Electronic Supplementary Information

Novel method for preparing stable near-infrared absorbers: a new phthalocyanine family based on rhenium(I) complexes

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1. Experimental details

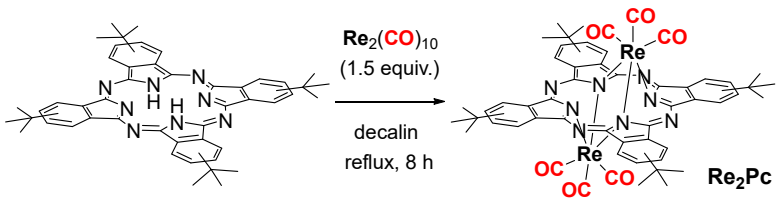
General procedures

Materials: $Re_2(CO)_{10}$ was purchased from Merck KGaA. The precursor, tetra-*tert*-butyl-29H,31H-phthalocyanine, was synthesized according to a literature procedure.[1] Here, *tert*-butyl groups were introduced to the macrocycle to just improve the solubility in organic solvents, and it was reasonably assumed that the electronic structures of the Pc ring were almost unchanged. Chloroform, decalin, and pyridine were purchased from Wako Pure Chemical Industries, Ltd.. Toluene was purchased from Kanto Chemical Co., Inc.. All of the chemicals were used as received without further purification.

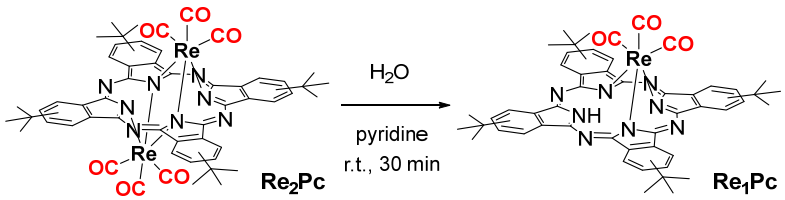
Photophysical Measurements: UV-Vis absorption spectra were recorded with a V-570 UV/visible/NIR spectrophotometer (JASCO Co., Ltd.). MCD spectra for the Q band (> 500 nm) and B band (< 500 nm) regions were measured with a JASCO E-250 instrument equipped with a JASCO electromagnet (+1.35 to −1.35 T) and a JASCO J-720 spectrodichrometer equipped with a JASCO permanent magnet (0.47 T), respectively. ESI-MS spectra were measured with a Bruker HCT Ultra 125 spectrometer with chloroform/MeOH eluent. FT-IR spectra were measured with a JASCO FT/IR 4100typeA spectrometer using KBr pellets. NMR spectra were measured with a JEOL Resonance ECS 400 spectrometer.

Theoretical Study: DFT and TD-DFT calculations were performed with the Gaussian 16 package using the B3LYP functional.[2] The LANL2DZ and 6-31G(d,p) basis sets were used for the Re atom and other atoms, respectively.[3] To address solvent effects, the polarizable continuum model (PCM, toluene) was used for excited states.[4] For validation, the vibrational frequencies were calculated for the optimized geometry of the ground state. The orbital plots and graphical representations were produced with Molekel.[5] For the strong ligand-field of CO, $[Re(CO)_3]^+$ complexes are known to show diamagnetism, which are consistent with the NMR data of **Re_2Pc** and **Re_1Pc** (shown below). Thus, the DFT and TD-DFT calculations were carried out using S = 0.

Preparations



(Tetra-*tert*-butyl-phthalocyaninato)bis(tricarbonylrhenium(I) (**Re_2Pc**): Under a nitrogen atmosphere, a mixture of tetra-*tert*-butyl-29H,31H-phthalocyanine (60.7 mg, 0.0821 mmol) and $Re_2(CO)_{10}$ (80.7 mg, 0.124 mmol) was refluxed in decalin (10 mL) for 8 h. The crude product was purified by silica-gel column chromatography (*n*-hexane → $CHCl_3$/*n*-hexane = 2/3 eluents) to give an analytically pure product of **Re_2Pc** (93.4 mg, 0.0731 mmol, 89.0% yield). UV–Vis (toluene, λ_{max}/nm (10^{-4} ε /L mol^{-1} cm^{-1})): 362 (4.52), 599 (1.06), 798 (7.24) nm. IR (KBr pellet, ν(CO)/cm^{-1}): 1915, 2026. ESI-MS: *m/z* = 1278 $[M]^+$. ^{1}H NMR (400 MHz, $CDCl_3$, r.t., δ /ppm): δ 9.57, 9.54 (s, 4 H, Pc), 9.51–9.43 (m, 4 H, Pc), 8.42 (d, J = 8.0 Hz, 4 H, Pc), 1.81–1.79 (m, 36 H, ^{t}Bu). Anal. found (calcd for $C_{54}H_{48}N_8O_6Re_2$): C 49.81 (50.77), H 3.79 (3.79), N 8.00 (8.77).



(Tetra-*tert*-butyl-phthalocyaninato)tricarbonylrhenium(I) (**Re_1Pc**): Under air, **Re_2Pc** (77.5 mg, 0.0606 mmol) was dissolved in pyridine and then the solution was stirred at room temperature for 30 min. After removal of the solvent, the crude product was purified by gel-permeation chromatography ($CHCl_3$ eluent) to give an analytically pure product of **Re_1Pc** (52.9 mg, 0.0525 mmol, 87.3% yield). UV–Vis (toluene, λ_{max}/nm (10^{-4} ε /L mol^{-1} cm^{-1})): 349 (4.76), 553 (0.861), 745 (11.1). IR (KBr pellet, ν(CO)/cm^{-1}): 1908, 2023. ESI-MS: *m/z* = 1008 $[M]^+$. ^{1}H NMR (400 MHz, $CDCl_3$, r.t., δ /ppm): δ 9.59–9.16 (m, 8 H, Pc), 8.42–8.23 (m. 4 H, Pc), 1.79–1.73 (m, 36 H, ^{t}Bu), -1.28−-1.42 (m, 1 H, N–H). Anal. found (calcd for $C_{51}H_{49}N_8O_3Re$): C 59.97 (60.76), H 5.09 (4.90), N 10.16 (11.11).

2. Spectroscopic observations

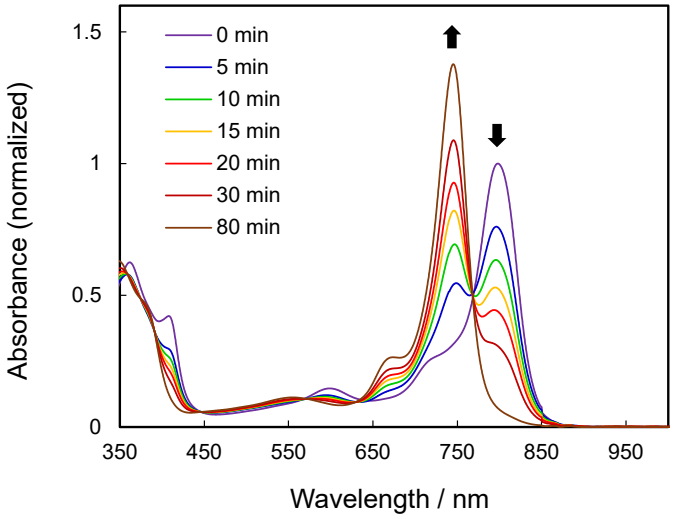


Fig. S1 Electronic absorption spectral changes during the demetallation reaction of **Re_2Pc** to form **Re_1Pc**: Time course after the addition of pyridine (150 μL) to a toluene solution of **Re_2Pc** (0.01 mM, 3mL). An isosbestic point was observed at 759 nm.

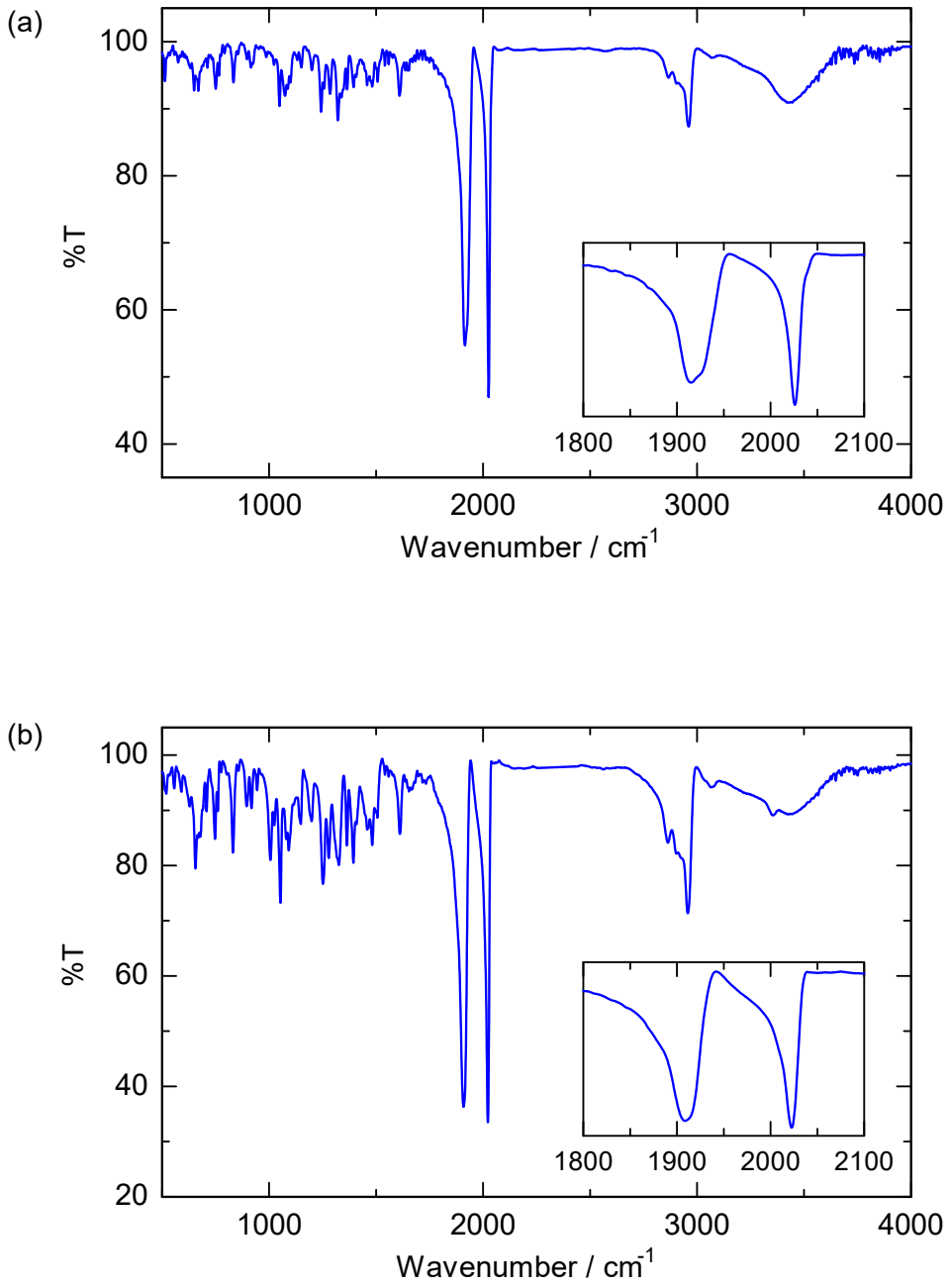
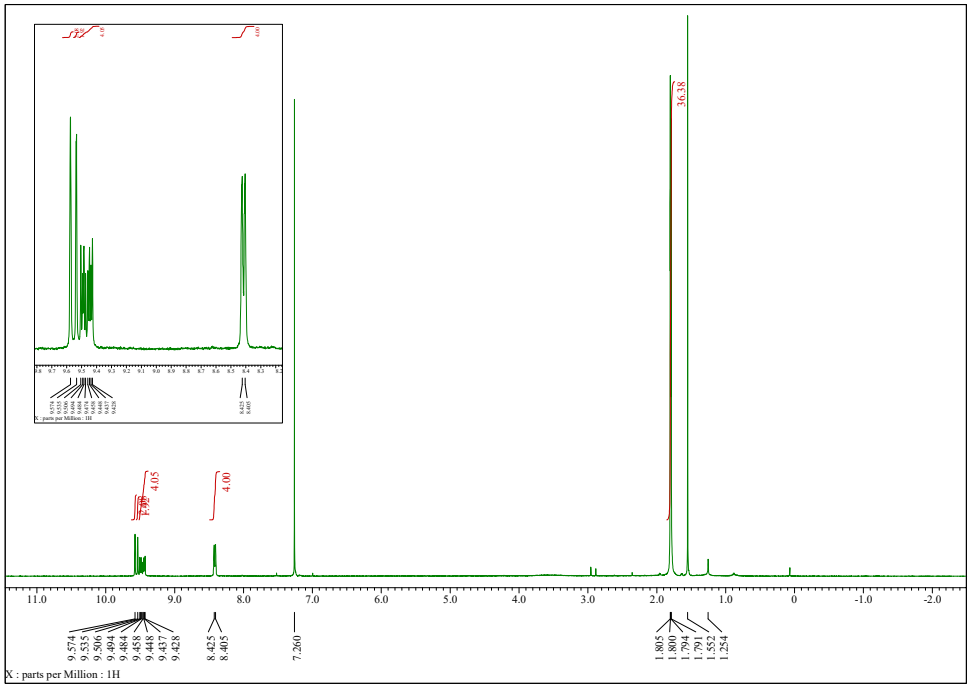


Fig. S2 FT-IR spectra of (a) **Re_2Pc** and (b) **Re_1Pc** (KBr pellet).

(a)



(b)

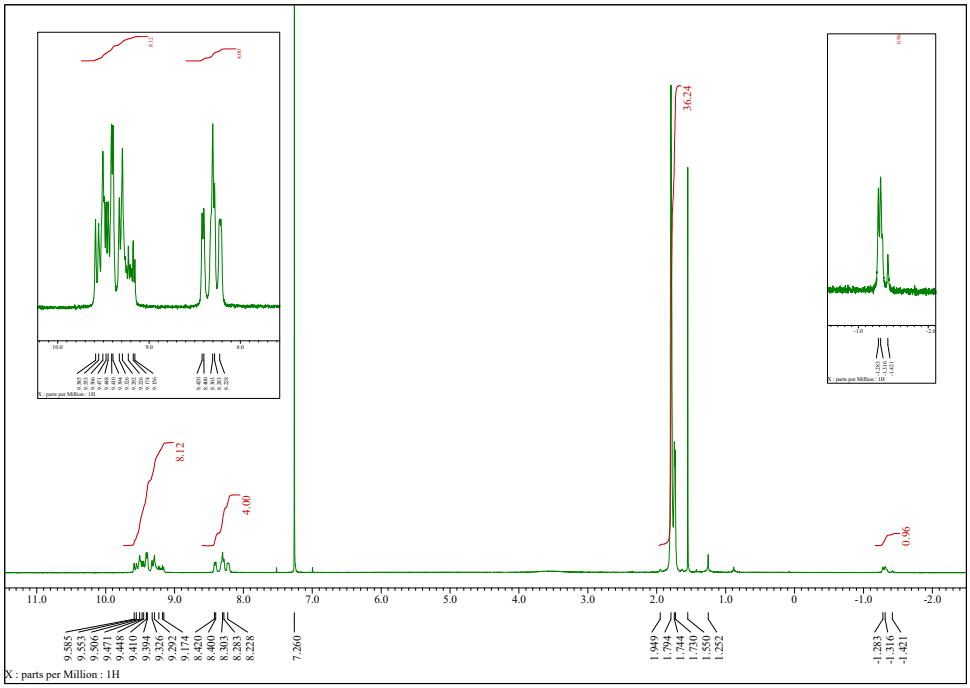


Fig. S3 ^{1}H NMR spectra of (a) **Re_2Pc** and (b) **Re_1Pc** (400 MHz, $CDCl_3$, r.t.).

3. Electrochemistry

Table S1 Electrochemical data (vs. Fc/Fc^{+}) of the Pc complexes.[a]

Complex	$E^{1+/0}$ / V	$E^{0/1-}$ / V	$E^{1-/2-}$ / V
Re_2Pc	+0.52 (0.08)	-0.96 (0.08)	-1.36 (0.08)
Re_1Pc	+0.32 (0.08)	-1.17 (0.07)	-1.56 (0.08)
ZnPc	+0.11 (0.07)	-1.20 (0.06)	-1.67 (0.08)

[a]Obtained in CH_2Cl_2 with 0.1 M [*n*-Bu_4N](PF_6). The numbers in parentheses are the differences between the anodic and cathodic waves (V).

4. Tolerance to oxidation

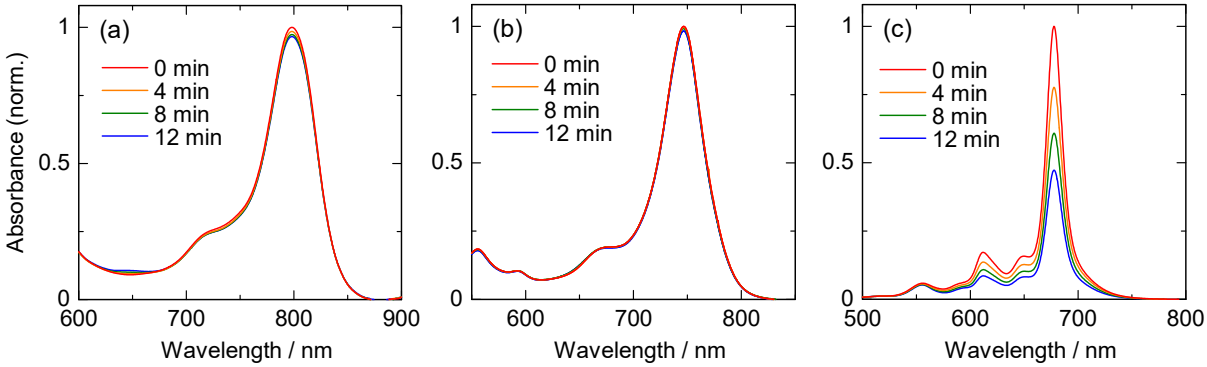


Fig. S4 Electronic absorption spectral changes in the Q band region of (a) **Re_2Pc**, (b) **Re_1Pc** and (c) **ZnPc** under light irradiation ($\lambda_{irr.}$ = 425 nm) in the presence of germanium tetraphenylporphyrin dihydroxide (**GeTPP(OH)$_2$**) as a singlet oxygen generator. Condition: A toluene solution of the corresponding Pc (5×10^{-6} M) and **GeTPP(OH)$_2$** (absorbance at 425 nm: 1.4) was irradiated by blue LED under air. After the light irradiation for 12 min, the bleaching (53 %) of the Q band was observed in **ZnPc**, those were negligibly small in **Re_1Pc** and **Re_2Pc**.

4. DFT analyses

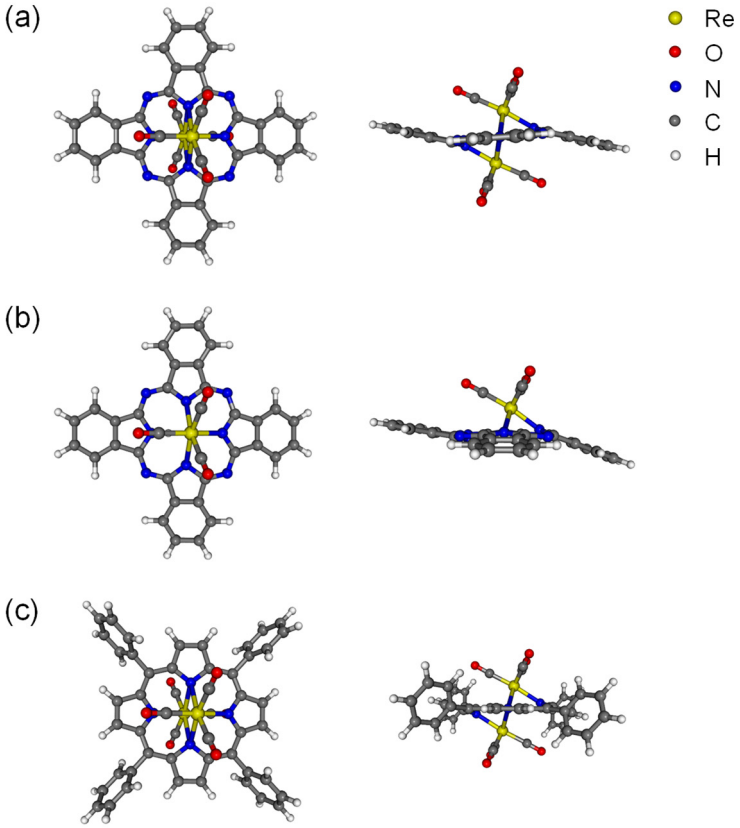


Fig. S5 Top and side views of the optimized structures of (a) **Re_2Pc'**, (b) **Re_1Pc'** and (c) **Re_2TPP** obtained by DFT.

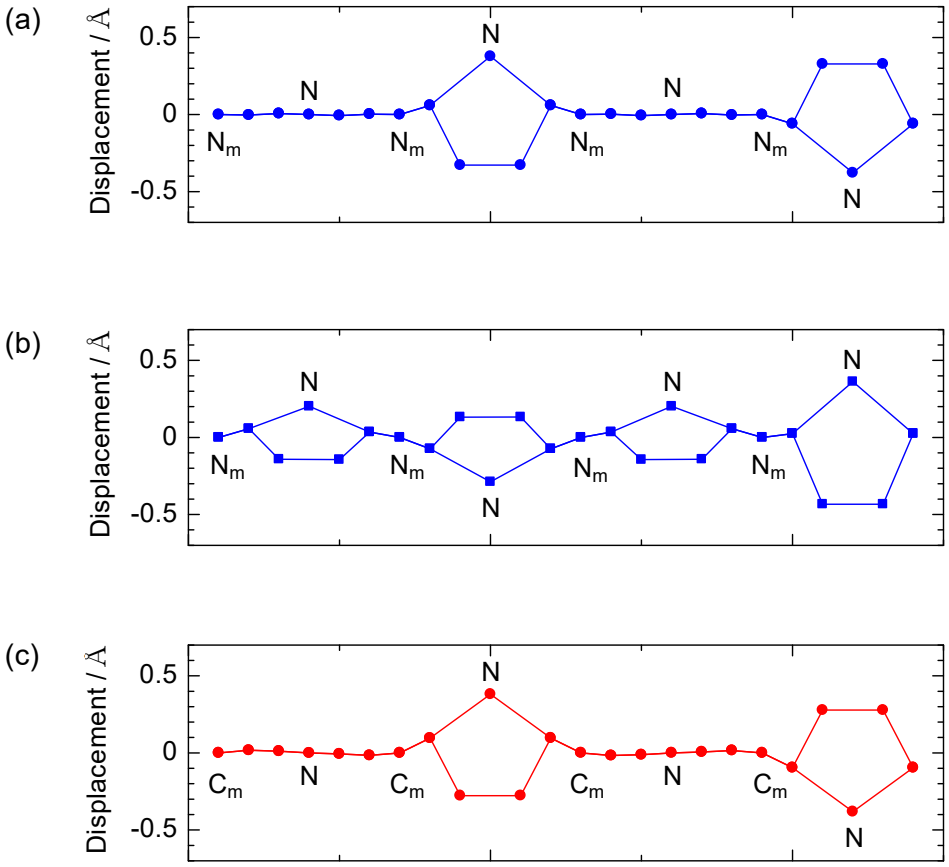
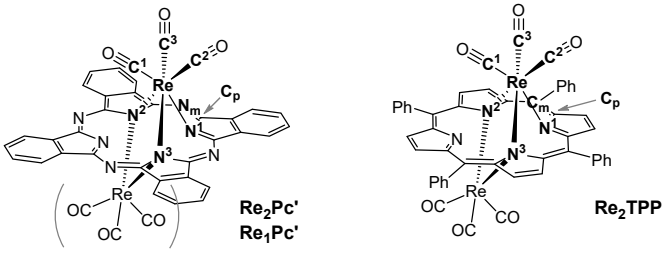


Fig. S6 Plots of the skeletal deviation of the atoms from the $4N_m$ / $4C_m$ mean plane for (a) **Re_2Pc'**, (b) **Re_1Pc'** and (c) **Re_2TPP**. "N" indicates a nitrogen atom in pyrrol units, and "N_m" and "C_m" indicate nitrogen and carbon atoms at *meso*-positions, respectively.

Table S2 Selected bond lengths and a dihedral angle of the rhenium coordination environment in the rhenium phthalocyanine and porphyrin complexes.

Complex	Bond Length / Å						Dihedral Angle / °
	l (Re-N1)	*l* (Re-N2)	*l* (Re-N3)	*l* (Re-C1)	*l* (Re-C2)	*l* (Re-C3)	θ (X_m-C_p-N1-Re)[c]
Re_2Pc'[a]	2.175	2.429	2.429	1.935	1.907	1.907	26.3
Re_1Pc'[a]	2.156	2.396	2.396	1.936	1.913	1.913	25.4
Re_2TPP[a]	2.190	2.459	2.461	1.935	1.902	1.903	28.9
Re_2TPP (exp)[b]	2.169	2.382	2.407	1.868	1.847	1.854	28.5

[a]Based on the optimized structure calculated at B3LYP/LanL2DZ (for Re), 6-31G(d,p) (for other atoms) level. [b]Based on the structure experimentally obtained by X-ray single crystal structure analysis.[6] [c]X_m: nitrogen / carbon atoms at *meso*-positions. C_p: β-pyrrolic carbon atoms adjacent to the pyrrolic nitrogens.



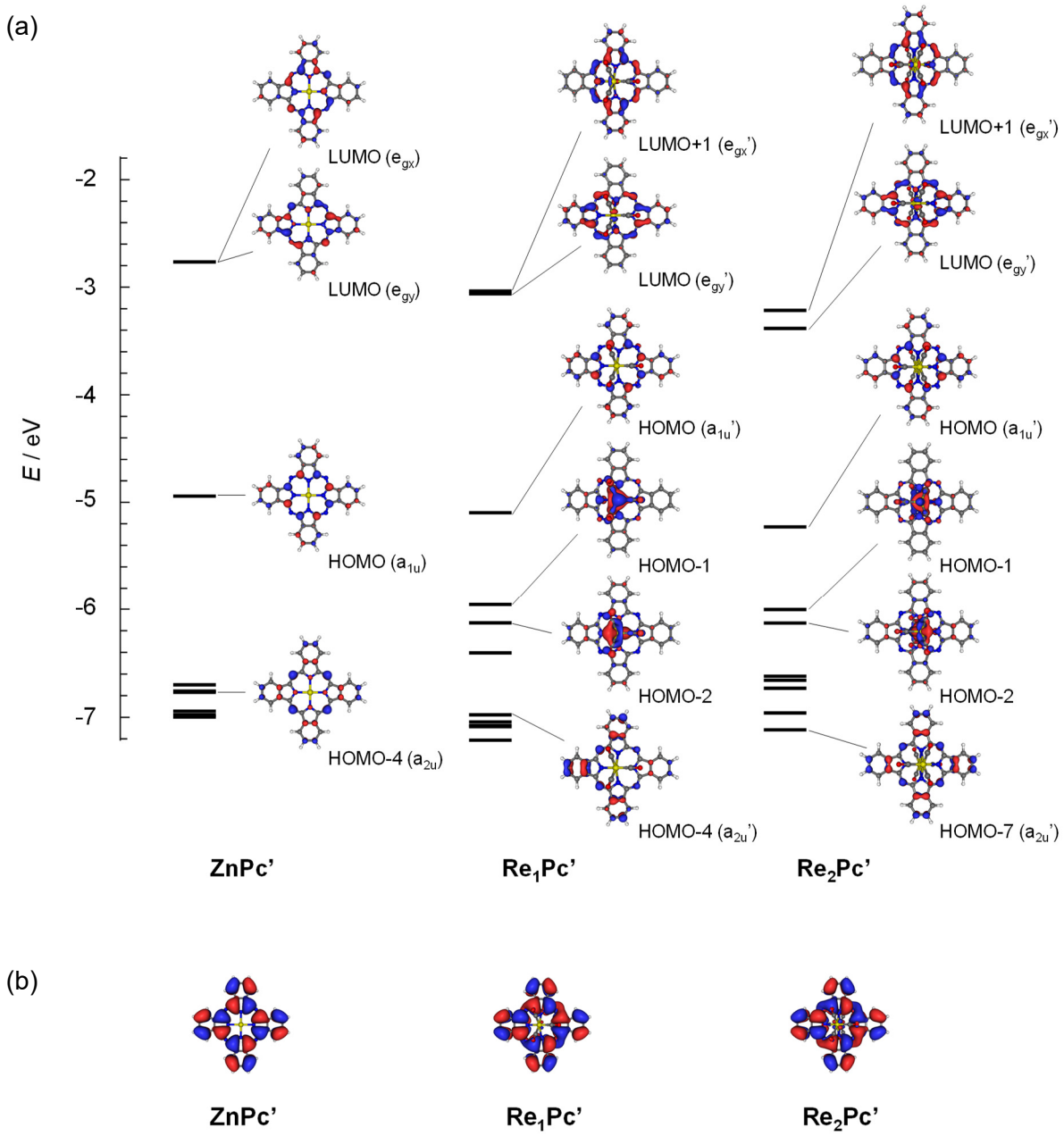


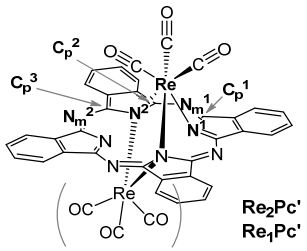
Fig. S7 (a) Molecular orbital energies and distributions (isosurface value: 0.03), and (b) HOMO distributions (isosurface value: 0.008) of **ZnPc'**, **Re$_1$Pc'** and **Re$_2$Pc'** calculated by DFT. For **ZnPc'**, the a_{1u}, a_{2u}, e_{gx} and e_{gy} orbitals in the Gouterman's four orbital model were calculated to be the HOMO, HOMO-4 and degenerate LUMOs, respectively. The notations of a_{1u}', a_{2u}', e_{gy}' and e_{gx}' are used for the a_{1u}- and a_{2u}-like π orbitals and e_{gy}- and e_{gx}-like π* orbitals of **Re$_1$Pc'** and **Re$_2$Pc'**, respectively.

Table S3 Selected natural atomic orbital (NAO) charges and Mulliken charges of the optimized structures of **ZnPc'**, **Re_1Pc'** and **Re_2Pc'** calculated by DFT.[a]

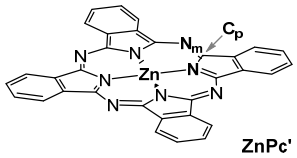
Complex	Natural Atomic Orbital Charges							
	M	N1	N2	$C_p^{1\,b}$	$C_p^{2\,b}$	$C_p^{3\,b}$	$N_m^{1\,c}$	$N_m^{2\,c}$
ZnPc'	+1.337	-0.697	---	+0.446	---	---	-0.495	---
Re_1Pc'	-0.782	-0.502	-0.549	+0.469	+0.456	+0.452	-0.488	-0.492
Re_2Pc'	-0.717	-0.514	-0.563	+0.468	+0.470	+0.471	-0.484	-0.484

Complex	Mulliken Atomic Charges							
	M	N1	N2	$C_p^{1\,b}$	$C_p^{2\,b}$	$C_p^{3\,b}$	$N_m^{1\,c}$	$N_m^{2\,c}$
ZnPc'	+1.156	-0.704	---	+0.380	---	---	-0.433	---
Re_1Pc'	+0.435	-0.576	-0.563	+0.383	+0.381	+0.372	-0.429	-0.424
Re_2Pc'	+0.489	-0.557	-0.627	+0.371	+0.400	+0.400	-0.424	-0.424

[a]Analysis based on the optimized structures calculated at B3LYP/LanL2DZ (for Re), 6-31G(d,p) (for other atoms) level. [b]β-pyrrolic carbon aoms adjascent to the pyrrolic nitrogens. [c]nitrogen atoms at *meso*-positions.



Re_2Pc'
Re_1Pc'



ZnPc'

Table S4 Excitation energies and compositions of the selected excited singlet states of **ZnPc'**, **Re_1Pc'** and **Re_2Pc'** calculated by TD-DFT (transition percentage ≥ 10% except for the S_{1x} and S_{1y} states).[a]

Complex	State	*E* / eV	*f*	Compositions[a]	
ZnPc′	S_{1x}	1.997	0.6161	96%	HOMO (π(Pc), a_{1u}) → LUMO (π^*(Pc), e_{gy})
				4%	HOMO-4 (π(Pc), a_{2u}) → LUMO (π^*(Pc), e_{gx})
	S_{1y}	1.997	0.6161	96%	HOMO (π(Pc), a_{1u}) → LUMO (π^*(Pc), e_{gx})
				4%	HOMO-4 (π(Pc), a_{2u}) → LUMO (π^*(Pc), e_{gy})
	S_{9x}	3.614	0.3172	45%	HOMO-7 (π(Pc)) → LUMO (π^*(Pc), e_{gx})
				42%	HOMO-4 (π(Pc), a_{2u}) → LUMO (π^*(Pc), e_{gx})
	S_{9y}	3.614	0.3172	45%	HOMO-7 (π(Pc)) → LUMO (π^*(Pc), e_{gx})
				42%	HOMO-4 (π(Pc), a_{2u}) → LUMO (π^*(Pc), e_{gy})
	S_{13x}	3.690	0.7305	53%	HOMO-8 (π(Pc)) → LUMO (π^*(Pc), e_{gx})
				18%	HOMO-4 (π(Pc), a_{2u}) → LUMO (π^*(Pc), e_{gx})
				11%	HOMO-7 (π(Pc)) → LUMO (π^*(Pc), e_{gx})
	S_{13y}	3.690	0.7307	53%	HOMO-8 (π(Pc)) → LUMO (π^*(Pc), e_{gy})
				18%	HOMO-4 (π(Pc), a_{2u}) → LUMO (π^*(Pc), e_{gy})
				11%	HOMO-7 (π(Pc)) → LUMO (π^*(Pc), e_{gy})
Re_1Pc′	S_{1x}	1.817	0.4442	93%	HOMO (π(Pc), a_{1u}') → LUMO (π^*(Pc), e_{gy}')
				5%	HOMO-1 (dπ(Re)) → LUMO+1 (π^*(Pc), e_{gx}')
	S_{1y}	1.819	0.4017	95%	HOMO (π(Pc), a_{1u}') → LUMO+1 (π^*(Pc), e_{gx}')
				2%	HOMO-1 (dπ(Re)) → LUMO (π^*(Pc), e_{gy}')
	S_{2x}	2.303	0.0172	97%	HOMO-1 (dπ(Re)) → LUMO (π^*(Pc), e_{gy}')
	S_{2y}	2.358	0.0837	93%	HOMO-1 (dπ(Re)) → LUMO+1 (π^*(Pc), e_{gx}')
	S_{3x}	2.455	0.0425	98%	HOMO-2 (dπ(Re)) → LUMO (π^*(Pc), e_{gy}')
	S_{3y}	2.478	0.0243	98%	HOMO-2 (dπ(Re)) → LUMO+1 (π^*(Pc), e_{gx}')
	S_{9x}	3.392	0.0173	41%	HOMO-7 (π(Pc)) → LUMO (π^*(Pc), e_{gy}')
				33%	HOMO-6 (π(Pc) + dπ(Re)) → LUMO+1 (π^*(Pc), e_{gx}')
				13%	HOMO-11 (π(Pc)) → LUMO (π^*(Pc), e_{gy}')
	S_{9y}	3.414	0.1109	31%	HOMO-7 (π(Pc)) → LUMO+1 (π^*(Pc), e_{gx}')
				24%	HOMO-8 (π(Pc)) → LUMO (π^*(Pc), e_{gy}')
				16%	HOMO-11 (π(Pc)) → LUMO+1 (π^*(Pc), e_{gx}')
				15%	HOMO-4 (π(Pc), a_{2u}') → LUMO (π^*(Pc), e_{gy}')
	S_{12x}	3.469	0.1773	62%	HOMO-4 (π(Pc), a_{2u}') → LUMO (π^*(Pc), e_{gy}')
				13%	HOMO-7 (π(Pc)) → LUMO+1 (π^*(Pc), e_{gx}')
				11%	HOMO-11 (π(Pc)) → LUMO+1 (π^*(Pc), e_{gx}')
	S_{12y}	3.501	0.4672	83%	HOMO-4 (π(Pc), a_{2u}') → LUMO+1 (π^*(Pc), e_{gx}')
Re_2Pc′	S_{1x}	1.640	0.3595	96%	HOMO (π(Pc), a_{1u}') → LUMO (π^*(Pc), e_{gy}')
	S_{1y}	1.691	0.2320	88%	HOMO (π(Pc), a_{1u}') → LUMO+1 (π^*(Pc), e_{gx}')
				6%	HOMO-2 (dπ(Re)) → LUMO (π^*(Pc), e_{gy}')
				5%	HOMO-1 (dπ(Re)) → LUMO (π^*(Pc), e_{gy}')
	S_{2x}	1.971	0.0077	94%	HOMO-1 (dπ(Re)) → LUMO (π^*(Pc), e_{gy}')
	S_{3x}	2.135	0.1079	91%	HOMO-2 (dπ(Re)) → LUMO (π^*(Pc), e_{gy}')
	S_{2y}	2.160	0.0220	94%	HOMO-1 (dπ(Re)) → LUMO+1 (π^*(Pc), e_{gx}')
	S_{3y}	2.278	0.0286	96%	HOMO-2 (dπ(Re)) → LUMO+1 (π^*(Pc), e_{gx}')
	S_{10x}	3.278	0.3573	81%	HOMO-7 (π(Pc), a_{2u}') → LUMO (π^*(Pc), e_{gy}')
				13%	HOMO (π(Pc), a_{1u}') → LUMO+5 (dπ(Re) + π^*(Pc))
	S_{17}	3.410	0.1652	79%	HOMO (π(Pc), a_{1u}') → LUMO+5 (dπ(Re) + π^*(Pc))
				11%	HOMO-7 (π(Pc), a_{2u}') → LUMO (π^*(Pc), e_{gy}')
	S_{10y}	3.474	0.6296	76%	HOMO-7 (π(Pc), a_{2u}') → LUMO+1 (π^*(Pc), e_{gx}')
				16%	HOMO (π(Pc), a_{1u}') → LUMO+3 (π^*(Pc))

[a]In the TD-DFT calculation for **ZnPc'**, the a_{1u}, a_{2u}, e_{gx} and e_{gy} orbitals in the Gouterman's four orbital model were calculated to be the HOMO, HOMO-4 and degenerate LUMOs, respectively. The notations of a_{1u}', a_{2u}', e_{gy}' and e_{gx}' are used for the a_{1u}- and a_{2u}-like π orbitals and e_{gy}- and e_{gx}-like π^* orbitals of **Re_1Pc'** and **Re_2Pc'**, respectively.

Table S5 Cartesian coordinates and ZPE corrected total energy of the optimized structures.

Re_2Pc(S_0) E_{tot} = -2505.5545 a.u.

Re	0.22229	-0.00001	-1.63371
Re	-0.22227	0.00003	1.63366
O	1.01979	-2.13071	-3.69274
C	0.70907	-1.33506	-2.90585
C	-1.55739	-0.00005	-2.39387
N	-0.00005	1.78411	-0.00008
N	2.12007	0.00000	-0.57052
N	0.00002	-1.78414	0.00004
C	0.70908	1.33498	-2.90591
O	-2.61854	-0.00001	-2.86225
C	-1.12386	2.63719	0.10407
C	1.12376	2.63720	-0.10413
C	2.87714	1.10870	-0.31898
C	2.87717	-1.10868	-0.31898
C	1.12383	-2.63721	-0.10408
C	-1.12379	-2.63723	0.10415
O	1.01978	2.13058	-3.69287
C	-0.70903	-1.33496	2.90588
C	-0.70904	1.33509	2.90580
C	1.55740	0.00006	2.39385
C	0.69874	4.01850	-0.05624
C	-0.69884	4.01849	0.05617
C	4.25235	-0.70584	-0.05361
C	4.25233	0.70589	-0.05361
N	2.41058	2.34349	-0.21707
C	-0.69876	-4.01852	0.05624
C	0.69882	-4.01851	-0.05618
N	2.41063	-2.34348	-0.21707
N	-2.12008	-0.00002	0.57051
N	-2.41065	2.34347	0.21709
N	-2.41059	-2.34352	0.21713
O	-1.01972	-2.13056	3.69284
O	-1.01975	2.13074	3.69270
O	2.61856	0.00010	2.86218
C	-2.87716	-1.10872	0.31902
C	-2.87718	1.10866	0.31900
C	-1.42371	-5.21494	0.11749
C	1.42379	-5.21491	-0.11744
C	5.41226	-1.42735	0.22590
C	5.41223	1.42742	0.22591
C	1.42369	5.21490	-0.11748
C	-1.42381	5.21489	0.11742
C	-4.25238	0.70582	0.05368
C	-4.25236	-0.70592	0.05369
C	-0.70445	-6.40229	0.05720
C	0.70455	-6.40228	-0.05716
C	6.57853	-0.70357	0.47584
C	6.57851	0.70367	0.47585
C	0.70444	6.40227	-0.05720
C	-0.70456	6.40226	0.05715
H	-2.50444	-5.20102	0.20549
H	2.50452	-5.20098	-0.20544
H	5.40202	-2.51201	0.24277
H	5.40196	2.51209	0.24279
H	2.50443	5.20098	-0.20546
H	-2.50454	5.20096	0.20541
C	-5.41230	1.42731	-0.22581
C	-5.41226	-1.42745	-0.22578
H	-1.23023	-7.35159	0.09797
H	1.23034	-7.35157	-0.09795
H	7.50405	-1.23327	0.68072
H	7.50402	1.23339	0.68073
H	1.23022	7.35156	-0.09797
H	-1.23035	7.35156	0.09792
C	-6.57857	0.70353	-0.47570
C	-6.57855	-0.70371	-0.47569
H	-5.40206	2.51198	-0.24269
H	-5.40200	-2.51212	-0.24264
H	-7.50410	1.23323	-0.68056
H	-7.50407	-1.23343	-0.68054

Re_1Pc(S_0) E_{tot} = -2086.9435 a.u.

Re	0.21911	0.00003	1.11654
O	1.06994	2.13173	3.16091
C	0.73880	1.34240	2.37619
C	0.73869	-1.34258	2.37599
C	-1.54979	0.00025	1.90295
N	-0.05913	-1.86977	-0.35533
N	-0.05913	1.86978	-0.35534
N	2.05271	0.00001	-0.01811
O	1.06976	-2.13215	3.16051
O	-2.61805	0.00000	2.35809
C	1.06776	-2.68577	-0.40665
C	-1.14612	-2.68568	-0.61277
C	-1.14614	2.68568	-0.61278
C	1.06774	2.68579	-0.40667
C	2.79771	1.11081	-0.29511
C	2.79772	-1.11078	-0.29512
C	-0.71926	-4.07161	-0.75684
C	0.67671	-4.06942	-0.63862
N	-2.43466	-2.37087	-0.75565
C	0.67668	4.06944	-0.63862
C	-0.71929	4.07160	-0.75685
N	-2.43468	2.37085	-0.75566
C	4.15678	-0.70499	-0.64201
C	4.15678	0.70504	-0.64201
N	2.35413	-2.35666	-0.35723
N	2.35411	2.35669	-0.35723
C	-2.88690	-1.14282	-0.86755
C	-2.88691	1.14280	-0.86755
C	1.41827	5.24535	-0.76553
C	-1.42463	5.24940	-1.01024
C	5.29943	-1.42667	-0.98506
C	5.29942	1.42673	-0.98505
C	-1.42459	-5.24941	-1.01024
C	1.41832	-5.24532	-0.76554
C	-4.26758	0.70791	-0.77528
C	-4.26758	-0.70795	-0.77527
N	-2.13344	-0.00001	-1.01913
C	0.71562	6.42588	-1.00026
C	-0.68844	6.42796	-1.11968
C	6.45009	-0.70358	-1.30168
C	6.45009	0.70365	-1.30167
C	-0.68838	-6.42796	-1.11968
C	0.71568	-6.42586	-1.00027
H	2.49957	5.22967	-0.68067
H	-2.50485	5.23888	-1.10927
H	5.28760	2.51153	-0.99780
H	2.49961	-5.22963	-0.68068
H	5.28761	-2.51148	-0.99781
H	-2.50481	-5.23890	-1.10927
C	-5.45947	1.42738	-0.65133
C	-5.45946	-1.42743	-0.65132
H	1.25643	7.36285	-1.09595
H	-1.20279	7.36705	-1.30185
H	7.36285	-1.23360	-1.55739
H	7.36284	1.23368	-1.55738
H	-1.20272	-7.36706	-1.30186
H	1.25650	-7.36282	-1.09597
H	-1.12600	-0.00001	-1.11364
C	-6.64401	0.70527	-0.54658
C	-6.64401	-0.70532	-0.54658
H	-5.45003	2.51202	-0.63783
H	-5.45001	-2.51206	-0.63782
H	-7.58807	1.23422	-0.45689
H	-7.58806	-1.23427	-0.45689

Re2TPP(S_0) E_{tot} = -2750.9958 a.u.

C	-2.99901	1.12563	0.12395
C	-2.47158	2.42019	0.02393
C	-3.52277	-3.46947	-0.13116
C	-3.60503	-4.22495	-1.31254
C	-4.56844	-5.22416	-1.45070
C	-5.46357	-5.48536	-0.41085
C	-5.39273	-4.73903	0.76688
C	-4.43277	-3.73574	0.90468
C	-3.45566	3.53610	-0.12916
C	-4.36984	3.81098	0.90081
C	-5.31097	4.83183	0.76217
C	-4.33848	0.72298	-0.23728
C	-5.35867	5.58768	-0.41064
C	-4.45931	5.31825	-1.44473
C	-3.51476	4.30136	-1.30572
C	1.32637	-0.01449	2.45599
C	-0.96840	1.34153	2.80416
C	-0.99371	-1.32744	2.80212
C	-4.35162	-0.63975	-0.23743
C	-3.02010	-1.06811	0.12332
C	-2.51747	-2.37232	0.02181
C	-1.14405	-2.69817	-0.00841
C	-0.72011	-4.06171	-0.00770
C	0.64186	-4.07481	-0.00212
C	-1.09200	2.71978	-0.00459
N	-2.24417	0.02132	0.40159
N	-0.01773	-1.84309	-0.00059
O	2.34753	-0.02401	3.00818
O	-1.33472	2.13969	3.56759
O	-1.37523	-2.11982	3.56419
Re	-0.39803	0.00231	1.57901
C	1.09199	-2.71967	0.00431
C	-0.64191	4.07495	0.00144
N	0.01772	1.84328	0.00045
Re	0.39815	-0.00237	-1.57902
C	2.47154	-2.42010	-0.02405
C	0.72006	4.06188	0.00698
C	1.14401	2.69833	0.00816
C	-1.32631	0.01457	-2.45583
C	0.96816	-1.34192	-2.80392
C	0.99391	1.32703	-2.80252
N	2.24425	-0.02117	-0.40154
C	2.99900	-1.12550	-0.12379
C	3.45562	-3.53604	0.12884
C	2.51747	2.37248	-0.02169
O	-2.34744	0.02417	-3.00808
O	1.33432	-2.14034	-3.56715
O	1.37521	2.11931	-3.56478
C	3.02011	1.06825	-0.12298
C	4.33838	-0.72290	0.23782
C	4.36981	-3.81068	-0.90119
C	3.51470	-4.30157	1.30522
C	3.52272	3.46960	0.13149
C	4.35151	0.63984	0.23814
C	5.31094	-4.83155	-0.76277
C	4.45926	-5.31847	1.44401
C	3.60346	4.22638	1.31216
C	4.43426	3.73459	-0.90333
C	5.35864	-5.58765	0.40987
C	4.56684	5.22556	1.45059
C	5.39421	4.73785	-0.76526
C	5.46351	5.48546	0.41175
H	-2.91740	-4.01565	-2.12667
H	-4.62337	-5.79411	-2.37372
H	-6.21259	-6.26445	-0.51896
H	-6.08281	-4.93857	1.58160
H	-4.37252	-3.16089	1.82408
H	-4.32760	3.22868	1.81649
H	-6.00442	5.03763	1.57247
H	-5.13107	1.39536	-0.52946
H	-6.09304	6.38050	-0.51942
H	-4.49646	5.89553	-2.36408
H	-2.82416	4.08571	-2.11565
H	-5.15703	-1.29675	-0.52961
H	-1.38322	-4.91231	0.00698
H	1.28846	-4.93794	-0.02086
H	-1.28851	4.93808	0.01994
H	1.38315	4.91248	-0.00801
H	5.13089	-1.39530	0.53017
H	4.32756	-3.22817	-1.81674
H	2.82407	-4.08611	2.11517
H	5.15684	1.29677	0.53067
H	6.00441	-5.03715	-1.57311
H	4.49641	-5.89596	2.36323
H	2.91464	4.01811	2.12554
H	4.37523	3.15877	-1.82220
H	6.09304	-6.38048	0.51849
H	4.62056	5.79652	2.37307
H	6.08549	4.93638	-1.57922
H	6.21252	6.26454	0.52007

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