Supporting Information for:

Strain-Induced Stereoselective Formation of Blue-Emitting Cyclostilbenes

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1. General Information

All reactions were performed in flame-dried round bottom flasks, unless otherwise noted. The flasks were fitted with rubber septa and reactions were conducted under a positive pressure of argon, unless otherwise noted. Anhydrous solvents were obtained from a Schlenk manifold with purification columns packed with activated alumina and supported copper catalyst (Glass Contour, Irvine, CA). Stainless steel syringes were used to transfer air- and moisture-sensitive liquids. Chromatography was performed on a Teledyne ISCO Combiflash RF using Redisep RF silica gel columns.

The following reagents were purchased from Sigma-Aldrich: dichloro(1,5-cyclooctadiene)platinum(II), *n*-butyllithium (1.6 M in hexanes), trimethyltin chloride solution (1.0 M in THF), triphenylphosphine. *trans*-4,4'-dibromostilbene was purchased from TCI America. All chemicals purchased from commercial sources were used without further purification unless otherwise specified.

Proton nuclear magnetic resonance (^{1}H NMR) spectra, carbon nuclear magnetic resonance (^{13}C NMR) spectra, tin nuclear magnetic resonance (^{119}Sn NMR) were recorded on a Bruker DRX300 (300 MHz) and Bruker DRX500 (500 MHz) spectrometer. Chemical shifts for protons are reported in parts per million downfield from tetramethylsilane and are referenced to NMR solvent ($CDCl_3$: δ 7.26; CD_2Cl_2: δ 5.32). Chemical shifts for carbon are reported in parts per million downfield from tetramethylsilane and referenced to the carbon resonances of the solvent ($CDCl_3$: δ 77.2; CD_2Cl_2: δ 53.8). Spectra were analyzed with MestraNova software (Version 7.1). Data are represented as follows: chemical shift, multiplicity (s = singlet, d = doublet, t = triplet, m = multiplet), coupling constants in Hertz (Hz), and integration. High-resolution mass spectrometry (HRMS) was performed on a Waters XEVO G2XS instrument equipped with a UPC2 SFC inlet, electrospray ionization, and a QToF mass spectrometer. Absorption spectra were obtained on a Shimadzu UV 1800 UV-Vis spectrophotometer and emission spectra were recorded on a Fluorolog-3 spectrophotometer.

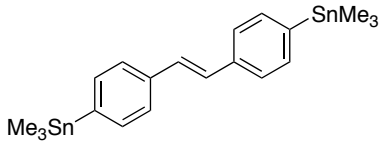
In the transient absorption measurement, the pump laser light (~100 fs pulse width)

comes from an optical parametric amplifier (TOPAS) pumped by a Ti:sapphire femtosecond regenerative amplifier (800 nm, 1 kHz rep-rate). The probe light is a white-light supercontinuum (450-850 nm and 900-1600 nm wavelength range, ~100 fs pulse width). The pump and probe beams overlapped under a small angle in a cuvette of 2 mm path length. The detection consists of a pair of high-resolution multichannel detector arrays coupled to a high-speed data acquisition system (Ultrafast Systems). The pump intensity was 2.5 $\mu J/cm^2$.

Time resolved photoluminescence (PL) decay kinetics were measured using a home-built epifluorescence microscope setup (Olympus, IX73 inverted microscope). The 402 nm excitation light was generated from doubling the fundamental output (805 nm, 100 fs, 250 kHz) from a regenerative amplifier (Coherent RegA amplifier seeded by Coherent Mira oscillator). The light was focused into diluted sample solution in 1cm cuvette by a 50X, NA=0.5 objective (Olympus LMPLFLN50X) and time resolved photoluminescence (TRPL) decay kinetics with emission wavelength between 450 nm and 550 nm were collected using a TCSPC module (B&H, SPC130) and a SPAD detector (IDQ, id100-50) with an instrument response function of ~ 100 ps (FWHM).

2. Synthetic Procedures

Synthesis of *trans*-1,2-bis(4-(trimethylstannyl)phenyl)ethane (4b)



A 250 mL round bottom flask was charged with *trans*-4,4'-dibromostilbene (2.76 g, 8.2 mmol) and 100 mL anhydrous THF. The solution was cooled down to -78 °C and *n*-BuLi (1.6 M, 12.3 mL, 19.6 mmol) was added dropwise, during which a light yellow suspension formed. After stirring for 3 h, trimethyltin chloride solution in THF (1.0 M, 19.6 mL, 19.6 mmol) was slowly added, and the reaction was warmed to room temperature overnight. The light yellow reaction mixture was quenched with water and extracted with DCM three times, dried over $MgSO_4$, then concentrated under reduced pressure. The residue was recrystallized from hot hexanes to yield **4b** as white solid (3.24 g, 78%).

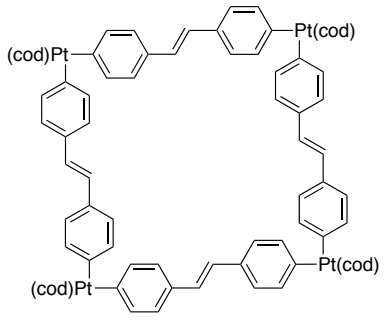
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.44-7.57 (m, 8H), 7.12 (s, 2H), 0.31 (s, 9H).

^{13}C NMR (100 MHz, CDCl3): δ 142.2, 137.4, 136.3, 128.9, 126.2, -9.4.

^{119}Sn NMR (112 MHz, $CDCl_3$): δ 27.5.

HRMS (ASAP+): calculated m/z for $[C_{20}H_{28}Sn_2]^+$ is 508.0235, found 508.0235.

Synthesis of platinum macrocycle 5



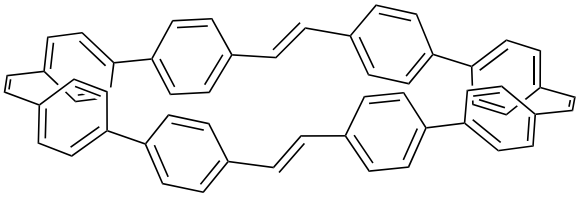
A solution of **4b** (1.01 g, 2.0 mmol) and Pt(cod)Cl_2 (0.75 g, 2.0 mmol) in 1,2-dichloroethane (200 mL) was degassed under N_2 for 30 minutes. The mixture was heated to 75 °C for 20 hours, during which a precipitate formed and was collected by filtration.

The precipitate was thoroughly washed by hexanes and dried to give **5** (0.81 g, 84%) as an off-white solid.

^{1}H NMR (400 MHz, $C_2D_2Cl_4$): δ 7.24 (d, J = 8.4 Hz, 16H), 7.12 (d, J = 8.4 Hz, 16H), 6.84 (s, 8H), 5.13 (s, 16H), 2.55 (s, 32H).

^{13}C NMR could not be obtained due to poor solubility.

Synthesis of cyclostilbene 1-CTCT



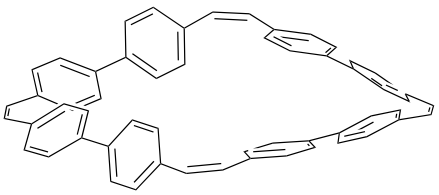
A suspension of **5** (0.48 g, 0.25 mmol) and PPh_3 (2.62 g, 10 mmol) in toluene (100 mL) was degassed under N_2 for 30 minutes. The mixture was stirred at room temperature for 30 minutes, and then heated to 100 °C for 24 hours. The reaction was filtered to collect a yellow precipitate, which was extracted with DCM (3 × 50 mL) and concentrated under reduced pressure. The residue was recrystallized from DCM/MeOH to yield **1** (49 mg, 28%) as a light yellow solid.

^{1}H NMR (500 MHz, CD_2Cl_2): δ 7.44 (d, J = 8.5 Hz, 8H), 7.42 (d, J = 8.5 Hz, 8H), 7.23 (d, J = 8.5 Hz, 8H), 6.94-6.96 (m, 16H).

^{13}C NMR (125 MHz, CD_2Cl_2): δ 140.6, 139.4, 137.7, 136.8, 133.0, 130.2, 128.6, 127.7, 127.1, 126.7.

HRMS (ASAP+): calculated m/z for $[C_{56}H_{40}]^+$ is 712.3130, found 713.3124.

Synthesis of cyclostilbene 2-CCCC



In a 100 mL round bottom flask, all-*trans* cyclostilbene **1** (25 mg, 0.035 mmol) was dissolved in anhydrous THF (35 mL) and degassed under N_2 for 20 minutes. The solution was irradiated using a 450 W mercury lamp for 1 hour, then concentrated under reduced

pressure. The resultant solid was recrystallized from DCM/hexanes to give **2** (19 mg, 79%) as a light yellow solid. This compound is known and agrees with spectroscopic data in literature.[1]

^{1}H NMR (500 MHz, CD_2Cl_2): δ 7.48 (d, J = 8.0 Hz, 16H), 7.36 (d, J = 8.0 Hz, 16H), 6.66 (s, 8H).

^{13}C NMR (125 MHz, CDCl3): δ 139.7, 136.8, 130.3, 129.8, 127.0.

HRMS (ASAP+): calculated m/z for $[C_{56}H_{40}]^{+}$ is 712.3130, found 713.3132.

3. ^{1}H and ^{13}C NMR Spectra

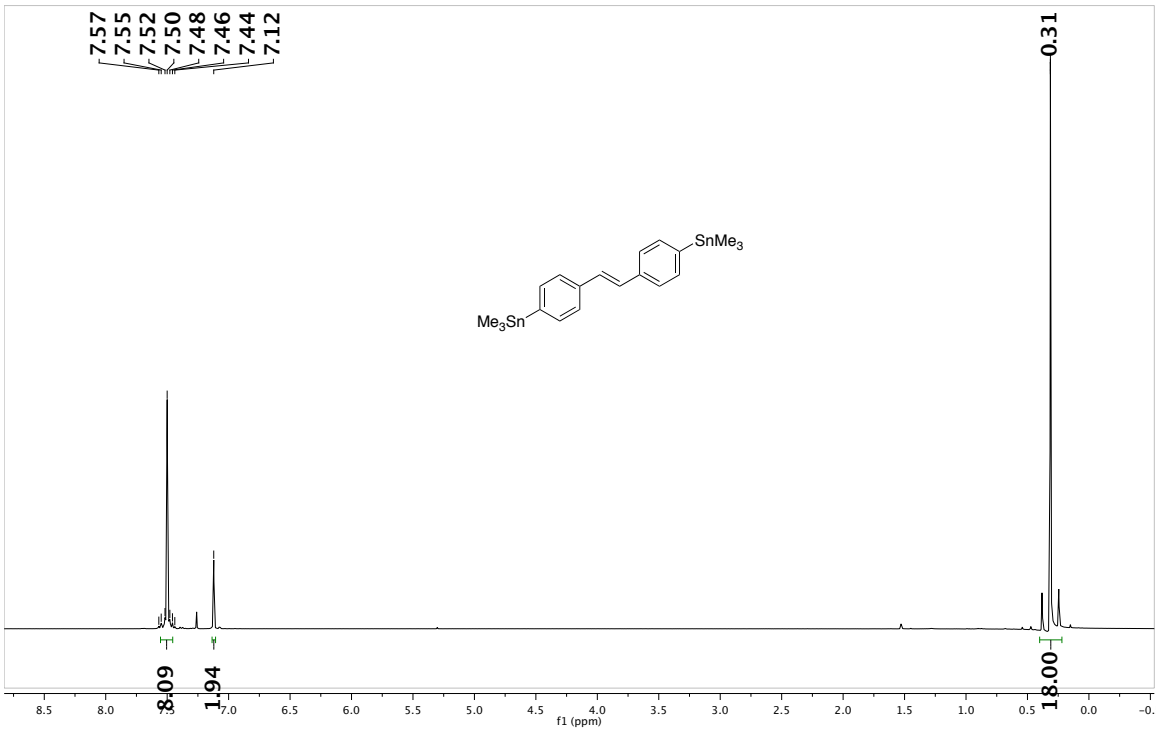


Figure S1. ^{1}H NMR spectrum (400 MHz) of **4b** in $CDCl_3$.

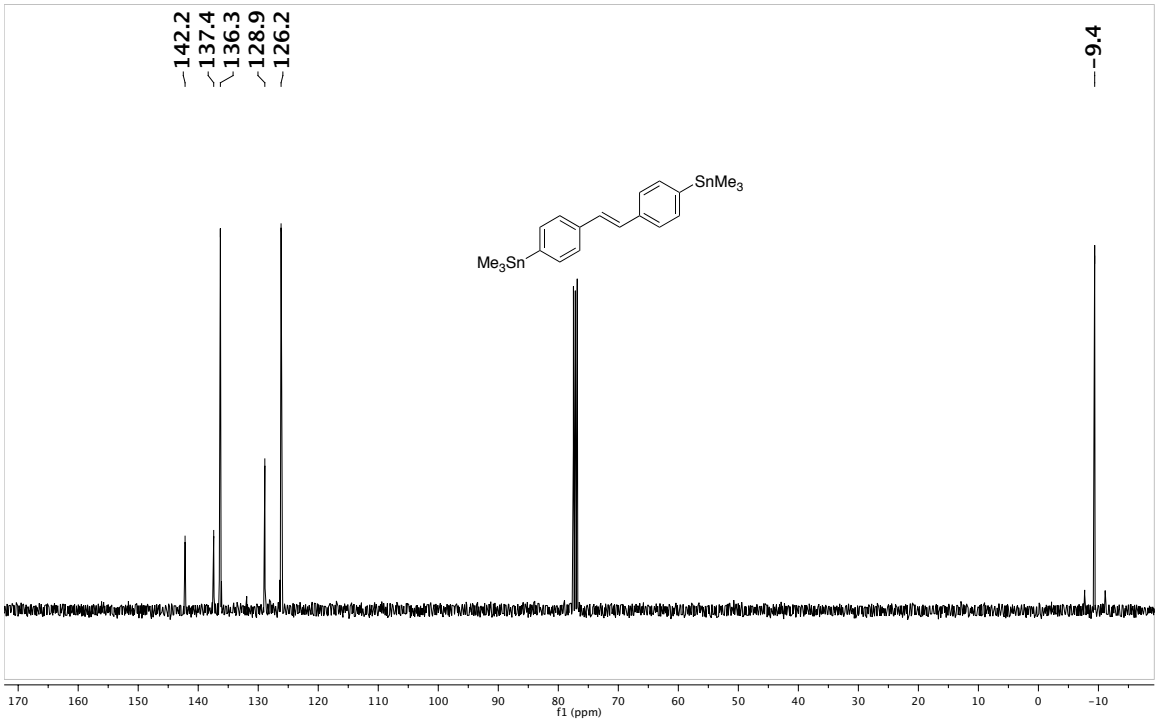


Figure S2. ^{13}C NMR spectrum (100 MHz) of **4b** in $CDCl_3$.

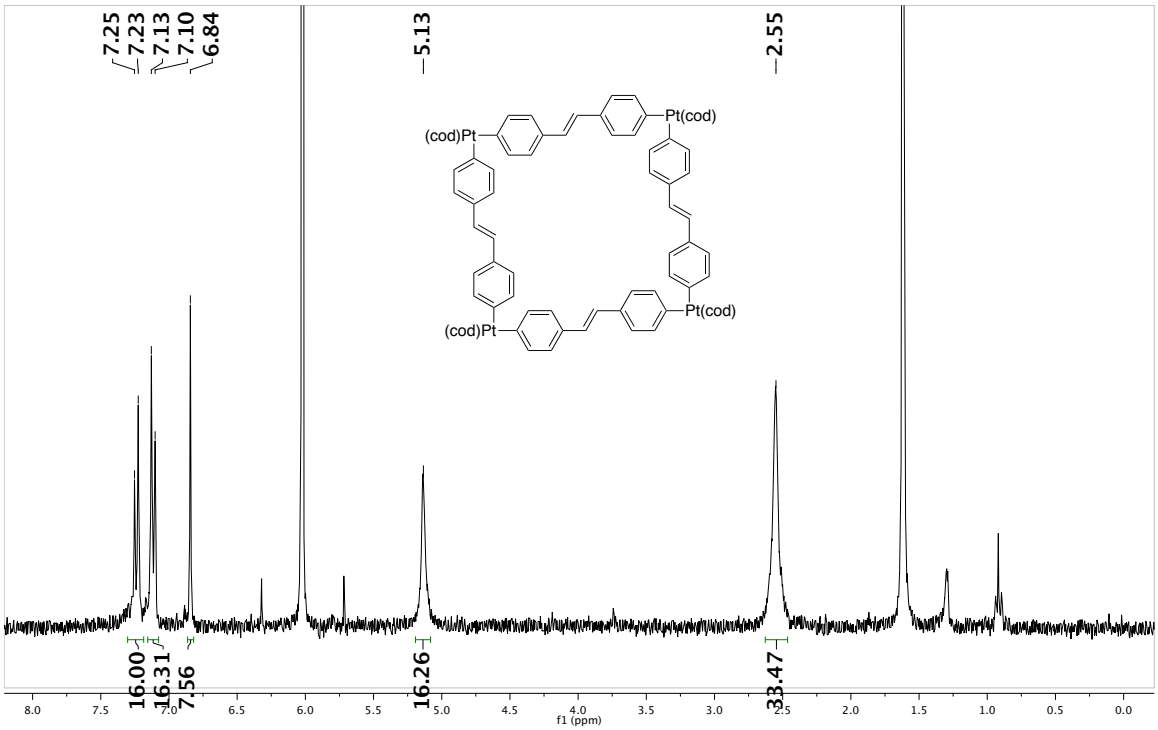


Figure S3. ^{1}H NMR spectrum (400 MHz) of **5** in $C_2D_2Cl_4$.

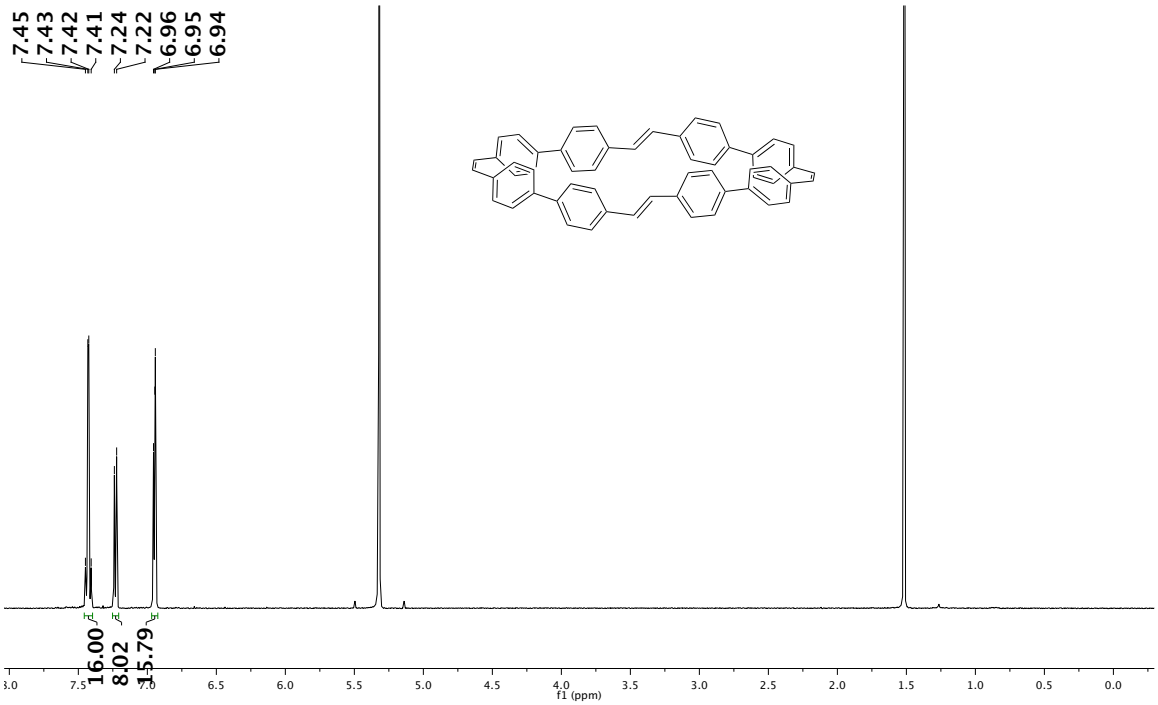


Figure S4. ^{1}H NMR spectrum (500 MHz) of **1-CTCT** in CD_2Cl_2.

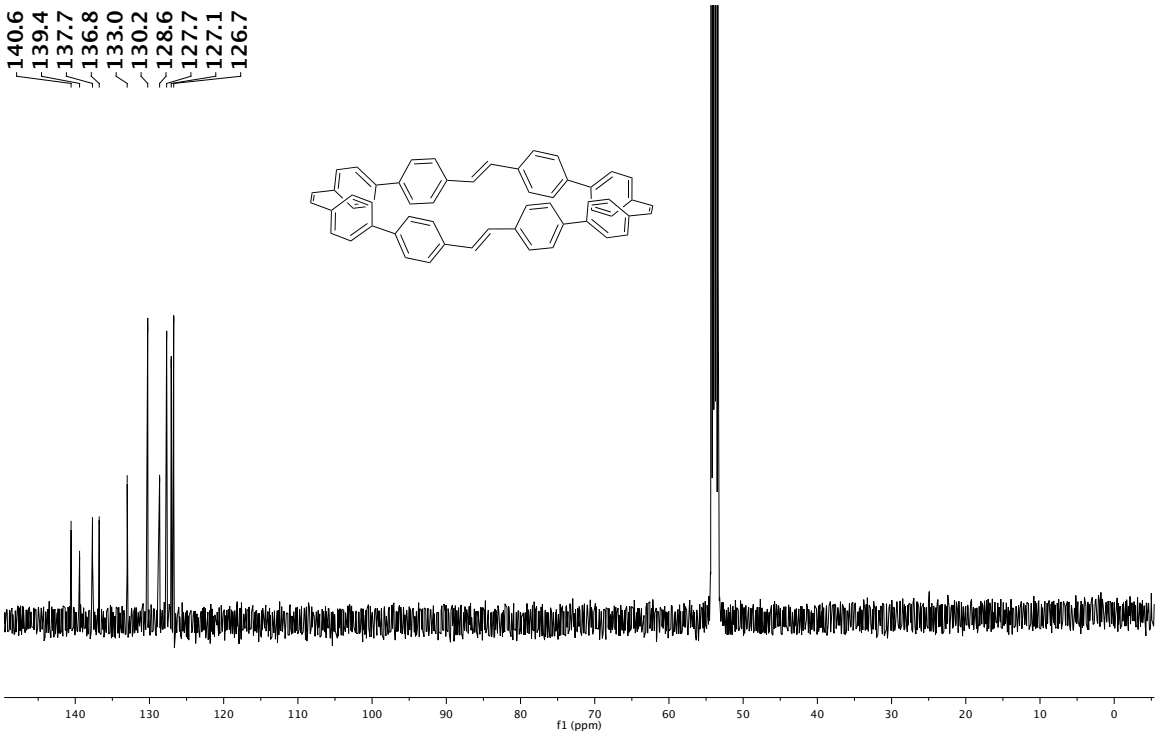


Figure S5. ^{13}C NMR spectrum (125 MHz) of **1-CTCT** in CD_2Cl_2.

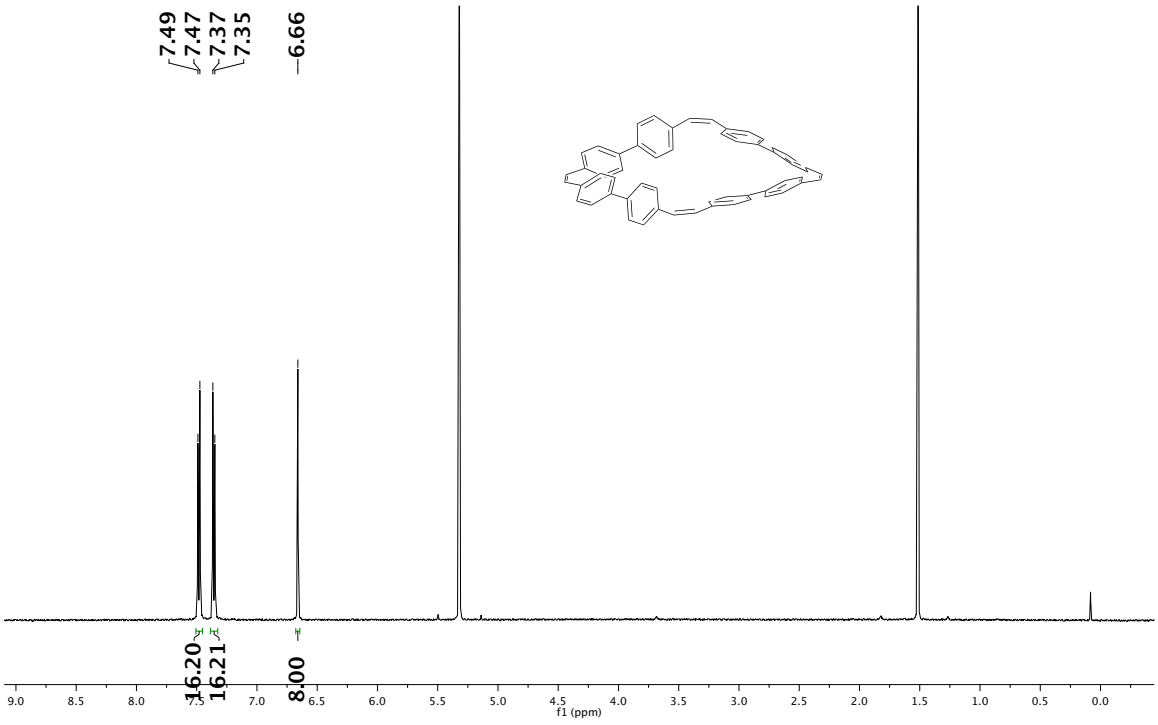


Figure S6. ^{1}H NMR spectrum (500 MHz) of **2-CCCC** in CD_2Cl_2.

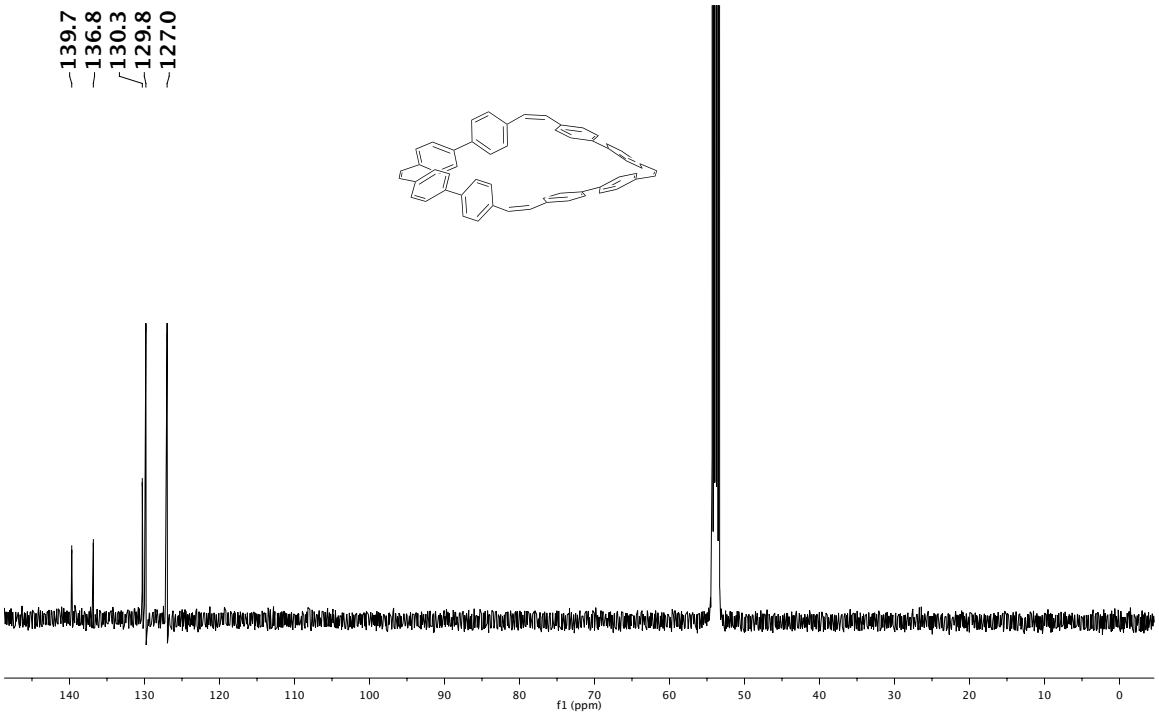


Figure S7. ^{13}C NMR spectrum (125 MHz) of **2-CCCC** in CD_2Cl_2.

4. Thermal Gravimetric Analysis

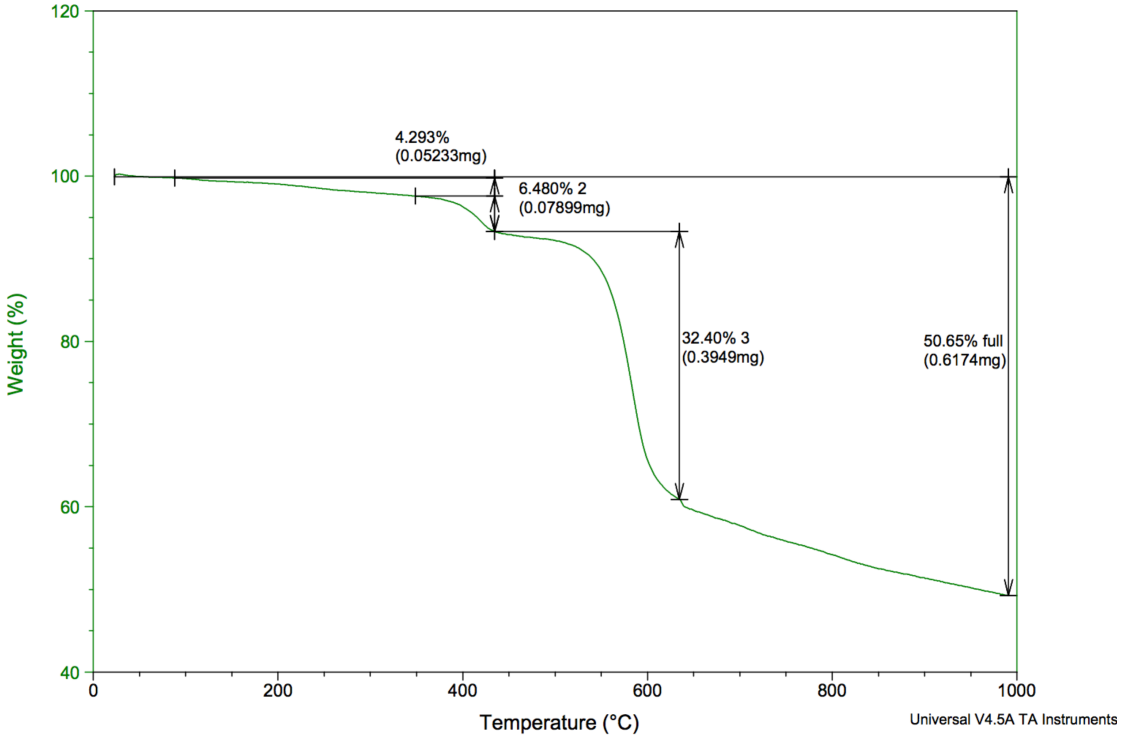


Figure S8. TGA analysis of **1-CTCT**.

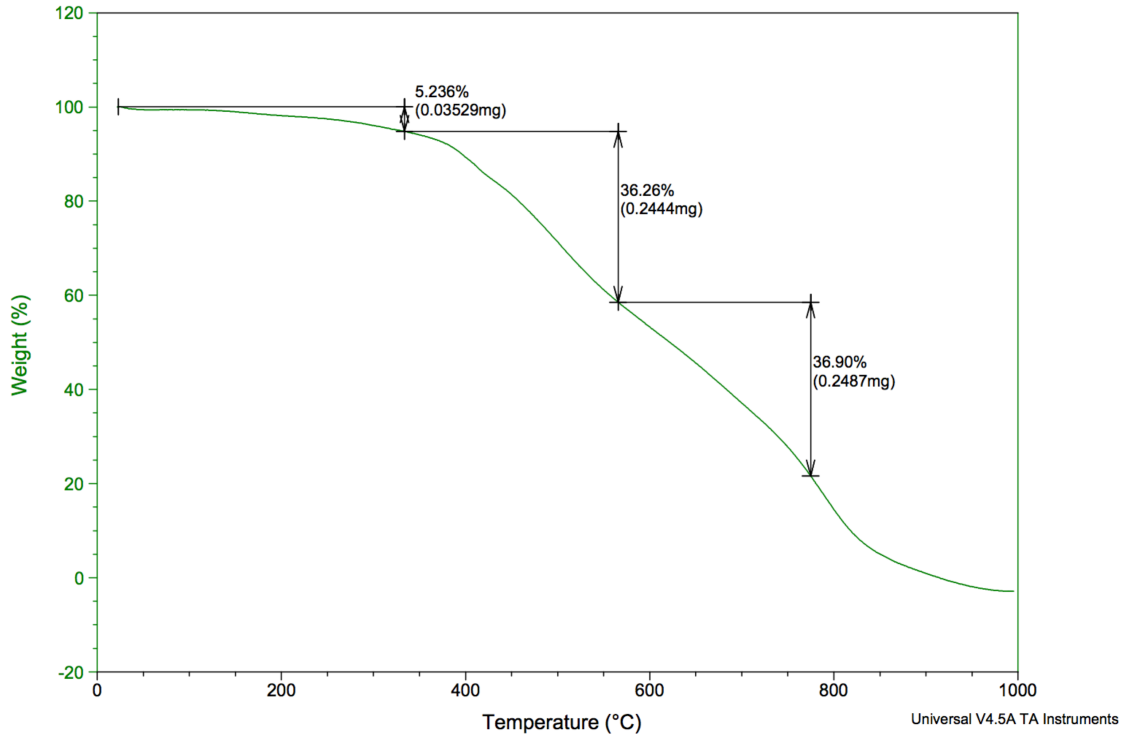


Figure S9. TGA analysis of **2-CCCC**.

5. Crystallographic Characterization

Data for all compounds was collected on an Agilent SuperNova diffractometer using mirror-monochromated Cu Kα or Mo Kα radiation. Data collection, integration, scaling (ABSPACK) and absorption correction (face-indexed Gaussian integration[2] or numeric analytical methods[3]) were performed in CrysAlisPro.[4] Structure solution was performed using ShelXS,[5] ShelXT,[6] or SuperFlip.[7] Subsequent refinement was performed by full-matrix least-squares on F^2 in ShelXL.[5] Olex2[8] was used for viewing and to prepare CIF files. PLATON[9] was used extensively for SQUEEZE,[10] ADDSYM[11] and TwinRotMat. Many disordered solvent molecules were modeled as rigid fragments from the Idealized Molecular Geometry Library.[12] ORTEP graphics were prepared in CrystalMaker.[13] Thermal ellipsoids are rendered at the 50% probability level.

A THF solution of **1-CTCT** was layered with toluene. Part of a crystal (.17 x .06 x .02 mm) was separated carefully, mounted with STP oil treatment, and cooled to 100 K on the diffractometer. Complete data (99.9%) were collected to 0.833 Å. 32409 reflections were collected.

The lattice was very nearly orthorhombic, with β approximately 90.6° and clear signs of twinning by rotation around [100]. There were absences for 2_1 axes in all three directions, indicating a twin in $P2_1$ that very closely approximated $P2_12_12_1$. Twin decomposition in CrysAlisPro and solution in $P2_1$ resulted in poor refinements with numerous NPD atoms. When the data were processed assuming an orthorhombic lattice, the structure solved easily in $P2_12_12_1$.

For the orthorhombic data set, there were 8679 unique data (6394 observed) with R(int) 12.7% and R(sigma) 11.5% after multiscan absorption correction.

For the solution in $P2_12_12_1$, all non-solvent C atoms were located readily in Fourier maps and refined anisotropically with a rigid-bond restraint on all anisotropic ADPs. A toluene molecule in the cavity of the macrocycle was disordered over two positions in a 70:30

ratio; these were refined with SAME and FLAT restraints on their geometry and with anisotropic ADPs for only the major component of the disorder. All hydrogen atoms were placed in calculated positions and refined with riding coordinates and ADPs.

The final refinement (8679 data, 597 restraints, 599 parameters) converged with R_1 ($F_o > 4\sigma(F_o)$) = 12.6%, wR_2 = 28.5%, S = 1.04. The largest Fourier features were 0.51 and -0.41 $e^- A^{-3}$ and are explained by deviation from strict orthorhombic symmetry. The absolute structure was undetermined; the Flack parameter for the final refinement was -1.8(10).

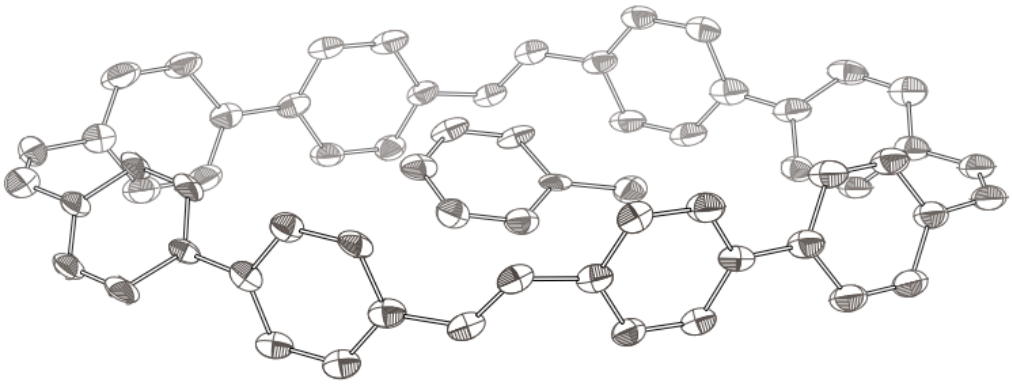


Figure S10. Molecular structure of **1-CTCT•**toluene. Hydrogen atoms and the minor position of the disordered toluene molecule are omitted for clarity.

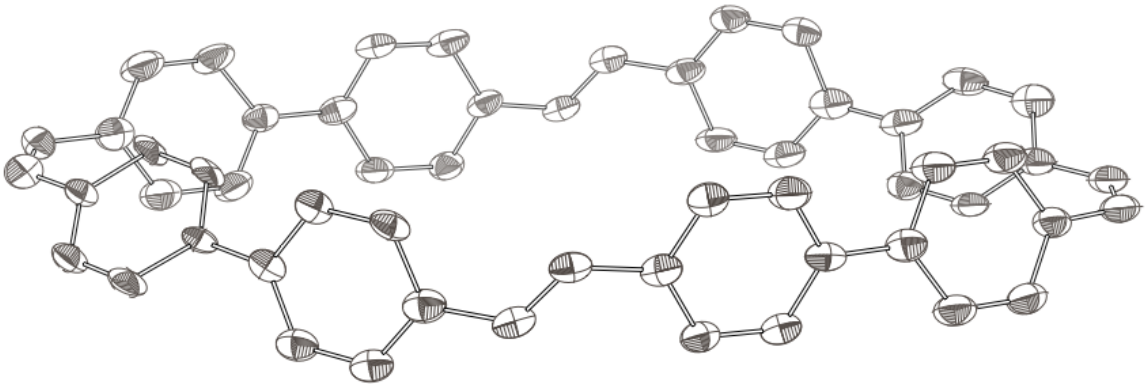


Figure S11. Molecular structure of **1-CTCT**. Hydrogen atoms and a disordered toluene molecule are omitted for clarity.

Table S1. Crystal data for compound **1-CTCT**.

Compound	CTCT . PhMe
Formula	$C_{63}H_{48}$
MW	805.01
Space group	$P2_12_12_1$
a (Å)	8.9270(14)
b (Å)	17.389(2)
c (Å)	28.757(4)
α (°)	90
β (°)	90
γ (°)	90
V (Å^3)	4464.1(11)
Z	4
ρ_{calc} (g cm^{-3})	1.198
T (K)	100
λ (Å)	1.54184
$2\theta_{min}$, $2\theta_{max}$	10.174, 147.6
Nref	32409
R(int), R(σ)	.1269, .1147
μ(mm^{-1})	0.510
Size (mm)	.17 x .06 x .02
T_{max}, T_{min}	.964, .992 (calc.)
Data	8679
Restraints	597
Parameters	599
R_1(obs)	0.1265
wR_2(all)	0.2849
S	1.040
Peak, hole (e$^-$ Å^{-3})	0.51, -0.41
Flack	-1.8(10)

A DCM solution of **2-CCCC** was layered with MeOH. The crystals disintegrated rapidly in contact with the mounting oil. A crystal was mounted successfully by cooling the microscope slide with dry ice and cooling the mounted crystal continuously with cold N_2

gas. Part of a crystal (.12 x .07 x .04 mm) was separated carefully, mounted with STP oil treatment, and cooled to 100 K on the diffractometer. Complete data (99.7%) were collected to 0.815 Å. 73051 reflections were collected (8941 unique, 8090 observed) with R(int) 4.6% and R(sigma) 2.2% after analytical absorption correction (Tmax .908, Tmin .773).

The space group assignment was not completely obvious. There were clean absences for a 2_1 axis and weakly violated absences for a *c* glide (<I> 1.4 vs. 27.3 for the full data set). ShelXT and Superflip gave good solutions in $P2_1/c$. A refinement in $P2_1$ was difficult and unstable, as expected for a (pseudo-)centrosymmetric structure, and this possibility was not explored further.

The macrocycle was located readily in the initial solution and refined with no restraints. A molecule of dichloromethane outside the macrocycle was disordered over two independent positions that were introduced as rigid fragments from the IMGL and subsequently refined with SAME and RIGU restraints.

The macrocycle crystallizes in columns aligned along the *c* axis, forming a continuous channel that is filled with disordered dichloromethane. The disorder is extensive and no satisfactory discrete model could be constructed. Therefore the solvent-filled channel was treated with Platon Squeeze, which recovered 215 electrons per unit cell (corresponding to approximately 1.25 DCM molecules per formula unit).

Hydrogen atoms were placed in calculated positions and refined with riding coordinates and ADPs. The final refinement (8941 data, 37 restraints, 560 parameters) converged with R_1 ($F_o > 4\sigma(F_o)$) = 6.3%, wR_2 = 16.1%, S = 1.13. The final R indices are slightly high compared to R(int) and R(sigma), which may indicate a slight deviation from strict centrosymmetry.
The largest Fourier features were 0.40 and -0.46 $e^- A^{-3}$.

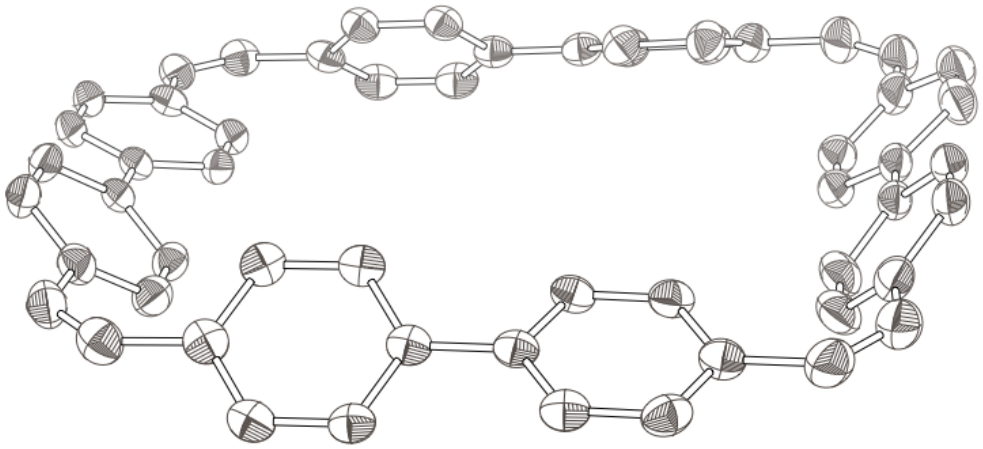


Figure S12. Molecular structure of **2-CCCC**. Hydrogen atoms are omitted for clarity.

Table S2. Crystal data for compound **2-CCCC**.

Compound	**cccc * CH_2Cl_2**
Formula	$C_{57}H_{42}Cl_2$
MW	797.8
Space group	$P2_1/c$
***a* (Å)**	14.73721(18)
***b* (Å)**	33.7850(3)
***c* (Å)**	9.62683(10)
***α* (°)**	90
***β* (°)**	106.5877(12)
***γ* (°)**	90
V (Å^3)	4593.69(9)
Z	4
ρ_{calc} (g cm^{-3})	1.154
T (K)	100
λ (Å)	1.54184
$2\theta_{min}$, $2\theta_{max}$	9.938, 143.2
Nref	73051
R(int), R(σ)	.0460, .0223
μ(mm^{-1})	1.535
Size (mm)	.12 x .07 x .04
T_{max}, T_{min}	.908, .773

Data	8941
Restraints	37
Parameters	560
R_1(obs)	0.0627
wR_2(all)	0.1606
S	1.137
Peak, hole (e^- $Å^{-3}$)	0.40, -0.46
Flack	

Single crystals of the platinum macrocycle **5** were grown by vapor diffusion of methanol into tetrachloroethane solution to afford small, colorless blocks. A small single crystal (.11 x .06 x .04 mm) was separated carefully, mounted with STP oil treatment, and cooled to 100 K on the diffractometer. Complete data (99.8%) were collected to 0.800 Å. 110111 reflections were collected (11973 unique, 10859 observed) out to 0.72 Å resolution but the data set was ultimately truncated to 0.800 Å resolution, with 6661 unique data within this limit. R(int) was 5.8% and R(sigma) 3.0% after analytical absorption correction (Tmax .853, Tmin .674).

The space group was assigned as $P2_1/c$ based on the systematic absences. The structure solved readily in ShelXT with ½ macrocycle in the asymmetric unit. All non-H, non-solvent atoms were located rapidly in Fourier maps. The saturated C_2H_4 bridges of the two independent cyclooctadiene ligands were each disordered over two positions, which were located in difference maps and refined using SAME and RIGU restraints.

The asymmetric unit contains four tetrachloroethane molecules. Two were fully ordered, one was disordered over two positions and refined with similarity restraints for geometry and ADPs, and one was extensively disordered over multiple positions. This molecule was ultimately modeled as a diffuse contribution to the overall scattering using Platon Squeeze. The unaccounted electron density was estimated as 379 e^- per unit cell (4 $C_2H_2Cl_4$ = 328 e^-).

All hydrogen atoms were placed in calculated positions and refined with riding coordinates and ADPs. The final refinement (6661 data, 574 restraints, 706 parameters)

converged with R_1 ($F_o > 4\sigma(F_o)$) = 3.7%, wR_2 = 8.5%, S = 1.09. The largest Fourier features were 2.50 and -0.80 $e^- A^{-3}$; the large positive feature occurred near a Pt atom.

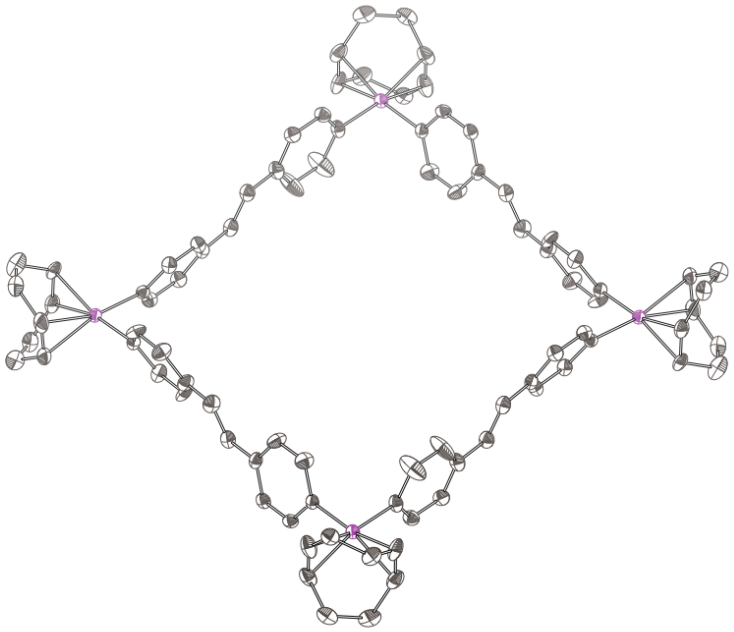


Figure S13. Molecular structure of **5**. Black, carbon; purple, platinum. Solvent molecules, hydrogen atoms and the minor positions of the disordered cod ligands are omitted for clarity.

Table S3. Crystal data for compound **5**.

Compound	**Pt-cycle-3(TCE)**
Formula	$C_{100}H_{100}Cl_{24}Pt_4$
MW	2392.95
Space group	$P2_1/c$
***a* (Å)**	18.3098(3)
***b* (Å)**	26.5227(4)
***c* (Å)**	12.8182(2)
***α* (°)**	90
***β* (°)**	109.301(2)
***γ* (°)**	90
V (Å^3)	5874.99(19)
Z	2
ρ_{calc} (g cm^{-3})	1.658

T (K)	100
λ (Å)	0.71073
$2\theta_{min}$, $2\theta_{max}$	6.582, 52.74
Nref	110111
R(int), R(σ)	.0580, .0296
$\mu(mm^{-1})$	5.334
Size (mm)	.11 x .06 x .04
T_{max}, T_{min}	.853, .674
Data	6661
Restraints	574
Parameters	706
R_1(obs)	0.0367
wR_2(all)	0.0846
S	1.089
Peak, hole (e^- $Å^{-3}$)	2.50, -0.80
Flack	

6. 2D-NMR analysis of intermediate 6-Pt_2

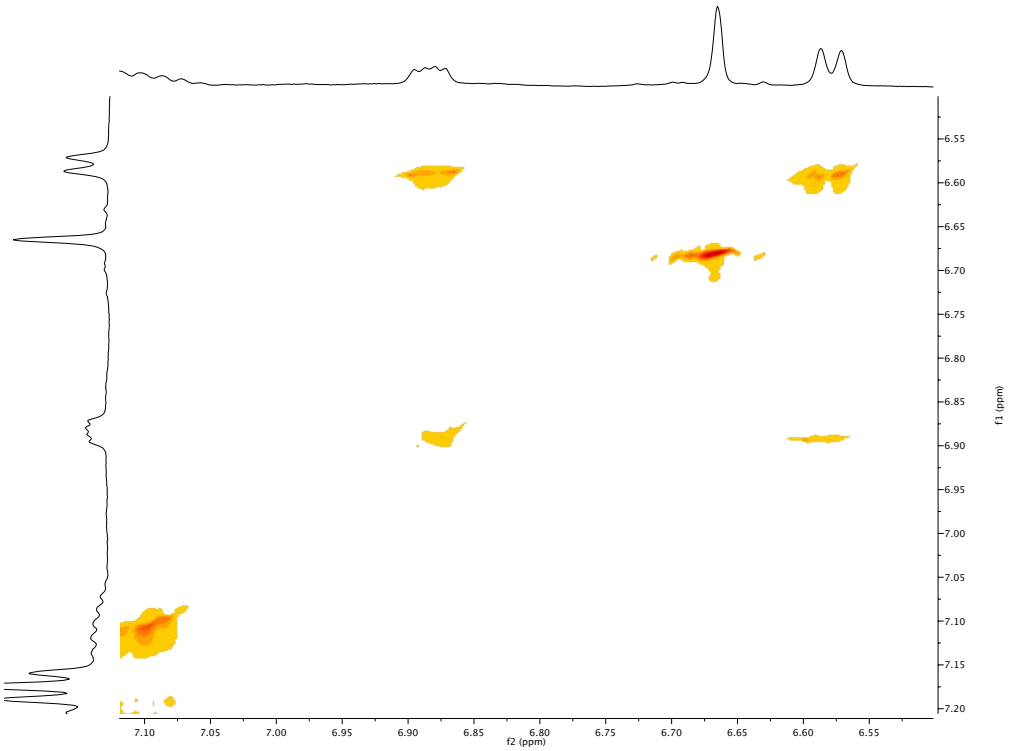


Figure S14. COSY spectrum of intermediate **6-Pt_3**.

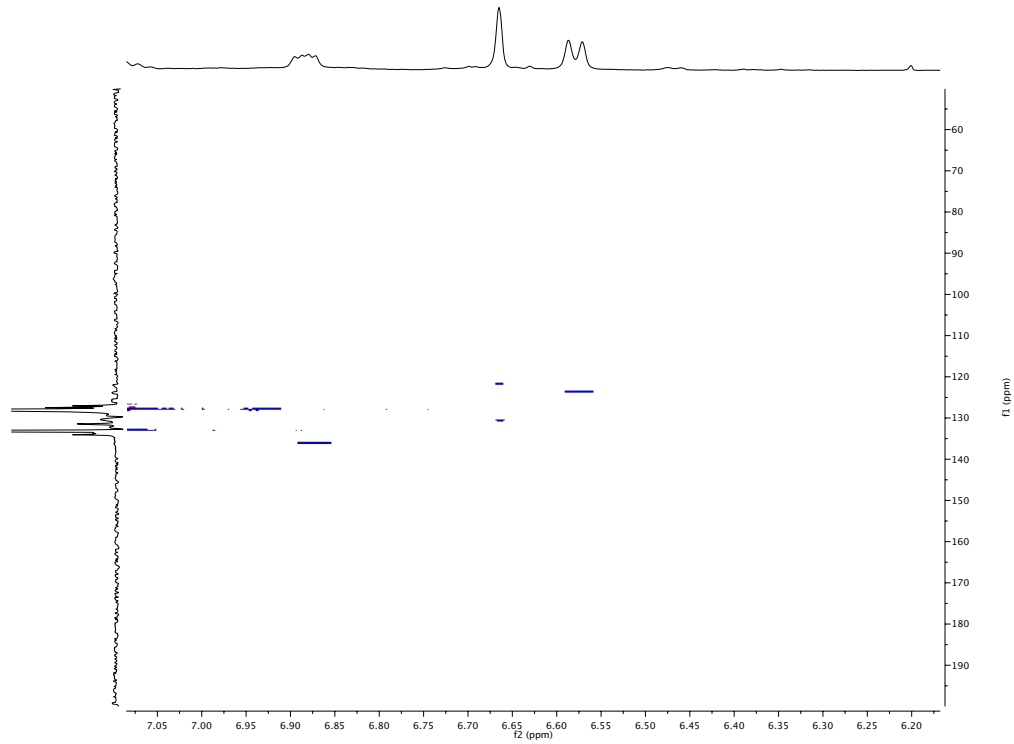


Figure S15. HSQC spectrum of intermediate **6-Pt_3**.

7. NMR kinetic experiments

Platinum complex **5** (7.20×10^{-7} mol), PPh_3 (2.88×10^{-6} mol), and 1,3,5-trimethoxybenzene (1.08×10^{-6} mol, internal standard) were dissolved in $C_2D_2Cl_4$ (0.6 mL) in a screw-capped NMR tube. The tube was heated to 90°C in the NMR probe, and the decay of **6-Pt$_3$** (Figure S12) and formation of product **1-CTCT** (Figure S13) over time were monitored by ^{1}H NMR spectroscopy.

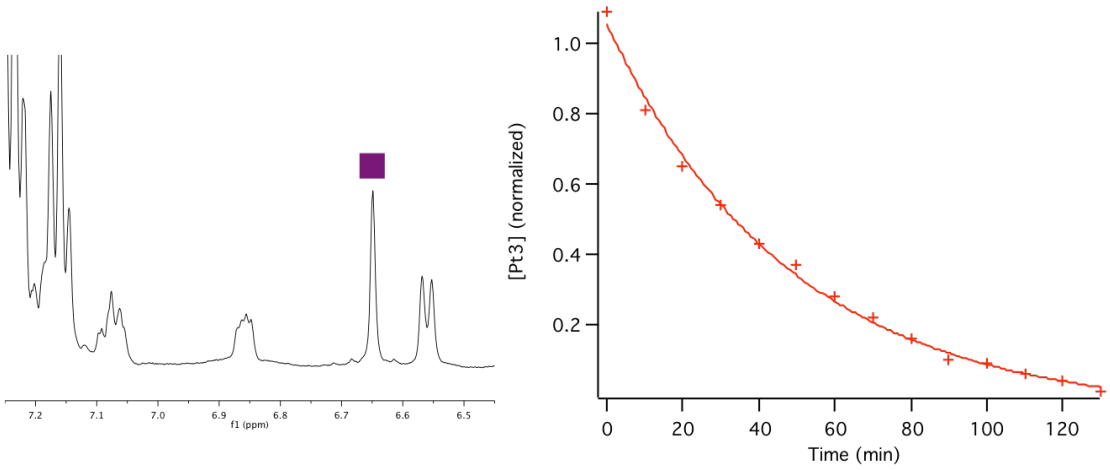


Figure S16. Decay of **6-Pt$_3$** over time monitored by ^{1}H NMR spectroscopy.

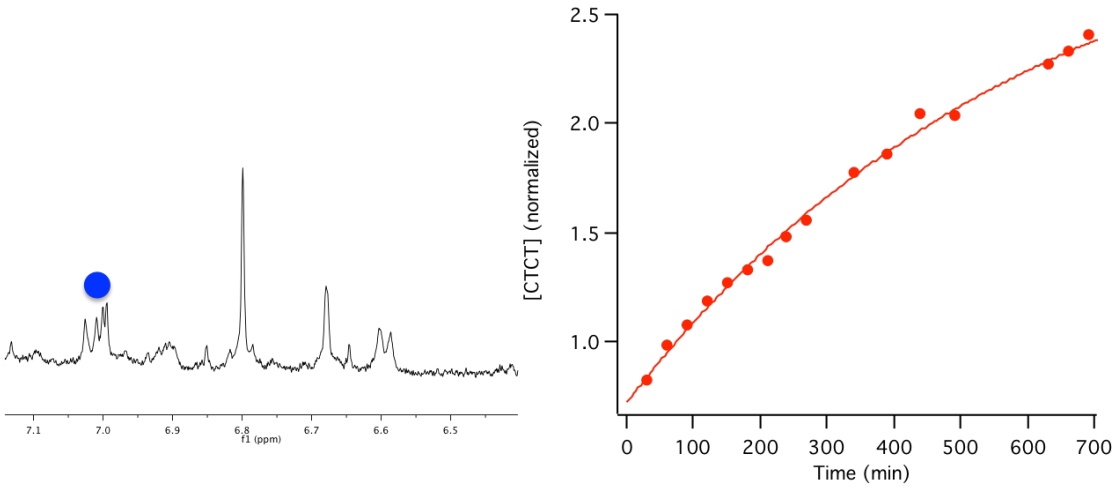


Figure S17. Formation of **1-CTCT** over time monitored by ^{1}H NMR spectroscopy.

8. Cyclic Voltammetry

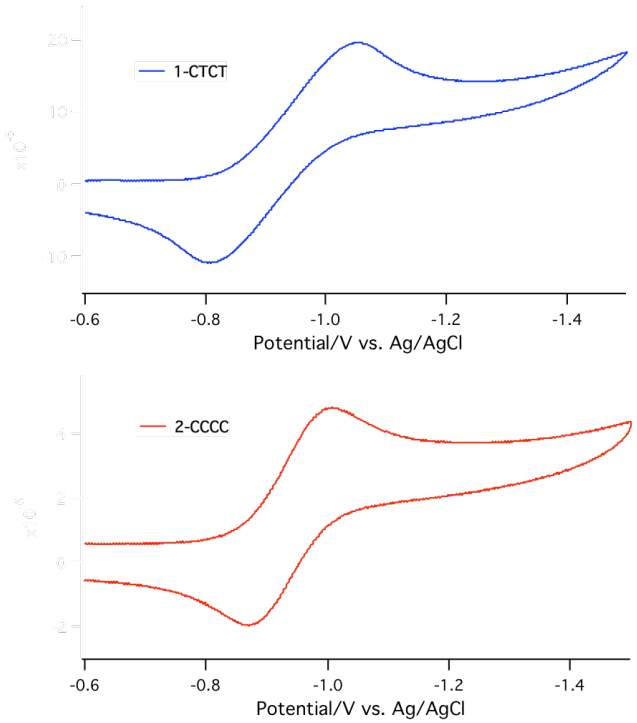


Figure S18. Cyclic voltammograms for **1-CTCT** (blue) and **2-CCCC** (red).

Reduction potentials were estimated from peak onset values. Ferrocene/ferrocenium (Fc/Fc+) was used for calibration. The redox potential of Fc/Fc+ was located at 0.42V to Ag/AgCl reference electrode under the same condition. Therefore, reduction onset potentials (E_{red}) were estimated to be –1.26 V for **1-CTCT** and -1.28 V for **2-CCCC**. The absolute energy level for Fc/Fc+ redox potential is -4.80eV to vacuum level. The energy levels of the lowest unoccupied molecular orbitals (LUMO) can be calculated according to the following equation: $E_{LUMO}=-(E_{red}+4.80)$ (eV). The LUMO energies from DFT calculations (Figure S23) are nearly identical for the two isomers, as are the values determined by cyclic voltammetry.

9. PLQY measurements.

We performed photoluminescence quantum yield (PLQY) measurements using absolute and relative methods. In the relative method, we used coumarin 1 as a reference. The advantages of the coumarin 1 are high QY and the good overlapping of the absorption and emission spectra to that of **1-CTCT** and **2-CCCC**. Coumarin 1 was dissolved in EtOH in air with the known QY of 79%.[14] **1** and **2** were dissolved in chloroform inside a nitrogen-filled glovebox. To avoid re-absorption we chose an optical density in the range of 0.1 to 0.2 for all solutions. The relative emission QY was calculated using equation[15]:

$$\Phi_S = \Phi_R \frac{I_S}{I_R} \frac{1-10^{A_R}}{1-10^{A_S}} \frac{n_S}{n_R}$$

where Φ, *I, A,* and *n* denotes the quantum yield, integrated PL intensity, optical density at the excitation wavelength, and reflective index, respectively. The abbreviations S and R refer to sample and reference, respectively. Using the above method we obtained relative QYs of 56 ± 6 and 55 ± 2 % for **1** and **2**, respectively. The results were averaged from three different measurements with the excitation wavelengths of 340, 350 and 360 nm. The errors are the standard deviation obtained from these measurements. We also performed the absolute PLQY measurements. At the excitation of 350 nm, the QY are 63 ± 5 and 60 ± 5 % for **1** and **2**, respectively. The QY results obtained from two methods are quantitatively in agreement.

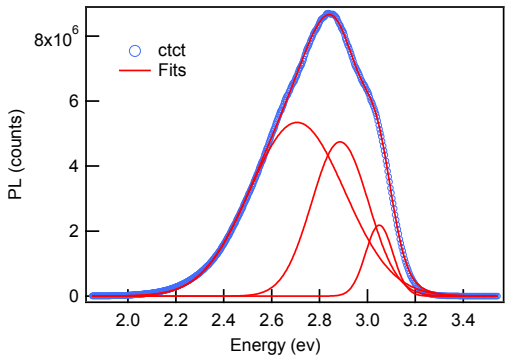


Figure S19. Emission spectrum (blue) of **1-CTCT** decomposed into three different Gaussian peaks (red).

10. Time resolved photoluminescence (PL) decay kinetics

The PL decay kinetics for 1-CTCT and 2-CCCC molecules in DCM solutions (see Fig. 5b, main text) were fitted by a stretched exponential function $I(t) = A\exp[-(t/\tau)^{\alpha}]$, which yields τ of 1.26 ns and 0.78 ns, α of 0.92 and 0.86 for **1-CTCT** and **2-CCCC**, respectively.

To test the possible isomerization process of as synthesized molecules, **1-CTCT** and **2-CCCC** are also prepared in polystyrene film and time resolved PL of them were measured as a function of temperature (88K~ 293K). No significant difference of PL emission spectra between molecules in DCM and in polymer matrix were observed (Fig. S20) and more importantly, the PL lifetime of both **1-CTCT** (Fig. S21a) and **2-CCCC** (Fig. S21a) depends very weekly on the temperature, indicating the absence of isomerization of **1-CTCT** and **2-CCCC**.

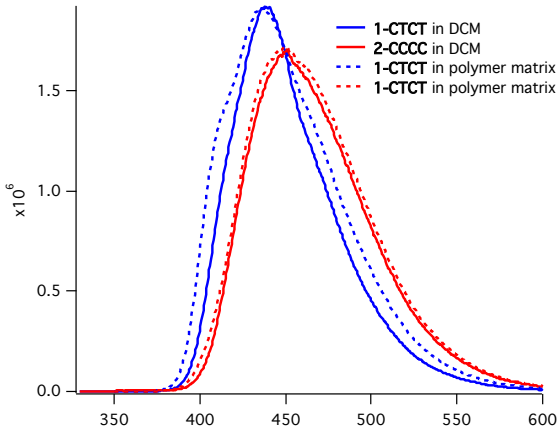


Figure S20. Fluorescence spectra of **1-CTCT**, 1×10^{-6} M in DCM (blue) and in a polystyrene film (blue, dashed line); **2-CCCC**, 1×10^{-6} M in DCM (red) and in a polystyrene film (red, dashed line). All samples were excited at 320 nm.

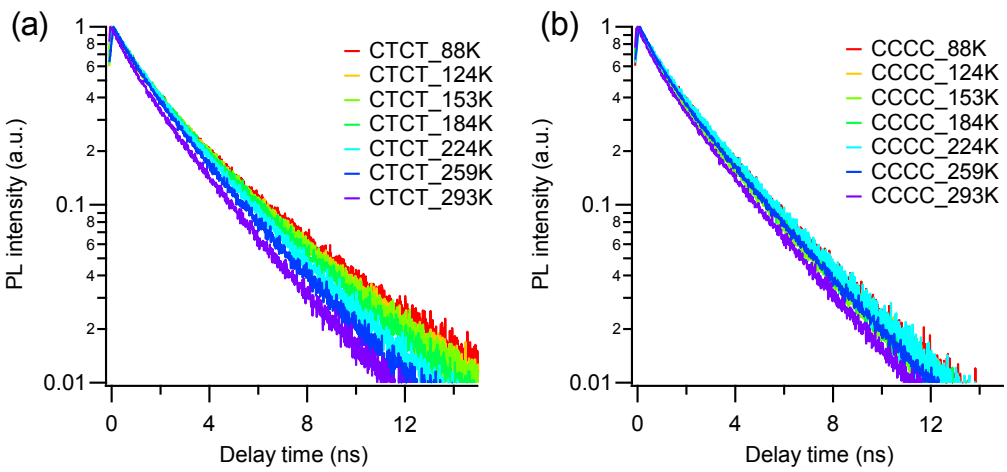


Figure S21. Temperature dependent fluorescence decay lifetime of (a) **1-CTCT** and (b) **2-CCCC** in a polymer matrix.

11. Transient Absorption

The samples were dissolved in chloroform in cuvettes with the path length of 2 mm for transient absorption measurements. The laser beam from a Ti:sapphire femtosecond regenerative amplifier at 800 nm wavelength and 1 kHz repetition rate was split into two paths. The first path was directed into an optical parametric amplifier to generate tunable pump laser (UV to near IR). The second path was focused onto a sapphire crystal to produce the white-light super-continuum (visible: 450 nm − 900 nm, near IR: 850 nm – 1600 nm) as probe. The probe spot was located within the pump spot on the sample cuvette. The transmitted probe beam was focused onto a fiber coupled high-speed multichannel detector and collected by a high speed spectrometer (HELIOS, Ultrafast Systems).

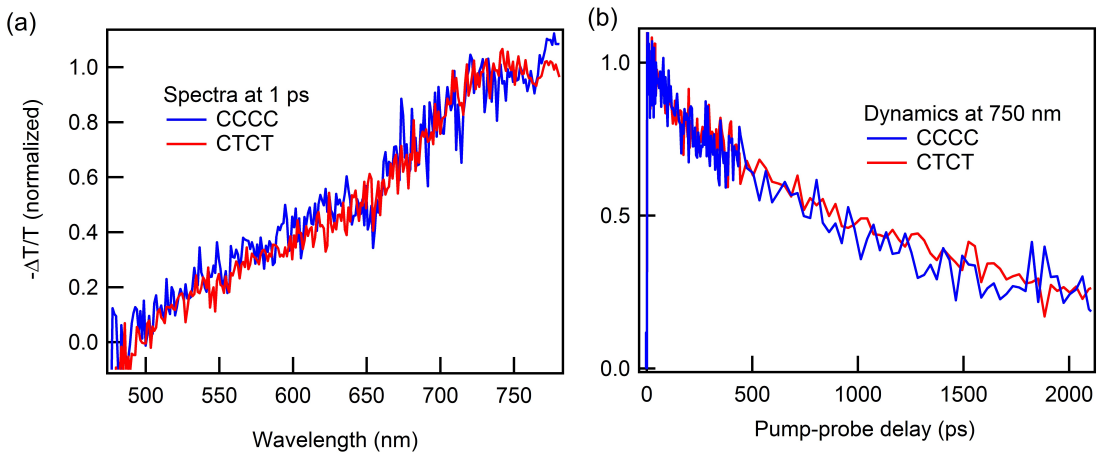


Figure S22. Transient absorption spectra in the visible range (a) and the dynamics (b) of **1-CTCT** and **2-CCCC** upon 325 nm excitation.

12. DFT computation details

All quantum chemical calculations were performed using Jaguar, version 8.3, Schrodinger, Inc., New York, NY, 2014.[16] Geometries were optimized using the B3LYP functional and the 6-31G** and LACVP (for platinum intermediates) basis set. All orbital surfaces shown are plotted at a 0.03 isovalue. At the optimized geometry, excited singlet states were calculated using the TD-DFT method that is included in the Jaguar package.

I) Orbital images

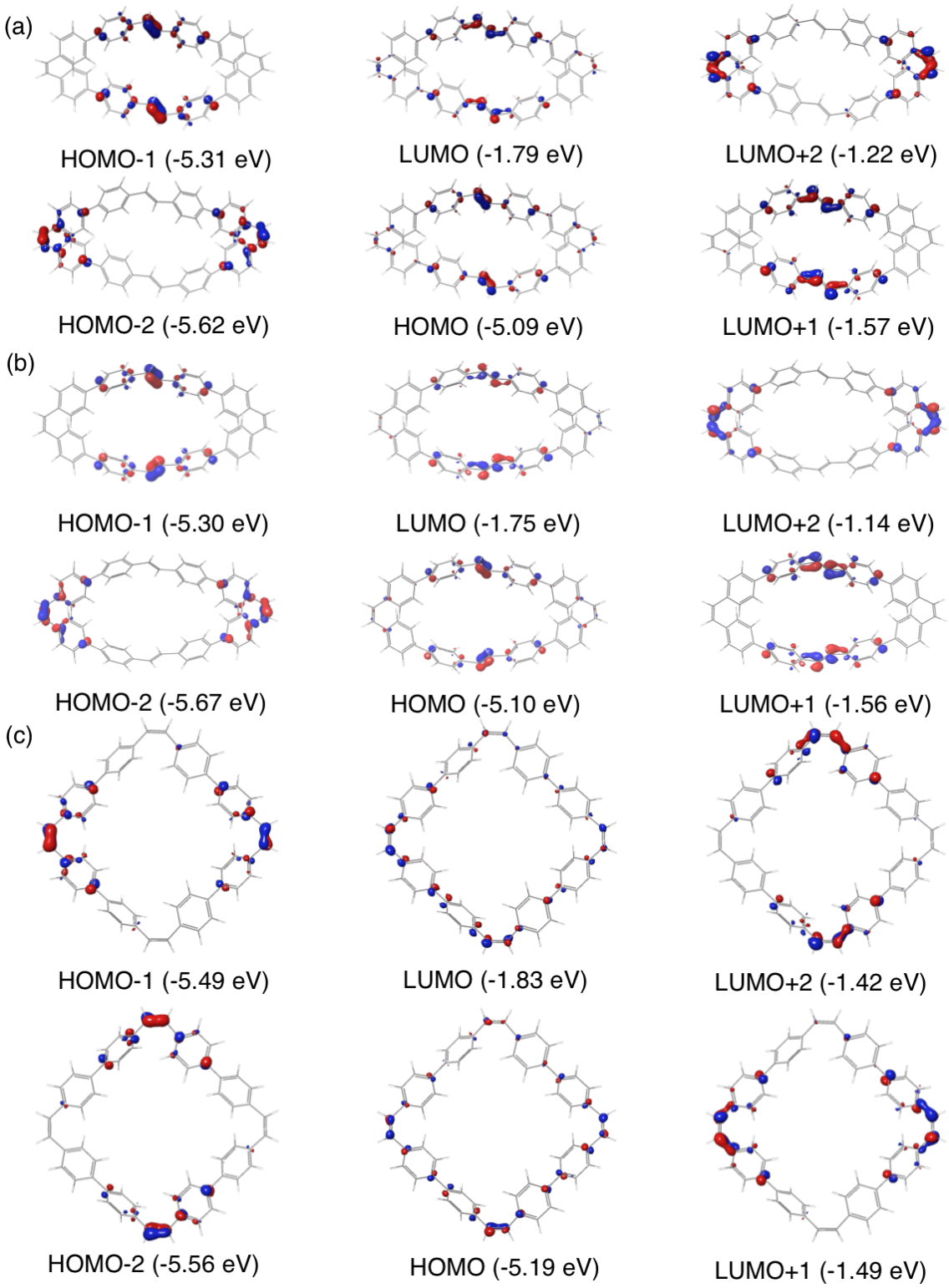
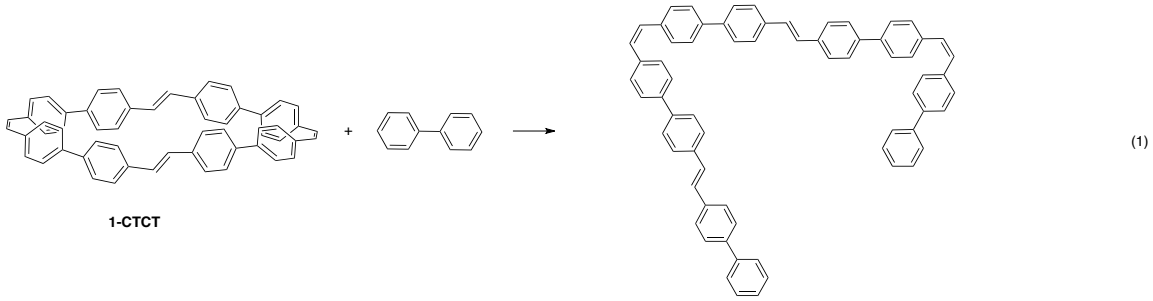
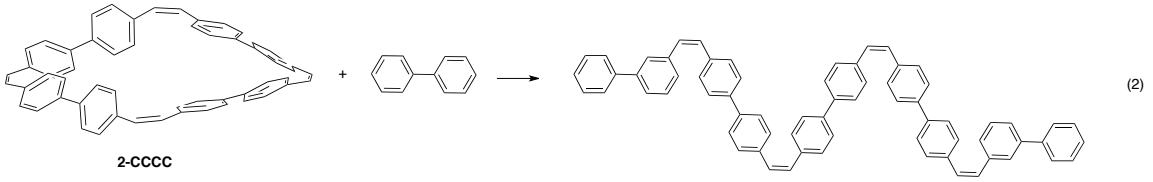


Figure S23. DFT calculated molecular frontier orbitals of a) **1-CTCT** b) **1-CTCT** C2 conformer and c) **2-CCCC** at the B3LYP/6-31G** level, plotted at 0.05 isovalue.

II) Calculation of strain energies

Strain energies of cyclostilbenes **1-CTCT** and **2-CCCC** were estimated by the following isodesmic reactions (1) and (2):





The energies are summarized below.

Table S4. DFT calculated energies of components relevant to the isodesmic reactions.

	Biphenyl	2 × benzene	**1-CTCT**	**CTCT-acyclic**	**2-CCCC**	**CCCC-acyclic**
Energy (h)	-463.3215	-464.5164	-2158.0947	-2159.3167	-2158.1049	-2159.3001

III) Optimized geometries

Cyclostilbene **1-CTCT**

B3LYP/6-31G** optimized geometry

Final total energy = -2158.0947 hartrees

Final geometry:

angstroms

atom	x	y	z
C1	-0.1879000000	0.5740000000	0.2529000000
C2	-0.2737000000	0.1113000000	1.5753000000
C3	0.8656000000	-0.5101000000	2.1205000000
C4	2.0220000000	-0.6924000000	1.3762000000

C5	2.0993000000	-0.2554000000	0.0420000000
C6	0.9782000000	0.4058000000	-0.4895000000
C7	-1.5103000000	0.2018000000	2.3859000000
C8	-2.7848000000	-0.0131000000	1.8272000000
C9	-3.9177000000	-0.1354000000	2.6239000000
C10	-3.8245000000	-0.0528000000	4.0270000000
C11	-2.5677000000	0.2749000000	4.5708000000
C12	-1.4390000000	0.3958000000	3.7749000000
C13	-4.8737000000	-0.4415000000	4.9683000000
C14	-6.0407000000	-1.0757000000	4.7237000000
C15	-6.8106000000	-1.7852000000	5.7515000000
C16	-7.6719000000	-2.8312000000	5.3716000000
C17	-8.1425000000	-3.7590000000	6.2989000000
C18	-7.7673000000	-3.6769000000	7.6488000000
C19	-7.0408000000	-2.5400000000	8.0519000000
C20	-6.5839000000	-1.6110000000	7.1319000000
C21	-7.9602000000	-4.8117000000	8.5841000000
C22	-9.1227000000	-5.5955000000	8.6332000000
C23	-9.1889000000	-6.7247000000	9.4483000000
C24	-8.0863000000	-7.1352000000	10.2167000000
C25	-6.9388000000	-6.3256000000	10.1987000000
C26	-6.8824000000	-5.1884000000	9.4063000000
C27	-8.1356000000	-8.3632000000	11.0387000000
C28	-7.1963000000	-9.3260000000	11.1347000000
C29	-5.9707000000	-9.5017000000	10.3302000000
C30	-4.8110000000	-10.0480000000	10.9081000000
C31	-3.6474000000	-10.2379000000	10.1656000000
C32	-3.6037000000	-9.9171000000	8.7997000000
C33	-4.7765000000	-9.4035000000	8.2156000000
C34	-5.9294000000	-9.1963000000	8.9585000000
C35	-2.3820000000	-10.0487000000	7.9711000000

C36	-2.4754000000	-10.4241000000	6.6214000000
C37	-1.3769000000	-10.3465000000	5.7783000000
C38	-0.1292000000	-9.8813000000	6.2341000000
C39	-0.0090000000	-9.6133000000	7.6124000000
C40	-1.1093000000	-9.6959000000	8.4576000000
C41	0.8698000000	-9.5335000000	5.2247000000
C42	2.0058000000	-8.8248000000	5.3940000000
C43	2.7260000000	-8.1223000000	4.3286000000
C44	2.4329000000	-8.2711000000	2.9575000000
C45	2.8819000000	-7.3443000000	2.0289000000
C46	3.6622000000	-6.2375000000	2.4143000000
C47	4.0786000000	-6.1740000000	3.7525000000
C48	3.6209000000	-7.0974000000	4.6864000000
C49	3.8911000000	-5.0982000000	1.4941000000
C50	5.0866000000	-4.3637000000	1.4700000000
C51	5.1979000000	-3.2031000000	0.7080000000
C52	4.1095000000	-2.7121000000	-0.0318000000
C53	2.9329000000	-3.4792000000	-0.0549000000
C54	2.8310000000	-4.6487000000	0.6865000000
C55	4.2078000000	-1.4329000000	-0.7661000000
C56	3.3175000000	-0.4204000000	-0.7747000000
H57	-2.8762000000	-0.1570000000	0.7550000000
H58	5.9366000000	-4.7038000000	2.0541000000
H59	-4.8723000000	-0.3568000000	2.1553000000
H60	-2.7702000000	-10.6614000000	10.6471000000
H61	1.8034000000	-9.0889000000	2.6208000000
H62	6.1325000000	-2.6476000000	0.7133000000
H63	-2.4740000000	0.3856000000	5.6482000000
H64	-7.9004000000	-2.9713000000	4.3178000000
H65	1.8935000000	-5.1964000000	0.6892000000
H66	2.6018000000	-7.4582000000	0.9856000000

H67	-9.9848000000	-5.3159000000	8.0336000000
H68	-3.4285000000	-10.7584000000	6.2245000000
H69	3.8921000000	-6.9753000000	5.7323000000
H70	2.0864000000	-3.1359000000	-0.6403000000
H71	2.3358000000	-8.5848000000	6.4034000000
H72	-6.8079000000	-2.4057000000	9.1043000000
H73	2.8755000000	-1.1817000000	1.8301000000
H74	-1.4929000000	-10.5987000000	4.7272000000
H75	-5.9679000000	-4.6041000000	9.3809000000
H76	-10.1014000000	-7.3154000000	9.4694000000
H77	-4.7692000000	-9.1299000000	7.1651000000
H78	-0.4830000000	0.6232000000	4.2367000000
H79	0.5444000000	-9.7378000000	4.2065000000
H80	3.5217000000	0.4045000000	-1.4569000000
H81	-6.0815000000	-6.6059000000	10.8009000000
H82	-8.7229000000	-4.6099000000	5.9540000000
H83	0.8280000000	-0.8907000000	3.1364000000
H84	-0.9988000000	-9.4103000000	9.5000000000
H85	-4.5695000000	-0.3398000000	6.0080000000
H86	-9.0293000000	-8.4824000000	11.6508000000
H87	-6.0027000000	-0.7647000000	7.4846000000
H88	-4.8210000000	-10.3205000000	11.9608000000
H89	5.1040000000	-1.3079000000	-1.3735000000
H90	4.6934000000	-5.3419000000	4.0835000000
H91	-6.8110000000	-8.7944000000	8.4736000000
H92	0.9402000000	-9.2758000000	8.0186000000
H93	-6.3575000000	-1.2458000000	3.6961000000
H94	-7.3647000000	-10.1015000000	11.8816000000
H95	1.0203000000	0.7842000000	-1.5080000000
H96	-1.0348000000	1.0880000000	-0.1929000000

Cyclostilbene **1-CTCT** C2 conformer

B3LYP/6-31G** optimized geometry

Final total energy = -2158.0943 hartrees

Final geometry:

angstroms

atom	x	y	z
C1	-0.1399417513	0.1807958631	0.1354522723
C2	-0.1084742472	0.2069935468	1.5422078482
C3	1.1507610083	0.1870967448	2.1592904346
C4	2.3234412297	0.1948557503	1.4056253237
C5	2.2899443472	0.2537109456	0.0037728815
C6	1.0275679106	0.2040009189	-0.6149121896
C7	-1.3755798661	0.3523571581	2.2997629341
C8	-1.4695288625	1.2186241075	3.3974796460
C9	-2.7036665194	1.5543834205	3.9414574906
C10	-3.9062543489	1.0409244031	3.4230628818
C11	-3.7978326634	0.0717830512	2.4074272069
C12	-2.5660789036	-0.2608695857	1.8618918471
C13	-5.1734502577	1.6402835737	3.8469587271
C14	-6.3894389729	1.4196138331	3.3018025747
C15	-7.6123873447	2.2009767754	3.5168020759
C16	-7.7327154925	3.2848321678	4.4100351401
C17	-8.8132687106	4.1574884343	4.3374494609
C18	-9.8304366765	3.9902976060	3.3769053175
C19	-9.7716410075	2.8420264891	2.5717044832
C20	-8.6946868299	1.9680193322	2.6466314291
C21	-10.8226211698	5.0602627567	3.1126366038
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C24	-12.4348750412	7.3257379410	2.4852520400
C25	-11.9245057325	6.4920203085	1.4754053819

C26	-11.1443466620	5.3866223183	1.7823913208
C27	-13.2030000916	8.5464334030	2.1469808400
C28	-12.8771907468	9.4833812536	1.2312203067
C29	-11.5977379774	9.5985525763	0.4954844151
C30	-11.5609662553	9.8287120591	-0.8897452597
C31	-10.3534403598	9.8604324767	-1.5854122591
C32	-9.1311518372	9.6985245744	-0.9158425608
C33	-9.1678494551	9.5449524539	0.4812117786
C34	-10.3698102533	9.4909682767	1.1702841327
C35	-7.8280680114	9.5962167354	-1.6117815138
C36	-6.6616069388	10.1166995678	-1.0301958462
C37	-5.4115648937	9.8282472880	-1.5569574650
C38	-5.2617772806	8.9951679724	-2.6811427016
C39	-6.4366280738	8.5612324156	-3.3245784208
C40	-7.6888665720	8.8557696698	-2.7998371465
C41	-3.9140015812	8.5303621515	-3.0043999824
C42	-3.5639896802	7.5334910209	-3.8430478946
C43	-2.2569016218	6.8753529706	-3.8848428456
C44	-1.1455861241	7.3053855333	-3.1330005268
C45	-0.0239136555	6.5041943585	-2.9944115609
C46	0.0539493572	5.2373719056	-3.6031503757
C47	-0.9981086543	4.8613895702	-4.4511985081
C48	-2.1264071394	5.6632455224	-4.5866872856
C49	1.1217132651	4.2806522339	-3.2303193322
C50	1.5164058248	4.1975335026	-1.8834119650
C51	2.3846466340	3.2091469118	-1.4458524483
C52	2.9084343373	2.2594619496	-2.3378703245
C53	2.5869259342	2.3954178255	-3.6982441237
C54	1.6973639924	3.3750885519	-4.1348276837
C55	3.7687385969	1.1554353726	-1.8523332237
C56	3.5345215825	0.3462832783	-0.7973128510

H57	-0.5736280361	1.7005924518	3.7766380054
H58	1.4464613786	3.4380306962	-5.1900735412
H59	-2.7482325588	2.2852060565	4.7454732563
H60	-10.3599148365	10.0185895588	-2.6605099965
H61	-1.1724928953	8.2617102150	-2.6198082948
H62	3.0115292424	1.7006116185	-4.4187068837
H63	-4.6907444994	-0.3987043559	2.0070386966
H64	-6.9440618512	3.4866722816	5.1288310791
H65	1.0873909888	4.8840536247	-1.1602749806
H66	0.8041583255	6.8518243349	-2.3836154966
H67	-11.2078975760	5.6022846229	5.1660266194
H68	-6.7374360971	10.7366006465	-0.1425108935
H69	-2.9569044422	5.3142611299	-5.1954548097
H70	2.6433004575	3.1491706653	-0.3941535967
H71	-4.3313130839	7.0647154973	-4.4572101180
H72	-10.5664080659	2.6471589133	1.8577328507
H73	0.9677602987	0.2087888883	-1.6974708044
H74	-4.5228027479	10.2125446196	-1.0625562513
H75	-10.7217464994	4.7998612181	0.9738202269
H76	-12.6115255561	7.5457306322	4.6234513128
H77	-8.2376256000	9.4126686804	1.0250090428
H78	-2.5248474886	-0.9920641652	1.0611165906
H79	-3.1405908400	8.9693729645	-2.3767576559
H80	4.3331890473	-0.3377506023	-0.5118709259
H81	-12.1210990480	6.7351582620	0.4374862986
H82	-8.8324813677	5.0296314072	4.9845196791
H83	-1.0971660437	0.1981026656	-0.3753602772
H84	-8.5746350162	8.4470438689	-3.2781362183
H85	-14.1383141052	8.6863162114	2.6879436672
H86	-8.6562054812	1.1153514796	1.9724010572
H87	-12.4931350498	9.9536214742	-1.4352909900

H88	4.6969149860	1.0011158172	-2.4015952986
H89	-0.9694402906	3.8938794201	-4.9442526701
H90	-10.3655024420	9.3413789296	2.2438942424
H91	-6.3704236312	7.9425171825	-4.2149275199
H92	-13.6149280657	10.2566164227	1.0185741735
H93	3.2840967569	0.1845000536	1.9147553049
H94	1.2150588916	0.1638707609	3.2436722074
H95	-6.4888286657	0.6631298759	2.5230536970
H96	-5.0826644112	2.4181642824	4.6041894309

Cyclostilbene **2-CCCC**

B3LYP/6-31G** optimized geometry

Final total energy = -2158.1049 hartrees

Final geometry:

angstroms

atom	x	y	z
C1	-1.0040000000	0.3550000000	0.8690000000
C2	-1.7070000000	-0.4020000000	1.8210000000
C3	-1.5010000000	-1.7950000000	1.8180000000
C4	-0.6260000000	-2.3990000000	0.9240000000
C5	0.0830000000	-1.6380000000	-0.0230000000
C6	-0.1440000000	-0.2510000000	-0.0380000000
C7	-2.6360000000	0.2340000000	2.7810000000
C8	-3.3270000000	1.4150000000	2.4630000000
C9	-4.1840000000	2.0160000000	3.3790000000
C10	-4.4160000000	1.4540000000	4.6450000000
C11	-3.7190000000	0.2740000000	4.9670000000
C12	-2.8500000000	-0.3150000000	4.0590000000
C13	-5.2970000000	2.1510000000	5.5990000000
C14	-6.0610000000	1.6330000000	6.5800000000
C15	-6.3320000000	0.2070000000	6.8580000000

C16	-6.7270000000	-0.6780000000	5.8400000000
C17	-6.9790000000	-2.0170000000	6.1100000000
C18	-6.8350000000	-2.5330000000	7.4090000000
C19	-6.4720000000	-1.6420000000	8.4320000000
C20	-6.2400000000	-0.2970000000	8.1650000000
C21	-7.0380000000	-3.9740000000	7.6880000000
C22	-8.0640000000	-4.7090000000	7.0700000000
C23	-8.2370000000	-6.0620000000	7.3420000000
C24	-7.3770000000	-6.7490000000	8.2170000000
C25	-6.3570000000	-6.0110000000	8.8400000000
C26	-6.1950000000	-4.6550000000	8.5830000000
C27	-7.6250000000	-8.1700000000	8.5230000000
C28	-6.7570000000	-9.1830000000	8.7240000000
C29	-5.2980000000	-9.2610000000	8.5370000000
C30	-4.5710000000	-10.2240000000	9.2600000000
C31	-3.2070000000	-10.4060000000	9.0630000000
C32	-2.5030000000	-9.6470000000	8.1140000000
C33	-3.2300000000	-8.6860000000	7.3880000000
C34	-4.5900000000	-8.4960000000	7.5920000000
C35	-1.0600000000	-9.8660000000	7.8600000000
C36	-0.5270000000	-9.7400000000	6.5630000000
C37	0.8220000000	-9.9430000000	6.3090000000
C38	1.7160000000	-10.2780000000	7.3450000000
C39	1.1770000000	-10.4360000000	8.6340000000
C40	-0.1750000000	-10.2270000000	8.8890000000
C41	3.1510000000	-10.5380000000	7.1310000000
C42	3.9930000000	-10.0450000000	6.2000000000
C43	3.7440000000	-8.9970000000	5.1950000000
C44	4.2530000000	-9.1310000000	3.8930000000
C45	3.9850000000	-8.1820000000	2.9120000000
C46	3.2070000000	-7.0460000000	3.1920000000

C47	2.7560000000	-6.8800000000	4.5130000000
C48	3.0230000000	-7.8270000000	5.4920000000
C49	2.8430000000	-6.0760000000	2.1340000000
C50	2.6110000000	-4.7170000000	2.4210000000
C51	2.2300000000	-3.8210000000	1.4300000000
C52	2.0700000000	-4.2390000000	0.0950000000
C53	2.3320000000	-5.5890000000	-0.1950000000
C54	2.6940000000	-6.4880000000	0.8000000000
C55	1.7340000000	-3.3310000000	-1.0130000000
C56	0.9630000000	-2.2250000000	-1.0450000000
H57	-3.2080000000	1.8600000000	1.4800000000
H58	2.7620000000	-4.3490000000	3.4310000000
H59	-4.6990000000	2.9330000000	3.1040000000
H60	-2.6890000000	-11.1800000000	9.6210000000
H61	4.8510000000	-10.0040000000	3.6420000000
H62	2.0800000000	-2.7780000000	1.6840000000
H63	-3.8360000000	-0.1660000000	5.9500000000
H64	-6.8250000000	-0.3060000000	4.8260000000
H65	2.8370000000	-7.5310000000	0.5410000000
H66	4.3960000000	-8.3200000000	1.9170000000
H67	-8.7510000000	-4.2060000000	6.3960000000
H68	-1.1900000000	-9.5160000000	5.7340000000
H69	2.6480000000	-7.6760000000	6.4990000000
H70	2.2270000000	-5.9410000000	-1.2180000000
H71	-6.3890000000	-2.0050000000	9.4520000000
H72	-0.5140000000	-3.4770000000	0.9370000000
H73	1.1850000000	-9.8660000000	5.2920000000
H74	-5.3860000000	-4.1160000000	9.0670000000
H75	-9.0540000000	-6.6020000000	6.8700000000
H76	-2.7160000000	-8.0700000000	6.6560000000
H77	-2.2970000000	-1.1990000000	4.3590000000

H78	0.9660000000	-1.6750000000	-1.9860000000
H79	-5.6890000000	-6.5070000000	9.5350000000
H80	-7.2570000000	-2.6830000000	5.2980000000
H81	-2.0630000000	-2.4190000000	2.5050000000
H82	-0.5450000000	-10.3240000000	9.9060000000
H83	-8.6800000000	-8.4240000000	8.6200000000
H84	-5.9660000000	0.3730000000	8.9760000000
H85	-5.0930000000	-10.8500000000	9.9790000000
H86	2.2060000000	-3.6030000000	-1.9570000000
H87	2.1540000000	-6.0140000000	4.7700000000
H88	-5.1160000000	-7.7570000000	7.0000000000
H89	1.8370000000	-10.7120000000	9.4530000000
H90	-7.2000000000	-10.1250000000	9.0470000000
H91	0.3800000000	0.3620000000	-0.7680000000
H92	-1.1170000000	1.4350000000	0.8510000000
H93	-6.5500000000	2.3390000000	7.2490000000
H94	-5.3000000000	3.2360000000	5.4990000000
H95	4.9940000000	-10.4750000000	6.1760000000
H96	3.5770000000	-11.2580000000	7.8300000000

Cyclostilbene **3-TTTT**

B3LYP/6-31G** optimized geometry

Final total energy = -2158.0514 hartrees

Final geometry:

angstroms

atom	x	y	z
C1	0.1060000000	0.2010000000	0.0660000000
C2	-0.0470000000	0.2360000000	1.4700000000
C3	1.1380000000	0.2530000000	2.2290000000
C4	2.3770000000	0.0510000000	1.6350000000

C5	2.4990000000	-0.2090000000	0.2570000000
C6	1.3420000000	-0.0180000000	-0.5280000000
C7	-1.3470000000	-0.0190000000	2.1400000000
C8	-1.5430000000	0.2220000000	3.5180000000
C9	-2.5530000000	-0.4070000000	4.2320000000
C10	-3.4370000000	-1.3090000000	3.6040000000
C11	-3.3590000000	-1.3910000000	2.2000000000
C12	-2.3410000000	-0.7700000000	1.4860000000
C13	-4.2510000000	-2.3080000000	4.3020000000
C14	-4.1870000000	-2.6400000000	5.6120000000
C15	-4.5770000000	-3.9220000000	6.2090000000
C16	-4.1100000000	-4.2210000000	7.5040000000
C17	-4.1020000000	-5.5190000000	7.9980000000
C18	-4.5550000000	-6.5990000000	7.2180000000
C19	-5.1820000000	-6.2740000000	5.9950000000
C20	-5.2010000000	-4.9740000000	5.5060000000
C21	-4.1910000000	-8.0030000000	7.5370000000
C22	-4.8360000000	-9.1160000000	6.9650000000
C23	-4.2540000000	-10.3800000000	6.9900000000
C24	-3.0060000000	-10.6140000000	7.6010000000
C25	-2.4440000000	-9.5320000000	8.3080000000
C26	-3.0140000000	-8.2690000000	8.2690000000
C27	-2.2550000000	-11.8350000000	7.2810000000
C28	-1.0010000000	-12.1320000000	7.6930000000
C29	-0.0210000000	-12.9650000000	6.9910000000
C30	-0.3150000000	-13.8400000000	5.9230000000
C31	0.6690000000	-14.2080000000	5.0140000000
C32	1.9900000000	-13.7180000000	5.1140000000
C33	2.3210000000	-13.0330000000	6.2970000000
C34	1.3400000000	-12.6750000000	7.2140000000
C35	2.8990000000	-13.6470000000	3.9420000000

C36	4.2870000000	-13.4110000000	4.0550000000
C37	5.0290000000	-12.9090000000	2.9910000000
C38	4.4190000000	-12.6240000000	1.7510000000
C39	3.0860000000	-13.0480000000	1.5890000000
C40	2.3430000000	-13.5340000000	2.6550000000
C41	4.9570000000	-11.7370000000	0.7170000000
C42	5.9760000000	-10.8560000000	0.8340000000
C43	6.1560000000	-9.6430000000	0.0290000000
C44	5.2710000000	-9.2530000000	-0.9970000000
C45	5.2520000000	-7.9530000000	-1.4770000000
C46	6.1250000000	-6.9630000000	-0.9790000000
C47	7.1090000000	-7.3910000000	-0.0700000000
C48	7.1190000000	-8.6920000000	0.4220000000
C49	5.8510000000	-5.5290000000	-1.2480000000
C50	6.1660000000	-4.5510000000	-0.2830000000
C51	5.6220000000	-3.2770000000	-0.3290000000
C52	4.7130000000	-2.9050000000	-1.3400000000
C53	4.5240000000	-3.8300000000	-2.3860000000
C54	5.0820000000	-5.1020000000	-2.3460000000
C55	3.7970000000	-1.7660000000	-1.2230000000
C56	3.7070000000	-0.9150000000	-0.1760000000
H57	4.8690000000	-5.7900000000	-3.1580000000
H58	5.8310000000	-2.5960000000	0.4900000000
H59	6.7670000000	-4.8230000000	0.5780000000
H60	4.4790000000	-7.6760000000	-2.1860000000
H61	4.5230000000	-9.9480000000	-1.3660000000
H62	7.8510000000	-8.9660000000	1.1770000000
H63	7.8500000000	-6.6870000000	0.2970000000
H64	6.0790000000	-12.6740000000	3.1450000000
H65	4.7820000000	-13.5650000000	5.0090000000
H66	1.2840000000	-13.7170000000	2.5080000000

H67	2.5940000000	-12.8870000000	0.6330000000
H68	0.3920000000	-14.8320000000	4.1690000000
H69	-1.3360000000	-14.1720000000	5.7600000000
H70	1.6130000000	-12.0480000000	8.0590000000
H71	3.3290000000	-12.6590000000	6.4410000000
H72	-4.7470000000	-11.1980000000	6.4700000000
H73	-5.7790000000	-8.9850000000	6.4440000000
H74	-2.4750000000	-7.4490000000	8.7320000000
H75	-1.4900000000	-9.6490000000	8.8110000000
H76	-3.6850000000	-5.7000000000	8.9830000000
H77	-3.6760000000	-3.4250000000	8.1050000000
H78	-5.6250000000	-4.7940000000	4.5230000000
H79	-5.5710000000	-7.0690000000	5.3670000000
H80	-2.6150000000	-0.2430000000	5.3040000000
H81	-0.8550000000	0.8680000000	4.0530000000
H82	-2.2550000000	-0.9720000000	0.4240000000
H83	-4.0520000000	-2.0400000000	1.6710000000
H84	-0.7700000000	0.2860000000	-0.5700000000
H85	1.3980000000	-0.1140000000	-1.6090000000
H86	3.2560000000	-0.0340000000	2.2680000000
H87	1.0870000000	0.3050000000	3.3110000000
H88	3.8690000000	-3.5640000000	-3.2120000000
H89	-0.5680000000	-11.5290000000	8.4880000000
H90	-2.6950000000	-12.4320000000	6.4830000000
H91	-3.6170000000	-1.9990000000	6.2810000000
H92	-4.8060000000	-2.9630000000	3.6330000000
H93	4.4990000000	-0.9280000000	0.5700000000
H94	2.9950000000	-1.7650000000	-1.9590000000
H95	6.6250000000	-10.9170000000	1.7060000000
H96	4.3100000000	-11.6520000000	-0.1540000000

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B3LYP/LACVP optimized geometry

Final total energy = -3883.0093 hartrees

Final geometry:

	angstroms		
atom	x	y	z
C1	1.3508455771	5.7411654068	-3.6556021929
C2	-1.3508455771	-5.7411654068	3.6556021929
C3	6.9976377761	-2.7570905220	-0.8091795757
C4	-6.9976377761	2.7570905220	0.8091795757
C5	2.2613424801	5.8210868199	-2.5827305454
C6	-2.2613424801	-5.8210868199	2.5827305454
C7	7.2689424336	-3.9782907129	-1.4518885087
C8	-7.2689424336	3.9782907129	1.4518885087
C9	3.6274008220	5.6110287496	-2.7660051512
C10	-3.6274008220	-5.6110287496	2.7660051512
C11	7.3113523781	-5.1860046947	-0.7528190460
C12	-7.3113523781	5.1860046947	0.7528190460
C13	4.1696634547	5.3278133027	-4.0347802000
C14	-4.1696634547	-5.3278133027	4.0347802000
C15	7.0711901150	-5.2361012028	0.6314949363
C16	-7.0711901150	5.2361012028	-0.6314949363
C17	3.2593342516	5.2306744355	-5.1027015514
C18	-3.2593342516	-5.2306744355	5.1027015514
C19	6.8080223604	-4.0117928224	1.2767642109
C20	-6.8080223604	4.0117928224	-1.2767642109
C21	-1.8912696664	-5.4299854006	4.9166525631
C22	1.8912696664	5.4299854006	-4.9166525631
C23	6.7841836934	-2.8050172259	0.5833272040
C24	-6.7841836934	2.8050172259	-0.5833272040
C25	7.0187337151	-9.3249521691	1.9960471314

C26	-7.0187337151	9.3249521691	-1.9960471314
C27	6.3735676477	7.5058778142	-4.7416243455
C28	-6.3735676477	-7.5058778142	4.7416243455
C29	7.3856412830	-8.7916461690	3.2126694121
C30	-7.3856412830	8.7916461690	-3.2126694121
C31	6.2371483795	6.9649067734	-6.0009939988
C32	-6.2371483795	-6.9649067734	6.0009939988
C33	5.0793169685	-6.7650662150	1.9097771051
C34	-5.0793169685	6.7650662150	-1.9097771051
C35	6.2297866688	3.4141184166	-3.3853697499
C36	-6.2297866688	-3.4141184166	3.3853697499
C37	8.7960732076	-8.7411019208	3.7817059193
C38	-8.7960732076	8.7411019208	-3.7817059193
C39	7.3609425070	6.7104281094	-6.9948952954
C40	-7.3609425070	-6.7104281094	6.9948952954
C41	4.5188631628	-6.6547973443	3.1989218586
C42	-4.5188631628	6.6547973443	-3.1989218586
C43	6.2701161914	2.1734890123	-4.0530574989
C44	-6.2701161914	-2.1734890123	4.0530574989
C45	9.5752519896	-7.4471640610	3.4367313115
C46	-9.5752519896	7.4471640610	-3.4367313115
C47	7.9933833958	5.2990584405	-6.8951093831
C48	-7.9933833958	-5.2990584405	6.8951093831
C49	3.1473713457	-6.4862562375	3.3927074269
C50	-3.1473713457	6.4862562375	-3.3927074269
C51	6.4200213119	0.9695832701	-3.3646594331
C52	-6.4200213119	-0.9695832701	3.3646594331
C53	9.3957929156	-6.9395470412	2.0206622701
C54	-9.3957929156	6.9395470412	-2.0206622701
C55	8.2026439358	4.7781530466	-5.4876038386
C56	-8.2026439358	-4.7781530466	5.4876038386

C57	2.2534490260	-6.4298056621	2.3056234378
C58	-2.2534490260	6.4298056621	-2.3056234378
C59	6.5316361632	0.9406898989	-1.9607429999
C60	-6.5316361632	-0.9406898989	1.9607429999
C61	9.2460398464	-7.6899940901	0.8736450759
C62	-9.2460398464	7.6899940901	-0.8736450759
C63	8.5517608828	5.5015443156	-4.3679629671
C64	-8.5517608828	-5.5015443156	4.3679629671
C65	2.8147508588	-6.5578001487	1.0208959124
C66	-2.8147508588	6.5578001487	-1.0208959124
C67	6.4688492281	2.1779680904	-1.2944561948
C68	-6.4688492281	-2.1779680904	1.2944561948
C69	9.3032059545	-9.2078836766	0.7802097115
C70	-9.3032059545	9.2078836766	-0.7802097115
C71	8.8766826746	6.9875820277	-4.3275096357
C72	-8.8766826746	-6.9875820277	4.3275096357
C73	4.1863673975	-6.7038777556	0.8264876161
C74	-4.1863673975	6.7038777556	-0.8264876161
C75	6.3213535425	3.3803569812	-1.9842255909
C76	-6.3213535425	-3.3803569812	1.9842255909
C77	7.9290285785	-9.9072808510	0.9340207679
C78	-7.9290285785	9.9072808510	-0.9340207679
C79	7.6571142846	7.8990230651	-4.0400050443
C80	-7.6571142846	-7.8990230651	4.0400050443
C81	0.8040661445	-6.2319697044	2.4248426042
C82	-0.8040661445	6.2319697044	-2.4248426042
C83	6.6805278351	-0.2808498815	-1.1649658073
C84	-6.6805278351	0.2808498815	1.1649658073
C85	0.0969395606	-5.9528989032	3.5401327115
C86	-0.0969395606	5.9528989032	-3.5401327115
C87	6.9091942672	-1.5332947535	-1.6107736116

C88	-6.9091942672	1.5332947535	1.6107736116
Pt89	7.0918743460	-7.0152550703	1.6357706899
Pt90	-7.0918743460	7.0152550703	-1.6357706899
Pt91	6.1805989538	5.1967163878	-4.3822150762
Pt92	-6.1805989538	-5.1967163878	4.3822150762
H93	9.3577319292	-9.6209509690	3.4557892114
H94	8.7309454318	-8.8173790317	4.8726941659
H95	10.6458567470	-7.5965439609	3.6447671051
H96	9.2470491065	-6.6473865748	4.1101537573
H97	7.3928105032	-9.8455709294	-0.0194475664
H98	8.0829056155	-10.9803152027	1.1251471526
H99	10.0108367681	-9.5970586388	1.5171178062
H100	9.7141935961	-9.4782049726	-0.1986385115
H101	5.9593082569	-9.5178646706	1.8429588373
H102	6.5799994307	-8.5756163265	3.9093822004
H103	9.5871521587	-5.8765429791	1.8907937866
H104	9.2987739120	-7.1493078476	-0.0680723065
H105	7.5068962022	-6.1003971249	-1.3092056911
H106	7.4369944016	-3.9802858605	-2.5279106097
H107	6.5603324401	-1.8930503239	1.1294654403
H108	6.5918445982	-4.0025227583	2.3419130463
H109	7.0292835545	-1.6902729592	-2.6821701753
H110	6.5882874851	-0.1221273300	-0.0914575742
H111	6.4279385453	0.0401587413	-3.9275410265
H112	6.1704782436	2.1401642689	-5.1361316759
H113	6.2757114413	4.3045997415	-1.4126091681
H114	6.5382510179	2.1931060364	-0.2079853434
H115	8.9480887239	5.2859983396	-7.4429563907
H116	7.3420651348	4.5839856990	-7.4104104061
H117	8.1308987607	7.4795560613	-6.8868553367
H118	6.9599941618	6.8315468799	-8.0073157046

H119	9.3601129385	7.2845637459	-5.2624516778
H120	9.6201716141	7.1569834803	-3.5409382158
H121	7.4534040439	7.8878073621	-2.9634425746
H122	7.9112355172	8.9408871808	-4.2882701723
H123	8.8100970281	4.9298675496	-3.4798539475
H124	8.2510769588	3.6944679108	-5.4045477911
H125	5.4644795219	7.8525795676	-4.2551039672
H126	5.2253255073	6.8989623270	-6.3925630257
H127	4.2801135769	5.6668403697	-1.8986533800
H128	3.6160021642	4.9885080297	-6.1018019597
H129	1.2205917535	5.3434178268	-5.7702784455
H130	1.8987404214	6.0462544137	-1.5834343128
H131	-0.6342021273	5.8566417972	-4.4831802538
H132	-0.2697470090	6.3056973757	-1.4785055472
H133	-2.1571055761	6.5144460190	-0.1543106949
H134	-2.7700524321	6.3985907101	-4.4083992136
H135	-5.1617590032	6.6799051941	-4.0766921212
H136	-4.5666143697	6.7533010645	0.1900786070
H137	-8.7309454318	8.8173790317	-4.8726941659
H138	-9.3577319292	9.6209509690	-3.4557892114
H139	-9.2470491065	6.6473865748	-4.1101537573
H140	-10.6458567470	7.5965439609	-3.6447671051
H141	-8.0829056155	10.9803152027	-1.1251471526
H142	-7.3928105032	9.8455709294	0.0194475664
H143	-9.7141935961	9.4782049726	0.1986385115
H144	-10.0108367681	9.5970586388	-1.5171178062
H145	-5.9593082569	9.5178646706	-1.8429588373
H146	-6.5799994307	8.5756163265	-3.9093822004
H147	-9.2987739120	7.1493078476	0.0680723065
H148	-9.5871521587	5.8765429791	-1.8907937866
H149	-6.5918445982	4.0025227583	-2.3419130463

H150	-6.5603324401	1.8930503239	-1.1294654403
H151	-7.4369944016	3.9802858605	2.5279106097
H152	-7.5068962022	6.1003971249	1.3092056911
H153	-7.0292835545	1.6902729592	2.6821701753
H154	-6.5882874851	0.1221273300	0.0914575742
H155	-6.5382510179	-2.1931060364	0.2079853434
H156	-6.2757114413	-4.3045997415	1.4126091681
H157	-6.1704782436	-2.1401642689	5.1361316759
H158	-6.4279385453	-0.0401587413	3.9275410265
H159	-7.9112355172	-8.9408871808	4.2882701723
H160	-7.4534040439	-7.8878073621	2.9634425746
H161	-9.6201716141	-7.1569834803	3.5409382158
H162	-9.3601129385	-7.2845637459	5.2624516778
H163	-8.8100970281	-4.9298675496	3.4798539475
H164	-8.2510769588	-3.6944679108	5.4045477911
H165	-7.3420651348	-4.5839856990	7.4104104061
H166	-8.9480887239	-5.2859983396	7.4429563907
H167	-6.9599941618	-6.8315468799	8.0073157046
H168	-8.1308987607	-7.4795560613	6.8868553367
H169	-5.2253255073	-6.8989623270	6.3925630257
H170	-5.4644795219	-7.8525795676	4.2551039672
H171	-4.2801135769	-5.6668403697	1.8986533800
H172	-3.6160021642	-4.9885080297	6.1018019597
H173	-1.2205917535	-5.3434178268	5.7702784455
H174	-1.8987404214	-6.0462544137	1.5834343128
H175	0.6342021273	-5.8566417972	4.4831802538
H176	0.2697470090	-6.3056973757	1.4785055472
H177	2.7700524321	-6.3985907101	4.4083992136
H178	5.1617590032	-6.6799051941	4.0766921212
H179	4.5666143697	-6.7533010645	-0.1900786070
H180	2.1571055761	-6.5144460190	0.1543106949

6-Pt_3

B3LYP/LACVP optimized geometry

Final total energy = -3451.7645 hartrees

Final geometry:

angstroms

atom	x	y	z
C1	2.1860000000	5.6670000000	-4.0160000000
C2	-2.0550000000	-5.4630000000	3.9360000000
C3	6.5730000000	-2.2010000000	-1.2590000000
C4	-6.6110000000	1.8060000000	0.7560000000
C5	3.1000000000	5.8090000000	-2.9530000000
C6	-3.0260000000	-5.4640000000	2.9150000000
C7	6.2710000000	-3.4380000000	-1.8550000000
C8	-6.2580000000	3.0720000000	1.2650000000
C9	4.4710000000	5.8550000000	-3.1720000000
C10	-4.3870000000	-5.4570000000	3.2030000000
C11	6.1610000000	-4.6080000000	-1.1060000000
C12	-5.4490000000	3.9480000000	0.5530000000
C13	5.0150000000	5.7840000000	-4.4680000000
C14	-4.8690000000	-5.4700000000	4.5260000000
C15	6.3410000000	-4.6030000000	0.2860000000
C16	-4.9310000000	3.5990000000	-0.7080000000
C17	4.1060000000	5.6740000000	-5.5330000000
C18	-3.9010000000	-5.4330000000	5.5450000000
C19	6.6380000000	-3.3650000000	0.8870000000
C20	-5.4080000000	2.4020000000	-1.2790000000
C21	-2.5360000000	-5.4270000000	5.2570000000
C22	2.7290000000	5.6070000000	-5.3110000000
C23	6.7560000000	-2.1970000000	0.1390000000
C24	-6.2310000000	1.5340000000	-0.5750000000

C25	6.0620000000	-8.6490000000	1.7630000000
C26	7.1410000000	8.1350000000	-4.9400000000
C27	-6.6060000000	-7.9910000000	5.3700000000
C28	6.5010000000	-8.1130000000	2.9500000000
C29	7.1050000000	7.6770000000	-6.2370000000
C30	-6.5600000000	-7.4060000000	6.6130000000
C31	4.2760000000	-5.9780000000	1.7070000000
C32	-3.7820000000	4.3230000000	-1.3020000000
C33	7.0640000000	3.9730000000	-3.8670000000
C34	-7.2260000000	-3.9790000000	3.9090000000
C35	7.9290000000	-8.1390000000	3.4700000000
C36	8.2960000000	7.5480000000	-7.1740000000
C37	-7.6980000000	-7.3490000000	7.6190000000
C38	3.8000000000	-5.8590000000	3.0280000000
C39	-3.4630000000	4.2850000000	-2.6750000000
C40	6.5350000000	2.8120000000	-4.4610000000
C41	-7.0990000000	-2.6900000000	4.4630000000
C42	8.7780000000	-6.9070000000	3.0690000000
C43	8.9870000000	6.1620000000	-7.1400000000
C44	-8.5870000000	-6.0860000000	7.5070000000
C45	2.4450000000	-5.7150000000	3.3140000000
C46	-2.2450000000	4.7600000000	-3.1520000000
C47	6.5460000000	1.5830000000	-3.8060000000
C48	-7.2490000000	-1.5410000000	3.6900000000
C49	8.5850000000	-6.4190000000	1.6490000000
C50	9.1420000000	5.5480000000	-5.7660000000
C51	-8.9090000000	-5.6410000000	6.0960000000
C52	1.4790000000	-5.6870000000	2.2910000000
C53	-1.2800000000	5.3080000000	-2.2810000000
C54	7.0710000000	1.4560000000	-2.5050000000
C55	-7.5200000000	-1.6200000000	2.3080000000

C56	8.3460000000	-7.1790000000	0.5260000000
C57	9.3860000000	6.1990000000	-4.5790000000
C58	-9.1250000000	-6.4360000000	4.9940000000
C59	1.9580000000	-5.7800000000	0.9710000000
C60	-1.6450000000	5.4300000000	-0.9280000000
C61	7.6070000000	2.6150000000	-1.9170000000
C62	-7.7250000000	-2.9060000000	1.7760000000
C63	8.3020000000	-8.6970000000	0.4650000000
C64	9.6360000000	7.6890000000	-4.4040000000
C65	-9.1650000000	-7.9560000000	4.9790000000
C66	3.3160000000	-5.9100000000	0.6850000000
C67	-2.8530000000	4.9470000000	-0.4510000000
C68	7.6110000000	3.8390000000	-2.5800000000
C69	-7.5890000000	-4.0540000000	2.5540000000
C70	6.8940000000	-9.3030000000	0.6810000000
C71	8.3590000000	8.5220000000	-4.1290000000
C72	-7.8000000000	-8.6290000000	4.6930000000
C73	0.0340000000	-5.5860000000	2.5210000000
C74	0.0930000000	5.6610000000	-2.6390000000
C75	7.0540000000	0.2230000000	-1.7160000000
C76	-7.4080000000	-0.4940000000	1.3800000000
C77	-0.6090000000	-5.5150000000	3.7050000000
C78	0.7450000000	5.4890000000	-3.8080000000
C79	6.6450000000	-1.0030000000	-2.0980000000
C80	-7.1440000000	0.7970000000	1.6730000000
Pt81	6.2570000000	-6.3410000000	1.3450000000
Pt82	7.0350000000	5.8070000000	-4.7600000000
Pt83	-6.8600000000	-5.6900000000	4.9580000000
H84	8.4220000000	-9.0600000000	3.1490000000
H85	7.8980000000	-8.1860000000	4.5640000000
H86	9.8430000000	-7.1240000000	3.2450000000

H87	8.5270000000	-6.0740000000	3.7340000000
H88	6.3280000000	-9.2240000000	-0.2540000000
H89	6.9870000000	-10.3810000000	0.8860000000
H90	9.0090000000	-9.1160000000	1.1850000000
H91	8.6600000000	-9.0140000000	-0.5210000000
H92	4.9870000000	-8.7730000000	1.6460000000
H93	5.7350000000	-7.8330000000	3.6680000000
H94	8.8330000000	-5.3720000000	1.4900000000
H95	8.3910000000	-6.6610000000	-0.4290000000
H96	5.9190000000	-5.5360000000	-1.6200000000
H97	6.1150000000	-3.4780000000	-2.9320000000
H98	6.9630000000	-1.2630000000	0.6550000000
H99	6.7590000000	-3.3060000000	1.9670000000
H100	6.3210000000	-1.1490000000	-3.1290000000
H101	7.4080000000	0.3490000000	-0.6940000000
H102	6.1070000000	0.7190000000	-4.3000000000
H103	6.0770000000	2.8740000000	-5.4450000000
H104	8.0210000000	4.7070000000	-2.0660000000
H105	8.0170000000	2.5510000000	-0.9100000000
H106	9.9710000000	6.2310000000	-7.6280000000
H107	8.4020000000	5.4600000000	-7.7440000000
H108	9.0200000000	8.3380000000	-6.9600000000
H109	7.9520000000	7.7300000000	-8.1980000000
H110	10.1630000000	8.0810000000	-5.2780000000
H111	10.3190000000	7.8280000000	-3.5580000000
H112	8.0910000000	8.4180000000	-3.0720000000
H113	8.5790000000	9.5900000000	-4.2790000000
H114	9.6200000000	5.5720000000	-3.7220000000
H115	9.2320000000	4.4640000000	-5.7590000000
H116	6.1910000000	8.4130000000	-4.4880000000
H117	6.1230000000	7.6040000000	-6.6980000000

H118	5.1330000000	5.9070000000	-2.3120000000
H119	4.4710000000	5.6040000000	-6.5560000000
H120	2.0580000000	5.4910000000	-6.1610000000
H121	2.7390000000	5.8270000000	-1.9280000000
H122	0.1920000000	5.1320000000	-4.6770000000
H123	0.6680000000	6.0430000000	-1.7970000000
H124	-0.9320000000	5.8590000000	-0.2280000000
H125	-2.0260000000	4.6740000000	-4.2130000000
H126	-4.1710000000	3.8530000000	-3.3780000000
H127	-3.0430000000	4.9820000000	0.6160000000
H128	-5.0430000000	2.0960000000	-2.2560000000
H129	-6.4930000000	0.5840000000	-1.0300000000
H130	-6.5770000000	3.3410000000	2.2700000000
H131	-5.1720000000	4.8960000000	1.0070000000
H132	-7.1730000000	1.1110000000	2.7160000000
H133	-7.4070000000	-0.7910000000	0.3320000000
H134	-7.9490000000	-3.0060000000	0.7150000000
H135	-7.7170000000	-5.0240000000	2.0770000000
H136	-6.8220000000	-2.5800000000	5.5090000000
H137	-7.0780000000	-0.5720000000	4.1540000000
H138	-7.8530000000	-9.6940000000	4.9640000000
H139	-7.6120000000	-8.6040000000	3.6140000000
H140	-9.8700000000	-8.2760000000	4.2040000000
H141	-9.5770000000	-8.3230000000	5.9230000000
H142	-9.5020000000	-5.9390000000	4.1030000000
H143	-9.1630000000	-4.5880000000	5.9990000000
H144	-8.0780000000	-5.2520000000	8.0020000000
H145	-9.5210000000	-6.2440000000	8.0680000000
H146	-7.2710000000	-7.3740000000	8.6270000000
H147	-8.3100000000	-8.2510000000	7.5350000000
H148	-5.5740000000	-7.1490000000	6.9900000000

H149	-5.6540000000	-8.1710000000	4.8760000000
H150	-5.0920000000	-5.4400000000	2.3760000000
H151	-4.2060000000	-5.4010000000	6.5890000000
H152	-1.8200000000	-5.4040000000	6.0780000000
H153	-2.7140000000	-5.4700000000	1.8740000000
H154	-0.0130000000	-5.5150000000	4.6180000000
H155	-0.5610000000	-5.5870000000	1.6080000000
H156	2.1370000000	-5.6270000000	4.3530000000
H157	4.5020000000	-5.8680000000	3.8600000000
H158	3.6300000000	-5.9550000000	-0.3550000000
H159	1.2430000000	-5.7470000000	0.1500000000

7-Pt_2

B3LYP/LACVP optimized geometry

Final total energy = -3020.5276 hartrees

Final geometry:

angstroms

atom	x	y	z
C1	2.7417816369	5.5023445321	-4.0134382684
C2	-2.5340174076	-5.7426407709	4.0947095886
C3	6.1688307957	-1.2549625306	-0.7861846186
C4	-5.7094242611	1.3199281477	1.4397715181
C5	3.6442139093	6.2138488276	-3.1983655266
C6	-3.4432680607	-6.2070173008	3.1226637656
C7	5.7141656380	-2.4626647428	-1.3506611120
C8	-5.1973965831	2.5053698455	2.0032609543
C9	4.9822338474	6.3604287731	-3.5530520057
C10	-4.7922670987	-6.3828601023	3.4139607483
C11	4.8148111300	-3.2886764349	-0.6897450945
C12	-4.3380836149	3.3425074933	1.3006696129
C13	5.4959923635	5.8200595945	-4.7482066042

C14	-5.3125676140	-6.1247867491	4.6973029564
C15	4.3062886562	-2.9535068319	0.5782661240
C16	-3.9241413139	3.0326594602	-0.0086290818
C17	4.5843579670	5.1648754980	-5.5932444194
C18	-4.3987762592	-5.7208019917	5.6848512667
C19	4.8475138510	-1.8057282093	1.1922918986
C20	-4.5174923371	1.9034785148	-0.6085600684
C21	-3.0457766464	-5.5348634105	5.3885728842
C22	3.2422564556	5.0146617572	-5.2348080499
C23	5.7567886139	-0.9823752224	0.5359461057
C24	-5.3881993639	1.0744070028	0.0878577889
C25	7.3261044882	8.2006977980	-5.8249164836
C26	-7.2155424342	-8.6145064721	5.2558559217
C27	7.2720293932	7.4842937632	-7.0017084372
C28	-7.1644804886	-8.1438434784	6.5512157472
C29	3.1547060596	-3.6899384202	1.1582576024
C30	-2.8080286785	3.7574791015	-0.6660959094
C31	7.7109148424	4.3164654351	-3.9905985423
C32	-7.4737542800	-4.4634238645	4.1671021910
C33	8.4244859050	7.2911976429	-7.9768769324
C34	-8.3261262277	-8.1119072685	7.5335958297
C35	2.9039577978	-3.7831091089	2.5424144390
C36	-2.6470077669	3.8158745965	-2.0662080686
C37	7.7399400125	3.0039134210	-4.5043367233
C38	-7.2124982206	-3.2510923008	4.8370817152
C39	9.2755957475	6.0216514820	-7.7188167981
C40	-9.1391630453	-6.7925856928	7.5187736935
C41	1.7376986243	-4.3585359783	3.0405414033
C42	-1.5054710027	4.3524551606	-2.6544606281
C43	7.6930409630	1.8874671203	-3.6690381167
C44	-7.1243922365	-2.0389073672	4.1530379426

C45	9.5487722679	5.7068753512	-6.2619246645
C46	-9.3878104308	-6.1976686552	6.1475430385
C47	0.7510186304	-4.8745151521	2.1744150725
C48	-0.4531774894	4.8658707776	-1.8684366725
C49	7.6076335411	2.0303919545	-2.2691671347
C50	-7.2802242886	-1.9809595088	2.7526665538
C51	9.7738515541	6.6035807027	-5.2387808415
C52	-9.6243496107	-6.8762101375	4.9709883446
C53	1.0327398312	-4.8303678925	0.7952337878
C54	-0.6491544466	4.8711608911	-0.4736363145
C55	7.6921773886	3.3391057043	-1.7574593766
C56	-7.6400326774	-3.1765242842	2.1026952470
C57	9.8779664782	8.1151076400	-5.3866290696
C58	-9.7597076366	-8.3849550893	4.8200971467
C59	2.1920996711	-4.2523302881	0.3005121624
C60	-1.7841084744	4.3276021760	0.1115106107
C61	7.7369412874	4.4534672934	-2.5927006589
C62	-7.7355064464	-4.3861562184	2.7884967942
C63	8.5365622569	8.8704494952	-5.2074104187
C64	-8.4307440735	-9.1170390373	4.5035057891
C65	-0.5661133469	-5.3758646349	2.5763583568
C66	0.8454718188	5.3205613797	-2.3744325296
C67	7.2563596994	0.9511739616	-1.3412778991
C68	-6.9253687745	-0.8288175828	1.9197987328
C69	-1.1388616214	-5.3893806131	3.7993753906
C70	1.3649799184	5.1812169251	-3.6135638022
C71	6.8793817048	-0.3080924792	-1.6507346395
C72	-6.3884060063	0.3491334380	2.3048648706
Pt73	7.4920567669	5.9624365542	-5.1902103471
Pt74	-7.3193948940	-6.2969984363	5.0670204790
H75	4.4794922435	-4.1976166121	-1.1797637119

H76	6.0418261167	-2.7302547721	-2.3529599894
H77	6.0894475829	-0.0752953938	1.0324690492
H78	4.4898921221	-1.5091648404	2.1741885332
H79	6.9704016767	-0.6377767592	-2.6851057567
H80	7.1613631214	1.2773457432	-0.3063788945
H81	7.6604231567	0.8975177140	-4.1176434762
H82	7.7406686596	2.8433631454	-5.5805386446
H83	7.7318620743	5.4421219287	-2.1404959982
H84	7.6528031869	3.4842117215	-0.6792075845
H85	10.2261645147	6.1004531624	-8.2678760786
H86	8.7547153703	5.1562873563	-8.1437273315
H87	9.0602994613	8.1810165845	-7.9729970394
H88	8.0127722421	7.2240973883	-8.9896791290
H89	10.3220085661	8.3583681398	-6.3556709942
H90	10.5811655381	8.4881284362	-4.6342745699
H91	8.3330950072	8.9795235399	-4.1363344521
H92	8.6371655335	9.8934661110	-5.6004865772
H93	10.1140254119	6.1894425352	-4.2927070479
H94	9.7595560940	4.6606763633	-6.0514971943
H95	6.3755509343	8.4674979655	-5.3688692890
H96	6.2822664393	7.2176507833	-7.3650332630
H97	5.6430818600	6.8856958735	-2.8673378198
H98	4.9240517229	4.7312841466	-6.5311467933
H99	2.5726804084	4.4704437675	-5.8990656896
H100	3.3029553218	6.6431641317	-2.2603898863
H101	0.7608051109	4.7123732479	-4.3897120463
H102	1.4858687533	5.7434803326	-1.6015763317
H103	0.1376431761	5.2663990613	0.1649923004
H104	-1.4260720342	4.3614930125	-3.7383498426
H105	-3.4322663693	3.4290326502	-2.7093882967
H106	-1.8482024412	4.2894999767	1.1946960949

H107	-4.2257662618	1.6208935439	-1.6156899294
H108	-5.7527735513	0.1767100871	-0.4025649764
H109	-5.4517714508	2.7505145972	3.0322942016
H110	-3.9587853247	4.2349868029	1.7888021572
H111	-6.3288010736	0.5773317112	3.3686535518
H112	-7.0004083570	-1.0285531469	0.8515835179
H113	-7.7878241387	-3.1636858341	1.0239961810
H114	-7.9585752316	-5.2880912731	2.2225610974
H115	-7.0135734272	-3.2571608091	5.9061400331
H116	-6.8635317857	-1.1408026439	4.7076318449
H117	-8.5555228302	-10.1961266101	4.6784929672
H118	-8.2145779969	-9.0104508974	3.4345179422
H119	-10.4619522433	-8.5888587222	4.0045368370
H120	-10.2179082641	-8.8050696421	5.7194170877
H121	-9.9403469564	-6.2786838606	4.1190589164
H122	-9.5684720270	-5.1248141939	6.1409033377
H123	-8.5997496604	-6.0397214227	8.1040916514
H124	-10.0978507850	-6.9474498475	8.0365632132
H125	-7.9280537802	-8.2546748136	8.5439813722
H126	-8.9852055325	-8.9649205032	7.3507908261
H127	-6.1747451510	-7.9810866344	6.9703402221
H128	-6.2641872505	-8.8154115271	4.7677540797
H129	-5.4576722643	-6.6955055388	2.6127968474
H130	-4.7430529736	-5.5105785131	6.6950270392
H131	-2.3736656625	-5.1864249611	6.1713068800
H132	-3.1018056237	-6.4047316291	2.1105133499
H133	-0.5640781088	-5.0426881263	4.6576720453
H134	-1.1693109850	-5.7096644998	1.7333207432
H135	1.5849065412	-4.3909494348	4.1160484236
H136	3.6370910756	-3.3943086593	3.2437341576
H137	2.3258886389	-4.1819421322	-0.7745102719

H138	0.2957682843	-5.2201609868	0.0966071295

8-Pt_2

B3LYP/LACVP optimized geometry

Final total energy = -3020.5291 hartrees

Final geometry:

angstroms

atom	x	y	z
C1	2.7519003356	4.6526318176	-2.6216403128
C2	-2.4744461618	-4.2117704549	3.4077780111
C3	7.3079454051	-0.6405759167	-0.1500881626
C4	-6.7107218451	1.2251672456	1.7451742066
C5	3.9629334434	4.6166813903	-1.9047922227
C6	-3.0547792696	-5.2218147288	2.6155548409
C7	6.9962900655	-1.9961757405	0.0601077799
C8	-5.5594134494	0.6213491171	2.2850338464
C9	5.1843336092	4.8358587536	-2.5413472579
C10	-4.2956399624	-5.7675170830	2.9379630762
C11	5.7025982837	-2.4086896926	0.3500959096
C12	-4.2886438370	0.9621310908	1.8348435877
C13	5.2727233180	5.1050368101	-3.9261437435
C14	-5.0302953173	-5.3301299867	4.0590895330
C15	4.6539413451	-1.4809133641	0.4760775040
C16	-4.0894584893	1.9096616471	0.8121013564
C17	4.0492986819	5.1955673627	-4.6188127053
C18	-4.4259083588	-4.3619739349	4.8795279823
C19	4.9648061883	-0.1238722346	0.2836794901
C20	-5.2428558536	2.4929313826	0.2546140340
C21	-3.1767440477	-3.8278867232	4.5657218452
C22	2.8256889255	4.9861322208	-3.9847860801
C23	6.2574462336	0.2880178681	-0.0307257960

C24	-6.5115551013	2.1711760281	0.7213381462
C25	6.6825246227	7.4228833342	-5.7647526301
C26	-6.4836664923	-8.3054247816	4.2700378515
C27	6.3118528221	6.6047539953	-6.8082850521
C28	-6.3639639716	-7.8674792351	5.5724471685
C29	3.2924452830	-1.9585586666	0.8179015542
C30	-2.7317227283	2.3058971978	0.3621537717
C31	7.7618799793	3.7803712063	-3.7203388081
C32	-7.4853964819	-4.0550029401	3.8696784649
C33	7.1383126795	6.2680777288	-8.0395036741
C34	-7.4003830455	-7.9575021308	6.6735481521
C35	2.4685902042	-1.3032941694	1.7538689163
C36	-2.4995441566	3.5746945596	-0.2042107420
C37	7.1772152575	2.5006359181	-3.6746246326
C38	-7.0791172522	-3.4437945392	2.6664725940
C39	8.0012088664	4.9935183523	-7.8854445217
C40	-8.8703301832	-7.7841403213	6.2162478852
C41	1.2360613666	-1.8347660148	2.1299340662
C42	-1.2402815451	3.9617623279	-0.6415869353
C43	7.6503659172	1.5096963841	-2.8174939559
C44	-7.4359861620	-2.1343257035	2.3526440199
C45	8.6985872925	4.8490923050	-6.5498610456
C46	-9.0745360672	-6.6938572418	5.1748254216
C47	0.7637470802	-3.0437165974	1.5781229391
C48	-0.1304677217	3.1033624101	-0.5291074931
C49	8.7302934478	1.7526220641	-1.9503684844
C50	-8.2088029826	-1.3578799930	3.2346945469
C51	9.2137847551	5.8534957421	-5.7554919718
C52	-9.0478750809	-6.8573850739	3.8066503006
C53	1.5657910879	-3.6586653982	0.5983764218
C54	-0.3507475815	1.8500403217	0.0732572582

C55	9.3353638833	3.0191589977	-2.0139882137
C56	-8.6333540453	-1.9704741581	4.4263714198
C57	9.2498391743	7.3398485491	-6.0806271935
C58	-8.7412051701	-8.1252328550	3.0371216863
C59	2.8001171353	-3.1390241976	0.2361028389
C60	-1.6179363564	1.4558240847	0.4929742505
C61	8.8580263405	4.0131316411	-2.8690654395
C62	-8.2739363327	-3.2819619058	4.7416897758
C63	8.0125122716	8.1239242045	-5.5777424720
C64	-7.6734328297	-9.0473036702	3.6772128221
C65	-0.4878596389	-3.7060757224	1.9521266951
C66	1.2017473212	3.4637131571	-1.0306482492
C67	-8.6639066997	0.0093619777	2.9268565245
C68	-1.2236668176	-3.5245769197	3.0679552918
C69	1.4440070216	4.3215513093	-2.0440444517
C70	8.7202456686	-0.2793667714	-0.3728260278
C71	-8.0759976671	1.0273505327	2.2603234661
Pt72	7.0596774758	5.2572515136	-4.9373283482
Pt73	-6.9494970520	-5.9744993376	4.3368377222
H74	5.5042662302	-3.4627576370	0.5234997735
H75	7.7916841681	-2.7359270177	0.0009586827
H76	6.4592568382	1.3439675268	-0.1760681310
H77	4.1770831090	0.6201538403	0.3629414661
H78	7.1764309798	0.5328055664	-2.8189881256
H79	6.3241266972	2.2765969600	-4.3084908853
H80	9.3399360331	4.9874914361	-2.8477149729
H81	10.1859358699	3.2325591160	-1.3688074246
H82	8.7432668287	4.9485506845	-8.6973028523
H83	7.3602388364	4.1141525377	-8.0143874524
H84	7.7640269663	7.1209409159	-8.3142429147
H85	6.4533924619	6.1172976484	-8.8811183232

H86	9.3822974771	7.4836212863	-7.1563419356
H87	10.1402652937	7.7728805108	-5.6118971234
H88	8.1287236392	8.3180647781	-4.5058200609
H89	7.9790683721	9.1111804229	-6.0623900312
H90	9.8406601067	5.5337697201	-4.9278183340
H91	8.9852471863	3.8306204811	-6.2968228831
H92	5.8915406001	7.7573854979	-5.0971395170
H93	5.2622466985	6.3359333607	-6.8658257851
H94	6.0909038232	4.7756164925	-1.9486827434
H95	4.0313644959	5.3963247998	-5.6857371534
H96	1.9074123252	5.0385958718	-4.5670975511
H97	3.9466203571	4.4135376805	-0.8363660446
H98	0.5893356255	4.7578917361	-2.5606725792
H99	2.0391221098	2.9301062054	-0.5824897307
H100	0.4812185712	1.1574570864	0.1825768917
H101	-1.1050285488	4.9606771285	-1.0473203275
H102	-3.3146106086	4.2881977325	-0.2720153380
H103	-1.7450763441	0.4587043838	0.9050267959
H104	-5.1494782649	3.2031380836	-0.5605709501
H105	-7.3778424720	2.6614428981	0.2822877458
H106	-5.6594560284	-0.0951515241	3.0930380634
H107	-3.4295694726	0.5073180061	2.3181336499
H108	-9.2466604766	-1.4021787868	5.1237152413
H109	-8.6056439759	-3.6923777760	5.6928152359
H110	-6.4592496176	-3.9941937247	1.9653177375
H111	-7.1131181272	-1.7048489211	1.4090526389
H112	-8.1292630798	-9.6845211054	4.4399406843
H113	-7.3043749039	-9.7281434032	2.9025298920
H114	-8.3976730004	-7.8233505923	2.0415521090
H115	-9.6697108171	-8.6933306107	2.8764911304
H116	-9.4618719112	-6.0497554007	3.2071055007

H117	-9.4794624358	-5.7546136062	5.5412243901
H118	-9.4728649601	-7.5364738135	7.0970103985
H119	-9.2670927130	-8.7320122046	5.8425197444
H120	-7.1637258310	-7.1759704835	7.4042466091
H121	-7.2921064376	-8.9135071913	7.2081345458
H122	-5.3664975433	-7.5922883050	5.9074841073
H123	-5.5736871705	-8.3093242521	3.6750750866
H124	-4.7153490879	-6.5193909844	2.2729869232
H125	-4.9526654366	-3.9845351709	5.7516056824
H126	-2.7490718038	-3.0612584246	5.2099706381
H127	-2.5457042779	-5.5752630631	1.7235430165
H128	-0.8879390518	-2.7953178689	3.8046856891
H129	-0.8143470556	-4.4593368799	1.2371559111
H130	0.6345208545	-1.3077001401	2.8648204574
H131	2.8187766620	-0.3870789640	2.2224302028
H132	3.3914275686	-3.6459028282	-0.5214727616
H133	1.2131613442	-4.5743963126	0.1289280954
H134	-9.6694192222	0.2209789340	3.2933351020
H135	-8.7133009950	1.8974606691	2.0987788204
C136	9.2993577864	0.7304395785	-1.0558548699
H137	10.3826125378	0.8010036841	-0.9489262289
H138	9.4126304655	-0.9546761452	0.1310960798

III) TD-DFT calculations

1-CTCT

Restricted Singlet Excited State 1: 2.8403 eV 436.52 nm

excitation	X coeff.
186 => 191	-0.16190
187 => 190	0.18274

188 => 189 0.96605

Transition dipole moment (debye):

X= 0.0098 Y= 0.1461 Z= -0.1425 Tot= 0.2043

Oscillator strength, f= 0.0004

Restricted Singlet Excited State 2: 3.2182 eV 385.26 nm

excitation	X coeff.
187 => 189	-0.72095
188 => 190	0.68883

Transition dipole moment (debye):

X= -0.1162 Y= -0.4217 Z= 0.2625 Tot= 0.5101

Oscillator strength, f= 0.0032

Restricted Singlet Excited State 3: 3.3269 eV 372.67 nm

excitation	X coeff.
187 => 189	0.69020
188 => 190	0.72204

Transition dipole moment (debye):

X= 10.2379 Y= 5.5929 Z= -9.0027 Tot= 14.7358

Oscillator strength, f= 2.7396

Restricted Singlet Excited State 4: 3.4178 eV 362.76 nm

excitation	X coeff.
186 => 191	0.15104
187 => 190	-0.95731
188 => 189	0.21595

Transition dipole moment (debye):

X= 0.1937 Y= 0.2298 Z= -0.1215 Tot= 0.3242

Oscillator strength, f= 0.0014

Restricted Singlet Excited State 5: 3.4871 eV 355.55 nm

excitation	X coeff.
186 => 189	-0.93223
188 => 191	0.34275

Transition dipole moment (debye):

X= 4.0878 Y= -5.7778 Z= 0.3970 Tot= 7.0888

Oscillator strength, f= 0.6645

Restricted Singlet Excited State 6: 3.5421 eV 350.03 nm

excitation X coeff.

---

186 => 189 -0.33862

188 => 191 -0.92991

Transition dipole moment (debye):

X= -1.2592 Y= 3.0727 Z= -0.7642 Tot= 3.4075

Oscillator strength, f= 0.1560

Restricted Singlet Excited State 7: 3.6556 eV 339.16 nm

excitation X coeff.

---

186 => 190 0.75679

187 => 191 0.64193

Transition dipole moment (debye):

X= 0.0907 Y= 0.0653 Z= -0.0913 Tot= 0.1443

Oscillator strength, f= 0.0003

Restricted Singlet Excited State 8: 3.8689 eV 320.47 nm

excitation X coeff.

---

184 => 189 -0.10011

186 => 190 0.63799

187 => 191 -0.75048

Transition dipole moment (debye):

X= 0.1247 Y= -0.0390 Z= 0.0121 Tot= 0.1312

Oscillator strength, f= 0.0003

Restricted Singlet Excited State 9: 3.9563 eV 313.38 nm

excitation	X coeff.
185 => 189	-0.77586
188 => 192	0.61470

Transition dipole moment (debye):

X= -0.0200 Y= -0.0135 Z= 0.0375 Tot= 0.0445

Oscillator strength, f= 0.0000

Restricted Singlet Excited State 10: 4.0846 eV 303.54 nm

excitation	X coeff.
186 => 191	0.95152
187 => 190	0.19080
188 => 189	0.13273

Transition dipole moment (debye):

X= -0.1672 Y= 0.1130 Z= -0.1874 Tot= 0.2754

Oscillator strength, f= 0.0012

Restricted Singlet Excited State 11: 4.1290 eV 300.28 nm

excitation	X coeff.
185 => 189	0.59212
186 => 191	-0.15709
188 => 192	0.74631

Transition dipole moment (debye):

X= -0.0397 Y= -0.0362 Z= -0.1542 Tot= 0.1633

Oscillator strength, f= 0.0004

Restricted Singlet Excited State 12: 4.1668 eV 297.55 nm

excitation	X coeff.
184 => 191	-0.12701
185 => 190	0.75230
187 => 192	-0.60436

Transition dipole moment (debye):

X= 0.4607 Y= 0.6108 Z= -0.3975 Tot= 0.8621

Oscillator strength, f= 0.0117

Restricted Singlet Excited State 13: 4.1733 eV 297.09 nm

excitation	X coeff.
184 => 189	0.82246
188 => 193	0.52525

Transition dipole moment (debye):

X= 0.0298 Y= 0.0246 Z= 0.0082 Tot= 0.0395

Oscillator strength, f= 0.0000

Restricted Singlet Excited State 14: 4.2773 eV 289.87 nm

excitation	X coeff.
177 => 189	-0.18238
178 => 190	-0.12704
179 => 189	0.17597
179 => 190	0.11708
180 => 190	-0.12601
182 => 191	0.10620
183 => 189	-0.23584
185 => 190	-0.44066
186 => 194	-0.15250
187 => 192	-0.39279
187 => 197	0.20834
187 => 198	0.15869
188 => 194	-0.45500

188 => 195 0.16521

188 => 196 0.21541

Transition dipole moment (debye):

X= -0.9144 Y= -1.0727 Z= 0.8660 Tot= 1.6543

Oscillator strength, f= 0.0444

Restricted Singlet Excited State 15: 4.3002 eV 288.32 nm

excitation	X coeff.
178 => 189	0.11579
178 => 190	-0.14599
179 => 189	-0.15004
180 => 189	-0.10124
182 => 189	-0.36538
183 => 189	-0.17310
183 => 191	0.18239
185 => 190	0.23566
186 => 194	-0.21673
186 => 195	0.10093
187 => 192	0.29251
187 => 198	-0.18947
188 => 194	-0.47642
188 => 195	-0.33765
188 => 196	-0.16517
188 => 199	0.14685

Transition dipole moment (debye):

X= 0.7864 Y= 0.8412 Z= -0.7680 Tot= 1.3842

Oscillator strength, f= 0.0312

2-CCCC

Restricted Singlet Excited State 1: 2.8726 eV 431.61 nm

excitation	X coeff.
186 => 191	0.17886
187 => 190	-0.20258
188 => 189	-0.96033

Transition dipole moment (debye):

X= 0.4966 Y= 0.8011 Z= 0.3765 Tot= 1.0150

Oscillator strength, f= 0.0112

Restricted Singlet Excited State 2: 3.3594 eV 369.07 nm

excitation	X coeff.
187 => 189	0.98257
188 => 190	0.15357

Transition dipole moment (debye):

X= -2.2058 Y= 6.7296 Z= -5.2988 Tot= 8.8448

Oscillator strength, f= 0.9966

Restricted Singlet Excited State 3: 3.3939 eV 365.32 nm

excitation	X coeff.
187 => 189	0.14930
188 => 190	-0.98171

Transition dipole moment (debye):

X= 1.6217 Y= -4.8554 Z= 3.8698 Tot= 6.4172

Oscillator strength, f= 0.5300

Restricted Singlet Excited State 4: 3.4228 eV 362.23 nm

excitation	X coeff.
186 => 189	-0.99138

Transition dipole moment (debye):

X= -4.2468 Y= -5.0302 Z= -4.5157 Tot= 7.9831

Oscillator strength, f= 0.8272

Restricted Singlet Excited State 5: 3.4528 eV 359.08 nm

excitation	X coeff.
188 => 191	-0.99068

Transition dipole moment (debye):

X= 3.6856 Y= 4.3812 Z= 3.9015 Tot= 6.9282

Oscillator strength, f= 0.6285

Restricted Singlet Excited State 6: 3.6298 eV 341.57 nm

excitation	X coeff.
186 => 191	0.41344
187 => 190	-0.86567
188 => 189	0.26353

Transition dipole moment (debye):

X= -0.3316 Y= -0.8068 Z= -0.3852 Tot= 0.9535

Oscillator strength, f= 0.0125

Restricted Singlet Excited State 7: 3.6534 eV 339.37 nm

excitation	X coeff.
186 => 190	0.69280
187 => 191	0.70700

Transition dipole moment (debye):

X= 0.1092 Y= 0.2048 Z= 0.0975 Tot= 0.2517

Oscillator strength, f= 0.0009

Restricted Singlet Excited State 8: 3.8439 eV 322.55 nm

excitation	X coeff.
186 => 190	0.14667
186 => 191	-0.86605
187 => 190	-0.43211
187 => 191	-0.14592

Transition dipole moment (debye):

X= -0.0124 Y= 0.9090 Z= -0.7149 Tot= 1.1565

Oscillator strength, f= 0.0195

Restricted Singlet Excited State 9: 3.8805 eV 319.50 nm

excitation	X coeff.
184 => 189	0.15188
185 => 189	-0.10290
186 => 190	-0.68204
186 => 191	-0.17536
187 => 190	-0.10529
187 => 191	0.66577

Transition dipole moment (debye):

X= -0.9055 Y= -1.5476 Z= -0.0330 Tot= 1.7934

Oscillator strength, f= 0.0473

Restricted Singlet Excited State 10: 4.0253 eV 308.01 nm

excitation	X coeff.
184 => 189	-0.10934
185 => 189	0.84404
188 => 192	-0.47354
188 => 193	-0.14094

Transition dipole moment (debye):

X= -0.1475 Y= 0.0432 Z= 0.1591 Tot= 0.2213

Oscillator strength, f= 0.0007

Restricted Singlet Excited State 11: 4.0904 eV 303.11 nm

excitation	X coeff.
184 => 189	-0.82262
185 => 189	-0.16233
188 => 193	-0.49938

Transition dipole moment (debye):

X= -0.0248 Y= 0.1468 Z= 0.0765 Tot= 0.1674

Oscillator strength, f= 0.0004

Restricted Singlet Excited State 12: 4.2012 eV 295.12 nm

excitation	X coeff.
185 => 189	0.46015
188 => 192	0.83330
188 => 193	-0.14989

Transition dipole moment (debye):

X= -0.4385 Y= 0.3478 Z= 0.1817 Tot= 0.5885

Oscillator strength, f= 0.0055

Restricted Singlet Excited State 13: 4.2360 eV 292.69 nm

excitation	X coeff.
181 => 191	-0.17149
182 => 189	0.38367
182 => 190	-0.21287
183 => 189	0.33600
183 => 190	0.10899
186 => 196	0.20579
187 => 194	0.13901
187 => 195	0.26177
188 => 194	-0.64944
188 => 196	-0.15250

Transition dipole moment (debye):

X= 0.0116 Y= 0.1527 Z= -0.0639 Tot= 0.1659

Oscillator strength, f= 0.0004

Restricted Singlet Excited State 14: 4.2676 eV 290.52 nm

excitation	X coeff.
179 => 191	-0.10797
180 => 190	-0.13819
182 => 189	-0.35249
183 => 189	0.38827
183 => 190	0.27583
186 => 198	0.12153
187 => 194	-0.30827
187 => 195	0.14648
187 => 197	-0.13513
188 => 195	0.60040

Transition dipole moment (debye):

X= -0.0557 Y= -0.0511 Z= 0.2039 Tot= 0.2174

Oscillator strength, f= 0.0008

Restricted Singlet Excited State 15: 4.3043 eV 288.05 nm

excitation	X coeff.

179 => 190 -0.13611

180 => 189 0.13841

180 => 191 0.15447

181 => 189 -0.51099

182 => 191 0.15288

183 => 191 0.16615

184 => 190 -0.11453

186 => 194 0.28813

186 => 197 -0.12078

187 => 195 -0.12450

187 => 198 -0.15483

188 => 194 0.10671

188 => 196 -0.56707

188 => 197 0.13707

Transition dipole moment (debye):

X= -0.1760 Y= 0.0222 Z= 0.0006 Tot= 0.1774

Oscillator strength, f= 0.0005

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