

Electronic Supplementary Information

Molecular Assembly-induced Charge Transfer between Mixed (Phthalocyaninato)(porphyrinato) Yttrium Triple-decker and Fullerene

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Experimental Section

General remarks. All the reagents and solvents were used as received. The compound of sandwich-type triple-decker mixed (phthalocyaninato)(porphyrinato) yttrium(III) [(TCIPP)Y(Pc)Y(TCIPP)] (**1**) was prepared according to the published procedure.¹ ¹H NMR spectra were recorded on a Bruker DPX 400 spectrometer in CDCl₃. Spectra were referenced against tetramethylsilane (TMS, $\delta = 0$ for ¹H NMR). Electronic absorption spectra were recorded on a Hitachi U-4100 spectrophotometer. Steady-state fluorescence spectroscopic studies were performed on an F 4500 (Hitachi). Electrochemical measurements were carried out with a BAS CV-50W voltammetric analyzer. The cell comprised inlets for a glassy carbon-disk working electrode with a diameter of 2.0 mm and a silver wire counter electrode. The reference electrode was Ag⁺/Ag (a solution of 0.01 M AgNO₃ and 0.1 M TBAP in *o*-dichlorobenzene), which was connected to the solution by a Luggin capillary, whose tip was placed close to the working electrode. It was corrected for junction potentials by being referenced internally to the ferrocenium/ferrocene (Fc⁺/Fc) couple [$E_{1/2}(\text{Fc}^+/\text{Fc}) = 0.229$ V for C₆₀ and 0.210 V for **1**]. Typically, a 0.1 M solution of [NBu₄][ClO₄] in *o*-dichlorobenzene containing a 1 mM sample was purged with nitrogen for 10 min, and then the voltammograms were recorded at ambient temperature. Crystal data of the compound **2** was collected on a Oxford Diffraction Gemini E diffractometer with Mo *K* α radiation ($\lambda = 0.7107$ Å) at 150 K. Final unit cell parameters were derived by global refinements of reflections obtained from integration of all the frame data. The collected frames were integrated by using the preliminary cell-orientation matrix. CrysAlisPro Agilent Technologies software was used for collecting frames of data, indexing reflections, and determination of lattice

constants; CrysAlisPro Agilent Technologies for integration of intensity of reflections and scaling, SCALE3 ABSPACK for absorption correction, The structures were solved by the direct method (*SHELXS-97*) and refined by full-matrix least-squares (*SHELXL-97*) on F^2 .² Anisotropic thermal parameters were used for the nonhydrogen atoms and isotropic parameters for the hydrogen atoms. Hydrogen atoms were added geometrically and refined using a riding model. ‘Crystallographic data and other pertinent information for all the complexes are summarized in Table S3. Selected structural information is listed in the Table S4. CCDC 1001326 for **2**, contains the supplementary crystallographic data for this paper. These data can be obtained free of charge from the Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif.

Synthesis of [(TCIPP)Y(Pc)Y(TCIPP)]·C₆₀ (2**)** Single crystals of cocrystallized fullerene-mixed(phthalocyaninato)(porphyrinato) yttrium **2** were obtained by simple diffusion of the *n*-hexane (15 mL) into the chloroform/*o*-dichlorobenzene (1:1) solution (5 mL) containing mixed (phthalocyaninato)(porphyrinato) yttrium(III) triple-decker complex **1** (0.004 mmol) and C₆₀ (2.8 mg, 0.002 mmol) with the yield of 23-41% (computed on the basis of **1**).

Photocurrent measurement. Photoelectric conversions were conducted on the CHI 760E workstation (CH Instruments, Inc.) with a three-electrode photoelectric conversion cell. The three-electrode system was filled with alcohol solution of tetra-*n*-butylammonium hexafluorophosphate (0.10 M). ITO modified by nanofilms was served as a working electrode, an Ag⁺/Ag electrode (a solution of 0.01 M AgNO₃ and 0.1 M tetra-*n*-butylammonium hexafluorophosphate in alcohol) employed as reference

electrode which was connected to the solution by a Luggin capillary and a platinum wire was employed as counter electrode. The working electrode was fixed at 0 V versus Ag⁺/Ag. The cell was purged with N₂ for 20 min, and light from a xenon lamp equipped with a 365 nm cut-off filter was illuminated to the modified ITO electrode to extract photocurrent. The monochromatic light was extracted from xenon lamp (PLS-SXE 300) by optical band-pass filters (for example CEL-QD 365, 365 ± 10 nm).

Computational detail. All structures were optimized at B3LYP-D3(BJ)/BSI level in the gas phase, where BSI represent a basis set with 6-311G(d) for C, H, N, Cl and LanL2DZ for Y atoms.³⁻⁷ Visual Molecular Dynamics (VMD) software package was employed to visualize the reduced density gradient (RDG) and static charge transfer isosurface.^{8,9} All calculations were carried out by Gaussian 09 D.01 and Multiwfn 3.4 version.^{10,11}

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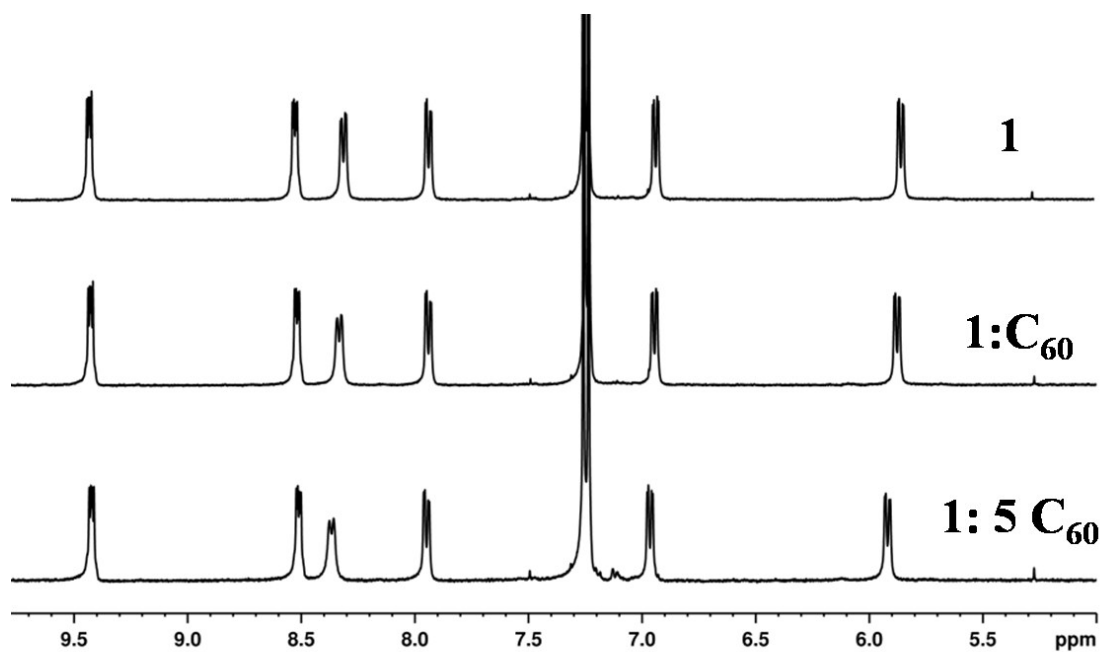


Figure S1. The downfield region of the ^1H NMR spectra (400 MHz) of the solutions of **1**, **1** + C_{60} , and **1** + 5 C_{60} , in $\text{CDCl}_3/\text{CS}_2$ (2:1, v:v).

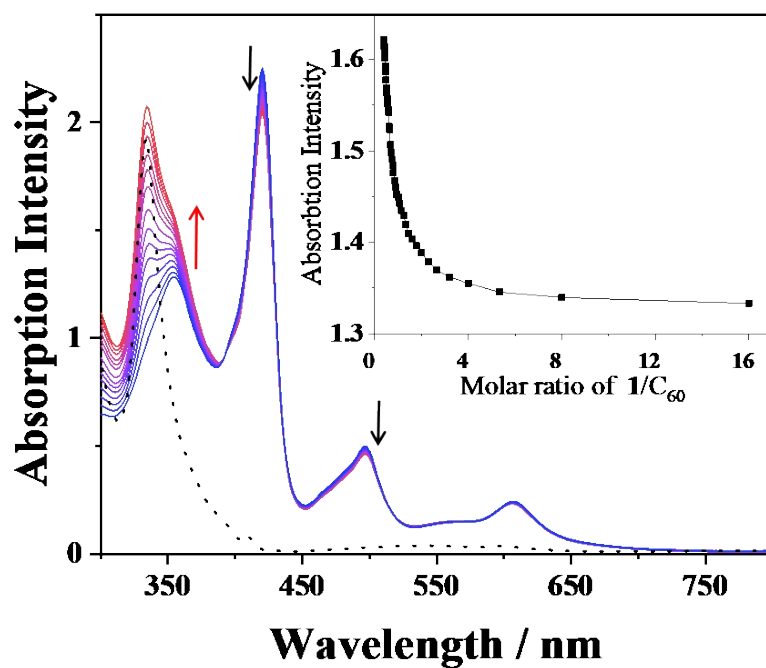


Figure S2. Electronic absorption spectrum of **1** in *o*-dicholobenzene with the concentration of 8.0×10^{-6} M upon addition of C₆₀. Changed intensity at 354 nm is shown in the insert diagram. The absorption of C₆₀ is drawn by dash line.

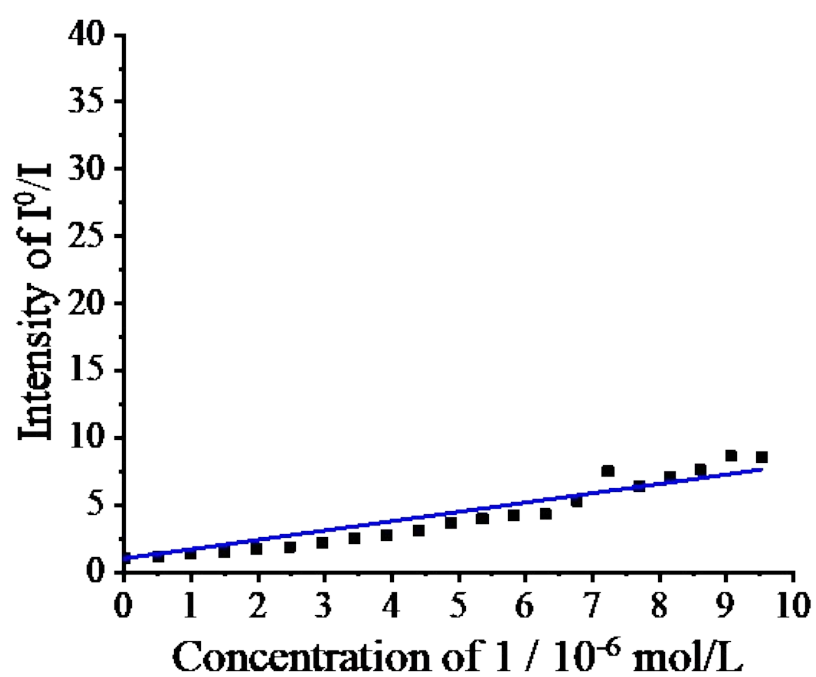


Figure S3. Stern-Volmer plot for the fluorescent spectral change of C_{60} at 450 nm upon addition of 1.

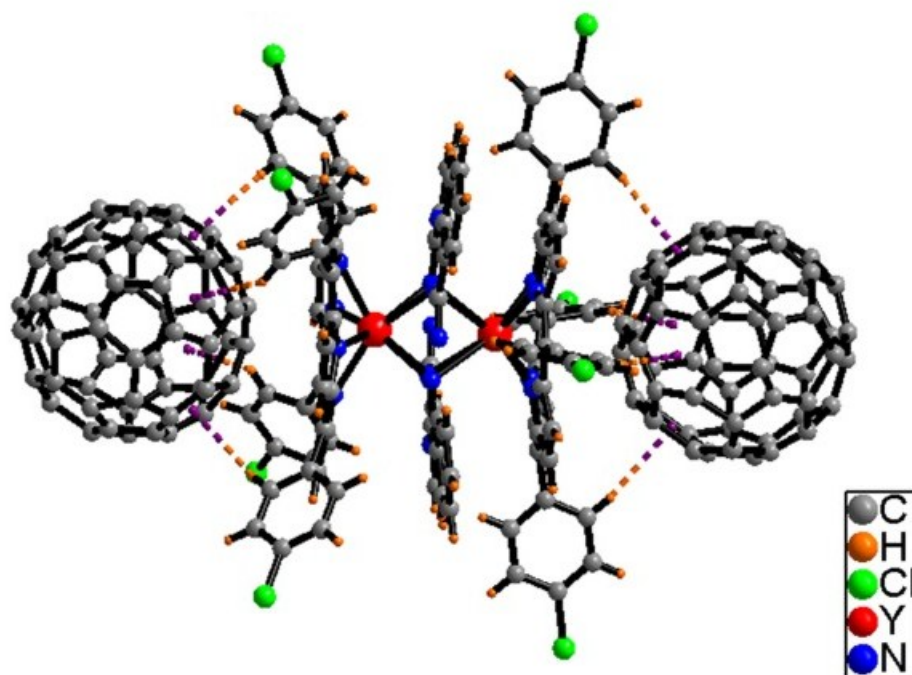


Figure S4. Molecular structure of **2** with the detailed C-H... π interaction. Selected hydrogen atoms and all solvent molecules omitted for clarity.

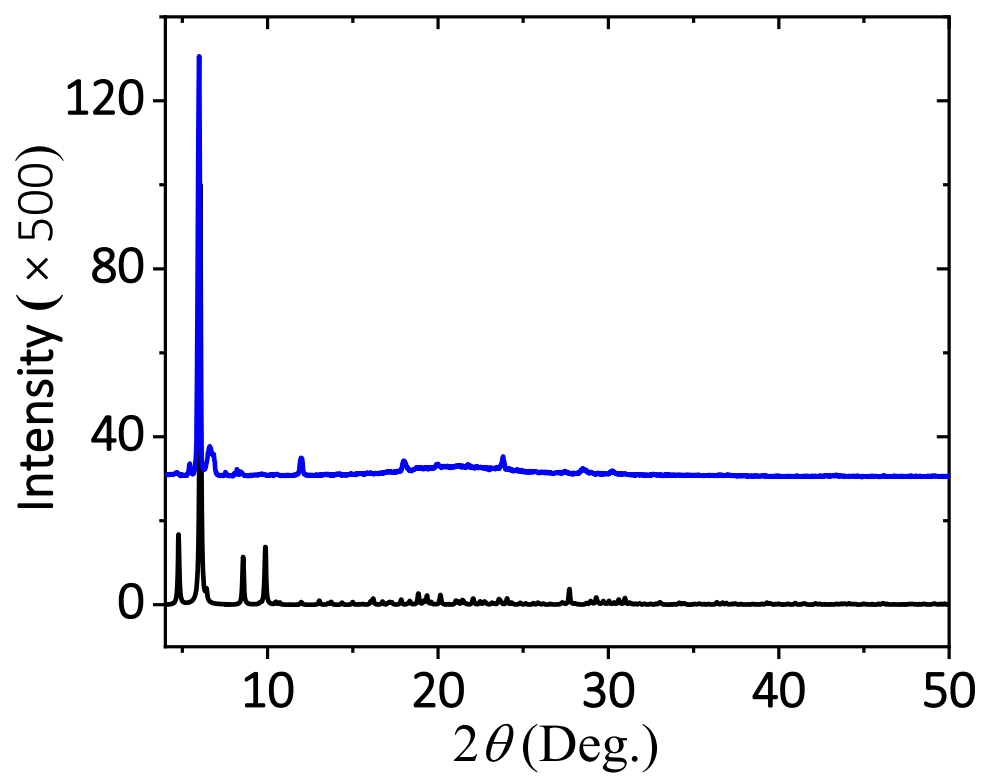


Figure S5. Powder X-ray diffraction of **2**. The experimental and simulated results are shown in blue and black, respectively.

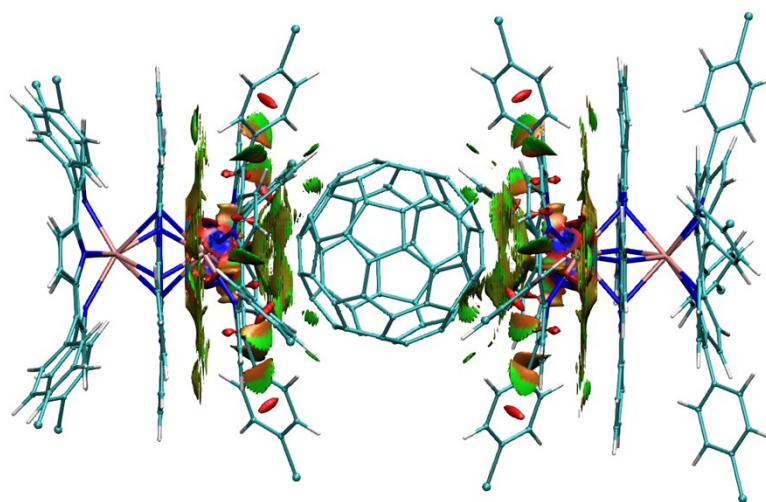


Figure S6. The RDG analysis of **2**. The isosurface between C₆₀ and porphyrin suggests the strong interaction between two molecules and the isosurface between the porphyrin and phthalocyanine in triple-decker molecule suggests the presence of intramolecular π - π interaction between these two kinds of macrocycles.

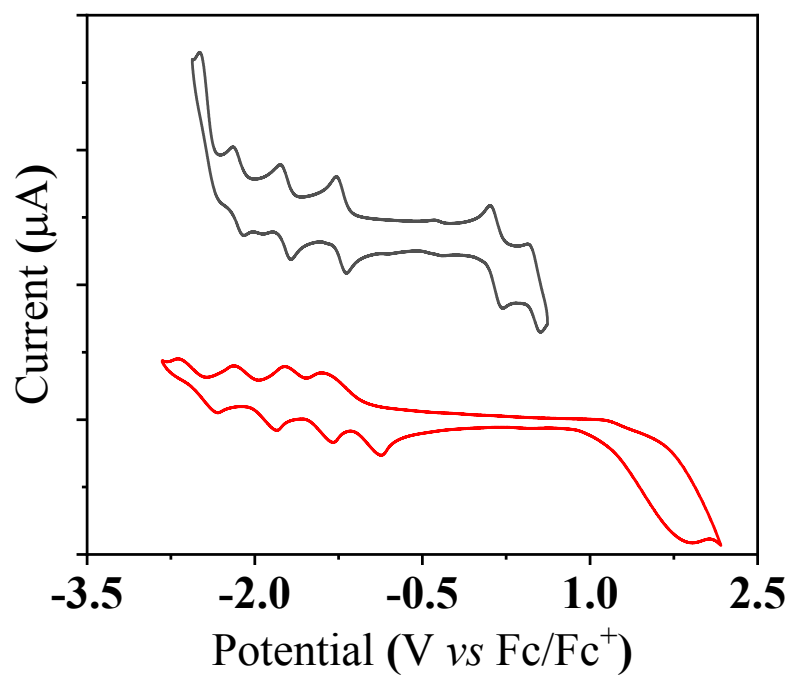


Figure S7. Cyclic voltammogram of **1** (grey) and C₆₀ (red) in o-dichlorobenzene containing 0.1 M [NBu₄][ClO₄] at a scan rate of 40 mV/s.

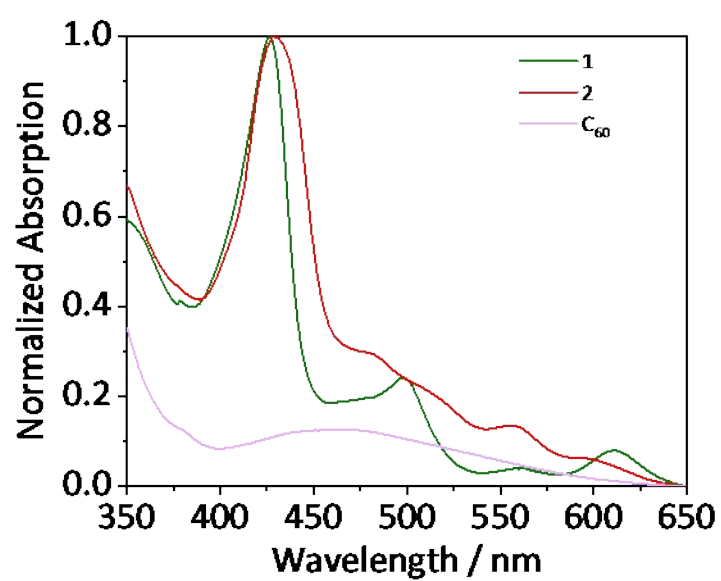


Figure S8. Solid UV-vis absorption spectra of **1**, **2** and C₆₀.

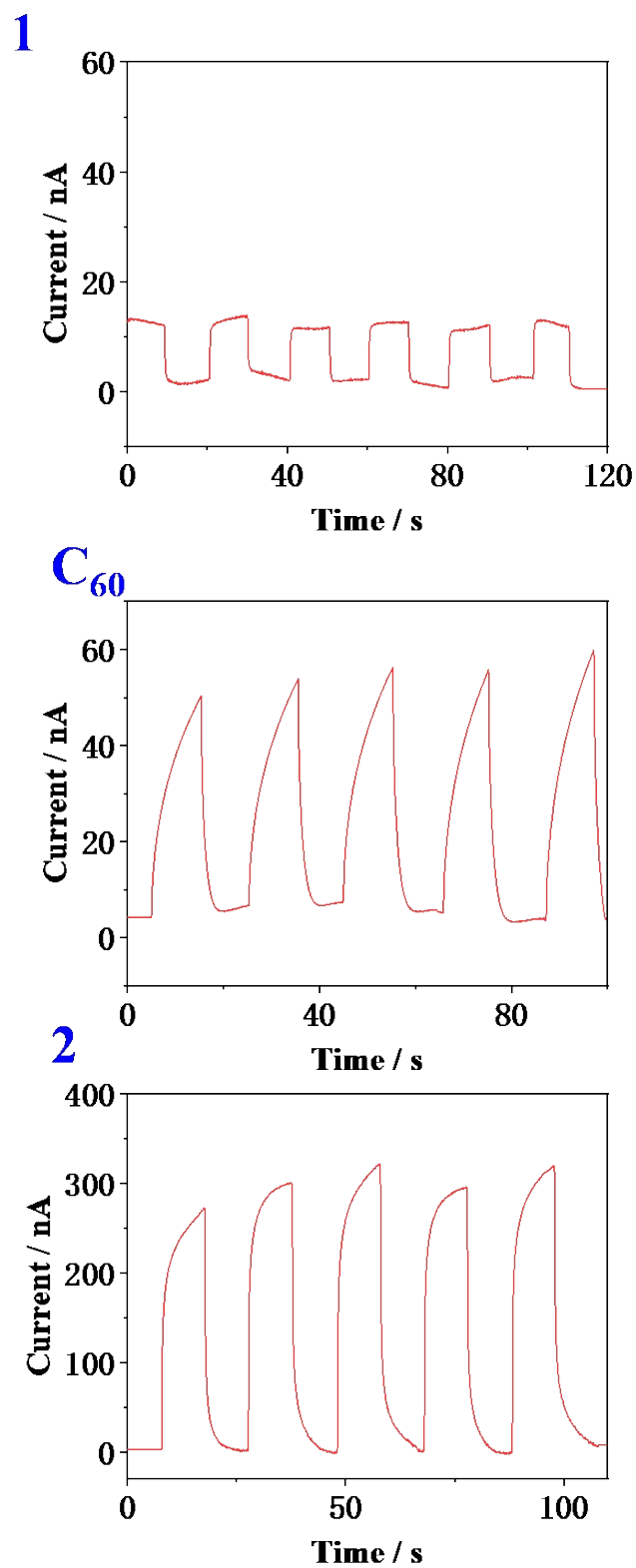


Figure S9. Photoelectric conversion response upon irradiation of **1**, C₆₀ and **2** with 365 nm monochromatic light.

Table S1. ^1H NMR data (δ) and assignments of the sandwich-type mixed (phthalocyaninato)(porphyrinato) triple-decker complex in the solution of **1**, **1** + C_{60} , **1** + 5C_{60} , in $\text{CDCl}_3/\text{CS}_2$.

Compound	Pc^{inner}	
	H^{α}	H^{β}
1	9.43 (dd)	8.52(dd)
1 + C_{60}	9.42 (dd)	8.52 (dd)
1 + 5C_{60}	9.41 (dd)	8.50 (dd)

Compound [a]	$\text{TCIPP}^{\text{outer}}$				
	$\text{H}^{\text{endo-ortho}}$	$\text{H}^{\text{endo-meta}}$	$\text{H}^{\text{exo-ortho}}$	$\text{H}^{\text{exo-meta}}$	$\text{H}^{\beta\text{-pyrrole}}$
1	8.31 (dd)	7.93 (dd)	6.92 (dd)	5.84 (dd)	7.23 (s) ^[c]
1 + C_{60}	8.33 (dd)	7.93 (dd)	6.93 (dd)	5.87 (dd)	7.24 (s) ^[c]
1 + 5C_{60}	8.36 (dd)	7.94 (dd)	6.96 (dd)	5.91 (dd)	7.24 (s) ^[c]

[a] Multiplicities: s = singlet, d = doublet, dd = double doublet, b broad

[b] Overlapped signal between the H^{β} of the Pc^{inner} ring and $\text{H}^{\text{endo-meta}}$ of the TCIPP ring.

[c] Obscured by the strong residual CHCl_3 signal at δ 7.26.

Table S2. Cyclic voltammogram derived and DFT calculated energy level data of **1** and C₆₀.

Compound	HOMO _{CV} ^a	LUMO _{CV}	HOMO _{Cal} ^b	LUMO _{Cal}
1	-4.96	-3.58	-5.06	-3.52
C ₆₀	-6.34	-3.66	-6.41	-3.65

^a The HOMO_{CV} is derived from cyclic voltammogram analysis result. ^b The HOMO_{Cal} is calculated on the level of B3LYP-D3(BJ)/6-311G(d)/LanL2DZ.

Table S3. Crystal data and structure refinement of complex **2**.

complex	2
Formula	C ₁₈₀ H ₆₄ Cl ₈ N ₁₆ Y ₂
F.W.	2911.89
system	tetragonal
space group	<i>P4/ncc</i>
<i>a</i>	20.6353(3)
<i>b</i>	20.6353(3)
<i>c</i>	36.9677(9)
α	90
β	90
γ	90
<i>Z</i>	4
volume	15741.4(5)
absorption coefficient mm ⁻¹	0.926
<i>F</i> 000	9290
<i>R</i> _{int} <i>I</i> >2 θ	0.0720
<i>R</i> _{w2} <i>I</i> >2 θ	0.1911
<i>R</i> _{int} all	0.1359
<i>R</i> _{w2} all	0.2123
<i>S</i>	1.005

^a $R_1 = \Sigma |F_o - |F_c|| / \Sigma |F_o|$, ^b $R_{w2} = [\Sigma w(F_o^2 - F_c^2)^2 / \Sigma w(F_o^2)^2]^{1/2}$.

Table S4. Crystallographic data and selected structural information for **2**.

complex	2
average Y-N(TCIPP) bond distance (Å)	2.37/2.39
average Y-N(Pc) bond distance (Å)	2.60/2.75
Y-N ₄ (Pc) plane distance (Å)	1.74/1.96
Y-N ₄ (TCIPP) plane distance (Å)	1.18
interplanar distance (Å)	2.92/3.14
dihedral angle between the adjacent two N ₄ planes (°)	0/3.1
dihedral angle ϕ for the Pc ring (°) ^a	7.4
dihedral angle ϕ for the TCIPP ring (°) ^a	11.1/14.5
twist angle (°) ^b	2.4/32.0
dihedral angle θ between the benzene rings and the N ₄ plane of TCIPP (°)	59.9/81.4
separation of 6:6 ring juncture and mean N ₄ plane of Pc (Å)	no
separation of 6:6 ring juncture and mean N ₄ plane of TCIPP (Å)	2.75

^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 S5. Quantum yields for photoelectric conversion (ϕ) of **1**, **2** and C₆₀.

compound	ϕ (‰)
1	0.004
2	0.115
C ₆₀	0.042

Table S6. Cartesian coordinates (Å) and SCF energies, at 298.15 K and 1 atm for the optimized structures.

All energies are given in Hartree and on the basis of B3LYP-D3(BJ)/BSI.

[(TCIPP)Y(Pc)Y(TCIPP)] · C₆₀ · [(TCIPP)Y(Pc)Y(TCIPP)](2)

SCF Energy: -20782.09239740

Atoms	X	Y	Z
C	-9.20561497	1.13036405	-2.75755900
C	-9.35106596	2.39577605	-3.45798299
C	-9.59827196	2.70889206	-4.79281499
H	-9.67984196	1.93149306	-5.53993499
C	-9.74172595	4.05043406	-5.13026798
H	-9.94239295	4.32497207	-6.16016698
C	-9.61945495	5.05935006	-4.16022798
H	-9.71733694	6.09700806	-4.45961397
C	-9.38059695	4.74835405	-2.82631298
H	-9.28972695	5.52404705	-2.07667898
C	-9.26687796	3.40437505	-2.48070999
C	-9.12475996	2.72653004	-1.20236299
C	-9.13959096	2.75439403	1.12659301
C	-9.29828296	3.45720402	2.39025101
C	-9.43112396	4.80639102	2.70847402
H	-9.35718595	5.56791603	1.94425502
C	-9.67172996	5.14143102	4.03658402
H	-9.78636095	6.18375402	4.31260703
C	-9.77049296	4.15213701	5.02937502
H	-9.96615496	4.44700601	6.05464502
C	-9.61412697	2.80622301	4.71810301
H	-9.67620497	2.04337601	5.48305301
C	-9.37361197	2.46789102	3.38824201
C	-9.22249397	1.19000602	2.71377200
N	-9.07766497	1.35929204	-1.40064700

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C	-5.87877996	2.41399003	-2.46840199
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C	-5.90430696	4.24399302	-0.73766998
H	-5.83094095	5.08773803	-1.40437097
C	-5.90932996	4.26321802	0.62150902
H	-5.84166495	5.12511801	1.26502103
C	-6.02582396	2.89350902	1.06640202
C	-5.89268397	2.48241901	2.40299201
C	-5.92975797	1.15401301	2.86225301
C	-5.47556598	0.74930800	4.17259801
H	-5.13176598	1.41514999	4.94741601
C	-4.26169295	4.13382003	-3.31312298
H	-3.64669495	3.94280902	-2.44363698
C	-5.46236396	3.43122904	-3.47810598
C	-6.22637995	3.68375905	-4.61916198
H	-7.15313495	3.14941205	-4.76579398
C	-5.82124395	4.61874405	-5.56555698
H	-6.42938194	4.81671806	-6.43954398
C	-4.62643994	5.30179004	-5.37380597
C	-3.83684795	5.06432503	-4.25402597
H	-2.90071994	5.59273903	-4.12344997
C	-5.48581496	3.52861200	3.38707602
C	-6.25972996	3.81084900	4.51452402
H	-7.18480597	3.27625500	4.67048302
C	-5.86805596	4.77699499	5.43494303
H	-6.48464396	4.99757399	6.29754103
C	-4.67663896	5.46248499	5.23134503
C	-3.87698696	5.19584799	4.12539703

H	-2.94343396	5.72635899	3.98517803
C	-4.28865896	4.23427200	3.21043602
H	-3.66647496	4.02335600	2.35122102
Cl	-4.17088796	6.68443298	6.39040004
Cl	-4.10263194	6.48222205	-6.56742496
N	-6.21484997	-0.02344597	-2.11159800
N	-6.16897597	2.06781602	-0.02818499
N	-6.23225898	0.03478101	2.11636100
Y	-7.36668198	-0.00367497	-0.00209200
N	-9.13265996	3.36908103	-0.04543899
N	-9.25587297	-0.04114795	-3.37058200
N	-9.27968398	0.03238902	3.35214800
C	-9.20272198	-1.19832095	-2.73071401
C	-9.35619998	-2.47599695	-3.40465702
C	-9.60372798	-2.81416094	-4.73334502
H	-9.67275898	-2.05109894	-5.49733201
C	-9.75685199	-4.16035494	-5.04489103
H	-9.95730399	-4.45498093	-6.06929803
C	-9.64905799	-5.15004294	-4.05336403
H	-9.76112000	-6.19260694	-4.32952904
C	-9.40304699	-4.81510095	-2.72622603
H	-9.32187500	-5.57676695	-1.96289303
C	-9.27337999	-3.46564895	-2.40758202
C	-9.11345699	-2.76257496	-1.14396702
C	-9.11621899	-2.73489897	1.18507398
C	-9.28156799	-3.41277198	2.46079598
C	-9.40330400	-4.75650398	2.80505697
H	-9.29800400	-5.53284798	2.05793697
C	-9.66896500	-5.06642598	4.13412697
H	-9.77284401	-6.10389198	4.43213996
C	-9.81100900	-4.05688999	5.10082198
H	-10.03308800	-4.33070399	6.12651397

C	-9.66140699	-2.71576699	4.76523298
H	-9.75934299	-1.93768499	5.50962699
C	-9.38564099	-2.40371598	3.43567598
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N	-9.07199598	-1.36794297	1.38410999
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C	-4.24717599	-4.20279497	-3.25932002
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H	-7.19462698	-3.26794795	-4.62509502
C	-5.89425799	-4.76085195	-5.42971902
H	-6.53755599	-4.98608495	-6.27130102
C	-4.69188999	-5.43739496	-5.26487302
C	-3.85807099	-5.16221597	-4.18670002
H	-2.91568199	-5.68446897	-4.07747902
C	-5.50328000	-3.41430000	3.51069998

C	-6.30698300	-3.62305700	4.63404198
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C	2.19486903	1.11814897	2.60143202
C	1.19898403	2.17718098	2.57813002
C	1.41337904	2.96967898	1.37705703

C	0.32523704	3.48239599	0.67397903
C	0.31702604	3.44295700	-0.77958197
C	-1.04022296	3.15769501	-1.21530998
C	-1.25845196	2.33292101	-2.31683498
C	0.10082102	-1.91960499	-2.93881800
C	-1.84729697	0.15428902	-2.98563899
C	3.46304203	0.08439798	-0.70627298

[(TCIPP)Y(Pc)Y(TCIPP)] (1)(Upper)

SCF Energy: -9247.53175488

Atoms	X	Y	Z
C	-9.20561497	1.13036405	-2.75755900
C	-9.35106596	2.39577605	-3.45798299
C	-9.59827196	2.70889206	-4.79281499
H	-9.67984196	1.93149306	-5.53993499
C	-9.74172595	4.05043406	-5.13026798
H	-9.94239295	4.32497207	-6.16016698
C	-9.61945495	5.05935006	-4.16022798
H	-9.71733694	6.09700806	-4.45961397
C	-9.38059695	4.74835405	-2.82631298
H	-9.28972695	5.52404705	-2.07667898
C	-9.26687796	3.40437505	-2.48070999
C	-9.12475996	2.72653004	-1.20236299
C	-9.13959096	2.75439403	1.12659301
C	-9.29828296	3.45720402	2.39025101
C	-9.43112396	4.80639102	2.70847402
H	-9.35718595	5.56791603	1.94425502
C	-9.67172996	5.14143102	4.03658402
H	-9.78636095	6.18375402	4.31260703
C	-9.77049296	4.15213701	5.02937502
H	-9.96615496	4.44700601	6.05464502
C	-9.61412697	2.80622301	4.71810301

H	-9.67620497	2.04337601	5.48305301
C	-9.37361197	2.46789102	3.38824201
C	-9.22249397	1.19000602	2.71377200
N	-9.07766497	1.35929204	-1.40064700
N	-9.08799997	1.39169403	1.35318800
C	-5.46189197	0.63051004	-4.18974999
H	-5.12279196	1.27336304	-4.98569499
C	-5.91521897	1.07348104	-2.89078599
C	-5.87877996	2.41399003	-2.46840199
C	-6.01882396	2.86209203	-1.14468998
C	-5.90430696	4.24399302	-0.73766998
H	-5.83094095	5.08773803	-1.40437097
C	-5.90932996	4.26321802	0.62150902
H	-5.84166495	5.12511801	1.26502103
C	-6.02582396	2.89350902	1.06640202
C	-5.89268397	2.48241901	2.40299201
C	-5.92975797	1.15401301	2.86225301
C	-5.47556598	0.74930800	4.17259801
H	-5.13176598	1.41514999	4.94741601
C	-4.26169295	4.13382003	-3.31312298
H	-3.64669495	3.94280902	-2.44363698
C	-5.46236396	3.43122904	-3.47810598
C	-6.22637995	3.68375905	-4.61916198
H	-7.15313495	3.14941205	-4.76579398
C	-5.82124395	4.61874405	-5.56555698
H	-6.42938194	4.81671806	-6.43954398
C	-4.62643994	5.30179004	-5.37380597
C	-3.83684795	5.06432503	-4.25402597
H	-2.90071994	5.59273903	-4.12344997
C	-5.48581496	3.52861200	3.38707602
C	-6.25972996	3.81084900	4.51452402
H	-7.18480597	3.27625500	4.67048302

C	-5.86805596	4.77699499	5.43494303
H	-6.48464396	4.99757399	6.29754103
C	-4.67663896	5.46248499	5.23134503
C	-3.87698696	5.19584799	4.12539703
H	-2.94343396	5.72635899	3.98517803
C	-4.28865896	4.23427200	3.21043602
H	-3.66647496	4.02335600	2.35122102
Cl	-4.17088796	6.68443298	6.39040004
Cl	-4.10263194	6.48222205	-6.56742496
N	-6.21484997	-0.02344597	-2.11159800
N	-6.16897597	2.06781602	-0.02818499
N	-6.23225898	0.03478101	2.11636100
Y	-7.36668198	-0.00367497	-0.00209200
N	-9.13265996	3.36908103	-0.04543899
N	-9.25587297	-0.04114795	-3.37058200
N	-9.27968398	0.03238902	3.35214800
C	-9.20272198	-1.19832095	-2.73071401
C	-9.35619998	-2.47599695	-3.40465702
C	-9.60372798	-2.81416094	-4.73334502
H	-9.67275898	-2.05109894	-5.49733201
C	-9.75685199	-4.16035494	-5.04489103
H	-9.95730399	-4.45498093	-6.06929803
C	-9.64905799	-5.15004294	-4.05336403
H	-9.76112000	-6.19260694	-4.32952904
C	-9.40304699	-4.81510095	-2.72622603
H	-9.32187500	-5.57676695	-1.96289303
C	-9.27337999	-3.46564895	-2.40758202
C	-9.11345699	-2.76257496	-1.14396702
C	-9.11621899	-2.73489897	1.18507398
C	-9.28156799	-3.41277198	2.46079598
C	-9.40330400	-4.75650398	2.80505697
H	-9.29800400	-5.53284798	2.05793697

C	-9.66896500	-5.06642598	4.13412697
H	-9.77284401	-6.10389198	4.43213996
C	-9.81100900	-4.05688999	5.10082198
H	-10.03308800	-4.33070399	6.12651397
C	-9.66140699	-2.71576699	4.76523298
H	-9.75934299	-1.93768499	5.50962699
C	-9.38564099	-2.40371598	3.43567598
C	-9.22421398	-1.13885698	2.73836099
N	-9.06442598	-1.40011196	-1.37068001
N	-9.07199598	-1.36794297	1.38410999
N	-9.10793499	-3.37745897	0.02804798
C	-5.45627997	-0.72877596	-4.17044400
H	-5.11124197	-1.39195396	-4.94706600
C	-5.90272698	-1.13802797	-2.85844600
C	-5.84573098	-2.46588397	-2.39902901
C	-5.96752599	-2.87920397	-1.06104301
C	-5.83589699	-4.24780098	-0.61657302
H	-5.74799900	-5.10754597	-1.26059902
C	-5.84706899	-4.23090998	0.74278898
H	-5.77073700	-5.07540999	1.40816398
C	-5.98231299	-2.85087099	1.15126999
C	-5.87242499	-2.40092299	2.47817099
C	-5.92530398	-1.05823499	2.89697700
C	-5.47438498	-0.60998300	4.19490300
H	-5.12845799	-1.24885101	4.99102300
C	-4.24717599	-4.20279497	-3.25932002
H	-3.59789199	-3.98266498	-2.42331302
C	-5.45526799	-3.50869896	-3.39548102
C	-6.26265699	-3.79700896	-4.49748202
H	-7.19462698	-3.26794795	-4.62509502
C	-5.89425799	-4.76085195	-5.42971902
H	-6.53755599	-4.98608495	-6.27130102

C	-4.69188999	-5.43739496	-5.26487302
C	-3.85807099	-5.16221597	-4.18670002
H	-2.91568199	-5.68446897	-4.07747902
C	-5.50328000	-3.41430000	3.51069998
C	-6.30698300	-3.62305700	4.63404198
H	-7.21896600	-3.05660000	4.74553398
C	-5.96188600	-4.55365801	5.60735998
H	-6.60279901	-4.71616601	6.46501698
C	-4.78545201	-5.27862401	5.46317598
C	-3.95559500	-5.08413501	4.36469498
H	-3.03300501	-5.64355601	4.27166298
C	-4.32118000	-4.15641800	3.39600398
H	-3.67212800	-4.00068600	2.54468798
Cl	-4.33744201	-6.45612502	6.68996997
Cl	-4.21567600	-6.65728295	-6.43857303
N	-6.12834298	-2.05655798	0.03367899
C	-12.71368499	-2.82972597	3.18687698
H	-12.90463699	-3.06159797	4.22178298
C	-12.47252299	-1.50776196	2.65647398
C	-12.54592498	-0.32523397	3.40518499
C	-12.48647898	0.97737803	2.88891000
C	-12.76333597	2.16805203	3.65811400
H	-12.98835997	2.18974103	4.71233000
C	-12.70931097	3.22295204	2.80140801
H	-12.86151596	4.26459404	3.03242901
C	-12.42314497	2.69121304	1.49015701
C	-12.42512296	3.44849705	0.31006301
C	-12.39058896	2.92937705	-0.99246999
C	-12.65574196	3.70633406	-2.18104399
H	-12.81892095	4.77179206	-2.20425898
C	-13.99899999	-0.86115897	5.39608799
H	-14.81286999	-1.09315196	4.71832198

C	-12.76809198	-0.45247597	4.87668399
C	-11.73435798	-0.14245598	5.76413399
H	-10.77714998	0.15652201	5.35686500
C	-11.91579299	-0.24223999	7.13974299
H	-11.11000799	-0.00718200	7.82470199
C	-13.14984599	-0.65460399	7.63014199
C	-14.19693499	-0.96544998	6.77004298
H	-15.15358299	-1.27824498	7.16971798
C	-12.57355095	4.92960605	0.43582802
C	-11.49260395	5.76408004	0.14047102
H	-10.55148595	5.31164904	-0.14500498
C	-11.61014394	7.14716604	0.23485203
H	-10.76870694	7.79205304	0.01133603
C	-12.82518794	7.69798805	0.62596503
C	-13.91826595	6.89088805	0.92042102
H	-14.85980094	7.33725405	1.21539803
C	-13.78513195	5.50897305	0.82173002
H	-14.63533996	4.87221405	1.03922701
Cl	-12.98376393	9.44505805	0.74708604
Cl	-13.39069199	-0.78278099	9.36697299
N	-12.23110298	-1.59493796	1.30031598
N	-12.24424897	1.32483004	1.57683900
N	-12.22749797	1.60409705	-1.33617500
Y	-11.07054498	0.00614604	-0.01405901
C	-12.66643599	-3.69736896	2.14096997
H	-12.82895900	-4.76293896	2.16279797
C	-12.38998299	-2.92033996	0.95484498
C	-12.41437099	-3.43926095	-0.34811003
C	-12.40661598	-2.68177894	-1.52828902
C	-12.68890299	-3.21359994	-2.84016202
H	-12.83988299	-4.25530993	-3.07143003
C	-12.73990598	-2.15886093	-3.69734202

H	-12.96169898	-2.18094292	-4.75220302
C	-12.46570298	-0.96802494	-2.92757801
C	-12.52216397	0.33467507	-3.44428001
C	-12.45507896	1.51699606	-2.69480800
C	-12.69127896	2.83886207	-3.22759899
H	-12.87168596	3.07050407	-4.26446999
C	-13.77396400	-5.49856494	-0.86483804
H	-14.62279199	-4.86095294	-1.08523504
C	-12.56313000	-4.92036195	-0.47478203
C	-11.48397500	-5.75582895	-0.17593204
H	-10.54306300	-5.30472996	0.11228997
C	-11.60264901	-7.13884095	-0.27058104
H	-10.76254201	-7.78447896	-0.04422904
C	-12.81689301	-7.68848095	-0.66562605
C	-13.90818300	-6.88029494	-0.96386804
H	-14.84913301	-7.32578093	-1.26203705
C	-12.73327097	0.46261508	-4.91734401
C	-11.69315097	0.15282608	-5.79748501
H	-10.73902597	-0.14703393	-5.38359801
C	-11.86451596	0.25360108	-7.17432001
H	-11.05389796	0.01868308	-7.85360401
C	-13.09477696	0.66684009	-7.67339301
C	-14.14778996	0.97814309	-6.82077101
H	-15.10116796	1.29217210	-7.22721901
C	-13.95988596	0.87309008	-5.44548501
H	-14.77830396	1.10613008	-4.77361801
Cl	-13.32312796	0.79603310	-9.41187201
Cl	-12.97702602	-9.43539594	-0.78692406
N	-12.22812198	-1.31531894	-1.61455901

[(TCIPP)Y(Pc)Y(TCIPP)] (1)(Lower)

SCF Energy: -9247.53161902

Atoms	X	Y	Z
C	9.18919203	1.15854597	-2.74422697
C	9.33230604	2.42814297	-3.43543696
C	9.56555504	2.75029098	-4.77056596
H	9.63157804	1.97787298	-5.52578697
C	9.70877005	4.09300398	-5.10078296
H	9.89657005	4.37560898	-6.13095195
C	9.60749805	5.09462697	-4.12091495
H	9.71146206	6.13399897	-4.41197295
C	9.37899705	4.77559097	-2.78677695
H	9.30570805	5.54602196	-2.03143295
C	9.25766504	3.42977397	-2.44992496
C	9.11280104	2.74199896	-1.17631196
C	9.12565404	2.74358295	1.15320604
C	9.29216204	3.43784694	2.41954004
C	9.41545204	4.78619594	2.74427105
H	9.31201805	5.55182794	1.98608605
C	9.68077404	5.11521093	4.06872605
H	9.78677905	6.15669993	4.35150605
C	9.81937804	4.11928893	5.05010004
H	10.04011004	4.40758892	6.07211405
C	9.66739203	2.77365093	4.73409704
H	9.76131803	2.00703092	5.49065603
C	9.39415503	2.44225094	3.40847004
C	9.23310103	1.16810194	2.72768103
N	9.06530603	1.37653796	-1.38533397
N	9.08249403	1.37939395	1.37008103
C	12.68381402	-2.86862104	-3.20948699
H	12.85928902	-3.11033704	-4.24494899
C	12.44699502	-1.54153905	-2.68996098

C	12.50758403	-0.36741804	-3.45241497
C	12.45172503	0.94070195	-2.95019397
C	12.71485104	2.12348996	-3.73610696
H	12.92727504	2.13369196	-4.79320396
C	12.66516104	3.18811595	-2.89119796
H	12.81004905	4.22765895	-3.13581995
C	12.39536004	2.67046095	-1.57071796
C	12.40906604	3.44099394	-0.39939296
C	12.39390604	2.93639294	0.90916104
C	12.67105704	3.72715093	2.08585605
H	12.83079704	4.79337193	2.09526005
C	13.93900003	-0.91534904	-5.45608998
H	14.76495703	-1.12842605	-4.78678597
C	12.71127603	-0.51248404	-4.92521197
C	11.66017203	-0.22922003	-5.80090697
H	10.70600803	0.06500697	-5.38238897
C	11.82247303	-0.34848602	-7.17749698
H	11.00383504	-0.13415701	-7.85401598
C	13.05396003	-0.75385002	-7.67981998
C	14.11768403	-1.03870203	-6.83104298
H	15.07166403	-1.34702503	-7.24040798
C	12.55470205	4.92115194	-0.54450095
C	11.47518505	5.75916395	-0.25441094
H	10.53532105	5.31080195	0.04164305
C	11.59261206	7.14098495	-0.36678694
H	10.75240806	7.78877195	-0.14698494
C	12.80549906	7.68672494	-0.77136593
C	13.89689706	6.87585294	-1.06173394
H	14.83667406	7.31825094	-1.36806293
C	13.76395905	5.49533894	-0.94492994
H	14.61248405	4.85549394	-1.15996794
Cl	12.96335007	9.43209194	-0.91589692

Cl	13.27039403	-0.90760902	-9.41785398
N	12.22680402	-1.61387505	-1.32975498
N	12.22216503	1.30259195	-1.63959197
N	12.23863703	1.61439493	1.26991804
Y	11.07216702	-0.00291105	-0.02015797
N	9.11449404	3.37122595	-0.01194996
N	9.23956503	-0.00654403	-3.36995698
N	9.28989602	0.00473594	3.35581802
C	9.19590302	-1.17014103	-2.74157198
C	9.34064902	-2.44427603	-3.42644399
C	9.57765802	-2.77550602	-4.75888799
H	9.64829002	-2.00921602	-5.51827599
C	9.72456301	-4.12104702	-5.07851400
H	9.91771201	-4.40915802	-6.10614400
C	9.61499501	-5.11702003	-4.09354300
H	9.71578400	-6.15832603	-4.37882901
C	9.38414501	-4.78808103	-2.76256600
H	9.30220600	-5.55355504	-2.00157401
C	9.26674001	-3.43997503	-2.43517999
C	9.12777301	-2.74608004	-1.16517699
C	9.14987501	-2.74465905	1.16431501
C	9.30992301	-3.43167406	2.43663501
C	9.44393900	-4.77666406	2.77183800
H	9.37058100	-5.54721606	2.01664000
C	9.68703300	-5.09445307	4.10375000
H	9.80289499	-6.13306207	4.39304599
C	9.78779100	-4.09256407	5.08348200
H	9.98585900	-4.37401008	6.11204700
C	9.63038801	-2.75070907	4.75525901
H	9.69422201	-1.97825308	5.51065601
C	9.38612401	-2.42980406	3.42184901
C	9.23275802	-1.16065506	2.73181402

N	9.07725602	-1.38194704	-1.38092698
N	9.09687402	-1.37947505	1.37400402
N	9.14070601	-3.37388805	-0.00010499
C	12.65599801	-3.72436105	-2.15306199
H	12.82135701	-4.78971305	-2.16516400
C	12.39493801	-2.93501505	-0.97166699
C	12.43418901	-3.43959106	0.33636801
C	12.43398601	-2.66935307	1.50800501
C	12.72381001	-3.18570908	2.82478401
H	12.87663800	-4.22449108	3.06772501
C	12.77935501	-2.12093608	3.66914202
H	13.00598201	-2.13049309	4.72328102
C	12.50085802	-0.93919707	2.88684602
C	12.55915602	0.36933792	3.38804103
C	12.48233303	1.54314793	2.62627504
C	12.72178803	2.87144892	3.14151904
H	12.91317903	3.11430692	4.17385904
C	13.80526900	-5.48869207	0.86144200
H	14.65449100	-4.84569107	1.06383701
C	12.58803500	-4.91906106	0.47884800
C	11.50773800	-5.76123906	0.20413400
H	10.56209100	-5.31611205	-0.07804800
C	11.63195099	-7.14262306	0.31456299
H	10.79115599	-7.79355305	0.10674399
C	12.85265299	-7.68372007	0.70147699
C	13.94508299	-6.86870307	0.97601599
H	14.89089999	-7.30760308	1.26844399
C	12.78423402	0.51472391	4.85763203
C	11.74971302	0.22111991	5.74952303
H	10.79142402	-0.08056608	5.34612602
C	11.93263702	0.33988791	7.12353403
H	11.12658901	0.11743891	7.81241703

C	13.16830102	0.75532790	7.60706803
C	14.21599702	1.05032290	6.74202004
H	15.17377202	1.36604189	7.13664504
C	14.01676502	0.92708391	5.36985603
H	14.83049502	1.14757291	4.68808704
Cl	13.41068802	0.90842589	9.34170603
Cl	13.01918598	-9.42845907	0.84384898
N	12.25536302	-1.30225707	1.57941702
C	5.49040102	0.68972395	4.19774602
H	5.14698302	1.34603695	4.98080302
C	5.93359303	1.10960095	2.88782402
C	5.88090003	2.44218596	2.44026303
C	5.99669904	2.86511496	1.10454003
C	5.88408004	4.23891397	0.67113004
H	5.82093105	5.09569696	1.32186804
C	5.88162504	4.23181497	-0.68822196
H	5.81814705	5.08290098	-1.34636996
C	5.98885304	2.85266597	-1.10803797
C	5.85355104	2.41260298	-2.43636397
C	5.89367003	1.07216898	-2.86523598
C	5.41854303	0.63325899	-4.15772898
H	5.05452004	1.27715700	-4.94147598
C	4.31930104	4.20963996	3.30753304
H	3.67393804	4.02220297	2.45992904
C	5.50623204	3.47947695	3.44686604
C	6.30827703	3.72864294	4.56274704
H	7.22428603	3.17219594	4.69143704
C	5.95599904	4.68778894	5.50569504
H	6.59529304	4.88227193	6.35791004
C	4.77497504	5.40027595	5.33743604
C	3.94672504	5.16527196	4.24552204
H	3.02084704	5.71581996	4.13410704

C	5.46521504	3.43419599	-3.45276997
C	6.22292505	3.62949699	-4.61011196
H	7.11997204	3.04820699	-4.76000296
C	5.85127005	4.56656300	-5.56724996
H	6.45659005	4.71953100	-6.45211096
C	4.69459206	5.31151700	-5.37214196
C	3.91078505	5.13230800	-4.23769996
H	3.00395206	5.70886400	-4.10381196
C	4.30312205	4.19846499	-3.28622396
H	3.69840805	4.05518399	-2.40093196
Cl	4.21357906	6.49631601	-6.57901595
Cl	4.31915304	6.61507694	6.52431805
N	6.24101402	0.00099296	2.13051102
N	6.13535003	2.04855497	0.00255903
N	6.21445603	-0.02673002	-2.09848398
Y	7.37105902	-0.00524104	0.00826202
C	5.49614902	-0.66972505	4.20627001
H	5.16011301	-1.31910005	4.99826301
C	5.94447602	-1.10226805	2.90244301
C	5.90481401	-2.43953104	2.47052401
C	6.03516101	-2.87811404	1.14299800
C	5.91772601	-4.25720604	0.72768300
H	5.85019000	-5.10536904	1.38939999
C	5.91030501	-4.26697203	-0.63157700
H	5.83697300	-5.12450102	-1.28019001
C	6.02095701	-2.89392103	-1.06795500
C	5.87202102	-2.47245002	-2.39951599
C	5.90091802	-1.14028202	-2.84820099
C	5.42321703	-0.72612501	-4.14683299
H	5.06645803	-1.38631400	-4.92059199
C	4.28381700	-4.15562404	3.31449799
H	3.66275100	-3.95311103	2.45206799

C	5.49132000	-3.46389405	3.47477300
C	6.26469100	-3.73395106	4.60511300
H	7.19780500	-3.20954306	4.74663700
C	5.86103600	-4.67442506	5.54687099
H	6.47628399	-4.88601007	6.41268499
C	4.65834999	-5.34511605	5.36110699
C	3.86024400	-5.09112804	4.25098199
H	2.91869999	-5.61079504	4.12432899
C	5.45387201	-3.51081201	-3.38669200
C	6.21269401	-3.78251801	-4.52701500
H	7.13496102	-3.24531501	-4.69134500
C	5.80950601	-4.74159500	-5.44982801
H	6.41429901	-4.95414700	-6.32273001
C	4.62177601	-5.43030800	-5.23551501
C	3.83666301	-5.17338300	-4.11694201
H	2.90562901	-5.70610400	-3.96860601
C	4.25955501	-4.21869301	-3.19981801
H	3.64789401	-4.01460401	-2.33120901
Cl	4.10160900	-6.64323099	-6.39760102
Cl	4.13570699	-6.53135906	6.54941498
N	6.17496402	-2.07604703	0.03082901

C₆₀(Center of 2)

SCF Energy: -2286.90677233

Atoms	X	Y	Z
C	-3.45845598	-0.07744499	0.79000500
C	-3.46781197	-0.11663299	-0.66152000
C	-3.01822298	-1.24886799	-1.33148800
C	-2.53766698	-2.39281399	-0.57507501
C	-2.52942499	-2.35458100	0.81599499
C	-3.00171198	-1.17190500	1.51523800
C	-3.09294097	1.26735400	1.20094701

C	-2.87961497	2.06140501	0.00262102
C	-3.10752897	1.20412401	-1.14844599
C	-2.31833197	1.33781102	-2.28473699
C	-2.19037498	-1.11131498	-2.51739300
C	-1.40879099	-2.96273199	-1.29241301
C	-0.32050499	-3.47531400	-0.58987501
C	-0.31229999	-3.43597901	0.86351999
C	-1.39238399	-2.88595001	1.54993499
C	-1.16454399	-2.03046001	2.70456300
C	-2.15996798	-0.97121701	2.68223900
C	-1.81270498	0.31761099	3.07885201
C	-2.29076697	1.46136599	2.31936701
C	-1.87128796	3.01903200	-0.02893598
C	-1.02681596	3.22086699	1.13934702
C	-1.23159497	2.45656499	2.28599802
C	-0.09641997	1.92646598	3.02278302
C	-0.45525298	0.60423198	3.51090201
C	0.49950402	-0.41001703	3.53150501
C	0.13589801	-1.75615402	3.11951300
C	1.26308601	-2.32611402	2.40060000
C	1.04499601	-3.15075702	1.29898200
C	-1.19451398	-2.17031799	-2.49392900
C	3.09763002	-1.26054001	-1.11727799
C	2.29503902	-1.45424000	-2.23536599
C	1.81685003	-0.31055100	-2.99473899
C	2.16418803	0.97832300	-2.59825298
C	3.00589403	1.17895099	-1.43113198
C	3.47194002	0.12344698	0.74517702
C	3.11215202	-1.19744403	1.23215401
C	2.88441602	-2.05477702	0.08080900
C	1.87615601	-3.01268901	0.11233700
C	1.03139101	-3.21425000	-1.05565301

C	1.23592302	-2.44958100	-2.20205700
C	0.45964303	-0.59731999	-3.42706999
C	-0.49507697	0.41692301	-3.44786099
C	-0.13137796	1.76306801	-3.03592698
C	1.16902604	2.03754700	-2.62080298
C	1.39685804	2.89295800	-1.46615597
C	2.53359204	2.36145199	-0.73183797
C	2.54211103	2.39978198	0.65944703
C	3.02286703	1.25570797	1.41551302
C	2.32283902	-1.33101803	2.36843601
C	1.85173402	-0.14745303	3.06939701
C	2.19486903	1.11814897	2.60143202
C	1.19898403	2.17718098	2.57813002
C	1.41337904	2.96967898	1.37705703
C	0.32523704	3.48239599	0.67397903
C	0.31702604	3.44295700	-0.77958197
C	-1.04022296	3.15769501	-1.21530998
C	-1.25845196	2.33292101	-2.31683498
C	0.10082102	-1.91960499	-2.93881800
C	-1.84729697	0.15428902	-2.98563899
C	3.46304203	0.08439798	-0.70627298

H₂TCIPP·C₆₀·H₂TCIPP

SCF Energy: -9792.72053075

C	-5.71352200	0.64597900	-4.21478000
H	-5.52404700	1.28655100	-5.06039000
C	-5.96695700	1.11132900	-2.88373000
C	-5.94402300	2.43837300	-2.44651000
C	-6.03120700	2.85764700	-1.10867400
C	-6.02991000	4.26345800	-0.71839200
H	-6.03572600	5.10532500	-1.39264100
C	-6.04113900	4.28436400	0.63409400

H	-6.05831400	5.14668600	1.28172300
C	-6.04767900	2.89122200	1.06747900
C	-5.97737700	2.51293500	2.41841400
C	-5.99885900	1.19947700	2.89534100
C	-5.75857400	0.77565700	4.24265400
H	-5.58105100	1.44235000	5.07051700
C	-4.50471500	4.19291400	-3.50479300
H	-3.75643200	3.99304800	-2.74725100
C	-5.70608300	3.47543800	-3.49117800
C	-6.65413000	3.73672700	-4.48438000
H	-7.59221600	3.19298000	-4.48174400
C	-6.41667300	4.69147100	-5.46841700
H	-7.15731100	4.89716100	-6.23123600
C	-5.21314400	5.38729500	-5.45907600
C	-4.25125000	5.14677800	-4.48410400
H	-3.31608700	5.69272000	-4.49502100
C	-5.76140400	3.58261800	3.43468900
C	-6.72613200	3.86713000	4.40520700
H	-7.66013000	3.31638700	4.40552300
C	-6.51061800	4.85388400	5.36234700
H	-7.26429000	5.07751900	6.10713300
C	-5.31236100	5.55869600	5.34899000
C	-4.33402500	5.29522400	4.39658500
H	-3.40331000	5.84878400	4.40425000
C	-4.56556300	4.30930100	3.44398700
H	-3.80456700	4.09160300	2.70424100
Cl	-5.02952000	6.80340800	6.55631700
Cl	-4.90243000	6.59093400	-6.70075500
N	-6.13577800	-0.00767200	-2.10238600
N	-6.07297000	2.04929300	-0.00829100
N	-6.15407800	0.05657100	2.14651300
C	-5.70981800	-0.72148500	-4.19425200

H	-5.51602200	-1.38613400	-5.02010100
C	-5.95778300	-1.14812200	-2.84909000
C	-5.91534900	-2.46152200	-2.37242500
C	-5.98160800	-2.84304900	-1.02159800
C	-5.95890500	-4.23655000	-0.58855200
H	-5.95457000	-5.09866000	-1.23669800
C	-5.96411800	-4.21599500	0.76389500
H	-5.96484600	-5.05820400	1.43771800
C	-5.98963000	-2.80993100	1.15438100
C	-5.93368000	-2.38752600	2.49345500
C	-5.98086200	-1.05990100	2.92940200
C	-5.74850300	-0.59180900	4.26340100
H	-5.56030500	-1.23030200	5.11083700
C	-4.49285800	-4.24138300	-3.41631800
H	-3.72764100	-4.02054400	-2.68205600
C	-5.69531200	-3.52673700	-3.39306800
C	-6.66637400	-3.81706500	-4.35559600
H	-7.60529400	-3.27485700	-4.34549100
C	-6.45028500	-4.79803400	-5.31846200
H	-7.20859100	-5.02594700	-6.05722500
C	-5.24507400	-5.49105900	-5.31908000
C	-4.26053400	-5.22135000	-4.37491100
H	-3.32440700	-5.76545100	-4.39346600
C	-5.72397300	-3.42090900	3.54821300
C	-6.70082400	-3.67580100	4.51506800
H	-7.63714900	-3.12994700	4.48341600
C	-6.49367900	-4.62654700	5.50963000
H	-7.25629600	-4.82716100	6.25189300
C	-5.29188900	-5.32493800	5.53790300
C	-4.30200400	-5.09063000	4.58988600
H	-3.36865600	-5.63828700	4.63008000
C	-4.52541100	-4.14062900	3.59962400

H	-3.75647300	-3.94678500	2.86177000
Cl	-5.01936100	-6.52355000	6.79321500
Cl	-4.96133600	-6.72823400	-6.53386700
N	-6.02846600	-2.00252400	0.05360600
C	5.74576500	0.69146600	4.22275400
H	5.55677600	1.34977400	5.05475500
C	5.98718200	1.12845700	2.87976800
C	5.94024200	2.44565800	2.41406600
C	5.99050300	2.83716500	1.06541100
C	5.95975500	4.23356600	0.64232100
H	5.96201100	5.09121500	1.29637100
C	5.94759200	4.22234600	-0.71021200
H	5.93780800	5.06912700	-1.37821200
C	5.97144400	2.81911600	-1.11068700
C	5.90192000	2.40626800	-2.45210000
C	5.94874900	1.08216900	-2.89879000
C	5.71228800	0.62370000	-4.23553000
H	5.51820200	1.26808900	-5.07716100
C	4.53054500	4.21963400	3.48624500
H	3.75712500	4.00790000	2.75786700
C	5.73104300	3.50254600	3.44545800
C	6.71157600	3.78220600	4.40172200
H	7.64908200	3.23798400	4.37807900
C	6.50673600	4.75498500	5.37519100
H	7.27234300	4.97459100	6.10893800
C	5.30320900	5.45076200	5.39306100
C	4.30950800	5.19165200	4.45564800
H	3.37478300	5.73752100	4.48772000
C	5.68235100	3.44709500	-3.49766800
C	6.65368600	3.71206400	-4.46745200
H	7.59174200	3.16878300	-4.44426200
C	6.43894300	4.66920900	-5.45414200

H	7.19732500	4.87744000	-6.19863600
C	5.23490700	5.36411600	-5.47156600
C	4.25059600	5.12007100	-4.52031600
H	3.31551500	5.66535300	-4.55180700
C	4.48150700	4.16361200	-3.53785600
H	3.71630300	3.96350400	-2.79769800
Cl	4.95267400	6.57073400	-6.71700500
Cl	5.03343300	6.67759700	6.62139000
N	6.16007800	-0.00632500	2.12312700
N	6.02550700	2.00419300	-0.01604500
N	6.12951400	-0.03971000	-2.12562000
C	5.74696900	-0.67606800	4.23235100
H	5.56005500	-1.32285700	5.07376700
C	5.99322400	-1.13139600	2.89644700
C	5.96415100	-2.45498400	2.44920500
C	6.04172800	-2.86455600	1.10756700
C	6.03604200	-4.26756000	0.70707000
H	6.04530800	-5.11430600	1.37511800
C	6.03826600	-4.27866000	-0.64556700
H	6.04952300	-5.13626000	-1.29958300
C	6.04328400	-2.88250400	-1.06885400
C	5.96399100	-2.49433300	-2.41618500
C	5.97638700	-1.17713200	-2.88289300
C	5.72868400	-0.74385000	-4.22579300
H	5.55123100	-1.40501600	-5.05811300
C	4.52592200	-4.21565800	3.49822500
H	3.77669300	-4.01074500	2.74302300
C	5.72799700	-3.49915800	3.48708600
C	6.67756900	-3.76798300	4.47684000
H	7.61627200	-3.22530300	4.47601300
C	6.44081700	-4.72870900	5.45519800
H	7.18264400	-4.94012300	6.21528800

C	5.23645600	-5.42307000	5.44368400
C	4.27314700	-5.17538600	4.47190500
H	3.33739800	-5.72034800	4.48094500
C	5.75003700	-3.55703900	-3.44053800
C	6.71783800	-3.83443700	-4.40995700
H	7.65139600	-3.28297300	-4.40386300
C	6.50575200	-4.81497200	-5.37427600
H	7.26168600	-5.03317000	-6.11838500
C	5.30791400	-5.52055300	-5.36904300
C	4.32643900	-5.26371100	-4.41807400
H	3.39605300	-5.81769400	-4.43234800
C	4.55448000	-4.28378700	-3.45838400
H	3.79073800	-4.07054100	-2.72015800
Cl	5.02945700	-6.75768400	-6.58520500
Cl	4.92657000	-6.63409200	6.67834700
N	6.07674600	-2.04833100	0.01311800
C	-3.46446900	-0.01633900	0.73341000
C	-3.44784900	-0.05234500	-0.71646700
C	-3.01410000	-1.19294200	-1.38109600
C	-2.57519900	-2.35065200	-0.62025000
C	-2.59089700	-2.31554400	0.77132800
C	-3.04639300	-1.12200800	1.46349700
C	-3.08494300	1.32024500	1.15445900
C	-2.83494600	2.11248900	-0.03750200
C	-3.05795900	1.26202800	-1.19441100
C	-2.24919300	1.38254400	-2.31830100
C	-2.16560500	-1.07021700	-2.55307700
C	-1.44644300	-2.94212000	-1.31968400
C	-0.38085100	-3.47581900	-0.59765500
C	-0.39778300	-3.43934700	0.85604100
C	-1.47919500	-2.87098300	1.52533000
C	-1.25364900	-2.02144500	2.68566800

C	-2.22553000	-0.94090400	2.64738500
C	-1.86020000	0.34076400	3.05281700
C	-2.30243300	1.49661700	2.28932600
C	-1.80827200	3.04918200	-0.04879400
C	-0.98099300	3.23115900	1.13476700
C	-1.22268700	2.47113500	2.27734600
C	-0.11144300	1.91503600	3.03158100
C	-0.50523200	0.59883100	3.50946600
C	0.42694100	-0.43569100	3.54507300
C	0.04407100	-1.77413300	3.12456500
C	1.17253500	-2.36708700	2.42594700
C	0.95678700	-3.18243000	1.31661500
C	-1.19336100	-2.15093800	-2.51496000
C	3.08798300	-1.33011400	-1.05789700
C	2.30554600	-1.50650100	-2.19273300
C	1.86335300	-0.35070500	-2.95646100
C	2.22853700	0.93097000	-2.55098300
C	3.04890200	1.11195500	-1.36689700
C	3.45077300	0.04249900	0.81282300
C	3.06120100	-1.27194800	1.29096700
C	2.83809600	-2.12241700	0.13402900
C	1.81130000	-3.05901000	0.14530600
C	0.98411200	-3.24115100	-1.03828000
C	1.22576900	-2.48103600	-2.18079900
C	0.50840500	-0.60874700	-3.41316000
C	-0.42383500	0.42583800	-3.44876500
C	-0.04099400	1.76431300	-3.02826000
C	1.25673900	2.01159200	-2.58937400
C	1.48225600	2.86106700	-1.42889700
C	2.59386500	2.30551800	-0.67491100
C	2.57828700	2.34079500	0.71661700
C	3.01735700	1.18315600	1.47757400

C	2.25233000	-1.39246200	2.41487200
C	1.79228700	-0.19990700	3.10819600
C	2.16877900	1.06039200	2.64954800
C	1.19652900	2.14111300	2.61140100
C	1.44958900	2.93229500	1.41607900
C	0.38395700	3.46590700	0.69409000
C	0.40082900	3.42941200	-0.75960400
C	-0.95375500	3.17266500	-1.22017800
C	-1.16941600	2.35726400	-2.32947600
C	0.11460300	-1.92493800	-2.93520900
C	-1.78913000	0.19004100	-3.01177700
C	3.46741100	0.00645900	-0.63703600
H	6.22160100	-0.03131900	-1.11783700
H	6.24833700	-0.01334900	1.11500400
H	-6.23019900	0.00724600	-1.09488100
H	-6.23893300	0.04019300	1.13820200

C₆₀ (Center of H₂TCIPP·C₆₀·H₂TCIPP)

SCF Energy: -2286.90663706

C	-5.34358031	-0.67811934	0.00000000
C	-6.36434831	0.35160966	-0.03749100
C	-7.62555331	0.06556666	-0.54579400
C	-7.92014831	-1.26824134	-1.04176200
C	-6.94001231	-2.25618034	-1.00600000
C	-5.62262431	-1.95450634	-0.47253500
C	-4.06567931	-0.05554234	-0.29520500
C	-4.29671331	1.36210766	-0.51386300
C	-5.71928631	1.61274866	-0.35599400
C	-6.36199031	2.53726766	-1.17082700
C	-8.29763331	1.02777966	-1.40077900
C	-8.77129131	-1.13087534	-2.21215400
C	-8.60778631	-1.98908534	-3.29769000

C	-7.58407431	-3.02128034	-3.25981100
C	-6.76795031	-3.15112834	-2.13842000
C	-5.34356131	-3.40481734	-2.29882700
C	-4.63620731	-2.66558034	-1.26598400
C	-3.40958431	-2.06976334	-1.55043200
C	-3.11832431	-0.73540934	-1.05128100
C	-3.57239431	2.04451766	-1.48404900
C	-2.58523931	1.33447766	-2.28385500
C	-2.36431831	-0.02491734	-2.07224000
C	-2.19259731	-0.92050134	-3.20423900
C	-2.83922931	-2.18297434	-2.88195200
C	-3.51708931	-2.88991634	-3.87250100
C	-4.79613831	-3.51426434	-3.57406000
C	-5.64781431	-3.37851934	-4.74423700
C	-7.01187831	-3.13814634	-4.59094900
C	-9.00521331	0.28855166	-2.43399700
C	-7.18939331	-0.07576334	-6.64075000
C	-8.13673431	0.60407266	-5.88474700
C	-7.84567631	1.93856066	-5.38564200
C	-6.61902431	2.53434566	-5.66994400
C	-5.63258231	1.82303066	-6.46289900
C	-4.89085531	-0.48275334	-6.89834900
C	-5.53581731	-1.74407934	-6.58016500
C	-6.95842031	-1.49342534	-6.42220500
C	-7.68268331	-2.17575934	-5.45189200
C	-8.66997031	-1.46581034	-4.65218700
C	-8.89078531	-0.10639834	-4.86375800
C	-8.41604631	2.05182666	-4.05414200
C	-7.73814231	2.75880766	-3.06352100
C	-6.45907331	3.38317966	-3.36193100
C	-5.91168031	3.27371866	-4.63718000
C	-4.48724431	3.01988466	-4.79756000

C	-4.31527731	2.12487066	-5.92989400
C	-3.33504731	1.13708666	-5.89424200
C	-3.62950531	-0.19674734	-6.39037300
C	-4.89310631	-2.66861034	-5.76522700
C	-3.57587131	-2.36858834	-5.22726600
C	-2.95746331	-1.15898534	-5.53530800
C	-2.24990431	-0.41973534	-4.50208400
C	-2.48385831	0.99972366	-4.72390500
C	-2.64740131	1.85784366	-3.63833400
C	-3.67113131	2.89002066	-3.67615500
C	-4.24320531	3.00700266	-2.34499200
C	-5.60728431	3.24731366	-2.19179400
C	-9.06262331	0.78931466	-3.73184000
C	-7.67929131	2.23739266	-1.70880700
C	-5.91163431	0.54693966	-6.93585900

H₂TCIPP (Lower)

SCF Energy: -3752.85692223

C	-1.31103070	-0.28028933	0.00000000
H	-0.75719870	-1.18611633	0.18448600
C	-0.71638870	1.00000067	-0.24440200
C	0.64725330	1.30412667	-0.21756100
C	1.19647430	2.59464867	-0.29570800
C	2.63390430	2.84444067	-0.29074600
H	3.40522230	2.09054267	-0.30027100
C	2.78803230	4.18832367	-0.29316400
H	3.71001230	4.74789467	-0.30543600
C	1.44440030	4.75695467	-0.29800300
C	1.20100930	6.13812267	-0.21922100
C	-0.05901270	6.74232367	-0.23865500
C	-0.34831770	8.12328867	0.01004600
H	0.39647130	8.88025167	0.19348200

C	2.28686930	0.06887267	1.21624200
H	2.16156730	0.83762767	1.96927400
C	1.57595830	0.16082167	0.01441300
C	1.73944430	-0.84721833	-0.93986300
H	1.19995530	-0.78500133	-1.87834700
C	2.59220630	-1.92207133	-0.70804400
H	2.72277330	-2.69670133	-1.45346100
C	3.28383030	-1.98905733	0.49607800
C	3.13919830	-1.00129333	1.46409800
H	3.68005930	-1.07194833	2.39960800
C	2.36534030	7.04260667	0.00421300
C	2.74551330	7.98649967	-0.95395600
H	2.19882730	8.04707067	-1.88837300
C	3.82149130	8.84031467	-0.73143100
H	4.11853130	9.56423167	-1.48006500
C	4.51983030	8.74988967	0.46727800
C	4.16236030	7.82186067	1.43918900
H	4.71264030	7.76897367	2.37037800
C	3.08767930	6.97258467	1.20067100
H	2.79703430	6.25305167	1.95666600
Cl	5.87707230	9.82681067	0.75896200
Cl	4.35877430	-3.34529433	0.79967700
N	-1.75268370	1.88890467	-0.40903600
N	0.50057630	3.76959867	-0.33096300
N	-1.26993670	6.11080867	-0.39965600
C	-2.66981670	-0.12509233	0.00274100
H	-3.41290670	-0.88262533	0.19063000
C	-2.96143370	1.25713067	-0.23681400
C	-4.22151570	1.86065767	-0.19233500
C	-4.46794570	3.24290967	-0.25011500
C	-5.81200970	3.81105167	-0.22571400
H	-6.73381170	3.25102767	-0.22628500

C	-5.65824470	5.15489167	-0.22211700
H	-6.42993570	5.90844267	-0.21913800
C	-4.22050370	5.40503367	-0.24396100
C	-3.66825170	6.69556367	-0.17896700
C	-2.30405570	6.99881367	-0.22224900
C	-1.70709270	8.27866367	0.01915500
H	-2.25921970	9.18368967	0.21234700
C	-6.09764570	0.98822167	1.22191100
H	-5.80661170	1.69223267	1.99206300
C	-5.38245870	0.94859967	0.02020700
C	-5.76484670	0.02560367	-0.95732600
H	-5.22293270	-0.01178633	-1.89572500
C	-6.83625270	-0.83723833	-0.74828900
H	-7.13478070	-1.54507633	-1.51156500
C	-7.52769770	-0.77724433	0.45633600
C	-7.16765770	0.12942867	1.44721100
H	-7.71228470	0.15861367	2.38276100
C	-4.59294170	7.84568567	0.03676500
C	-4.74988870	8.83918067	-0.93398200
H	-4.20846570	8.75986267	-1.87005500
C	-5.59827370	9.92127167	-0.72113700
H	-5.72365270	10.68455367	-1.47907200
C	-6.29220670	10.01056567	0.48025100
C	-6.15390470	9.03776267	1.46413800
H	-6.69627570	9.12577767	2.39728800
C	-5.30581370	7.96012767	1.23505900
H	-5.18674570	7.20186067	1.99933800
Cl	-7.36164370	11.37614667	0.75997400
Cl	-8.87899070	-1.86595333	0.73117700
N	-3.52547070	4.23030267	-0.28930700
H	-1.63839870	2.89061567	-0.49689200
H	-1.38549670	5.10958567	-0.49107900

H₂TCIPP (Upper)

SCF Energy: -3752.85698922

C	-0.69620251	0.26220614	0.00000000
H	0.23974049	-0.23764686	0.18833700
C	-0.83193751	1.66773014	-0.24276100
C	0.18992849	2.62056814	-0.19815000
C	0.01047049	4.01334014	-0.24968500
C	1.12194249	4.95870614	-0.22137200
H	2.16937649	4.70137814	-0.22468400
C	0.57176749	6.19434114	-0.20984100
H	1.08151749	7.14483914	-0.20173100
C	-0.87470651	6.00136114	-0.23164300
C	-1.78861151	7.06654114	-0.16210400
C	-3.18100951	6.94749714	-0.20703100
C	-4.13466551	7.99036114	0.02951900
H	-3.87955751	9.01946514	0.22217100
C	2.24622449	2.34717014	1.20922600
H	1.76232249	2.93131414	1.98263300
C	1.57093649	2.09702514	0.00985600
C	2.20782049	1.33083014	-0.97066300
H	1.69820749	1.13425414	-1.90730900
C	3.48858449	0.82681614	-0.76691000
H	3.98185649	0.24089914	-1.53251400
C	4.13518849	1.08946814	0.43551200
C	3.52468749	1.84659814	1.42917500
H	4.03917249	2.03609914	2.36304200
C	-1.25139651	8.44090614	0.05529900
C	-1.39680851	9.43479614	-0.91692400
H	-1.88686451	9.19565614	-1.85410000
C	-0.91282151	10.72176914	-0.70418600
H	-1.02005251	11.48667814	-1.46325700
C	-0.28110251	11.01643514	0.49873000

C	-0.12388851	10.04790414	1.48388700
H	0.36468549	10.29545114	2.41808000
C	-0.60895451	8.76506614	1.25497700
H	-0.49599751	8.00738214	2.02085500
Cl	0.32841749	12.64030414	0.77843500
Cl	5.75070649	0.45326414	0.70391700
N	-2.17464251	1.90830714	-0.41420700
N	-1.18499751	4.67235614	-0.28387700
N	-3.90122551	5.79057414	-0.38563200
C	-1.94622651	-0.29248386	0.00098600
H	-2.20313551	-1.32193786	0.18933800
C	-2.89728251	0.75034714	-0.24518300
C	-4.28933651	0.63209514	-0.21421000
C	-5.20051451	1.69863014	-0.29177700
C	-6.64675251	1.50579214	-0.28404100
H	-7.15645051	0.55526514	-0.29163300
C	-7.19687751	2.74155514	-0.28689800
H	-8.24427051	2.99885714	-0.29709900
C	-6.08575451	3.68696514	-0.29435100
C	-6.26757751	5.07733114	-0.21632600
C	-5.24618951	6.03102814	-0.23105100
C	-5.38466751	7.43552014	0.01531400
H	-6.32289151	7.93492014	0.19342300
C	-5.48307051	-1.03099386	1.22733500
H	-5.59569851	-0.25596486	1.97587300
C	-4.83210851	-0.73606686	0.02411100
C	-4.68470651	-1.75187886	-0.92455400
H	-4.18866451	-1.53550686	-1.86412300
C	-5.17472751	-3.03215386	-0.68579700
H	-5.06609951	-3.81425186	-1.42691900
C	-5.81443051	-3.29747186	0.51966700
C	-5.97402351	-2.30656486	1.48211200

H	-6.46888351	-2.53138086	2.41873500
C	-7.65057151	5.59255414	-0.00116600
C	-8.29311451	6.36961314	-0.96898800
H	-7.78624851	6.58315114	-1.90342400
C	-9.57680551	6.86259114	-0.75579900
H	-10.07486051	7.45692914	-1.51174100
C	-10.22011851	6.57743314	0.44316700
C	-9.60377051	5.80909914	1.42468700
H	-10.11621451	5.60205314	2.35595100
C	-8.32250751	5.32010414	1.19554200
H	-7.83133051	4.72919214	1.95929700
Cl	-11.83952151	7.19896314	0.72301600
Cl	-6.43153551	-4.91257986	0.83208100
N	-4.88906651	3.02788214	-0.32862600
H	-3.49136351	4.86981514	-0.47724800
H	-2.58361751	2.82972814	-0.50293900