Supplementary Information for:

"Dual molecular tweezers extending from a nanohoop"

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Experimental section

General considerations. Manipulations involving air sensitive reactions were performed under an atmosphere of dry, oxygen-free N_2 by means of standard Schlenk or glovebox techniques (MBraun glovebox equipped with a –35 °C freezer). All glassware was oven dried for a minimum of 10 h and cooled in an evacuated antechamber prior to use in the drybox. Anhydrous and anaerobic tetrahydrofuran (THF), diethyl ether (Et_2O), hexanes, dimethylformamide (DMF), and 1,4-dioxane were dried and deoxygenated on dual high-performance columns within a Glass Contour 800L Solvent Purification System and stored over 4 Å molecular sieves prior to use. Chemicals and solvents were purchased from commercial suppliers and used as received.

^{1}H- and ^{13}C- nuclear magnetic resonance (NMR) spectra were obtained on any of the following instruments: a) Bruker Avance 400 spectrometer at 400 and 100 MHz b) Bruker Avance 500 spectrometer at 500 and 125 MHz and c) Bruker Avance 600 spectrometer at 600 and 150 MHz, respectively. Chemical shifts for protons are reported in parts per million (ppm) downfield from tetramethylsilane (TMS) and are referenced to residual protium in the NMR solvent ($CHCl_3$: δ 7.26; CH_2Cl_2: δ 5.32). Chemical shifts for carbon are reported in ppm downfield from TMS and are referenced to the carbon resonances of the solvent ($CHCl_3$: δ 77.2 and CH_2Cl_2: δ 54.0). Data are presented as follows: chemical shift, multiplicity (s = singlet, d = doublet, t = triplet, m = multiplet, br = broad), coupling constants in Hertz, and integration.

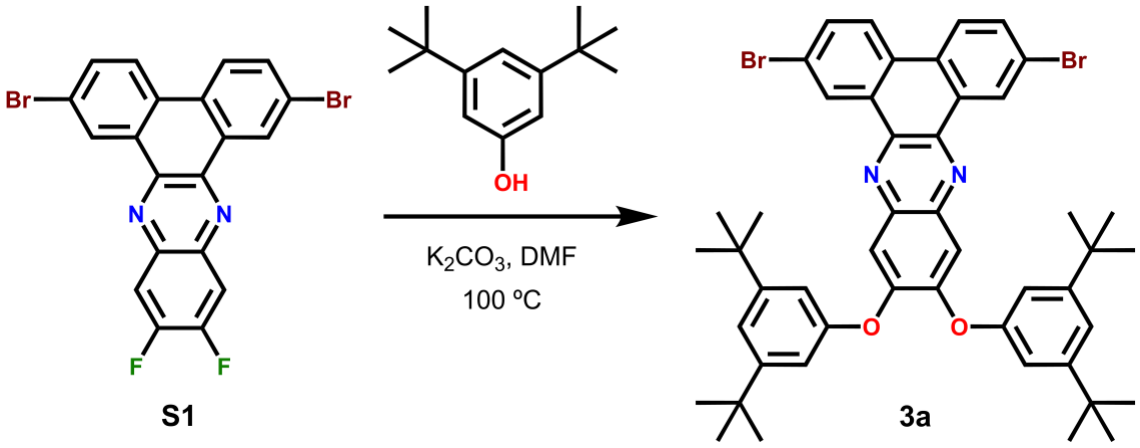
High-resolution mass spectrometry (HRMS) was performed on a (1) Thermo Scientific Q-Exactive Oribtrap instrument equipped with a Dionex Ultimate 3000 (RSLC) inlet system, and electrospray (ESI) and atmospheric pressure chemical (APCI) ionization sources; or (2) a Bruker Daltonics UltrafleXtreme MALDI TOF/TOF MS instrument using dithranol (DIT) matrix.
Absorption spectra were obtained on a Cary 60 UV-Vis spectrophotometer and emission spectra were recorded in an Agilent Cary Eclipse Fluorescence spectrophotometer.

Quantum yield determination. Fluorescence quantum yields of the molecules **1** and **3b** were determined using the relative method as described by Williams and co-workers.[1]

$$\phi_x = \phi_r \times \frac{\mathrm{Grad}_x}{\mathrm{Grad}_r} \times \frac{\eta_x^2}{\eta_r^2}$$

Where ϕ is the quantum yield, x stands for the measured sample, and r for the standard fluorescent compound, Grad (gradient) is the slope of the fitted line in the integrated emission area vs absorption plots $\left(\text{Grad} = \frac{E}{A}\right)$, and η is the refractive index of the solvent. About five solutions in dichloromethane of each compound were prepared with absorption values ranging from 0.01 to 0.1 at 400 nm. Fluorescence data was collected using 400 nm as the excitation wavelength. The same procedure was used for the standard fluorophore (Coumarin 153, C153). Gradient plots are shown in Figure S15. The quantum yield of coumarin 153 (0.544) was obtained from the literature and data herein was collected in anhydrous ethanol (η = 1.36).[2] For molecules **1** and **3b**, anhydrous DCM (η = 1.42) has been use as the solvent.

Synthetic details.

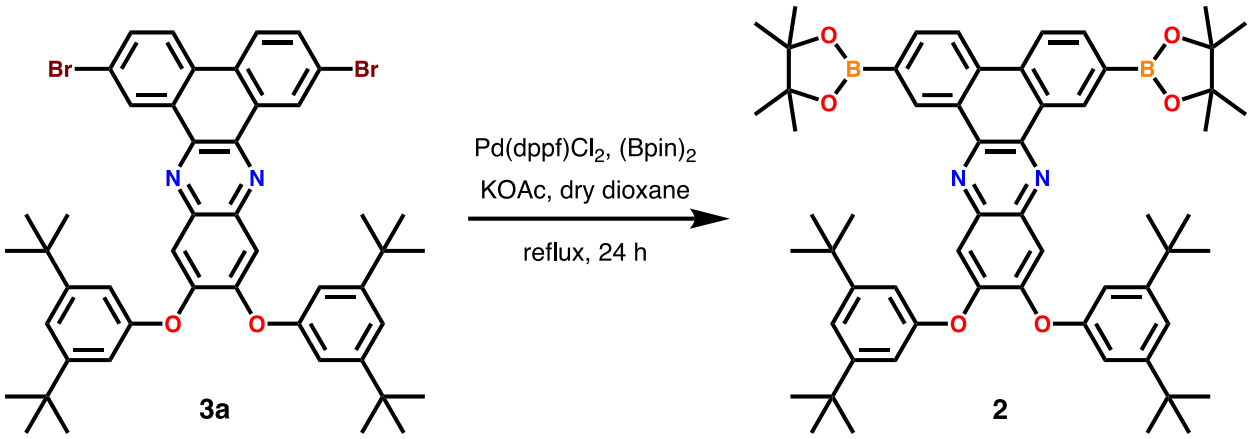


Compound **3a**. Compound **S1** was prepared according to the reported procedure.[3] A 500 mL round bottom flask was loaded with 1.5 g of **S1** (3.18 mmol), 1.6 g of 3,5-di-*tert*-butylphenol (7.9 mmol, 2.5 eq), and 5.0 g of K_2CO_3 in 200 mL of DMF. The reaction mixture was stirred vigorously at 100 °C for ~16 h. Then, the reaction mixture was cooled down to room temperature and 250 mL DI water was added to the flask and stirred for 5 min. The precipitate was filtered and washed with copious amounts of DI water. Subsequently, the pure product (light yellow solid) was obtained by washing the precipitate with 300 mL of MeOH. Yield: 93% (2.7 g, 3.2 mmol).

^{1}H NMR (400 MHz, $CDCl_3$, 20 °C): 9.29 (d, J = 2.2 Hz, 1H), 8.24 (d, J = 8.7 Hz, 1H), 7.75 (dd, J = 6.4 and 2.2 Hz, 1H), 7.50 (s, 1H), 7.38 (t, J = 1.6 Hz, 1H), 7.17 (d, J = 1.6 Hz, 2H), and 1.39 (s, 18H).

^{13}C NMR (100 MHz, $CDCl_3$, 20 °C): 154.6, 153.9, 153.4, 140.4, 139.4, 132.7, 131.9, 129.5, 128.5, 124.6, 122.7, 119.5, 115.1, 112.0, 35.3, and 31.7.

HRMS (APCI), $C_{48}H_{50}Br_2N_2O_2$, $[M+H]^+$ calc.: 845.2312; exp.: 845.2319.

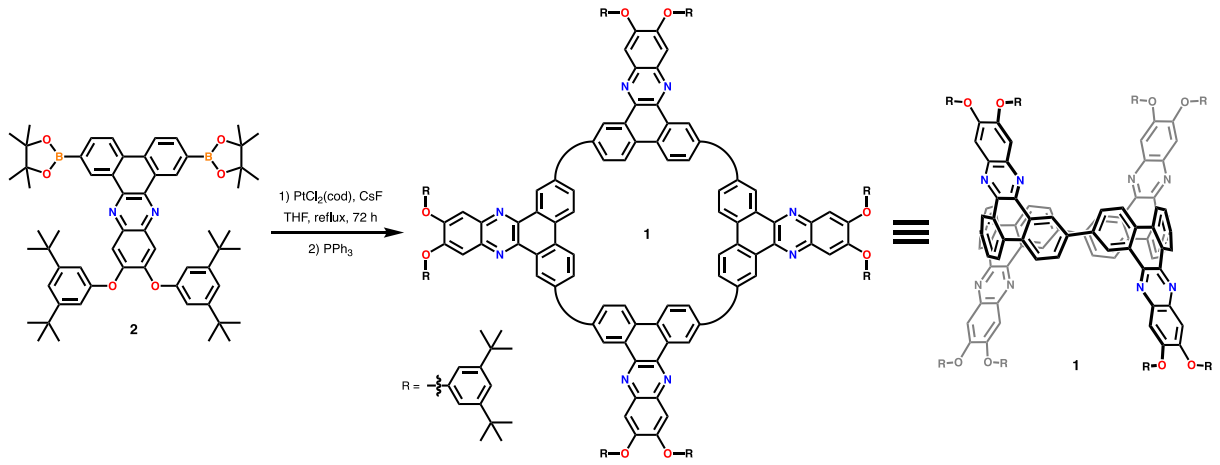


Compound **2**. A 250 mL Pyrex Schlenk flask was loaded with 1.5 g of **3a** (1.8 mmol), 0.9 g of bis(pinacolato)diboron (3.9 mmol, 2.2 eq), and 1.5 g of KOAc. The flask was left under high vacuum for 4 hours at room temperature. The flask was then back filled with nitrogen gas. Around 0.13 g (10% mmol) of $Pd(dppf)Cl_2$ and 100 mL of dry dioxane was added to the flask. The solution was degassed for an additional 10 minutes while gradually increasing the temperature to reflux. Then, the reaction mixture was refluxed under N_2 for 24 h. The solvent was removed under vacuum and the black solid was passed through a pack of silica gel using pure DCM. The DCM was removed, and the pure final product (light yellow solid) was obtained after washing with MeOH. Yield: 64% (1.1 g, 1.1 mmol).

^{1}H NMR (400 MHz, $CDCl_3$, 20 °C): 9.70 (d, J = 0.7 Hz, 1H), 8.59 (d, J = 8.2 Hz, 1H), 8.16 (dd, J = 7.0 and 1.0 Hz, 1H), 7.66 (s, 1H), 7.38 (t, J = 1.5 Hz, 1H), 7.16 (d, J = 1.5 Hz, 2H), 1.42 (s, 12H), and 1.39 (s, 18H).

^{13}C NMR (100 MHz, $CDCl_3$, 20 °C): 155.0, 153.2, 153.0, 141.0, 140.1, 135.5, 133.8, 132.8, 130.2, 128.7, 122.6, 119.3, 115.0, 112.9, 84.2, 35.3, 31.7, and 25.1.

HRMS (APCI), $C_{60}H_{74}B_2N_2O_6$, $[M+H]^+$ calc.: 941.5806; exp.: 941.5865.

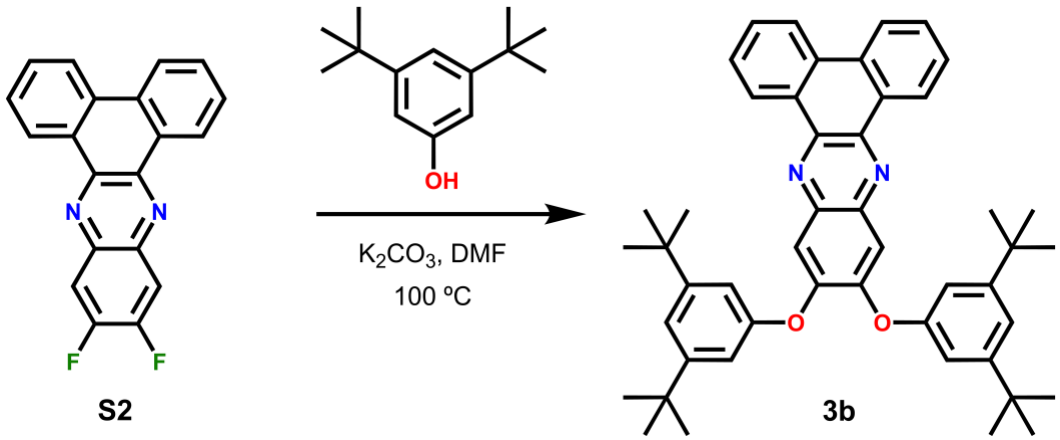


Compound **1**. A 150 mL pressure flask inside the nitrogen filled glovebox, containing a magnetic stirring bar was added **2** (0.3 g, 0.3 mmol), CsF (0.9 g, 20 eq), $Pt(cod)Cl_2$ (0.12 g, 0.33 mmol, 1.1 eq) and anhydrous THF (60 mL). Then the mixture was stirred at 80 °C for 48 hours. After cooling down to room temperature, the solvent was removed under high vacuum. Anhydrous toluene (50 mL) and triphenylphosphine (1.0 g, 4.0 mmol, 40 eq) were added to this brown solid material. The mixture was stirred at 120 °C for 24 hours. After the reaction mixture was cooled down to room temperature, the solvent was removed and the brown solid was washed with MeOH to remove CsF and PPh_3. The crude product was purified by silica gel column chromatography using a gradient of 40-80% DCM in hexanes. The final product (yellowish-orange solid) was purified further by prep-TLC using 50% DCM in hexanes.

From preparatory TLC, the orange band was scrapped off, filtered, and washed with DCM. The solvent was removed and the resulting orange solid was crystallized by slow diffusion of acetonitrile into a 1:1 solution of **1** in DCM:*ortho*-dichlorobenzene (*o*DCB). Yield: 9% (19 mg, 0.007 mmol)

^{1}H NMR (400 MHz, CD_2Cl_2, 20 °C): 8.77 (d, J = 1.7 Hz, 1H), 8.24 (dd, J = 7.3 and 1.7 Hz, 1H), 8.10 (d, J = 9.0 Hz, 1H), 7.57 (s, 1H), 7.42 (s, 1H), 7.14 (d, J = 1.5 Hz, 2H), and 1.41 (s, 18H).
^{13}C NMR (100 MHz, CD_2Cl_2, 20 °C): 155.4, 153.8, 153.1, 142.6, 150.5, 136.4, 131.8, 130.5, 126.8, 124.3, 119.6, 114.8, 113.5, 35.5, and 31.7.

^{1}H NMR (400 MHz, 1,1,2,2-tetrachloroethane-d_2, 20 °C): 8.53 (d, J = 8.9 Hz, 1H), 8.29 (d, J = 8.9, 1H), 8.14 (d, J = 9.1, 1H), 7.60 (s, 1H), 7.41 (s, 1H), 7.15 (s, 2H), and 1.44 (s, 18H).
HRMS (APCI), $C_{192}H_{200}N_8O_8$, $[M+H]^+$ calc.: 2746.5561; exp.: 2746.5557.



Compound **3b**. Compound **S2** has previously been reported.[4] A 500 mL round bottom flask was loaded with 0.5 g of **S2** (1.6 mmol), 0.7 g of 3,5-di-*tert*-butylphenol (3.47 mmol, 2.2 eq), and 0.9 g of K_2CO_3 in 100 mL of DMF. The reaction mixture was stirred vigorously at 100 °C for ~16 hours. Then, the reaction mixture was cooled down to room temperature and 250 mL DI water was added to the flask and stirred for 5 min. The precipitate was filtered and washed with copious amounts of DI water. Subsequently, the pure product (light yellow solid) was obtained by washing the precipitate with 300 mL of MeOH. Yield: 70% (0.7 g, 1.0 mmol).

^{1}H NMR (500 MHz, $CDCl_3$, 20 °C): 9.31 (d, J = 7.9 Hz, 1H), 8.56 (d, J = 8.0 Hz, 1H), 7.76 (t, J = 7.0 Hz, 1H), 7.70 (t, J = 7.7 Hz, 1H), 7.63 (s, 1H), 7.35 (s, 1H), 7.14 (d, J = 1.5 Hz, 2H), and 1.37 (s, 18H).

^{13}C NMR (125 MHz, $CDCl_3$, 20 °C): 154.9, 155.3, 153.3, 140.8, 139.9, 131.8, 130.2, 130.0, 128.0, 126.1, 123.0, 119.3, 115.0, 112.4, 35.3, and 31.6.

HRMS (APCI), $C_{48}H_{52}N_2O_2$, $[M+H]^+$ calc.: 689.4102; exp.: 689.4105.

Single crystal data for **1** was collected on a Rigaku Synergy-S diffractometer equipped with dual-beam microfocus Cu Kα and Mo Kα X-ray radiation sources paired with a Rigaku's HyPix-Arc150 detector. Temperature was maintained using an Oxford Cryosystem nitrogen flow apparatus. Single crystals suitable for X-ray structure analysis were coated with Paratone N-oil and mounted on MiTeGen Kapton loops (polyimide). Data from Rigaku's diffractometer was integrated and corrected using CrysAlisPro V42. Space group assignments were determined by examination of systematic absences, E-statistics, and successive refinement of the structures. The program PLATON[5-6] was employed to confirm the absence of higher symmetry in the crystal. The positions of the heavy atoms were determined using intrinsic phasing methods using the program SHELXT[7] and SHELXL[8] with Olex2[9] interface. Successive cycles of least-square refinement followed by difference Fourier syntheses revealed the positions of the remaining non-hydrogen atoms. Non-hydrogen atoms were refined with anisotropic displacement parameters, and hydrogen atoms were added in idealized positions. Crystallographic data for **1** is given in Table S1.

The crystal structure of **1** contains at least 8 well-defined molecules of *o*DCB. A region of electron density contains is observed in the structure that may contain heavily disorder DCM, *o*DCB, or MeCN (solvents used during crystallization). Thus, a solvent mask was used to facilitate the structure modeling (solvent r = 1.2 Å and truncation = 1.2 Å). All *tert*-butyl groups present disorder, therefore C–C distances within this group where restrained.

Computational details. All calculations were carried out using Gaussian 16 software package.[10] B3LYP[11] functional of density functional theory (DFT) is used for all optimizations and subsequent studies of neutral molecules. The frequency calculations were carried out for optimized structures to ensure the absence of any imaginary frequencies for the ground state molecules. In order to include the dispersion effects, the D3 version of Grimme with Becke-Johnson damping factors (D3BJ) were used.[12] The implicit solvation effects were included using the polarizable continuum model (PCM) with standard parameters of CH_2Cl_2.[13] The gauge-independent atomic orbital (GIAO) method[14] was used for ^{1}H NMR chemical shift calculations. The DFT calculated ^{1}H NMR chemical shifts assisted in assigning the experimental spectra. In order to decrease the computational costs, the solubilizing groups (3,5-di-*tert*-butylphenyl) were replaced with methyl groups. For complete structures, the atoms comprising the 3,5-di-*tert*-butylphenyl groups were

fixed and their positions frozen during geometry optimization and followed by analytical frequency calculations performed at 3–21G(d) basis set. The optimized geometry of **1** complexed with two molecules of C_{60} was further used to generate the wavefunction file for the visualization of weak interactions based on the independent gradient model using Hirshfeld partition of molecular density (IGMH) method.[15] The isosurface map was rendered by VMD 1.9.3 program[16] based on the cube files generated by MultiWFN 3.8.[17]

Table S1. Crystallographic data for compound **1**.

	1
CCDC Number	2385495
Chemical formula	$C_{192}H_{200}N_8O_8 \cdot 8(C_6H_4Cl_2)$
Formula weight	3923.52
Space group	*P–1*
***a* (Å)**	14.7048(4)
***b* (Å)**	23.2163(8)
***c* (Å)**	32.0917(9)
***α* (deg)**	81.364(3)
***β* (deg)**	79.536(2)
***γ* (deg)**	89.251(2)
***V* (Å^3)**	10650.3(6)
Z	2
μ (mm^{-1})	2.36
T (K)	100
R_{int}	0.079
***R*1[a] (*wR*2[b])**	0.279 (0.667)
Reflections	41997
Radiation type	Cu *Kα*

[a]$R1 = [\Sigma w(F_o - F_c)^2/\Sigma wF_o^2]^{1/2}$; [b]$wR2 = [\Sigma[w(F_o^2 - F_c^2)^2]/\Sigma w(F_o^2)^2]^{1/2}]$, $w = 1/[\sigma^2(F_o^2) + (aP)^2 + bP]$, where $P = [\max(F_o^2,0) + 2(F_c^2)]/3$

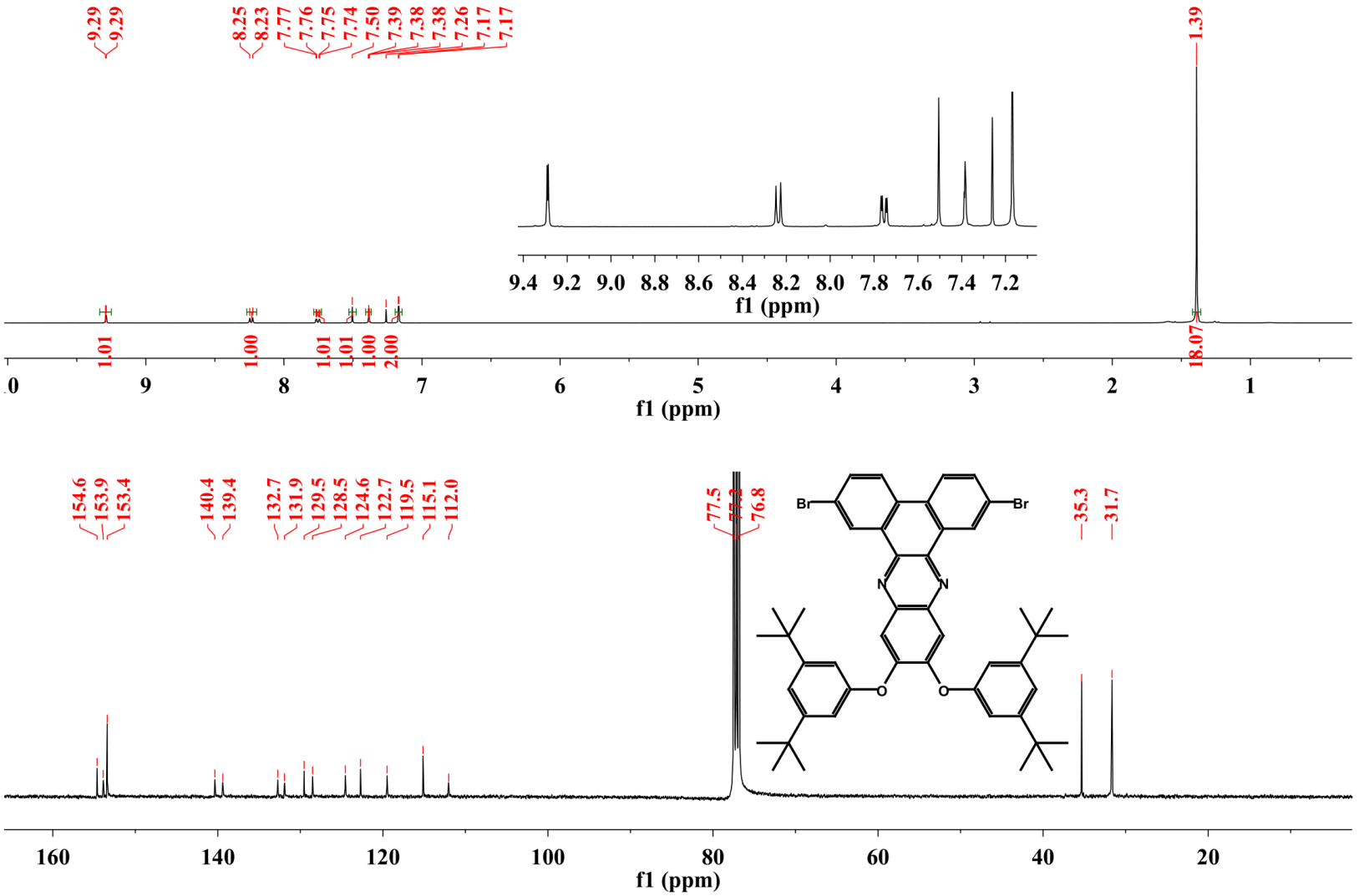


Figure S1. ^{1}H and ^{13}C NMR spectra of **3a**. Data collected in $CDCl_3$ at 20 ºC.

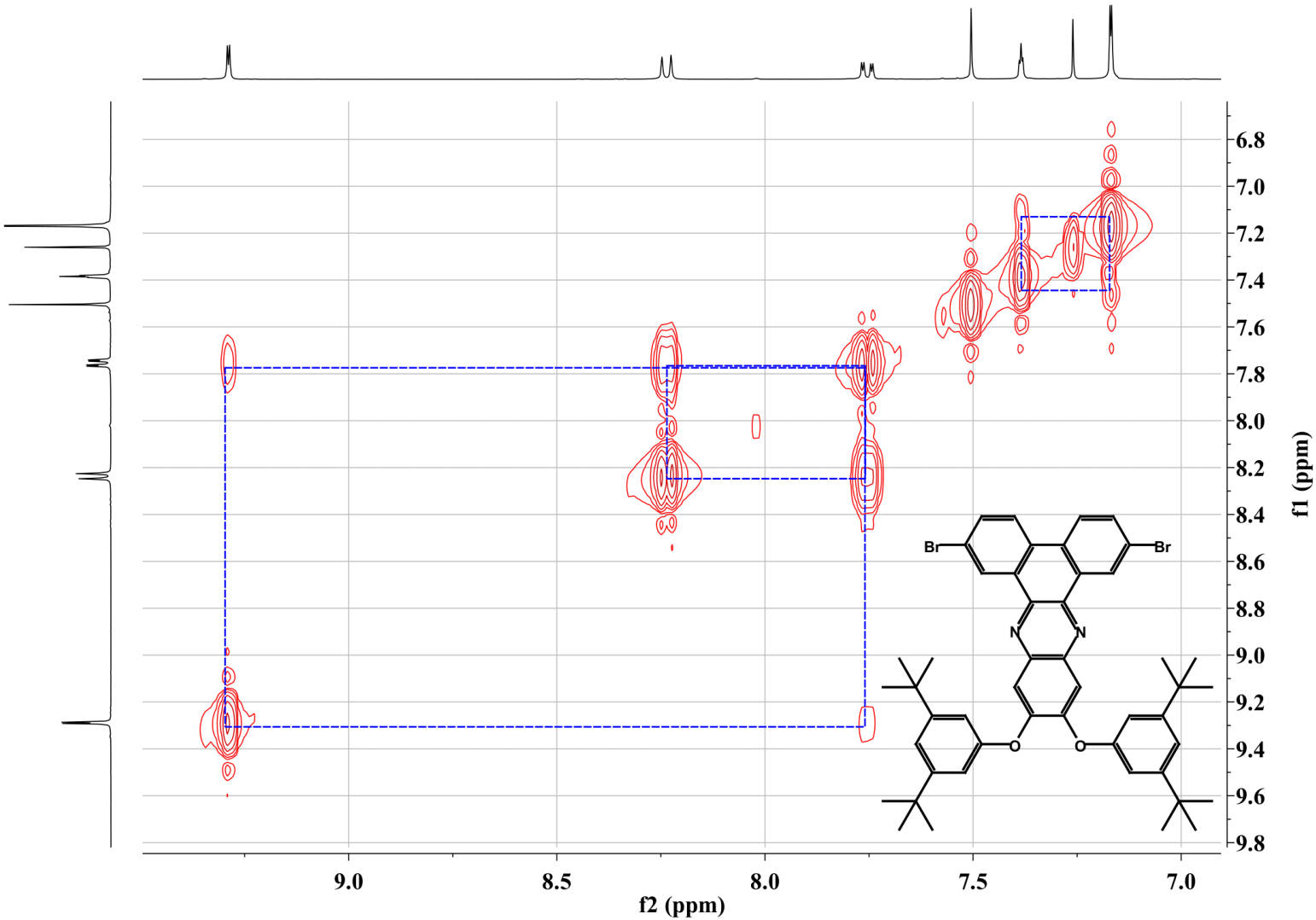


Figure S2. COSY NMR spectrum of **3a**. Data collected in $CDCl_3$ at 20 ºC.

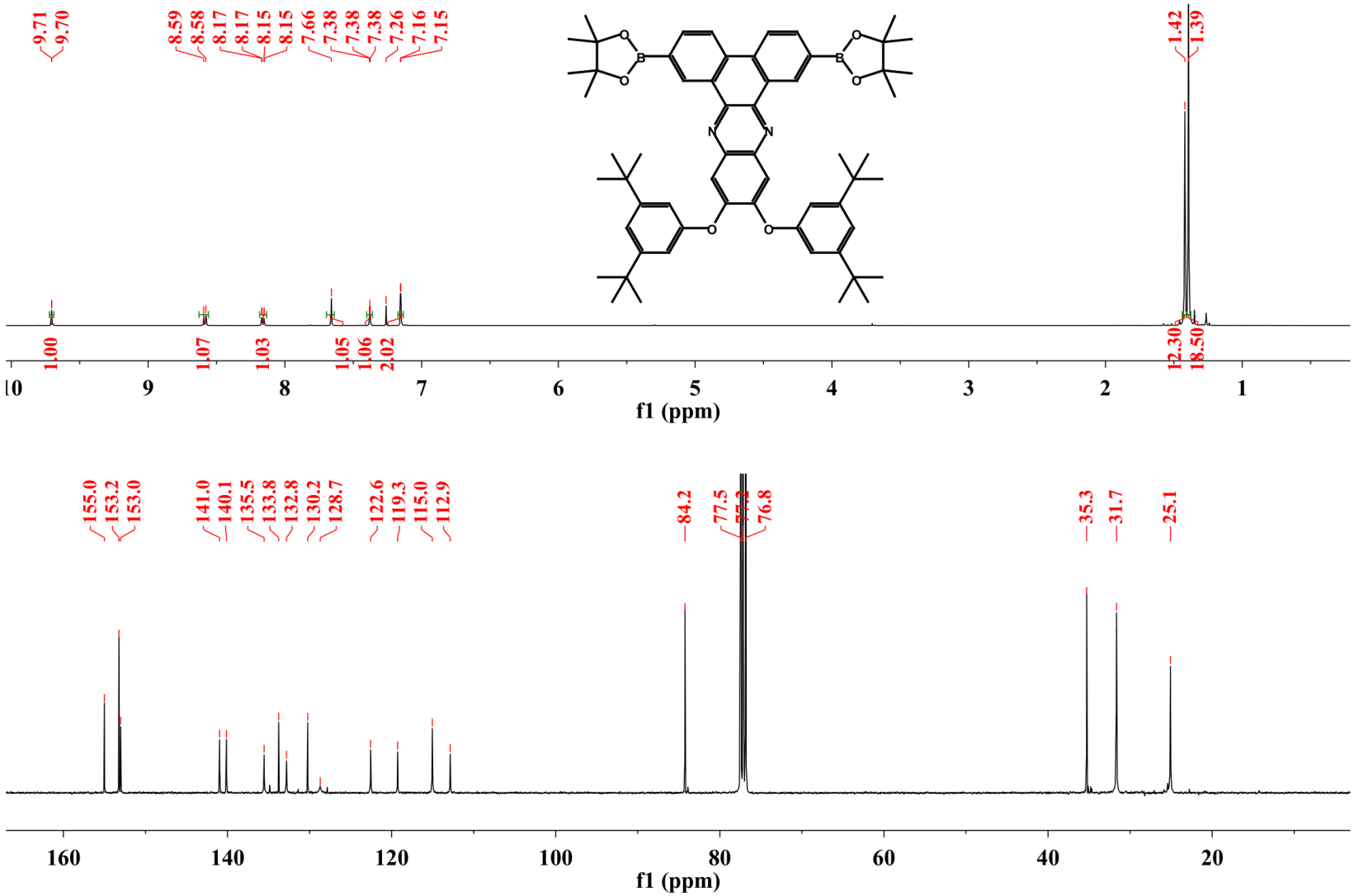


Figure S3. ^{1}H and ^{13}C NMR spectra of **2**. Data collected in $CDCl_3$ at 20 ºC.

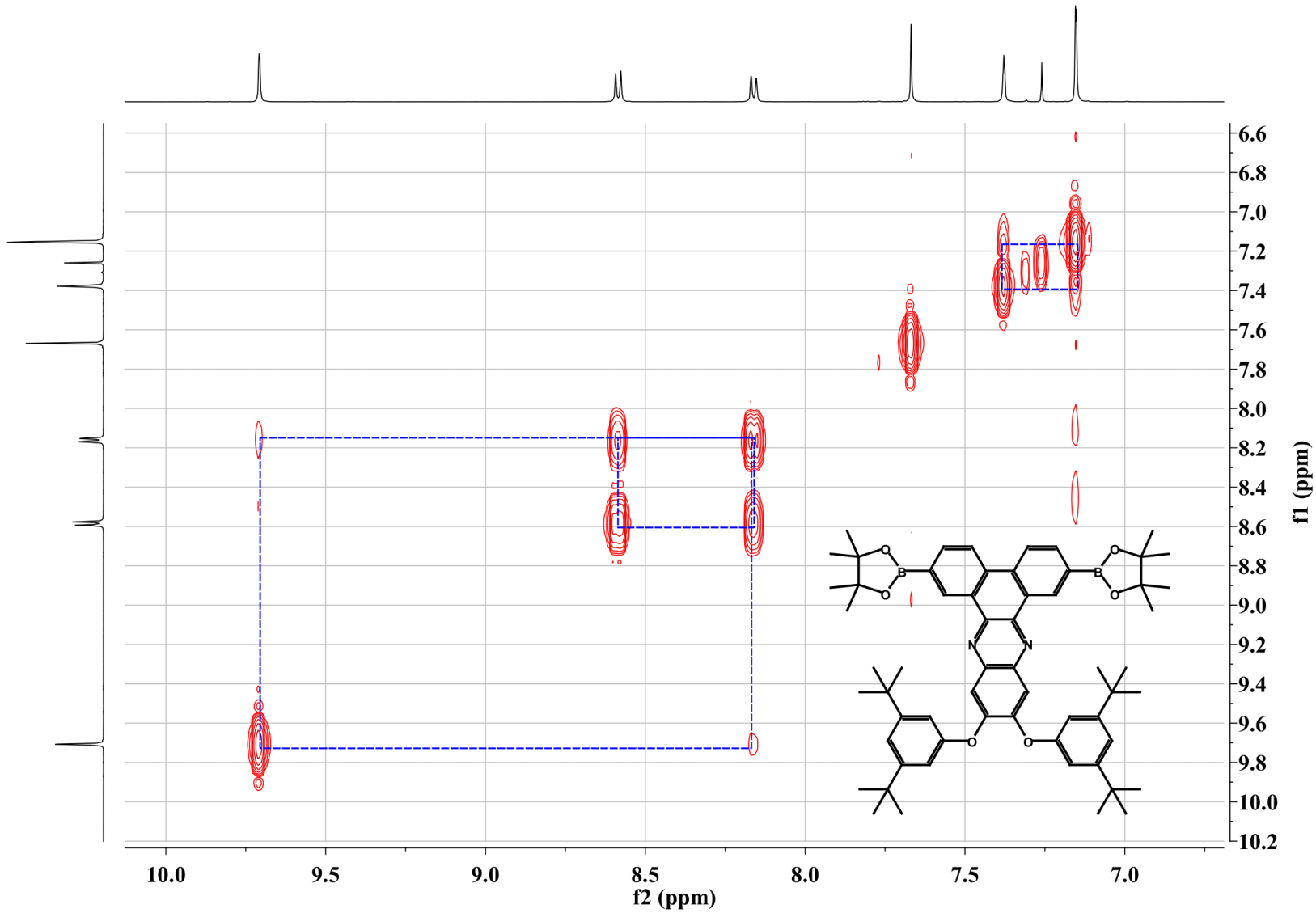


Figure S4. COSY NMR spectrum of **2**. Data collected in $CDCl_3$ at 20 ºC.

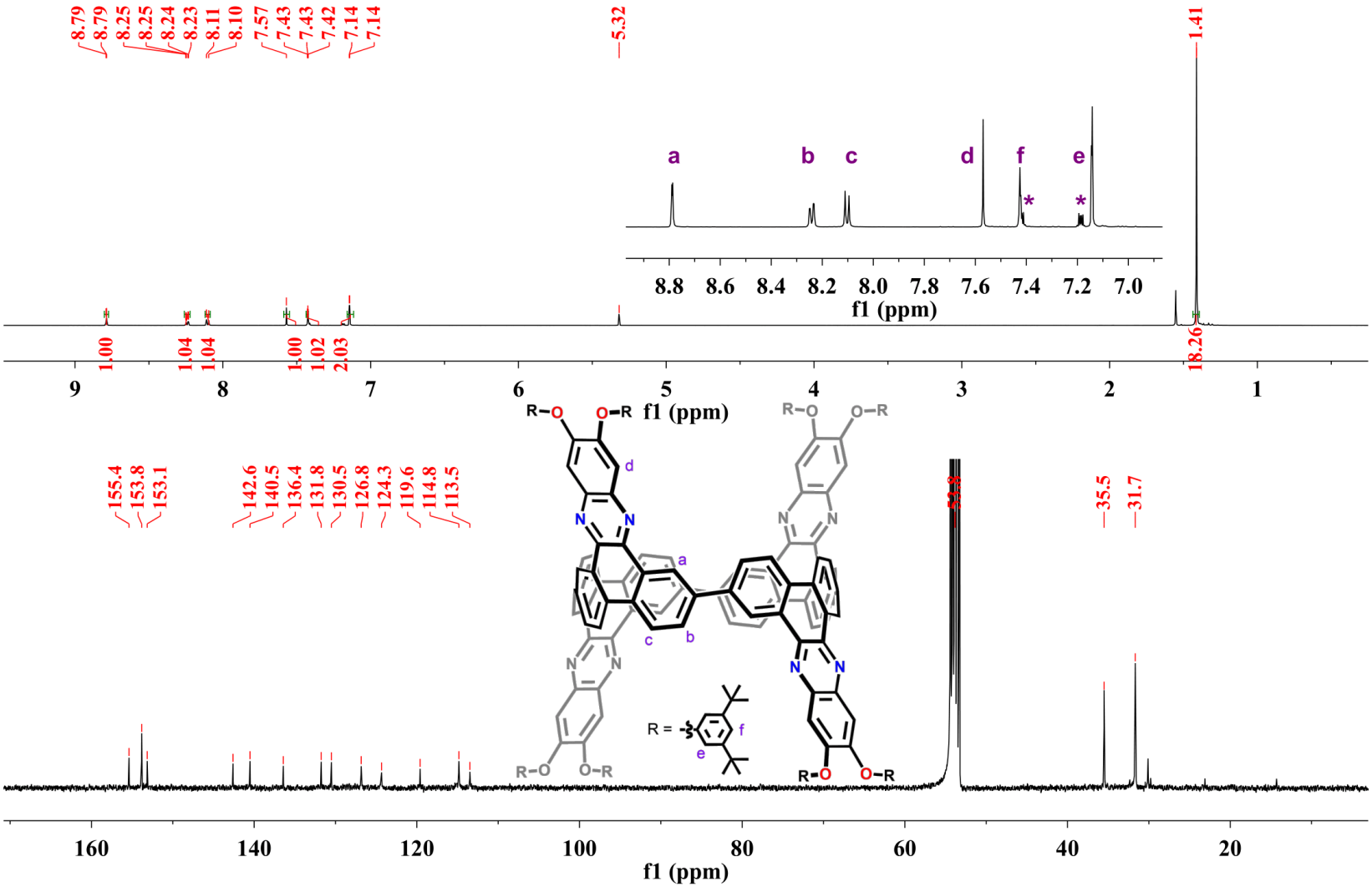


Figure S5. ^{1}H and ^{13}C NMR spectra of **1**. Data collected in CD_2Cl_2 at 20 ºC (* = *o*DCB).

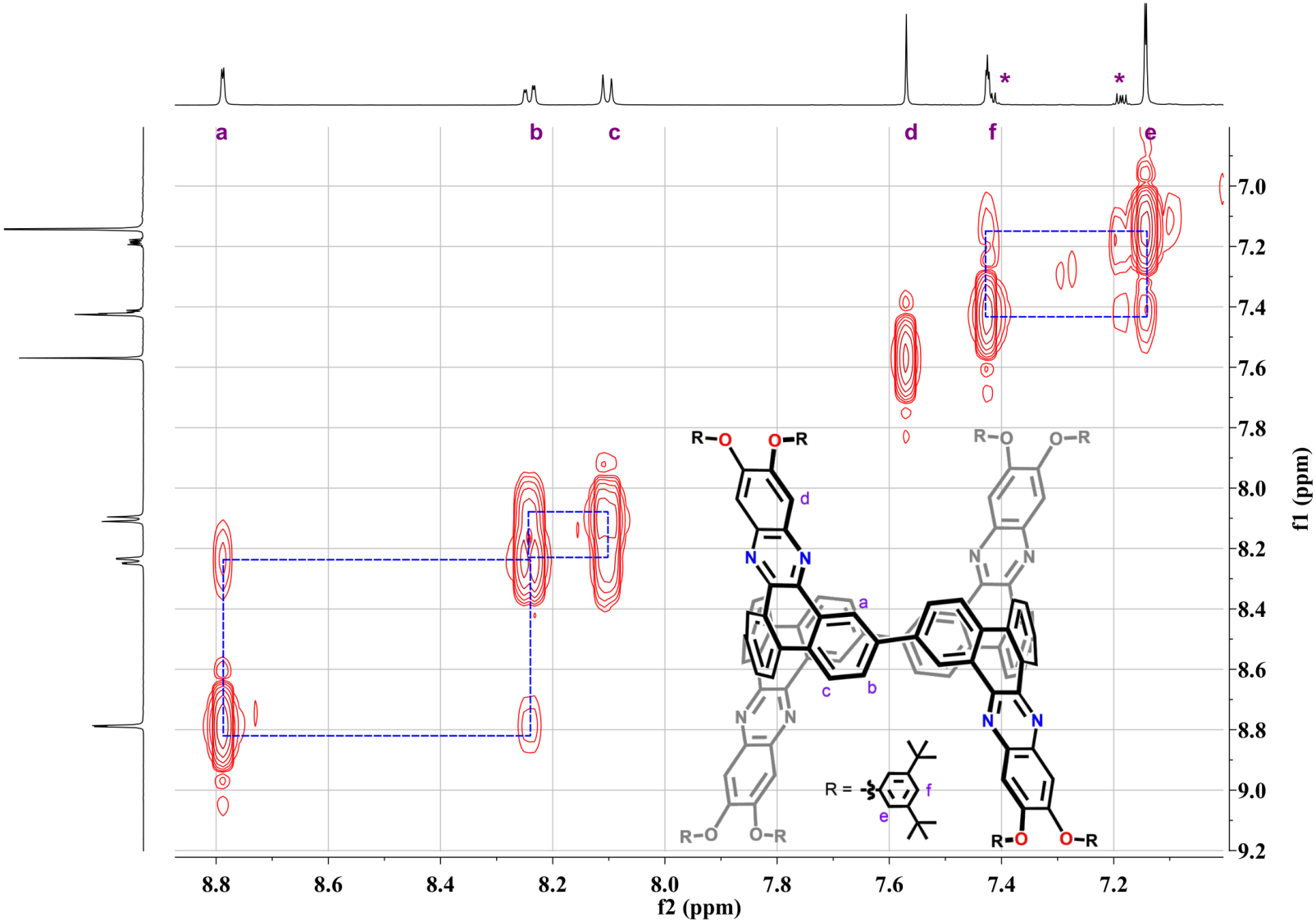


Figure S6. COSY NMR spectrum of **1**. Data collected in CD_2Cl_2 at 20 ºC (* = *o*DCB).

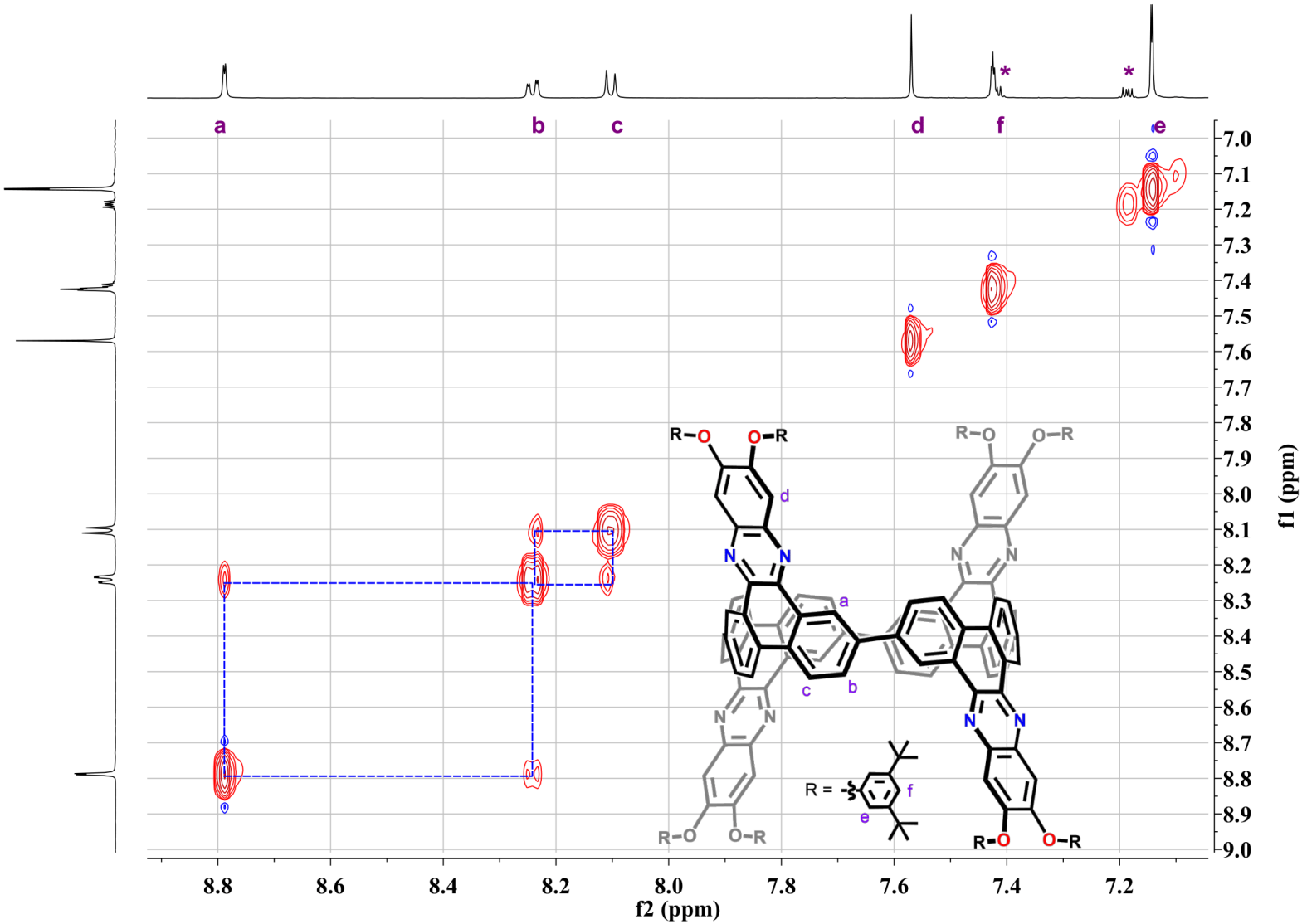


Figure S7. NOESY NMR spectrum of **1**. Data collected in CD_2Cl_2 at 20 ºC (* = *o*DCB).

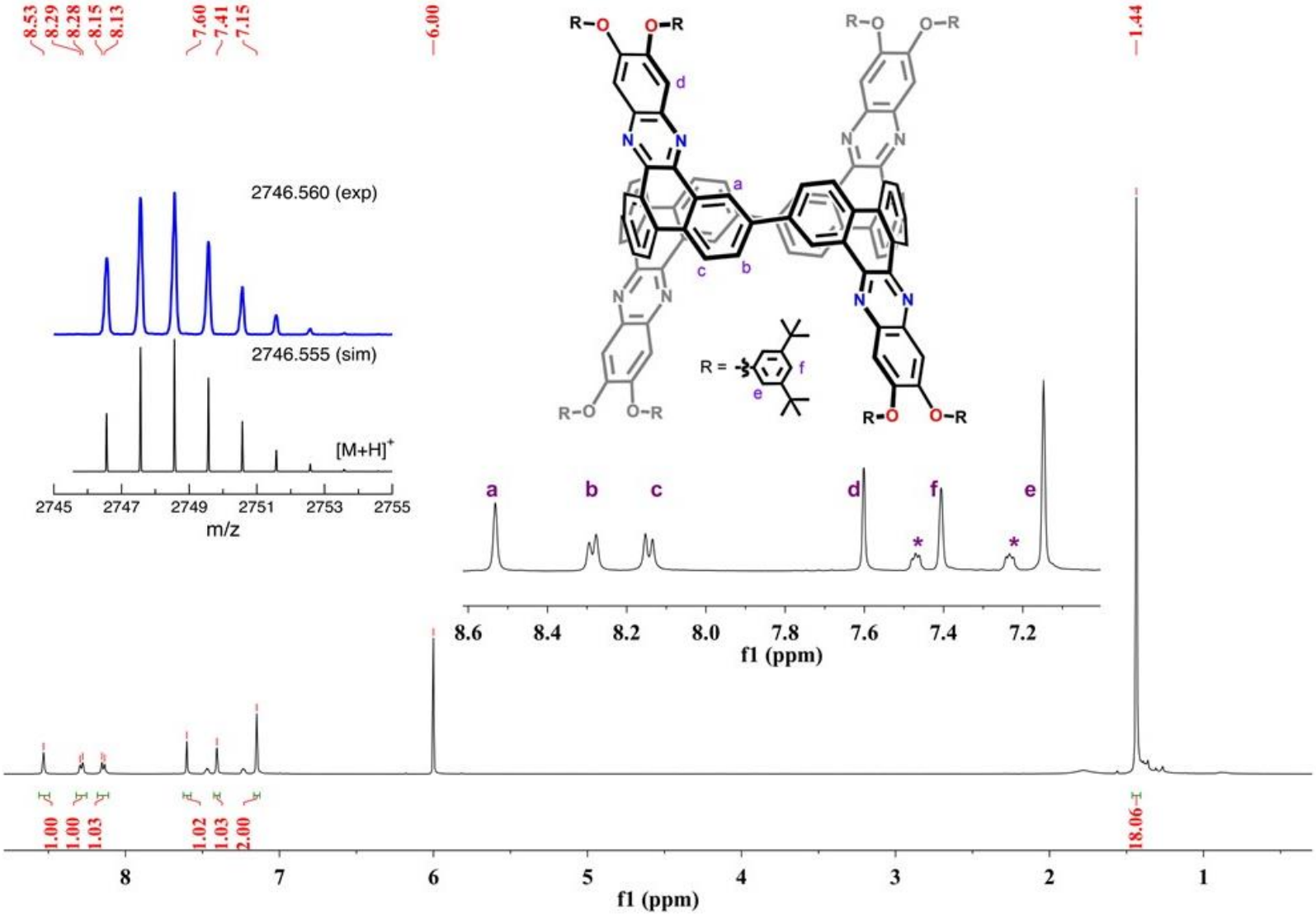


Figure S8. ^{1}H NMR spectrum of **1**. Data collected in 1,1,2,2-tetrachloroethane-d_2 at 20 ºC (* = *o*DCB). Inset: Experimental MALDI MS molecular ion peaks of **1** (blue trace). Black trace represents simulation of $[M+H]^+$ isotopic distribution (same as Figure 2b).

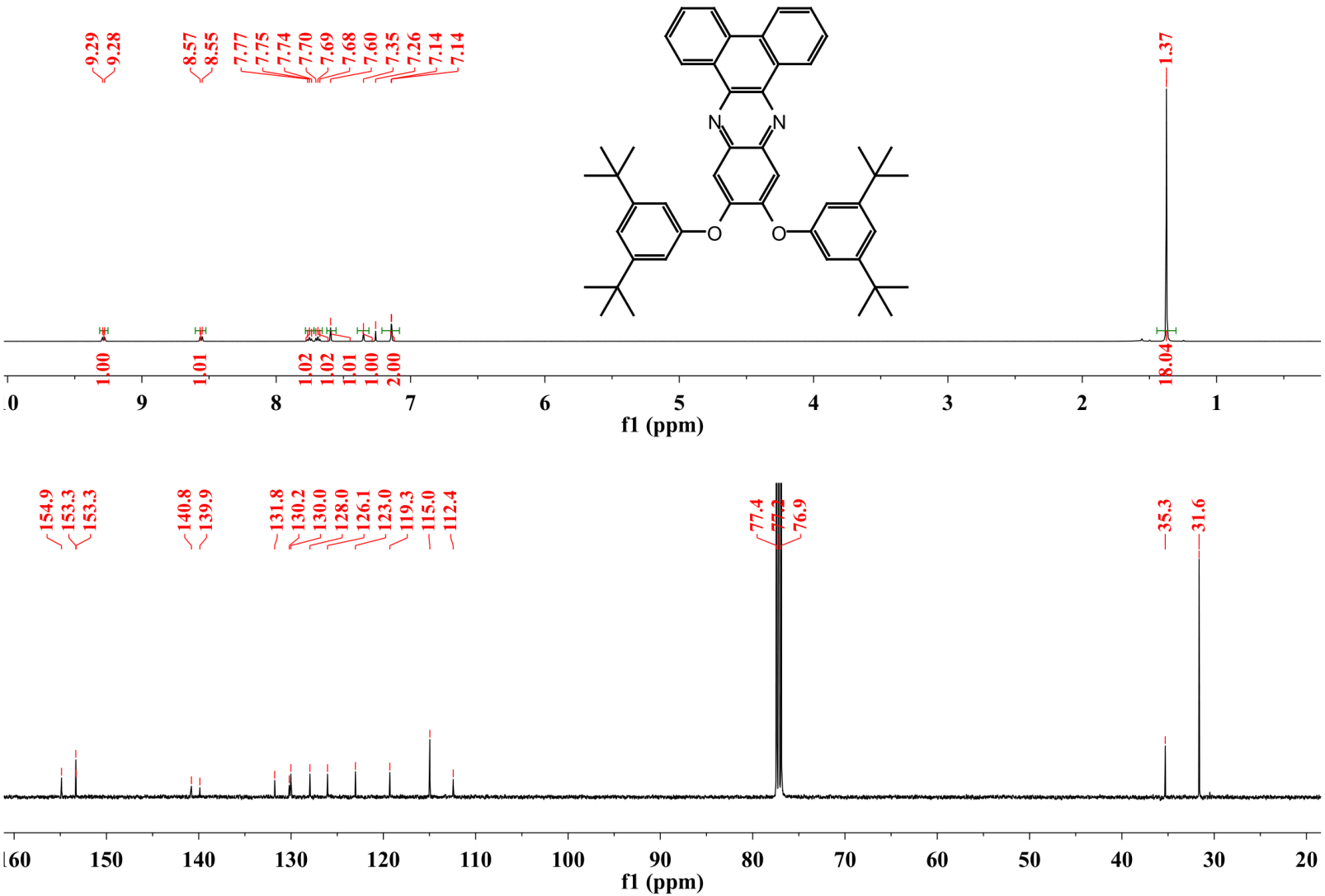


Figure S9. ^{1}H and ^{13}C NMR spectra of **3b**. Data collected in $CDCl_3$ at 20 ºC.

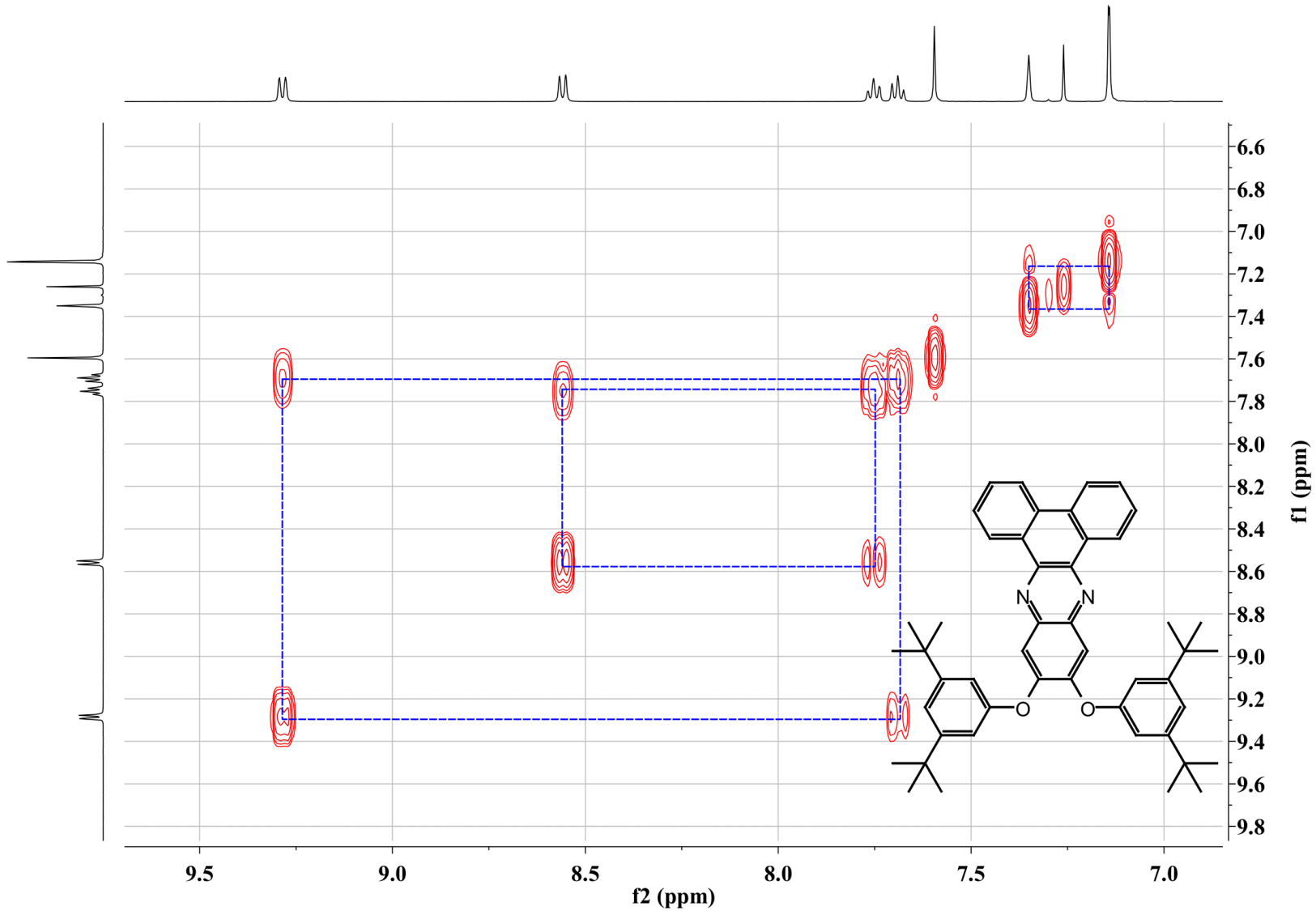


Figure S10. COSY NMR spectrum of **3b**. Data collected in $CDCl_3$ at 20 ºC.

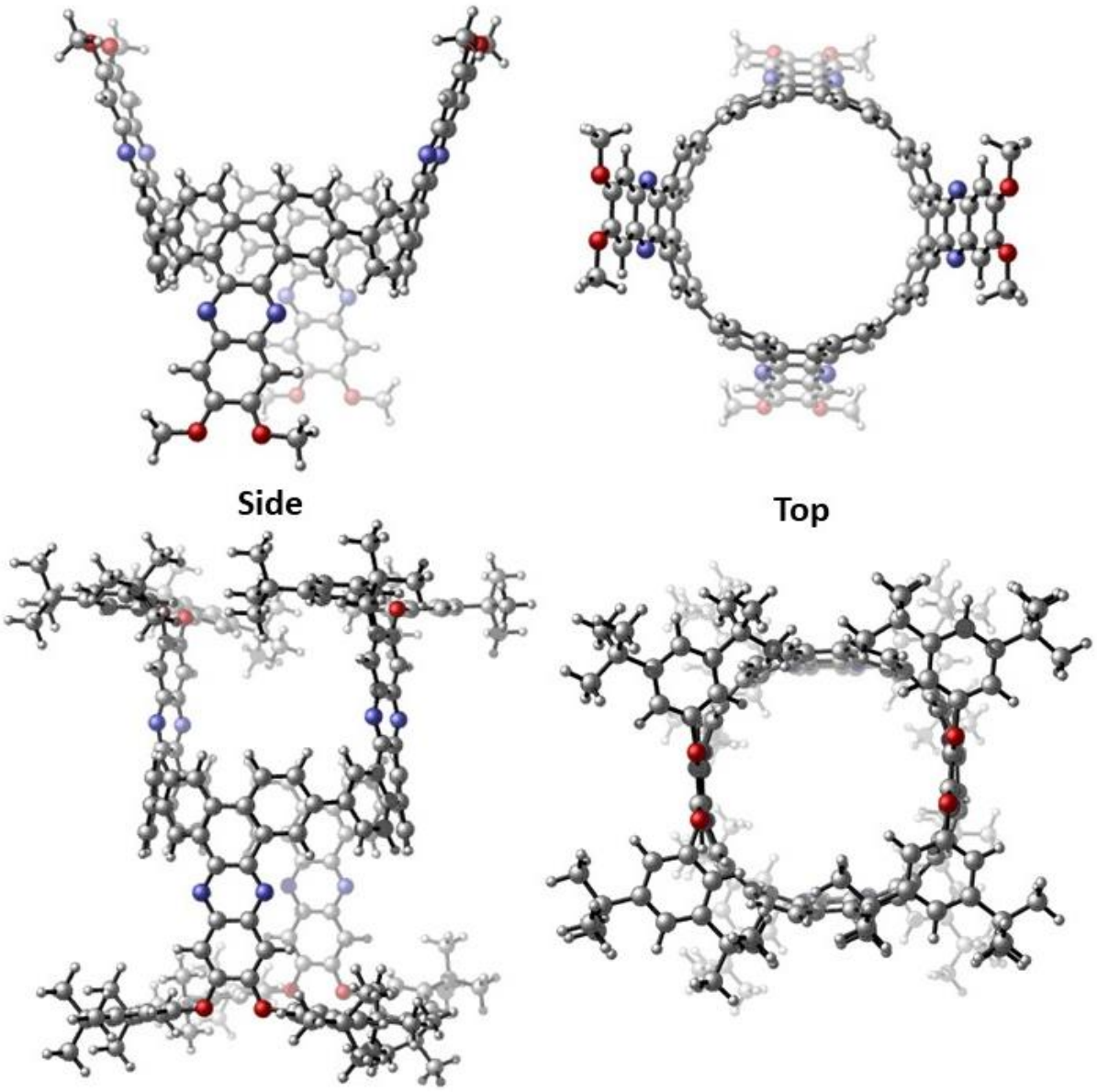


Figure S11. DFT optimized structure of (*top*) **1'** (R = Me) and (*bottom*) **1''** (R = 1,3-di-*tert*-butylphenyl) at the B3LYP/6-31G(d) and /3-21G(d) level of theory, respectively.

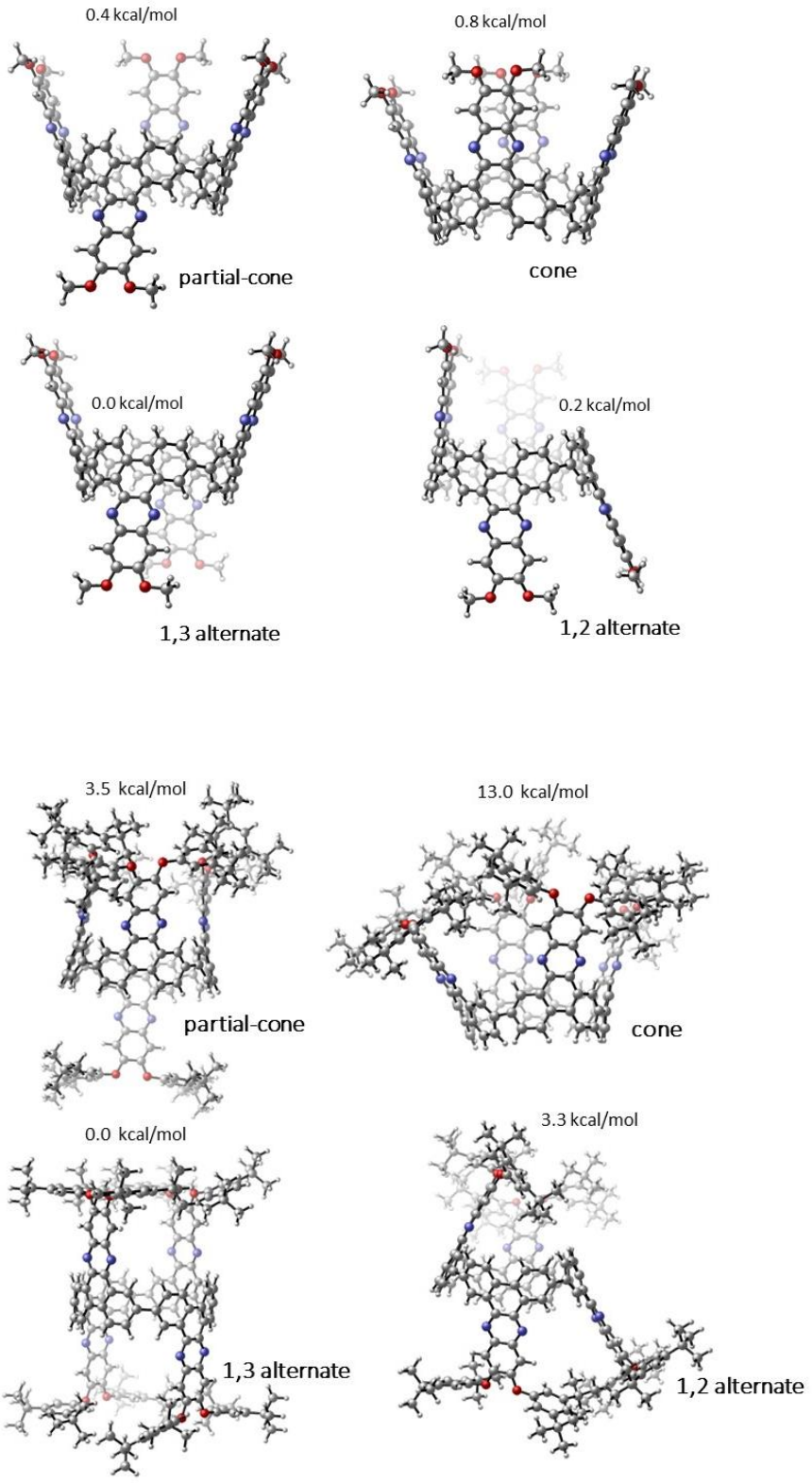


Figure S12. DFT conformational analysis of (*top*) **1'** (R = Me) and (*bottom*) **1''** (R = 1,3-di-*tert*-butylphenyl) at the B3LYP/6-31G(d) and /3-21G(d) level of theory, respectively.

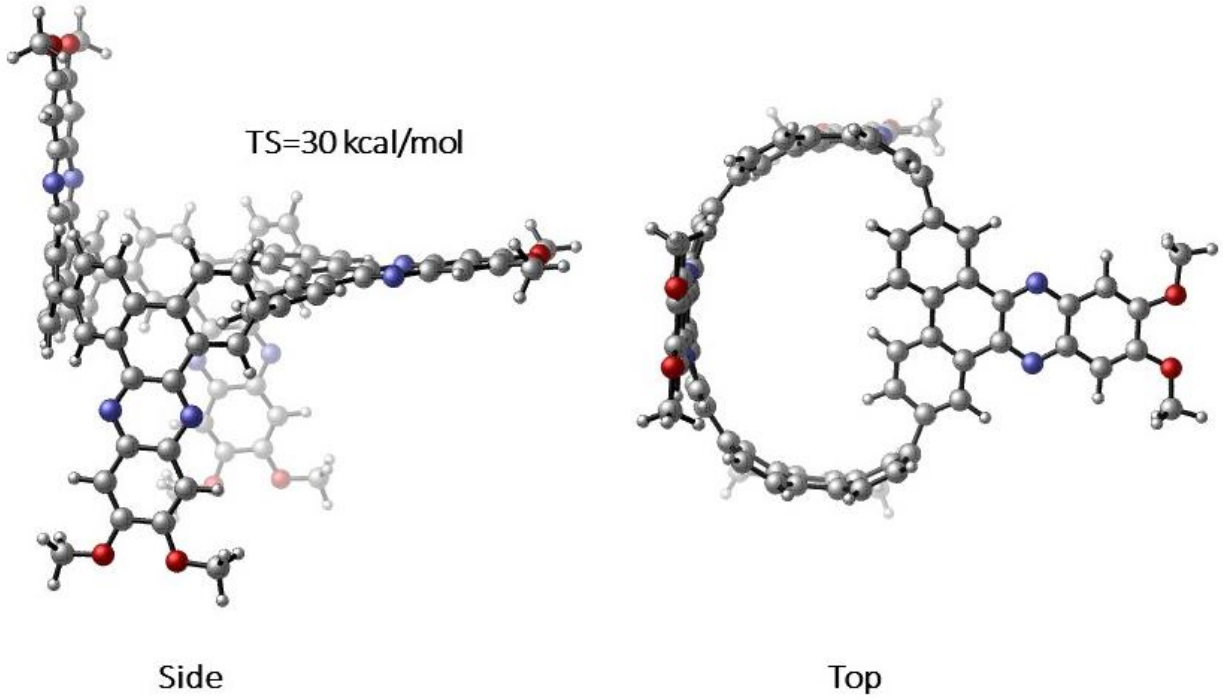


Figure S13. Dibenzo[*a*,*c*]phenazine rotational barrier in **1'** (R = Me). DFT calculations performed at the B3LYP/6-31G(d) level of theory.

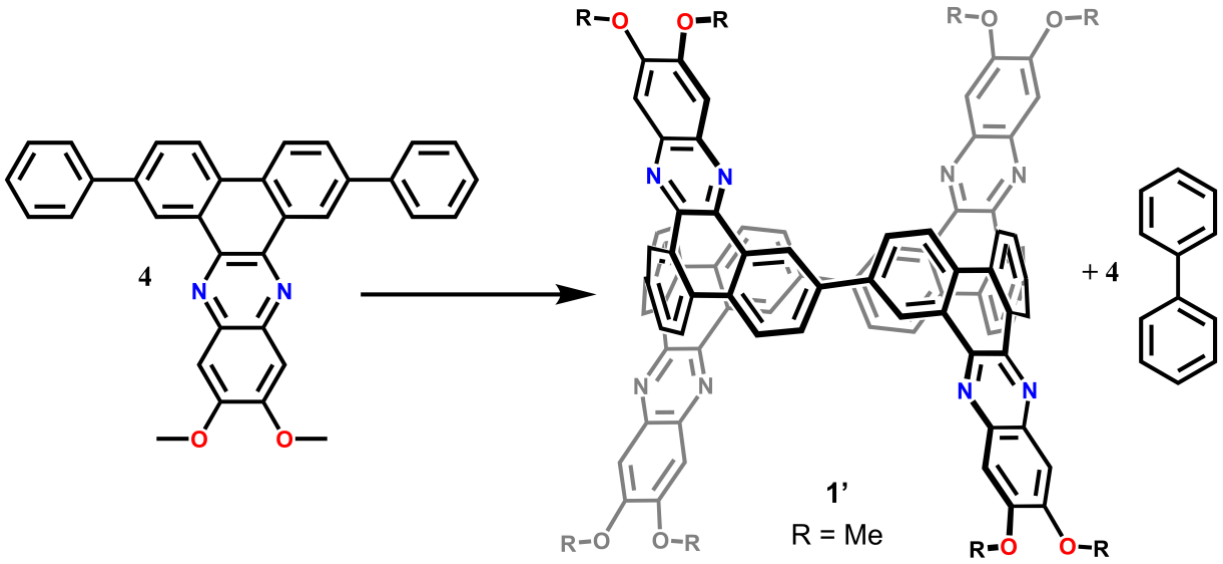


Figure S14. Homodesmotic reaction for the calculation of strain energy (ΔH) of **1'** (R = Me). Strain energy of **1'** was calculated at B3LYP/6-31G(d) level of theory to be 77.0 kcal/mol.

Table S2. Calculated absorption energies (λ, nm), oscillator strengths (*f*), and main contributions with its percentages for **1'** (R = Me) at time-dependent (TD) DFT/ 6-31G* level of theory. Except for the HOMO-to-LUMO transition, only major and intense transitions are provided. H and L stands for HOMO and LUMO, respectively.

1'			
	λ (nm)	*f*	Major contributes
B3LYP-D3BJ	527.2	0.000	H→L (96%)
	474.0	0.130	H→L+1 (94%)
	406.2	0.698	H-1→L (72%)
	406.2	0.698	H-2→L (72%)
	393.1	1.366	H-6→L (58%)
CAM-B3LYP-D3BJ	395.6	0.000	H→L (71%)
	352.9	1.025	H→L+1 (43%)
	352.9	1.026	H→L+2 (43%)
***ω*B97XD**	344.3	0.000	H→L (62%)
	451.3	1.170	H-4→L (10%)
	451.2	1.180	H-3→L+1 (21%)

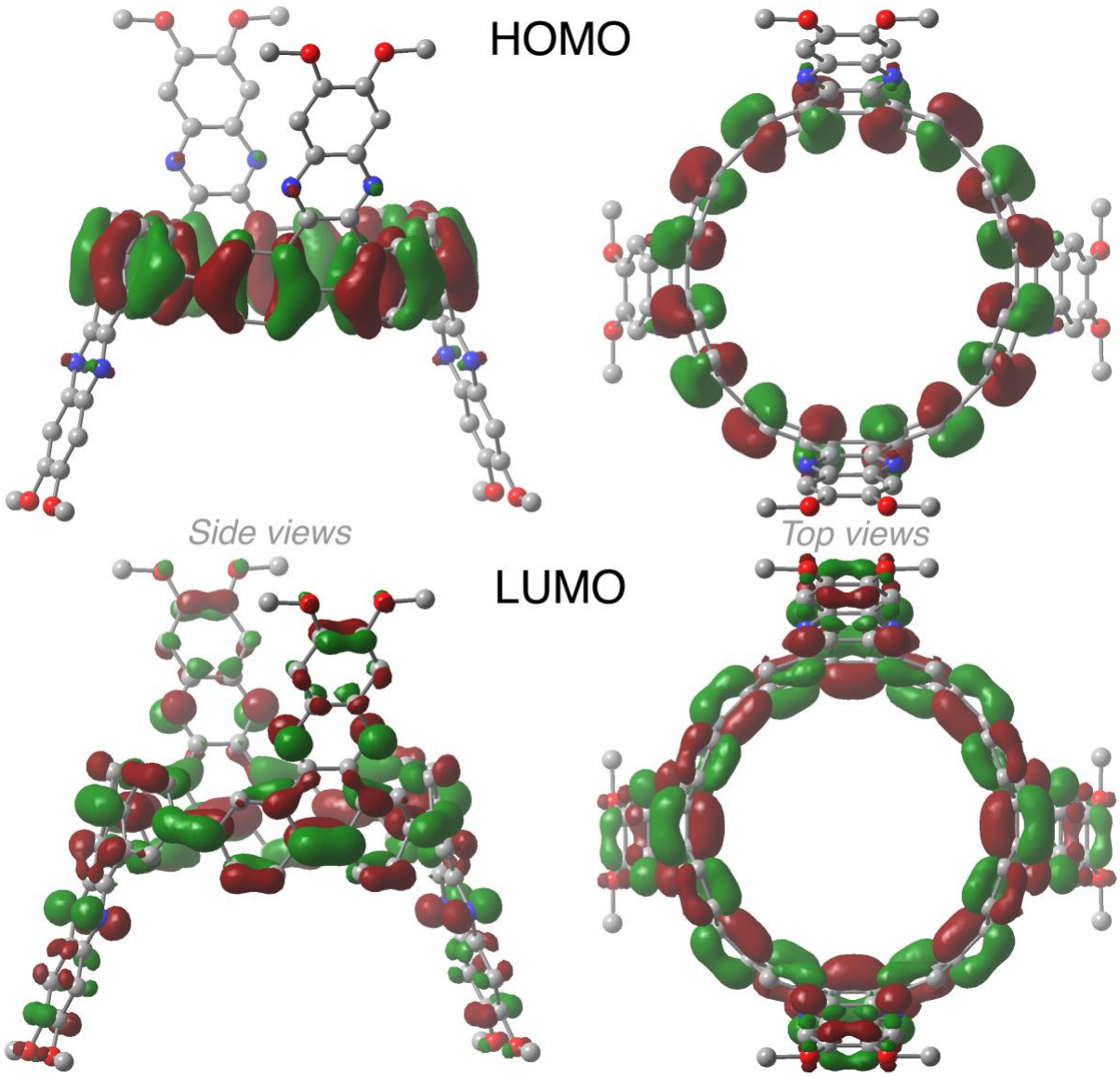


Figure S15. HOMO and LUMO (±0.02 au) of **1'** (R = Me) calculated by DFT at the B3LYP/6-31G(d) level of theory

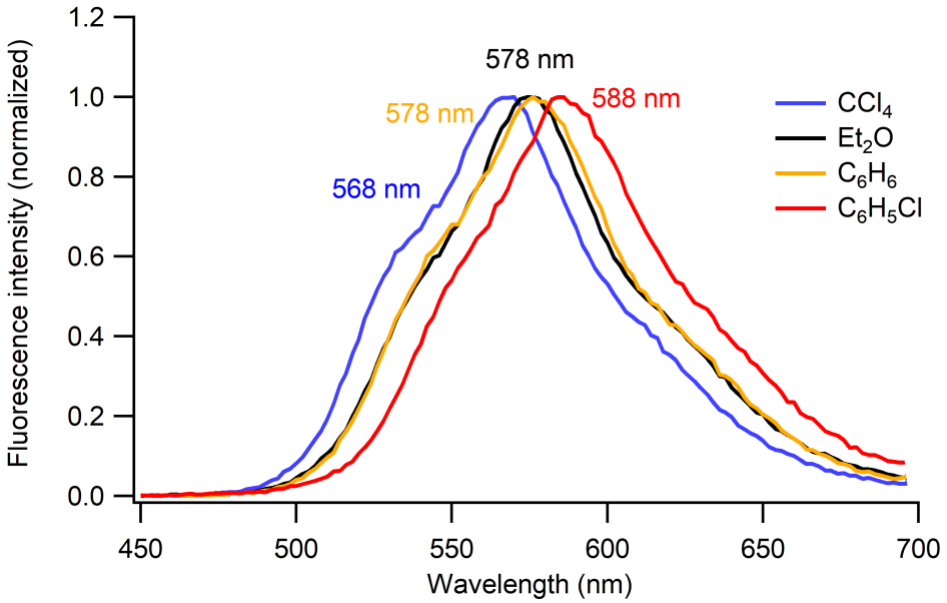


Figure S16. Emission profile of **1** in a variety of solvents. Peak maximum is indicated by the numbers in the plot and color-coded according to solvent. The samples were excited at 350 nm. Dielectric constants: CCl_4, 2.24; Et_2O, 4.267; C_6H_6, 2.28; C_6H_5Cl, 5.69; and CH_2Cl_2, 9.08 (this last solvent is in the main text).[18]

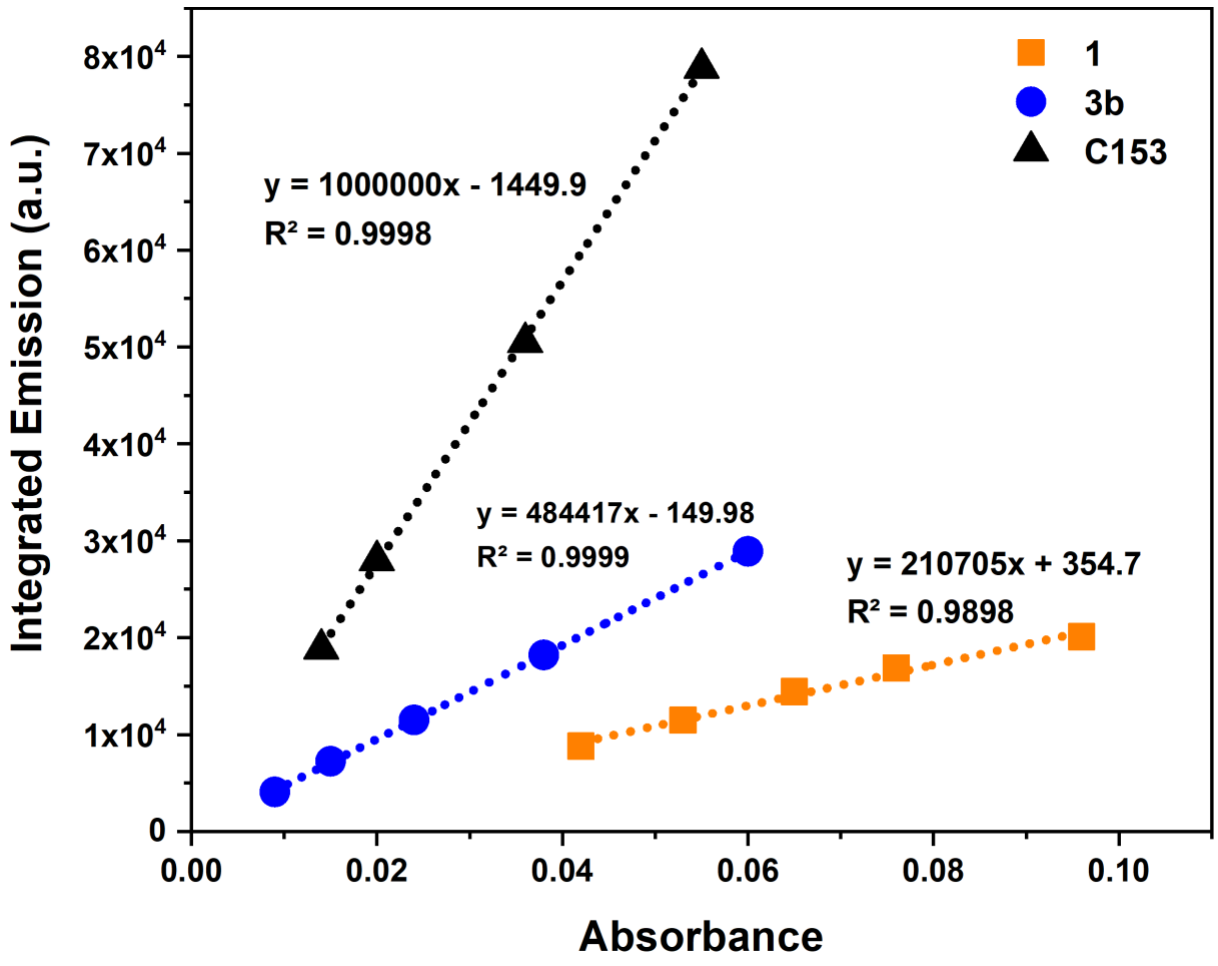


Figure S17. Linear plots used to obtain the gradient values for quantum yield determination of **1** and **3b**. Quantum yield determination equation and details are provided in the experimental section.

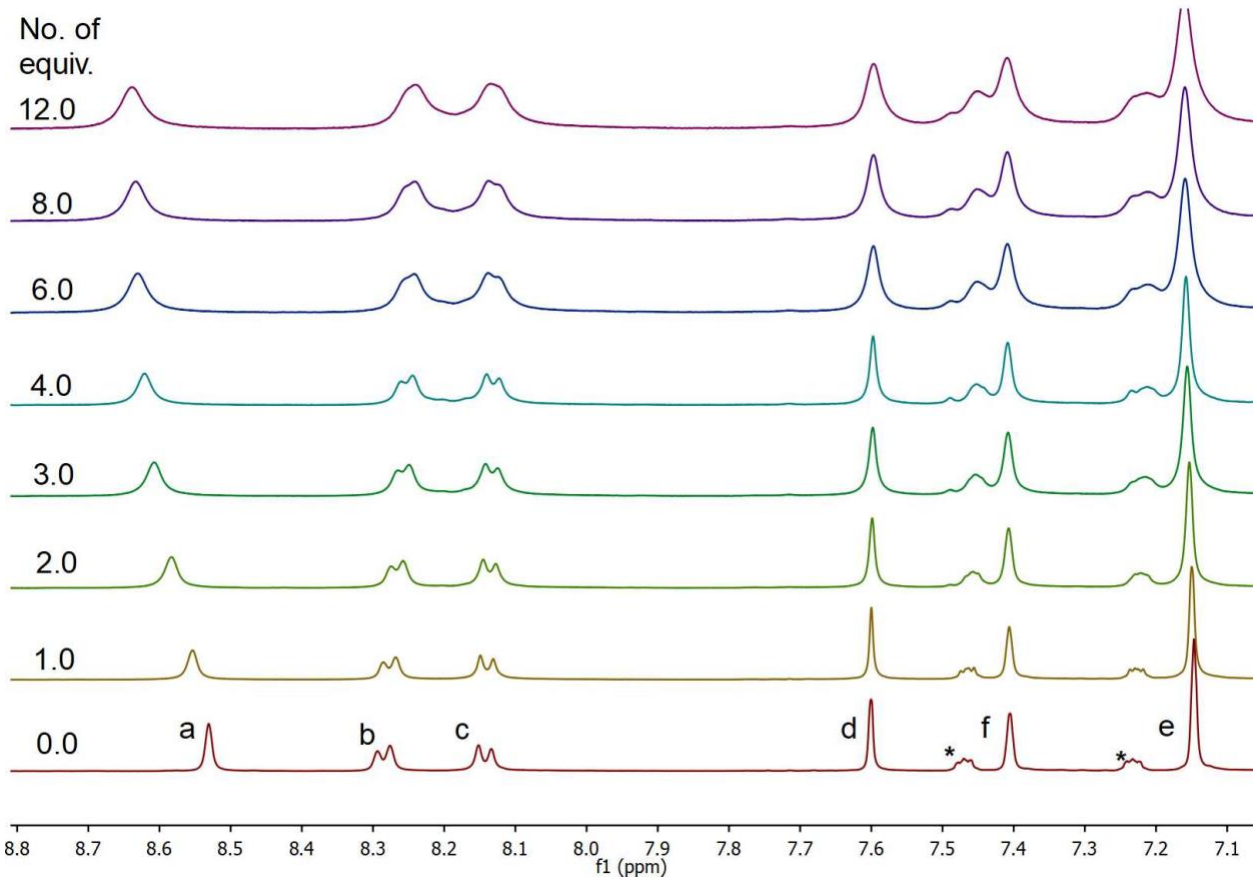


Figure S18. ^{1}H NMR titration spectra (500 MHz, 298 K) of C_{60} into **1** (1 mM) in 1,1,2,2-tetrachloroethane-d_2. The number of C_{60} equivalents relative to **1** are indicated on the left-hand side of the stacked plot (* = *o*DCB).

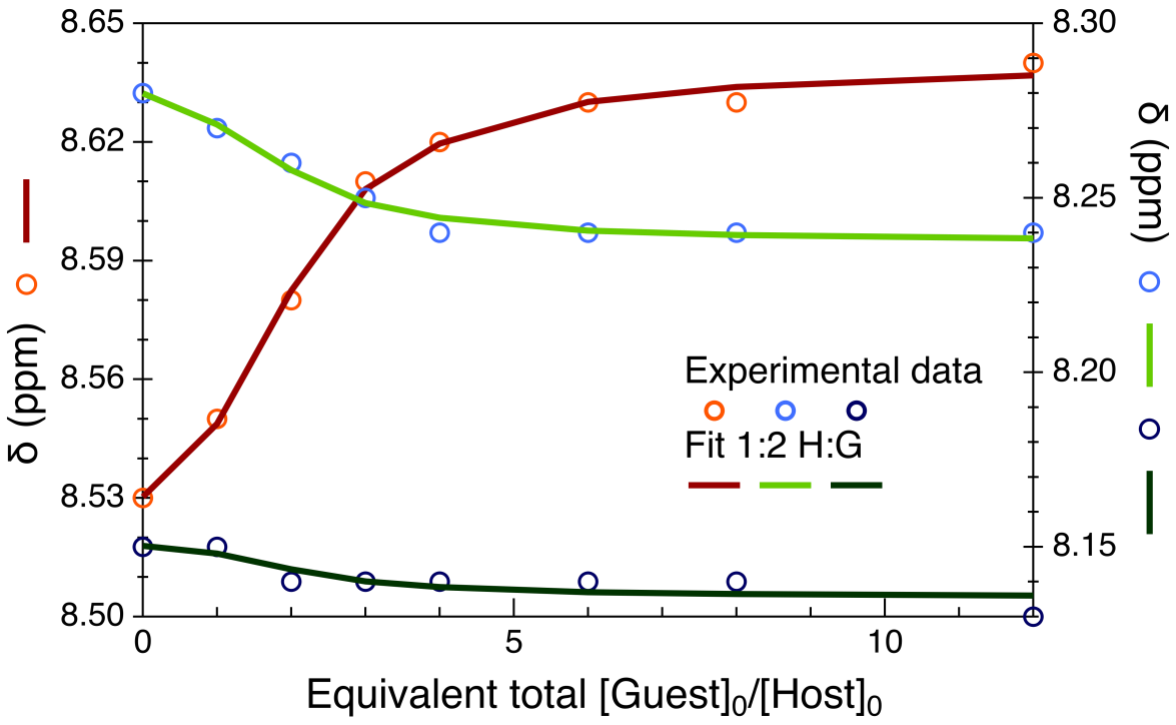
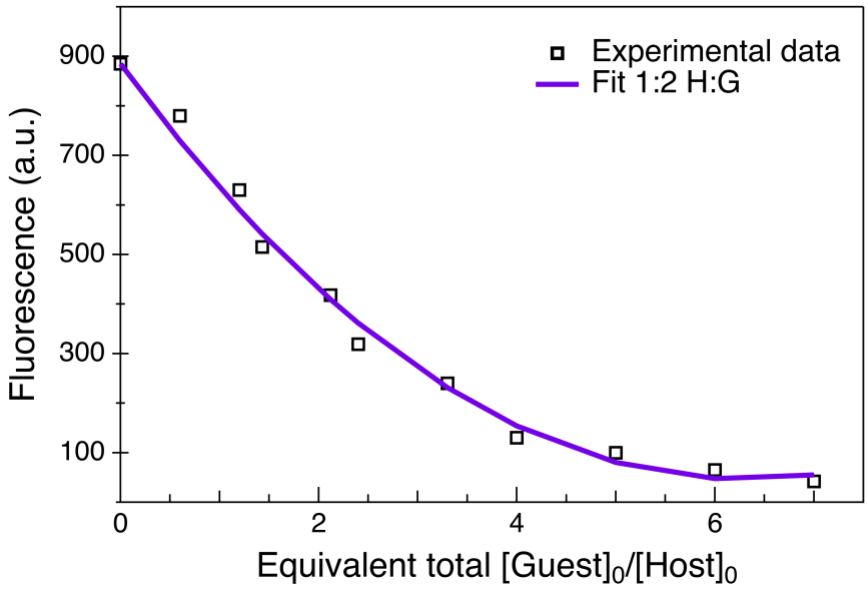


Figure S19. Non-linear curve fitting of ^{1}H NMR resonance "a", "b" and "c" of **1** upon titration with C_{60}. Experimental data is shown as open circles, while the fit to a 1:2 H:G model is shown as continuous traces. Data was fit using Bindfit.[19] Fitting to 1:2 H:G model provides the following parameters: L-BFGS-B, K_1 = 149 M^{-1} (±146%), K_2 = 1021 M^{-1}(±32%).



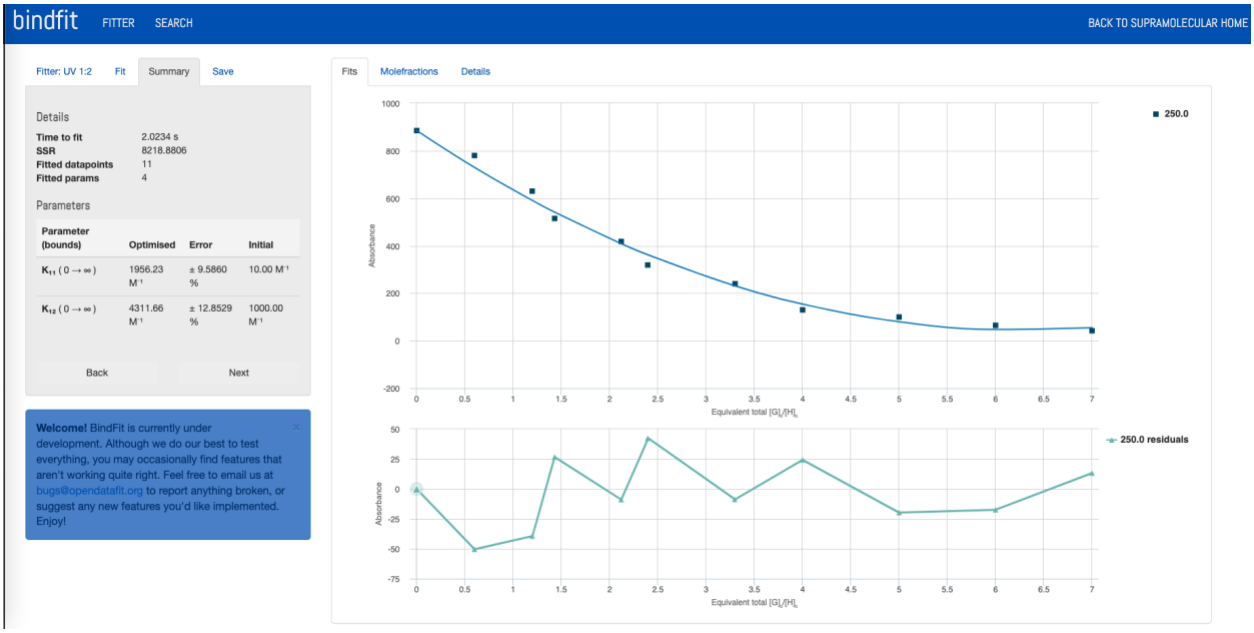


Figure S20. Non-linear curve fitting of fluorescence quenching titration of **1** upon addition of C_{60}. Experimental data is shown in the black open squares, while the fit to a 1:2 H:G model is shown in purple. Data was fit using Bindfit. For 1:2 H:G model: L-BFGS-B, K_1 = 1956 M^{-1} (±9.6%), K_2 = 4311 M^{-1} (±12.8%).

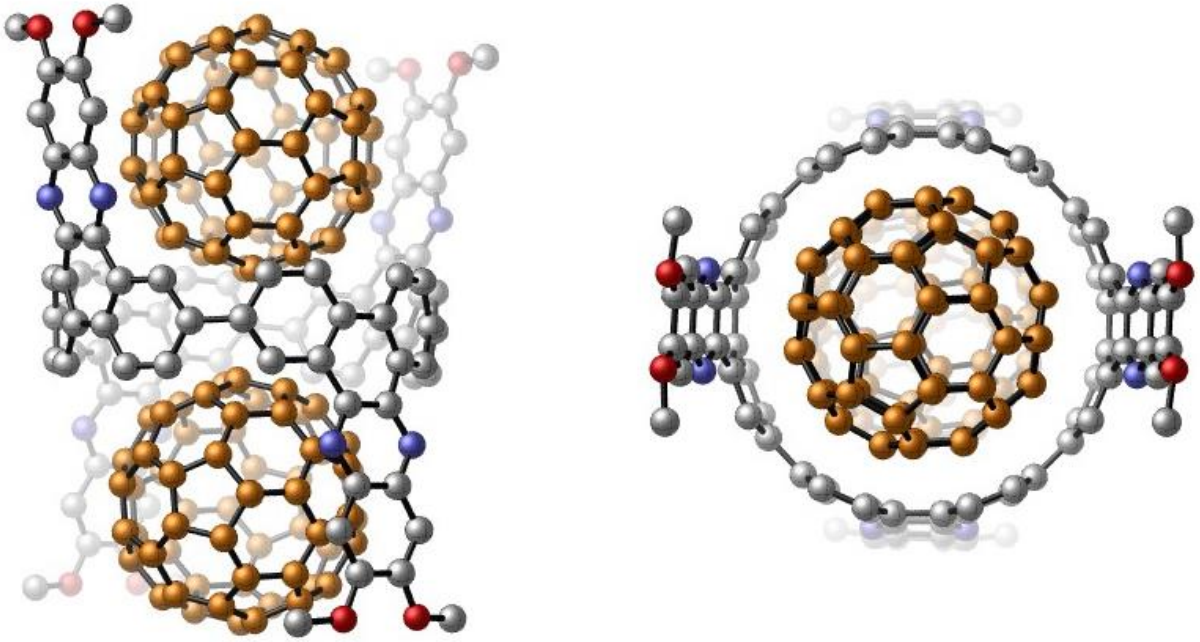


Figure S21. DFT optimized structure of [$(C_{60})_2$ ⊂**1'**] at the B3LYP/6-31G(d) level of theory. Hydrogens are omitted for clarity.

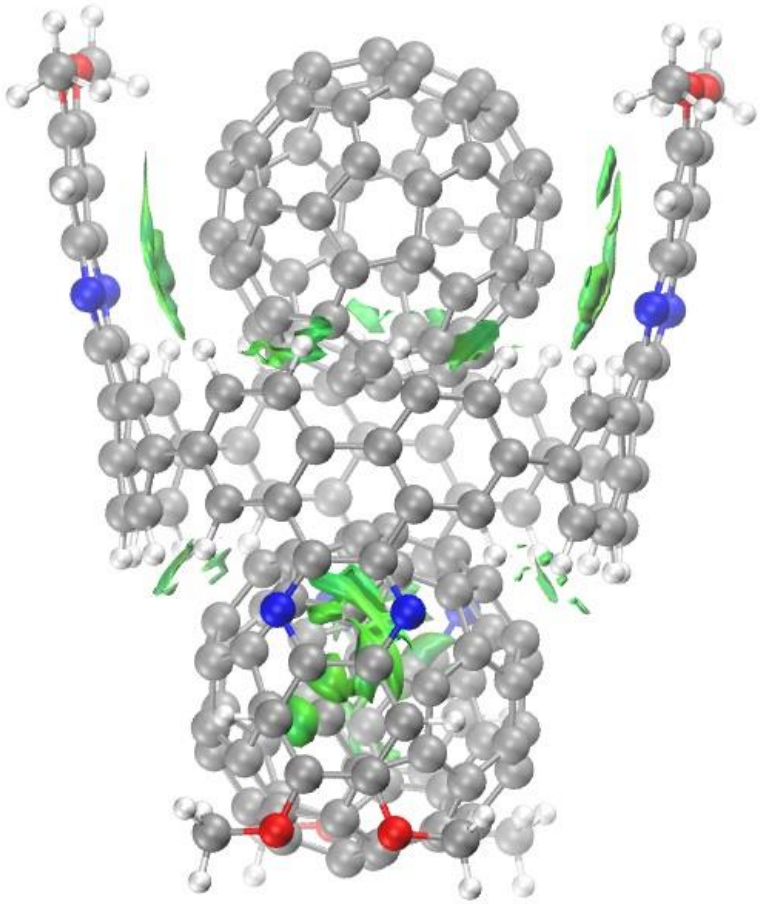


Figure S22. Sign(λ_2)ρ colored IGMH of δg^{inter} = 0.003 a.u. isosurfaces showing non-covalent interactions in [$(C_{60})_2$⊂**1'**].

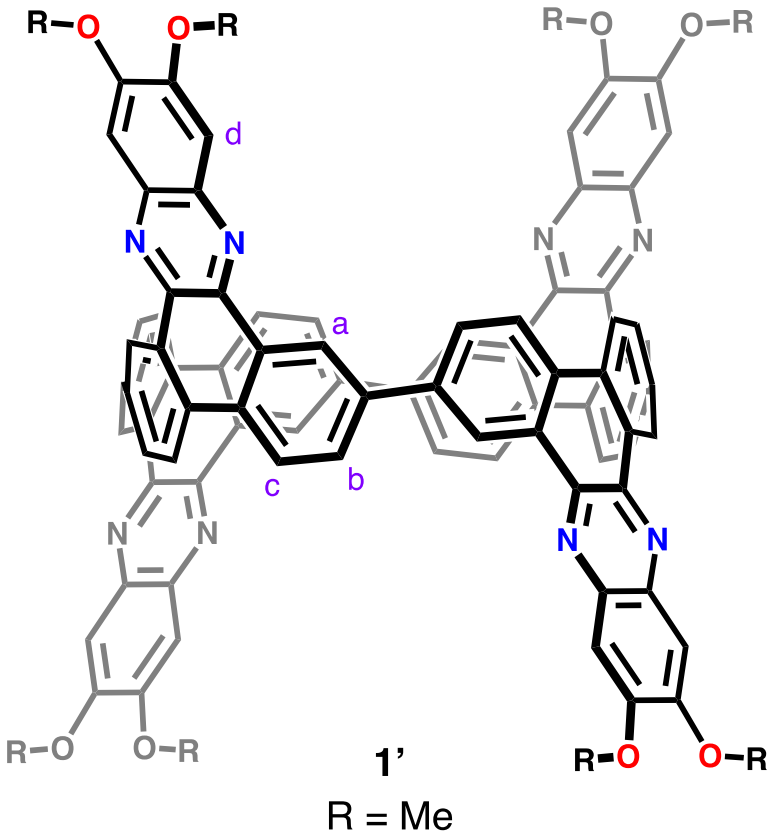


Table S3. DFT calculated ^{1}H NMR data of **1’** (R = Me) using DFT/6-31G*+PCM(CH_2Cl_2) level of theory.

	B3LYP	***ω*B97XD**	**Exp.** (CD_2Cl_2)
a	9.68	9.06	8.77
b	8.58	7.82	8.24
c	8.28	7.37	8.10
d	7.65	6.92	7.57

Cartesian Coordinates of optimized molecules

(B3LYP/6-31G* or 3-21G*)

1' (1,3-alternate, R = Me)

Zero-point correction= 1.238311 (Hartree/Particle)
Thermal correction to Energy= 1.318127
Thermal correction to Enthalpy= 1.319071
Thermal correction to Gibbs Free Energy= 1.119914
Sum of electronic and zero-point Energies= -4425.685982
Sum of electronic and thermal Energies= -4425.606066
Sum of electronic and thermal Enthalpies= -4425.605522
Sum of electronic and thermal Free Energies= -4425.803979

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C	-9.29404600	5.47484000	2.03029500
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C	-8.95004300	3.27398800	3.08539400
C	-9.33598700	3.83671500	4.33443500
C	-9.68761200	5.16265900	4.42431000
C	-3.40855700	-9.66000500	2.47299300
C	-4.04713600	-8.48648200	2.79687800
C	-3.29744900	-7.32066900	3.12027200
C	-1.86648900	-7.37920500	3.10354200
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C	5.09173300	3.24451400	4.17787000
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C	4.65451100	3.54635600	1.77101300
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1’ (1,2-alternate, R = Me)

Zero-point correction= 1.238231 (Hartree/Particle)
Thermal correction to Energy= 1.317945
Thermal correction to Enthalpy= 1.318889
Thermal correction to Gibbs Free Energy= 1.120053
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Sum of electronic and thermal Energies= -4425.605905
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Sum of electronic and thermal Free Energies= -4425.803797

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C	15.71470200	4.38337200	5.03444400
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C	11.81822100	12.09644500	-2.41132500
C	9.92141900	10.72178400	-0.58350900
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C	15.82823600	2.42442000	-5.50788300
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C	9.12651000	3.01715000	-0.45278100
C	8.49755700	5.64070900	0.87211400

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O	16.07301700	12.29750300	6.64992800
O	16.62035300	4.77225300	5.96430900
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C	12.08032000	14.08041400	-11.58601300
C	13.31469000	9.39851100	-13.98157100
C	16.40898900	6.01853900	6.61212700
C	17.48501600	1.25073900	4.31344700
C	5.71682500	3.30822700	-8.48608400
C	9.15312300	5.86981600	-11.77273800
H	17.01454800	13.53127100	2.41519900
H	13.78742400	11.30158700	5.50223900
H	14.34833900	6.04898100	5.10386800
H	15.35221100	1.65040300	2.96761700
H	7.78845100	2.72329800	-7.11257400
H	10.96651200	5.07799600	-10.15795500
H	14.39439200	8.77883100	-11.75209400
H	13.28180600	13.11761800	-9.54910200
H	15.58028900	6.64009900	-8.52001000
H	15.44292100	12.46984400	-1.15255900
H	10.23384200	2.14341800	-3.94967700
H	11.47684600	7.36902500	2.59326700
H	8.45769300	9.19622500	-0.38412300
H	8.98931500	1.77934800	-2.18429400
H	17.67829800	3.44929000	-5.76870300
H	16.64658400	11.17536000	-2.31323600
H	11.34846300	9.52449500	2.79497700
H	7.59597000	7.56688200	0.73686500
H	12.60099700	12.19874200	-4.38190800
H	14.23516900	12.24314400	-5.72253900
H	17.99732200	5.48850500	-5.14318700
H	14.25709900	5.07233900	-7.81996600
H	13.44722800	0.41475900	-1.66279000
H	12.77835300	1.83815300	-0.13886400
H	10.80691000	11.99195900	-2.78923800
H	9.50532000	11.03516200	-1.53485400
H	18.28504100	7.80583100	-4.55124100
H	17.86787300	9.60204000	-3.66650000
H	16.28737900	1.69255900	-4.85094200
H	14.94841900	0.74281000	-3.53751000

H	8.09856800	3.34706600	-0.56433000
H	7.65243900	5.17299000	0.37712500
H	15.68565800	11.80825700	8.56354600
H	14.22611200	12.22753700	7.61887800
H	15.02423100	10.64538300	7.37690800
H	19.50259800	14.39115600	4.92533200
H	19.10070000	13.41553700	3.48167800
H	18.27665200	14.97856000	3.76351100
H	11.54421200	14.61247700	-12.37336600
H	11.42826500	13.96428500	-10.71084200
H	12.97266900	14.65078400	-11.29829500
H	12.89291300	9.52672800	-14.97968000
H	14.39878000	9.24544100	-14.05681800
H	12.86039900	8.52273200	-13.50020100
H	17.24192300	6.13663500	7.30697600
H	16.40974200	6.84718800	5.89248600
H	15.46256000	6.02332900	7.16802900
H	18.40790900	0.95277400	4.81338300
H	16.70656400	0.49992900	4.49998000
H	17.66062400	1.32806600	3.23279900
H	4.75507200	3.48339100	-8.97064500
H	5.90690300	2.22904000	-8.42499900
H	5.70034100	3.72992800	-7.47291000
H	8.48835700	6.27123200	-12.53922100
H	9.68262300	6.69340200	-11.27685900
H	9.88543300	5.19655300	-12.23666100

1’ (partial cone, R = Me)

Zero-point correction= 1.238247 (Hartree/Particle)
Thermal correction to Energy= 1.317997
Thermal correction to Enthalpy= 1.318941
Thermal correction to Gibbs Free Energy= 1.120032
Sum of electronic and zero-point Energies= -4425.684810
Sum of electronic and thermal Energies= -4425.605059
Sum of electronic and thermal Enthalpies= -4425.604115
Sum of electronic and thermal Free Energies= -4425.803025

C	-4.67004900	0.38410700	-5.05537100
C	-5.65941200	-0.55807900	-4.90200300
C	-6.26617600	-0.76951800	-3.63201400
C	-5.83175000	0.00542600	-2.50899900
C	-4.80667700	0.97684100	-2.68622100
C	-4.23546800	1.17184500	-3.92125900
C	0.47466600	-2.75925800	1.03949700

C	-0.74909000	-2.30269400	1.46757600
C	-1.46724300	-3.00003500	2.47939900
C	-0.90183100	-4.18573100	3.05121500
C	0.36669300	-4.64327300	2.59591200
C	1.04588600	-3.95779900	1.61709500
C	1.94313800	-11.76385400	2.33076500
C	1.03246300	-11.24813500	3.22200800
C	-0.36338400	-11.44348100	3.02387000
C	-0.81368000	-12.18540700	1.88492700
C	0.14324300	-12.70700000	0.96949800
C	1.48791200	-12.50849700	1.17583200
C	-14.56252900	-12.74560000	-1.13808100
C	-13.19770700	-12.88579400	-1.05175500
C	-12.33381800	-11.86060900	-1.52969400
C	-12.89976300	-10.67582500	-2.10183300
C	-14.31498100	-10.54688700	-2.18122500
C	-15.13467200	-11.54788100	-1.71649100
N	-12.11265600	-9.68103400	-2.55996800
N	-7.23812100	-1.69604800	-3.50297500
N	-6.37554300	-0.17424200	-1.28782400
N	-2.67025200	-2.54099400	2.87951300
N	-1.55603600	-4.87681000	4.00642500
N	-1.24073900	-10.92490400	3.90737100
N	-2.12845700	-12.39435700	1.66694000
N	-10.99755300	-12.01549400	-1.43263300
C	-10.22750100	-11.04050700	-1.91149500
C	-10.79450200	-9.85347900	-2.48475300
C	-9.90507300	-8.78052800	-2.93658300
C	-8.52679500	-9.05730300	-3.11813800
C	-7.79135900	-1.84506300	-2.30127500
C	-7.34929700	-1.07455600	-1.17398600
C	-7.93843100	-1.32960500	0.14310200
C	-9.15541200	-2.05307700	0.22444300
C	-3.29935100	-3.22050900	3.83645900
C	-2.73453300	-4.40426200	4.40777600
C	-3.50088300	-5.14665500	5.40977400
C	-4.61186400	-4.53376500	6.04318700
C	-2.53479600	-11.15486400	3.69706500
C	-2.98613000	-11.90603300	2.56043100
C	-4.42421900	-12.08813800	2.34703800
C	-5.31774200	-11.82774900	3.41615000
C	-8.77177800	-11.15311600	-1.79055800
C	-8.20603900	-12.01148700	-0.83244100
C	-7.94740900	-10.27014300	-2.53215400
C	-6.83560800	-11.99417200	-0.55283700
C	-6.29309300	-12.34904800	0.78913400

C	-8.83215900	-2.85889000	-2.11250000
C	-8.94697300	-3.93291300	-3.01146900
C	-9.61439000	-2.83148800	-0.93075700
C	-9.79638600	-5.01430100	-2.75466800
C	-9.51390800	-6.38692000	-3.26185800
C	-3.52285000	-10.57496900	4.61046800
C	-3.19208500	-9.45725800	5.39453300
C	-4.85837300	-11.05028200	4.57182200
C	-4.16502600	-8.76414500	6.12245900
C	-4.05575100	-7.30779400	6.41448400
C	-4.62808600	-2.78529000	4.26949000
C	-5.40419000	-1.98624900	3.41723400
C	-5.19199500	-3.31874100	5.45630500
C	-6.73943900	-1.68755400	3.69939700
C	-7.67418600	-1.41589100	2.57215900
C	-8.99852400	-1.90821300	2.64790500
C	-4.98510400	-6.62843700	7.23867200
C	-7.15875100	-12.33832800	1.90928700
C	-8.20191000	-6.71249000	-3.68252300
C	-7.22810400	-1.00629100	1.31115100
C	-7.19514400	-2.00049800	5.00282400
C	-10.73868300	-4.84302300	-1.71208200
C	-10.37948000	-7.46107100	-3.03048900
C	-6.01313500	-11.29448800	-1.46839900
C	-4.92101900	-12.36215900	1.06133700
C	-5.42154300	-9.39841300	6.26680200
C	-3.24360200	-6.51177600	5.60302400
C	-10.65731800	-3.77687400	-0.83567500
C	-9.72162200	-2.20638000	1.50696300
C	-6.55370800	-10.46883200	-2.43667000
C	-7.72832900	-8.01012800	-3.62494300
C	-6.68299300	-12.09819400	3.18495300
C	-5.75322900	-10.51577500	5.52182000
C	-5.25442500	-5.28167000	7.05521600
C	-6.44241100	-2.79412000	5.85340500
O	-16.48908100	-11.53246700	-1.74354600
O	-15.47532600	-13.65459300	-0.71863900
O	-4.02735900	0.66956200	-6.21364400
O	-3.25938400	2.06896200	-4.20427700
O	1.24161400	-2.17891000	0.08499500
O	2.25340000	-4.30250500	1.10799000
O	3.29019300	-11.64344700	2.42347700
O	2.48261000	-12.95992800	0.37400700
C	-2.79896100	2.89953000	-3.14825000
C	-4.40413100	-0.05640900	-7.37534500
C	-17.12682900	-10.39228600	-2.30184500

C	-14.99218100	-14.86061100	-0.14372400
C	0.74520800	-1.00219800	-0.53670300
C	2.87530100	-5.47373100	1.61695200
C	3.81585400	-10.95027500	3.54608200
C	2.11628300	-13.70749700	-0.77728500
H	-6.01207900	-1.16216600	-5.72865300
H	-4.50705200	1.54745200	-1.81596500
H	-1.20795200	-1.41217300	1.05653600
H	0.76181200	-5.54414700	3.04849800
H	1.33631600	-10.68646200	4.09659600
H	-0.23279800	-13.26234600	0.11929600
H	-12.73537300	-13.76781900	-0.62640800
H	-14.70795200	-9.63844800	-2.62049500
H	-8.89390300	-12.59806900	-0.23388700
H	-8.25963700	-3.94551300	-3.84990900
H	-2.17984400	-9.07690300	5.31303800
H	-4.97394500	-1.74195800	2.45357500
H	-9.41717300	-2.18840800	3.60903800
H	-5.56534600	-7.18014900	7.97290500
H	-8.23242900	-12.38950000	1.76338200
H	-7.50312000	-5.92200800	-3.93466200
H	-6.25757200	-0.53864600	1.18736300
H	-8.18676000	-1.69111300	5.32083700
H	-11.46475700	-5.62218200	-1.50605400
H	-11.42491000	-7.29877400	-2.79335100
H	-4.93625500	-11.29539100	-1.33774500
H	-4.19156800	-12.46276900	0.26549300
H	-6.19625300	-8.93328000	6.86766100
H	-2.48388000	-6.95781300	4.97271100
H	-11.34185800	-3.75144700	0.00533200
H	-10.68972600	-2.68149600	1.62299200
H	-5.87560000	-9.87774700	-3.04266600
H	-6.68431100	-8.18538300	-3.86107100
H	-7.40298100	-11.99856500	3.99008100
H	-6.76621800	-10.89696400	5.59240000
H	-6.04594900	-4.82948800	7.64437200
H	-6.87753300	-3.08875400	6.80310600
H	-2.03647300	3.54419800	-3.58821100
H	-3.61137600	3.51494000	-2.74132300
H	-2.35602000	2.30676400	-2.33738500
H	-3.77558500	0.32602700	-8.18101200
H	-4.22604800	-1.13199600	-7.24890900
H	-5.46051500	0.10798900	-7.62314900
H	-18.19806800	-10.58541200	-2.22736800
H	-16.87753700	-9.48170400	-1.74213900
H	-16.84976300	-10.25609800	-3.35498000

H	-15.87860500	-15.44064700	0.11744300
H	-14.37993000	-15.42563300	-0.85808000
H	-14.40231800	-14.66316300	0.76052000
H	1.50432600	-0.70770400	-1.26304000
H	-0.20373700	-1.19420700	-1.05356900
H	0.60223800	-0.19544500	0.19371700
H	3.81862400	-5.56732200	1.07664200
H	3.07473500	-5.38386700	2.69257100
H	2.25821000	-6.36325800	1.43680100
H	4.90064400	-10.98061900	3.43267900
H	3.47736300	-9.90620100	3.56586400
H	3.53011100	-11.43872300	4.48634800
H	3.05318800	-13.97055500	-1.27067800
H	1.57524900	-14.62216200	-0.50333700
H	1.49616100	-13.11167900	-1.45922100

1' (cone, R = Me)

Zero-point correction= 1.238120 (Hartree/Particle)
Thermal correction to Energy= 1.317826
Thermal correction to Enthalpy= 1.318770
Thermal correction to Gibbs Free Energy= 1.120053
Sum of electronic and zero-point Energies= -4425.684505
Sum of electronic and thermal Energies= -4425.604799
Sum of electronic and thermal Enthalpies= -4425.603855
Sum of electronic and thermal Free Energies= -4425.802572

C	-19.58784700	-6.47131800	-5.34532600
C	-18.68188900	-7.49729700	-5.21721200
C	-18.90345000	-8.54472000	-4.27933900
C	-20.08029400	-8.51977100	-3.46449100
C	-21.00575300	-7.44798300	-3.60830000
C	-20.77764700	-6.44607300	-4.52156200
C	-19.52244400	-4.26157200	3.06113100
C	-19.98330600	-5.52207200	2.76457400
C	-19.66279000	-6.62517500	3.60489000
C	-18.85288500	-6.41049500	4.76697600
C	-18.38493200	-5.09831200	5.05836800
C	-18.70416800	-4.04458000	4.23561300
C	-11.83406400	-4.07511100	8.31862100
C	-12.58379700	-5.21573500	8.48212500
C	-12.19990200	-6.43053200	7.84752200
C	-11.02378700	-6.45481700	7.03159100
C	-10.26158600	-5.26358400	6.87076900
C	-10.64517700	-4.09958300	7.49352800
C	-12.05190700	-4.18510600	-0.37615000

C	-11.42410000	-5.24514300	0.23325500
C	-11.57004000	-6.56432800	-0.28073400
C	-12.37958200	-6.77943700	-1.44300300
C	-13.02200600	-5.66975300	-2.06074000
C	-12.87003300	-4.40251200	-1.55065800
N	-12.54628800	-8.01566900	-1.95493400
N	-18.00340700	-9.54376600	-4.17112400
N	-20.32383600	-9.49455000	-2.56423400
N	-20.11925100	-7.85507900	3.29323800
N	-18.52329200	-7.43210300	5.58297100
N	-12.94803500	-7.53937500	8.02271500
N	-10.62878000	-7.58733700	6.41408800
N	-10.95113800	-7.59182300	0.33519900
C	-11.10640600	-8.80551800	-0.19008800
C	-11.91485200	-9.02031900	-1.35076300
C	-12.10111700	-10.38513900	-1.84570500
C	-11.23647300	-11.41832500	-1.40299800
C	-18.26469400	-10.51544100	-3.29998900
C	-19.44458800	-10.49036700	-2.48279600
C	-19.65663900	-11.55452300	-1.49799700
C	-18.90575100	-12.75254300	-1.60795900
C	-19.80439300	-8.85326900	4.11637100
C	-18.99550600	-8.63890000	5.27682400
C	-18.62828700	-9.78492200	6.11001100
C	-19.33047700	-11.00920600	5.97164800
C	-12.53655800	-8.65874200	7.43195100
C	-11.35713300	-8.68317400	6.61403000
C	-10.97873800	-9.92776000	5.93947400
C	-11.55511800	-11.14821900	6.37470500
C	-10.48805700	-9.95659800	0.46951400
C	-10.14563300	-9.87334100	1.82717500
C	-10.40614900	-11.19770700	-0.21171000
C	-9.71495500	-10.98954800	2.54851900
C	-9.96210700	-11.04352900	4.01613100
C	-17.29914700	-11.60462500	-3.13106500
C	-15.95668300	-11.42737200	-3.50505800
C	-17.70006300	-12.77821200	-2.44329600
C	-14.97950700	-12.37549800	-3.18365200
C	-13.55354800	-12.00903900	-2.95949400
C	-13.33581500	-9.87873000	7.57319500
C	-14.69670100	-9.80033600	7.91289300
C	-12.76081400	-11.12313900	7.21002600
C	-15.52442900	-10.92733400	7.87000300
C	-16.98328600	-10.83708800	7.58447500
C	-20.24189000	-10.21258300	3.79497700
C	-20.56693000	-10.53870400	2.47006000

C	-20.16078200	-11.22932300	4.78025400
C	-20.82207400	-11.85456800	2.07614900
C	-20.54207000	-12.25725600	0.66995000
C	-19.99138800	-13.53688900	0.42280500
C	-17.83841700	-11.96357100	7.65025300
C	-10.33130300	-12.27759600	4.60143700
C	-12.54744200	-12.98121200	-2.74226800
C	-20.47279600	-11.33141700	-0.37656200
C	-20.99992100	-12.80170000	3.11341700
C	-15.44090400	-13.63373200	-2.73002100
C	-13.23656900	-10.69433800	-2.60892800
C	-9.38537200	-12.14127200	1.79387500
C	-10.18113800	-9.89449400	4.78350500
C	-14.88212700	-12.18259900	7.75355700
C	-17.47520000	-9.71931000	6.90594400
C	-16.76478800	-13.83171400	-2.38134600
C	-19.20603800	-13.77970200	-0.68971000
C	-9.72378500	-12.24056800	0.45397500
C	-11.42402200	-12.69230000	-1.98450200
C	-11.09553400	-12.32765200	5.75331900
C	-13.53720000	-12.27675200	7.44417500
C	-18.97673200	-12.04545600	6.86459900
C	-20.67632400	-12.49610000	4.42553600
O	-13.43400200	-3.27810200	-2.05464300
O	-11.98436200	-2.89286400	0.02625100
O	-19.48077800	-5.42944600	-6.20631000
O	-21.59090400	-5.38459700	-4.74538200
O	-19.76350100	-3.14382000	2.33389500
O	-18.31396200	-2.75930300	4.41498300
O	-12.10242800	-2.86962900	8.87809200
O	-9.99404500	-2.91297800	7.41462900
C	-22.79522400	-5.30574700	-3.99667400
C	-18.35450100	-5.40033800	-7.07108800
C	-14.25975900	-3.41067000	-3.20252600
C	-11.20759500	-2.59948700	1.17849300
C	-20.55201900	-3.27663200	1.16014800
C	-17.50024900	-2.46700300	5.54172200
C	-13.23690600	-2.77341900	9.72714000
C	-8.80010400	-2.86453300	6.64695000
H	-17.78289100	-7.55079300	-5.81857800
H	-21.88613100	-7.46363000	-2.97788600
H	-20.59522100	-5.72197700	1.89388200
H	-17.77359200	-4.97386700	5.94340100
H	-13.47686200	-5.23556500	9.09431300
H	-9.37662500	-5.32000900	6.24916700
H	-10.80697300	-5.12048700	1.11424000

H	-13.62793300	-5.87008800	-2.93552000
H	-10.37979500	-8.94420100	2.33257000
H	-15.68540300	-10.47219600	-3.94101900
H	-15.10797500	-8.81230700	8.08804200
H	-20.45678400	-9.75184900	1.73366700
H	-20.06609600	-14.31266700	1.17784500
H	-17.56252500	-12.82053200	8.25824800
H	-10.13343300	-13.20600700	4.07568000
H	-12.68852000	-13.99809000	-3.09752500
H	-20.94871100	-10.36040100	-0.29497500
H	-21.31255700	-13.81478200	2.87660100
H	-14.73034600	-14.42639100	-2.51947700
H	-13.94187700	-9.89021700	-2.78056600
H	-8.93742700	-13.00163700	2.28304100
H	-9.84544500	-8.92201800	4.44053200
H	-15.47006700	-13.09448600	7.77154100
H	-16.89317700	-8.80759800	6.84609700
H	-17.04193700	-14.78257700	-1.93915900
H	-18.72190600	-14.74660300	-0.77453900
H	-9.54038600	-13.18114500	-0.05569400
H	-10.73113800	-13.49763300	-1.76216900
H	-11.43985000	-13.29651800	6.09860300
H	-13.12073100	-13.26146700	7.26153300
H	-19.54517500	-12.97002800	6.87550700
H	-20.73459600	-13.28558200	5.16810900
H	-23.29692200	-4.39805200	-4.33572200
H	-23.43925600	-6.17429600	-4.18419100
H	-22.59294400	-5.23376000	-2.92012300
H	-18.46929700	-4.50101800	-7.67822200
H	-17.41621200	-5.34383500	-6.50410200
H	-18.32845900	-6.28329400	-7.72226100
H	-14.60854100	-2.40323200	-3.43496100
H	-13.69608700	-3.81069300	-4.05523000
H	-15.12066700	-4.06103200	-3.00144200
H	-11.29117000	-1.52158800	1.32599800
H	-11.59271700	-3.12301400	2.06289700
H	-10.15431500	-2.86971800	1.02877000
H	-20.61793000	-2.27507200	0.73220100
H	-20.08064300	-3.95528700	0.43778800
H	-21.55952700	-3.64297100	1.39588500
H	-17.30176800	-1.39510900	5.49419000
H	-18.01830800	-2.70393600	6.47997900
H	-16.55239000	-3.01893200	5.50301300
H	-13.26111200	-1.73936100	10.07456400
H	-14.16342200	-3.00053600	9.18397000
H	-13.14974900	-3.44893900	10.58759600

H	-8.43778100	-1.83832400	6.72558600
H	-8.04309000	-3.55354900	7.04255100
H	-8.99177800	-3.10705800	5.59362500

1' – transition state (Figure S13)

Zero-point correction= 1.237291 (Hartree/Particle)
Thermal correction to Energy= 1.316311
Thermal correction to Enthalpy= 1.317255
Thermal correction to Gibbs Free Energy= 1.120297
Sum of electronic and zero-point Energies= -4425.636131
Sum of electronic and thermal Energies= -4425.557112
Sum of electronic and thermal Enthalpies= -4425.556168
Sum of electronic and thermal Free Energies= -4425.753125

C	-3.48398600	-0.34589100	-3.75631200
C	-4.58704300	-1.13973300	-3.96469200
C	-5.65067200	-1.16264600	-3.01973000
C	-5.56149300	-0.35064000	-1.84314400
C	-4.41167000	0.46295900	-1.64283100
C	-3.39394200	0.47451100	-2.56725000
C	-6.31854700	-1.14518400	10.51988700
C	-6.73603100	-1.15695900	9.21019100
C	-6.57846800	-2.32484300	8.41180600
C	-5.97367800	-3.48946600	8.98346100
C	-5.55053900	-3.46082000	10.34223300
C	-5.71321100	-2.32557600	11.10017500
C	2.05317800	-10.85266900	1.93533300
C	1.11804100	-10.64727400	2.92216000
C	-0.22479700	-11.08405100	2.74834500
C	-0.59755600	-11.74037300	1.53110100
C	0.38269800	-11.94235300	0.51963500
C	1.67666300	-11.51614200	0.70530900
C	-14.42337100	-11.94229800	0.36049900
C	-13.08217300	-12.20800400	0.21984100
C	-12.24139200	-11.31904100	-0.50770700
C	-12.80623100	-10.14014700	-1.09413100
C	-14.19709400	-9.88048700	-0.93693100
C	-14.99431800	-10.75012200	-0.23173200
N	-12.04023500	-9.27574300	-1.78802200
N	-6.72282400	-1.95264400	-3.24205300
N	-6.54492800	-0.35306800	-0.91777700
N	-7.00896400	-2.32235500	7.13455800
N	-5.79066000	-4.60645000	8.25162100
N	-1.12845000	-10.86461900	3.72762600
N	-1.86359600	-12.16291400	1.32625200

N	-10.92841600	-11.59456400	-0.63276500
C	-10.18190200	-10.74305100	-1.33534100
C	-10.74646000	-9.56608700	-1.92246600
C	-9.88031000	-8.63858700	-2.65241000
C	-8.55905400	-9.02614100	-2.99167400
C	-7.70175500	-1.92086600	-2.34157100
C	-7.60998000	-1.11066400	-1.16301900
C	-8.67273400	-1.21349900	-0.16035600
C	-9.94471700	-1.70839600	-0.54557700
C	-6.84360300	-3.43065300	6.41484300
C	-6.19995600	-4.59992700	6.98442600
C	-5.92612900	-5.77969800	6.15427300
C	-6.34460700	-5.72372000	4.80836800
C	-2.36372200	-11.31528600	3.52876300
C	-2.73736000	-11.97439600	2.31161100
C	-4.13373100	-12.37757700	2.12833100
C	-4.96909000	-12.50707600	3.26639800
C	-8.74593700	-10.99544600	-1.46875300
C	-8.12019800	-11.90393800	-0.60103200
C	-7.97847800	-10.23025200	-2.38340500
C	-6.73506800	-12.09164400	-0.58618900
C	-6.05439700	-12.62842800	0.62903300
C	-8.87138600	-2.78523400	-2.51477100
C	-8.76037800	-3.97888200	-3.24722600
C	-10.04950500	-2.51133500	-1.77526100
C	-9.79543300	-4.91824900	-3.28231800
C	-9.49939300	-6.36416800	-3.48974100
C	-3.40411300	-11.04112900	4.52292900
C	-3.35309600	-9.84737200	5.26637500
C	-4.59741100	-11.80717200	4.50626700
C	-4.47470500	-9.39357200	5.96389800
C	-4.91234600	-7.96627000	5.75405300
C	-7.38788600	-3.46789300	5.05180400
C	-8.07506600	-2.37715900	4.45031900
C	-7.22526300	-4.66966800	4.33229500
C	-8.67199300	-2.52836000	3.20096800
C	-9.23638000	-1.56353100	2.18382300
C	-10.59044800	-1.69715600	1.80035900
C	-5.17417700	-7.77985900	4.37225700
C	-6.79732900	-13.06357100	1.75553200
C	-8.26458000	-6.82247100	-4.01023900
C	-8.33921600	-1.13138100	1.20487200
C	-8.66043600	-3.81454200	2.60255000
C	-11.05513300	-4.47907100	-2.80385400
C	-10.32095500	-7.32961600	-2.90158600
C	-6.01334500	-11.47994300	-1.64125700

C	-4.68380000	-12.43978400	0.83725300
C	-5.49184700	-10.33991000	6.22930000
C	-5.25276800	-6.93673500	6.63147300
C	-11.17684700	-3.31100000	-2.07058500
C	-10.94101300	-1.74744300	0.45816400
C	-6.61568300	-10.58113800	-2.50632300
C	-7.81133300	-8.10861800	-3.76412000
C	-6.27033200	-13.00496200	3.03397600
C	-5.54198100	-11.53356100	5.52313500
C	-5.88906100	-6.70369900	3.91371200
C	-7.93881900	-4.84976500	3.13696500
O	-16.32430800	-10.60429600	-0.02088700
O	-15.31340600	-12.71534100	1.02734300
O	-2.41849400	-0.24518800	-4.58733700
O	-2.25868600	1.20846000	-2.47879900
O	-6.41926600	-0.09395400	11.36888300
O	-5.34763600	-2.18595300	12.39743700
O	3.35469200	-10.48119300	1.99480000
O	2.68758500	-11.65814300	-0.18568000
C	-2.09569200	2.03978900	-1.33813100
C	-2.43313000	-1.01904500	-5.77842500
C	-16.96030600	-9.45963900	-0.57204700
C	-14.83144300	-13.90561200	1.63533900
C	-7.00336700	1.10252300	10.87351300
C	-4.74460900	-3.30126800	13.03818500
C	3.80214700	-9.82515200	3.17298400
C	2.39821100	-12.30424700	-1.41721600
H	-4.68815600	-1.76557800	-4.84258500
H	-4.37809500	1.06244700	-0.74169500
H	-7.19608600	-0.29431100	8.74457000
H	-5.09838400	-4.36009300	10.74159800
H	1.36344400	-10.15431500	3.85454300
H	0.06604000	-12.44260100	-0.38707200
H	-12.62208200	-13.08959500	0.64841900
H	-14.59023600	-8.98080700	-1.39363300
H	-8.75869300	-12.37000000	0.13844100
H	-7.78171600	-4.20921700	-3.65177500
H	-2.51915600	-9.17791900	5.07993800
H	-8.10754800	-1.43301900	4.98398900
H	-11.33659300	-1.94855900	2.55017200
H	-4.86322000	-8.54535400	3.67062800
H	-7.83681000	-13.35340500	1.64507400
H	-7.61941900	-6.14113500	-4.55671600
H	-7.29408900	-0.97775900	1.45430900
H	-9.18398000	-3.96126700	1.66390700
H	-11.93105100	-5.10882800	-2.92530400

H	-11.29292200	-7.06653900	-2.50349200
H	-4.94587900	-11.64745200	-1.74066200
H	-4.01853500	-12.18896300	0.01963600
H	-6.34471800	-10.05098300	6.83855600
H	-5.01808100	-6.99429000	7.68937000
H	-12.14022500	-3.07724000	-1.62829900
H	-11.96413000	-2.00359900	0.20146500
H	-5.99270600	-10.08392900	-3.24285100
H	-6.82345100	-8.38124800	-4.12134000
H	-6.92179900	-13.23711100	3.87051300
H	-6.42219800	-12.15911500	5.63233300
H	-6.09318100	-6.61674600	2.85306700
H	-7.93085600	-5.80796000	2.63094900
H	-1.13084100	2.53286300	-1.46604900
H	-2.88979400	2.79493900	-1.27836000
H	-2.08764100	1.44997000	-0.41268200
H	-1.49810200	-0.79055700	-6.29221300
H	-2.47751500	-2.09291100	-5.55595500
H	-3.28123600	-0.74785800	-6.42006700
H	-18.01089000	-9.53875900	-0.28857800
H	-16.53764200	-8.53310700	-0.16287900
H	-16.87447200	-9.44389100	-1.66603800
H	-15.69841100	-14.36882900	2.10875800
H	-14.40904800	-14.59124200	0.88975700
H	-14.07116400	-13.68520200	2.39553300
H	-6.98523000	1.80810900	11.70555300
H	-6.42672700	1.50973600	10.03315400
H	-8.04019500	0.93765600	10.55361300
H	-4.53338500	-2.97859500	14.05883900
H	-5.42222400	-4.16440000	13.05805600
H	-3.80871900	-3.58842400	12.54202500
H	4.86171500	-9.61940800	3.01359100
H	3.26430500	-8.88199400	3.33309300
H	3.68030300	-10.46490500	4.05632100
H	3.33612000	-12.31415800	-1.97460400
H	2.05489800	-13.33419300	-1.25647500
H	1.63775000	-11.75493500	-1.98697400

$[(C_{60})_2 \subset \mathbf{1'}]$

Zero-point correction= 1.999241 (Hartree/Particle)
Thermal correction to Energy= 2.122814
Thermal correction to Enthalpy= 2.123759
Thermal correction to Gibbs Free Energy= 1.849991
Sum of electronic and zero-point Energies= -8998.524277

Sum of electronic and thermal Energies= -8998.400703
Sum of electronic and thermal Enthalpies= -8998.399759
Sum of electronic and thermal Free Energies= -8998.673526

C	6.87804500	-6.13521200	2.48335600
C	5.69551800	-5.84134000	3.11822400
H	5.66190300	-5.49980300	4.14435200
C	4.46525500	-5.89599800	2.40946600
C	4.46459100	-6.30043200	1.03471600
C	5.68929300	-6.66814900	0.41543800
H	5.65076100	-6.94830900	-0.62894300
C	6.87405600	-6.56679200	1.10274500
C	-6.89264600	-2.62455700	-6.23580000
C	-5.69847600	-3.23740600	-5.94216200
H	-5.63975300	-4.27814500	-5.65158600
C	-4.49086900	-2.48873400	-5.92965100
C	-4.51778600	-1.10292400	-6.28914500
C	-5.75645900	-0.49568500	-6.62591700
H	-5.74340900	0.56056800	-6.85987300
C	-6.92286700	-1.22064200	-6.57813600
C	6.79942500	6.19694900	-2.56346100
C	5.60504600	5.92133100	-3.18459600
H	5.55255600	5.60142300	-4.21691800
C	4.38995900	5.94906400	-2.44957500
C	4.41097500	6.33644300	-1.07153000
C	5.64918300	6.67098400	-0.46012200
H	5.62992400	6.92590100	0.59130500
C	6.82251100	6.57395400	-1.16806700
C	-6.81419200	2.55622500	6.27114900
C	-5.62413800	3.17999800	5.98244000
H	-5.57342800	4.22297400	5.69866400
C	-4.41001900	2.44218700	5.97012300
C	-4.42859500	1.05175000	6.31287700
C	-5.66228000	0.43415500	6.64917000
H	-5.64143300	-0.62353800	6.87598700
C	-6.83422000	1.15133100	6.60800100
N	-3.30791900	0.30469700	6.25078500
N	3.33285000	-5.48624500	3.01637800
N	3.33841800	-6.25408800	0.29645000
N	-3.35388500	-3.07317700	-5.49989500
N	-3.40381100	-0.34477900	-6.22766600
N	3.25346900	5.51815100	-3.03476500
N	3.29225200	6.29206200	-0.31896300
N	-3.27467400	3.04103600	5.55745800
C	-2.17990800	2.28953100	5.47410700
C	-2.19356300	0.90168800	5.83424500

C	-0.98000700	0.10696400	5.65477400
C	0.25826100	0.77572200	5.48772700
C	2.22850300	-5.43592500	2.27801400
C	2.23272200	-5.81813000	0.89536100
C	1.01164400	-5.65884400	0.11031200
C	-0.22436400	-5.51461200	0.78788100
C	-2.26625900	-2.31176700	-5.41672800
C	-2.28850400	-0.92677500	-5.79300600
C	-1.08110500	-0.12137900	-5.61243800
C	0.16140400	-0.78521900	-5.45582000
C	2.16075000	5.45513100	-2.27880600
C	2.18134300	5.84983400	-0.89956200
C	0.97510900	5.67638500	-0.09377700
C	-0.27024800	5.51907400	-0.75113200
C	-0.96408100	2.86341700	4.90404000
C	-1.04267100	3.97823000	4.05396700
C	0.26549600	2.18464100	5.08626500
C	0.07643000	4.45364000	3.36227700
H	-2.03263200	4.37649200	3.87145700
C	-0.04853400	5.19433800	2.07592400
C	1.00531200	-4.88715500	2.85888600
C	1.07946000	-4.02429000	3.96278000
C	-0.22755500	-5.09932800	2.19367800
C	-0.04744900	-3.34882900	4.44370100
H	2.07090200	-3.81842700	4.34620000
C	0.06419700	-2.05426100	5.17277000
C	0.93464800	4.88804000	-2.83685500
C	0.99392900	4.01830400	-3.93694300
C	-0.29061000	5.10516000	-2.15811800
C	-0.14061700	3.34071200	-4.40117300
H	1.97982500	3.81332900	-4.33438300
C	-0.04076500	2.04347500	-5.12891400
C	-1.04173000	-2.87802600	-4.85559400
C	-1.09717100	-3.99126000	-4.00206100
C	0.18161200	-2.19727600	-5.06634900
C	0.03956200	-4.45903000	-3.33186800
H	-2.08118300	-4.39349600	-3.79747800
C	-0.05569200	-5.19839800	-2.04259300
C	-1.30055300	-5.35926700	-1.38865700
H	-2.22456500	-5.23970900	-1.94153100
C	1.21257000	1.39988300	-5.26671000
H	2.12759500	1.96369200	-5.13549900
C	-1.30662600	5.33959000	1.44377800
H	-2.21981100	5.20218500	2.01029900
C	1.31714900	-1.40729500	5.30158800
H	2.23460100	-1.96619700	5.16264500

C	1.08053900	-5.50052700	-1.28189600
H	2.07046100	-5.50802500	-1.71950800
C	1.28105500	-3.94066400	-3.77340000
H	2.20838600	-4.31798200	-3.35896600
C	-1.29649400	-3.78531600	3.94082400
H	-2.21418900	-3.36296700	4.33127500
C	-1.06064500	-1.28551200	5.49413700
H	-2.05354800	-1.71716700	5.51922300
C	1.32893900	3.93647700	3.77437900
H	2.24331500	4.32720300	3.34635700
C	1.07044900	5.51122800	1.29591400
H	2.06822900	5.52547800	1.71605500
C	-1.38194400	3.78703100	-3.88929700
H	-2.30633400	3.36560800	-4.26332900
C	-1.16612400	1.27122300	-5.44416700
H	-2.16031800	1.70083400	-5.46114500
H	-2.36438000	-4.82993700	2.43154400
H	-2.36147300	-5.53370100	0.44451600
H	2.39434100	0.41886200	5.44937100
H	2.40077200	2.42030200	4.80604500
H	-2.40195200	5.49657300	-0.36859600
H	-2.43039900	4.86116700	-2.38682600
H	2.29590300	-0.42106900	-5.40913900
H	2.32283400	-2.43496900	-4.84550200
C	-1.38414900	-4.63111300	2.84891500
C	-1.38133100	-5.52036300	-0.01543900
C	1.42078800	2.83807300	4.61037400
C	1.41071300	-0.03558300	5.45798300
C	-1.41342600	5.50355400	0.07252000
C	-1.45504800	4.64374400	-2.80421000
C	1.31060300	0.02931200	-5.42392200
C	1.34860100	-2.85073500	-4.62258700
O	-8.06852100	0.64557000	6.83100400
O	-8.03295600	3.14118700	6.23539000
O	8.10850100	-6.02986500	3.03349400
O	8.10142500	-6.80244700	0.58677100
O	-8.10702100	-3.21963500	-6.20635100
O	-8.16124800	-0.72461300	-6.80116700
O	8.01961600	6.10686700	-3.13932200
O	8.06108900	6.77005000	-0.66111300
C	8.18379600	-7.04907900	-0.81078400
H	9.24740200	-7.14095500	-1.03351000
H	7.66922600	-7.97882200	-1.08352800
H	7.75428100	-6.21520200	-1.38032300
C	8.19784600	-5.42321800	4.31629400
H	7.75761700	-4.41825800	4.30207900

H	7.69809800	-6.03013000	5.08147000
H	9.26329800	-5.35869500	4.53996600
C	-8.17358400	-0.76079600	7.00752300
H	-7.65078200	-1.08972800	7.91424800
H	-9.23973600	-0.96874800	7.10425200
H	-7.76686300	-1.29536000	6.13979200
C	-8.10134000	4.47378500	5.74568000
H	-7.69534700	4.53670400	4.72809300
H	-9.16059500	4.73312500	5.73856100
H	-7.55717600	5.16784300	6.39823200
C	-8.16428800	-4.55869800	-5.73457400
H	-9.22058600	-4.82998600	-5.73856000
H	-7.60722200	-5.23794800	-6.39190500
H	-7.76519900	-4.63135800	-4.71491000
C	-8.27499700	0.67914600	-6.99155700
H	-9.34274800	0.88037000	-7.08532100
H	-7.86673700	1.22465700	-6.13147400
H	-7.75827300	1.00144900	-7.90420200
C	8.08097800	5.56984800	-4.45389800
H	7.56190600	6.21493700	-5.17365800
H	9.14108300	5.52065600	-4.70505700
H	7.64332300	4.56400700	-4.48585900
C	8.16873400	6.93530900	0.74675300
H	9.23717800	6.99531600	0.95725000
H	7.67672200	7.85738800	1.08041200
H	7.73235700	6.07730000	1.27364800
C	4.40732200	2.02482600	2.78842300
C	3.77381700	2.77293200	1.71312300
C	2.64492400	2.25590700	1.07264800
C	2.09828700	0.97034700	1.48115100
C	2.70943100	0.25204400	2.50766200
C	3.88613400	0.79069500	3.17507000
C	5.84752000	2.20631400	2.68119500
C	6.10644000	3.06657700	1.53658800
C	4.82465900	3.41128600	0.94009700
C	4.70770800	3.49401300	-0.44491000
C	2.51855200	2.35812900	-0.37145300
C	1.63675300	0.27605200	0.28707100
C	1.80027900	-1.10585100	0.17528300
C	2.43459200	-1.85181400	1.25207700
C	2.87822200	-1.18699000	2.39353800
C	4.16054100	-1.53728700	2.99223500
C	4.78212800	-0.31422600	3.47775200
C	6.16442600	-0.14112000	3.37422500
C	6.70740600	1.14486000	2.96581000
C	7.21651100	2.83091600	0.72228800

C	8.11144400	1.72191400	1.01790300
C	7.86377100	0.89786900	2.11667900
C	8.03642400	-0.54183500	1.99945300
C	6.98626800	-1.18398200	2.77849500
C	6.39103600	-2.35542200	2.31106500
C	4.95008300	-2.53005600	2.41669600
C	4.49289000	-3.21037000	1.21756200
C	3.26070900	-2.89048200	0.65198200
C	1.89246500	1.13563200	-0.85977800
C	4.50340300	-2.17039800	-2.75044200
C	3.64499900	-1.10611000	-3.02625700
C	4.18821700	0.17739600	-3.43717000
C	5.56881400	0.34952900	-3.55103900
C	6.46522200	-0.75641700	-3.25411900
C	6.57577800	-2.73836500	-1.78737200
C	5.52521900	-3.37781400	-1.01205600
C	4.24241800	-3.03208900	-1.60725800
C	3.13379900	-2.79085500	-0.79356000
C	2.23217200	-1.68613000	-1.08835300
C	2.48303300	-0.85990600	-2.18375900
C	3.36559000	1.21911100	-2.84088600
C	3.96105000	2.38842000	-2.37836200
C	5.40147700	2.56703200	-2.49023200
C	6.19009800	1.57348700	-3.06763800
C	7.47138800	1.22336900	-2.46901900
C	7.64016400	-0.21699300	-2.58479100
C	8.24509000	-0.93394700	-1.55162200
C	7.70355000	-2.22162700	-1.14491200
C	5.64566600	-3.46010400	0.37290000
C	6.82117700	-2.93510400	1.04486800
C	7.82921100	-2.32356900	0.30099600
C	8.44851900	-1.09907500	0.78859100
C	8.70571900	-0.24100900	-0.35744100
C	8.54143000	1.14014800	-0.24534000
C	7.91196000	1.88709900	-1.32311700
C	7.09164000	2.92995700	-0.72476900
C	5.86165400	3.25125100	-1.29252100
C	2.30896600	0.57823100	-2.06798600
C	3.53279900	2.96192500	-1.11166500
C	5.94361300	-1.99015400	-2.86358900
C	-5.56949200	1.67705100	3.12174100
C	-6.04368600	2.67961000	2.18215800
C	-7.23358600	2.46826600	1.48353900
C	-7.99843800	1.24936100	1.70320500
C	-7.54372000	0.29362000	2.61332000
C	-6.30403900	0.51389200	3.33999800

C	-4.12134000	1.61350500	3.01641000
C	-3.69340200	2.57740700	2.01950500
C	-4.88304100	3.23576600	1.49840100
C	-4.96180300	3.55414600	0.14293400
C	-7.31353200	2.80126800	0.06873100
C	-8.55010800	0.82911500	0.42434800
C	-8.62713400	-0.52767100	0.10813100
C	-8.15440100	-1.52391200	1.05754800
C	-7.62442800	-1.12229600	2.28403600
C	-6.43402600	-1.77510000	2.81065200
C	-5.61727300	-0.76399000	3.46237200
C	-4.22667900	-0.82055200	3.36365400
C	-3.46195600	0.39569000	3.13678000
C	-2.62733300	2.27242900	1.17250000
C	-1.93313300	0.99863500	1.29706700
C	-2.34436800	0.07852800	2.26238300
C	-2.42725600	-1.33584200	1.93277400
C	-3.59133500	-1.88892600	2.61298600
C	-4.37556000	-2.85926300	1.98861400
C	-5.82517200	-2.80313900	2.08847800
C	-6.37992600	-3.22225100	0.81021500
C	-7.52055100	-2.59670500	0.30564400
C	-8.12779800	1.78801700	-0.58560400
C	-6.11637800	-1.60618600	-2.96474500
C	-6.77527800	-0.38371200	-3.08782500
C	-6.00799900	0.83539800	-3.30616200
C	-4.61647400	0.77620400	-3.38733500
C	-3.93349200	-0.49820700	-3.25180700
C	-4.18952300	-2.66273900	-2.11267600
C	-5.34876100	-3.22267500	-1.43336600
C	-6.54003700	-2.56959300	-1.96019900
C	-7.60284100	-2.26329000	-1.10871300
C	-8.28683300	-0.98462300	-1.23063800
C	-7.88198900	-0.06518100	-2.19951200
C	-6.64304900	1.90631900	-2.55411500
C	-5.86046800	2.87649800	-1.92512200
C	-4.41030600	2.81315700	-2.01968000
C	-3.79907300	1.78598900	-2.73853100
C	-2.60453700	1.13540600	-2.21454600
C	-2.68722900	-0.27884800	-2.53925400
C	-2.22536400	-1.23570600	-1.63703400
C	-3.00010800	-2.44841000	-1.41545000
C	-5.27097000	-3.54093900	-0.07765000
C	-4.03236400	-3.31277700	0.65070400
C	-2.92346600	-2.77562800	-0.00253500
C	-2.09582300	-1.77387300	0.65175600

C	-1.66962500	-0.81626900	-0.35884700
C	-1.59197200	0.54119600	-0.04312100
C	-2.06938600	1.53698500	-0.99218000
C	-2.71356300	2.60123200	-0.23971300
C	-3.85508600	3.22698200	-0.74199000
C	-7.80090600	1.35042500	-1.86946200
C	-6.20273900	3.33323800	-0.58706400
C	-4.66605200	-1.66145000	-3.05035200

1'' (1,3-alternate, R= 3,5-di-*tert*-butylphenyl)

Zero-point correction= 3.478261 (Hartree/Particle)
Thermal correction to Energy= 3.668941
Thermal correction to Enthalpy= 3.669885
Thermal correction to Gibbs Free Energy= 3.222534
Sum of electronic and zero-point Energies= -8427.058721
Sum of electronic and thermal Energies= -8426.868041
Sum of electronic and thermal Enthalpies= -8426.867097
Sum of electronic and thermal Free Energies= -8427.314448

C	16.11265800	10.85098300	4.24672200
C	16.02945500	11.19605800	2.92439400
C	14.79581800	11.10019200	2.23186400
C	13.64174300	10.61109800	2.92261200
C	13.75439100	10.24687800	4.28838500
C	14.95037300	10.36878100	4.94387600
C	5.12666500	5.22753800	-7.03788000
C	5.90101600	4.41678400	-6.24968900
C	6.35138800	4.86139100	-4.98156000
C	5.99527000	6.17208600	-4.53077100
C	5.20195900	6.99802500	-5.36582900
C	4.76772900	6.54311000	-6.58293500
C	18.66866900	1.22401900	1.07183100
C	18.57347800	1.68451000	-0.21449400
C	17.35560300	1.57257600	-0.93220200
C	16.21325700	1.00088500	-0.28786700
C	16.33056100	0.53874900	1.04711100
C	17.52240800	0.63547300	1.71404500
C	13.21352400	8.80320200	-11.76400600
C	14.09385600	8.06037200	-11.02395200
C	14.53576400	8.52035900	-9.75736900
C	14.06413800	9.77929400	-9.26599000
C	13.12592400	10.51475800	-10.03407800
C	12.70810400	10.04922300	-11.25187700
N	14.50673400	10.26708200	-8.07472300

N	14.71290100	11.47878000	0.92667500
N	12.44551900	10.50145600	2.28097200
N	7.12773300	4.05143400	-4.20926500
N	6.42464600	6.62879700	-3.32240200
N	17.28020700	2.00365800	-2.22151300
N	15.02572900	0.89960000	-0.94618500
N	15.39598100	7.76815400	-9.01733600
C	15.83513300	8.26873700	-7.85667900
C	15.40274900	9.54710700	-7.38893400
C	15.89925600	10.04521600	-6.10840400
C	16.98904900	9.40002300	-5.47133300
C	13.51869100	11.41913800	0.32612500
C	12.37009300	10.91641400	1.01112700
C	11.10903000	10.78843200	0.28465100
C	10.93553200	11.46212200	-0.94979300
C	7.51542500	4.50147400	-3.01048800
C	7.15727500	5.80941700	-2.55980000
C	7.67154000	6.28878300	-1.27941800
C	8.26155200	5.38049300	-0.36601600
C	16.12247200	1.84674000	-2.87392400
C	14.97551700	1.29652500	-2.22294900
C	13.70658600	1.24045000	-2.94465200
C	13.68777500	1.40264400	-4.35203200
C	16.70128900	7.45747700	-7.00458400
C	16.68106700	6.06311700	-7.15271800
C	17.38436500	8.05533800	-5.91725000
C	17.31075400	5.22057700	-6.23350200
C	11.26768300	1.35159500	-2.84013100
C	13.39773900	11.81139800	-1.07579800
C	14.54650000	11.83762500	-1.87919400
C	12.11499700	11.99243100	-1.65016800
C	14.46903900	12.03478800	-3.25988300
C	15.52176600	11.46100600	-4.15262500
C	16.00689200	2.30613900	-4.25580000
C	16.93028900	3.24200500	-4.74384000
C	14.87746100	1.93987900	-5.02959500
C	16.76969000	3.84617900	-5.99318800
C	8.40121600	8.20055800	0.05674800
C	8.39003700	3.67643200	-2.18011200
C	9.12418000	2.64599700	-2.78508100
C	8.63142000	4.03440800	-0.83019200
C	10.11657600	1.94803400	-2.09294700
C	9.02151300	9.55929000	-0.02995000
C	8.73655400	10.42439400	-1.11710900
C	8.76801400	7.28359000	1.07433100
C	11.25553700	1.26099800	-4.25536600

C	16.75120100	10.98396300	-3.63208500
C	10.15744200	9.85755900	0.72667000
C	10.17391800	2.14977700	-0.69045900
C	13.21758300	12.45796100	-3.77454500
C	15.18807000	11.05653200	-5.44713300
C	18.18976600	5.83618900	-5.30636100
C	12.50915200	1.21139200	-2.21492000
C	15.78724900	3.28497200	-6.84838100
C	7.74269200	7.67080000	-1.05502300
C	12.07555000	12.43490200	-2.99192400
C	9.66779600	11.34610100	-1.56368800
C	18.22504200	7.21214700	-5.15503700
C	17.46017800	9.98160300	-4.27246600
C	12.43052900	1.28666500	-4.98735100
C	14.86851800	2.36193300	-6.37834800
C	8.69938800	5.91578300	0.86712900
C	9.45312900	3.16252000	-0.08004100
O	11.78387000	10.68076900	-12.07433700
O	12.74174200	8.46235900	-13.02506700
O	17.26372200	10.92882600	5.02116600
O	15.16094500	10.06787400	6.28389800
O	4.64789500	4.90187400	-8.30037300
O	4.02119300	7.30378000	-7.47817500
O	19.80297500	1.28000000	1.86932100
O	17.74743700	0.19307600	3.01167000
H	16.89124900	11.56465000	2.38778000
H	12.87233700	9.88747000	4.79758100
H	6.18022900	3.42437300	-6.57079600
H	4.94030600	7.98558700	-5.01430200
H	19.42211100	2.12367900	-0.71751500
H	15.46164300	0.10179700	1.51664100
H	14.47456700	7.11779000	-11.38891100
H	12.76201100	11.45190900	-9.63944700
H	16.03058400	5.67721400	-7.92519900
H	15.47278500	11.55889500	-1.39619200
H	17.68842900	3.56977700	-4.04620700
H	8.97667300	2.52039500	-3.84862900
H	7.81534600	10.30536100	-1.67371800
H	9.19602100	7.64827100	1.99996500
H	10.31239000	1.26373300	-4.78736000
H	17.10626900	11.34305500	-2.67396600
H	10.42285600	9.28423300	1.60420300
H	10.85881100	1.56494900	-0.08912700
H	13.12679700	12.72108600	-4.82119500
H	14.29096200	11.40643200	-5.93877800
H	18.77843600	5.22501300	-4.63358600

H	12.60784300	1.21803000	-1.13826600
H	15.68694300	3.64613400	-7.86429800
H	7.38884100	8.30000200	-1.85958100
H	11.12559500	12.67466000	-3.45276600
H	9.44762300	11.91451800	-2.45849300
H	18.83648900	7.63101400	-4.36584000
H	18.34569900	9.58400200	-3.79269600
H	12.36793800	1.31465600	-6.06787100
H	14.07715700	2.03403300	-7.04061600
H	9.07914100	5.25548600	1.63659800
H	9.60137100	3.33909500	0.97783700
C	3.20700400	8.35468400	-6.97641000
C	2.00077100	8.05058100	-6.34600700
C	3.61113100	9.66335400	-7.18449300
C	1.17092100	9.08390000	-5.90778800
H	1.73070900	7.01283100	-6.21776000
C	2.79324300	10.72457400	-6.75838700
H	4.55133100	9.83804000	-7.69016300
C	1.58826000	10.41181400	-6.12277800
H	0.94811700	11.21447000	-5.78520400
C	4.80487700	3.58605900	-8.80877200
C	3.67114500	2.78690500	-8.89305700
C	6.05052200	3.14261900	-9.24197800
C	3.76656600	1.50188600	-9.44114300
H	2.73370200	3.19111400	-8.54179800
C	6.17793300	1.85586900	-9.78040500
H	6.89790200	3.80731200	-9.16184800
C	5.02642500	1.05993100	-9.87182800
H	5.11311900	0.06564000	-10.29259400
C	7.53082000	1.30489500	-10.27493000
C	2.54291900	0.57330700	-9.57606000
C	2.79428200	-0.72704300	-8.76612100
H	3.68216300	-1.25391700	-9.12960000
H	2.94080300	-0.49188900	-7.70648000
H	1.93159600	-1.39696000	-8.86222800
C	1.24893200	1.23226700	-9.04439000
H	1.33682000	1.47583200	-7.97972200
H	1.01172800	2.14577400	-9.60092400
H	0.41492400	0.53228800	-9.16609100
C	2.33056100	0.22401700	-11.07379800
H	2.14786300	1.13514600	-11.65350400
H	3.20824400	-0.28076200	-11.48972300
H	1.46574300	-0.44147800	-11.18117000
C	7.85879800	-0.01179600	-9.52067700
H	7.08887500	-0.77036900	-9.69212800
H	8.81847000	-0.41018400	-9.87072700

H	7.92721300	0.17438900	-8.44349400
C	7.43776100	1.02535300	-11.79909800
H	6.65139400	0.29599000	-12.01815400
H	7.21259100	1.95020600	-12.34095900
H	8.39206000	0.62586800	-12.16371100
C	8.68949000	2.29950900	-10.03144300
H	8.53255600	3.23602100	-10.57793100
H	8.80139500	2.52401200	-8.96476100
H	9.62487000	1.85373300	-10.38729800
C	3.24973300	12.17618600	-7.00818500
C	4.62055700	12.40883900	-6.31786300
H	5.38059800	11.72463500	-6.70813800
H	4.95822500	13.43679300	-6.49847000
H	4.53470700	12.25215600	-5.23720200
C	3.39051900	12.40574700	-8.53698200
H	3.72494500	13.43243000	-8.73095100
H	4.12162100	11.71749600	-8.97269800
H	2.42827100	12.24890600	-9.03595100
C	2.24621700	13.21273400	-6.45204300
H	2.62471200	14.22077600	-6.65471200
H	1.26660600	13.11419000	-6.93274500
H	2.12489600	13.10546100	-5.36837900
C	-0.17594900	8.81607200	-5.20655500
C	-0.14585300	9.44287700	-3.78640900
H	0.65611900	8.99413000	-3.19056200
H	0.02142000	10.52350900	-3.83475700
H	-1.10234700	9.26361200	-3.28118700
C	-1.32148700	9.45572900	-6.03657800
H	-1.18160400	10.53672200	-6.13635700
H	-1.35407700	9.01643800	-7.03940000
H	-2.28333300	9.27614200	-5.54169500
C	-0.46867800	7.30458800	-5.06202200
H	-0.52497900	6.81643300	-6.04142900
H	0.29955700	6.80783700	-4.45909700
H	-1.43353100	7.17342100	-4.55981900
C	18.46450800	11.40477900	4.42878600
C	18.74276500	12.76980000	4.46797200
C	19.35017600	10.49397700	3.87615700
C	19.94595300	13.24446000	3.94050900
H	18.01732300	13.43089100	4.91834800
C	20.57151600	10.94146800	3.34457700
H	19.08701500	9.44477800	3.88339600
C	20.84252300	12.31294000	3.38303600
H	21.77574400	12.67524600	2.97553000
C	14.07134800	9.60164400	7.06779600
C	13.85466100	8.23295600	7.17341600

C	13.28050300	10.52647100	7.73989500
C	12.81980700	7.75717800	7.98871100
H	14.50604600	7.56407700	6.63090900
C	12.23657000	10.07928900	8.55947000
H	13.50056400	11.57699100	7.62138100
C	12.02652800	8.69608200	8.66466500
H	11.22179700	8.33899200	9.29570400
C	11.32648400	11.05246300	9.33579700
C	11.44222200	10.75879100	10.85580700
H	10.79356200	11.44231400	11.41644300
H	11.14026300	9.73173700	11.08400800
H	12.47527600	10.89887700	11.19164100
C	9.85704700	10.85524400	8.87513700
H	9.19993200	11.53764900	9.42718200
H	9.76327900	11.06632000	7.80451400
H	9.52024900	9.82968200	9.05678300
C	11.71449400	12.53032700	9.09740800
H	12.73951100	12.72962600	9.42941000
H	11.62374300	12.79877700	8.03902100
H	11.03900200	13.17443100	9.67114700
C	12.53452200	6.25129800	8.15855000
C	13.52260100	5.37765000	7.35226700
H	13.45075800	5.58348700	6.27845300
H	14.55538100	5.54254600	7.67890500
H	13.28110400	4.32108800	7.51174600
C	11.09589800	5.94469700	7.66220700
H	10.35281800	6.51425000	8.22920800
H	10.99681800	6.20476000	6.60284800
H	10.87957600	4.87654300	7.78444300
C	12.66301900	5.87130400	9.65820800
H	13.67637900	6.08088700	10.01692400
H	11.95479900	6.43702100	10.27159600
H	12.45663600	4.80237200	9.78971900
C	21.56681600	9.91133700	2.77392000
C	20.31593800	14.74119700	3.95348300
C	19.21315600	15.60939500	4.60260500
H	18.26875200	15.52695900	4.05324400
H	19.04503200	15.32151000	5.64638200
H	19.52718400	16.65887500	4.58482500
C	21.62716900	14.93717700	4.76139800
H	22.45278400	14.37140300	4.31830200
H	21.90186900	15.99866700	4.77128100
H	21.49022200	14.59931200	5.79423400
C	20.52298700	15.22948600	2.49431700
H	19.60124500	15.10133100	1.91675600
H	20.79387500	16.29196100	2.49337800

H	21.32271200	14.66925800	1.99966800
C	20.87625800	9.07487400	1.66353200
H	20.55864500	9.72382500	0.84022200
H	21.57749500	8.32768000	1.27299300
H	19.99689700	8.55009400	2.04937700
C	22.82102500	10.57967700	2.16449800
H	23.48096700	9.80171600	1.76462800
H	22.55120900	11.25416700	1.34414800
H	23.37942200	11.14248300	2.92072700
C	22.02360900	8.97480200	3.92512200
H	22.51917800	9.55483800	4.71108900
H	21.16994000	8.45180200	4.36787400
H	22.72626600	8.22614800	3.54107900
C	13.18277400	7.25526600	-13.63110100
C	14.32238600	7.28067100	-14.42699900
C	12.43419600	6.09775000	-13.45347000
C	14.73651200	6.11395000	-15.08144100
H	14.85862900	8.21216200	-14.53129800
C	12.82178600	4.91755600	-14.10113600
H	11.55407200	6.14262000	-12.82937500
C	13.97334900	4.95063900	-14.90146600
H	14.28336800	4.04282300	-15.40441300
C	11.20633700	11.90787600	-11.65054000
C	10.01079400	11.86757900	-10.94299600
C	11.82461600	13.10683500	-11.98437200
C	9.39020000	13.06282700	-10.56060600
H	9.57958500	10.90382500	-10.71695600
C	11.22728700	14.31867900	-11.61295600
H	12.75154100	13.07556400	-12.53748700
C	10.01713200	14.26997500	-10.90419800
H	9.54715400	15.20158100	-10.61333100
C	15.98809700	6.07608100	-15.98150700
C	16.69557400	7.44918200	-16.05530500
H	17.57394700	7.36459200	-16.70463800
H	16.03344400	8.21438100	-16.47559600
H	17.03379500	7.77471100	-15.06529300
C	15.57123000	5.66590100	-17.41961900
H	14.86316000	6.39313900	-17.83116600
H	16.45571300	5.62996500	-18.06669700
H	15.09765200	4.67909100	-17.42740700
C	16.99534200	5.04037800	-15.41319800
H	16.55344900	4.03970100	-15.37402600
H	17.88619700	4.99997100	-16.05114800
H	17.30086400	5.32417700	-14.40042200
C	12.02642000	3.60382000	-13.96217500
C	12.94196300	2.51488100	-13.34097900

H	12.38844700	1.57295600	-13.24643000
H	13.82278600	2.33604800	-13.96567000
H	13.28042300	2.82588000	-12.34673300
C	10.78368200	3.76751300	-13.05714000
H	11.06825400	4.06255500	-12.04093200
H	10.09272400	4.51395100	-13.46466100
H	10.25427700	2.81024600	-12.99732300
C	11.54653000	3.14533900	-15.36570100
H	10.89677500	3.90614200	-15.81122500
H	12.39379000	2.97708300	-16.03781500
H	10.98352400	2.20848000	-15.27805300
C	8.05737000	13.08120900	-9.78500100
C	8.26465500	13.80166000	-8.42555800
H	7.32096700	13.82041900	-7.86738800
H	9.01574500	13.27409200	-7.82779400
H	8.60048400	14.83315200	-8.57212600
C	7.53104400	11.65459700	-9.50212400
H	7.34352900	11.10865000	-10.43331500
H	8.23847700	11.08394200	-8.89024200
H	6.58572200	11.72568000	-8.95339500
C	6.98950600	13.83737400	-10.62050000
H	6.83528700	13.33561500	-11.58173800
H	6.03728200	13.85638400	-10.07707700
H	7.29817800	14.86958500	-10.81424300
C	11.85558500	15.68401000	-11.95888100
C	10.86768400	16.49050400	-12.84425000
H	10.66474100	15.94996500	-13.77496400
H	9.91785300	16.65594000	-12.32600000
H	11.30178300	17.46673600	-13.09095900
C	12.13912800	16.46435500	-10.64706900
H	12.84073400	15.90653500	-10.01761200
H	12.57829900	17.44083800	-10.88332700
H	11.21868600	16.62889600	-10.07801500
C	13.18733500	15.53543500	-12.73071200
H	13.58805900	16.53180100	-12.94759200
H	13.93067000	14.99086900	-12.13790600
H	13.03816400	15.01356200	-13.68253000
C	21.04768900	1.70953900	1.34730700
C	21.64054400	2.80551700	1.97174700
C	21.67311000	1.03967200	0.30540900
C	22.89454300	3.25076300	1.55050800
H	21.10539600	3.27460400	2.78348700
C	22.92752100	1.47812100	-0.15189800
C	23.51434600	2.57943100	0.47985300
H	24.47914900	2.92765900	0.13952700
C	16.68219100	-0.41734000	3.72721400

C	15.86567700	0.36725600	4.52492700
C	16.51133800	-1.79744500	3.63320200
C	14.84196800	-0.23196300	5.27857600
H	16.04432100	1.43358800	4.56106500
C	15.50158000	-2.42026400	4.37023000
H	17.18027500	-2.35694100	2.99630600
C	14.67934200	-1.61751900	5.18381800
H	13.89639200	-2.09466600	5.75608000
C	23.60108900	4.45264100	2.20865000
C	25.00389000	4.01697400	2.71133700
H	25.62896800	3.66071900	1.88674700
H	25.50873100	4.86836900	3.18305600
H	24.90922000	3.21201100	3.44790400
C	22.80822500	5.00353000	3.41617000
H	21.82073000	5.36749300	3.11183500
H	22.68289900	4.23751400	4.18937900
H	23.35771700	5.84473800	3.85291400
C	23.75168600	5.58959600	1.16202000
H	22.76552200	5.92296800	0.81971200
H	24.27485000	6.44263200	1.61157600
H	24.32418300	5.25156600	0.29234000
C	13.94738300	0.65354000	6.16870300
C	13.22022200	1.69812700	5.27957400
H	13.93692300	2.32633400	4.74147700
H	12.58230100	1.19350000	4.54589600
H	12.59427900	2.34725800	5.90344800
C	12.87762700	-0.16532800	6.92759500
H	13.34053300	-0.90373700	7.59166400
H	12.27614600	0.51461300	7.54116000
H	12.20560400	-0.68119700	6.23273700
C	14.83335000	1.38343100	7.21371400
H	15.34022600	0.65604700	7.85684200
H	15.59277900	2.00170000	6.72511200
H	14.21099700	2.03417300	7.83953600
C	15.26503900	-3.94290100	4.31851300
C	16.25942200	-4.65619800	3.37318000
H	17.29392000	-4.51263700	3.70451600
H	16.04683500	-5.73096500	3.37527500
H	16.16026500	-4.29130100	2.34481600
C	15.43820600	-4.53551200	5.74305100
H	15.26566400	-5.61806000	5.71817400
H	16.45305300	-4.34915100	6.11047200
H	14.72771100	-4.08903000	6.44587100
C	13.82518500	-4.22031900	3.80826200
H	13.07788400	-3.76625800	4.46666100
H	13.69405200	-3.81133200	2.80071900

H	13.64508100	-5.30137700	3.77532700
C	23.60436200	0.72979100	-1.31818200
C	24.96241500	1.35777000	-1.70912100
H	25.39330500	0.78752800	-2.53945000
H	24.83884400	2.39606800	-2.03687400
H	25.66997500	1.32927900	-0.87303300
C	22.67576400	0.77221000	-2.56180700
H	21.70916100	0.30351500	-2.35234500
H	22.49853200	1.80872800	-2.86853200
H	23.14526700	0.23514000	-3.39440700
C	23.85124600	-0.74518200	-0.90123000
H	24.51001000	-0.78743100	-0.02718900
H	22.91121500	-1.24675200	-0.65051800
H	24.32442600	-1.29044800	-1.72648500
H	21.18543200	0.18481600	-0.14369100

D 6 92 208 210 F
D 6 92 208 5 F
D 1 91 199 200 F
D 1 91 199 2 F
D 18 96 347 349 F
D 18 96 347 17 F
D 13 95 399 341 F
D 13 95 399 14 F
D 19 90 269 270 F
D 19 90 269 20 F
D 24 89 278 280 F
D 24 89 278 23 F
D 7 93 138 140 F
D 7 93 138 8 F
D 12 94 129 130 F
D 12 94 129 11 F

1’’ (1,2-alternate, R=3,5-di-*tert*-butylphenyl)

Zero-point correction= 3.478270 (Hartree/Particle)
Thermal correction to Energy= 3.666586
Thermal correction to Enthalpy= 3.667530
Thermal correction to Gibbs Free Energy= 3.234085
Sum of electronic and zero-point Energies= -8427.051090
Sum of electronic and thermal Energies= -8426.862774
Sum of electronic and thermal Enthalpies= -8426.861830
Sum of electronic and thermal Free Energies= -8427.295274

C	8.70463400	13.58233700	-6.45503300

C	8.92257300	12.57362300	-5.55471400
C	10.23351300	12.29829400	-5.08792900
C	11.33072600	13.05624600	-5.60554700
C	11.07212700	14.14406800	-6.47577800
C	9.79566600	14.41081100	-6.89344500
C	10.87096700	2.05195400	4.58799100
C	10.82958200	3.05854500	3.66033100
C	10.80177900	2.75485200	2.27416400
C	10.86960900	1.38735100	1.85920900
C	10.83770500	0.36192700	2.83710200
C	10.83089700	0.67571300	4.16944900
C	20.10175900	2.19813300	0.00857000
C	20.00910700	2.32041200	-1.34837500
C	18.95286400	1.68771300	-2.05111900
C	17.95677100	0.95662400	-1.32817400
C	18.09003500	0.82096800	0.08119600
C	19.11715300	1.44147400	0.74037500
C	12.37045900	6.56169900	-11.47815200
C	13.49151300	5.93856100	-10.99657500
C	14.48978800	6.67788200	-10.31571700
C	14.31060900	8.08350700	-10.11029400
C	13.18148500	8.72187600	-10.68306100
C	12.22271800	7.98307300	-11.33356800
N	15.18774300	8.78325200	-9.33555100
N	10.44293000	11.32715600	-4.15633200
N	12.61153600	12.73975500	-5.26585600
N	10.67935300	3.75138600	1.35321900
N	10.93340400	1.06753300	0.53652800
N	18.89197600	1.78912700	-3.40394900
N	16.88560900	0.42283600	-1.98213100
N	15.59731400	6.04716300	-9.84276600
C	16.48381700	6.75982400	-9.13932200
C	16.24678200	8.13519500	-8.83519000
C	17.11271200	8.79814400	-7.85952100
C	18.35800600	8.21953300	-7.50336600
C	11.69813400	11.09160300	-3.75727500
C	12.80321800	11.77149700	-4.36458800
C	14.16296100	11.33092300	-4.05602000
C	14.39092000	10.58114400	-2.87554900
C	10.62908200	3.41471400	0.05913100
C	10.81557100	2.05541800	-0.35562600
C	10.93937200	1.75718200	-1.78128300
C	10.42800600	2.68963700	-2.71718900
C	17.87212400	1.20288700	-4.03979700
C	16.83273000	0.54338700	-3.31602000
C	15.65003800	0.08732500	-4.04901300

C	15.70079500	-0.04041900	-5.46209800
C	17.66282900	6.09220700	-8.59704700
C	17.70110200	4.69102500	-8.60778700
C	18.65514700	6.83292100	-7.90737800
C	18.69625300	3.98342100	-7.93691200
C	13.22323700	-0.18592900	-4.07913500
C	11.95140800	10.08817700	-2.72453900
C	10.95141800	9.16177400	-2.38617800
C	13.25111100	9.97605300	-2.16804300
C	11.21774800	8.09549100	-1.52287100
C	17.24854800	10.35237700	-5.97972100
C	17.78395400	1.32018700	-5.49115700
C	18.55140100	2.30251000	-6.13369700
C	16.80502100	0.58955700	-6.20753200
C	18.36534500	2.60155200	-7.48174800
C	11.97612000	0.46174700	-3.56548600
C	10.40593400	4.44915700	-0.94991400
C	10.57774700	5.80618200	-0.62816900
C	10.11444500	4.05903800	-2.28198300
C	10.48750300	6.79613800	-1.61131100
C	16.42280900	10.86641500	-4.84208500
C	16.70778200	10.33091500	-3.56191500
C	11.27026400	1.26662000	-4.49335700
C	13.32694400	-0.59138200	-5.43246600
C	18.59354200	9.94806400	-5.79695900
C	15.17916400	11.47957600	-5.01734800
C	9.98718500	6.41131500	-2.87832700
C	12.44317500	8.12286500	-0.81517600
C	16.58032900	9.85287600	-7.09958500
C	19.78318100	4.72187500	-7.41288900
C	14.41585600	0.01478700	-3.37960000
C	17.53740600	1.73597200	-8.23553000
C	11.69620600	0.65080200	-2.20933600
C	13.42591800	9.04755200	-1.12013600
C	15.72221000	10.20463600	-2.60014000
C	19.76338100	6.10897400	-7.40800700
C	19.13210500	8.91144100	-6.54281300
C	14.53566300	-0.51925700	-6.10420100
C	16.78519500	0.75142500	-7.61302200
C	10.50815300	2.34315000	-4.08123000
C	9.79434100	5.08060700	-3.19943600
O	11.08153100	8.52771700	-11.89230200
O	11.33541600	5.92300500	-12.14414600
O	7.46291400	13.92308200	-6.98687300
O	9.42405400	15.50392800	-7.66925800
O	10.86842500	2.23062500	5.96838100

O	10.66424500	-0.23577900	5.20566800
O	21.07852000	2.77230400	0.81299400
O	19.38096900	1.39036400	2.10115900
H	8.10678900	11.97263800	-5.18082700
H	11.90531700	14.74868400	-6.80240100
H	10.79475000	4.09541600	3.96130600
H	10.80533800	-0.66477500	2.50309600
H	20.73919300	2.87819900	-1.91566400
H	17.34535200	0.24893100	0.61631500
H	13.63521600	4.87463700	-11.11455800
H	13.07238100	9.78958500	-10.55879600
H	16.84298500	4.18356500	-9.02746400
H	10.00428500	9.25069600	-2.90362500
H	19.17664800	2.92301200	-5.50577200
H	10.87495300	6.03940600	0.38685100
H	17.67459600	9.87800700	-3.38113100
H	11.44708500	1.12944300	-5.55263000
H	12.43162200	-0.86600500	-5.97968000
H	19.18232600	10.38881800	-5.00004400
H	14.91830200	11.96926300	-5.94772500
H	9.86977500	7.16048300	-3.65104500
H	12.66560300	7.33193100	-0.10966800
H	15.55714000	10.13780600	-7.30640300
H	20.60856200	4.19843600	-6.94340000
H	14.40446000	0.29587900	-2.33435300
H	17.42955900	1.89534600	-9.30258300
H	12.14790100	0.02651500	-1.44789800
H	14.38102700	8.97289400	-0.61680300
H	15.96065900	9.68485300	-1.68162500
H	20.58116200	6.63744600	-6.93450300
H	20.13045300	8.56582700	-6.30612200
H	14.55504200	-0.73662300	-7.16467400
H	16.10524900	0.16061600	-8.21368100
H	10.08352400	2.99303700	-4.83494700
H	9.49725900	4.82889800	-4.20906200
C	10.48379900	-1.61278100	4.89383900
C	11.57533200	-2.46415300	4.78083800
C	9.17707300	-2.06689300	4.74269400
C	11.35992200	-3.82629800	4.52284100
H	12.56825100	-2.05989500	4.90807500
C	8.93379900	-3.41949900	4.48238200
H	8.37290200	-1.35342700	4.84378700
C	10.03992600	-4.27499200	4.37549400
H	9.86807800	-5.32487200	4.17241300
C	10.81962400	3.54973000	6.50053100
C	12.00101800	4.21510700	6.80459500

C	9.57339300	4.11413400	6.75090700
C	11.94856700	5.48905000	7.38687000
H	12.94035800	3.72523100	6.59847000
C	9.49013900	5.38634300	7.32912200
H	8.69069200	3.54493200	6.50001000
C	10.68748500	6.05051100	7.63424500
H	10.63599100	7.03520300	8.08227000
C	8.13951500	6.06475100	7.63430600
C	13.21944500	6.27943600	7.75963300
C	14.51300100	5.50645500	7.41556400
H	14.56741400	4.55779600	7.96096600
H	14.58168300	5.30252000	6.34147800
H	15.37898100	6.11314200	7.70288400
C	13.23438100	7.62148100	6.97899400
H	13.24305800	7.43295500	5.90009700
H	12.35483400	8.22775700	7.21719100
H	14.13092700	8.19461200	7.24340200
C	13.21492800	6.56237200	9.28623700
H	12.33483200	7.14398000	9.57796300
H	13.20932900	5.62112700	9.84629300
H	14.11152200	7.13056600	9.56104400
C	8.04182700	6.34648700	9.15788100
H	8.85220100	7.00244500	9.49127000
H	7.08663000	6.83482100	9.38455200
H	8.10056000	5.40926500	9.72161900
C	8.04967000	7.40054800	6.84824000
H	8.86100000	8.07971500	7.12860500
H	8.11198100	7.21236600	5.77108800
H	7.09516900	7.89490300	7.06440500
C	6.93760600	5.18123300	7.22678400
H	6.94528400	4.97273700	6.15115500
H	6.93931000	4.23214100	7.77437600
H	6.00808100	5.71016200	7.46450900
C	7.50892100	-3.98291900	4.31182000
C	7.25490500	-5.06546200	5.39516100
H	7.34312900	-4.62878300	6.39575400
H	6.24578800	-5.47823000	5.27846100
H	7.97511700	-5.88537600	5.31056500
C	6.42724700	-2.88749800	4.45824400
H	5.43853000	-3.34134000	4.32843600
H	6.46261400	-2.42554000	5.45120100
H	6.54687200	-2.10796500	3.69764200
C	7.37400000	-4.61369700	2.89973200
H	6.36531000	-5.02389400	2.77116900
H	7.54685900	-3.85645200	2.12756600
H	8.09636200	-5.42375000	2.75798100

C	12.51864200	-4.83399800	4.39275900
C	12.50167000	-5.45053000	2.96793200
H	11.55592700	-5.96572400	2.77232700
H	12.63163100	-4.66709500	2.21370800
H	13.31817700	-6.17535900	2.86665900
C	13.89482800	-4.17047000	4.61636000
H	14.08664800	-3.38744200	3.87469700
H	13.96449500	-3.73621900	5.62060500
H	14.67795700	-4.92947000	4.51787100
C	12.34583900	-5.95665900	5.45114100
H	12.35777100	-5.53159500	6.46055300
H	11.40094600	-6.49100900	5.31188200
H	13.16643500	-6.67854700	5.36281200
C	6.31773800	13.18048200	-6.57858700
C	5.94818600	12.04752300	-7.29381500
C	5.58108400	13.64008400	-5.49324500
C	4.79383900	11.34400600	-6.92516800
H	6.55977800	11.73767400	-8.12777000
C	4.42026500	12.95928500	-5.10550300
H	5.91899300	14.52794400	-4.97981600
C	4.05102500	11.81866200	-5.83393600
H	3.15559100	11.28339300	-5.54268900
C	10.42823700	16.42870400	-8.07166000
C	10.66679100	17.52613600	-7.25067600
C	11.11111700	16.24366900	-9.26687300
C	11.60918800	18.48835600	-7.63059200
H	10.10174700	17.61383400	-6.33467300
C	12.06360500	17.18989700	-9.67057000
H	10.88608300	15.37322500	-9.86410300
C	12.29279600	18.29623200	-8.84021800
H	13.02683300	19.03184100	-9.14543900
C	12.85707900	17.04972600	-10.98431300
C	14.37560400	16.99891000	-10.66503800
H	14.94741600	16.90360000	-11.59573600
H	14.70250300	17.90838200	-10.15137500
H	14.60059600	16.13934900	-10.02476500
C	12.55422000	18.26864900	-11.89686800
H	13.12016200	18.18263300	-12.83212900
H	11.48561100	18.30875100	-12.13400000
H	12.83543000	19.20680000	-11.40825100
C	12.48362700	15.76384000	-11.75373400
H	12.70275400	14.86602700	-11.16520800
H	11.42218100	15.75711200	-12.02583700
H	13.07092200	15.71667000	-12.67721300
C	11.91205900	19.73018600	-6.76852300
C	11.06606100	19.76233900	-5.47440800

H	9.99466400	19.79492700	-5.70171400
H	11.27086400	18.88912800	-4.84509500
H	11.32078500	20.66160900	-4.90276400
C	11.59622400	21.01017600	-7.58827400
H	12.19950700	21.05370100	-8.50058100
H	10.53829700	21.02793000	-7.87134900
H	11.81500900	21.90017000	-6.98632200
C	13.41208200	19.72178100	-6.36841500
H	13.64435200	18.82445800	-5.78497900
H	14.05723700	19.73635200	-7.25253200
H	13.63907600	20.60561500	-5.76050100
C	3.55326500	13.42253800	-3.91753600
C	4.32317200	10.08328500	-7.67844400
C	5.29242700	9.68492000	-8.81561200
H	5.37107500	10.47609600	-9.56907800
H	6.29210100	9.46542700	-8.42375900
H	4.91380300	8.78276400	-9.30863700
C	4.23053500	8.89383700	-6.68496400
H	3.52227900	9.10482700	-5.87772700
H	3.89219000	7.99509700	-7.21399400
H	5.21141400	8.69229800	-6.24126000
C	2.92671900	10.35531400	-8.29993300
H	2.98314000	11.18803600	-9.00918500
H	2.57547200	9.46287500	-8.83144800
H	2.19437000	10.60840000	-7.52668700
C	4.11996700	14.69303900	-3.24209000
H	4.15934800	15.53218800	-3.94558800
H	3.46718400	14.97675700	-2.40920300
H	5.12445600	14.51518400	-2.84221900
C	2.12018500	13.73917000	-4.42367800
H	1.49332000	14.06366300	-3.58461600
H	2.15003800	14.53937500	-5.17095800
H	1.65803300	12.85746900	-4.87878000
C	11.22133000	4.51140600	-12.12223800
C	11.27564600	3.85050600	-13.34361100
C	11.00094500	3.83241200	-10.92741900
C	11.10014200	2.46179600	-13.38948500
H	11.43974900	4.44036300	-14.23368300
C	10.82758600	2.44340700	-10.94387100
H	10.96139100	4.39378500	-10.00575100
C	10.88467300	1.78290100	-12.18083200
H	10.75338000	0.70799200	-12.20371400
C	10.98128200	9.88307000	-12.27113600
C	9.90096800	10.59609200	-11.76648600
C	11.86795700	10.44612000	-13.18239500
C	9.69377300	11.92244700	-12.16776100

H	9.23382100	10.08680300	-11.08071300
C	11.65956700	11.75445600	-13.63504900
H	12.69823000	9.85439900	-13.54381300
C	10.57595300	12.47668500	-13.10918000
H	10.41343000	13.48936500	-13.44266300
C	11.14247000	1.67240600	-14.71349900
C	12.29101700	0.62982500	-14.65170400
H	12.32396300	0.05744300	-15.58633400
H	13.25375000	1.13364600	-14.51380800
H	12.14464300	-0.07044500	-13.82326200
C	11.38752200	2.59131000	-15.93296600
H	12.34878700	3.11076700	-15.85145200
H	11.40585900	1.98121400	-16.84282300
H	10.58884000	3.33418200	-16.03621400
C	9.78628000	0.94502900	-14.91828700
H	8.96936400	1.67292600	-14.96699200
H	9.80765800	0.37599600	-15.85533800
H	9.58243500	0.25048800	-14.09722800
C	10.58397400	1.63382500	-9.65327900
C	11.75749400	0.63712100	-9.45114400
H	11.59442700	0.05050200	-8.53840300
H	11.83727400	-0.05346000	-10.29674600
H	12.70344900	1.18077200	-9.35412100
C	10.49845200	2.54087300	-8.40339500
H	11.43331300	3.08911500	-8.24330900
H	9.67341300	3.25674300	-8.49017000
H	10.31582800	1.91534800	-7.52211000
C	9.24851900	0.85253300	-9.77678800
H	8.41442100	1.54784500	-9.91921500
H	9.27069000	0.16051800	-10.62432200
H	9.07152800	0.27282500	-8.86306200
C	8.55416900	12.73645800	-11.51991600
C	7.19987400	12.00765000	-11.72095500
H	6.39859800	12.57965200	-11.23775600
H	6.97112800	11.91315100	-12.78810300
H	7.21936000	11.00526000	-11.28147500
C	8.42918300	14.15720900	-12.11717100
H	9.34340200	14.73892800	-11.95658300
H	8.21615600	14.11928000	-13.19159800
H	7.60649600	14.68167800	-11.61941100
C	8.86638500	12.86515600	-10.00405000
H	9.84776900	13.33011400	-9.86439600
H	8.12399400	13.48184800	-9.48548700
H	8.89548900	11.87760300	-9.53049700
C	12.62298500	12.34608600	-14.68551000
C	12.15683000	13.72818000	-15.19949500

H	11.15972400	13.66531300	-15.64945100
H	12.13786500	14.46893900	-14.39417100
H	12.85784700	14.07866300	-15.96539000
C	14.02901100	12.50319300	-14.04625500
H	14.40907200	11.53840900	-13.69498100
H	14.73312500	12.90626400	-14.78419700
H	13.98306900	13.18774100	-13.19253800
C	12.71127800	11.39137000	-15.90713000
H	13.38980000	11.81503500	-16.65695700
H	13.09249800	10.40710500	-15.61912200
H	11.72254600	11.26157300	-16.36007600
C	22.11853200	3.53596600	0.21336600
C	23.11923100	2.81218400	-0.44505700
C	22.15088900	4.93120300	0.32829500
C	24.21690500	3.44345800	-1.02632600
H	23.01333900	1.73716000	-0.47533400
C	23.27716700	5.55088200	-0.25290800
C	24.27217800	4.84329500	-0.91365500
H	23.37490200	6.62665400	-0.18067800
H	25.10602100	5.38802500	-1.34074400
C	18.53795100	0.68489700	2.99937900
C	18.92821600	-0.58783100	3.39704700
C	17.41621800	1.31055400	3.53010500
C	18.19416800	-1.26149600	4.37979700
H	19.81659200	-1.01401800	2.95581800
C	16.65933700	0.65792800	4.51361600
H	17.16696300	2.30450600	3.18945500
C	17.06877600	-0.62085800	4.92063100
H	16.50156400	-1.12843300	5.69090700
C	25.33367500	2.67519800	-1.75554900
C	25.40938500	3.16330200	-3.22739800
H	25.61673300	4.23709300	-3.27650700
H	26.21050000	2.63185400	-3.75466100
H	24.46158800	2.96870500	-3.74077400
C	25.08422500	1.14932600	-1.76114500
H	25.04736200	0.75038700	-0.74124000
H	24.14830700	0.90234000	-2.27459700
H	25.90488700	0.65375000	-2.29149000
C	26.68730800	2.94694200	-1.04562500
H	26.64662500	2.60225800	-0.00681100
H	27.49243500	2.41207200	-1.56331000
H	26.92611400	4.01523700	-1.04696900
C	18.61998200	-2.64813400	4.90422600
C	19.88583200	-3.17986100	4.19230500
H	19.71832400	-3.28998300	3.11507700
H	20.74163500	-2.51523300	4.35427300

H	20.13772800	-4.16485700	4.60069100
C	18.92578800	-2.54286400	6.42297200
H	18.04546700	-2.20742300	6.98030300
H	19.22767400	-3.52339000	6.81013400
H	19.73858300	-1.82979300	6.59737000
C	17.47159200	-3.66293100	4.67309400
H	16.55952600	-3.34884100	5.18800400
H	17.25157300	-3.75116500	3.60369300
H	17.76317200	-4.64840800	5.05605400
C	15.43731700	1.32821100	5.17690500
C	15.02932900	2.62746900	4.44362700
H	14.80297000	2.43074800	3.39009200
H	14.12789400	3.03617300	4.90950600
H	15.81721200	3.38659500	4.50524700
C	14.21761200	0.36867500	5.16701000
H	13.35545700	0.84112500	5.65203600
H	13.94112600	0.11849800	4.13711900
H	14.43990000	-0.55883700	5.70510700
C	15.80803700	1.67677100	6.64404200
H	16.07154800	0.77296100	7.20327800
H	16.66276500	2.36138700	6.66815200
H	14.95654500	2.15679800	7.14132900
C	21.14161600	5.81916200	1.09503400
C	20.75265500	7.04589100	0.22263800
H	20.03267500	7.66240700	0.77309000
H	21.61621000	7.67233300	-0.01893300
H	20.28679100	6.71454400	-0.71160800
C	21.84780000	6.31230200	2.38878300
H	22.10667900	5.45981400	3.02544000
H	22.76544200	6.85912800	2.14638400
H	21.17848900	6.97839900	2.94657100
C	19.81878300	5.11791100	1.49853600
H	19.26900700	4.78664300	0.61128600
H	19.98917100	4.25477000	2.14140200
H	19.19863600	5.84962200	2.02990200
C	3.49526600	12.29198000	-2.85513200
H	3.06583000	11.37677900	-3.27471900
H	4.50144200	12.06513400	-2.48671600
H	2.87388300	12.60895600	-2.00918300

D 6 92 208 210 F
D 6 92 208 5 F
D 1 91 199 200 F
D 1 91 199 2 F
D 18 96 347 349 F
D 18 96 347 17 F

D 13 95 399 341 F
D 13 95 399 14 F
D 19 90 269 270 F
D 19 90 269 20 F
D 24 89 278 280 F
D 24 89 278 23 F
D 7 93 138 140 F
D 7 93 138 8 F
D 12 94 129 130 F
D 12 94 129 11 F

1’’ (partial cone, R=3,5-di-*tert*-butylphenyl)

Zero-point correction= 3.478991 (Hartree/Particle)
Thermal correction to Energy= 3.670818
Thermal correction to Enthalpy= 3.671762
Thermal correction to Gibbs Free Energy= 3.223297
Sum of electronic and zero-point Energies= -8427.054259
Sum of electronic and thermal Energies= -8426.862432
Sum of electronic and thermal Enthalpies= -8426.861487
Sum of electronic and thermal Free Energies= -8427.309952

C	5.06556900	8.31401200	-9.35038200
C	5.39289700	8.37837000	-8.02259700
C	6.65657200	8.87728700	-7.61602300
C	7.59061300	9.31059300	-8.61043500
C	7.23162300	9.23123400	-9.98008300
C	6.00459300	8.74970100	-10.35005000
C	13.81841500	4.96229500	2.93475300
C	12.76670200	5.54313700	2.28484400
C	11.91796200	4.76493300	1.46036200
C	12.17144200	3.36389500	1.30261000
C	13.26275400	2.77719100	2.00341300
C	14.07353100	3.55116900	2.79257400
C	17.91979700	-2.22626800	-2.59113300
C	17.58564200	-1.34428100	-3.58344000
C	16.22830700	-1.17114900	-3.95579200
C	15.21837100	-1.87135700	-3.22473900
C	15.59499400	-2.82880400	-2.25071800
C	16.91175000	-3.02764800	-1.94752400
C	19.97438700	8.24951900	-3.32911500
C	19.10193600	8.81616900	-4.21584100

C	18.32022900	7.99861800	-5.06573600
C	18.48947800	6.58059500	-5.04632700
C	19.39105400	6.01489100	-4.10223900
C	20.09596000	6.81354400	-3.25061200
N	17.82111800	5.78634500	-5.93334800
N	6.97763100	8.93296200	-6.29502000
N	8.81335600	9.78590600	-8.24937200
N	10.86341400	5.35634900	0.83889000
N	11.36907200	2.60743800	0.49926600
N	15.89200200	-0.35791000	-4.99613000
N	13.90081100	-1.63414800	-3.46690400
N	17.41857100	8.57651400	-5.91016100
C	16.78175900	7.78965200	-6.77795300
C	17.01422300	6.37597300	-6.82304500
C	16.33524800	5.58265000	-7.84867400
C	15.72487100	6.24902000	-8.94610600
C	8.17205400	9.43173100	-5.95308600
C	9.10249600	9.86547800	-6.94466700
C	10.42380100	10.32979200	-6.52995200
C	10.68531700	10.60990700	-5.16548600
C	10.05220600	4.59020600	0.10322600
C	10.31509300	3.19857500	-0.08065000
C	9.44888400	2.43630100	-0.98140400
C	8.18273600	2.96141100	-1.35183400
C	14.59543300	-0.21867000	-5.29641500
C	13.58460600	-0.81892200	-4.47637700
C	12.18384800	-0.47479500	-4.70209200
C	11.80717400	0.05199000	-5.95950800
C	15.75879200	8.36600800	-7.64464400
C	15.03775700	9.48145600	-7.19713300
C	15.36354300	7.66914000	-8.80850000
C	13.89664300	9.92410400	-7.87128200
C	9.98923000	0.02797400	-3.77342200
C	8.56408600	9.45557600	-4.54611100
C	7.87747500	8.63395700	-3.64064300
C	9.73101600	10.15221100	-4.14211900
C	8.31536300	8.46681400	-2.32609100
C	15.44940700	3.44219900	-8.61817000
C	14.19922100	0.56385200	-6.46749400
C	15.12599000	1.39504700	-7.12314300
C	12.84363400	0.52504500	-6.88810200
C	14.73728400	2.19782800	-8.20025900
C	9.23747200	0.66575300	-2.64901400
C	8.91823200	5.20739500	-0.57835200
C	8.93310900	6.59060000	-0.80962200
C	7.90947300	4.39390800	-1.14806000

C	7.96600700	7.20633600	-1.60560900
C	12.79057300	10.56275100	-7.09234500
C	12.99947000	11.07642700	-5.78746000
C	7.87397900	1.02201500	-2.79362800
C	9.56106500	0.34613200	-5.08623300
C	15.12268700	4.07213600	-9.84528500
C	11.46878600	10.31230600	-7.46493700
C	6.84040600	6.42699100	-1.97113000
C	9.34677500	9.32726600	-1.87603700
C	16.17361900	4.19627300	-7.68921600
C	13.67334800	9.38821300	-9.16496400
C	11.27433500	-0.50194600	-3.63056800
C	13.43608900	1.99752700	-8.72375300
C	9.95846600	1.30289700	-1.63520000
C	10.03184000	10.14552600	-2.76029600
C	11.97608300	11.09696400	-4.85378100
C	14.38763400	8.29150000	-9.62046700
C	15.24310300	5.44211500	-9.99797200
C	10.44127500	0.34455400	-6.15214200
C	12.52078600	1.17928400	-8.09197700
C	7.36315200	2.14373500	-2.16265700
C	6.81497000	5.05986900	-1.74718300
O	20.96880600	6.33585900	-2.25824000
O	20.86271800	8.92320100	-2.49340500
O	3.85783000	7.84765400	-9.85335400
O	5.55315000	8.63529000	-11.65866100
O	14.68405200	5.62217900	3.79799500
O	15.12413000	3.11612300	3.58001300
O	19.20992100	-2.43037700	-2.10907400
O	17.42485300	-3.99763400	-1.08502200
H	4.69964000	8.05551000	-7.26001800
H	7.94718100	9.56282300	-10.71793600
H	12.54929500	6.59510500	2.39460400
H	13.43096100	1.71440400	1.89981500
H	18.34160200	-0.77518900	-4.10419100
H	14.81355600	-3.39657300	-1.76756100
H	18.98340700	9.88678100	-4.29297900
H	19.50668200	4.93993100	-4.07523400
H	15.30464800	9.87125000	-6.22449700
H	7.08159700	8.02656700	-4.04938400
H	16.12712500	1.44166900	-6.71228400
H	9.80648300	7.12841900	-0.46662200
H	13.99360200	11.37903700	-5.48053000
H	7.24545100	0.46980500	-3.48328900
H	14.69018600	3.48788300	-10.64888500
H	11.21764700	9.95035000	-8.45226600

H	6.02006000	6.88886000	-2.50809800
H	9.66104200	9.29123000	-0.83946500
H	16.51300000	3.76048400	-6.75807800
H	12.86231500	9.77177300	-9.77230600
H	11.64708400	-0.82789400	-2.66727800
H	13.10703200	2.58391500	-9.57121200
H	10.99307900	1.04910200	-1.44422500
H	10.86867600	10.72382500	-2.38944000
H	12.20240700	11.41259300	-3.84309100
H	14.10615400	7.84492700	-10.56575700
H	14.88612700	5.90304300	-10.91074600
H	10.09074000	0.70135000	-7.11144900
H	11.51481700	1.12311700	-8.48670200
H	6.34662500	2.44706200	-2.37983100
H	5.97584700	4.48790100	-2.12275200
C	15.52842900	1.76296800	3.68922900
C	16.47938100	1.23266800	2.82524400
C	15.05618200	1.04678100	4.78313700
C	17.00201500	-0.04686300	3.07224400
H	16.83060200	1.83478500	1.99780700
C	15.56369700	-0.22661700	5.06033000
H	14.33143100	1.52150600	5.43057000
C	16.53131200	-0.75456400	4.19067100
H	16.94275100	-1.72904800	4.40112500
C	14.48464200	7.00677400	4.04252800
C	15.12778900	7.93650000	3.24355300
C	13.65940800	7.39051500	5.09855700
C	14.96748300	9.30813400	3.50242000
H	15.75267800	7.58267500	2.43456500
C	13.48595800	8.74679400	5.38273900
H	13.18256700	6.61933600	5.68509000
C	14.14821400	9.68685800	4.57020200
H	14.01544700	10.73818900	4.78325700
C	12.59874700	9.23705400	6.54438100
C	15.67838600	10.32778200	2.59239100
C	17.20883400	10.07166800	2.63275100
H	17.59018700	10.20580400	3.65071300
H	17.45028600	9.05640100	2.30361000
H	17.72045400	10.77824100	1.96934200
C	15.15286300	10.15131500	1.14155700
H	15.34882600	9.14014500	0.77140400
H	14.07233100	10.32856500	1.10751900
H	15.64842700	10.86591600	0.47526200
C	15.41904200	11.78832200	3.02873500
H	14.35162800	12.03218900	2.98571900
H	15.78594400	11.96930900	4.04526000

H	15.94992500	12.46372500	2.34868500
C	13.46485300	10.05911200	7.53666400
H	13.91546700	10.92615600	7.04341000
H	12.84174200	10.41753100	8.36470400
H	14.26812100	9.43620700	7.94457200
C	11.46130800	10.12998700	5.97929800
H	11.86619500	10.99879600	5.45073400
H	10.84067800	9.55754500	5.28160700
H	10.82877800	10.48882500	6.79991500
C	11.95362100	8.06548900	7.32060200
H	11.30848000	7.46574000	6.66899800
H	12.71667100	7.41551700	7.76316300
H	11.33762900	8.46952400	8.13158600
C	15.06599400	-0.97610000	6.31371300
C	15.26847000	-0.07995900	7.56609800
H	14.70584300	0.85479000	7.48388700
H	14.92121400	-0.61216100	8.45963900
H	16.32890400	0.16371600	7.69103300
C	13.55673000	-1.29777300	6.14517300
H	13.18129500	-1.81055100	7.03900800
H	12.97507700	-0.38182500	5.99935200
H	13.40207200	-1.94632200	5.27646300
C	15.82873800	-2.29952000	6.55097200
H	15.44886300	-2.77141000	7.46419900
H	15.68341900	-2.99929200	5.72246300
H	16.90176100	-2.11878600	6.67995900
C	18.08835600	-0.62034500	2.13617600
C	18.59408900	-2.00599500	2.60259800
H	19.04081000	-1.95110000	3.60175100
H	17.78520600	-2.74483000	2.61603100
H	19.35674700	-2.36080500	1.90141200
C	17.50924600	-0.77045100	0.70452600
H	16.60965400	-1.39455500	0.72221000
H	17.23710500	0.20392900	0.28509200
H	18.24320700	-1.24859500	0.04556700
C	19.30357600	0.34592400	2.10335000
H	19.01057300	1.33899400	1.74871900
H	19.73741100	0.44879700	3.10389300
H	20.07038000	-0.04906300	1.42565000
C	2.86064600	7.39383400	-8.94792100
C	2.84691800	6.05492000	-8.57469500
C	1.90791300	8.29614700	-8.48993600
C	1.83844200	5.58409900	-7.72433600
H	3.61318300	5.40181200	-8.96515300
C	0.88808800	7.85323200	-7.63805500
H	1.97070800	9.32349400	-8.81652100

C	0.87693100	6.49936400	-7.27044900
H	0.09287100	6.14593400	-6.61196500
C	6.40466100	9.04015100	-12.72203600
C	6.32589500	10.34804400	-13.18573000
C	7.26553600	8.10784400	-13.28944800
C	7.12117500	10.74830800	-14.26697600
H	5.63670300	11.02579300	-12.70439200
C	8.07201800	8.48014500	-14.37240300
H	7.28015500	7.10597400	-12.88675800
C	7.98311100	9.80036800	-14.83856600
H	8.60261200	10.09911700	-15.67535700
C	9.03877700	7.49168100	-15.05544400
C	10.48850000	8.03652700	-14.94819900
H	11.18297400	7.34410400	-15.43870300
H	10.57964500	9.01518600	-15.42972000
H	10.77782700	8.13975600	-13.89676600
C	8.64548500	7.34280900	-16.54990800
H	9.33088400	6.64617300	-17.04718400
H	7.62499700	6.95465200	-16.63627500
H	8.69467700	8.30516200	-17.06902600
C	8.99874900	6.09042000	-14.40255300
H	9.29337600	6.13551800	-13.34810900
H	7.99897300	5.64802900	-14.47456100
H	9.70117600	5.43185300	-14.92536700
C	7.07437600	12.18082300	-14.83590500
C	6.07046400	13.07834600	-14.07559300
H	5.05133800	12.68226700	-14.14687300
H	6.34367000	13.17225000	-13.01868200
H	6.07858100	14.07985300	-14.51970900
C	6.64393700	12.12444100	-16.32648200
H	7.34650600	11.52932500	-16.91838300
H	5.64858300	11.67649400	-16.41709200
H	6.61339400	13.13834400	-16.74283900
C	8.48316300	12.82314500	-14.72218800
H	8.79388000	12.87373700	-13.67312900
H	9.22788700	12.24332100	-15.27655700
H	8.46182000	13.83980500	-15.13221600
C	-0.20448900	8.80048800	-7.10227500
C	1.75887100	4.10898100	-7.28177900
C	2.90008000	3.25656600	-7.88380100
H	2.85899000	3.25598500	-8.97870100
H	3.88135400	3.62481100	-7.56418300
H	2.79461100	2.22218300	-7.53829600
C	1.85962100	4.03282100	-5.73445100
H	1.04896900	4.59263000	-5.25753800
H	1.79595800	2.98768700	-5.40890600

H	2.81431400	4.44977700	-5.39595700
C	0.40557600	3.50781600	-7.74795000
H	0.32653200	3.55349400	-8.83937100
H	0.33615800	2.45980500	-7.43304100
H	-0.43895000	4.05445600	-7.31671700
C	-0.02477700	10.24813400	-7.61538900
H	-0.08320900	10.29131800	-8.70867700
H	-0.82505800	10.87456500	-7.20619400
H	0.93470300	10.66729300	-7.29254200
C	-1.59545700	8.28973700	-7.56558500
H	-2.38062400	8.95355200	-7.18459300
H	-1.64837900	8.27342800	-8.65945100
H	-1.78878700	7.27824900	-7.19457900
C	20.86583800	10.35040600	-2.54562200
C	21.92193200	10.97327700	-3.19871300
C	19.83424600	11.07693000	-1.95853400
C	21.97583100	12.37136800	-3.26014500
H	22.68442600	10.35617000	-3.64518200
C	19.85093200	12.47690300	-2.02597800
H	19.03628500	10.54396500	-1.46242100
C	20.92889000	13.09636600	-2.67484100
H	20.95231700	14.17788700	-2.72625400
C	22.34825500	6.26826200	-2.56516400
C	23.15898100	5.78292400	-1.53587200
C	22.88166200	6.61379700	-3.79664600
C	24.53818900	5.68772900	-1.71872500
H	22.68044500	5.52595400	-0.60284700
C	24.26558100	6.50295400	-4.01683800
H	22.22465700	6.95894700	-4.58274100
C	25.07406100	6.05162100	-2.97053900
H	26.14160100	5.98068700	-3.11989500
C	23.13057000	13.12277500	-3.95261600
C	22.56097200	13.97693900	-5.11715300
H	23.37449300	14.52221600	-5.61017600
H	22.07071400	13.33347100	-5.85553500
H	21.82939300	14.70482100	-4.75234700
C	24.19093200	12.15857300	-4.53239600
H	23.75719200	11.50072500	-5.29340200
H	24.98795000	12.74476600	-5.00311700
H	24.63918300	11.54287800	-3.74447200
C	23.82914400	14.04694600	-2.91895500
H	24.23837100	13.45288000	-2.09482500
H	24.64919300	14.59111500	-3.40234000
H	23.12761900	14.77761900	-2.50418200
C	18.73619100	13.34842800	-1.41358600
C	18.08545500	14.20737400	-2.53128800

H	17.29403000	14.83460100	-2.10412300
H	18.82273300	14.86044300	-3.00839200
H	17.64673800	13.56175400	-3.29967700
C	17.62881400	12.49773000	-0.75359900
H	17.14942400	11.83438500	-1.48238000
H	18.03015500	11.89301100	0.06657500
H	16.86286000	13.16428500	-0.34097800
C	19.34751700	14.27603800	-0.32925700
H	19.80479700	13.67877600	0.46686600
H	20.11507500	14.92946300	-0.75557400
H	18.56257100	14.90476100	0.10775300
C	25.48418400	5.26012400	-0.57765100
C	24.71118300	4.73474600	0.65464400
H	25.42726400	4.41432600	1.41956400
H	24.07571900	5.51366100	1.08938100
H	24.08553000	3.87583400	0.38752300
C	26.31493100	6.49982900	-0.14537900
H	26.90309400	6.88454200	-0.98491400
H	25.64982800	7.29617100	0.20522800
H	26.99991800	6.22737300	0.66676400
C	26.44293600	4.13966900	-1.05778800
H	27.05180000	4.46663200	-1.90602800
H	27.11703100	3.85623100	-0.24085900
H	25.87327600	3.25606300	-1.36097400
C	24.83104600	6.87365100	-5.40334400
C	26.36767100	6.71557300	-5.47352400
H	26.86694900	7.36957500	-4.74986600
H	26.66805400	5.67918000	-5.28391900
H	26.71025200	6.99180800	-6.47700500
C	24.19746800	5.94444500	-6.47393100
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H	24.58784700	6.19850200	-7.46671500
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C	24.48178100	8.35121200	-5.72557600
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H	23.39836800	8.50879400	-5.72688800
H	24.92987000	9.01707700	-4.97988000
C	20.30593300	-1.86568500	-2.81869300
C	20.74330300	-2.46244400	-3.99628400
C	20.92592300	-0.74265500	-2.28692100
C	21.84672500	-1.92840500	-4.67259800
H	20.22335100	-3.33565200	-4.36161800
C	22.03499000	-0.19004700	-2.94012300
C	22.47104300	-0.79630100	-4.12729100
H	23.32339000	-0.37295500	-4.64417600
C	16.47991900	-4.90079300	-0.50960600

C	16.17704800	-6.07890300	-1.18910600
C	15.87889700	-4.58267700	0.69673500
C	15.27517800	-6.98847000	-0.63239700
H	16.64534100	-6.26058800	-2.14327200
C	14.97081300	-5.48005000	1.28424500
H	16.11767100	-3.63614000	1.16079200
C	14.68839800	-6.66976400	0.60632600
H	13.99018400	-7.37003300	1.04250400
C	22.38528600	-2.54330600	-5.98035400
C	22.31256600	-1.48274000	-7.11179300
H	22.90594200	-0.59744900	-6.86243400
H	22.70111800	-1.90789800	-8.04485700
H	21.27536900	-1.17008000	-7.27304400
C	21.56979400	-3.78019600	-6.42345300
H	21.60934700	-4.57278300	-5.66783500
H	20.52265800	-3.51826200	-6.61161700
H	21.99454400	-4.17437800	-7.35331200
C	23.85912500	-2.98295000	-5.76914200
H	23.92038000	-3.73542400	-4.97559600
H	24.25434900	-3.41517800	-6.69616900
H	24.48854600	-2.13246900	-5.48889200
C	14.90479700	-8.31195500	-1.33119700
C	15.64217000	-8.48706400	-2.67912200
H	15.38315200	-7.68558200	-3.37990600
H	16.72866300	-8.50031200	-2.53783700
H	15.34483300	-9.44113300	-3.12823000
C	15.28889800	-9.50078700	-0.40936000
H	14.76169000	-9.44467300	0.54824300
H	15.02377000	-10.44760600	-0.89471500
H	16.36641400	-9.49554300	-0.21281200
C	13.37700900	-8.33562900	-1.60627400
H	12.80636300	-8.25243800	-0.67597500
H	13.09626800	-7.50334200	-2.26052100
H	13.10272500	-9.27712000	-2.09684100
C	14.35814000	-5.14214900	2.65690200
C	15.49322700	-5.18880300	3.71490000
H	16.27992400	-4.46693700	3.47144400
H	15.09295600	-4.94685500	4.70641900
H	15.94061500	-6.18806000	3.74901800
C	13.72926500	-3.72395000	2.62490300
H	13.29034600	-3.49322400	3.60262600
H	14.47633800	-2.95477900	2.40685100
H	12.94077500	-3.67183200	1.86661000
C	13.25903800	-6.14728500	3.07368000
H	12.44493100	-6.16747700	2.34059700
H	13.66399900	-7.15905500	3.18617500

H	12.84344300	-5.84093400	4.04002100
C	-0.14574100	8.82378000	-5.55107300
H	-0.30512100	7.82421700	-5.13442300
H	0.83034300	9.18843500	-5.21355400
H	-0.92441000	9.48924600	-5.15989300
H	8.56225700	0.73478700	-5.23793800
H	20.53762100	-0.32478800	-1.37000500
C	22.76751000	1.05543000	-2.40322700
C	24.25959400	0.70344200	-2.16277500
H	24.74204400	0.37120600	-3.08709800
H	24.79325000	1.58780300	-1.79923000
H	24.34862300	-0.09380400	-1.41680000
C	22.16705600	1.55609700	-1.06887600
H	22.73436100	2.42860900	-0.72779000
H	21.12216400	1.86133000	-1.19271700
H	22.22447900	0.78498400	-0.29202000
C	22.65945500	2.20069200	-3.44658500
H	21.60741000	2.44635900	-3.62871900
H	23.16748600	3.09770000	-3.07580900
H	23.11478900	1.90865600	-4.39856500

D 6 92 207 209 F
D 6 92 207 5 F
D 1 91 198 199 F
D 1 91 198 2 F
D 18 96 346 348 F
D 18 96 346 17 F
D 13 95 398 340 F
D 13 95 398 14 F
D 19 90 268 269 F
D 19 90 268 20 F
D 24 89 273 274 F
D 24 89 273 23 F
D 7 93 137 139 F
D 7 93 137 8 F
D 12 94 128 129 F
D 12 94 128 11 F

1’’ (cone, R=3,5-di-*tert*-butylphenyl)

Zero-point correction= 3.479441 (Hartree/Particle)
Thermal correction to Energy= 3.668977
Thermal correction to Enthalpy= 3.669921
Thermal correction to Gibbs Free Energy= 3.234952

Sum of electronic and zero-point Energies= -8427.036813
Sum of electronic and thermal Energies= -8426.847277
Sum of electronic and thermal Enthalpies= -8426.846332
Sum of electronic and thermal Free Energies= -8427.281302

C	13.07894500	14.79058800	-2.26246800
C	12.88190900	14.24874200	-3.50398000
C	11.92215500	13.22509100	-3.69703000
C	11.15234300	12.76489600	-2.58387300
C	11.33375700	13.37971000	-1.32194500
C	12.28204200	14.35401500	-1.15026900
C	12.96952300	4.76519400	3.32930100
C	12.22055500	5.45568500	2.40554300
C	11.62314600	4.76667600	1.30836200
C	11.89492000	3.37069500	1.15272100
C	12.64157600	2.67813900	2.13211000
C	13.14581900	3.34062100	3.21096000
C	19.17412000	-0.39253100	-4.57670800
C	18.48360500	0.06648700	-5.66245000
C	17.07013900	0.10719900	-5.64050000
C	16.35503000	-0.31842700	-4.47658600
C	17.09499700	-0.77355200	-3.34981900
C	18.46872900	-0.81712900	-3.39709700
C	18.57545600	8.86776600	-4.72078400
C	17.71388100	9.42463400	-5.63165600
C	17.05954200	8.60199200	-6.58478700
C	17.36680900	7.20569600	-6.63629100
C	18.24291000	6.65118500	-5.66878700
C	18.80916100	7.44792200	-4.71567000
N	16.83150200	6.41086300	-7.60446800
N	11.73737000	12.68971600	-4.93337400
N	10.25491500	11.74911600	-2.72970900
N	10.74393800	5.39516000	0.46177000
N	11.36731800	2.66273000	0.11728500
N	16.41046300	0.54923000	-6.74232100
N	14.98523900	-0.30355400	-4.46831900
N	16.15020900	9.13806700	-7.45232200
C	15.62813600	8.34211500	-8.38994700
C	16.00668200	6.96616200	-8.49589700
C	15.42057900	6.13928900	-9.54861000
C	14.67922600	6.73935400	-10.59766000
C	10.81090300	11.73807000	-5.07742100
C	10.07174100	11.24059400	-3.95246000
C	9.13086500	10.13580900	-4.14385400
C	8.70117500	9.83781400	-5.46261400

C	10.12149400	4.64959600	-0.46272800
C	10.47311700	3.27239800	-0.65677000
C	9.81549100	2.49686400	-1.70208800
C	8.51280400	2.88510000	-2.08303200
C	15.07869100	0.52077700	-6.73556200
C	14.34624500	0.07749400	-5.58277900
C	12.87831100	0.07388200	-5.64490200
C	12.24882700	0.19796300	-6.91446600
C	14.56646100	8.84332900	-9.26242400
C	13.74125600	9.87614800	-8.79258400
C	14.21875000	8.12976500	-10.43708500
C	12.56366000	10.22125500	-9.45964300
C	10.70068300	0.17324400	-4.52489700
C	10.57797600	11.17804600	-6.40472700
C	11.54225500	11.33070800	-7.41537800
C	9.42684200	10.38342700	-6.61832500
C	11.39883800	10.68143300	-8.64395200
C	14.75544000	3.90918900	-10.28573900
C	14.37116600	1.02256200	-7.90756900
C	15.02521200	1.90450200	-8.78033600
C	12.99623500	0.73853300	-8.05803600
C	14.32186400	2.57243900	-9.78409300
C	9.88069000	0.77186800	-3.42192200
C	9.01036400	5.19180000	-1.26049000
C	8.88166900	6.56076500	-1.56494200
C	8.07660700	4.26092100	-1.80040900
C	7.80824800	7.02480500	-2.34093400
C	7.92322100	8.20701400	-3.25335600
C	7.36997500	8.03043600	-4.54816700
C	8.48795200	0.98514800	-3.59783600
C	10.10057000	0.02357000	-5.79958100
C	14.20748200	4.50020900	-11.44857000
C	8.73924300	9.32599100	-3.05691700
C	6.72244500	6.13304700	-2.53437300
C	10.14514500	10.08145500	-8.91862900
C	15.44909000	4.74598000	-9.40949700
C	12.39082400	9.70699200	-10.76828700
C	12.09941800	0.06513200	-4.47225900
C	12.99577700	2.14882600	-10.04123800
C	10.48500600	1.45706700	-2.36092500
C	9.18156000	9.94712100	-7.93663700
C	7.73589500	8.82527000	-5.61358200
C	13.19968700	8.68725500	-11.24316200
C	14.17499500	5.87863800	-11.59923700
C	10.85174100	0.03367500	-6.95744000
C	12.35656500	1.24310900	-9.21122900

C	7.82457500	2.01839800	-2.95730500
C	6.86432700	4.77935800	-2.29614300
O	19.60792000	6.93264800	-3.69015500
O	19.39795900	9.57137400	-3.84806000
O	14.01131100	15.78785300	-1.97633900
O	12.50941800	15.02826100	0.04746700
O	13.56101700	5.26127400	4.47607700
O	13.75636700	2.71813400	4.30283400
O	20.55864400	-0.44341300	-4.50486300
O	19.30614000	-1.30858300	-2.41064200
H	13.44877100	14.58776400	-4.35867900
H	10.71463200	13.05246500	-0.49995600
H	12.02622500	6.51320700	2.52076100
H	12.74691100	1.60808200	2.02719200
H	18.98976300	0.40391700	-6.55522300
H	16.55363000	-1.09785000	-2.47190600
H	17.51057300	10.48645300	-5.64471100
H	18.44012000	5.58868600	-5.69284900
H	13.95384700	10.26316600	-7.80478200
H	12.44400500	11.87441000	-7.16254000
H	16.06140700	2.13437200	-8.56802100
H	9.70007600	7.21786100	-1.29610600
H	6.73371400	7.17728200	-4.73830100
H	7.93490200	0.39246300	-4.31463800
H	9.02396200	0.01330400	-5.89433900
H	9.15173200	9.56352500	-2.08379600
H	5.80274100	6.50087000	-2.97356200
H	9.98427200	9.60076800	-9.87514400
H	15.90823200	4.35588400	-8.51139800
H	11.55344000	10.04102300	-11.37060900
H	12.63339400	0.07522700	-3.53013500
H	12.42622800	2.63094000	-10.82635900
H	11.52390200	1.29563100	-2.10495100
H	8.27841600	9.39922500	-8.17029100
H	7.34624300	8.58651300	-6.59394800
H	12.96911400	8.24484700	-12.20407800
H	13.67452300	6.29524500	-12.46429000
H	10.33882100	0.01328000	-7.91026900
H	11.31254800	1.02444600	-9.39245800
H	6.78994500	2.21060800	-3.21244800
H	6.06228500	4.10642600	-2.57386600
C	13.33035800	1.39213000	4.60496100
C	14.16700400	0.32028500	4.35025100
C	12.06775700	1.21779500	5.17517400
C	13.74547500	-0.98336600	4.67601600
H	15.13351900	0.51137600	3.90452700

C	11.62693700	-0.06064800	5.51272800
H	11.45845100	2.09189600	5.35073600
C	12.48323400	-1.14734000	5.25093200
H	12.14623000	-2.14250000	5.50331800
C	13.45750700	6.57687000	4.97807500
C	14.52445700	7.44692400	4.78972300
C	12.39349800	6.90004300	5.81319000
C	14.56053700	8.66601200	5.47933700
H	15.33936200	7.13373500	4.15110400
C	12.39990500	8.11223000	6.51470200
H	11.60256300	6.17470000	5.95020500
C	13.49139300	8.97774100	6.33527400
H	13.52261200	9.90089100	6.89275200
C	11.25834400	8.40947700	7.50963200
C	15.79066600	9.58314300	5.31868800
C	17.05917200	8.81113700	5.77465500
H	16.96733600	8.51691100	6.82569400
H	17.21019200	7.90850900	5.17464000
H	17.94211500	9.45163900	5.66326900
C	15.93837300	9.98880600	3.82862600
H	16.05777400	9.10869700	3.18913400
H	15.05423400	10.54112500	3.49432000
H	16.82025000	10.62817900	3.70257400
C	15.68322000	10.87130500	6.16759500
H	14.81566400	11.47102800	5.87337400
H	15.61172400	10.63808300	7.23587800
H	16.58372200	11.47572500	6.01172000
C	11.40591800	9.79374500	8.18315500
H	11.39303500	10.60190900	7.44370500
H	10.56545800	9.94803300	8.86897700
H	12.33350300	9.85785400	8.76256600
C	9.89559600	8.36952000	6.76982900
H	9.86258700	9.14291300	5.99640100
H	9.72890700	7.39823700	6.29390300
H	9.08075300	8.55092100	7.48067200
C	11.27499000	7.32782200	8.62504000
H	11.13160400	6.32736500	8.20519100
H	12.23270000	7.34570100	9.15604700
H	10.46913200	7.52189700	9.34294900
C	10.24763800	-0.31584200	6.15196300
C	10.44244900	-0.99323700	7.53522100
H	11.02260700	-0.34215400	8.19798300
H	9.46587800	-1.18483400	7.99565700
H	10.97066900	-1.94689200	7.43727600
C	9.45056700	0.99257000	6.36139800
H	8.48326300	0.75354100	6.81703500

H	9.98306400	1.67755200	7.03074600
H	9.26249800	1.49882800	5.40807900
C	9.41908800	-1.24644000	5.22566700
H	8.43751600	-1.43900300	5.67490100
H	9.27241000	-0.77544000	4.24785700
H	9.92385800	-2.20600300	5.07564000
C	14.67339600	-2.17485600	4.37241100
C	14.04177000	-3.53012000	4.76819400
H	13.83201200	-3.57259200	5.84282600
H	13.11371700	-3.71175100	4.21493200
H	14.74519200	-4.33463800	4.52654300
C	14.97200500	-2.20725000	2.84946600
H	14.03962400	-2.30993900	2.28380400
H	15.47937800	-1.29540100	2.52048900
H	15.62062100	-3.05771800	2.61148800
C	15.99251700	-2.00445900	5.17007600
H	16.49907300	-1.07407400	4.89720400
H	15.78858500	-1.98517600	6.24606300
H	16.66933400	-2.83890800	4.95371900
C	14.50812700	16.55646700	-3.07053700
C	15.77476200	16.29994500	-3.56780500
C	13.69248000	17.55259400	-3.60633100
C	16.26606500	17.06598000	-4.64150100
H	16.36288500	15.51273700	-3.11535700
C	14.15515100	18.32866800	-4.66939100
H	12.71337800	17.70396100	-3.17658000
C	15.44295900	18.06399200	-5.17166900
H	15.80460700	18.65660400	-5.99980100
C	11.55971500	14.83098600	1.09081400
C	10.40173200	15.60197600	1.08645900
C	11.82908000	13.91227100	2.09449800
C	9.46949300	15.46054900	2.12017400
H	10.25415200	16.30681700	0.28174500
C	10.89272000	13.72036900	3.11972700
H	12.74712000	13.34579200	2.04540800
C	9.73437700	14.50984700	3.11737700
H	9.01024900	14.37224600	3.91093600
C	11.07157700	12.63416600	4.19670800
C	9.88458600	11.63823500	4.08947500
H	9.99710400	10.84063200	4.83139300
H	8.92846800	12.14084400	4.26577900
H	9.86006400	11.18476200	3.09289400
C	11.08870400	13.28543200	5.60413100
H	11.19556300	12.50780600	6.36939400
H	11.92916700	13.98249600	5.69127800
H	10.16124800	13.83351500	5.79862400

C	12.38299800	11.84046800	4.00599600
H	12.40927000	11.35085900	3.02588100
H	13.25811300	12.49407100	4.10091300
H	12.45238400	11.05947700	4.76940700
C	8.17579700	16.29691400	2.18321300
C	8.06369200	17.28766100	1.00123700
H	8.89874500	17.99711800	0.99867600
H	8.04085300	16.75936600	0.04158300
H	7.13264200	17.85687700	1.09850600
C	8.15951100	17.11189100	3.50437100
H	8.20083000	16.45142400	4.37626300
H	9.01876500	17.79003300	3.54253400
H	7.23930200	17.70520300	3.56334300
C	6.94891800	15.34651500	2.13931800
H	6.94880300	14.76924700	1.20856800
H	6.96080000	14.64654300	2.98075400
H	6.02347400	15.93233300	2.19047000
C	13.30614600	19.44857900	-5.30298200
C	17.69184900	16.81490800	-5.17033000
C	17.92369700	15.29751200	-5.39775300
H	17.83524500	14.72712900	-4.46817900
H	17.19939600	14.90451700	-6.11940800
H	18.93305800	15.13754200	-5.79462400
C	17.95720300	17.54324100	-6.50978900
H	17.90485500	18.63122900	-6.39323000
H	18.96510200	17.29161100	-6.85778800
H	17.23958400	17.23080100	-7.27655100
C	18.69655400	17.34861500	-4.11444800
H	18.55914100	16.83740500	-3.15676000
H	19.72583100	17.18062500	-4.45351500
H	18.54664200	18.42237500	-3.95757300
C	11.92525300	19.59025000	-4.62156500
H	12.03095800	19.83998600	-3.55986600
H	11.36728800	20.39797300	-5.10799600
H	11.34078100	18.66818200	-4.71509300
C	14.05765900	20.80002300	-5.16464400
H	13.46427800	21.60288800	-5.61811100
H	14.22095000	21.03672200	-4.10775500
H	15.02998800	20.76440500	-5.66599900
C	18.92727500	10.66876900	-3.08272300
C	19.83353000	11.70193900	-2.87544000
C	17.66969400	10.68059900	-2.48873700
C	19.50479000	12.76882200	-2.03228100
H	20.79060200	11.64472700	-3.36959700
C	17.30143900	11.75073300	-1.65983200
H	16.99350000	9.85416800	-2.66115300

C	18.22925700	12.78234200	-1.44565800
H	17.95761500	13.60071000	-0.79773300
C	21.01564100	6.94757600	-3.82878100
C	21.72431400	6.40427600	-2.76557900
C	21.66610700	7.43268200	-4.96077500
C	23.12379500	6.34735200	-2.80820200
H	21.16221700	6.04330500	-1.91525700
C	23.06058600	7.38201400	-5.03245800
H	21.08131900	7.84020300	-5.77095400
C	23.77168100	6.83788200	-3.94847900
H	24.85025300	6.79797600	-4.00187200
C	20.57441900	13.83446800	-1.71394200
C	21.21550400	14.37085400	-3.02061000
H	21.97026200	15.12743400	-2.77552500
H	21.70763600	13.57023500	-3.58122900
H	20.45545700	14.82795600	-3.66121300
C	21.67311000	13.16451000	-0.84228700
H	22.12945600	12.32330900	-1.37375300
H	22.45545900	13.89409300	-0.59985400
H	21.23902500	12.78892100	0.09056300
C	19.99539200	15.03397400	-0.92815700
H	19.59821700	14.72184900	0.04356800
H	20.79330900	15.76313800	-0.74851700
H	19.19994900	15.53041100	-1.49390900
C	15.92765200	11.72530800	-0.95641500
C	14.80410900	11.43899400	-1.98581000
H	13.83352600	11.43277600	-1.47777800
H	14.78159300	12.21417700	-2.75697900
H	14.94157900	10.46669300	-2.46898000
C	15.95135800	10.59081900	0.10468800
H	16.15056700	9.62214600	-0.36526200
H	16.73188700	10.78243800	0.84897700
H	14.98245800	10.53819900	0.61572800
C	15.60382400	13.05778100	-0.23749200
H	16.33612700	13.27566800	0.54798800
H	15.55811900	13.90458300	-0.93061600
H	14.61975600	12.97977100	0.23747600
C	23.89189500	5.78396100	-1.59475500
C	23.36294500	4.36864700	-1.24227000
H	23.91075400	3.97412200	-0.37803500
H	22.29817300	4.39313300	-0.99104100
H	23.50092000	3.68580200	-2.08680300
C	23.67178400	6.73357600	-0.38561400
H	24.05133300	7.73468900	-0.61708800
H	22.60727600	6.81570900	-0.14430600
H	24.20188100	6.34908300	0.49435300

C	25.41184500	5.67721800	-1.85992300
H	25.85245500	6.66177100	-2.05179900
H	25.90053200	5.25391100	-0.97516800
H	25.61802000	5.02182300	-2.71348700
C	23.83225000	7.90407500	-6.26220500
C	24.78758600	9.04501600	-5.81978200
H	24.21393100	9.87134800	-5.38626900
H	25.50405200	8.69136000	-5.07183000
H	25.34669200	9.41969300	-6.68571000
C	24.65700400	6.74310800	-6.88027200
H	23.99103500	5.93466500	-7.20041000
H	25.21554400	7.10572900	-7.75166700
H	25.37043500	6.33711500	-6.15639400
C	22.88887100	8.46061100	-7.35402800
H	23.48911500	8.81627600	-8.19899900
H	22.20784500	7.68531200	-7.72214600
H	22.29817300	9.30249900	-6.97616000
C	21.38235400	-1.07600000	-5.47245600
C	20.83731600	-1.83178500	-6.50839400
C	22.77150800	-0.93077700	-5.29909000
C	21.65221600	-2.45069500	-7.46187800
H	19.76450100	-1.92947000	-6.56673900
C	23.57149400	-1.55513900	-6.26656100
C	23.03612500	-2.28542600	-7.32656000
H	24.64668600	-1.47134400	-6.19074100
H	23.71056900	-2.73760900	-8.04404800
C	18.99637100	-1.35701800	-1.03076400
C	19.04317400	-2.60448100	-0.42278700
C	18.81973100	-0.19093600	-0.29619700
C	18.94720900	-2.70676700	0.97000100
H	19.19949700	-3.47163400	-1.04952500
C	18.72514400	-0.26106800	1.10013100
H	18.80105600	0.75931500	-0.81271100
C	18.79144300	-1.52445900	1.71146100
H	18.73520000	-1.58659100	2.78682300
C	21.07540800	-3.28427800	-8.62215500
C	21.50580600	-2.64590600	-9.97030600
H	22.59629000	-2.60786400	-10.05716800
H	21.11171900	-3.23765400	-10.80526300
H	21.11625400	-1.62518100	-10.04785000
C	19.53085900	-3.34990900	-8.58710300
H	19.17486300	-3.81807200	-7.66251700
H	19.08766800	-2.35157500	-8.67373200
H	19.17840800	-3.95264600	-9.43152100
C	21.62674700	-4.73278000	-8.53269800
H	21.32519600	-5.19505700	-7.58660600

H	21.23146900	-5.33358400	-9.36062400
H	22.71979700	-4.74190200	-8.58937100
C	19.04871700	-4.09914400	1.62727400
C	17.82383100	-4.94976500	1.19663400
H	16.89751100	-4.47443600	1.53587900
H	17.78071600	-5.05105100	0.10743200
H	17.88831700	-5.95144800	1.63830900
C	20.35576800	-4.79797000	1.16290200
H	21.22797600	-4.20073300	1.44921400
H	20.43344500	-5.78453000	1.63494200
H	20.37170100	-4.93573200	0.07767600
C	19.07726500	-4.02267200	3.17111300
H	19.93039500	-3.43089200	3.52111300
H	18.15632100	-3.58473100	3.56857300
H	19.17277600	-5.03607000	3.57684400
C	18.54127500	1.04217800	1.90583300
C	19.63137300	2.07245700	1.50413100
H	19.57077300	2.32845400	0.44216200
H	19.49701500	2.99280500	2.08427200
H	20.62924300	1.66969400	1.70808100
C	17.13589500	1.62199200	1.59047900
H	16.97274800	2.54848500	2.15348100
H	17.03217300	1.83911100	0.52247400
H	16.35874400	0.90182200	1.86986600
C	18.64983900	0.81292000	3.43128400
H	17.86025400	0.14843200	3.79665600
H	19.62260400	0.38482700	3.69822400
H	18.54275500	1.77439400	3.94529700
C	23.37130000	-0.15351700	-4.11080800
C	22.92210800	1.33156600	-4.18107400
H	23.34793600	1.88823900	-3.33797600
H	23.27512700	1.78898800	-5.11233000
H	21.83529300	1.40088300	-4.13652300
C	24.91878600	-0.18326600	-4.12978900
H	25.29789400	-1.20885200	-4.05475300
H	25.32247000	0.28114600	-5.03632500
H	25.28840600	0.37992800	-3.26567700
C	22.90785800	-0.80050600	-2.77388000
H	21.82061000	-0.82770300	-2.70561300
H	23.29511600	-1.82397700	-2.70558200
H	23.31039500	-0.22237600	-1.93278400
C	13.07659600	19.12886600	-6.80481600
H	14.02682100	19.05443800	-7.34288000
H	12.54166600	18.17931600	-6.91329900
H	12.47945800	19.92418700	-7.26653500
H	13.74067400	3.87444900	-12.20097100

D 6 92 207 209 F
D 6 92 207 5 F
D 1 91 198 199 F
D 1 91 198 2 F
D 18 96 346 348 F
D 18 96 346 17 F
D 13 95 398 340 F
D 13 95 398 14 F
D 19 90 268 269 F
D 19 90 268 20 F
D 24 89 273 274 F
D 24 89 273 23 F
D 7 93 137 139 F
D 7 93 137 8 F
D 12 94 128 129 F
D 12 94 128 11 F

References

1. Williams, A. T. R.; Winfield, S. A.; Miller, J. N., Relative fluorescence quantum yields using a computer-controlled luminescence spectrometer. *Analyst* **1983,** *108,* 1067-1071.

2. Rurack, K.; Spieles, M., Fluorescence Quantum Yields of a Series of Red and Near-Infrared Dyes Emitting at 600−1000 nm. *Anal. Chem.* **2011,** *83,* 1232–1242.

3. Wang, K.; Jiang, P.; Zhang, Z.-G.; Fu, Q.; Li, Y., Synthesis and Photovoltaic Properties of D–A Copolymers Based on 11,12-Difluorodibenzo[a,c]phenazine Acceptor Unit. *Macromol. Chem. Phys.* **2013,** *214* (16), 1772-1779.

4. Si C, Sun D, Matulaitis T, Cordes D, Slawin A, Zysman-Colman E. Rational Molecular Design of Efficient Yellow-Red Dendrimer TADF for Solution-Processed OLEDs: A Combined Effect of Substitution Position and Strength of the Donors. ChemRxiv. 2023; doi:10.26434/chemrxiv-2023-93jq8 This content is a preprint and has not been peer-reviewed.

5. Spek, A., Single-crystal structure validation with the program PLATON. *J. Appl. Cryst.* **2003,** *36* (1), 7-13.

6. Spek, A., Structure validation in chemical crystallography. *Acta Cryst. D* **2009,** *65* (2), 148-155.

7. Sheldrick, G. M., SHELXT - Integrated space-group and crystal-structure determination. *Acta Cryst. A* **2015,** *71,* 3-8.

8. Sheldrick, G. M., Crystal structure refinement with SHELXL. *Acta Cryst. C* **2015,** *71,* 3-8.

9. Dolomanov, O. V.; Bourhis, L. J.; Gildea, R. J.; Howard, J. A. K.; Puschmann, H., OLEX2: a complete structure solution, refinement and analysis program. *J. Appl. Cryst.* **2009,** *42,* 339-341.

10. Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Petersson, G. A.; Nakatsuji, H.; Li, X.; Caricato, M.; Marenich, A. V.; Bloino, J.; Janesko, B. G.; Gomperts, R.; Mennucci, B.; Hratchian, H. P.; Ortiz, J. V.; Izmaylov, A. F.; Sonnenberg, J. L.; Williams; Ding, F.; Lipparini, F.; Egidi, F.; Goings, J.; Peng, B.; Petrone, A.; Henderson, T.; Ranasinghe, D.; Zakrzewski, V. G.; Gao, J.; Rega, N.; Zheng, G.; Liang, W.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Throssell, K.; Montgomery Jr., J. A.; Peralta, J. E.; Ogliaro, F.; Bearpark, M. J.; Heyd, J. J.; Brothers, E. N.; Kudin, K. N.; Staroverov, V. N.;

Keith, T. A.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A. P.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Millam, J. M.; Klene, M.; Adamo, C.; Cammi, R.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Farkas, O.; Foresman, J. B.; Fox, D. J. *Gaussian 16 Rev. C.01*, Wallingford, CT, 2016.

11. Becke, A. D., Density-functional exchange-energy approximation with correct asymptotic behavior. *Phys. Rev. A Gen. Phys.* **1988,** *38* (6), 3098-3100.

12. Grimme, S.; Ehrlich, S.; Goerigk, L., Effect of the damping function in dispersion corrected density functional theory. *J. Comput. Chem.* **2011,** *32* (7), 1456-1465.

13. Cancès, E.; Mennucci, B.; Tomasi, J., A new integral equation formalism for the polarizable continuum model: Theoretical background and applications to isotropic and anisotropic dielectrics. *J. Chem. Phys.* **1997,** *107* (8), 3032-3041.

14. Wolinski, K.; Hinton, J. F.; Pulay, P., Efficient implementation of the gauge-independent atomic orbital method for NMR chemical shift calculations. *J. Am. Chem. Soc.* **1990,** *112* (23), 8251-8260.

15. Lu, T.; Chen, Q., Independent gradient model based on Hirshfeld partition: A new method for visual study of interactions in chemical systems. *J. Comput. Chem.* **2022,** *43* (8), 539-555.

16. Humphrey, W.; Dalke, A.; Schulten, K., VMD: Visual molecular dynamics. *J. Mol. Graph.* **1996,** *14* (1), 33-38.

17. Lu, T.; Chen, F., Multiwfn: A multifunctional wavefunction analyzer. *J. Comput. Chem.* **2012,** *33* (5), 580-592.

18. Data obtained from: https://organicchemistrydata.org/solvents/ The data in the table was adapted by Dr. Brian J. Myers, Webmaster of ACS Division of Organic Division (DOC) from: Professor Murov's Organic solvent table. The values were obtained from the CRC (87th edition), or Vogel's Practical Organic Chemistry (5th ed.).

19. http://supramolecular.org/