Electronic Supplementary Material (ESI) for Inorganic Chemistry Frontiers.

Electronic Supplementary Information

High Mobility at Interface of Cocrystallized Sandwich-type Tetrapyrrole Metal Compound and Fullerene Layers

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Caption of Content

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) [(Pc)Y(Pc)Y(TClPP)] (**1**) was prepared according to the published procedure.[1] 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 $AgNO_3$ 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 [$E_{1/2}(Fc^+/Fc)$ = 0.229 V for C_{60} and 0.210 V for **1**]. Typically, a 0.1 M solution of $[NBu_4][ClO_4]$ 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 *Kα* radiation (λ = 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. Powder X-ray diffraction (XRD) patterns were recorded with a Japan Rigaku TTR3 powder X-ray diffractometer, using Cu Kα radiation (λ = 1.54 Å). Crystallographic data and other pertinent information for all the complexes are summarized in Table S3. Selected structural information is listed in the Table S2. CCDC 1001325 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 [(Pc)Y(Pc)Y(TClPP)]·C_{60} (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 C_{60} (2.8 mg, 0.002 mmol) with the yield of 23-41% (computed on the basis of **1**).

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 orbital populations.[8,9] All calculations were carried out by Gaussian 09 D.01 and Multiwfn 3.4 version.[10,11]

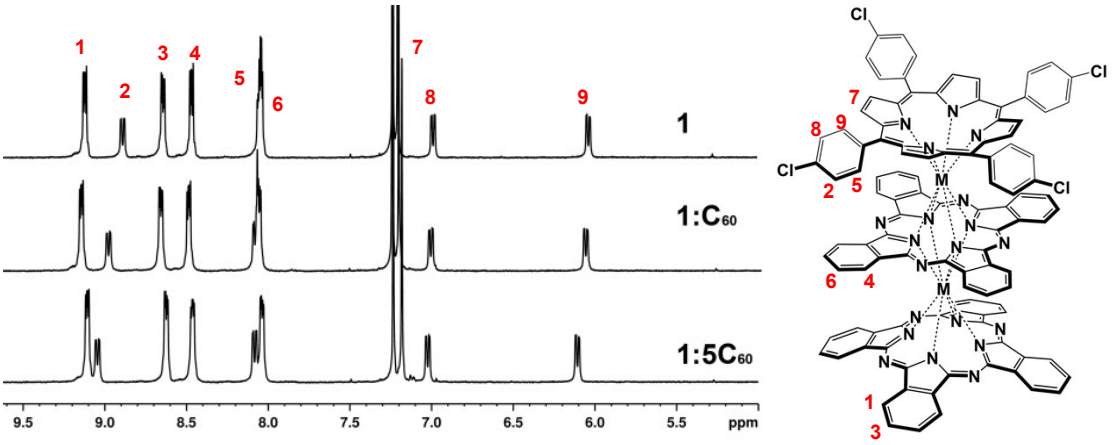

Figure S1. The downfield region of the ^{1}H NMR spectra (400 MHz, $CDCl_3/CS_2$ (2:1, v/v) solvent, 297K) of the solutions of **1**, **1** + C_{60}, and **1** + 5 C_{60}, along with the assignment of each peak.

Table S1. ^{1}H NMR data (δ) and assignments of the sandwich-type mixed (phthalocyaninato)(porphyrinato) triple-decker complexes in **1**, **1** + C_{60}, **1** + $5C_{60}$ (400 MHz, $CDCl_3/CS_2$ (2:1, v/v) solvent, 297K).

Compound	Pc^{inner}		Pc^{outer}	
	H^{α}	H^{β}	H^{α}	H^{β}
1	8.46 (d)	8.03 (m)[b]	9.11 (dd)	8.63 (d)
1+C_{60}	8.46 (d)	8.03 (m)[b]	9.11 (dd)	8.63 (d)
1+5C_{60}	8.45 (d)	8.03 (m)[b]	9.10 (dd)	8.61 (d)

Compound [a]	$TClPP^{outer}$				
	$H^{endo\text{-}ortho}$	$H^{endo\text{-}meta}$	$H^{exo\text{-}ortho}$	$H^{exo\text{-}meta}$	$H^{\beta\text{-}pyrrole}$
1	8.88 (dd)	8.03 (b)	6.97 (dd)	6.02 (dd)	7.20 (s)
1+C_{60}	8.94 (dd)	8.03 (b)	6.99 (dd)	6.04 (dd)	7.19 (s)
1+5C_{60}	9.03 (dd)	8.10 (dd)	7.01 (dd)	6.10 (dd)	7.18 (s)

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

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

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

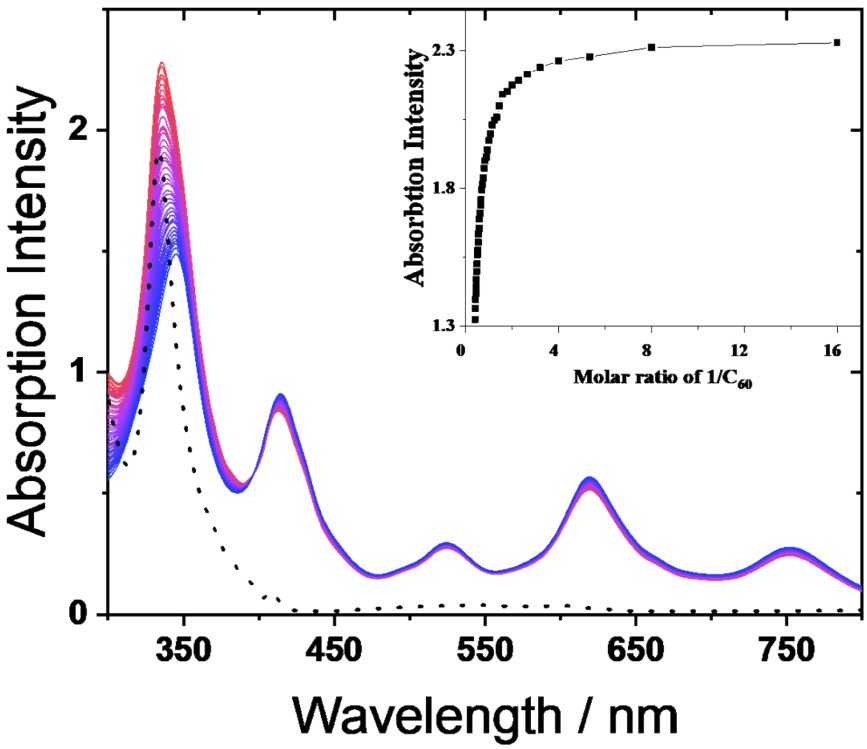

Figure S2. Electronic absorption spectrum of **1** in *o*-dicholobenzene with the concentration of 8.0×10^{-6} M upon addition of C_{60}. Changed intensity at 345 nm is shown in the insert diagram. The absorption of C_{60} is drawn by dash line.

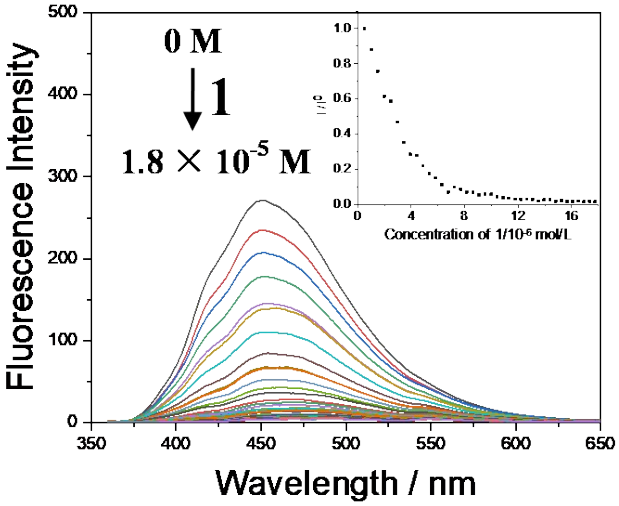

Figure S3. Fluorescent spectrum of C_{60} (*o*-dichlorobenzene, 1.0×10^{-5} M) upon addition of **1** (o-dichlorobenzene, 2.0×10^{-4} M) (λ_{ex} = 340 nm). Emission quenching upon addition of **1** curve is shown in the inserted diagram.

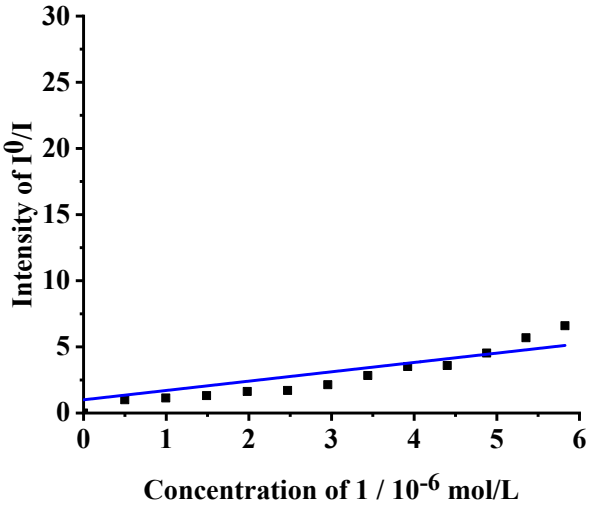

Figure S4. Stern-Volmer plot for the fluorescent spectral change of C_{60} at 450 nm upon addition of **1**.

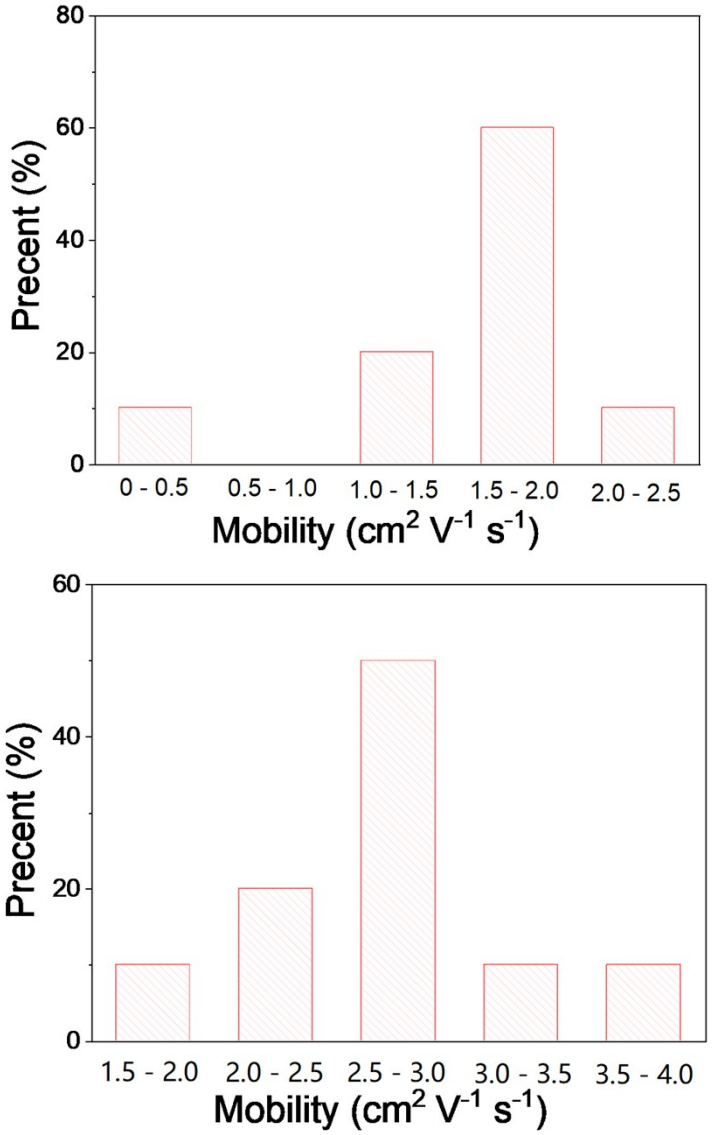

Figure S5. The distribution diagram of devices mobilities.

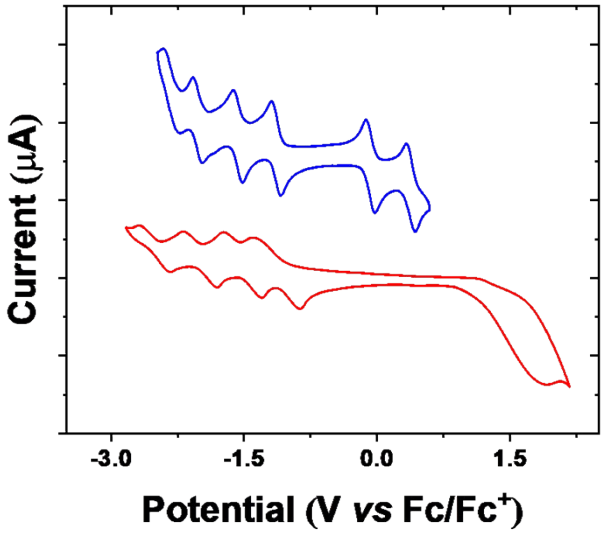

Figure S6. Cyclic voltammogram of **1** (blue) and C_{60} (red)[S12] in o-dichlorobenzene containing 0.1 M $[NBu_4][ClO_4]$ at a scan rate of 40 mV/s.

Table S2. Crystal data and structure refinement of complex **2.**

complex	**2**
Formula	C182H64Cl6N20O5Y2
F.W.	3001.05
system	Monoclinic
space group	*C*2/m
a	30.121(3)
b	25.7007(19)
c	18.6170(17)
α	90
β	105.358(10)
γ	90
Z	4
volume	13897(2)
absorption coefficient mm^{-1}	1.057
*F*000	6168
R_{int} *I>2θ*	0.1495
R_{w2} *I>2θ*	0.3900
R_{int} all	0.2364
R_{w2} all	0.4345
S	1.213

[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 S3. Crystallographic data and selected structural information for **2.**

complex	**2**
average Y-N(TClPP) bond distance (Å)	2.36
average Y-N(Pc) bond distance (Å)	2.34/2.59/2.64
Y-N_4(Pc) plane distance (Å)	1.25/1.74/1.81
Y-N_4(TClPP) plane distance (Å)	1.16
interplanar distance (Å)	2.97/3.00
dihedral angle between the adjacent two N_4 planes (°)	0.9
dihedral angle φ for the Pc ring (°)[a]	9.3/15.3
dihedral angle φ for the TClPP ring (°)[a]	14.2
twist angle (°)[b]	44.8
dihedral angle θ between the benzene rings and the N_4 plane of TClPP (°)	62.7
separation of 6:6 ring juncture and mean N_4 plane of Pc (Å)	2.87
separation of 6:6 ring juncture and mean N_4 plane of TClPP (Å)	2.88

[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. Cyclic voltammogram derived and DFT calculated energy level data of **1** and C_{60}.

Compound	$HOMO_{CV}$[a]	$LUMO_{CV}$	$HOMO_{Cal}$[b]	$LUMO_{Cal}$
1	-4.72	-3.66	-4.74	-3.47
C_{60}[3]	-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 S5. Comparison of the ambipolar mobilities of the reported systems and the present work.

	Compounds	Electron Mobility (μe) cm^2 /Vs	Hole Mobility (μh) cm^2 /Vs	HOMO Energy Level eV	LUMO Energy Level eV	References
1	CoTMPP-C_{60} nanosheet	10^{-5}	10^{-6}	-	-	13
2	DPTTA-DTTCNQ	0.24	0.77	-4.92	-4.53	14
3	Octanaphthoxy substituted tris(phthalocyaninato) europium	1.25	1.71	-5.07	-4.00	15
4	TPA-C_{60} Crystals	2.11 x 10^{-4}	3.37 x 10^{-4}	-5.20	-3.94	16
5	[Pc-(OPh)8]Eu[Pc(OPh)8]Eu [TP(C≡CCOOH)PP]	4×10^{-4}	0.11	-5.05	-3.89	17
6	CoTMPP- C_{70} cocrystals	0.02	4.21	-	-	18
7	dif-TES-ADT-BPE-PTCDI	0.43	0.32	-	-	19
8	Hexacene Diimides	2.17	0.30	-5.56	-4.41	20
9	PDBD-Se	7.71	8.90	-5.03	-3.85	21
10	TFT-CN-C6-DPA	0.87	0.82	-5.05	-4.55	22
11	(Pc)Y(Pc)Y (TClPP)	2.22	3.72	-4.72	-3.66	This work

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.

[(TClPP)Y(Pc)Y(TClPP)] ·C_{60} ·[(TClPP)Y(Pc)Y(TClPP)](**2**)

SCF Energy: -16614.01141320

C	3.73263906	0.52083333	0.00000000
C	4.02505406	1.70484933	-0.79728700
C	4.31249406	3.02234833	-0.45060000
H	4.32400906	3.32480933	0.58951100
C	4.57663706	3.91858633	-1.48084400
H	4.79714606	4.95514933	-1.24789600
C	4.58938106	3.49838233	-2.82338300
H	4.81116906	4.22478833	-3.59822000
C	4.31128606	2.18135633	-3.17288700
H	4.31654706	1.84787433	-4.20353500
C	4.02278306	1.28906333	-2.14380800
C	3.72995806	-0.13849767	-2.13477700
C	3.77504406	-2.21678367	-3.21115500
C	4.10051906	-3.01461567	-4.38557100
C	4.42967706	-2.66810067	-5.69289000
H	4.44440006	-1.62799467	-5.99553600
C	4.74186906	-3.69611367	-6.57671800
H	4.99913906	-3.45761767	-7.60347700
C	3.75753006	-0.57835467	2.06933400
C	4.07212606	-0.56847167	3.49149200
C	4.39373306	0.45869333	4.37327700
H	4.41039306	1.48775133	4.03501800
C	4.69446806	0.10581133	5.68450100
H	4.94620006	0.87754033	6.40432500
C	0.59780106	-0.51979767	2.00942900

C	0.76660606	0.89607533	2.27570000
C	1.05783606	1.59211333	3.44657600
H	1.13837606	1.06931433	4.39144900
C	1.26261806	2.96398633	3.34472300
H	1.49806206	3.53861233	4.23416300
C	1.17748106	3.62314533	2.10462000
H	1.34221906	4.69437733	2.06344900
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H	0.87215306	3.41932633	-0.03063800
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C	0.54289506	0.51529133	0.02581100
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H	1.54275606	-0.14457167	-7.36653500
C	1.09500106	-1.28146667	-5.60300200
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C	-2.61575294	0.62556933	-0.07911800
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H	-2.83773394	2.81641333	-0.53578000

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C	-4.32640794	2.50383933	1.72101300
H	-5.02110794	2.01007033	1.05131100
C	-3.08237994	1.91417833	1.97519600
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H	-1.25071594	2.11396233	3.07024900
C	-2.55355294	3.76382033	3.45593100
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C	-2.62389894	-5.38785167	6.35446200
H	-1.94130694	-5.40792867	7.19487300
C	-3.85859494	-6.01864567	6.43650900
C	-4.74485994	-6.00150067	5.36502100
H	-5.71031794	-6.48490567	5.44929100
C	-3.08303694	-6.81209267	-2.50726400
C	-2.20754994	-7.45744467	-3.38110100
H	-1.24374694	-7.01878267	-3.58826800
C	-2.55006394	-8.66341767	-3.98435600
H	-1.85566094	-9.16140267	-4.64954600
C	-3.79160394	-9.22511767	-3.71629300
C	-4.69242994	-8.59888467	-2.86166700
H	-5.66171294	-9.04319367	-2.67189500

C	-4.33130594	-7.39690467	-2.26288900
H	-5.02926094	-6.90060067	-1.59845300
Cl	-4.23385894	-10.75182367	-4.47096100
Cl	-4.30971994	-6.85173767	7.91921400
N	-2.47425294	-4.42198967	0.36168400
C	13.12498206	-1.81131667	-0.36626200
C	13.12095306	-3.15707967	-0.02763300
C	12.67418306	-4.14459367	-0.99515800
C	12.25663506	-3.74782467	-2.26011400
C	12.25980306	-2.33732567	-2.61266100
C	12.68106206	-1.39352067	-1.68283100
C	11.95705306	-0.14241167	-1.53618700
C	10.83831806	0.11286533	-2.32273800
C	10.39242606	-0.87622667	-3.29210600
C	11.08839006	-2.07501667	-3.43329200
C	10.36035806	-3.32465667	-3.58711600
C	11.08347306	-4.35874967	-2.86240800
C	9.66143306	0.73210033	-1.73410800
C	8.48812406	0.12250533	-2.33732800
C	8.93961006	-0.87220667	-3.29900000
C	8.24204906	-2.06920967	-3.44692900
C	8.96783606	-3.32183667	-3.59256700
C	8.23462906	-4.35343167	-2.87489000
C	8.92640506	-5.34360267	-2.18078300
C	10.38029806	-5.34576667	-2.17475300
C	10.81914306	-5.76105867	-0.85082300
C	11.94421606	-5.17560267	-0.27728500
C	7.36065206	-0.12515867	-1.56032300
C	6.64125506	-1.37777867	-1.70969500
C	7.06359006	-2.32624167	-2.63578000
C	7.05987006	-3.73679767	-2.28186100
C	6.63256406	-4.13448167	-1.02018400

C	7.34523006	-5.17260967	-0.29643600
C	8.47043606	-5.76108767	-0.86352200
C	9.64131806	-6.02094267	-0.04260400
C	6.18964006	-1.79441067	-0.39614300
C	6.18491906	-3.14308867	-0.05961900
C	12.66403406	-3.57287267	1.28509800
C	12.23852306	-2.62691567	2.21111100
C	12.24433106	-1.21629967	1.85856600
C	12.67441906	-0.82153867	0.59723600
C	11.95494606	0.21247333	-0.12719700
C	10.82752006	0.80330033	0.43590800
C	10.37543006	0.39017233	1.75616900
C	11.06824306	-0.60008467	2.44999900
C	10.33426906	-1.63104867	3.16815000
C	11.05834806	-2.88388867	3.02093600
C	9.65829106	1.06837033	-0.38278200
C	8.47921006	0.81374433	0.42791600
C	8.92159506	0.39433333	1.74925700
C	8.21947706	-0.59294567	2.43710100
C	8.94175606	-1.62777767	3.16115100
C	8.21176006	-2.87721567	3.00903000
C	8.90542906	-4.07717967	2.86717100
C	10.35831506	-4.07959167	2.87335900
C	10.80847806	-5.07077667	1.90807700
C	11.93559506	-4.82080667	1.13184700
C	7.35668906	0.22995533	-0.14910000
C	6.63315906	-0.80501367	0.56829900
C	7.04735106	-1.20453767	1.83371700
C	7.04163006	-2.61510667	2.18752900
C	6.62293406	-3.56175367	1.25787600
C	7.33821006	-4.81754467	1.11481900
C	8.45802006	-5.06989067	1.90153500

C	9.63402406	-5.68464767	1.30876000
C	22.02942506	0.50699433	0.13343400
C	22.21367006	1.74643833	-0.61236000
C	22.37797706	3.06874233	-0.21050000
H	22.39592906	3.32520633	0.84178600
C	22.50084206	4.03615233	-1.20338800
H	22.61913206	5.07828233	-0.92560200
C	22.47598306	3.68835133	-2.56541400
H	22.57512006	4.46880733	-3.31258100
C	22.32960206	2.36430333	-2.96809900
H	22.30861906	2.08411533	-4.01422700
C	22.19099806	1.39826433	-1.97582500
C	21.99676906	-0.04567767	-2.03034700
C	22.04504006	-2.06715967	-3.21456700
C	22.31127406	-2.80721667	-4.44123100
C	22.51912706	-2.40092667	-5.75686300
H	22.50185506	-1.34957667	-6.01761100
C	22.73648306	-3.38965967	-6.71154200
H	22.89239906	-3.10917567	-7.74816500
C	22.09638006	-0.69503267	2.14482700
C	22.37651806	-0.75505067	3.57401100
C	22.62051206	0.23358133	4.52303700
H	22.63352306	1.27801333	4.23598700
C	22.82988006	-0.17082267	5.83842400
H	23.01266306	0.57407733	6.60577600
C	18.93463906	-0.67997467	2.14062000
C	19.10559006	0.71668033	2.49228200
C	19.42567606	1.33675633	3.69742700
H	19.53189206	0.75416633	4.60388000
C	19.62213206	2.71349633	3.67935500
H	19.87951806	3.23079233	4.59745700
C	19.49460306	3.45118833	2.48842300

H	19.64842106	4.52458833	2.51327300
C	19.19501706	2.82924933	1.28081100
H	19.13072406	3.38497533	0.35370600
C	19.01345606	1.44912933	1.29370700
C	18.83984906	0.47754233	0.22735400
C	18.81323406	-0.08641767	-2.03019400
C	18.94300606	0.26942933	-3.43293900
C	19.08908506	1.49515933	-4.07646700
H	19.04229806	2.42040833	-3.51593100
C	19.32507706	1.47918333	-5.44695000
H	19.44629906	2.41593333	-5.98005000
C	19.42658606	0.26886733	-6.15683200
H	19.63199406	0.29595233	-7.22166500
C	19.27183406	-0.95668567	-5.51758700
H	19.36197006	-1.89554367	-6.04957900
C	19.01513806	-0.94050467	-4.14880900
C	18.88619306	-2.00796267	-3.17520300
N	18.80598706	-0.80025067	0.76631900
N	18.78181906	-1.46703567	-1.90377500
C	15.27532606	-0.88105067	3.73431000
H	14.99770606	-0.06191067	4.37798600
C	15.63581006	-0.76401967	2.34061200
C	15.57772706	0.44138833	1.61857800
C	15.66637906	0.56973033	0.22355400
C	15.45111706	1.80577733	-0.49264700
H	15.31041506	2.77366633	-0.03894400
C	15.44305506	1.50540733	-1.81932600
H	15.30139906	2.18519833	-2.64366900
C	15.64781706	0.07958133	-1.93623300
C	15.54751606	-0.64128867	-3.13821300
C	15.60067006	-2.04059767	-3.26332800
C	15.22462706	-2.75758967	-4.45942200

H	14.93372406	-2.30333167	-5.39264400
C	13.88818606	2.20105033	2.19613600
H	13.22025306	1.73652233	1.48366700
C	15.16807006	1.66353733	2.38408300
C	16.00936806	2.26599733	3.31768700
H	16.99253606	1.85980633	3.49125800
C	15.60016406	3.38386133	4.03906800
H	16.26638806	3.84907933	4.75489100
C	14.32763206	3.89760233	3.82846400
C	13.46017506	3.31194033	2.91271200
H	12.46512506	3.71370433	2.76715100
C	15.19568106	0.13015333	-4.37068700
C	16.07007006	0.19050133	-5.45740000
H	17.02326806	-0.31212467	-5.40010900
C	15.73812106	0.89116033	-6.61209400
H	16.43065706	0.93963233	-7.44315600
C	14.50801906	1.53257633	-6.68372100
C	13.61211806	1.48401633	-5.62176000
H	12.65127706	1.97839433	-5.69382300
C	13.96327006	0.78538333	-4.47221400
H	13.26619906	0.74629133	-3.64677500
Cl	14.07625406	2.41938733	-8.14107300
Cl	13.80152406	5.30992633	4.73773800
N	21.84424806	-2.95784267	-2.18453100
N	22.05985406	-0.74362567	-3.15412500
N	21.82706406	-0.52580567	-0.75236800
N	22.12120806	0.43437933	1.45230700
N	21.86643006	-1.96942167	1.67826200
N	15.89104506	-2.01767167	1.82534600
N	15.84971406	-0.45571467	-0.68155400
N	15.86585606	-2.94280567	-2.25415200
Y	20.57747406	-2.46709067	-0.24489700

Y	17.02353006	-2.47687667	-0.22190400
N	18.81787306	0.80600433	-1.05376800
N	18.97382506	-1.65482967	3.03259400
N	18.93662206	-3.28809067	-3.50148900
C	22.03206206	-4.88067467	1.52191500
C	22.23290806	-6.32364767	1.46491700
C	22.38957606	-7.28878567	2.45529300
H	22.38081206	-7.00871067	3.50166400
C	22.53749506	-8.61213867	2.05066100
H	22.65033406	-9.39207767	2.79645100
C	22.54656906	-8.95983667	0.68843300
H	22.66669906	-10.00136267	0.40911200
C	22.40603206	-7.99306867	-0.30281400
H	22.41195206	-8.24953267	-1.35526700
C	22.23981406	-6.67173067	0.10128900
C	22.03973006	-5.43323367	-0.64198700
C	22.07436906	-4.23105667	-2.65398600
C	22.33576306	-4.16975367	-4.08674600
C	22.57223006	-5.15707867	-5.03902200
H	22.59371806	-6.20150167	-4.75245100
C	22.76302706	-4.75156167	-6.35689700
H	22.93952906	-5.49550367	-7.12664000
C	22.08495506	-2.85906967	2.70546800
C	22.36294806	-2.11766267	3.92881100
C	22.58927406	-2.52272467	5.24175500
H	22.58006906	-3.57409767	5.50291200
C	22.81406706	-1.53278767	6.19351500
H	22.98428706	-1.81233067	7.22814800
N	22.11360406	-5.36029267	-1.96194400
N	21.84346806	-4.40142767	0.24630100
N	22.10548006	-4.18246167	2.64486100
C	18.92626506	-2.93524967	2.70694700

C	19.07237306	-4.00187367	3.67897800
C	19.34448806	-3.98371767	5.04468300
H	19.43533606	-3.04417867	5.57545900
C	19.51363106	-5.20826367	5.68234600
H	19.73137806	-5.23392467	6.74478800
C	19.41100906	-6.41922367	4.97380400
H	19.54385506	-7.35515267	5.50564700
C	19.15918606	-6.43685667	3.60604200
H	19.11124806	-7.36264667	3.04641400
C	18.99862106	-5.21218467	2.96408000
C	18.84994606	-4.85705767	1.56283300
C	18.85120906	-5.42088267	-0.69481000
C	19.01696106	-6.39161067	-1.76345100
C	19.20727506	-7.77051367	-1.75331000
H	19.15885606	-8.32699167	-0.82566100
C	19.49485306	-8.39045767	-2.96498500
H	19.65516506	-9.46287567	-2.99210800
C	19.60193406	-7.65190967	-4.15736100
H	19.85037706	-8.16745367	-5.07892200
C	19.39669406	-6.27640067	-4.17248700
H	19.48737006	-5.69293867	-5.08010500
C	19.08886006	-5.65867667	-2.96301600
C	18.91418906	-4.26315167	-2.60914800
N	18.80899506	-3.47681667	1.43689300
N	18.80269306	-4.14352867	-1.23326400
N	18.84758806	-5.74934567	0.58640800
C	15.28370406	-2.20627467	4.03994200
H	15.00950806	-2.66187967	4.97755500
C	15.64653206	-2.92118667	2.83842200
C	15.60143406	-4.32078067	2.71406300
C	15.68862006	-5.04085867	1.51081200
C	15.49216306	-6.46804167	1.39694700

H	15.36747906	-7.14878967	2.22331600
C	15.48339906	-6.76827767	0.07030600
H	15.34353606	-7.73721167	-0.38143300
C	15.67956506	-5.53065967	-0.64881200
C	15.56958106	-5.40332267	-2.04222100
C	15.61027406	-4.19795367	-2.76562500
C	15.22893206	-4.08292967	-4.15396100
H	14.94679806	-4.90351167	-4.79383800
C	14.05393206	-5.76086667	4.07647300
H	13.34150506	-5.72733367	3.26392300
C	15.27867106	-5.09505767	3.95270900
C	16.17350906	-5.14862167	5.02302000
H	17.12157006	-4.63835467	4.94834900
C	15.86874306	-5.85253767	6.18329300
H	16.57684406	-5.89566467	7.00146500
C	14.64560706	-6.50430167	6.27721200
C	13.72990906	-6.46290967	5.23195800
H	12.77483306	-6.96555667	5.32154800
C	15.15532906	-6.62888867	-2.79964400
C	15.98941106	-7.23289267	-3.73870300
H	16.96984606	-6.82474767	-3.92327800
C	15.57684406	-8.35535767	-4.45105000
H	16.23764506	-8.82188067	-5.17105000
C	14.30815206	-8.87223167	-4.22573400
C	13.44773206	-8.28526167	-3.30417900
H	12.45553306	-8.68974567	-3.14708100
C	13.87895906	-7.16972967	-2.59675300
H	13.21633106	-6.70511067	-1.87915100
Cl	13.77790606	-10.29047367	-5.12344600
Cl	14.24837806	-7.39551867	7.74176300
N	15.86833906	-4.50401567	0.25360200

C_{60}

Neutral SCF Energy: -2286.90674838

Negative SCF Energy: -2286.99677352

C	3.07291681	0.22569444	0.00000000
C	3.33413381	1.62631244	-0.28637800
C	4.26274181	1.97569744	-1.26215500
C	4.97167481	0.94002944	-1.99454100
C	4.72138381	-0.40121556	-1.72062900
C	3.75136681	-0.76634356	-0.70182100
C	2.86646881	0.09089644	1.43220800
C	3.00036781	1.40852644	2.03094600
C	3.28886781	2.35764144	0.96876000
C	4.17484681	3.40679544	1.19490000
C	5.18725281	3.07188944	-1.02652000
C	6.33444581	1.39552044	-2.21139100
C	7.38932881	0.49049844	-2.14425100
C	7.12839781	-0.91026856	-1.85838100
C	5.82310481	-1.34638756	-1.65095900
C	5.53450681	-2.29513756	-0.58884100
C	4.25407081	-1.93685756	-0.00237600
C	4.05637481	-2.06612656	1.36921400
C	3.34787781	-1.03022056	2.10190400
C	3.60995681	1.54896044	3.27411700
C	4.11240081	0.37849644	3.97329100
C	3.98428781	-0.88318956	3.40013600
C	5.08623081	-1.82804756	3.46985100
C	5.13091581	-2.55901656	2.21462900
C	6.35709281	-2.90184656	1.65284300
C	6.56324481	-2.76746156	0.22058200
C	7.92619881	-2.31200956	0.00394200
C	8.20284081	-1.40359556	-1.01340100
C	6.46786381	2.71288644	-1.61264500
C	9.87076381	1.15062744	1.06494900

C	9.38935481	2.27174244	0.39525400
C	8.68085881	3.30764844	1.12794200
C	8.48316381	3.17838144	2.49953200
C	8.98586781	2.00786844	3.19897800
C	9.40309981	-0.38478956	2.78353500
C	9.44836681	-1.11611856	1.52839500
C	9.73686581	-0.16700556	0.46621000
C	9.12727681	-0.30743956	-0.77696000
C	8.62483181	0.86302644	-1.47613600
C	8.75294381	2.12471244	-0.90298000
C	7.60631681	3.80053944	0.28252800
C	6.38014081	4.14336744	0.84431300
C	6.17398881	4.00898344	2.27657400
C	7.20272681	3.53666044	3.08599900
C	6.91412981	2.58791144	4.14811600
C	8.01584981	1.64273844	4.21778600
C	7.76555881	0.30149344	4.49169600
C	8.47449181	-0.73417356	3.75931000
C	8.56238681	-2.16527356	1.30225500
C	7.59269381	-2.53015156	2.32148600
C	7.54997981	-1.83036656	3.52367500
C	6.26936981	-1.47136356	4.10979900
C	6.40278681	-0.15399556	4.70854600
C	5.34790681	0.75102444	4.64140600
C	5.60883481	2.15179244	4.35553700
C	4.53439381	2.64511844	3.51055700
C	4.81103681	3.55353244	2.49321500
C	7.65100381	3.06956944	-0.97269500
C	5.14453881	3.77167344	0.17567100
C	9.66431681	1.01582844	2.49715500

C_{60}-relaxation in negative potential surface

Neutral SCF Energy: -2286.90418434

Negative SCF Energy: -2286.99921540

C	0.61728394	-0.92592591	0.00000000
C	-0.52329406	-0.33771491	0.56801700
C	-0.38992606	0.69660509	1.56371100
C	0.88459294	1.12386209	1.97371100
C	2.06802394	0.51102809	1.38975400
C	1.93927494	-0.48761791	0.42808400
C	2.81615894	-1.64499191	0.45822000
C	3.78862294	-1.76060391	1.45774100
C	3.92245194	-0.72191191	2.45933200
C	3.08129194	0.39393609	2.42638800
C	2.51149494	0.91242009	3.65459400
C	1.15476294	1.36629609	3.36929200
C	4.00777594	-3.03976491	2.10459200
C	4.27994294	-2.79243791	3.50958500
C	4.22644194	-1.35729191	3.72868900
C	3.68105294	-0.85544691	4.90971800
C	2.80287894	0.30416109	4.87324200
C	1.76188394	0.11881809	5.87006600
C	0.45367194	0.55441909	5.59208700
C	0.15146194	1.18195909	4.32930200
C	-1.17158606	0.73762709	3.90582600
C	-1.43180106	0.50105609	2.55851300
C	3.78632994	-3.66298191	4.47909800
C	3.21581494	-3.13853991	5.70818400
C	3.16481194	-1.76329191	5.91806700
C	1.98028294	-1.15514791	6.50977100
C	0.89405494	-1.96819991	6.86203300
C	-0.46272606	-1.51840491	6.57279200
C	-0.67322506	-0.28952391	5.95245300
C	-1.68663006	-0.16696091	4.91561800
C	2.08808794	-3.98102791	6.07837900

C	0.94749694	-3.39282291	6.64639200
C	-1.65102706	-1.18019991	0.93819900
C	-1.60003206	-2.55544591	0.72830400
C	-0.41550806	-3.16357391	0.13661200
C	0.67073694	-2.35054791	-0.21564000
C	2.02752094	-2.80033291	0.07357800
C	2.23800094	-4.02922091	0.69392200
C	1.11110694	-4.87315791	1.05429200
C	-0.19710406	-4.43755791	0.77632300
C	-1.23809406	-4.62289991	1.77313800
C	-2.11628106	-3.46330091	1.73666300
C	3.25141194	-4.15177491	1.73076200
C	2.73637494	-5.05635291	2.74055600
C	1.41332494	-5.50069291	2.31707900
C	0.41002594	-5.68503491	3.27709000
C	-0.94671406	-5.23116191	2.99178600
C	-1.51649706	-4.71266691	4.21999300
C	-2.35766306	-3.59681991	4.18705100
C	-2.66166006	-2.96145091	2.91768800
C	-2.71516706	-1.52630291	3.13679700
C	-2.22156206	-0.65574591	2.16727500
C	2.99657094	-4.81979091	4.08786400
C	1.95470894	-5.01534991	5.08268800
C	0.68019794	-5.44260591	4.67265600
C	-0.50323906	-4.82975891	5.25661800
C	-0.37449306	-3.83111991	6.21829600
C	-1.25136206	-2.67374291	6.18814300
C	-2.22383106	-2.55813091	5.18863900
C	-2.44299306	-1.27897091	4.54178200

[(Pc)Y(Pc)Y(TClPP)]

Neutral SCF Energy: -7163.50074456

Positive SCF Energy: -7163.29764072

Negative SCF Energy: -7163.59836114

C	2.77383267	1.83454506	-0.03630948
C	1.38788767	2.24529106	0.15616752
C	0.20844967	1.52367506	0.31361252
H	0.22254667	0.44049006	0.31154952
C	-0.97542633	2.24206706	0.45275952
H	-1.91516033	1.71153506	0.56511452
C	-0.97784733	3.64795106	0.45292652
H	-1.91939833	4.17521906	0.56543652
C	0.20354567	4.37047806	0.31405752
H	0.21398767	5.45372006	0.31220052
C	1.38546767	3.65295306	0.15647452
C	2.76992167	4.06859506	-0.03573448
C	4.43124967	5.72196006	0.01336452
C	4.84241267	7.09464506	0.28032852
C	4.12088267	8.26326706	0.50756952
H	3.03760367	8.24853406	0.50884052
C	4.83898667	9.43691006	0.71583852
H	4.30857667	10.36806306	0.88552952
C	4.44110467	0.18705406	0.01144552
C	4.85686667	-1.18445694	0.27705752
C	4.13928467	-2.35580094	0.50289752
H	3.05593767	-2.34449094	0.50454352
C	4.86131567	-3.52726194	0.70985352
H	4.33406467	-4.46042494	0.87830652
C	4.39422267	0.21661106	-3.13870848
C	3.12461667	-0.46792794	-2.98528748
C	2.81432267	-1.79564394	-2.70177748
H	3.59939467	-2.53539194	-2.60596548
C	1.47265467	-2.11936094	-2.52895948
H	1.19251267	-3.14255594	-2.30222248
C	0.46779867	-1.14145194	-2.64020348

H	-0.56858233	-1.43142594	-2.50528948
C	0.77959967	0.18895306	-2.90039648
H	0.01532767	0.95442106	-2.95106248
C	2.12251267	0.51721206	-3.06275848
C	2.80537567	1.79132006	-3.21127848
C	2.80218367	4.11871406	-3.20932248
C	2.11578767	5.39057706	-3.05947948
C	0.77188667	5.71446006	-2.89672448
H	0.00996467	4.94669806	-2.94814348
C	0.45594567	7.04361906	-2.63509748
H	-0.58131333	7.33019306	-2.49963048
C	1.45782867	8.02449706	-2.52324248
H	1.17456567	9.04663706	-2.29565248
C	2.80049367	7.70517906	-2.69683048
H	3.58314067	8.44741906	-2.60063648
C	3.11497667	6.37864706	-2.98137848
C	4.38665567	5.69774806	-3.13528248
N	4.17589067	1.58038706	-3.24890348
N	4.17208167	4.33350206	-3.24634948
C	4.88189167	-1.23800394	-6.84820148
H	4.22881367	-2.04276094	-7.14563848
C	4.45271967	0.08317306	-6.44976148
C	3.11607267	0.51846806	-6.48851348
C	2.68142267	1.84882506	-6.36482348
C	1.30470567	2.27256406	-6.48311148
H	0.45337467	1.61518406	-6.55523948
C	1.30202167	3.63224006	-6.48288248
H	0.44818567	4.28634206	-6.55484148
C	2.67701167	4.06127306	-6.36382548
C	3.10643167	5.39352206	-6.48646648
C	4.44116267	5.83401006	-6.44749248
C	4.86479567	7.15709906	-6.84519748

H	4.20824467	7.95938806	-7.14170348
C	1.40360667	-0.37922094	-8.08849048
H	1.63872767	0.44424606	-8.75279448
C	2.08172267	-0.49143694	-6.86838848
C	1.77878567	-1.57287094	-6.03975548
H	2.29586867	-1.68175094	-5.09899748
C	0.81496467	-2.50920594	-6.39833448
H	0.57895167	-3.33492194	-5.73865348
C	0.15215267	-2.36714494	-7.61063948
C	0.44162267	-1.30964194	-8.46606348
H	-0.07435433	-1.21946194	-9.41394648
C	2.06784567	6.39943006	-6.86523948
C	1.75851267	7.47742106	-6.03452948
H	2.27454967	7.58721306	-5.09325548
C	0.78918067	8.40872106	-6.39144748
H	0.54814367	9.23173106	-5.73023948
C	0.12761267	8.26519406	-7.60426648
C	0.42393667	7.21147806	-8.46203848
H	-0.09108733	7.12026806	-9.41033448
C	1.39133067	6.28605306	-8.08608148
H	1.63173967	5.46548806	-8.75207848
Cl	-1.10321133	9.43536006	-8.06426548
Cl	-1.07096033	-3.54434294	-8.07315448
N	5.54980467	4.95183206	-0.20647548
N	3.16549667	5.33042106	0.03779352
N	3.55107667	2.95297206	-0.22759448
N	3.17389767	0.57411506	0.03627852
N	5.55708767	0.96120606	-0.20764748
N	5.55764367	0.85809106	-6.17049148
N	3.48811567	2.95662606	-6.21612648
N	5.54906167	5.06343306	-6.16852348
Y	5.55367067	2.95680206	-1.48050948

Y	5.55347767	2.96018806	-5.03414248
N	2.17498967	2.95408106	-3.21275048
N	5.55776667	-0.40976094	-3.09872348
N	5.54853167	6.32705706	-3.09489048
C	8.33690967	1.84421006	-0.03601048
C	9.72142467	2.25974906	0.15601752
C	10.90346167	1.54217006	0.31255152
H	10.89304867	0.45893606	0.31001752
C	12.08487267	2.26464006	0.45149452
H	13.02649867	1.73732706	0.56317952
C	12.08239167	3.67053006	0.45234552
H	13.02214467	4.20102406	0.56470252
C	10.89843767	4.38896606	0.31420352
H	10.88429567	5.47214506	0.31295852
C	9.71894267	3.66741606	0.15674552
C	8.33294467	4.07826806	-0.03488848
C	6.66575267	5.72578806	0.01359752
C	6.24983767	7.09703706	0.28055152
C	6.96731267	8.26813906	0.50778752
H	8.05064267	8.25701706	0.50909052
C	6.24514267	9.43932806	0.71587252
H	6.77234467	10.37229806	0.88559952
C	6.67558267	0.19078506	0.01145652
C	6.26437667	-1.18215694	0.27699352
C	6.98576367	-2.35110594	0.50312952
H	8.06905967	-2.33636794	0.50500252
C	6.26756267	-3.52492494	0.71006052
H	6.79784267	-4.45633894	0.87866452
N	7.93290967	5.33869806	0.03837752
N	7.55565367	2.96001506	-0.22666748
N	7.94139567	0.58227506	0.03617952
C	6.71970867	0.21949306	-3.13874748

C	7.99116467	-0.46142794	-2.98477548
C	8.30563567	-1.78824994	-2.70130748
H	7.52302067	-2.53063394	-2.60591748
C	9.64822167	-2.10773994	-2.52789948
H	9.93149167	-3.13009794	-2.30128048
C	10.65013467	-1.12667094	-2.63842548
H	11.68734467	-1.41339194	-2.50290848
C	10.33417167	0.20270506	-2.89865848
H	11.09594467	0.97066506	-2.94900848
C	8.99034867	0.52666906	-3.06186948
C	8.30400667	1.79881006	-3.21090048
C	8.30091767	4.12604706	-3.20947548
C	8.98364767	5.40016306	-3.05996248
C	10.32663067	5.72823506	-2.89768148
H	11.09067667	4.96264606	-2.94930648
C	10.63855767	7.05829906	-2.63617848
H	11.67494267	7.34821406	-2.50118448
C	9.63368667	8.03609406	-2.52364348
H	9.91394067	9.05908006	-2.29608048
C	8.29202767	7.71261506	-2.69670248
H	7.50706867	8.45238406	-2.60010248
C	7.98158867	6.38517006	-2.98154848
C	6.71210767	5.70079006	-3.13542048
N	6.93436667	1.58386706	-3.24895748
N	6.93055167	4.33706906	-3.24659748
N	8.93109467	2.96334306	-3.21296348
C	6.24172767	-1.23529894	-6.84807748
H	6.89819267	-2.03728994	-7.14557348
C	6.66550167	0.08754106	-6.44983048
C	8.00037167	0.52809806	-6.48882148
C	8.42971567	1.86026806	-6.36539048
C	9.80471967	2.28951206	-6.48325848

H	10.65866567	1.63550806	-6.55486248
C	9.80196567	3.64917806	-6.48288048
H	10.65327367	4.30661506	-6.55450748
C	8.42521967	4.07277006	-6.36449848
C	7.99041167	5.40327806	-6.48706348
C	6.65386567	5.83847706	-6.44772548
C	6.22463567	7.15978606	-6.84567548
H	6.87767867	7.96474406	-7.14264748
C	9.71648067	-0.36282894	-8.08845248
H	9.47728967	0.45899506	-8.75334248
C	9.03881267	-0.47771294	-6.86837748
C	9.34701667	-1.55726094	-6.03916048
H	8.83022967	-1.66831194	-5.09852248
C	10.31603767	-2.48850594	-6.39678948
H	10.55636767	-3.31240494	-5.73639348
C	10.97863467	-2.34352894	-7.60892548
C	10.68356667	-1.28829494	-8.46518548
H	11.19937167	-1.19583694	-9.41294248
C	9.02469267	6.41358006	-6.86596948
C	9.32917667	7.49303406	-6.03542548
H	8.81312067	7.60019406	-5.09390348
C	10.29335467	8.42940606	-6.39289848
H	10.53045867	9.25367106	-5.73183448
C	10.95469767	8.28950706	-7.60626248
C	10.66336267	7.23425506	-8.46383048
H	11.17812267	7.14586006	-9.41253448
C	9.70104167	6.30374106	-8.08724448
H	9.46421467	5.48220206	-8.75332848
Cl	12.17874767	9.46642206	-8.06715448
Cl	12.20859967	-3.51408694	-8.07013848
N	7.61854767	2.96482906	-6.21679548

[(Pc)Y(Pc)Y(TClPP)]-relaxation in positive potential surface

Neutral SCF Energy: -7163.50074456

Positive SCF Energy: -7163.49904627

C	3.52173907	-0.73913042	0.00000000
C	2.13371507	-1.15696842	-0.18529800
C	0.95382307	-0.44046442	-0.33768400
H	0.96080607	0.64252458	-0.34255200
C	-0.22913693	-1.16783942	-0.47110400
H	-1.17120593	-0.64266442	-0.58351900
C	-0.22386493	-2.57049542	-0.47091000
H	-1.16195793	-3.10276742	-0.58315200
C	0.96458307	-3.28884242	-0.33726900
H	0.97982407	-4.37175542	-0.34222200
C	2.13900507	-2.56335342	-0.18501000
C	3.53014707	-2.97069042	0.00043400
C	5.19957907	-4.61510042	-0.04419400
C	5.61782907	-5.99097542	-0.30264700
C	4.90111707	-7.16014842	-0.52384700
H	3.81808507	-7.15195742	-0.53188500
C	5.62818207	-8.33346142	-0.72636300
H	5.10297207	-9.26702742	-0.89530400
C	5.17933007	0.91720158	-0.04431400
C	5.58730007	2.29619158	-0.30232300
C	4.86177907	3.46005958	-0.52291400
H	3.77881507	3.44386958	-0.53072900
C	5.57999007	4.63880658	-0.72542400
H	5.04779507	5.56850158	-0.89382900
C	5.12269307	0.89017358	3.05824700
C	3.84269807	1.56679158	2.92504500
C	3.51732307	2.89435058	2.66870500
H	4.29178307	3.64605158	2.57967800
C	2.16826707	3.20769258	2.52155600
H	1.87441807	4.23218358	2.32170200

C	1.17573607	2.22057558	2.63241000
H	0.13487607	2.50388458	2.52389800
C	1.50464507	0.88675458	2.86422200
H	0.74791907	0.11428958	2.91904800
C	2.85178907	0.57202858	2.99845500
C	3.54964307	-0.70018342	3.12121900
C	3.56682607	-3.02901642	3.12075700
C	2.88768007	-4.31127542	2.99643200
C	1.54581707	-4.64622942	2.85786500
H	0.77726807	-3.88541842	2.91097200
C	1.23769907	-5.98470542	2.62419900
H	0.20150207	-6.28334642	2.51218200
C	2.24496907	-6.95715742	2.51673500
H	1.96707807	-7.98585542	2.31566600
C	3.58879407	-6.62379842	2.66865900
H	4.37480707	-7.36371342	2.58243200
C	3.89332707	-5.29139842	2.92525800
C	5.16312907	-4.59616842	3.05932900
N	4.91912507	-0.47764742	3.15131500
N	4.93934307	-3.23143842	3.15247100
C	5.62591107	2.31322858	6.87331900
H	4.97333007	3.09379958	7.22902700
C	5.19749307	1.01736758	6.39649900
C	3.85509707	0.59120358	6.38644000
C	3.42297207	-0.73697242	6.21724800
C	2.04202807	-1.16625642	6.24402500
H	1.18467607	-0.51330442	6.25613300
C	2.04266807	-2.52511642	6.24431400
H	1.18593807	-3.17889742	6.25694400
C	3.42394007	-2.95296842	6.21741300
C	3.85689707	-4.28107742	6.38636000
C	5.19915607	-4.70647642	6.39641700

C	5.62836507	-6.00209542	6.87309000
H	4.97610407	-6.78333442	7.22796100
C	1.98335807	1.41555758	7.84799900
H	2.11196407	0.53687658	8.46881200
C	2.81400007	1.60092658	6.73443300
C	2.65500507	2.76621058	5.98022100
H	3.29661407	2.93753758	5.12944000
C	1.67983807	3.70454458	6.29547200
H	1.55641207	4.59548758	5.69247400
C	0.85700007	3.48461658	7.39400100
C	1.00824307	2.34795558	8.18205000
H	0.37642207	2.20053658	9.04899400
C	2.81623107	-5.29131042	6.73425100
C	2.65389007	-6.45362842	5.97619600
H	3.29203207	-6.62229742	5.12229000
C	1.67992107	-7.39293942	6.29215600
H	1.55413807	-8.28180442	5.68658500
C	0.86138507	-7.17670242	7.39465800
C	1.01533307	-6.04248442	8.18566100
H	0.38651607	-5.89764442	9.05521600
C	1.98933007	-5.10904742	7.85103100
H	2.12021607	-4.23215942	8.47393900
Cl	-0.37491993	-8.35233042	7.79804800
Cl	-0.38105993	4.65865958	7.79648800
N	6.31288607	-3.83633342	0.16701100
N	3.93114607	-4.23160242	-0.06782700
N	4.30777007	-1.85198242	0.18241900
N	3.91365907	0.52448458	-0.06851800
N	6.29834807	0.14671258	0.16677200
N	6.30548207	0.25752658	6.08453800
N	4.23878707	-1.84479142	6.11490200
N	6.30718307	-3.94573242	6.08491500

Y	6.30577007	-1.84469542	1.43916300
Y	6.30619307	-1.84424042	4.97694900
N	2.93028007	-1.86910342	3.11806000
N	6.28132107	1.52791658	3.02528500
N	6.33069607	-5.21696642	3.02610800
C	9.08101207	-0.71891842	-0.00041200
C	10.47211207	-1.12626742	-0.18618600
C	11.64648907	-0.40078442	-0.33888300
H	11.63122007	0.68213058	-0.34407100
C	12.83490907	-1.11913542	-0.47276300
H	13.77296307	-0.58686742	-0.58534900
C	12.84019307	-2.52179042	-0.47276500
H	13.78223607	-3.04697842	-0.58535000
C	11.65727107	-3.24916142	-0.33895000
H	11.65028907	-4.33215242	-0.34374600
C	10.47741007	-2.53265742	-0.18634800
C	9.08943407	-2.95047642	-0.00061800
C	7.43184607	-4.60680942	-0.04438900
C	7.02381507	-5.98576842	-0.30246200
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C	9.02309307	2.93454358	2.66585900
H	8.23705107	3.67442258	2.57957200
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H	10.64467907	4.29639858	2.31147500
C	11.37416707	2.29539758	2.62070400
H	12.41032107	2.59396858	2.50807600
C	11.06613507	0.95703558	2.85513900
H	11.83469507	0.19622158	2.90820400
C	9.72432607	0.62217458	2.99448500
C	9.04522807	-0.66002442	3.11958600
C	9.06241707	-2.98886342	3.12072300
C	9.76022707	-4.26113342	2.99815700
C	11.10735307	-4.57593042	2.86387300
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H	12.47704707	-6.19321942	2.52397500
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H	10.73743107	-7.92155342	2.32255800
C	9.09459607	-6.58356742	2.66932800
H	8.32012607	-7.33530442	2.58069700
C	8.76927907	-5.25590442	2.92521900
C	7.48932807	-4.57919842	3.05850000
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N	7.69294807	-3.21136042	3.15120000
N	9.68179407	-1.81994242	3.11706900
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C	10.57000107	-1.16323042	6.24318900
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[(Pc)Y(Pc)Y(TClPP)]-relaxation in negative potential surface

Neutral SCF Energy: -7163.49818130

Negative SCF Energy: -7163.60093179

C	0.40564373	-0.23809523	0.00000000
C	-0.98142627	-0.64546723	-0.19133500
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H	-2.14247227	1.16222677	-0.34504000
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C	-3.35087827	-2.04227923	-0.48587700
H	-4.29386627	-2.56723423	-0.59742200
C	-2.17107427	-2.76772423	-0.34859200
H	-2.16325427	-3.85101623	-0.34712300
C	-0.98724327	-2.05314123	-0.19207800
C	0.39643073	-2.47210123	-0.00123700
C	2.05388073	-4.12926923	-0.05128200
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C	1.73732273	-6.66955523	-0.54698900
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C	2.02990673	1.37663577	3.10031300
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C	0.45465473	3.39252677	2.66283400
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H	-1.16413127	4.74299877	2.26306200
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C	-0.24239727	1.08155177	3.02540200
C	0.43717473	-0.19416323	3.17434600
C	0.42857073	-2.52138723	3.17341100
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C	-1.60512727	-4.11292823	2.86141500
H	-2.36534027	-3.34346223	2.91312400
C	-1.92400027	-5.44138223	2.60004300
H	-2.96192527	-5.72580223	2.46491400
C	-0.92424227	-6.42446223	2.48786700
H	-1.20985627	-7.44600323	2.26040000
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C	-1.06415327	-0.66935823	6.44819700
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C	-1.07046027	-2.02906723	6.44762600
H	-1.92608527	-2.68083623	6.51990500
C	0.30331273	-2.46181223	6.32804300

C	0.72906573	-3.79521223	6.45059200
C	2.06270573	-4.23937623	6.41078600
C	2.48312473	-5.56393023	6.80716500
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C	-0.58172527	3.17341677	6.00269800
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C	-1.54318127	4.11216677	6.36158400
H	-1.77827827	4.93777377	5.70141400
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C	6.98841273	3.13858577	6.00048400
H	6.47263873	3.24988677	5.05922300
C	7.95973673	4.06769477	6.35778800
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C	8.62127373	3.92205677	7.57037400
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C	6.64467173	-4.83003123	6.83169900
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C	8.56909173	-6.71047723	7.57487900
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H	8.79517173	-5.56525223	9.37983000
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Cl	9.85424673	5.08963077	8.03107100
N	5.24767673	-1.37822923	6.17985000

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