQ). A chloroform/methanol (2/1, v/v) solution (30 mL) of DDQ was slowly added into the chloroform/methanol (1/1, v/v) solution (20 mL) of **1** (40 mg). The resulting mixture was then stirred for 30 min. The volatiles were removed under reduced pressure. Repeated column chromatography followed by recrystallization as detailed above provided pure neutral unprotonated double-decker complex **2** in the yield of 78-86%.

Single crystals growth. Single crystals of (R/S)-{DyH[Pc(OBNP)$_2$](TClPP)} (**1**) suitable for X-ray diffraction analysis were obtained by the diffusion of methanol into a solution of 6.0 mg (*R*)/(*S*)-{DyH[Pc(OBNP)$_2$](TClPP)} (**1a**, **1b**) in 8 mL *o*-dichlorohenzene/chloroform (1/1, v/v) with the help of 2.2 mg C_{60} led to single crystals of this double-decker species suitable for X-ray diffraction analysis. Due to the poor crystallinity and easy transformation of the neutral unprotonated double-decker complex into the reduced protonated analogue in solution, all the efforts towards crystallization of this compound by means of different kinds of organic solvents failed to provide single crystals of **2**. Fortunately, in the presence of the oxidation agent DDQ, single crystals of 3.0 mg (S)-{Dy[Pc(OBNP)$_2$](TClPP)} (**2b**) suitable for X-ray diffraction analysis were obtained by the diffusion of methanol into the solution of this compound in benzene/toluene (1/1, v/v).

Computation details. On the basis of the isostructural nature of the reduced protonated double-decker {DyH[Pc(α-OC$_5$H$_{11}$)$_4$](TClPP)} with its neutral unprotonated analogue {Dy[Pc(α-OC$_5$H$_{11}$)$_4$](TClPP)} [Pc(α-OC$_5$H$_{11}$)$_4$ = dianion of 1,8,15,22-tetrakis(3-pentyloxy)-phthalocyanine],[3] almost the same coordination geometry should be employed for the dysprosium ion in the neutral unprotoned compound {Dy[Pc(OBNP)$_2$](TClPP)} **2** as in reduced protonated species {DyH[Pc(OBNP)$_2$](TClPP)} **1**. As a consequence, density functional theory (DFT) calculations of these two double-deckers were performed on the basis of the crystal structure of neutral unprotonated complex (S)-{Dy[Pc(OBNP)$_2$](TClPP)} (**2b**) with the yttrium ion replacing the dysprosium ion to reduce the computing time. The total electron density and the fragment charge distribution of {YH[Pc(OBNP)$_2$](TClPP)} (**1b′**) and {Y[Pc(OBNP)$_2$](TClPP)} (**2b′**) were calculated at the level of M06-2X/LanL2DZ.[4] The electron density difference (EDD) between reduced protonated species **1b′** and neutral unprotonated **2b′** was calculated by $\rho_{diff} = \rho_N - \rho_P$, where ρ_P and ρ_N are the electron density of the double-deckers in the form of the reduced protonated species **1b′** and neutral unprotonated **2b′**.[5] In addition, the full natural bond orbital (NBO) analysis was carried out using NBO 3.1, revealing the almost unchanged and weak coordination interaction between the tetrapyrrole ligands and central yttrium(III) ion in terms of the covalent bond component.[6] As a consequence, the electrostatic interaction between Pc(OBNP)$_2$ (or TClPP) fragments and yttrium atom of double-deckers (which represents the total coordination interaction in the present case) in different oxidation state is calculated using the equation of $\sum_i \left(k \cos\theta \frac{q_i q_{\mathrm{Y}}}{r_{i\mathrm{Y}}^2} \right)$, where q_i is the NBO charge of any atom i belonging to Pc(OBNP)$_2$ or TClPP rings, q_{Y} is the NBO charge of yttrium atom, and $r_{i\mathrm{Y}}$ is the distance between i and yttrium atoms, and θ is the angle of atom i…Y…center of Pc (or TClPP) ligand, Figure S12 and Table S5 (Electronic Supplementary Information). All calculations were carried out using the Gaussian 09 D.01 software package.[7]

References

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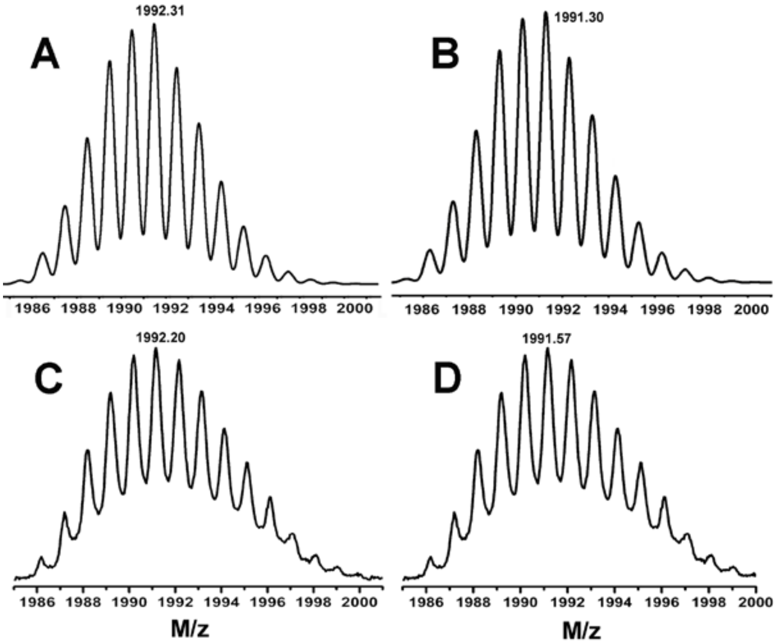

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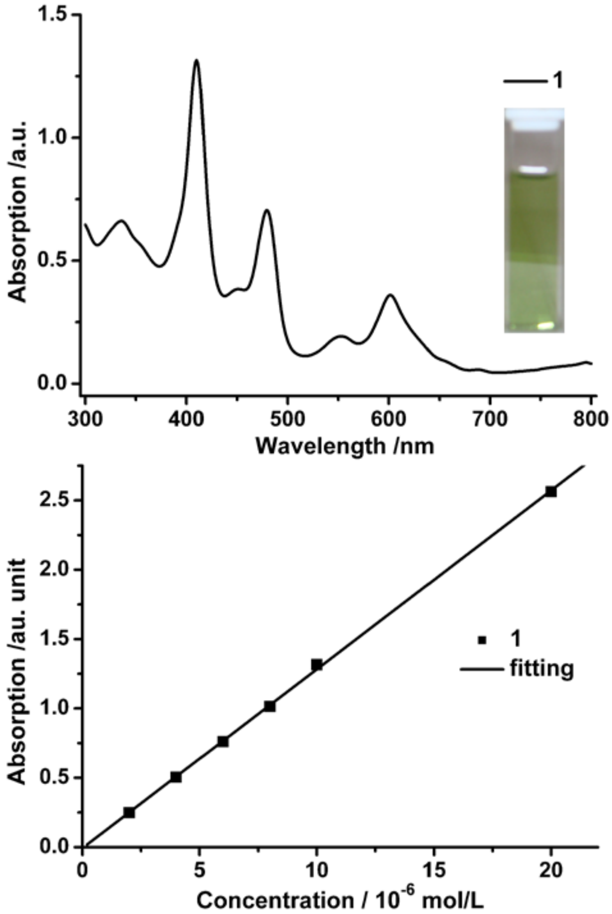


Figure S2. Electronic absorption spectrum of the reduced protonated double-decker complex {DyH[Pc(OBNP)$_2$](TClPP)} **1** with the concentration of 1.0 × 10^{-5} mol/L (top) and Beer-Lambert plot (bottom) recorded at 410 nm in chloroform.

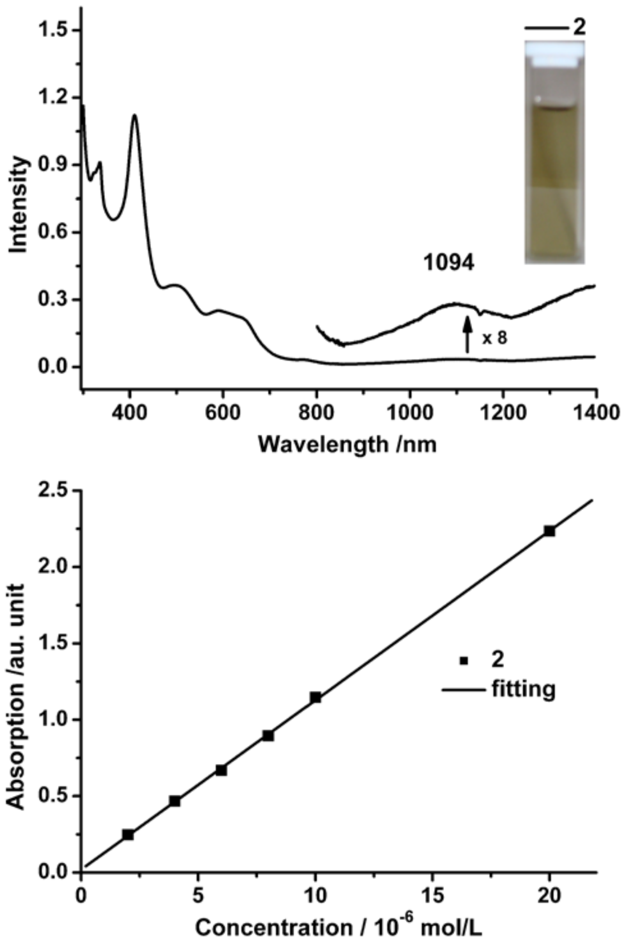
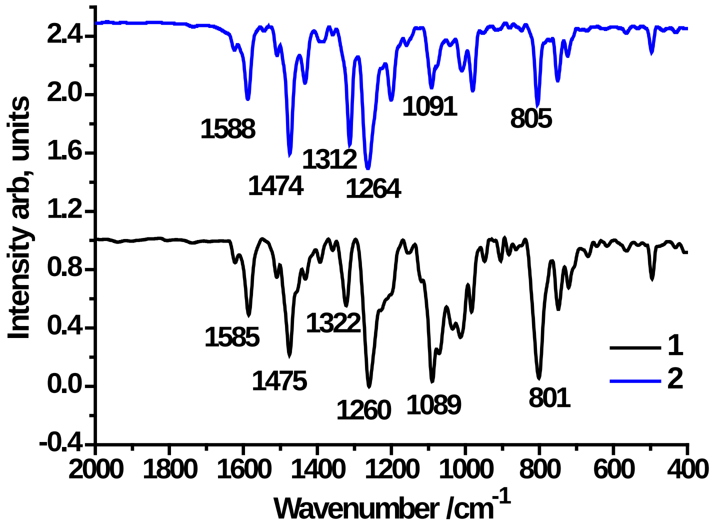


Figure S3. Electronic absorption spectrum of the neutral unprotonated complex {Dy[Pc(OBNP)$_2$](TClPP)} **2** with the concentration of 1.0×10^{-5} mol/L (top) and Beer-Lambert plot (bottom) recorded at 410 nm in chloroform.



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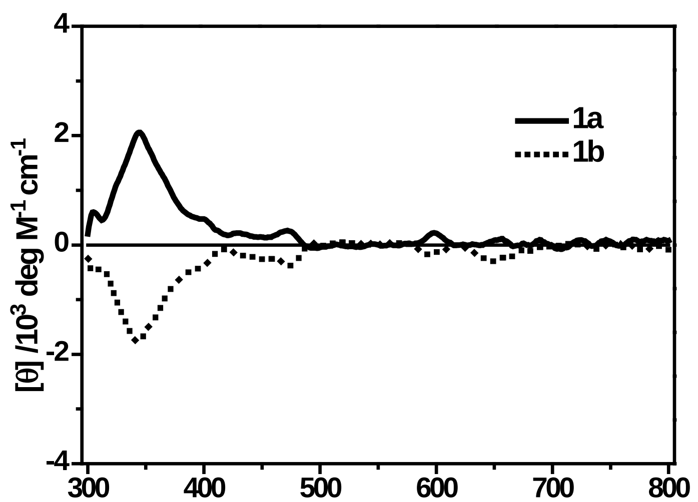


Figure S5. Circular dichroism (CD) spectra of chiral double-decker complex {DyH[Pc(OBNP)$_2$](TClPP)} (**1**) in chloroform.

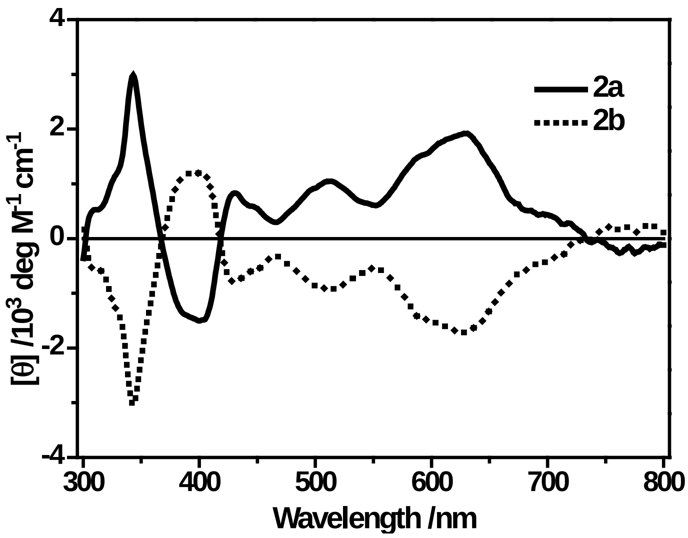


Figure S6. Circular dichroism (CD) spectra of chiral double-decker complex {Dy[Pc(OBNP)$_2$](TClPP)} (**2**) in chloroform.

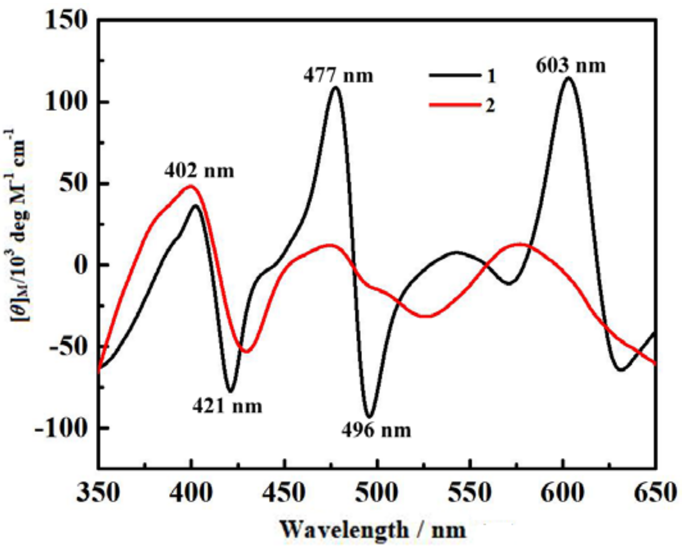


Figure S7. Magneto-chiral dichroism (MCD) spectra of double-decker complex **1** and **2** in chloroform at 25 °C, which were collected on a JASCO J-1500 CD spectrometer in the presence of a magnetic field (1.6 T).

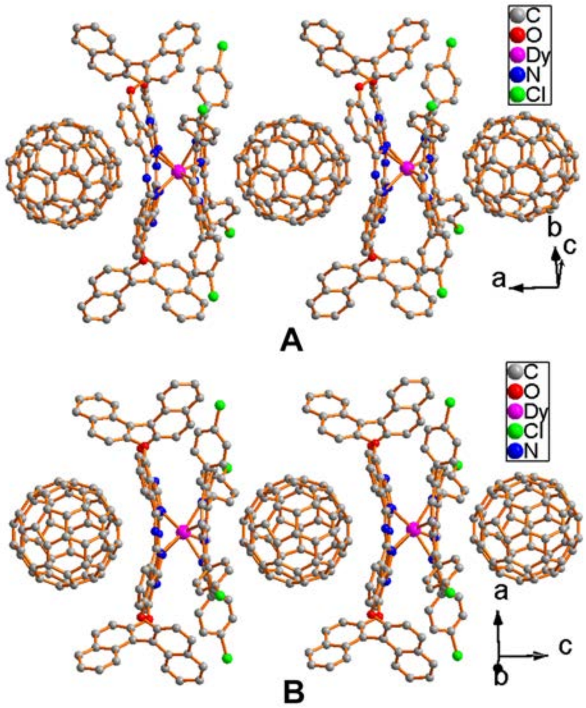


Figure S8. Packing plots of **1a** and **1b** (A and B) with all the hydrogen atoms and solvent molecules omitted for clarity.

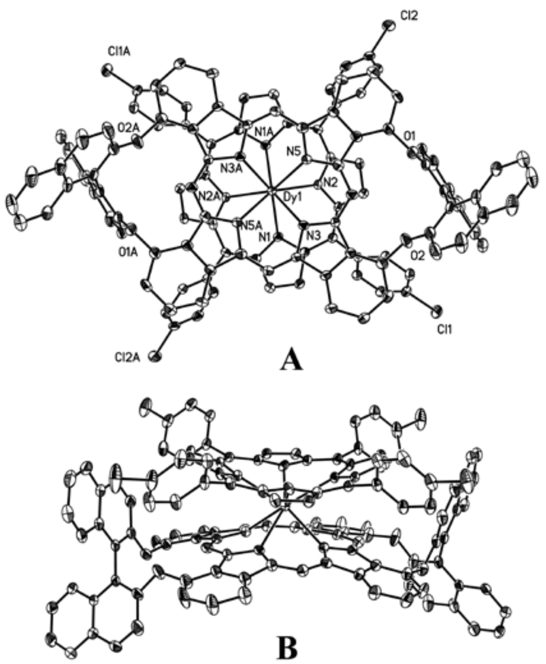


Figure S9. Molecular structure of **2b** in top view (A) and side view (B) with all the hydrogen atoms and solvent molecules omitted for clarity.

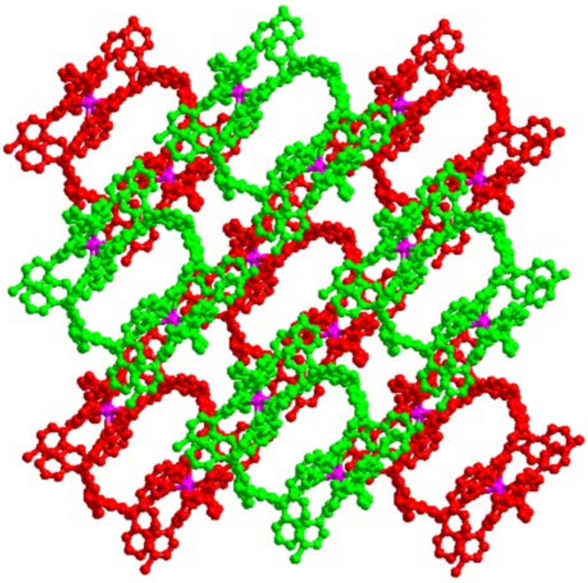


Figure S10. The packing diagram of (*S*)-{Dy[Pc(OBNP)$_2$](TClPP)} (**2b**) with all the hydrogen atoms and solvent molecules omitted for clarity.

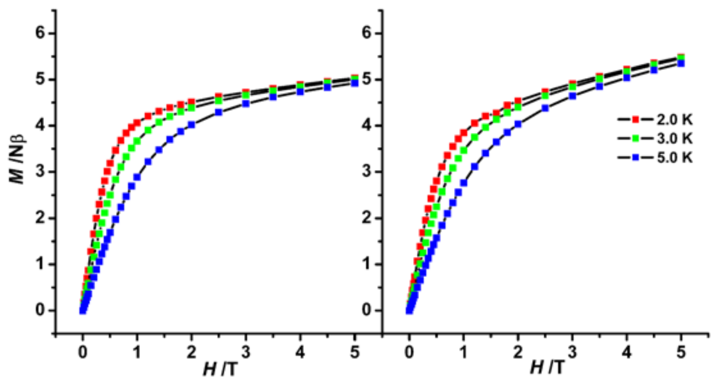


Figure S11. The *M vs. H* curves for **1** and **2** at 2.0, 3.0, and 5.0 K.

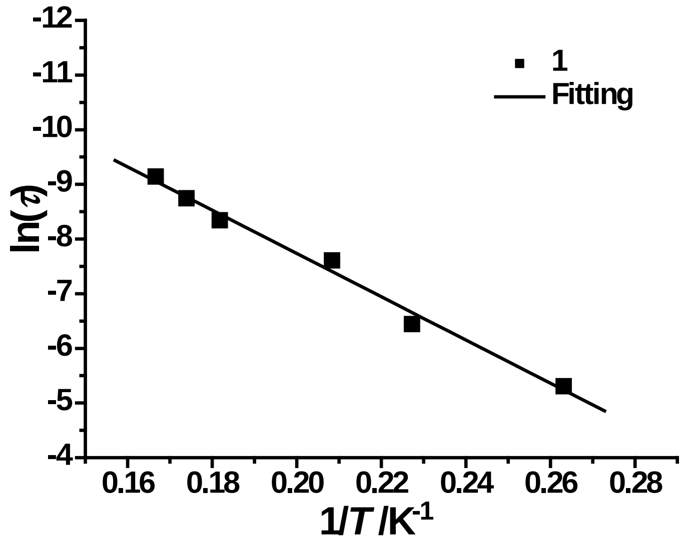
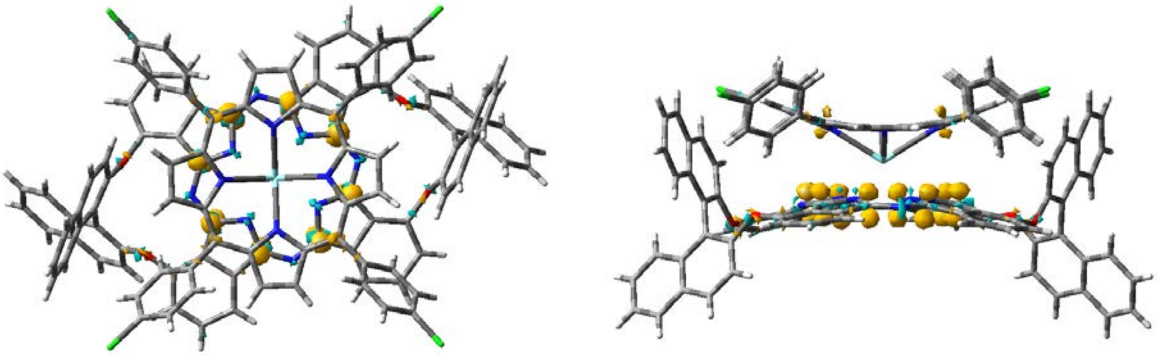
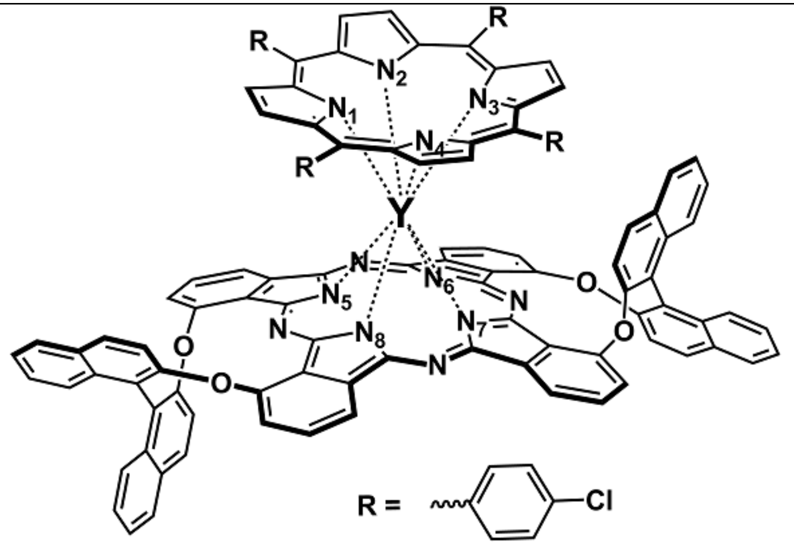


Figure S12. The plot of ln(τ) *vs.* 1/T for **1** under 2000 Oe applied magnetic field.



Top view **Side view**

Figure S13. Electron density difference plots between reduced protonated (*S*)-{YH[Pc(OBNP)$_2$](TClPP)} (**1b′**) and neutral unprotonated (*S*)-{Y[Pc(OBNP)$_2$](TClPP)} (**2b′**) (Isovalue: 2.0×10^{-3} e·a.u.^{3}). The loss of electron density is shown in the yellow color.



1b′		2b′	
Y-N$_1$	0.156	Y-N$_1$	0.154
Y-N$_2$	0.151	Y-N$_2$	0.148
Y-N$_3$	0.156	Y-N$_3$	0.154
Y-N$_4$	0.151	Y-N$_4$	0.148
Y-Por	0.614	Y-Por	0.604
Y-N$_5$	0.263	Y-N$_5$	0.265
Y-N$_6$	0.211	Y-N$_6$	0.215
Y-N$_7$	0.263	Y-N$_7$	0.265
Y-N$_8$	0.211	Y-N$_8$	0.215
Y-Pc	0.948	Y-Pc	0.960
Total	1.562	Total	1.564

Figure S14. Mayer bond order of reduced protonated **1b′** and **2b′**.

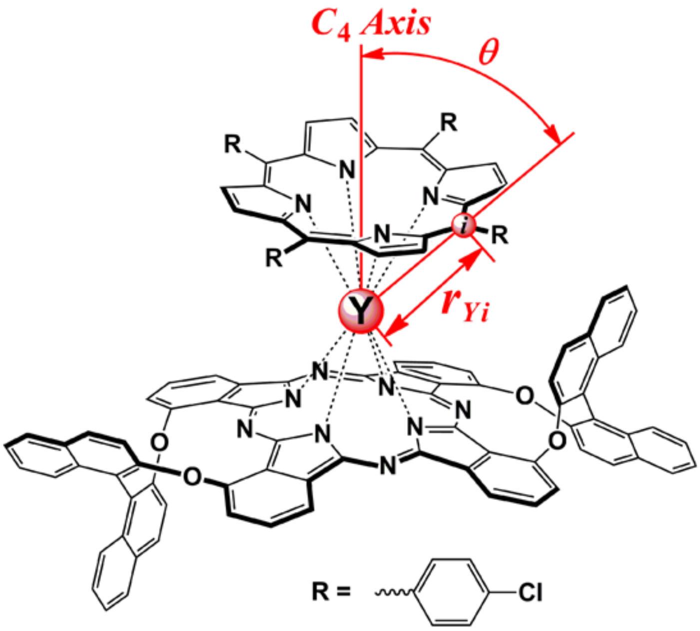


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Table S1. Mass spectroscopic and elemental analysis data for the sandwich-type double-decker complexes **1** and **2**.[a]

	Molecular formula	**M+H⁺ (*m/z*)**	(%) C	H	N
1a	$C_{116}H_{61}Cl_4DyN_{12}O_4$	1992.20	70.32 (69.97)	3.42 (3.08)	8.21 (8.44)
1b	$C_{116}H_{61}Cl_4DyN_{12}O_4$[b]		67.52 (67.06)	3.37 (3.44)	8.15 (7.68)
2a	$C_{116}H_{60}Cl_4DyN_{12}O_4$[c]	1991.57	68.81 (68.76)	3.22 (3.18)	8.32 (8.30)
2b	$C_{116}H_{60}Cl_4DyN_{12}O_4$[c]		68.36 (68.76)	3.32 (3.18)	8.01 (8.30)

[a] Calculated values given in parentheses. [b] Contain 4.0 equiv. of solvated H_2O. [c] Contain 2.0 equiv. of solvated H_2O.

Table S2. Crystal data and structure refinement of complex **1a**, **1b**, and **2b**.

complex	**1a**	**1b**	**2b**
Formula	$C_{182}H_{62}Cl_6DyN_{12}O_4$	$C_{188}H_{68}Cl_8DyN_{12}O_4$	$C_{128}H_{73}Cl_4DyN_{12}O_5$
F.W.	2855.64	3004.64	2163.34
system	orthorhombic	orthorhombic	orthorhombic
space group	$P2_12_12$	$P2_12_12$	$I222$
a /Å	20.0850(7)	21.7576(4)	21.6798(3)
b /Å	23.243(6)	21.4063(5)	21.8159(3)
c /Å	15.2100(10)	15.2756(3)	23.5650(4)
α /°	90	90	90
β /°	90	90	90
γ /°	90	90	90
Z	2	2	4
volume	7100.6(19)	7114.6(3)	11145.4(3)
D_{cald} / g cm^{-3}	1.336	1.403	1.289
F000	2876	4392	4392
R_{int} $I>2\theta$	0.1087	0.0892	0.0567
R_{w2} $I>2\theta$	0.2856	0.2385	0.1484
R_{int} all	0.1310	0.1038	0.0626
R_{w2} all	0.3039	0.2528	0.1526
S	1.281	1.057	1.027
Flack parameter	0.01(2)	-0.007(5)	-0.007(5)

Table S3. The structural data for **1a**, **1b**, and **2b**.

Structural parameter	**1a**	**1b**	**2b**
average M-N(Pc(OBNP)$_2$) bond distance (Å)	2.466	2.469	2.490
average M-N(TClPP) bond distance (Å)	2.433	2.437	2.432
M-N$_4$(Pc(OBNP)$_2$) plane distance (Å)	1.450	1.469	1.513
M-N$_4$(TClPP) plane distance (Å)	1.282	1.284	1.284
interplanar distance (Å)	2.732	2.752	2.797
average dihedral angle φ for the TClPP ring (°)[a]	10.39	9.00	27.83
average dihedral angle φ for the Pc(OBNP)$_2$ ring (°)[a]	17.95	16.59	13.93
average twist angle (°)[b]	33.95	31.11	34.63

[a] The average dihedral angle of the individual pyrrole or isoindole ring with respect to the corresponding N4 mean plane. [b] Defined as the rotation angle of one macrocycle away from the eclipsed conformation of the two macrocycles.

Table S4. Selected bond distances (Å) and bond angles (°) of **1a**, **1b**, and **2b**.

1a			
N(1)-Dy(1)	2.406(10)	Dy(1)-N(1)#1	2.406(10)
N(2)-Dy(1)	2.439(8)	Dy(1)-N(2)#1	2.439(8)
N(3)-Dy(1)	2.454(9)	Dy(1)-N(3)#1	2.454(9)
N(5)-Dy(1)	2.466(8)	Dy(1)-N(5)#1	2.466(8)
N(1)-Dy(1)-N(1)#1	114.6(5)	N(1)#1-Dy(1)-N(5)	152.1(3)
N(1)-Dy(1)-N(2)#1	73.5(3)	N(2)#1-Dy(1)-N(5)	133.7(3)
N(1)#1-Dy(1)-N(2)#1	73.6(3)	N(2)-Dy(1)-N(5)	86.1(3)
N(1)-Dy(1)-N(2)	73.6(3)	N(3)-Dy(1)-N(5)	70.1(3)
N(1)#1-Dy(1)-N(2)	73.5(3)	N(3)#1-Dy(1)-N(5)	70.0(3)
N(2)#1-Dy(1)-N(2)	116.8(4)	N(1)-Dy(1)-N(5)#1	152.1(3)
N(1)-Dy(1)-N(3)	133.9(3)	N(1)#1-Dy(1)-N(5)#1	76.0(3)
N(1)#1-Dy(1)-N(3)	85.8(3)	N(2)#1-Dy(1)-N(5)#1	86.1(3)
N(2)#1-Dy(1)-N(3)	151.8(3)	N(2)-Dy(1)-N(5)#1	133.7(3)
N(2)-Dy(1)-N(3)	73.8(3)	N(3)-Dy(1)-N(5)#1	70.0(3)
N(1)-Dy(1)-N(3)#1	85.8(3)	N(3)#1-Dy(1)-N(5)#1	70.1(3)
N(1)#1-Dy(1)-N(3)#1	133.9(3)	N(5)-Dy(1)-N(5)#1	107.2(4)
N(2)#1-Dy(1)-N(3)#1	73.8(3)	N(3)-Dy(1)-N(3)#1	109.9(4)
N(2)-Dy(1)-N(3)#1	151.8(3)	N(1)-Dy(1)-N(5)	76.0(3)
1b			
Dy(1)-N(2)#1	2.436(8)	Dy(1)-N(5)#1	2.463(8)
Dy(1)-N(2)	2.436(8)	Dy(1)-N(5)	2.463(8)
Dy(1)-N(1)#1	2.438(9)	Dy(1)-N(3)#1	2.475(8)
Dy(1)-N(1)	2.438(9)	Dy(1)-N(3)	2.475(8)
N(2)#1-Dy(1)-N(2)	117.4(4)	N(2)-Dy(1)-N(3)#1	87.0(3)
N(2)#1-Dy(1)-N(1)#1	74.0(3)	N(1)#1-Dy(1)-N(3)#1	153.4(3)
N(2)-Dy(1)-N(1)#1	73.8(3)	N(1)-Dy(1)-N(3)#1	75.2(3)
N(2)#1-Dy(1)-N(1)	73.8(3)	N(5)#1-Dy(1)-N(3)#1	68.1(2)
N(2)-Dy(1)-N(1)	74.0(3)	N(5)-Dy(1)-N(3)#1	70.4(3)
N(1)#1-Dy(1)-N(1)	115.4(4)	N(2)#1-Dy(1)-N(3)	87.0(3)
N(2)#1-Dy(1)-N(5)#1	154.5(3)	N(2)-Dy(1)-N(3)	132.2(3)
N(2)-Dy(1)-N(5)#1	73.3(3)	N(1)#1-Dy(1)-N(3)	75.2(3)
N(1)#1-Dy(1)-N(5)#1	88.5(3)	N(1)-Dy(1)-N(3)	153.4(3)
N(1)-Dy(1)-N(5)#1	131.4(3)	N(5)#1-Dy(1)-N(3)	70.4(3)
N(2)#1-Dy(1)-N(5)	73.3(3)	N(5)-Dy(1)-N(3)	68.1(2)
N(2)-Dy(1)-N(5)	154.5(3)	N(3)#1-Dy(1)-N(3)	106.7(4)
N(1)#1-Dy(1)-N(5)	131.4(3)	N(5)#1-Dy(1)-N(5)	107.2(3)
N(1)-Dy(1)-N(5)	88.5(3)	N(2)#1-Dy(1)-N(3)#1	132.2(3)
2b			
N(1)-Dy(1)	2.424(6)	Dy(1)-N(1)#1	2.424(6)
N(2)-Dy(1)	2.440(5)	Dy(1)-N(2)#1	2.440(5)

N(3)-Dy(1)	2.491(5)	Dy(1)-N(5)#1	2.489(5)
N(5)-Dy(1)	2.489(5)	Dy(1)-N(3)#1	2.491(5)
N(1)#1-Dy(1)-N(1)	116.3(3)	N(1)-Dy(1)-N(3)	76.71(19)
N(1)#1-Dy(1)-N(2)	73.77(19)	N(2)-Dy(1)-N(3)	86.31(18)
N(1)-Dy(1)-N(2)	73.91(19)	N(2)#1-Dy(1)-N(3)	135.00(17)
N(1)#1-Dy(1)-N(2)#1	73.91(19)	N(5)#1-Dy(1)-N(3)	68.82(17)
N(1)-Dy(1)-N(2)#1	73.77(19)	N(5)-Dy(1)-N(3)	67.86(17)
N(2)-Dy(1)-N(2)#1	116.3(3)	N(1)#1-Dy(1)-N(3)#1	76.71(19)
N(1)#1-Dy(1)-N(5)#1	134.48(17)	N(1)-Dy(1)-N(3)#1	150.82(18)
N(1)-Dy(1)-N(5)#1	86.5(2)	N(2)-Dy(1)-N(3)#1	135.00(17)
N(2)-Dy(1)-N(5)#1	151.45(18)	N(2)#1-Dy(1)-N(3)#1	86.31(18)
N(2)#1-Dy(1)-N(5)#1	76.13(18)	N(5)#1-Dy(1)-N(3)#1	67.86(17)
N(1)#1-Dy(1)-N(5)	86.5(2)	N(5)-Dy(1)-N(3)#1	68.82(17)
N(1)-Dy(1)-N(5)	134.48(17)	N(3)-Dy(1)-N(3)#1	104.9(3)
N(2)-Dy(1)-N(5)	76.13(18)	N(5)#1-Dy(1)-N(5)	105.5(3)
N(2)#1-Dy(1)-N(5)	151.45(18)	N(1)#1-Dy(1)-N(3)	150.82(18)

Symmetry transformations used to generate equivalent atoms: for **1a**, #1 -x, -y, z; for **1b**, #1 -x, -y+1, z; for **2b,** #1 -x+1, -y+1, z.

Table S5. The details of intramolecular electrostatic interaction for **1b′** and **2b′**.

Atom	Atom Number	Charge (e)	θ	Radius (Å)	Electrostatic Interaction (a.u) $\sum_i \left(k \cos\theta \frac{q_i q_Y}{r_{iY}^2} \right)$
1b′					
TClPP					0.09039
C	1	0.20567	59.269	3.4264	0.00422
C	2	-0.18898	60.281	4.6797	-0.00202
H	3	0.17389	61.211	5.5165	0.0013
C	4	-0.18995	61.009	4.6736	-0.00199
H	5	0.1839	62.44	5.5087	0.00132
C	6	0.21536	60.614	3.449	0.00419
C	7	-0.05514	65.565	3.7688	-7.57389E-4
C	8	0.19718	67.301	3.3769	0.00315
C	9	-0.19525	74.288	4.5162	-0.00122
H	10	0.18517	76.756	5.3286	7.04662E-4
C	11	-0.18486	75.175	4.508	-0.0011
H	12	0.18203	78.132	5.3177	6.24388E-4
C	13	0.2	69.348	3.3622	0.00294
C	14	-0.07026	62.974	3.7642	-0.00106
C	15	-0.01478	66.029	5.2504	-1.02736E-4
C	16	-0.14267	76.984	5.9614	-4.26445E-4
H	17	0.18289	84.406	5.6599	2.6248E-4
C	18	-0.18799	76.368	7.3374	-3.88147E-4
H	19	0.18864	81.225	7.9145	2.16684E-4
C	20	-0.00204	68.748	7.9926	-5.45935E-6
C	21	-0.19243	60.616	7.501	-7.91461E-4
H	22	0.18864	56.88	8.1618	7.29764E-4
C	23	-0.14609	57.786	6.172	-9.64223E-4
H	24	0.18629	50.503	6.0199	0.00154
C	25	-0.02681	69.259	5.2365	-1.63308E-4
C	26	-0.12942	79.436	5.906	-3.20827E-4
H	27	0.19338	85.946	5.5596	2.08611E-4
C	28	-0.18299	79.514	7.2982	-2.94897E-4
H	29	0.19384	84.137	7.8485	1.51608E-4
C	30	0.00468	72.726	7.9802	1.02921E-5
C	31	-0.19589	65.264	7.5402	-6.79973E-4
H	32	0.18569	61.967	8.2297	6.07735E-4
C	33	-0.15395	62.441	6.2109	-8.7086E-4
H	34	0.1838	56.293	6.1069	0.00129
N	89	-0.65896	60.073	2.4251	-0.02636

N	90	-0.65839	55.79	2.4405	-0.02931
Cl	97	-0.07138	73.826	9.7218	-9.92222E-5
Cl	98	-0.06165	69.813	9.7335	-1.0591E-4
C	100	0.20567	65.121	3.4264	0.00348
C	101	-0.18898	65.625	4.6797	-0.00168
H	102	0.17389	66.795	5.5165	0.00106
C	103	-0.18995	65.105	4.6736	-0.00173
H	104	0.1839	66.123	5.5087	0.00116
C	105	0.21536	63.694	3.449	0.00378
C	106	-0.05514	66.205	3.7688	-7.38722E-4
C	107	0.19718	65.421	3.3769	0.00339
C	108	-0.19525	71.249	4.5162	-0.00145
H	109	0.18517	74.166	5.3286	8.39237E-4
C	110	-0.18486	70.657	4.508	-0.00142
H	111	0.18203	73.286	5.3177	8.73152E-4
C	112	0.2	64.07	3.3622	0.00365
C	113	-0.07026	69.056	3.7642	-8.35985E-4
C	114	-0.01478	72.208	5.2504	-7.72687E-5
C	115	-0.14267	83.106	5.9614	-2.27274E-4
H	116	0.18289	90.513	5.6599	-2.41087E-5
C	117	-0.18799	82.485	7.3374	-2.1539E-4
H	118	0.18864	87.348	7.9145	6.57199E-5
C	119	-0.00204	74.818	7.9926	-3.9444E-6
C	120	-0.19243	66.586	7.501	-6.40982E-4
H	121	0.18864	62.761	8.1618	6.11308E-4
C	122	-0.14609	63.74	6.172	-8.00281E-4
H	123	0.18629	56.297	6.0199	0.00135
C	124	-0.02681	69.609	5.2365	-1.60671E-4
C	125	-0.12942	80.863	5.906	-2.77886E-4
H	126	0.19338	87.923	5.5596	1.06944E-4
C	127	-0.18299	80.83	7.2982	-2.58227E-4
H	128	0.19384	85.77	7.8485	1.09473E-4
C	129	0.00468	73.456	7.9802	9.86958E-6
C	130	-0.19589	65.361	7.5402	-6.77473E-4
H	131	0.18569	61.718	8.2297	6.12689E-4
C	132	-0.15395	62.334	6.2109	-8.73975E-4
H	133	0.1838	55.486	6.1069	0.00132
N	134	-0.65896	56.25	2.4251	-0.02936
N	135	-0.65839	60.57	2.4405	-0.02562
Cl	136	-0.07138	74.612	9.7218	-9.45199E-5
Cl	137	-0.06165	75.874	9.7335	-7.49026E-5

Y	1.68652

Pc(OBNP)$_2$					0.08177
C	35	0.46022	59.165	3.4464	0.00937
C	36	-0.03875	63.732	4.6626	-3.72059E-4
C	37	-0.13974	67.098	5.9321	-7.28856E-4
H	38	0.18485	67.987	6.2219	8.44125E-4
C	39	-0.15462	68.811	6.9606	-5.44038E-4
H	40	0.17332	70.053	7.8101	4.57189E-4
C	41	-0.22991	68.9	6.9624	-8.05291E-4
H	42	0.18523	70.181	7.8099	4.85622E-4
C	43	0.35679	67.3	5.9393	0.00184
C	44	-0.11243	64.048	4.6669	-0.00107
C	45	0.47087	59.861	3.4385	0.00943
C	46	0.37524	77.97	6.7574	8.07814E-4
C	47	-0.21595	88.584	6.7381	-5.54357E-5
H	48	0.1828	89.37	6.5682	2.19739E-5
C	49	-0.13361	97.057	7.3149	1.44689E-4
H	50	0.1739	103.178	7.529	-3.2986E-4
C	51	-0.05582	95.672	7.8999	4.16931E-5
C	52	-0.14603	102.614	8.6901	1.99169E-4
H	53	0.16852	108.07	8.8309	-3.16131E-4
C	54	-0.17481	100.589	9.4812	1.68543E-4
H	55	0.17147	104.234	10.0856	-1.95491E-4
C	56	-0.17473	92.797	9.5788	4.38285E-5
H	57	0.17451	92.033	10.2524	-2.77784E-5
C	58	-0.16115	86.064	8.9152	-6.56407E-5
H	59	0.17753	80.941	9.1986	1.55808E-4
C	60	-0.01743	86.507	7.9943	-7.83714E-6
C	61	-0.06644	77.505	7.4354	-1.22631E-4
C	62	-0.14191	54.939	9.3474	-4.40044E-4
H	63	0.17408	51.605	9.9547	5.14581E-4
C	64	-0.04761	58.219	9.7927	-1.23324E-4
C	65	-0.14943	56.165	11.0826	-3.195E-4
H	66	0.16817	53.048	11.6176	3.53272E-4
C	67	-0.18148	59.344	11.6449	-3.21841E-4
H	68	0.16819	58.269	12.5218	2.66079E-4
C	69	-0.16623	64.639	11.0729	-2.73886E-4
H	70	0.1694	66.577	11.6227	2.35109E-4
C	71	-0.1414	67.56	9.8444	-2.62679E-4
H	72	0.17718	71.997	9.5968	2.80432E-4
C	73	-0.02602	64.365	9.0942	-6.41971E-5
C	74	-0.06815	68.087	7.8972	-1.92342E-4
C	75	0.3765	64.366	7.4117	0.0014
C	76	-0.22801	57.388	8.2229	-8.57165E-4

H	77	0.18805	55.456	8.1108	7.64492E-4
C	78	0.46443	60.005	3.4581	0.00916
C	79	-0.1246	63.879	4.6815	-0.00118
C	80	0.34603	66.522	5.9836	0.00182
C	81	-0.20831	67.478	7.0113	-7.65542E-4
H	82	0.18404	68.648	7.868	5.10522E-4
C	83	-0.16536	67.027	6.9713	-6.26344E-4
H	84	0.17388	67.951	7.8193	5.03526E-4
C	85	-0.15329	65.669	5.9577	-8.3922E-4
H	86	0.19061	66.289	6.2389	9.2876E-4
C	87	-0.03564	63.375	4.6728	-3.45001E-4
C	88	0.45686	58.977	3.4413	0.00938
N	91	-0.64298	52.445	2.4923	-0.02976
N	92	-0.5239	62.5	3.8053	-0.00788
N	93	-0.64221	52.713	2.4881	-0.02964
N	94	-0.54502	60.992	3.8178	-0.00855
O	95	-0.58145	67.361	6.5484	-0.00246
O	96	-0.5827	70.203	6.3567	-0.0023
C	138	0.46022	59.165	3.4464	0.00937
C	139	-0.03875	63.732	4.6626	-3.72059E-4
C	140	-0.13974	67.098	5.9321	-7.28856E-4
H	141	0.18485	67.987	6.2219	8.44125E-4
C	142	-0.15462	68.811	6.9606	-5.44038E-4
H	143	0.17332	70.053	7.8101	4.57189E-4
C	144	-0.22991	68.9	6.9624	-8.05291E-4
H	145	0.18523	70.181	7.8099	4.85622E-4
C	146	0.35679	67.3	5.9393	0.00184
C	147	-0.11243	64.048	4.6669	-0.00107
C	148	0.47087	59.861	3.4385	0.00943
C	149	0.37524	77.97	6.7574	8.07814E-4
C	150	-0.21595	88.584	6.7381	-5.54357E-5
H	151	0.1828	89.37	6.5682	2.19739E-5
C	152	-0.13361	97.057	7.3149	1.44689E-4
H	153	0.1739	103.178	7.529	-3.2986E-4
C	154	-0.05582	95.672	7.8999	4.16931E-5
C	155	-0.14603	102.614	8.6901	1.99169E-4
H	156	0.16852	108.07	8.8309	-3.16131E-4
C	157	-0.17481	100.589	9.4812	1.68543E-4
H	158	0.17147	104.234	10.0856	-1.95491E-4
C	159	-0.17473	92.797	9.5788	4.38285E-5
H	160	0.17451	92.033	10.2524	-2.77784E-5
C	161	-0.16115	86.064	8.9152	-6.56407E-5
H	162	0.17753	80.941	9.1986	1.55808E-4
C	163	-0.01743	86.507	7.9943	-7.83714E-6

C	164	-0.06644	77.505	7.4354	-1.22631E-4
C	165	-0.14191	54.939	9.3474	-4.40044E-4
H	166	0.17408	51.605	9.9547	5.14581E-4
C	167	-0.04761	58.219	9.7927	-1.23324E-4
C	168	-0.14943	56.165	11.0826	-3.195E-4
H	169	0.16817	53.048	11.6176	3.53272E-4
C	170	-0.18148	59.344	11.6449	-3.21841E-4
H	171	0.16819	58.269	12.5218	2.66079E-4
C	172	-0.16623	64.639	11.0729	-2.73886E-4
H	173	0.1694	66.577	11.6227	2.35109E-4
C	174	-0.1414	67.56	9.8444	-2.62679E-4
H	175	0.17718	71.997	9.5968	2.80432E-4
C	176	-0.02602	64.365	9.0942	-6.41971E-5
C	177	-0.06815	68.087	7.8972	-1.92342E-4
C	178	0.3765	64.366	7.4117	0.0014
C	179	-0.22801	57.388	8.2229	-8.57165E-4
H	180	0.18805	55.456	8.1108	7.64492E-4
C	181	0.46443	60.005	3.4581	0.00916
C	182	-0.1246	63.879	4.6815	-0.00118
C	183	0.34603	66.522	5.9836	0.00182
C	184	-0.20831	67.478	7.0113	-7.65542E-4
H	185	0.18404	68.648	7.868	5.10522E-4
C	186	-0.16536	67.027	6.9713	-6.26344E-4
H	187	0.17388	67.951	7.8193	5.03526E-4
C	188	-0.15329	65.669	5.9577	-8.3922E-4
H	189	0.19061	66.289	6.2389	9.2876E-4
C	190	-0.03564	63.375	4.6728	-3.45001E-4
C	191	0.45686	58.977	3.4413	0.00938
N	192	-0.64298	52.445	2.4923	-0.02976
N	193	-0.5239	62.5	3.8053	-0.00788
N	194	-0.64221	52.713	2.4881	-0.02964
N	195	-0.54502	66.992	3.8178	-0.00689
O	196	-0.58145	67.361	6.5484	-0.00246
O	197	-0.5827	70.203	6.3567	-0.0023

2b′					
TClPP					0.08355
C	1	0.20343	59.269	3.4264	0.00417
C	2	-0.16868	60.281	4.6797	0.00217
H	3	0.17923	61.211	5.5165	0.00134
C	4	-0.18246	61.009	4.6736	-0.00191
H	5	0.18951	62.44	5.5087	0.00136
C	6	0.22386	60.614	3.449	0.00435
C	7	-0.03754	65.565	3.7688	-5.15398E-4

C	8	0.1937	67.301	3.3769	0.00309
C	9	-0.1825	74.288	4.5162	-0.00114
H	10	0.18978	76.756	5.3286	7.21867E-4
C	11	-0.18063	75.175	4.508	-0.00107
H	12	0.18722	78.132	5.3177	6.41889E-4
C	13	0.20458	69.348	3.3622	0.00301
C	14	-0.0502	62.974	3.7642	-7.58931E-4
C	15	-0.02787	66.029	5.2504	-1.93634E-4
C	16	-0.14812	76.984	5.9614	-4.42528E-4
H	17	0.17919	84.406	5.6599	2.57049E-4
C	18	-0.18312	76.368	7.3374	-3.77915E-4
H	19	0.19089	81.225	7.9145	2.19166E-4
C	20	0.00269	68.748	7.9926	7.19548E-6
C	21	-0.18301	60.616	7.501	-7.52364E-4
H	22	0.19301	56.88	8.1618	7.46319E-4
C	23	-0.14585	57.786	6.172	-9.62188E-4
H	24	0.18664	50.503	6.0199	0.00154
C	25	-0.03952	69.259	5.2365	-2.40617E-4
C	26	-0.13464	79.436	5.906	-3.33611E-4
H	27	0.19086	85.946	5.5596	2.05796E-4
C	28	-0.17818	79.514	7.2982	-2.87011E-4
H	29	0.19616	84.137	7.8485	1.53351E-4
C	30	0.00885	72.726	7.9802	1.94535E-5
C	31	-0.18665	65.264	7.5402	-6.47596E-4
H	32	0.19017	61.967	8.2297	6.22105E-4
C	33	-0.15246	62.441	6.2109	-8.62027E-4
H	34	0.18448	56.293	6.1069	0.00129
N	89	-0.65505	60.073	2.4251	-0.0262
N	90	-0.65602	55.79	2.4405	-0.02919
Cl	97	-0.05478	73.826	9.7218	-7.61116E-5
Cl	98	-0.04429	69.813	9.7335	-7.6051E-5
C	100	0.20343	65.121	3.4264	0.00344
C	101	-0.16868	65.625	4.6797	-0.0015
H	102	0.17923	66.795	5.5165	0.00109
C	103	-0.18246	65.105	4.6736	-0.00166
H	104	0.18951	66.123	5.5087	0.00119
C	105	0.22386	63.694	3.449	0.00393
C	106	-0.03754	66.205	3.7688	-5.02696E-4
C	107	0.1937	65.421	3.3769	0.00333
C	108	-0.1825	71.249	4.5162	-0.00136
H	109	0.18978	74.166	5.3286	8.59727E-4
C	110	-0.18063	70.657	4.508	-0.00139
H	111	0.18722	73.286	5.3177	8.97627E-4
C	112	0.20458	64.07	3.3622	0.00373

C	113	-0.0502	69.056	3.7642	-5.97023E-4
C	114	-0.02787	72.208	5.2504	-1.45634E-4
C	115	-0.14812	83.106	5.9614	-2.35846E-4
H	116	0.17919	90.513	5.6599	-2.36099E-5
C	117	-0.18312	82.485	7.3374	-2.09712E-4
H	118	0.19089	87.348	7.9145	6.64726E-5
C	119	0.00269	74.818	7.9926	5.19875E-6
C	120	-0.18301	66.586	7.501	-6.09319E-4
H	121	0.19301	62.761	8.1618	6.25176E-4
C	122	-0.14585	63.74	6.172	-7.98592E-4
H	123	0.18664	56.297	6.0199	0.00135
C	124	-0.03952	69.609	5.2365	-2.36731E-4
C	125	-0.13464	80.863	5.906	-2.88959E-4
H	126	0.19086	87.923	5.5596	1.05501E-4
C	127	-0.17818	80.83	7.2982	-2.51321E-4
H	128	0.19616	85.77	7.8485	1.10731E-4
C	129	0.00885	73.456	7.9802	1.86549E-5
C	130	-0.18665	65.361	7.5402	-6.45215E-4
H	131	0.19017	61.718	8.2297	6.27177E-4
C	132	-0.15246	62.334	6.2109	-8.65111E-4
H	133	0.18448	55.486	6.1069	0.00132
N	134	-0.65505	56.25	2.4251	-0.02917
N	135	-0.65602	60.57	2.4405	-0.02551
Cl	136	-0.05478	74.612	9.7218	-7.25046E-5
Cl	137	-0.04429	75.874	9.7335	-5.37856E-5
Y	1.68573				
$Pc(OBNP)_2$					0.07556
C	35	0.50518	59.165	3.4464	0.01028
C	36	-0.04508	63.732	4.6626	-4.32634E-4
C	37	-0.12432	67.098	5.9321	-6.48125E-4
H	38	0.18848	67.987	6.2219	8.60298E-4
C	39	-0.13571	68.811	6.9606	-4.77279E-4
H	40	0.17985	70.053	7.8101	4.74192E-4
C	41	-0.21119	68.9	6.9624	-7.39375E-4
H	42	0.19182	70.181	7.8099	5.02663E-4
C	43	0.37174	67.3	5.9393	0.00192
C	44	-0.11715	64.048	4.6669	-0.00111
C	45	0.51212	59.861	3.4385	0.01025
C	46	0.3663	77.97	6.7574	7.88199E-4
C	47	-0.22487	88.584	6.7381	-5.76984E-5
H	48	0.18036	89.37	6.5682	2.16705E-5
C	49	-0.13161	97.057	7.3149	1.42456E-4

H	50	0.17523	103.178	7.529	-3.32227E-4
C	51	-0.05565	95.672	7.8999	4.15467E-5
C	52	-0.1458	102.614	8.6901	1.98763E-4
H	53	0.17047	108.07	8.8309	-3.1964E-4
C	54	-0.16705	100.589	9.4812	1.60986E-4
H	55	0.1746	104.234	10.0856	-1.98966E-4
C	56	-0.16873	92.797	9.5788	4.23036E-5
H	57	0.1776	92.033	10.2524	-2.8257E-5
C	58	-0.16122	86.064	8.9152	-6.56385E-5
H	59	0.1789	80.941	9.1986	1.56937E-4
C	60	-0.01816	86.507	7.9943	-8.16155E-6
C	61	-0.06229	77.505	7.4354	-1.14917E-4
C	62	-0.13366	54.939	9.3474	-4.14268E-4
H	63	0.17728	51.605	9.9547	5.23795E-4
C	64	-0.04553	58.219	9.7927	-1.17881E-4
C	65	-0.14527	56.165	11.0826	-3.10459E-4
H	66	0.17127	53.048	11.6176	3.59616E-4
C	67	-0.17225	59.344	11.6449	-3.05329E-4
H	68	0.17207	58.269	12.5218	2.72089E-4
C	69	-0.15727	64.639	11.0729	-2.59001E-4
H	70	0.17226	66.577	11.6227	2.38966E-4
C	71	-0.14591	67.56	9.8444	-2.7093E-4
H	72	0.17659	71.997	9.5968	2.79368E-4
C	73	-0.02637	64.365	9.0942	-6.50302E-5
C	74	-0.06956	68.087	7.8972	-1.96229E-4
C	75	0.36776	64.366	7.4117	0.00137
C	76	-0.23485	57.388	8.2229	-8.82465E-4
H	77	0.18606	55.456	8.1108	7.56048E-4
C	78	0.50914	60.005	3.4581	0.01003
C	79	-0.12628	63.879	4.6815	-0.0012
C	80	0.35953	66.522	5.9836	0.00189
C	81	-0.18679	67.478	7.0113	-6.86134E-4
H	82	0.19059	68.648	7.868	5.28444E-4
C	83	-0.1439	67.027	6.9713	-5.44803E-4
H	84	0.18058	67.951	7.8193	5.22683E-4
C	85	-0.14248	65.669	5.9577	-7.79673E-4
H	86	0.19467	66.289	6.2389	9.48098E-4
C	87	-0.03825	63.375	4.6728	-3.70093E-4
C	88	0.50004	58.977	3.4413	0.01026
N	91	-0.65322	52.445	2.4923	-0.03022
N	92	-0.52303	62.5	3.8053	-0.00786
N	93	-0.65157	52.713	2.4881	-0.03006
N	94	-0.54817	60.992	3.8178	-0.0086
O	95	-0.57914	67.361	6.5484	-0.00245

O	96	-0.58369	70.203	6.3567	-0.00231
C	138	0.50518	59.165	3.4464	0.01028
C	139	-0.04508	63.732	4.6626	-4.32634E-4
C	140	-0.12432	67.098	5.9321	-6.48125E-4
H	141	0.18848	67.987	6.2219	8.60298E-4
C	142	-0.13571	68.811	6.9606	-4.77279E-4
H	143	0.17985	70.053	7.8101	4.74192E-4
C	144	-0.21119	68.9	6.9624	-7.39375E-4
H	145	0.19182	70.181	7.8099	5.02663E-4
C	146	0.37174	67.3	5.9393	0.00192
C	147	-0.11715	64.048	4.6669	-0.00111
C	148	0.51212	59.861	3.4385	0.01025
C	149	0.3663	77.97	6.7574	7.88199E-4
C	150	-0.22487	88.584	6.7381	-5.76984E-5
H	151	0.18036	89.37	6.5682	2.16705E-5
C	152	-0.13161	97.057	7.3149	1.42456E-4
H	153	0.17523	103.178	7.529	-3.32227E-4
C	154	-0.05565	95.672	7.8999	4.15467E-5
C	155	-0.1458	102.614	8.6901	1.98763E-4
H	156	0.17047	108.07	8.8309	-3.1964E-4
C	157	-0.16705	100.589	9.4812	1.60986E-4
H	158	0.1746	104.234	10.0856	-1.98966E-4
C	159	-0.16873	92.797	9.5788	4.23036E-5
H	160	0.1776	92.033	10.2524	-2.8257E-5
C	161	-0.16122	86.064	8.9152	-6.56385E-5
H	162	0.1789	80.941	9.1986	1.56937E-4
C	163	-0.01816	86.507	7.9943	-8.16155E-6
C	164	-0.06229	77.505	7.4354	-1.14917E-4
C	165	-0.13366	54.939	9.3474	-4.14268E-4
H	166	0.17728	51.605	9.9547	5.23795E-4
C	167	-0.04553	58.219	9.7927	-1.17881E-4
C	168	-0.14527	56.165	11.0826	-3.10459E-4
H	169	0.17127	53.048	11.6176	3.59616E-4
C	170	-0.17225	59.344	11.6449	-3.05329E-4
H	171	0.17207	58.269	12.5218	2.72089E-4
C	172	-0.15727	64.639	11.0729	-2.59001E-4
H	173	0.17226	66.577	11.6227	2.38966E-4
C	174	-0.14591	67.56	9.8444	-2.7093E-4
H	175	0.17659	71.997	9.5968	2.79368E-4
C	176	-0.02637	64.365	9.0942	-6.50302E-5
C	177	-0.06956	68.087	7.8972	-1.96229E-4
C	178	0.36776	64.366	7.4117	0.00137
C	179	-0.23485	57.388	8.2229	-8.82465E-4
H	180	0.18606	55.456	8.1108	7.56048E-4

C	181	0.50914	60.005	3.4581	0.01003
C	182	-0.12628	63.879	4.6815	-0.0012
C	183	0.35953	66.522	5.9836	0.00189
C	184	-0.18679	67.478	7.0113	-6.86134E-4
H	185	0.19059	68.648	7.868	5.28444E-4
C	186	-0.1439	67.027	6.9713	-5.44803E-4
H	187	0.18058	67.951	7.8193	5.22683E-4
C	188	-0.14248	65.669	5.9577	-7.79673E-4
H	189	0.19467	66.289	6.2389	9.48098E-4
C	190	-0.03825	63.375	4.6728	-3.70093E-4
C	191	0.50004	58.977	3.4413	0.01026
N	192	-0.65322	52.445	2.4923	-0.03022
N	193	-0.52303	62.5	3.8053	-0.00786
N	194	-0.65157	52.713	2.4881	-0.03006
N	195	-0.54817	66.992	3.8178	-0.00693
O	196	-0.57914	67.361	6.5484	-0.00245
O	197	-0.58369	70.203	6.3567	-0.00231