The Influence of Molecular Conformation on Electron Transport in Giant, Conjugated Macrocycles

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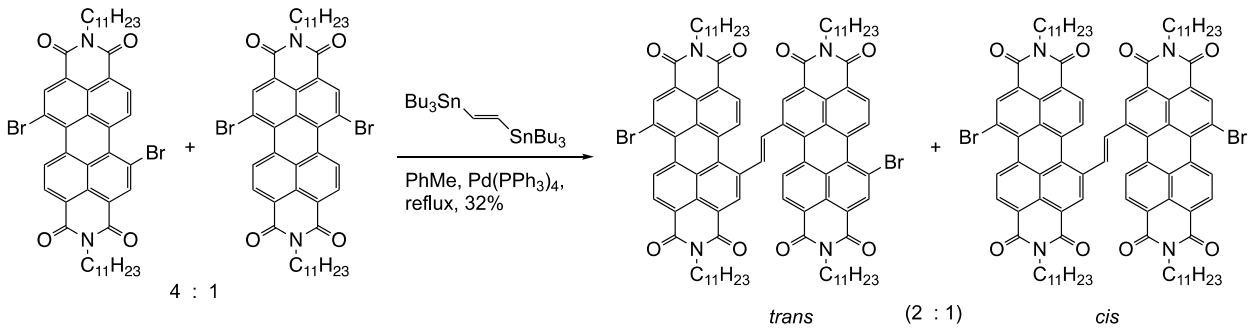
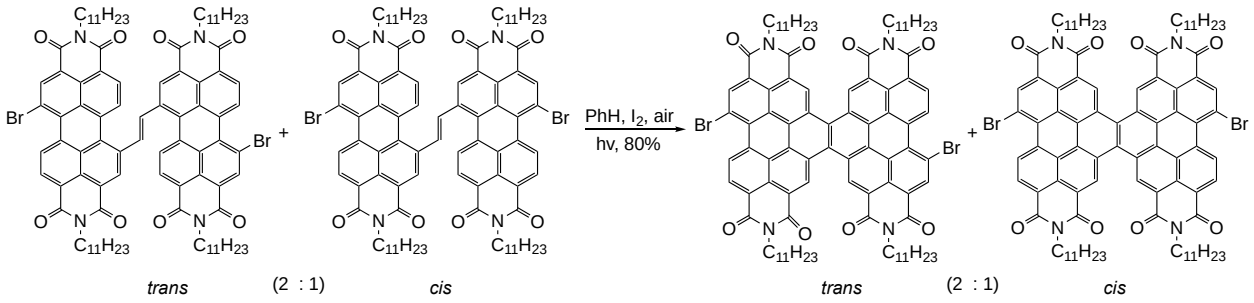
I. Figures and Tables Referenced in the Manuscript



A solution of dibromoPDI (4:1 trans/cis) (850 mg, 1.00 mmol, 4.00 equiv) and *trans*-1,2-bis(tributylstannyl)ethene (150 mg, 0.25 mmol, 1.00 equiv) in toluene (20 mL) was degassed under Argon for 30 minutes. Tetrakis(triphenylphosphine)palladium(0) (100 mg, 0.09 mmol) was added, and the resultant solution was degassed for 15 minutes. The mixture was refluxed for overnight under Argon. The black reaction mixture was filtered through celite. The solvent was removed under reduced pressure and the product was purified using silica gel column chromatography (DCM:hexane 6:4) to yield dark purple solid (126 mg, 0.08 mmol, 32%) as an inseparable 2:1 mixture of regioisomers. See ^{1}H NMR spectrum for regioisomeric distribution.



In standard photocyclization glassware, uncyclized dimer mixture (120 mg, 0.076mmol, 1.00 equiv) was dissolved in 150 mL toluene and iodine (150 mg, 0.59 mmol, 7.76 equiv) was added. The resultant purple solution was photoirradiated using 450W mercury lamp for 10 hours. The resultant pink reaction mixture extracted with saturated sodium bicarbonate (2 X 100 mL), brine (100 mL) and concentrated under reduced pressure. The residue was treated with 50 mL methanol to crash out dark red solid. The red solid was purified using silica gel column chromatography (gradient mobile phase: DCM:hexane 2:8 to DCM:hexane 6:4) to yield dark red solid (96 mg, 0.061 mmol, 80 %) that is spectroscopically identical to hPDI2Br$_2$ from dibromination of hPDI2.

Figure S1. The two dibromo hPDI2 isomers (**1a** and **2a**) are synthesized, creating an enriched mixture of **2a** (2:1 trans:cis).

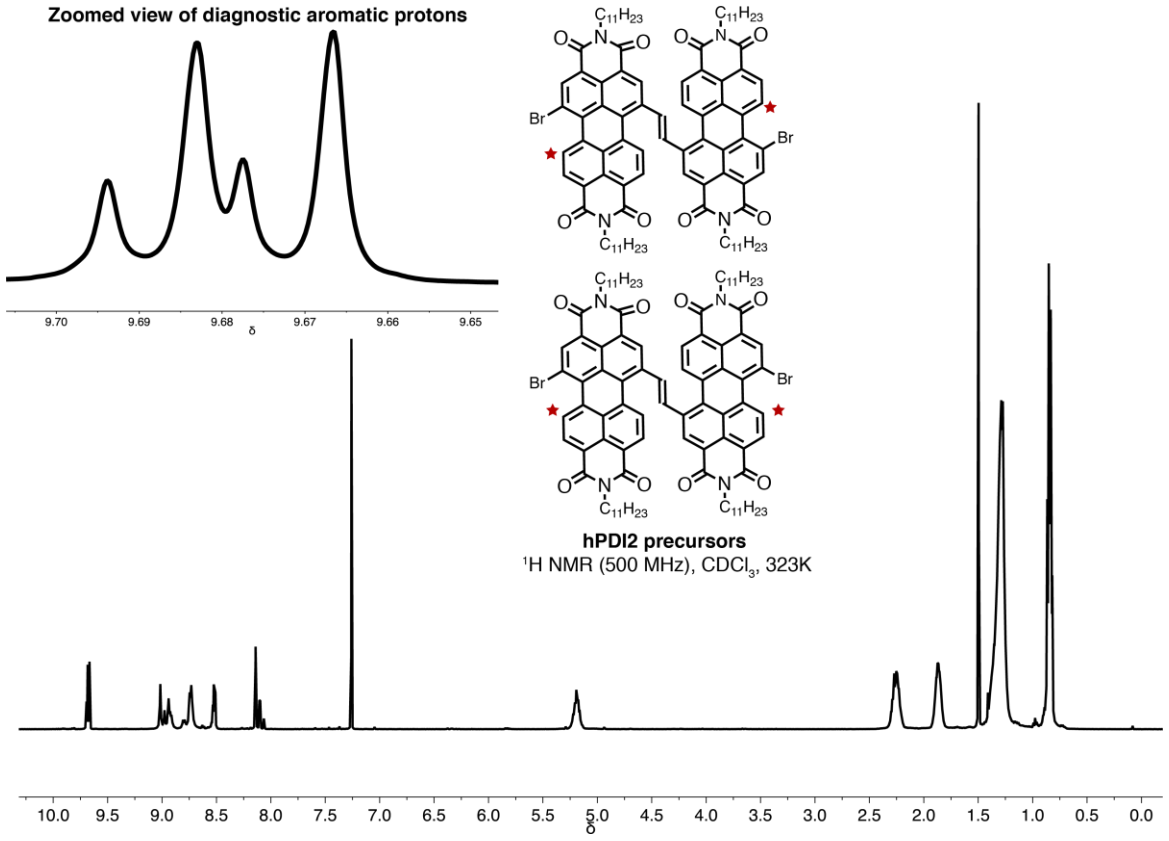


Figure S2. ^{1}HNMR spectrum of the enriched mixture of **2a**:**1a**'s precursors**,** showing an approximate 2:1 ratio of the downfield protons at 9.65-9.70 ppm. These correspond to the red starred protons.

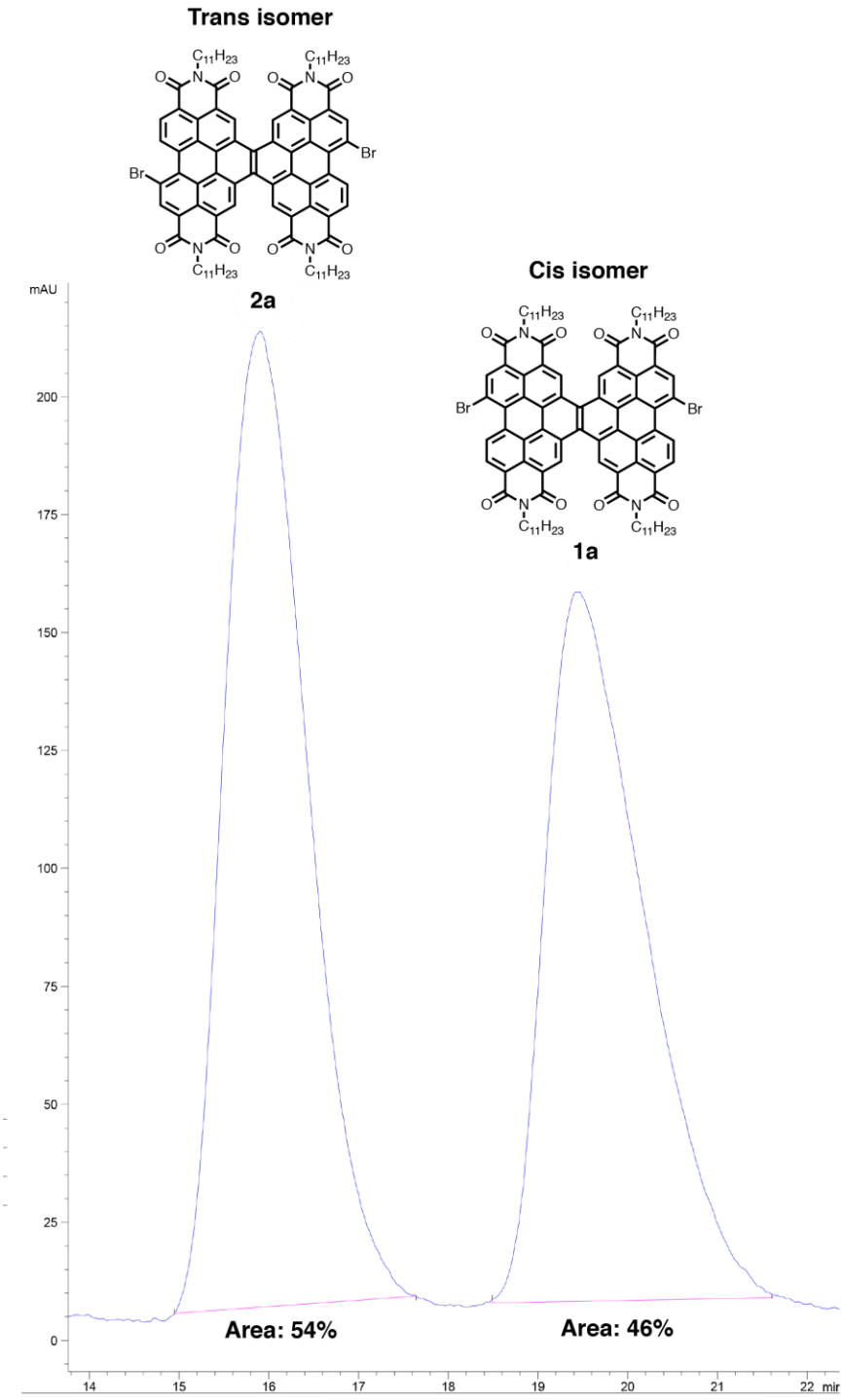


Figure S3. The two dibromo hPDI2 isomers are separated using a CHIRALPAK® IA-3 column (4.6 mm I.D. x 250 mm, 3 µm), using an isocratic method of 22% methylene chloride: 78% hexanes. Using an enriched mixture (2:1 trans isomer:cis isomer), we were able to confirm the first peak from HPLC is **2a**. This is consistent with the SCXRD structure obtained from crystals grown from the first peak (Figure S4 and Table S1).

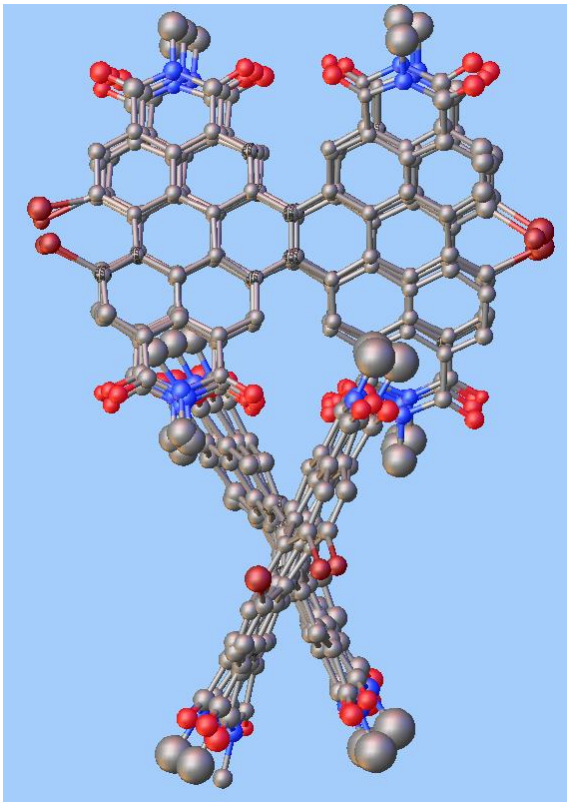


Figure S4. Thermal ellipsoid plot of **hPDI-Br_2**. The two independent sites are disordered over 4 and 3 positions. All atoms were refined with isotropic ADPs due to the extensive disorder. Thermal ellipsoids are depicted at the 40% level. The $C_{11}H_{23}$ side chains were omitted from the refinement. Hydrogen atoms are omitted for clarity.

Compound	**trans-hPDI-Br_2-2a**
Formula	$C_{54}H_{22}Br_2N_4O_8$ + side chains + solvent
MW	1014.57
Space group	P-1
***a* (Å)**	15.4448(11)
***b* (Å)**	19.9037(13)
***c* (Å)**	26.3807(18)
***α* (°)**	86.411(5)
***β* (°)**	82.181(6)
***γ* (°)**	79.782(6)
V (Å^3)	7900.6(9)
Z	4
ρ_{calc} (g cm^{-3})	0.853
T (K)	100
λ (Å)	1.54184

$2\theta_{min}$, $2\theta_{max}$	7, 90
Nref	41264
R(int), R(σ)	.0679, .0809
μ(mm^{-1})	1.600
Size (mm)	.12 x .04 x .03
T_{max}, T_{min}	.954, .831
Data	12531
Restraints	3167
Parameters	1940
R_1(obs)	0.1673
wR_2(all)	0.5119
S	1.846
Peak, hole (e^- $Å^{-3}$)	1.03, -0.81

Table S1. Crystallographic information for trans- **hPDI-Br_2**.

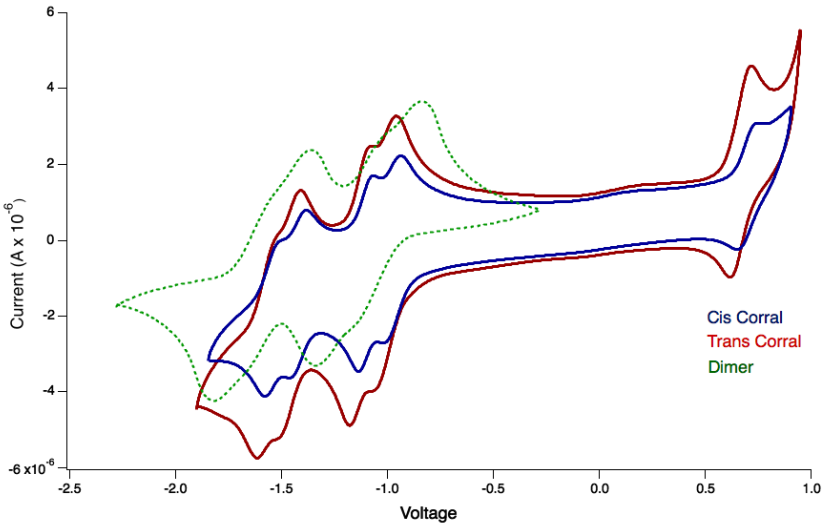


Figure S5. Cyclic Voltammogram for *cis*-**cDBDB** and *trans*-**cDBDB** relative to a hPDI monomer.

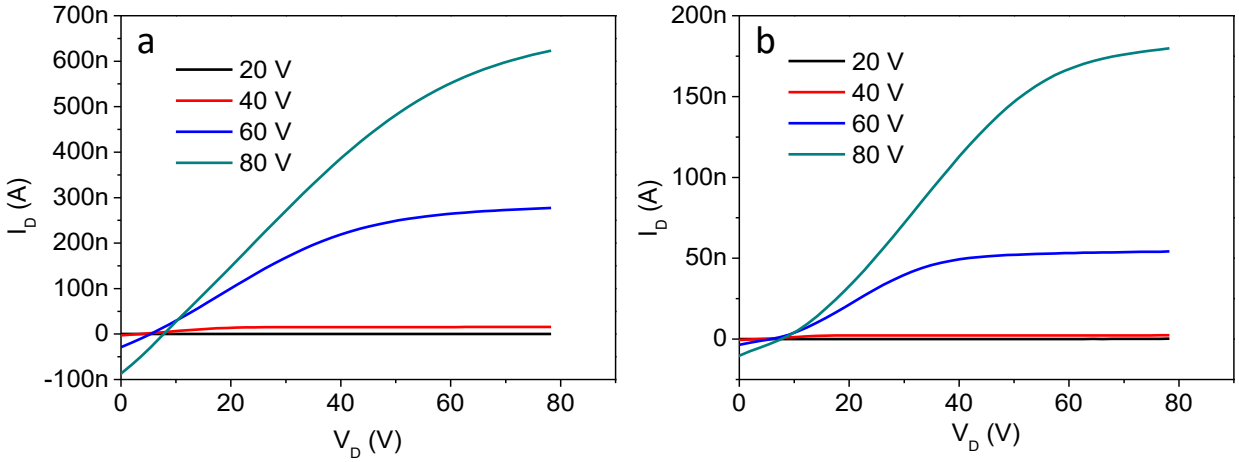


Figure S6. Output curves for a) *cis*-**cDBDB** and b) *trans*-**cDBDB**.

	***cis*-cDBDB** Highest/average	***trans*-cDBDB** Highest/average
Mobility (cm^2V^{-1})	4.1×10^{-3} / $2.7 \pm 1.2 \times 10^{-3}$	9.9×10^{-4} / $8.2 \pm 1.4 \times 10^{-4}$

Table S2. Summary of device mobilities of *cis*-**cDBDB** and *trans*-**cDBDB**.

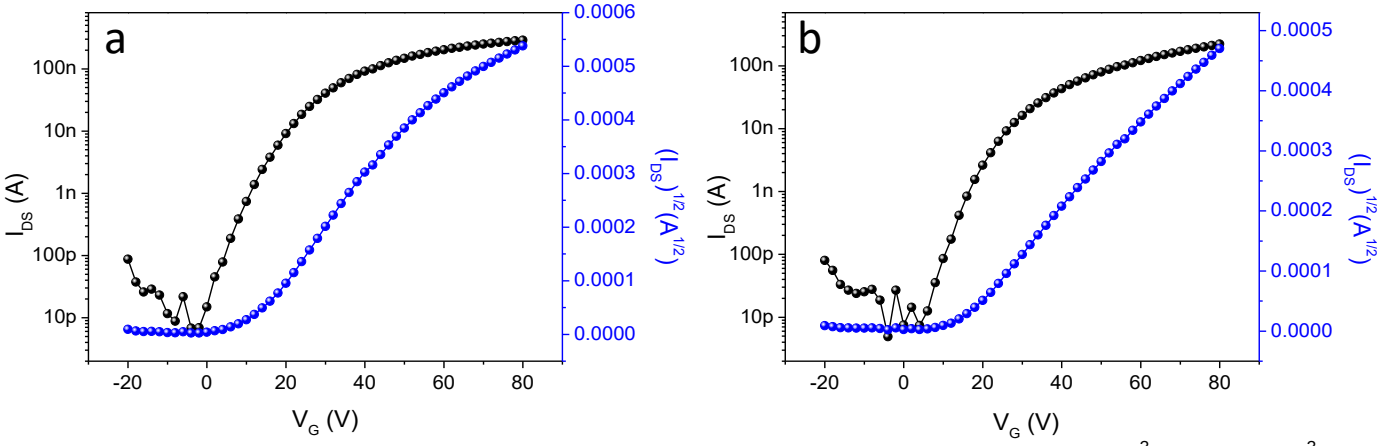


Figure S7. Transfer curves for a) **1a** and b) **2a**. The mobilities are essentially identical at 2.0×10^{-3} and 1.6×10^{-3} for **1a** and **2a**, respectively.

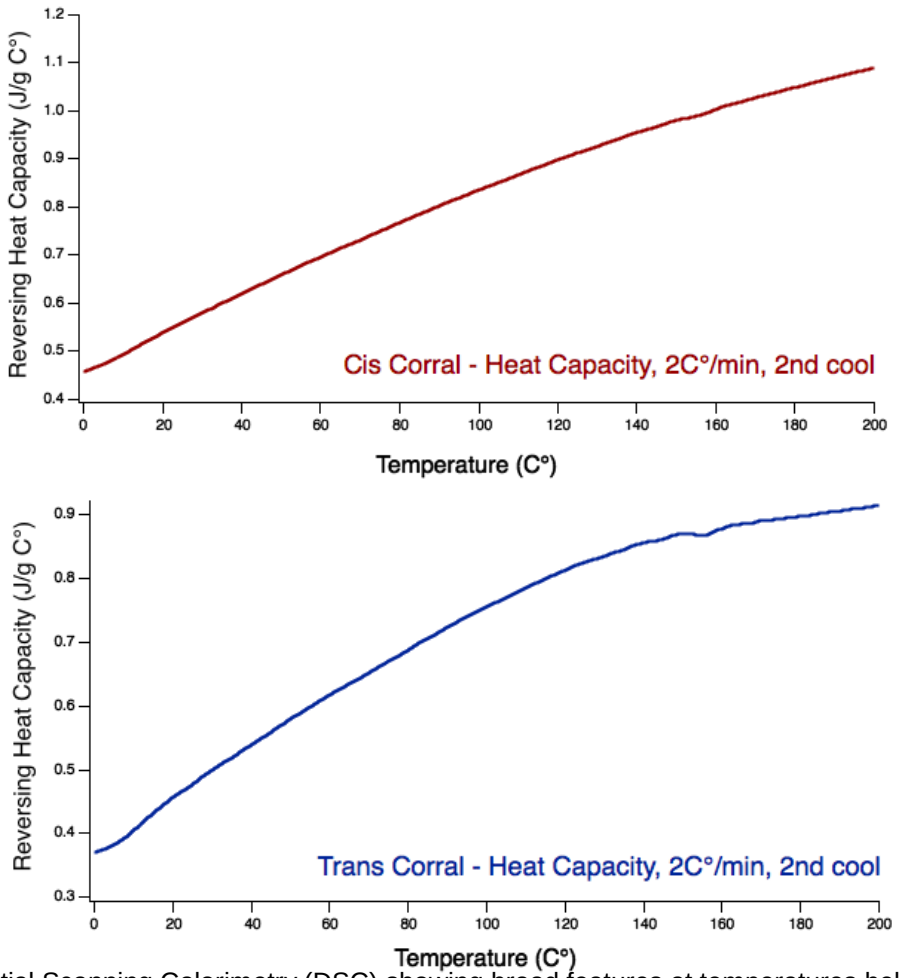
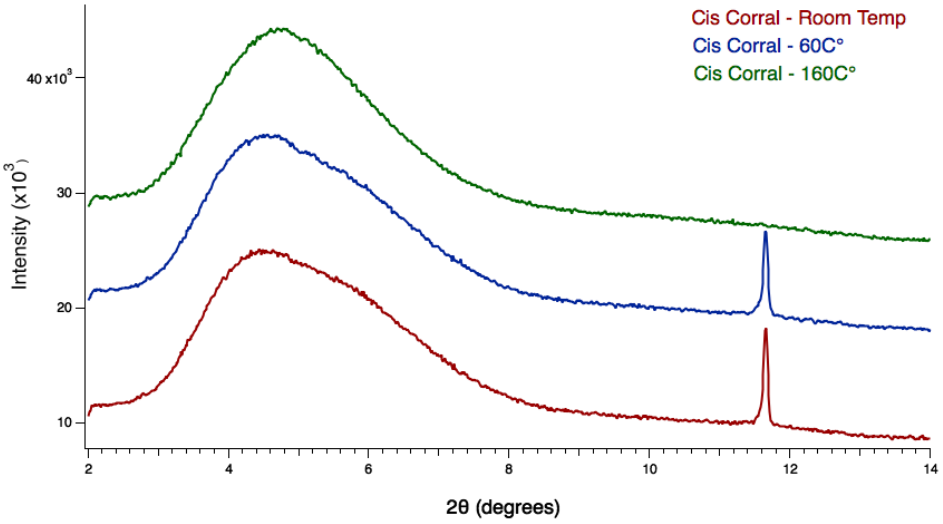


Figure S8. Differential Scanning Calorimetry (DSC) showing broad features at temperatures below 160 °C.



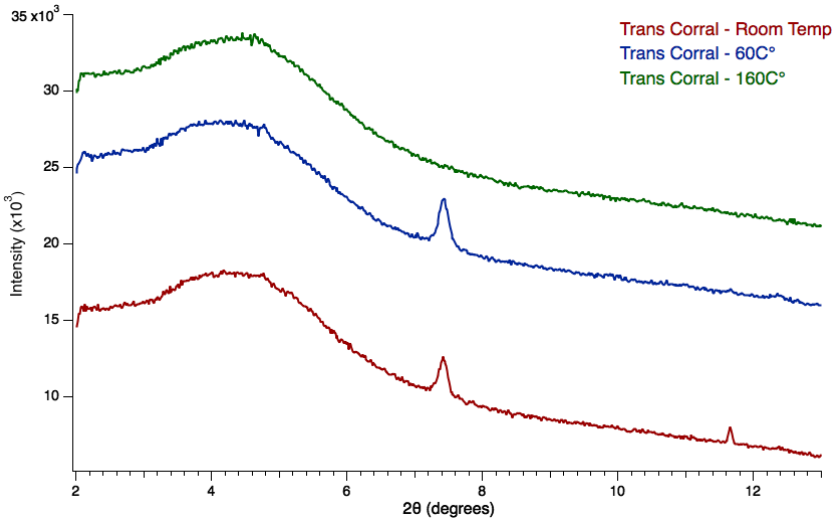


Figure S9. PXRD of *cis*-**cDBDB** and *trans*-**cDBDB** at three temperatures, showing the materials are amorphous at higher temperatures ~160 °C.

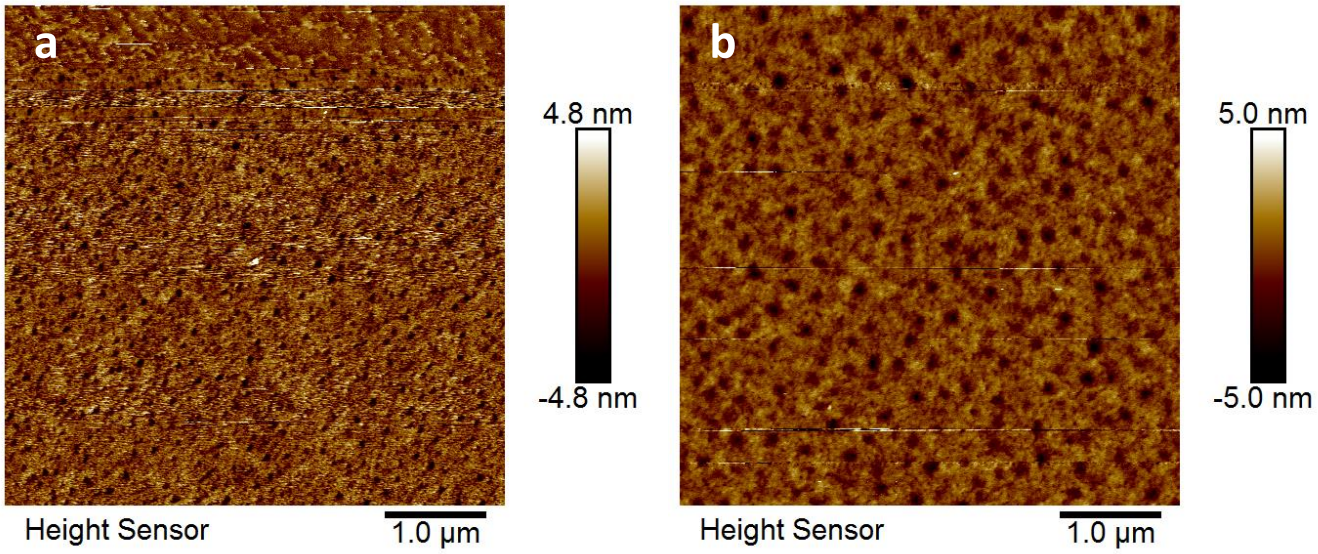


Figure S10. AFM of height images for a) *cis*-**cDBDB** and b) *trans*-**cDBDB** films from OFETs.

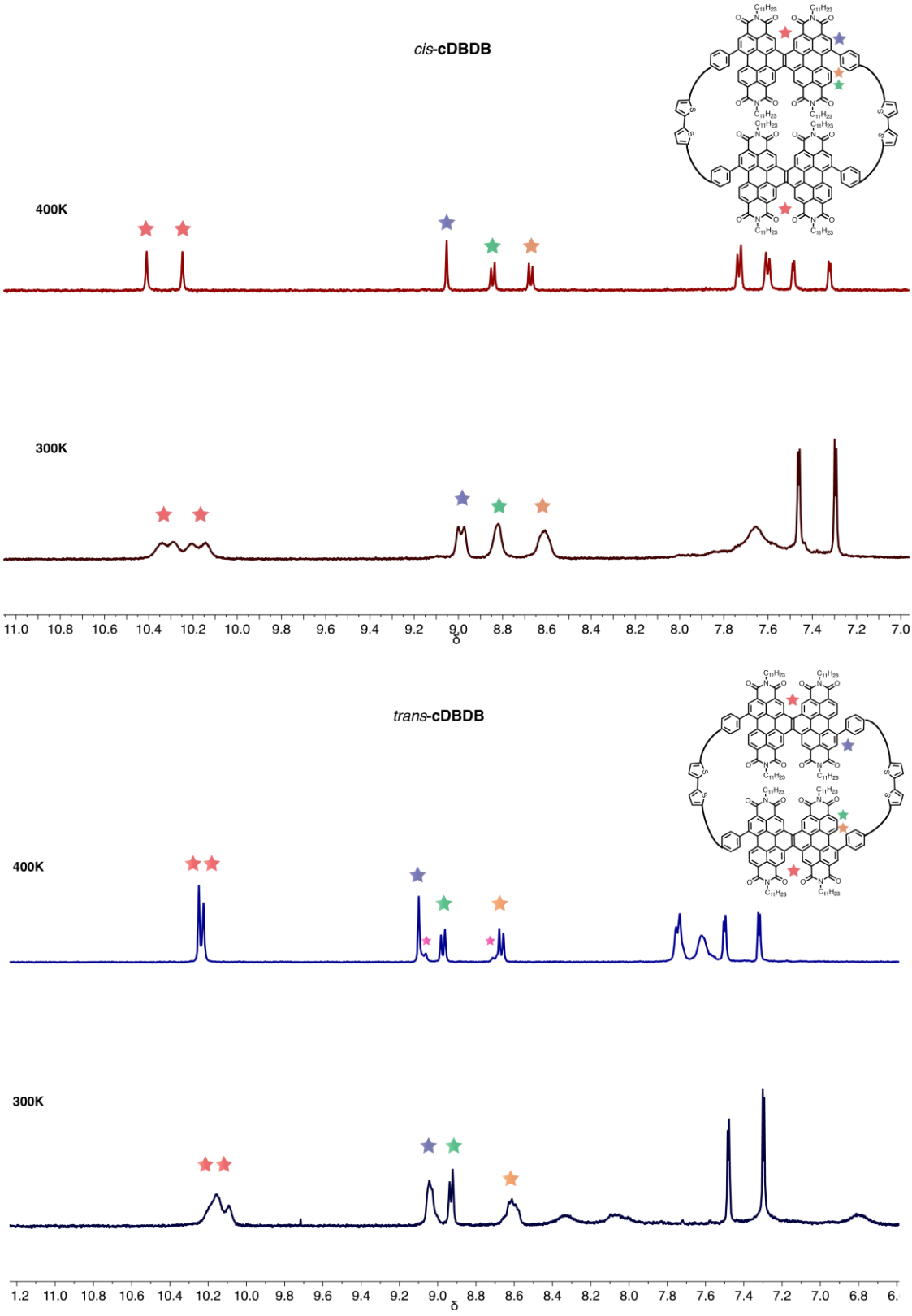


Figure S11. VT-NMR for *cis*-**cDBDB** and *trans*-**cDBDB**. Both room temperature specta show the presence of multiple conformers. Yet, at 400K, the spectrum for *cis*-**cDBDB** shows coalescence, while *trans*-**cDBDB** shows multiple peaks at 8.7 and 9.1 ppm, denoted with pink stars.

Figure S12. UV-vis and florescence spectrum for *trans*-**cDBDB**.

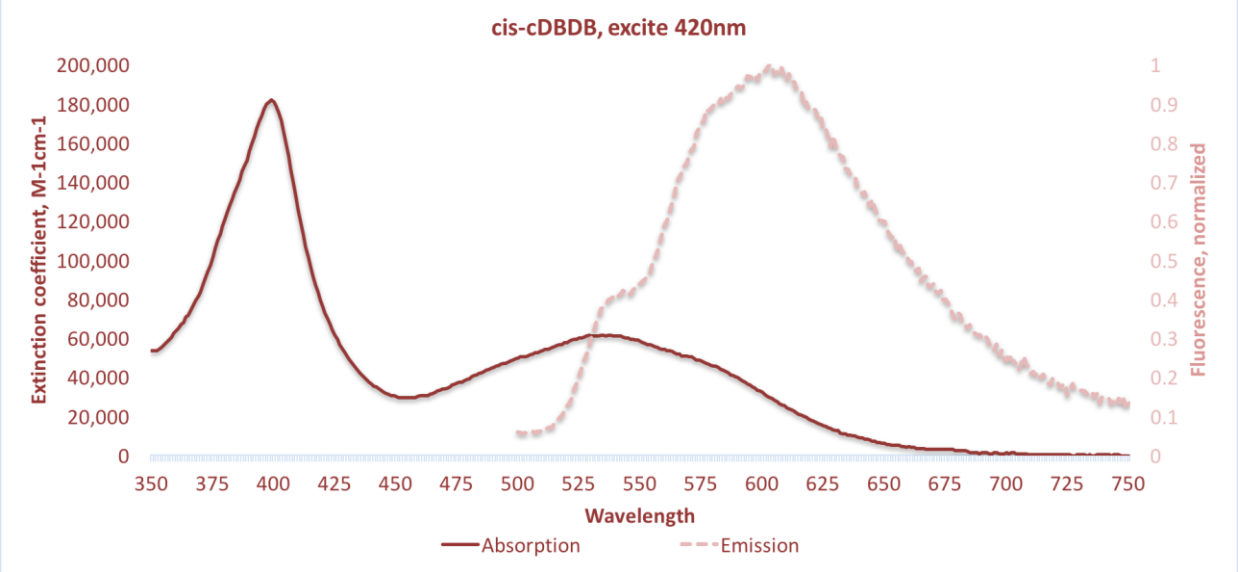


Figure S13. UV-vis and florescence spectrum for *cis*-**cDBDB**.

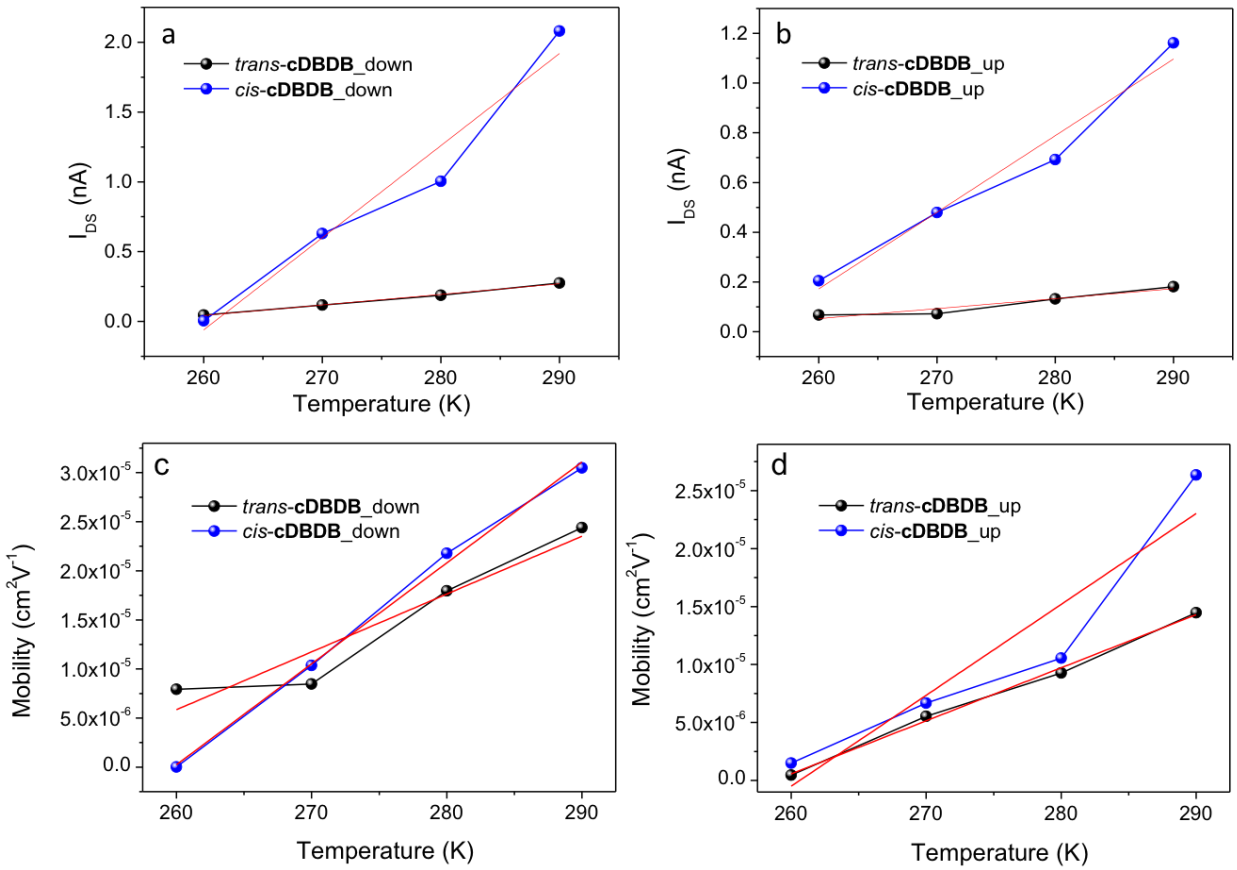


Figure S14. The dependence of source-drain current of the *cis*-**cDBDB** and *trans*-**cDBDB**-based OFET on temperature a) from 290 K to 250 K and b) from 250 K to 290 K, measured at gate voltage of 40V and bias voltage of 80V. The slope of the best fit line for the left graph is 6.6 x 10^{-2} and 7.6 x 10^{-3} for *cis*-**cDBDB** and *trans*-**cDBDB**, suggesting the cis corral is more temperature sensitive than the trans corral. The dependence of mobility of the *cis*-**cDBDB** and *trans*-**cDBDB**-based OFET on temperature c) from 290 K to 250 K and d) from 250 K to 290 K, measured at bias voltage of 80V.

II. General Experimental Information

Synthesis. All reactions were performed in oven-dried or flame-dried round bottom flasks unless otherwise noted. The flasks were fitted with rubber septa and reactions were conducted under a positive pressure of nitrogen unless otherwise noted. Anhydrous and anaerobic solvents were obtained from a Glass Contour solvent system consisting of a Schlenk manifold with purification columns packed with activated alumina and supported copper catalyst. Reaction monitoring by thin layer chromatography (TLC) was performed on J.T. Baker Baker-flex Silica Gel IB2-F (25 mm x 75 mm) TLC plates. TLC visualization was accomplished by visible observation and irradiation with a UV lamp.

Reagents. Commercial reagents were used without further purification. $Pt(COD)Cl_2$ was purchased from Strem Chemicals, and all other reagents were purchased from Sigma-Aldrich.

Purificaton. Automated flash chromatography was performed using a Teledyne Isco Combiflash Rf200 and Redisep Rf Silica columns. Preparative high performance liquid chromatography (HPLC) was performed on a Waters Prep150 instrument equipped with a UV-vis detector, an automated fraction collector, and a CHIRALPAK® IA SFC column (201mm I.D. x 250 mm, 5 µm) and/or COSMOSIL Buckyprep column (20 mm I.D. x 250 mm, 5 µm).

Spectrometers. ^{1}H NMR spectra were recorded on a Bruker 500 MHz or 400 MHz spectrometer. ^{13}C NMR spectra were recorded on a Bruker 125 MHz or 100 MHz spectrometer with complete proton decoupling. NMR spectra were recorded at 300 K unless otherwise noted. Chemical shifts for protons are reported in parts per million (ppm) downfield from tetramethylsilane (TMS) and are referenced to residual protium in the said NMR solvent. Chemical shifts for carbon are reported in ppm downfield from TMS and are referenced to the carbon resonances of the indicated solvent. Data are represented as follows: chemical shift, multiplicity (s = singlet, d = doublet, dd= doublet of doublets, t = triplet, m = multiplet, and br - broad), coupling constants in Hz, and integration.

High-resolution mass spectrometry (HRMS) was performed on (1) a Waters XEVO G2-XS QTOF instrument equipped with a UPC^2 SFC inlet, and electrospray (ESI) and atmospheric pressure chemical (APCI) ionization sources; or (2) a Bruker UltrafleXtreme MALDI TOF/TOF instrument using a dithranol matrix.

UV-vis absorption spectra were recorded on a Shimadzu UV-1800 spectrophotometer using a 1.0 cm quartz cell. Infrared (IR) spectra were recorded on a Perkin Elmer Spectrum400 FTIR spectrometer using a PIKE ATR attachment.

Atomic force microscopy. AFM measurements were carried out in scan analysis mode on a Bruker Multi-Mode AFM at ambient conditions. A commercial silicon cantilever (SCANASYST-AIR, Bruker) was used in this study with a typical radius of curvature of ~8nm and a nominal spring constant of ~0.4 Nm^{-1}.

Cyclic Voltammetry. Cyclic voltammograms (CVs) were recorded on a CH166 electrochemical workstation using an Ag/AgCl electrode as the reference electrode at room temperature. Experiments were performed in CH_2Cl_2 with NBu_4PF_6 as the supporting electrolyte at a scan rate of 0.1 V/s.[1]

Thin film transistors. To create the devices, we first silanize the substrate (300 nm of SiO_2 on a Si wafer) with octadecyltrichlorosilane (OTS). Au is deposited onto the substrate as bottom-contact source and drain electrodes (40 nm) with a width of 115 µm and length of 10 µm. Next, we spin-cast organic films onto the surface at 3,000 r.p.m. for 1 min, to form transistors using the silicon wafer as the global back gate for the device. Finally, the samples were annealed under inert atmosphere at 160℃ for 10 minutes to optimize device performance. The thin film transistors were tested on the Agilent 4155C semiconductor parameter analyzer.

The mobility is calculated in the saturation regime using $I_{DS} = (W/2L)Ci\mu(V_G - V_T)^2$, where W and L are the width and length of the channel, Ci (11.5 $nFcm^{-2}$), μ, and V_T correspond to the capacitance per unit area of the gate insulator, the field effect mobility, and the threshold voltage, respectively. W = 115 µm and L = 10 µm for transistor devices. The data is fitted using the methods developed by McCulloch[2] and Choi[3] to avoid overestimated mobilities.

Temperature dependence measurement. Temperature-dependent current-voltage measurements were realized in a vacuum cryogenic probe station (Lakeshore TTP4). Computer-controlled source units were used S3 to apply DC potentials (Yokogawa 7651). Current measurements were obtained using a current preamplifier (Stanford Research System SR570) and a digital multimeter (Keysight 34401A). All device measurements were performed in vacuum ($P < 1\times10^{-4}$ Torr) at different temperatures.

Single crystal X-ray diffraction. Data for all compounds was collected on an Agilent SuperNova diffractometer using mirror-monochromated Cu Kα radiation. Data collection, integration, scaling (ABSPACK) and absorption correction (multi-scan) were performed in CrysAlisPro.[4] Structure solution was performed using ShelXT.[5] Subsequent refinement was performed by full-matrix least-squares on F^4 in ShelXL.[6] Olex2[7] was used for viewing and to prepare CIF files. PLATON[8] was used extensively for SQUEEZE.[9]

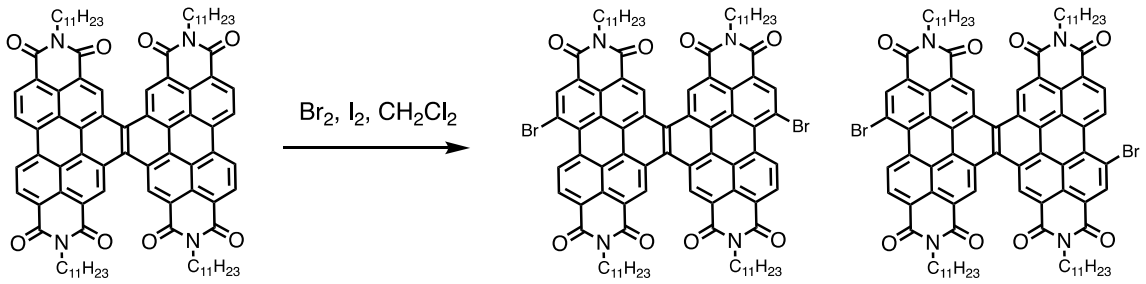
A toluene solution of $hPDI_2-Br_2$ - trans was diluted with methanol by vapor diffusion to afford bright red prisms. Part of a crystal (0.12 x 0.04 x 0.03 mm) was separated carefully, mounted with Paratone oil, and cooled to 100 K on the diffractometer. Complete data (99.7%) were collected to 1.1 Å, outside of which resolution there was little usable data. 41264 reflections were collected (12531 unique, 7287 observed) with R(int) 6.8% and R(sigma) 8.1% after multiscan absorption correction (Tmax 0.954, Tmin 0.831).

The structure solved readily in P-1 but showed signs of extensive disorder. Each of the two independent molecules was a mixture of PPP and PPM isomers (+ enantiomers) and was further disordered by a twofold rotation around the helical axis, which is not a point symmetry operator of the molecule but is an approximate symmetry of the van der Waals surface. For each site, these 4 possible isomers + orientations were introduced as fragments with DFT-optimized geometry and subsequently allowed to refine with all 1,2- and 1,3- distances restrained to match their DFT geometry. One site had all 4 possibilities occupied and the other had 3 of the 4 possibilities occupied.

The $C_{11}H_{23}$ side chains were not possible to locate in view of the extensive disorder of the hPDI cores. Thus they were modeled as methyl groups and the rest of the chains were treated as a diffuse contribution to the overall scattering using Platon SQUEEZE.

All ADPs were modeled isotropically because the data/parameters ratio was already poor due to the low resolution of the diffraction and the numerous overlapping disordered positions. All C-H hydrogens were placed in calculated positions and refined with riding coordinates and isotropic ADPs. The final refinement (12531 data, 3167 restraints, 1940 parameters) converged with R_1 ($F_o > 4\sigma(F_o)$) = 16.7%, wR_2 = 51.2%, S = 1.85. The largest Fourier features were 1.03 and -0.81 $e^- A^{-3}$.

III. Synthetic Procedures and Characterization Data



1a **2a**

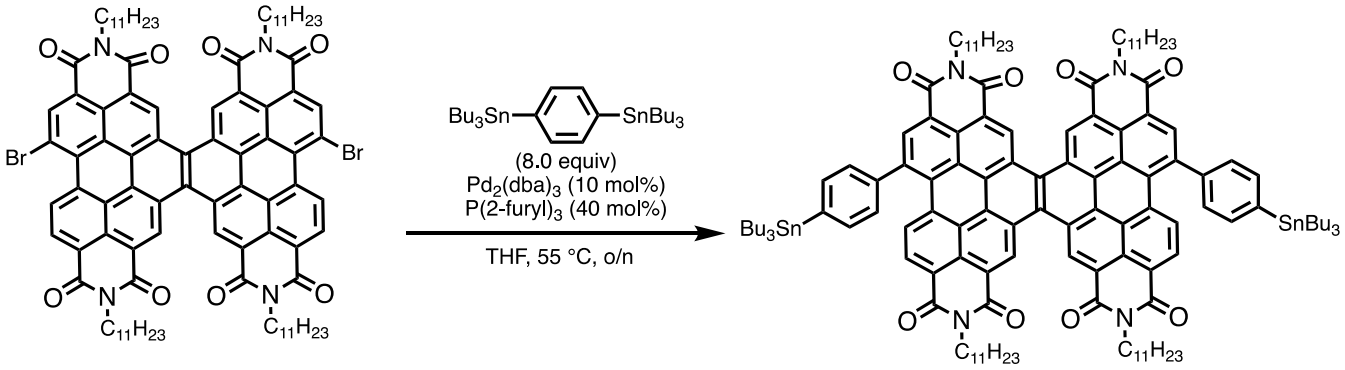
The synthesis for **1a** and **2a** was previously reported and characterized as a 1:1 mixture.[10] Separation of **1a** and **2a** through chiral chromatography is provided on S2.

1a

^{1}H NMR (400 MHz, $CDCl_3$, 323K) δ 10.74 (d, J = 8.6 Hz, 2H), 10.34 (s, 2H), 10.29 (s, 2H), 9.47 (s, 2H), 9.19 (d, J = 8.6 Hz, 2H), 5.31 (m, br, 4H), 2.35 (m, br, 8H), 1.97 (m, br, 8H), 1.35 (m, br, 48H), 0.85 (m, br, 24H). **^{13}C NMR** (100 MHz, $CDCl_3$, 323K): δ 164.0, 138.3, 133.8, 133.3, 133.0, 132.5, 129.3, 128.3,127.0, 126.8, 126.7, 126.6, 126.3, 125.9, 125.5, 125.3, 125.2, 124.1, 123.5, 122.6, 121.5, 55.4, 55.2, 32.4, 32.4, 31.7, 31.7, 26.7, 26.6, 22.5, 13.9. **IR** (cm^{-1}) 2955, 2924, 2859, 1704, 1662, 1593, 1323, 1264, 1261. **HRMS** (ESI+) calculated m/z for $[C_{94}H_{103}N_4O_8Br_2+H]^+$ is 1573.6122, found 1573.6143.

2a

^{1}H NMR (400 MHz, $CDCl_3$) δ 10.74 (d, J = 8.5 Hz, 2H), 10.35 (s, 2H), 10.28 (s, 2H), 9.47 (s, 2H), 9.19 (d, J = 8.5 Hz, 2H), 5.31 (m, br, 4H), 2.34 (m, br, 8H), 1.97 (m, br, 8H), 1.35 (m, br, 48H), 0.85 (m, br, 24H). **^{13}C NMR** (100 MHz, $CDCl_3$, 323K): δ 164.0, 138.3, 133.8, 133.3, 133.0, 132.5, 129.3, 128.3, 126.8, 126.6, 126.4, 126.0, 125.4, 125.4, 125.2, 124.1, 123.5, 122.6, 121.5, 55.4, 55.2, 32.4, 31.7, 26.6, 22.5, 13.9. **IR** (cm^{-1}) 2956, 2925, 2859, 1703, 1661, 1593, 1323, 1249. **HRMS** (ESI+) calculated m/z for $[C_{94}H_{103}N_4O_8Br_2+H]^+$ is 1573.6143, found 1573.6143.

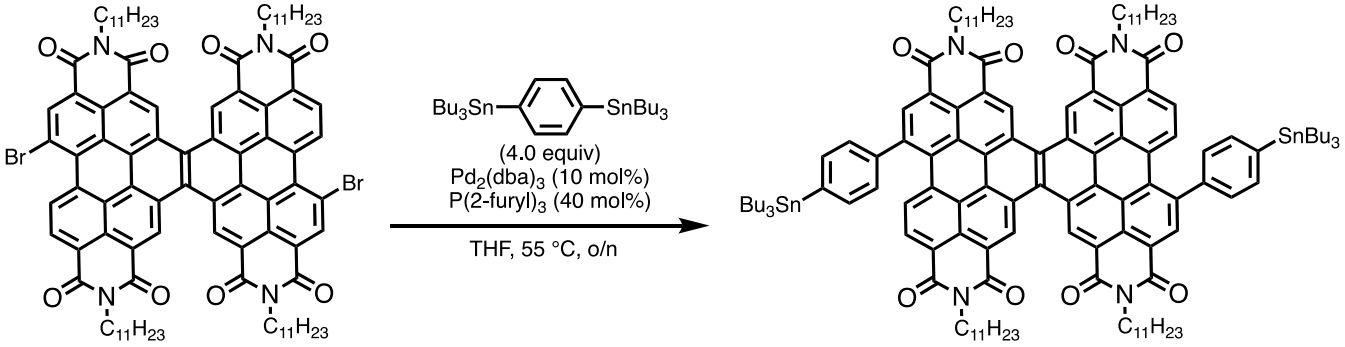


1a **1b**

Synthesis of Bis[4-(tributylstannyl)-phenyl]-hPDI2-Cis (1b). Regiopure **1a** (1.00 equiv, 0.196 mmol, 0.308 g), 1,4-bis(tributylstannyl)benzene (8.00 equiv, 1.56 mmol, 0.895 mL), tri(2-furyl)phosphine (0.400 equiv, 0.0784 mmol, 0.0180 g) and THF (24 mL) were added to an oven-dried two-neck 100 mL round bottom flask equipped with a stir bar. The mixture was degassed for thirty minutes. While under N_2, tris(dibenzylideneacetone)dipalladium (0.100 equiv, 0.0196 mmol, 0.0180 g) was added. The mixture was further degassed for ten minutes before being placed in a 55 °C oil bath and allowed to stir overnight. The crude mixture was concentrated and purified by column chromatography using a gradient from 0% to 80% CH_2Cl_2/hexanes to yield **1b** as a magenta solid (0.246 g, 0.115 mmol, 59% yield). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 10.29 (s, br, 4H), 9.05 (s, br, 2H), 8.69 (d, J = 8.5 Hz, 2H), 8.60 (d,br, 2H), 7.78* (d, J = 7.2 Hz, 4H), 7.66 (d, J = 7.1 Hz, 4H), 5.31 (m, 4H), 2.34 (m, br, 8H), 1.95 (m, br, 8H), 1.69* (m, 12H), 1.45** (m, 12H), 1.32** (m, br, 48H), 1.23*,** (m, 12H), 1.00 (tr, 18H), 0.84 (m, br, 24H).**^{13}C NMR** (100 MHz, $CDCl_3$) δ 164.9, 163.9, 143.2, 142.7, 142.6, 138.4*, 135.4, 134.8, 134.2, 133.9, 133.3, 131.8, 130.0*, 128.0, 126.9, 126.8, 126.3, 126.2, 126.1, 126.0, 125.9, 125.5, 123.8, 123.5, 122.1, 121.5, 55.1, 55.0, 32.4, 31.8, 29.2*, 27.4*, 26.7, 22.6, 14.1, 14.1, 13.8, 9.8*. **IR** (cm^{-1}) 2957, 2924, 2859, 1703, 1661, 1593, 1323, 1264, 126. **HRMS** (APCI+) calculated m/z for $[C_{136}H_{164}N_4O_8Sn_2+Na]^+$ is 2172.0547, found 2172.0491.

Broadening (br) of peaks in the ^{1}H NMR spectrum is due to rotational isomers about the imide side chains.[11,12]

*Tin satellite peaks visible. ** Overlapping peaks in the ^{1}HNMR.

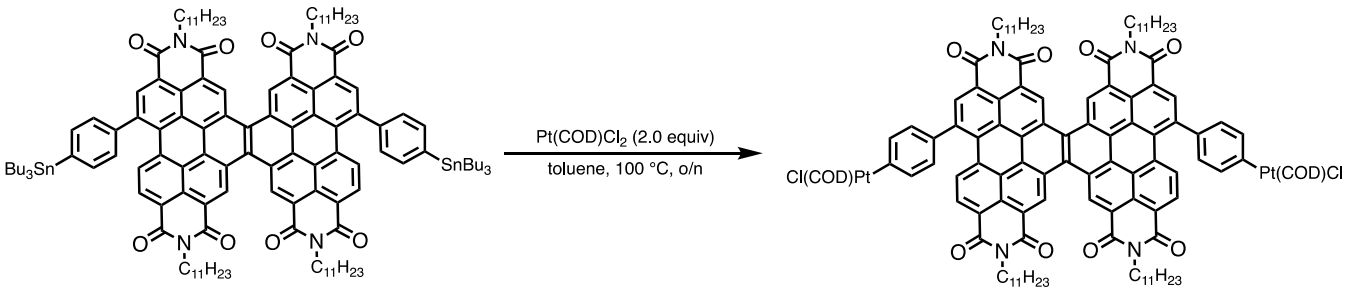


2a **2b**

Synthesis of Bis[4-(tributylstannyl)-phenyl]-hPDI2-Cis (2b). Regiopure **2a** (1.00 equiv, 0.451 mmol, 0.710 g), 1,4-bis(tributylstannyl)benzene (4.00 equiv, 1.80 mmol, 1.03 mL), tri(2-furyl)phosphine (0.400 equiv, 0.180 mmol, 0.0419 g) and THF (45 mL) were added to an oven-dried two-neck 100 mL round bottom flask equipped with a stir bar. The mixture was degassed for thirty minutes. While under N_2, tris(dibenzylideneacetone)dipalladium (0.100 equiv, 0.0451 mmol, 0.0413 g) was added. The mixture was further degassed for ten minutes before being placed in a 55 °C oil bath and allowed to stir overnight. The crude mixture was concentrated and purified by column chromatography using a gradient from 0% to 80% hexanes to CH_2Cl_2 to yield **2b** as a magenta solid (0.657 g, 0.306 mmol, 68% yield). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 10.30 (s, br, 4H), 9.05 (s, br, 2H), 8.69 (d, J = 8.5 Hz, 2H), 8.59 (d, br, 2H), 7.77* (d, J = 7.3 Hz, 4H), 7.66 (d, J = 7.2 Hz, 4H), 5.31 (m, 4H), 2.34 (m, br, 8H), 1.94 (m, br, 8H), 1.69* (m, 12H), 1.47 (m, 12H), 1.32 (m, br, 48H), 1.23* (m, 12H), 1.00 (tr, 18H), 0.84 (m, br, 24H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 164.9, 163.9, 143.2, 142.7, 142.5, 138.4*, 134.2, 133.9, 133.2, 131.8, 130.5, 130.0, 128.8, 128.0*, 126.9, 126.8, 126.7, 126.3, 126.3, 126.1, 126.0, 125.9, 125.5, 124.0, 123.4, 122.2, 121.5, 55.1, 55.0, 32.4, 31.8, 29.2*, 27.4*, 26.7, 22.6, 14.1, 14.1, 13.8, 9.8*. **IR** (cm^{-1}) 2955, 2924, 2855, 1701, 1661, 1597, 1322, 1268. **HRMS** (APCI+) calculated m/z for $[C_{136}H_{164}N_4O_8Sn_2+Na]^+$ is 2172.0542, found 2172.0491.

Broadening (br) of peaks in the ^{1}H NMR spectrum is due to rotational isomers about the imide side chains.[11,12]

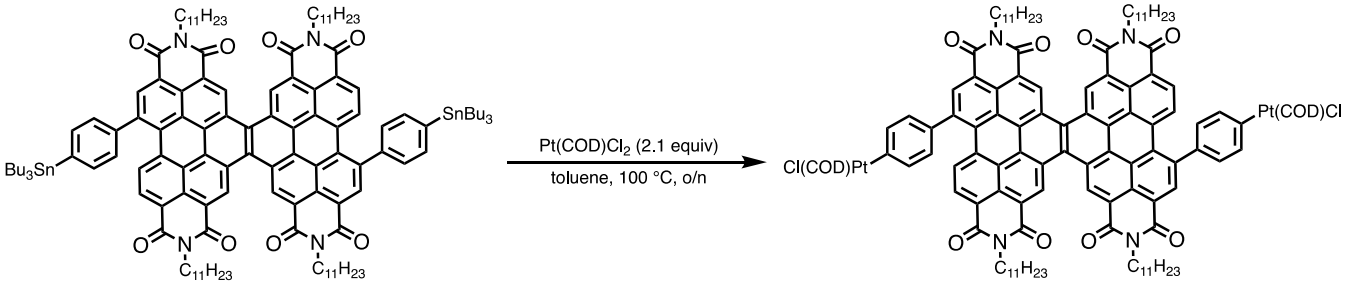
*Tin satellite peaks visible.



1b **1c**

Synthesis of Bis[4-(Pt(COD)Cl)-phenyl]-hPDI2-cis (1c): **1b** (1.00 equiv, 0.0700 mmol, 0.150 g) was added to an oven-dried two-neck, 100 mL round bottom flask equipped with a stir bar. Dichloro(1,5-cyclooctadiene)platinum(II) (2.00 equiv, 0.140 mmol, 0.0522 g) was added to the flask with anhydrous toluene (7.00 mL). The mixture was degassed for thirty minutes and then placed in a 100 °C oil bath and allowed to stir overnight. The crude mixture was allowed to cool to room temperature and concentrated *in vacuo*. The crude mixture is recrystallized from methanol before being purified by column chromatography using a gradient from 0% to 100% CH_2Cl_2/hexanes to elute the desired product. The product is a purple solid (0.100 g, 0.0445 mmol, 64% yield). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 10.26 (s, br, 4H), 9.04 (s, br, 2H), 8.68 (d, J = 8.5 Hz, 2H), 8.59 (d, br, 2H), 7.57 (d, J = 7.8 Hz, 4H), 7.44 (d, J = 7.6 Hz, 4H), 5.95 (s, 4H), 5.31 (m, br, 4H), 4.85 (s, 4H), 2.82 (m, br, 4H), 2.65 (m, br, 4H), 2.51 (m, br, 8H), 2.33 (m, br, 8H), 1.94 (m, br, 8H), 1.31 (m, br, 48H), 0.84 (m, br, 24H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 165.0, 163.9, 145.7, 142.9, 139.0, 136.0, 134.5, 133.9, 133.2, 131.7, 129.9, 128.5, 128.3, 126.8, 126.8, 126.2, 126.1, 126.1, 126.0, 125.9, 125.5, 123.9, 123.4, 122.0, 121.4, 116.0, 87.9, 55.0, 54.9, 32.4, 32.3, 31.8, 28.1, 26.7, 22.6, 14.1. **IR** (cm^{-1}) 2953, 2924, 2858, 1701, 1660, 1595, 1324, 1246. **HRMS** (ESI+) calculated m/z for $[C_{122}H_{134}Cl_2N_4O_8Pt_2+Na]^+$ is 2265.8772, found 2265.8774.

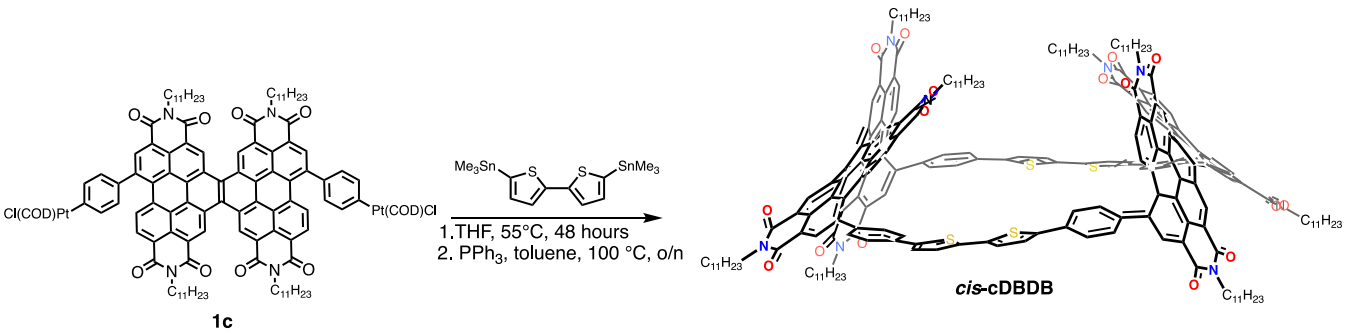
Broadening (br) of peaks in the ^{1}H NMR spectrum is due to rotational isomers about the imide side chains.[11,12]



2b **2c**

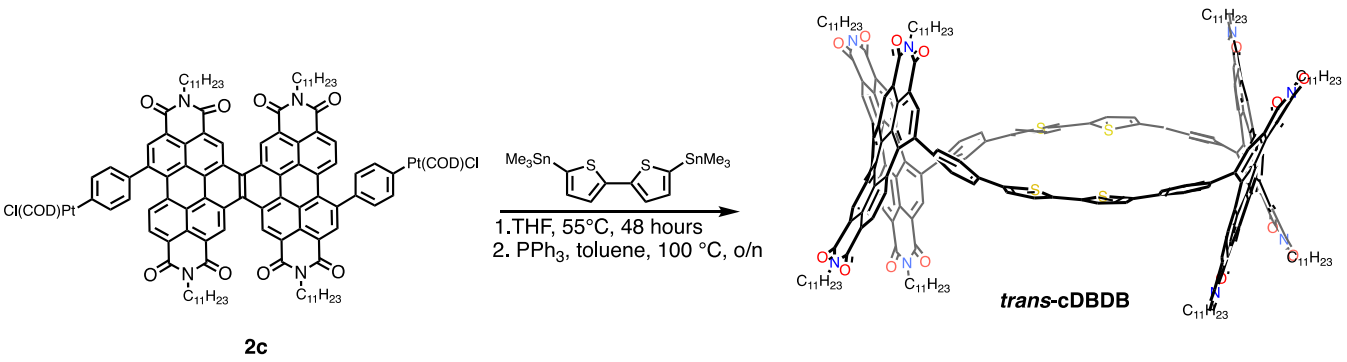
Synthesis of Bis[4-(Pt(COD)Cl)-phenyl]-hPDI2-trans (2c): **1b** (1.00 equiv, 0.0758 mmol, 0.163 g) was added to an oven-dried two-neck, 100 mL round bottom flask equipped with a stir bar. Dichloro(1,5-cyclooctadiene)platinum(II) (2.10 equiv, 0.159 mmol, 0.0596 g) was added to the flask with anhydrous toluene (8 mL). The mixture was degassed for thirty minutes and then placed in a 100 °C oil bath and allowed to stir overnight. The crude mixture was allowed to cool to room temperature and concentrated *in vacuo*. The crude mixture is recrystallized from methanol before being purified by column chromatography using a gradient from 0% to 100% CH_2Cl_2/hexanes to elute the desired product. The product is a purple solid (0.130 g, 0.0579 mmol, 76% yield). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 10.27 (s, br, 4H), 9.04 (s, br, 2H), 8.68 (d, J = 8.6 Hz, 2H), 8.58 (d, br, 2H), 7.57 (d, J = 7.7 Hz, 4H), 7.44 (d, J = 7.7 Hz, 4H), 5.95 (s, 4H), 5.30 (m, br, 4H), 4.84 (s, 4H), 2.82 (m, br, 4H), 2.65 (m, br, 4H), 2.51 (m, br, 8H), 2.33 (m, br, 8H), 1.94 (m, br, 8H), 1.31 (m, br, 48H), 0.85 (m, br, 24H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 165.0, 164.0, 145.7, 142.9, 139.0, 136.0, 134.5, 134.0*, 133.0*, 131.7, 129.9, 129.1, 128.3, 126.8, 126.8, 126.7, 126.3, 126.2, 126.0, 125.9, 125.9, 125.5, 124-121*, 116.0, 87.9, 55.0, 54.9, 32.4, 32.3, 31.8, 28.1, 26.7, 22.6, 14.1. **IR** (cm^{-1}) 2970, 2954, 2928, 2924, 2853, 1739, 1701, 1660, 1595, 1322, 1232. **HRMS** (ESI+) calculated m/z for $[C_{122}H_{134}Cl_2N_4O_8Pt_2+Na]^+$ is 2265.8772, found 2265.8772.

* Between 134-133 ppm and 124-121 ppm, there are broad signals that likely represent the quaternary carbons of the aromatic core of the dimer. Used the corresponding cis isomer (*cis*-**cDBDB**) as a guide. Broadening (br) of peaks in the ^{1}H NMR spectrum is due to rotational isomers about the imide side chains.[11,12]



***Synthesis of cis-cDBDB*.** Bis[4-(Pt(COD)Cl)-phenyl]-hPDI2-cis (**1c**) (1.00 equiv, 0.0771 mmol, 0.172 g), commercially available 5,5′-bis(trimethylstannyl)-2,2′-bithiophene (1.00 equivalent, 0.0771 mmol, 0.0379 grams) and THF (26.0 mL) were added to an oven-dried 50 mL round bottom flask. The mixture was degassed for thirty minutes, and stirred in a 55 °C oil bath for 48 h. The crude mixture was concentrated and triphenylphosphine (20.0 equiv, 1.54 mmol, 0.450 g) was added to the flask with toluene (26.0 mL). The mixture was degassed for ten minutes, then stirred for overnight in a 100 °C oil bath. The crude mixture was first purified by column chromatography (24 g Redisep Rf Silica) using a gradient from 0% to 100% CH_2Cl_2/hexanes at 35 mL/min. Fractions that contained *cis*-**cDBDB** were collected and further purified on by preparative TLC using 70%:30% CH_2Cl_2/hexanes. The solids were re-precipitated from methanol, followed by hexanes. The product is a dark purple solid (0.0150 g, 0.00448 mmol, 12% yield). **^{1}H NMR** (500 MHz, 400K, $C_2D_2Cl_4$) δ 10.41 (s, 4H), 10.25 (s, 4H), 9.05 (s, 4H), 8.85 (d, J = 8.4 Hz, 4H), 8.67 (d, J = 8.3 Hz, 4H), 7.73 (d, J = 8.1 Hz, 8H), 7.60 (d, J = 7.8 Hz, 8H), 7.49 (d, J = 4.0 Hz, 4H), 7.32 (d, J = 4.1 Hz, 4H), 5.37 (m, 4H), 5.23 (m, 4H), 2.41 (m, br, 8H), 2.28 (m, br, 8H), 2.05 (m, br, 8H), 1.94 (m, br, 8H), 1.33* (m, br, 96H), 0.93 (tr, 24H), 0.80 (tr, 24H). **^{13}C NMR** (100 MHz, 400K, $C_2D_2Cl_4$) δ□164.4, 164.3, 164.1, 142.7, 141.9, 141.7, 137.8, 134.4, 134.3, 133.5, 133.0, 132.7, 132.6, 130.5, 130.3, 128.9, 127.4, 127.2, 127.2, 127.1, 127.0, 126.6, 126.3, 126.2, 126.0, 125.9, 125.6, 125.0, 124.1, 124.0, 123.7, 123.4, 122.4, 122.4, 55.6, 55.3, 32.8, 32.6, 31.8, 31.6, 26.7, 26.6, 22.4, 22.3, 13.8, 13.7. **IR** (cm^{-1}) 2957, 2924, 2855, 1702, 1660, 1595, 1321. **HRMS** (MALDI-) calculated m/z for $[C_{228}H_{228}N_8O_{16}S_4]^-$ is 3461.6156, found 3461.6205.

*integration is higher due to overlapping peak with both H_20, and/or a small amount of grease.

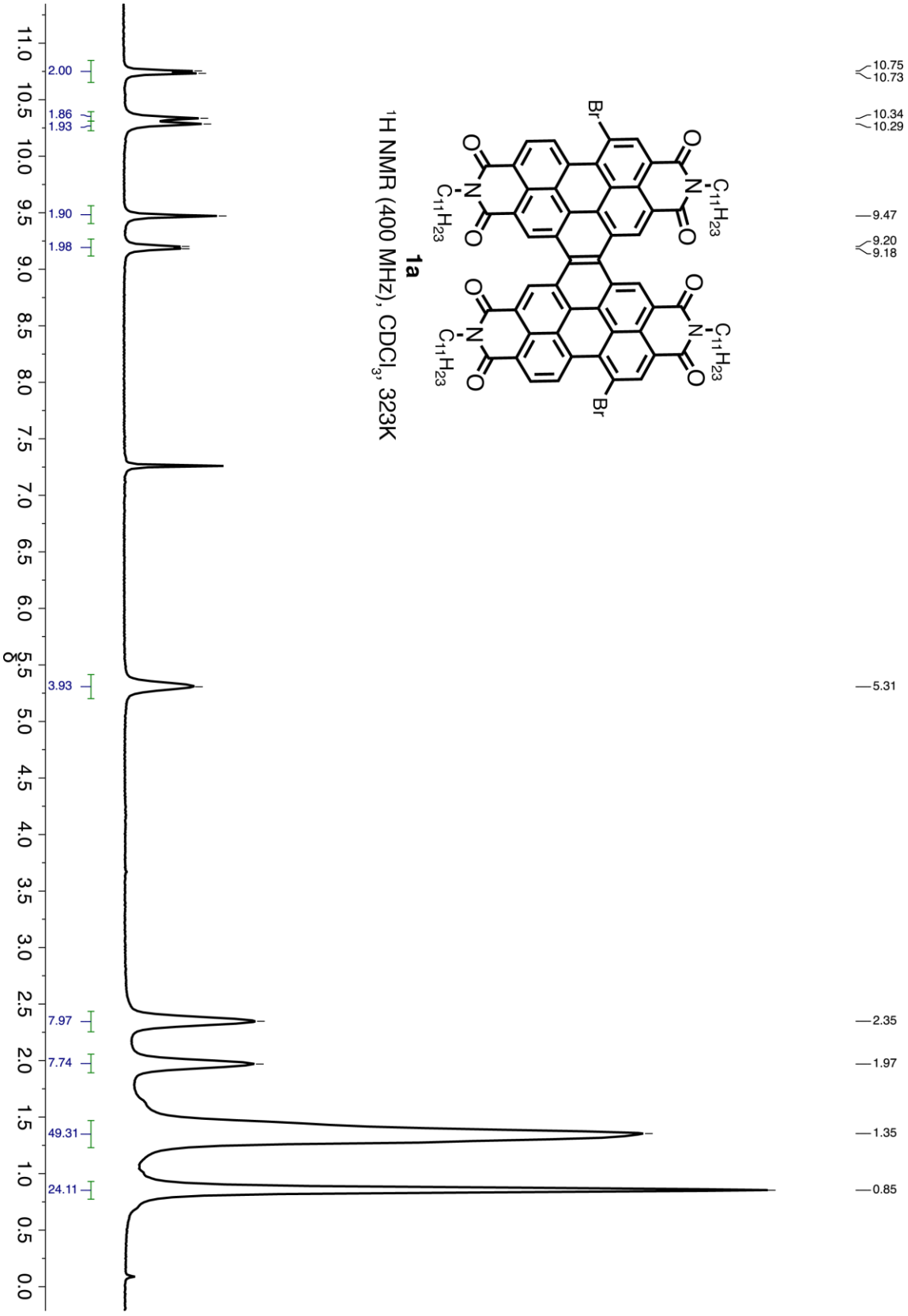


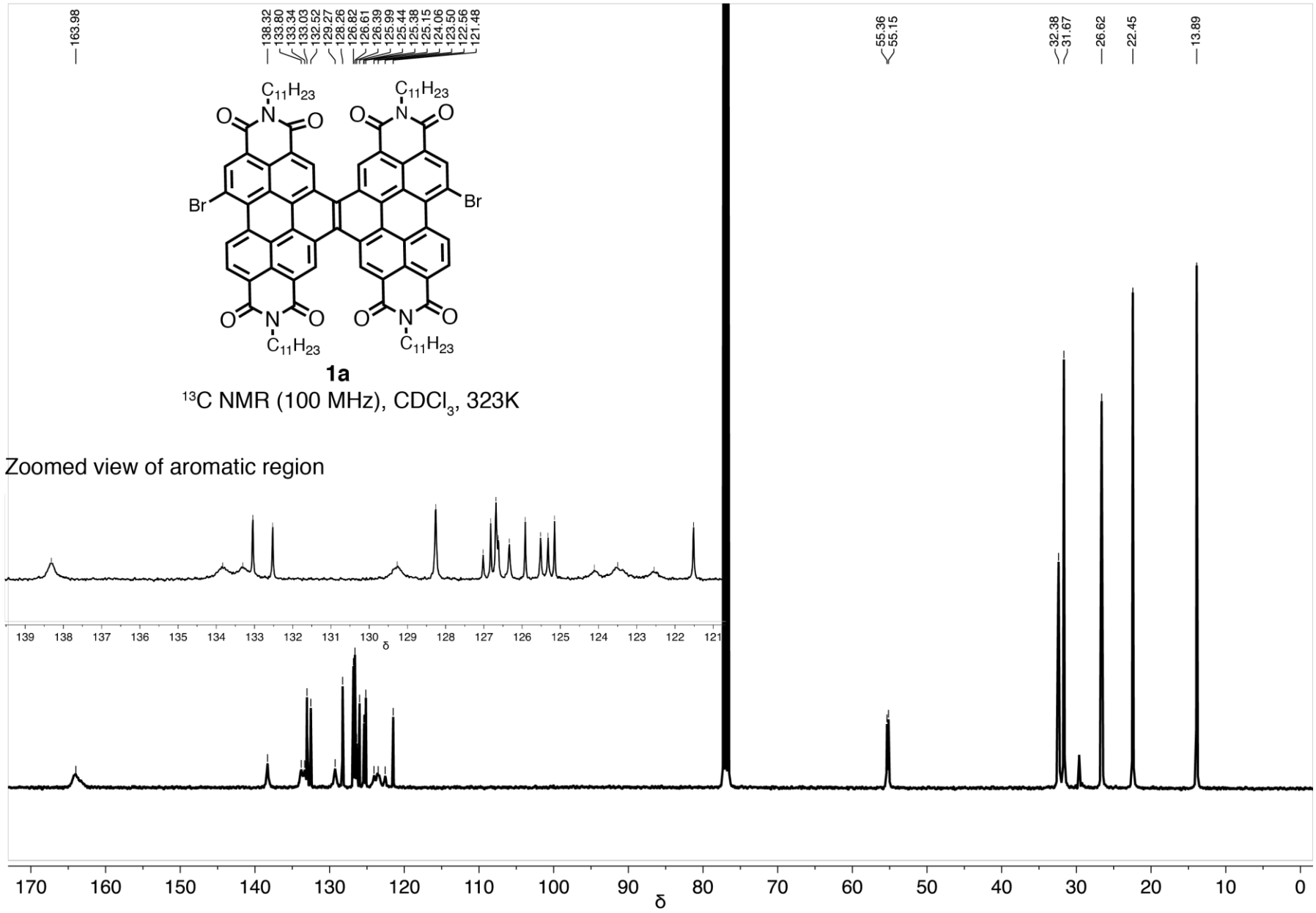
2c

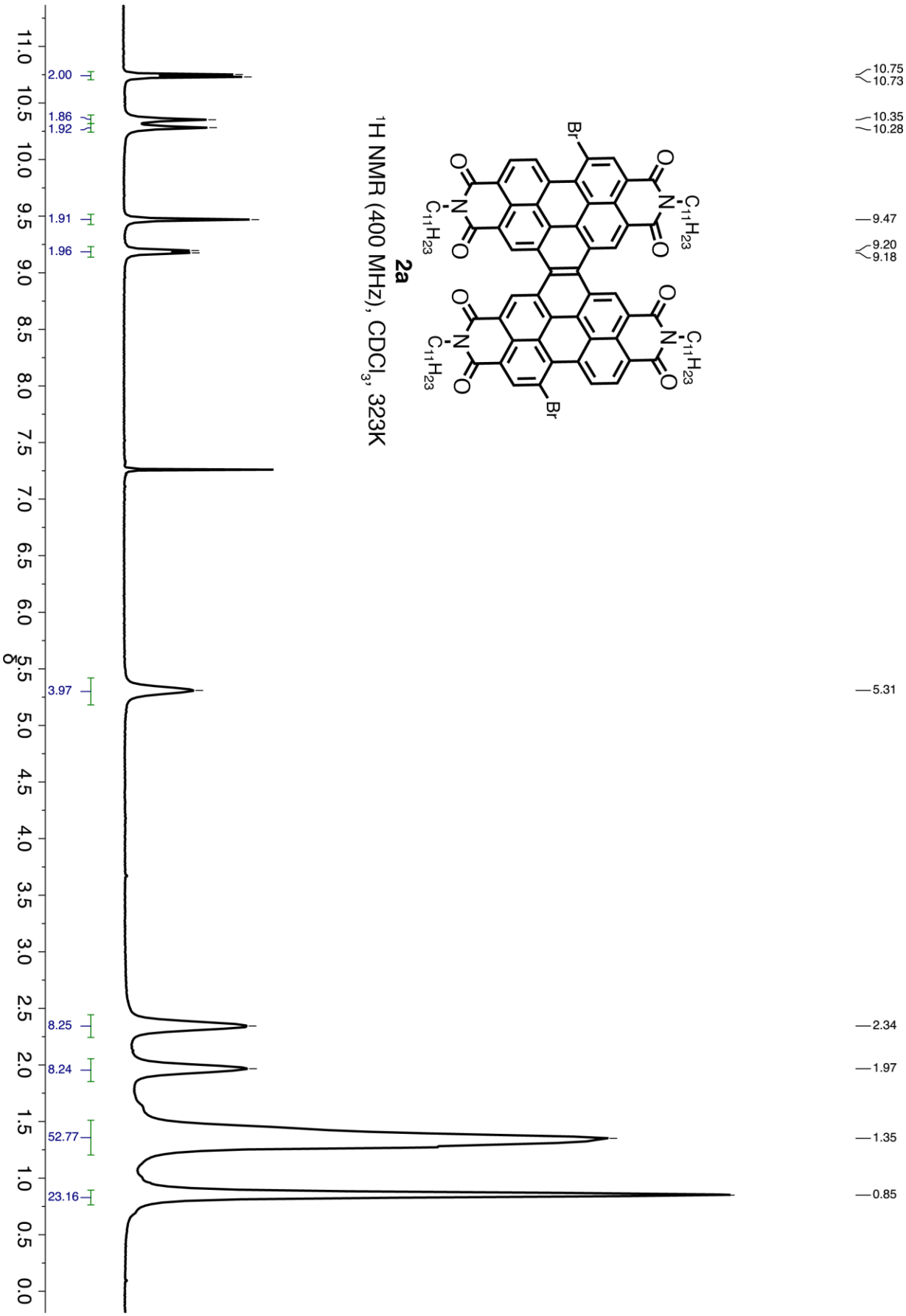
***Synthesis of trans-cDBDB*.** Bis[4-(Pt(COD)Cl)-phenyl]-hPDI2-trans (**2c**) (1.00 equiv, 0.0922 mmol, 0.207 g), commercially available 5,5′-bis(trimethylstannyl)-2,2′-bithiophene (1.00 equivalent, 0.0922 mmol, 0.0450 grams) and THF (31.0 mL) were added to an oven-dried 150. mL round bottom flask. The mixture was degassed for thirty minutes and, then, stirred in a 55 °C oil bath for 48 h. The crude mixture was concentrated and triphenylphosphine (20.0 equiv, 1.84 mmol, 0.538 g) was added to the flask with toluene (31.0 mL). The mixture was degassed for ten minutes, then stirred for overnight in a 100 °C oil bath. The crude mixture was first purified by column chromatography (24 g Redisep Rf Silica) using a gradient from 0% to 100% CH_2Cl_2/hexanes at 35 mL/min. Fractions that contained *trans*-**cDBDB** were collected and further purified on by preparative TLC using 70%:30% CH_2Cl_2/hexanes. To remove a small impurity, the product mixture was further purified using a COSMOSIL Buckyprep column (20 mm I.D. x 250 mm, 5 µm), using an isocratic method of 50% methylene chloride:50% hexanes. The solids were re-precipitated from methanol, followed by hexanes. The product is a dark purple solid (0.0100 g, 0.00289 mmol, 6% yield). **^{1}H NMR** (400 MHz, 400 K, $C_2D_2Cl_4$) □[*major stereoisomer*] 10.25 (s, 4H), 10.22 (s, 4H), 9.10 (s, 4H), 8.97 (d, J = 8.4 Hz, 4H), 8.67 (d, J = 8.4 Hz, 4H), 7.75 (d, J = 8.2 Hz, 8H), 7.61 (d, J = 8.1 Hz, 8H), 7.50 (d, J = 4.0 Hz, 4H), 7.32 (d, J = 3.9 Hz, 4H), 5.39 (m, 4H), 5.20 (m, 4H), 2.45 (m, br, 8H), 2.24 (m, br, 8H), 2.05 (m, br, 8H), 1.96 (m, br, 8H), 1.37* (m, br, 96H), 0.94* (tr, br, 24H), 0.83 (tr, br, 24H). [*distinguishable minor stereoisomer peaks*] 9.06, 8.71. **^{13}C NMR** (100 MHz, 400K, $C_2D_2Cl_4$) δ□164.4, 164.1, 164.0, 142.6, 142.0, 141.3, 137.4, 134.4, 134.2, 133.5, 132.7, 132.6, 132.5, 130.6, 130.4, 130.4, 130.4, 130.1, 128.9, 127.2, 127.1, 127.1, 127.0, 126.8, 126.5, 126.1, 125.2, 125.1, 124.9, 124.5, 124.2, 123.4, 122.8, 122.4, 122.1, 55.6, 55.3, 33.0, 32.8, 32.6, 32.4, 31.8, 31.7, 31.7, 26.7, 26.7, 26.7, 22.5, 22.4, 22.3, 13.9, 13.8, 13.7. **IR** (cm^{-1}) 2956, 2924, 2854, 1703, 1661, 1594, 1320. **HRMS** (MALDI-) calculated m/z for $[C_{228}H_{228}N_8O_{16}S_4]^-$ is 3461.61516, found 3461.6384.

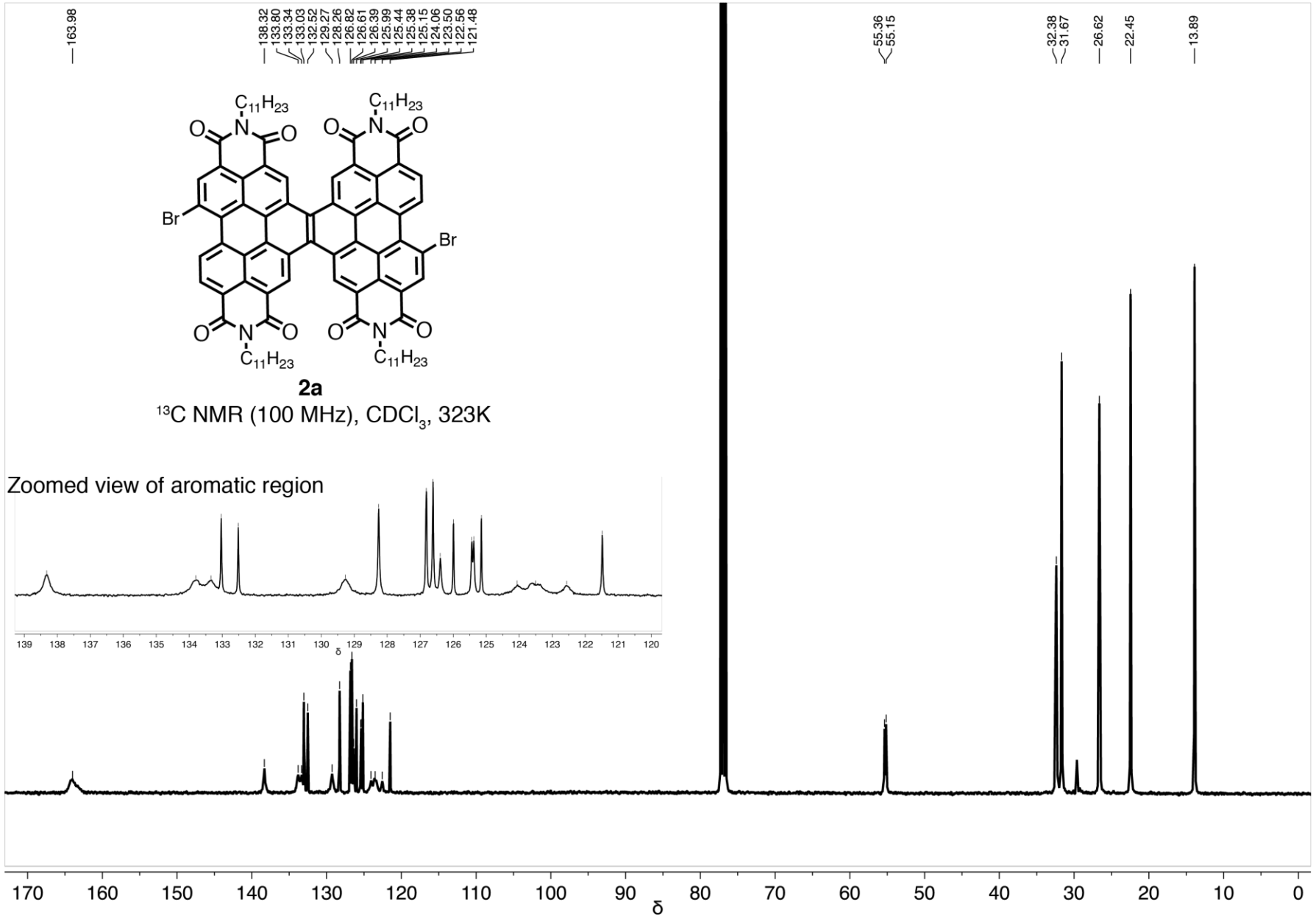
*integration is higher due to overlapping peak with both H_20, and/or a small amount of grease.

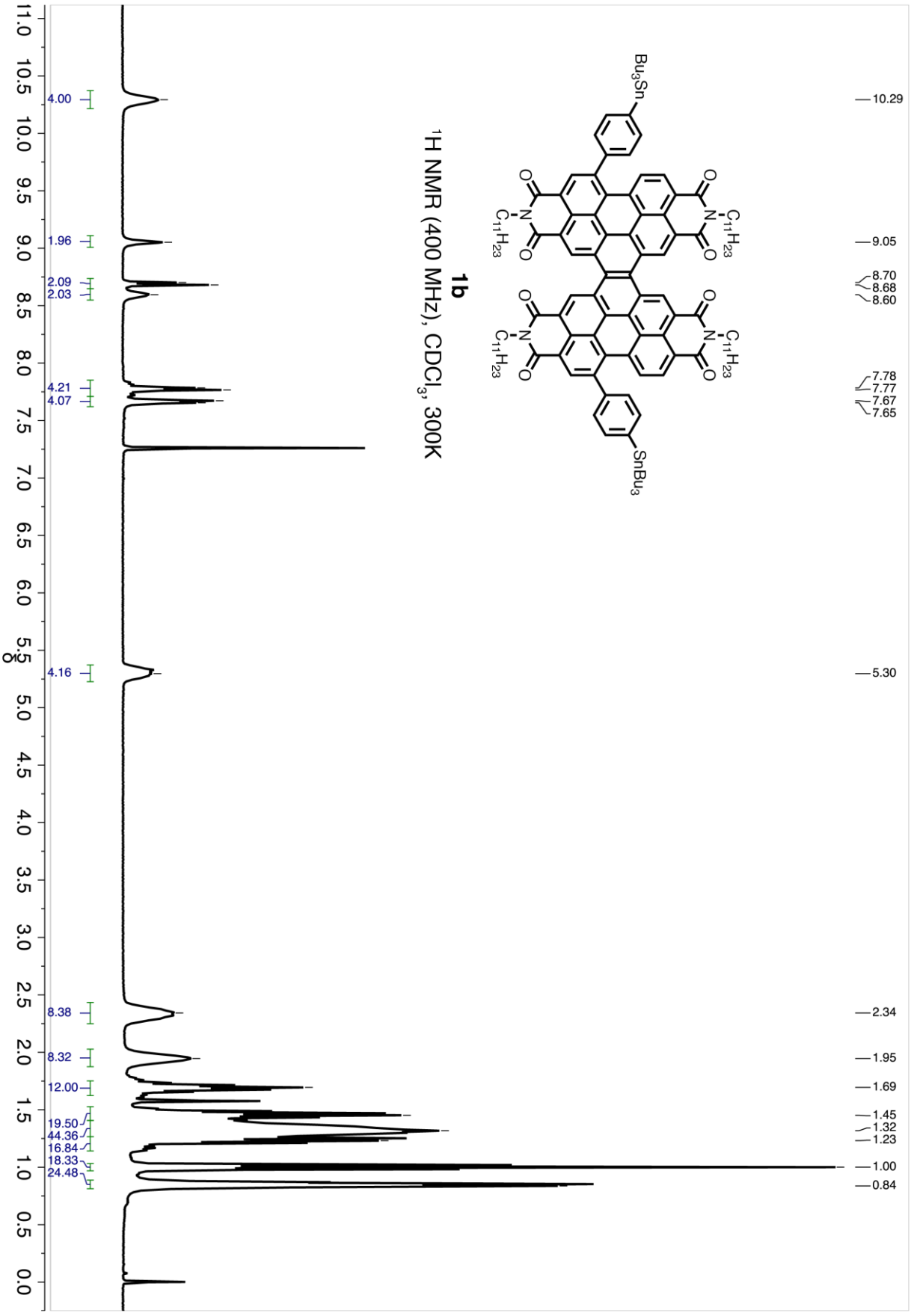
IV. ^{1}H NMR and ^{13}C NMR Spectra

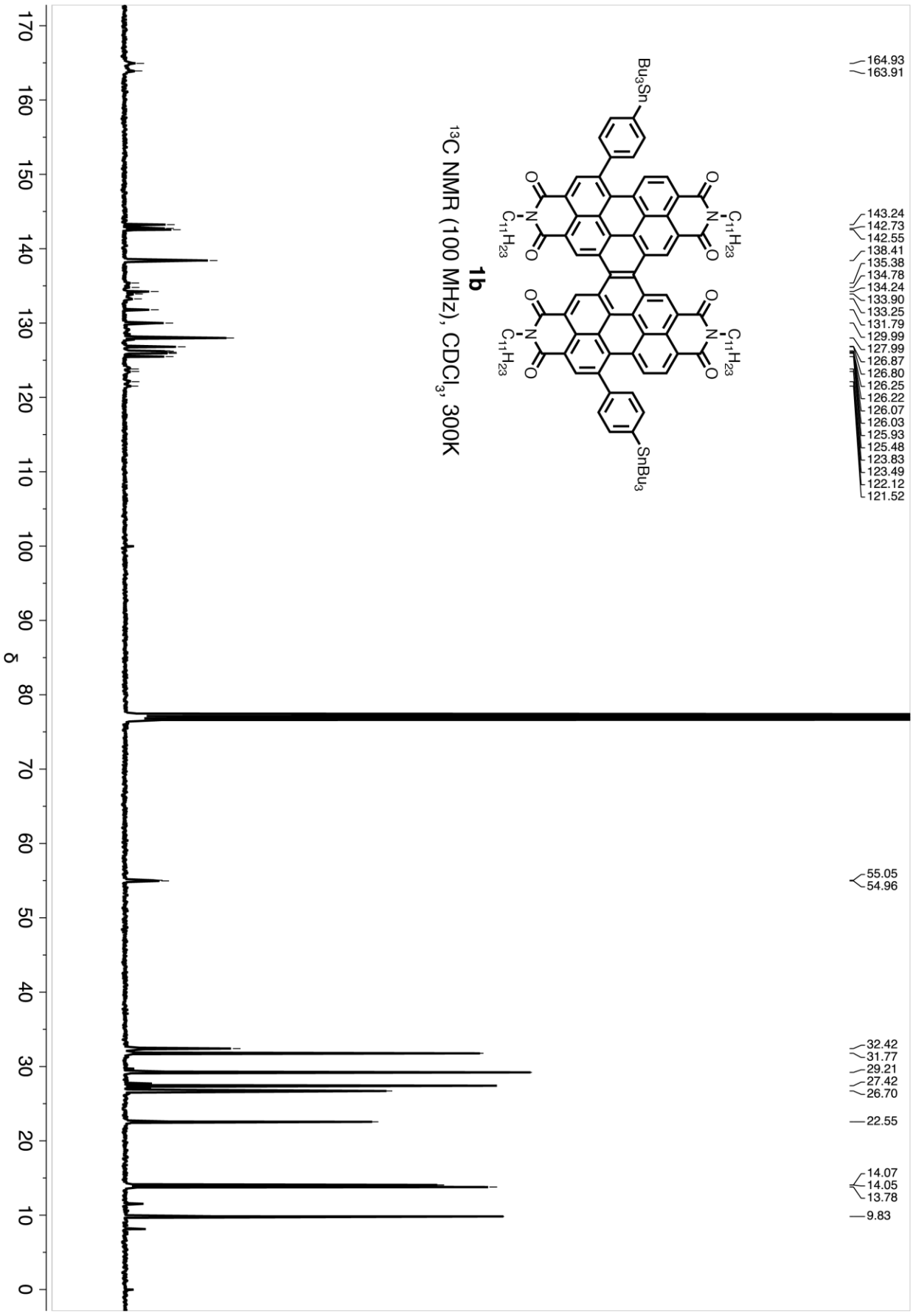


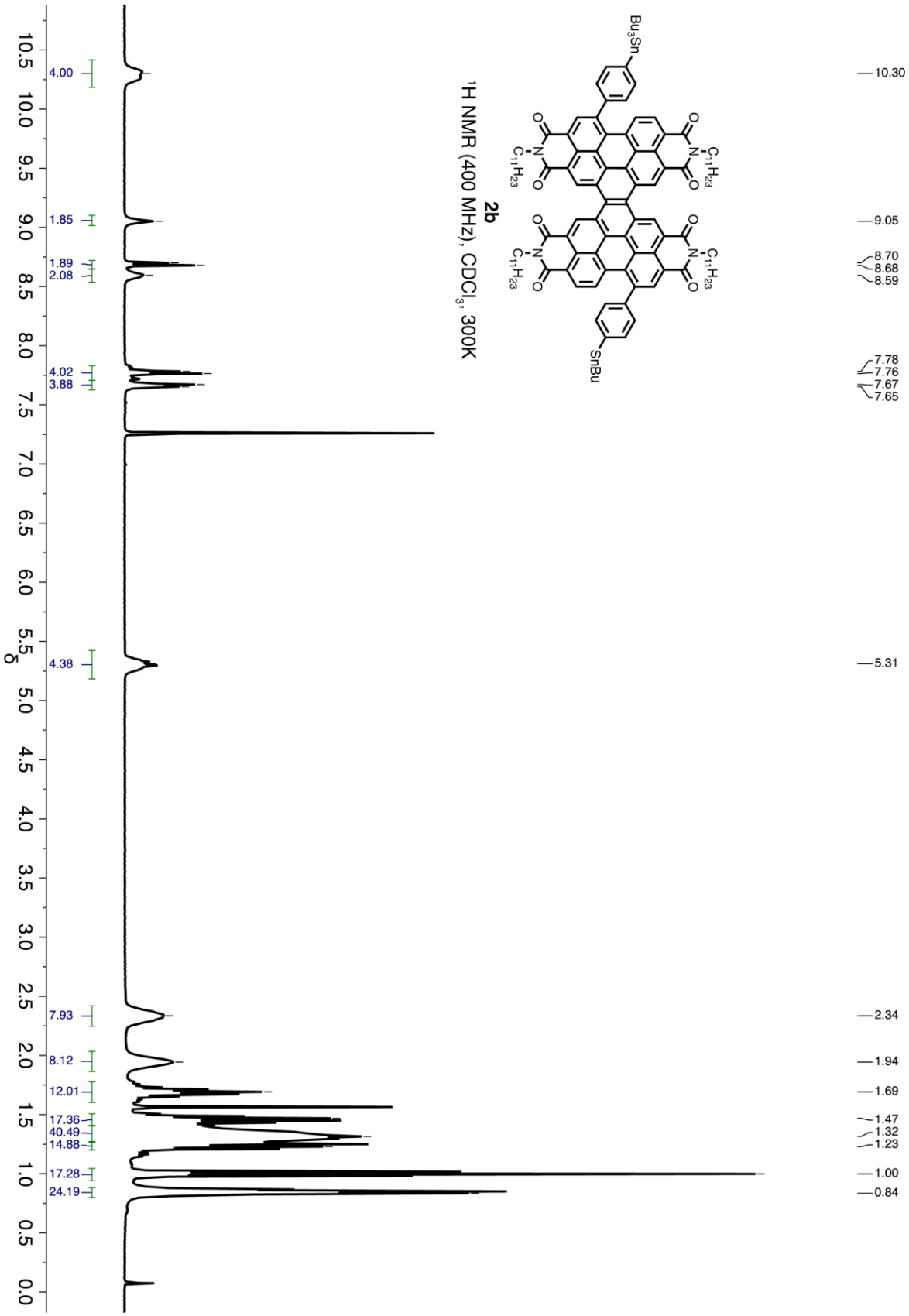

163.98
138.32
133.80
133.34
133.03
132.52
129.27
128.26
126.82
126.61
126.39
125.99
125.44
125.38
125.15
124.06
123.50
122.56
121.48
55.36
55.15
32.38
31.67
26.62
22.45
13.89
Br
Br
1a
13C NMR (100 MHz), CDCl3, 323K
Zoomed view of aromatic region
δ
δ

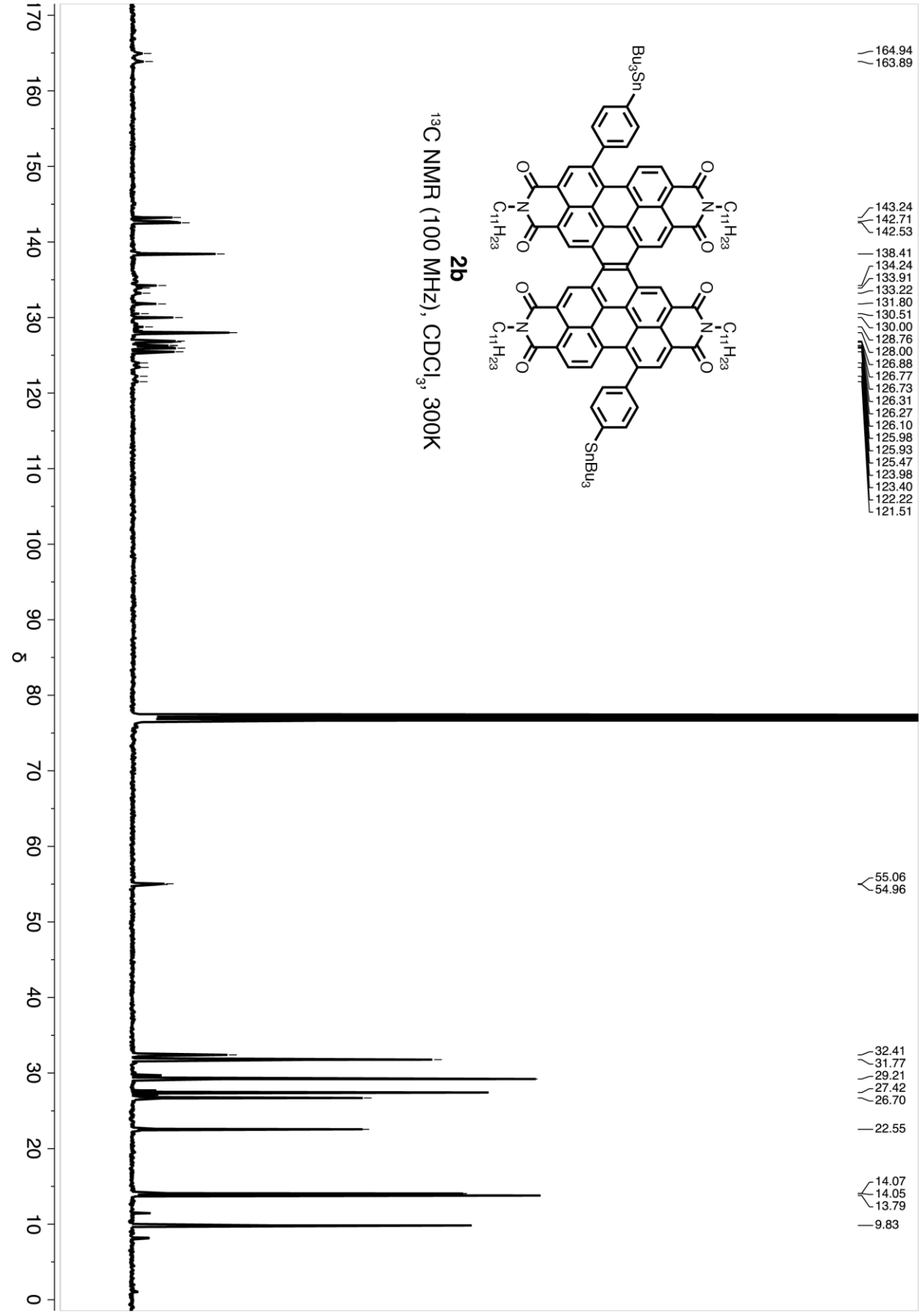

2a
^{1}H NMR (400 MHz), CDCl$_3$, 323K
δ
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
2.00
1.86
1.92
1.91
1.96
3.97
8.25
8.24
52.77
23.16
10.75
10.73
10.35
10.28
9.47
9.20
9.18
5.31
2.34
1.97
1.35
0.85
Br
Br
$C_{11}H_{23}$
$C_{11}H_{23}$
$C_{11}H_{23}$
$C_{11}H_{23}$


163.98
138.32
133.80
133.34
133.03
132.52
129.27
128.26
126.82
126.61
126.39
125.99
125.44
125.38
125.15
124.06
123.50
122.56
121.48
55.36
55.15
32.38
31.67
26.62
22.45
13.89
Br
Br
2a
13C NMR (100 MHz), CDCl3, 323K
Zoomed view of aromatic region
δ


1b
^{1}H NMR (400 MHz), $CDCl_3$, 300K
Bu_3Sn
$SnBu_3$
$C_{11}H_{23}$
δ
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
4.00
1.96
2.09
2.03
4.21
4.07
4.16
8.38
8.32
12.00
19.50
44.36
16.84
18.33
24.48
10.29
9.05
8.70
8.68
8.60
7.78
7.77
7.67
7.65
5.30
2.34
1.95
1.69
1.45
1.32
1.23
1.00
0.84


1b
^{13}C NMR (100 MHz), $CDCl_3$, 300K
Bu_3Sn
$SnBu_3$
$C_{11}H_{23}$
δ
164.93
163.91
143.24
142.73
142.55
138.41
135.38
134.78
134.24
133.90
133.25
131.79
129.99
127.99
126.87
126.80
126.25
126.22
126.07
126.03
125.93
125.48
123.83
123.49
122.12
121.52
55.05
54.96
32.42
31.77
29.21
27.42
26.70
22.55
14.07
14.05
13.78
9.83


3
2b
^{1}H NMR (400 MHz), $CDCl_3$, 300K
Bu_3Sn
SnBu
$C_{11}H_{23}$
δ
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
4.00
1.85
1.89
2.08
4.02
3.88
4.38
7.93
8.12
12.01
17.36
40.49
14.88
17.28
24.19
10.30
9.05
8.70
8.68
8.59
7.78
7.76
7.67
7.65
5.31
2.34
1.94
1.69
1.47
1.32
1.23
1.00
0.84


2b
^{13}C NMR (100 MHz), $CDCl_3$, 300K
δ
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
Bu_3Sn
$SnBu_3$
$C_{11}H_{23}$
164.94
163.89
143.24
142.71
142.53
138.41
134.24
133.91
133.22
131.80
130.51
130.00
128.76
128.00
126.88
126.77
126.73
126.31
126.27
126.10
125.98
125.93
125.47
123.98
123.40
122.22
121.51
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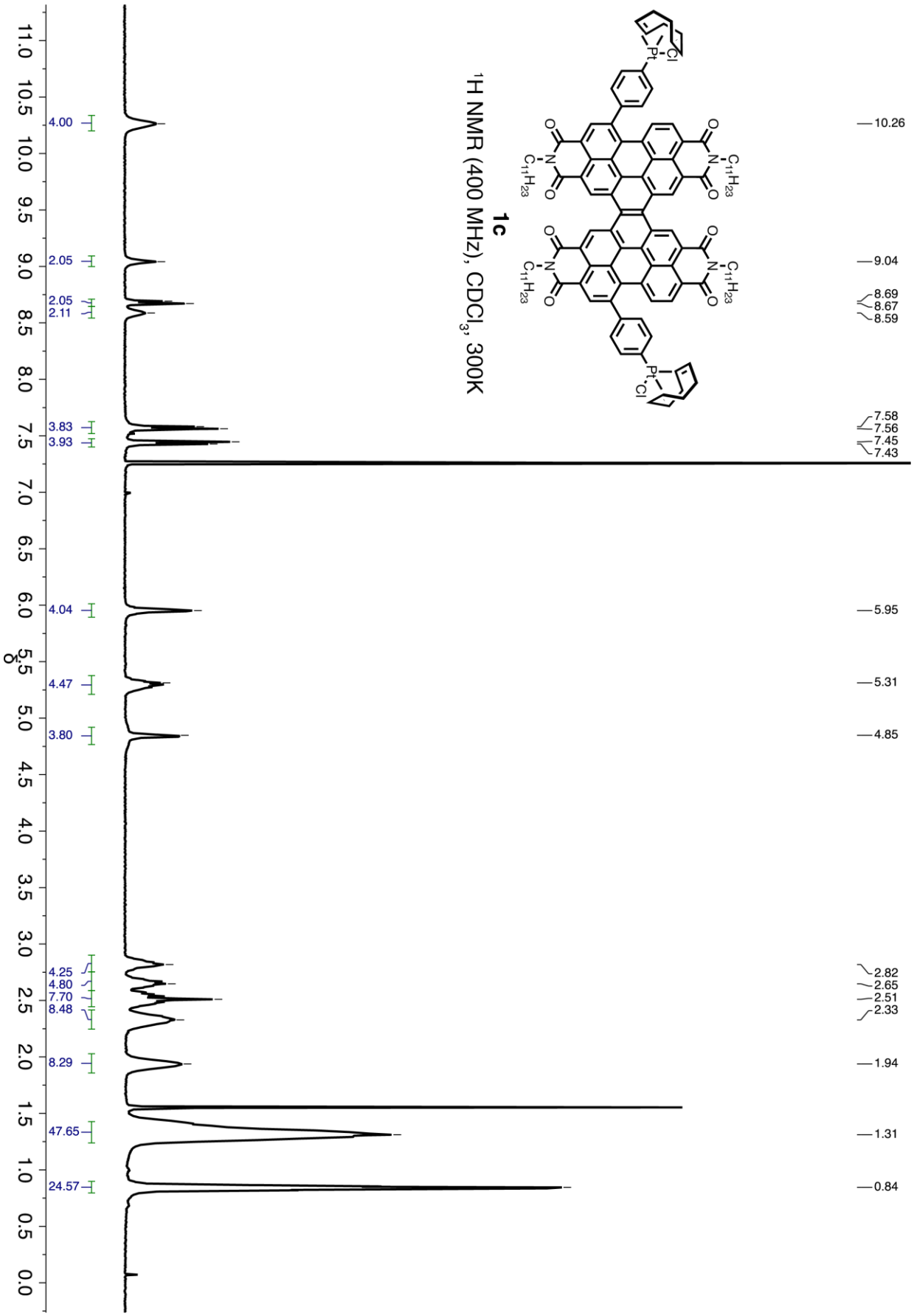
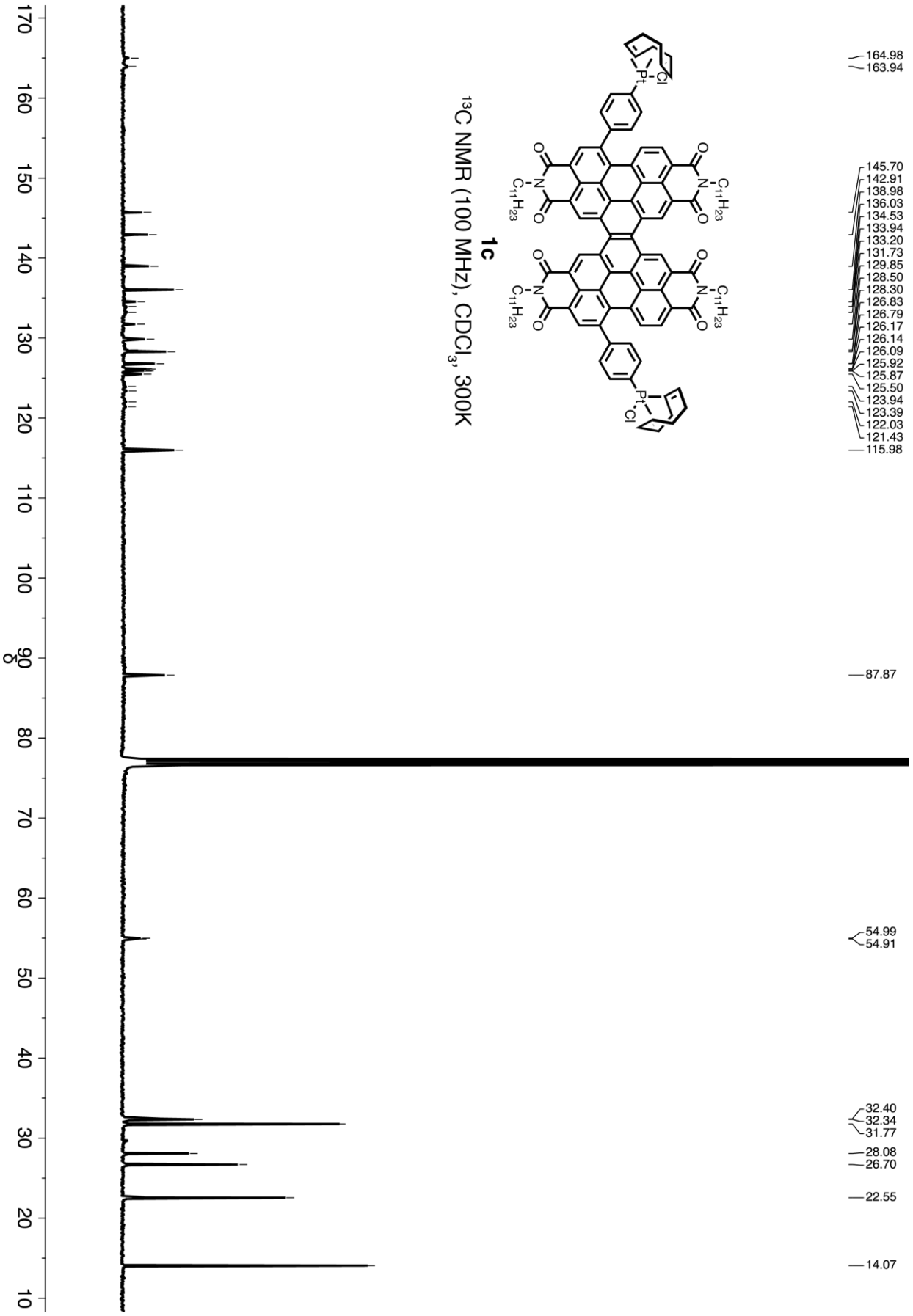
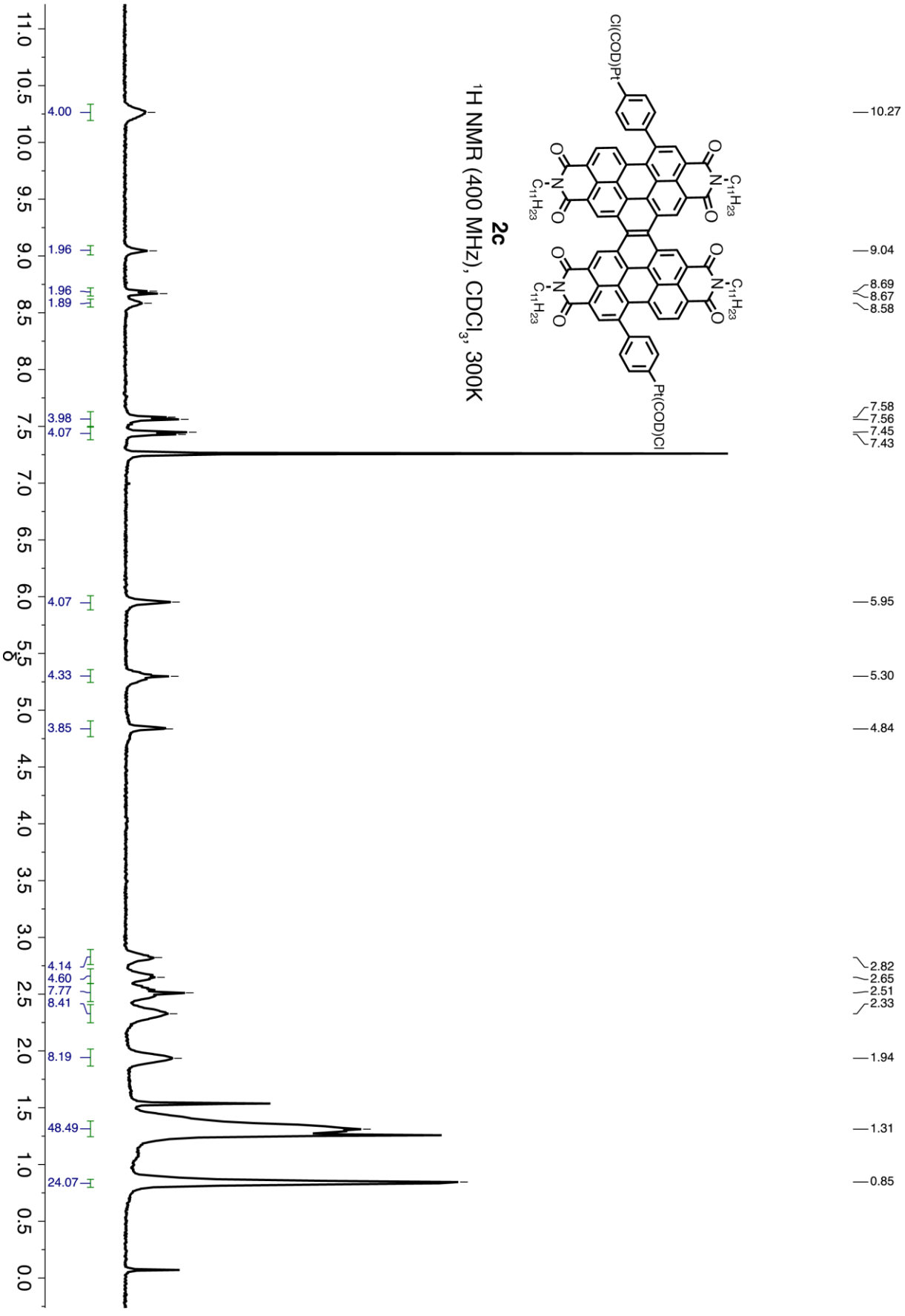
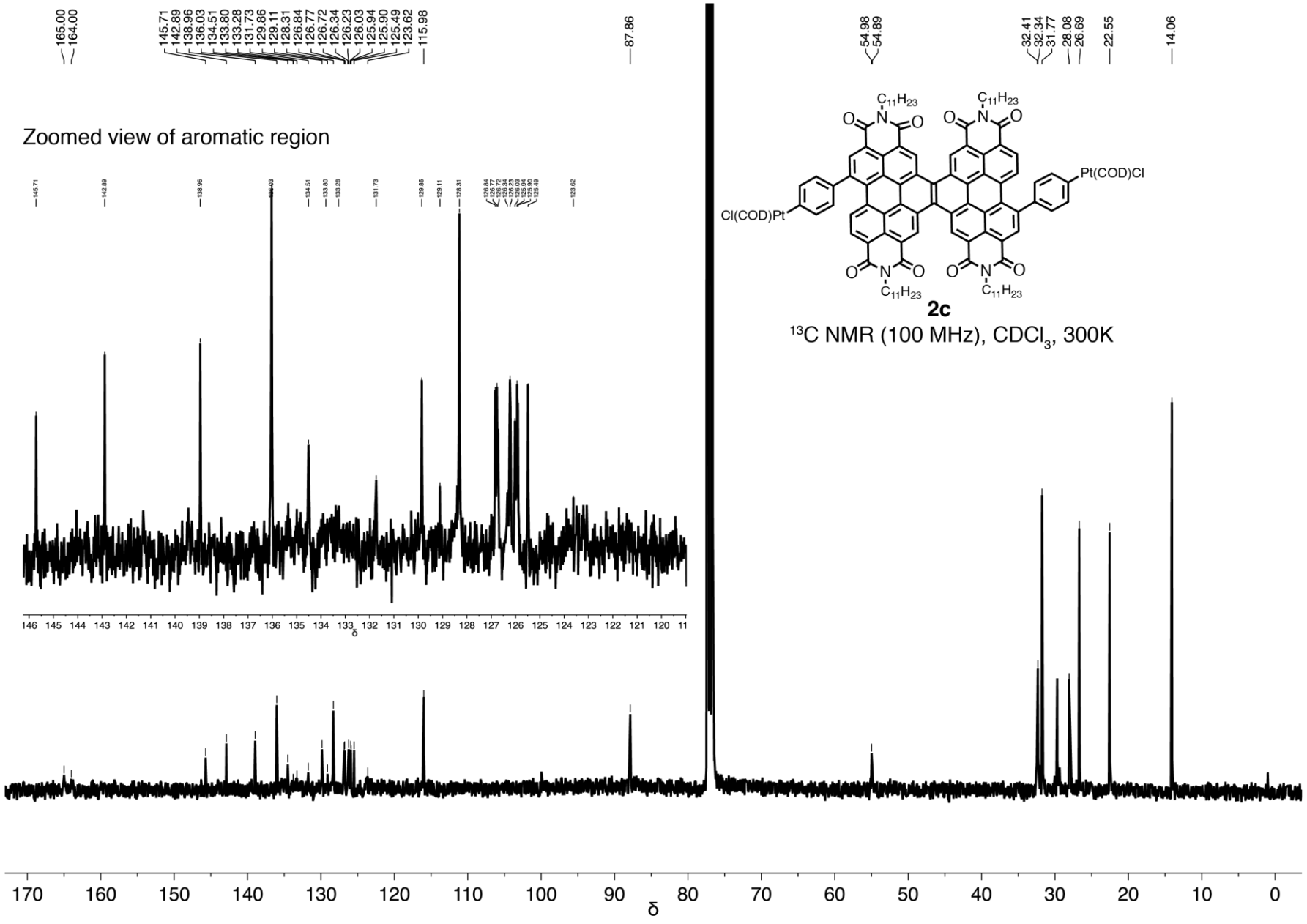
26.70
22.55
14.07
14.05
13.79
9.83


1c
^{1}H NMR (400 MHz), $CDCl_3$, 300K
δ
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
4.00
2.05
2.05
2.11
3.83
3.93
4.04
4.47
3.80
4.25
4.80
7.70
8.48
8.29
47.65
24.57
10.26
9.04
8.69
8.67
8.59
7.58
7.56
7.45
7.43
5.95
5.31
4.85
2.82
2.65
2.51
2.33
1.94
1.31
0.84


1c
^{13}C NMR (100 MHz), $CDCl_3$, 300K
164.98
163.94
145.70
142.91
138.98
136.03
134.53
133.94
133.20
131.73
129.85
128.50
128.30
126.83
126.79
126.17
126.14
126.09
125.92
125.87
125.50
123.94
123.39
122.03
121.43
115.98
87.87
54.99
54.91
32.40
32.34
31.77
28.08
26.70
22.55
14.07
δ


2c
^{1}H NMR (400 MHz), CDCl$_3$, 300K
Cl(COD)Pt
Pt(COD)Cl
$C_{11}H_{23}$
δ
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
4.00
1.96
1.96
1.89
3.98
4.07
4.07
4.33
3.85
4.14
4.60
7.77
8.41
8.19
48.49
24.07
10.27
9.04
8.69
8.67
8.58
7.58
7.56
7.45
7.43
5.95
5.30
4.84
2.82
2.65
2.51
2.33
1.94
1.31
0.85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164.00
145.71
142.89
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136.03
134.51
133.80
133.28
131.73
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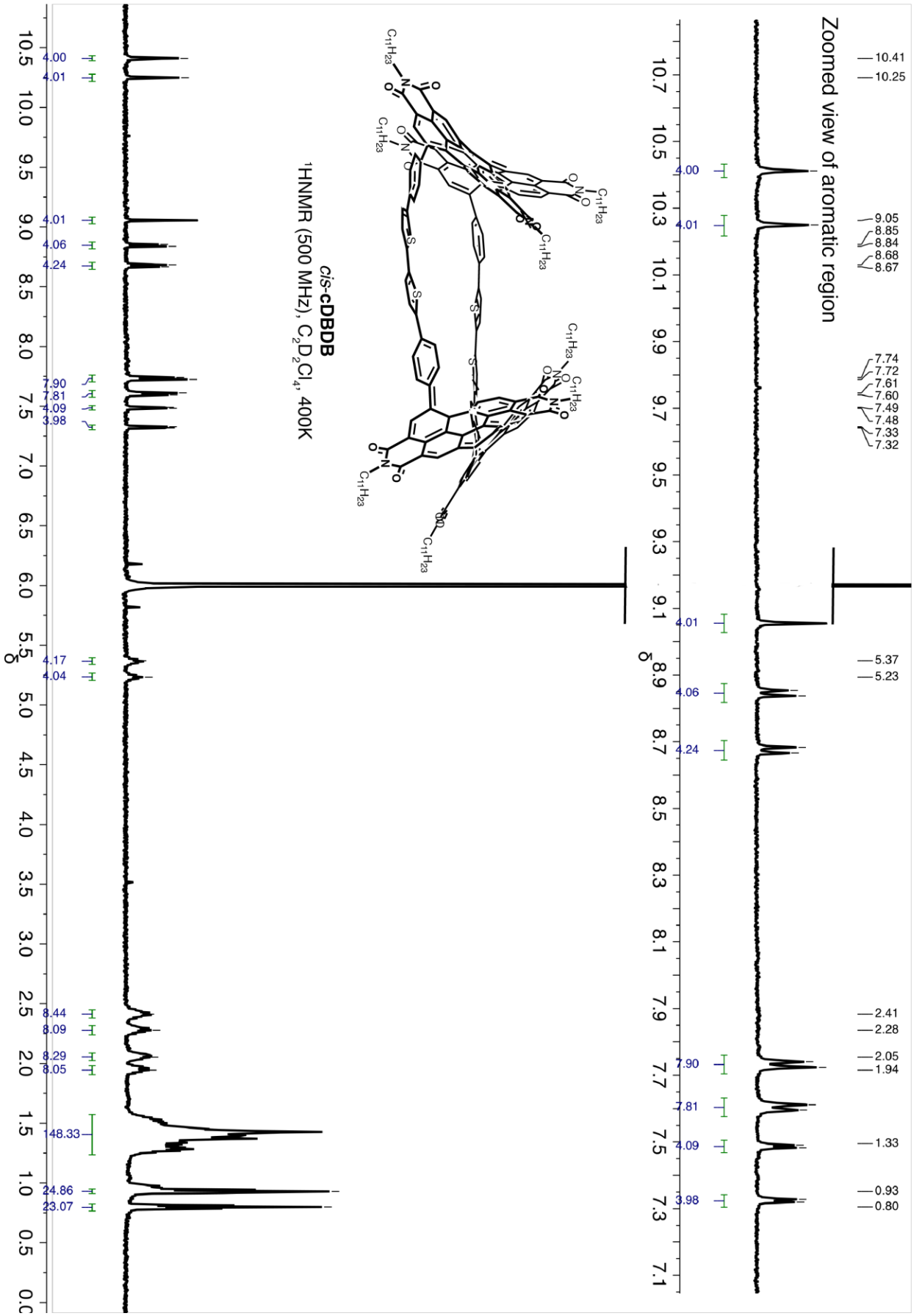
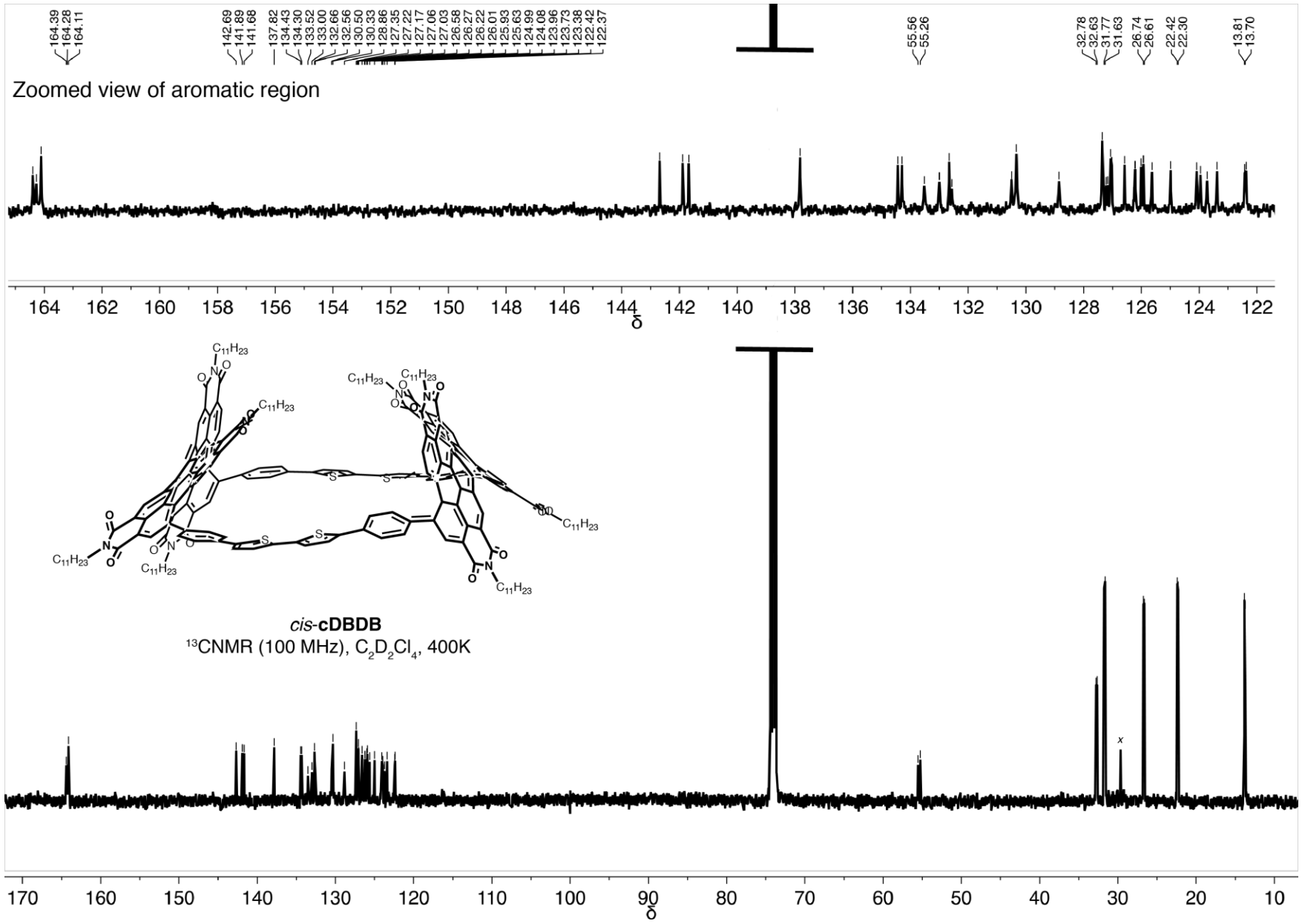
129.11
128.31
126.84
126.77
126.72
126.34
126.23
126.03
125.94
125.90
125.49
123.62
115.98
87.86
54.98
54.89
32.41
32.34
31.77
28.08
26.69
22.55
14.06
Zoomed view of aromatic region
Cl(COD)Pt
Pt(COD)Cl
C11H23
2c
13C NMR (100 MHz), CDCl3, 300K
δ


Zoomed view of aromatic region
10.41
10.25
9.05
8.85
8.84
8.68
8.67
7.74
7.72
7.61
7.60
7.49
7.48
7.33
7.32
5.37
5.23
2.41
2.28
2.05
1.94
1.33
0.93
0.80
4.00
4.01
4.06
4.24
7.90
7.81
4.09
3.98
4.17
4.04
8.44
8.09
8.29
8.05
48.33
24.86
23.07
cis-cDBDB
1HNMR (500 MHz), C2D2Cl4, 400K
δ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164.28
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142.69
141.89
141.68
137.82
134.43
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133.52
133.00
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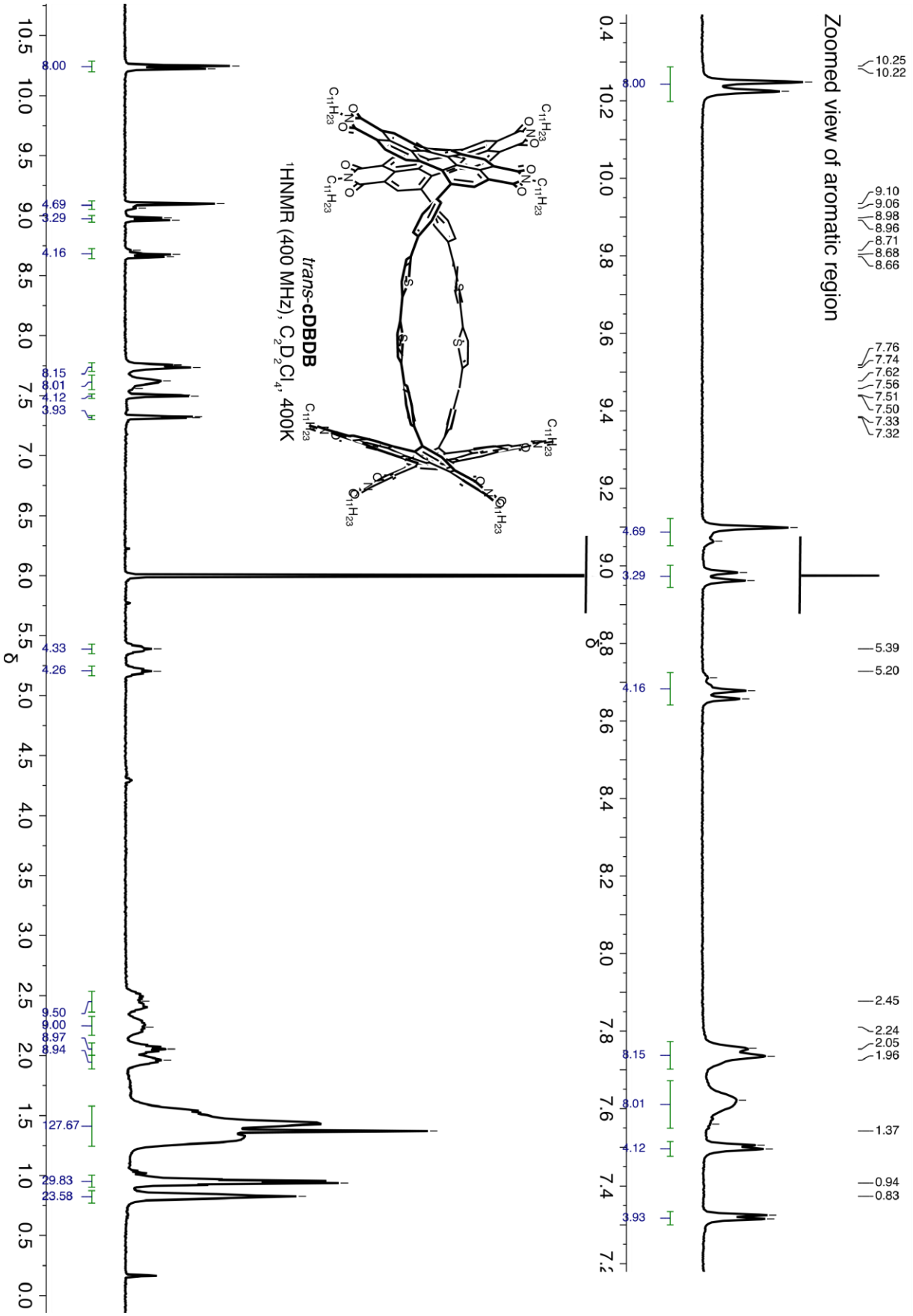
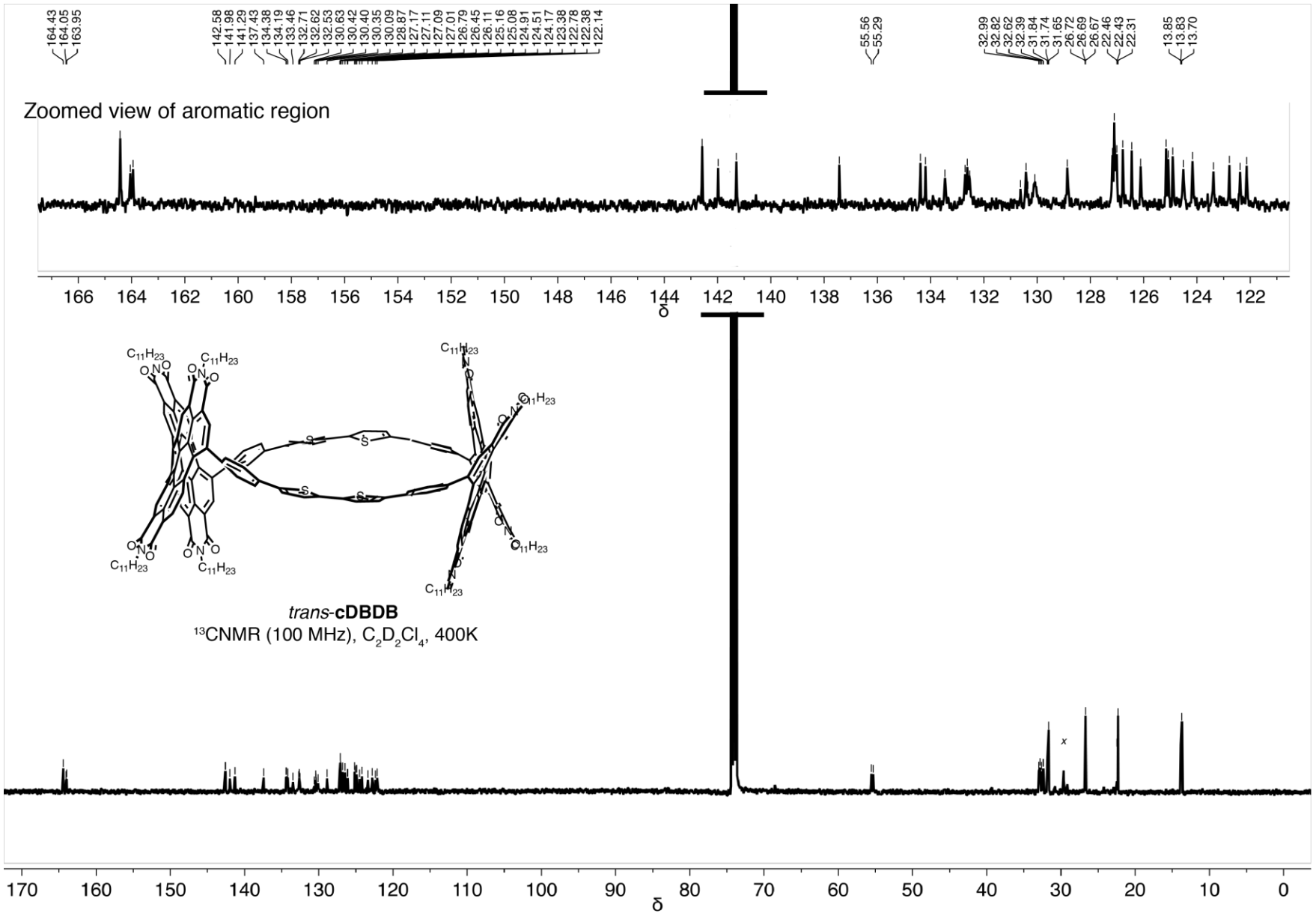
132.56
130.50
130.33
128.86
127.35
127.22
127.17
127.06
127.03
126.58
126.27
126.22
126.01
125.93
125.63
124.99
124.08
123.96
123.73
123.38
122.42
122.37
55.56
55.26
32.78
32.63
31.77
31.63
26.74
26.61
22.42
22.30
13.81
13.70
Zoomed view of aromatic region
164 162 160 158 156 154 152 150 148 146 144 142 140 138 136 134 132 130 128 126 124 122
δ
$C_{11}H_{23}$
S
cis-**cDBDB**
^{13}CNMR (100 MHz), $C_2D_2Cl_4$, 400K
x
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
δ


Zoomed view of aromatic region
trans-cDBDB
¹HNMR (400 MHz), C2D2Cl4, 400K
δ



trans-**cDBDB**

^{13}CNMR (100 MHz), $C_2D_2Cl_4$, 400K

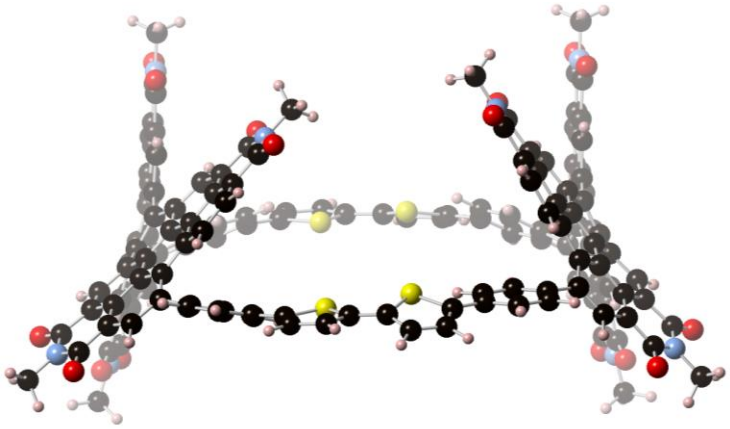
V. Density Functional Theory (DFT) calculations

All quantum chemical calculations were performed using Jaguar, version 8.2, Schrodinger, Inc., New York, NY, 2013. (See A. D. Bochevarov, E. Harder, T. F. Hughes, J. R. Greenwood, D. A. Braden, D. M. Philipp, D. Rinaldo, M. D. Halls, J. Zhang, R. A. Friesner, "Jaguar: A High Performance Quantum Chemistry Software Program with Strengths in Life and Materials Sciences", Int. J. Quantum Chem., 2013, 113(18), 2110-2142). All geometries were optimized using the B3LYP functional and the 6-31G** basis set. In the following pages, we include *cis*-cDBDB, *trans*-**cDBDB**, both acyclic corrals, and a bithiophene's minimized geometries as well as the homodesmotic calculations.

Optimized Geometries

Compound *cis*-**cDBDB**

Structure



Energy: -8915.8154 hartrees

angstroms

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C	5.413486	4.280325	-0.230142
C	5.381393	3.590375	1.015668
C	4.328930	3.833474	1.962325
C	4.148829	3.005598	3.116631
C	5.229062	2.076065	3.468296
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C	7.316604	0.242094	4.072982
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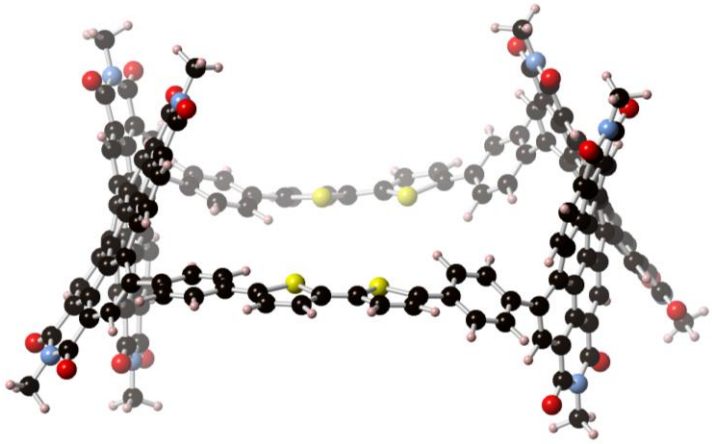
Compound *trans*-**cDBDB**

Structure



Energy: -8915.8024 hartrees

angstroms

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C	2.811642	3.998341	-1.760244
C	4.133593	3.843890	-1.248814
C	4.283949	3.643716	0.145784
C	3.153375	3.279393	0.945651
C	3.324421	2.761126	2.265085
C	4.623604	2.960361	2.910950
C	5.724914	3.433785	2.133183
C	5.578426	3.736689	0.742919
C	6.685924	4.181435	-0.030031
C	7.954539	4.250363	0.617210
C	8.105421	3.996331	1.957446
C	6.992087	3.611852	2.754602
C	4.815389	2.801234	4.293184
C	6.053738	3.007014	4.895908
C	7.153053	3.384393	4.133757
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N	9.551316	3.889446	3.940776
C	9.465749	4.102832	2.556624
C	0.940963	2.264969	2.324847
C	2.227208	2.082480	2.863417
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O	-1.630498	2.757343	1.192087
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C	6.533503	4.362170	-1.463480
H	8.856109	4.469144	0.065948
H	6.183987	2.870448	5.963982
C	10.857321	4.018195	4.594655
H	0.080144	1.809975	2.803434
H	2.642939	4.332026	-2.775354
C	-2.096074	3.823808	-1.214274
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C	9.676995	6.092217	-2.683535
C	9.866937	5.445053	-3.934044
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N	11.829853	7.230098	-2.983258
C	10.669035	7.088301	-2.201474
O	10.498879	7.747105	-1.185770
C	12.861604	8.172203	-2.537648
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C	6.659700	3.184353	-5.549336
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C	5.358535	3.534114	-3.465080
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C	4.366339	2.342470	-5.353611
C	5.533145	2.546941	-6.139401
C	5.580216	2.096589	-7.471849
C	6.733427	2.303469	-8.221576
C	7.855548	2.893768	-7.645064
C	3.209902	1.595220	-5.911132
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C	4.418431	1.405625	-8.084804
O	2.206838	1.334412	-5.260519
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O	4.421712	1.024434	-9.247555
H	6.742659	1.984875	-9.258248
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H	4.097157	-1.983640	3.974150
C	11.758888	0.203958	-8.090981
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N	1.283712	-12.995177	-3.056633
C	0.966355	-12.831644	-1.701166
C	2.010305	-13.218276	-0.719701
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C	0.247374	-12.592943	-4.012878
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C	11.071321	-13.636052	-3.437890
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C	15.106743	-13.373042	0.600911
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C	8.346400	-14.506028	-6.566680
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O	5.281812	-16.401903	-7.130523
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O	8.163592	-14.611534	-10.196104
H	10.163478	-13.450474	-9.229105
H	5.821953	-15.886621	-4.761802
C	2.652188	-10.296713	4.742941
C	1.582818	-11.193175	4.555277
C	1.651451	-12.208759	3.606369
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H	4.679268	-9.852697	4.143103
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C	11.374603	-10.153646	-5.932074
C	12.467357	-11.031876	-5.823725
C	13.639108	-10.717876	-6.527541
C	13.725968	-9.552388	-7.277471
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H	10.461715	-10.371849	-5.386826
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H	14.657456	-9.309432	-7.778232
C	12.822945	-7.383738	-8.060883
C	13.633386	-7.147024	-9.148785
C	13.655681	-5.798390	-9.563896
C	12.864701	-4.967405	-8.796180
S	12.059274	-5.892403	-7.540590
H	14.181631	-7.935968	-9.650419
H	14.243650	-5.442434	-10.399874
C	2.402970	-2.771857	5.965926
C	1.884136	-3.092969	7.200935
C	1.867059	-4.480725	7.475904
C	2.350469	-5.256857	6.441754
S	2.873112	-4.235849	5.116517
H	1.524318	-2.344771	7.897884
H	1.505265	-4.902414	8.406194
C	2.326563	-6.701465	6.340678
C	1.565228	-7.573690	7.094342
C	1.646638	-8.919205	6.663166
C	2.476176	-9.108367	5.580790
S	3.190337	-7.579950	5.094864
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H	1.101737	-9.730067	7.133083
H	11.638116	-12.654324	-7.423144
H	3.590028	-14.445478	3.888867
C	12.251459	-1.070801	-8.605704
C	13.147586	-1.333512	-9.618640
C	13.430531	-2.706535	-9.795977
C	12.751350	-3.531209	-8.919113
S	11.728995	-2.580844	-7.868464
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H	14.131073	-3.078756	-10.533572
H	8.736283	3.038125	-8.254330
H	3.981262	2.509877	4.915207
H	11.584126	4.286989	3.832555
H	10.804906	4.785603	5.369534
H	11.126801	3.072470	5.069410
H	-2.024846	4.265927	-2.204665
H	-2.600851	2.856640	-1.257837
H	-2.658425	4.472656	-0.539750

H	12.503583	8.648628	-1.628629
H	13.794050	7.635654	-2.350832
H	13.044136	8.913925	-3.317857
H	2.359696	0.243329	-8.830258
H	1.959722	-0.419365	-7.212460
H	1.259260	1.123331	-7.720478
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H	0.012516	-11.534591	-3.880976
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H	16.004314	-13.864456	0.220643
H	15.353277	-12.331073	0.815426
H	6.287583	-15.748955	-10.666445
H	5.781640	-17.111288	-9.616487
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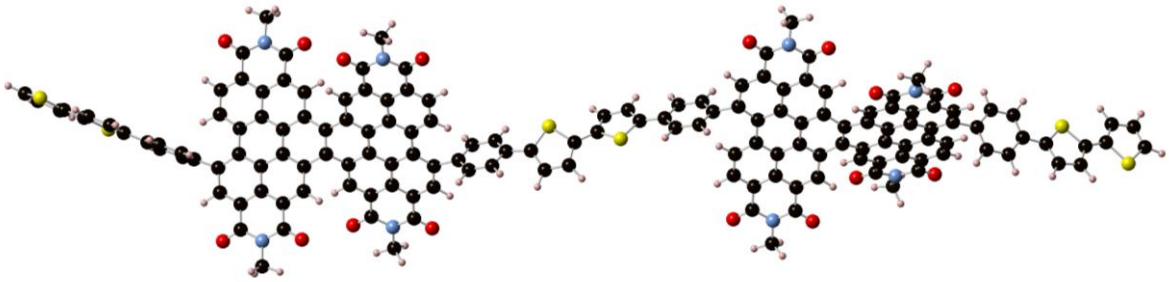
Compound *cis*-**cDBDB_Acyclic**

Structure



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C	23.102338	-2.396667	-1.536548
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C	24.794916	-1.239170	-0.084966
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C	24.032277	0.749605	1.196558
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C	26.299454	-0.006244	1.406880
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C	23.266673	2.732676	2.574452
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C	25.399039	-3.176432	-1.603430
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O	26.729060	2.119303	3.213218
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O	19.925914	-4.628425	-4.416291
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C	16.998108	2.604864	-1.063449
C	17.887611	1.480611	-0.972077
C	15.586900	2.442731	-1.308056
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C	15.389789	4.887227	-1.266943
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N	18.686386	6.521445	-0.733643
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C	14.125037	-1.617378	-1.682917
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C	13.326529	3.720902	-1.702741
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C	28.462100	-3.956560	1.043345
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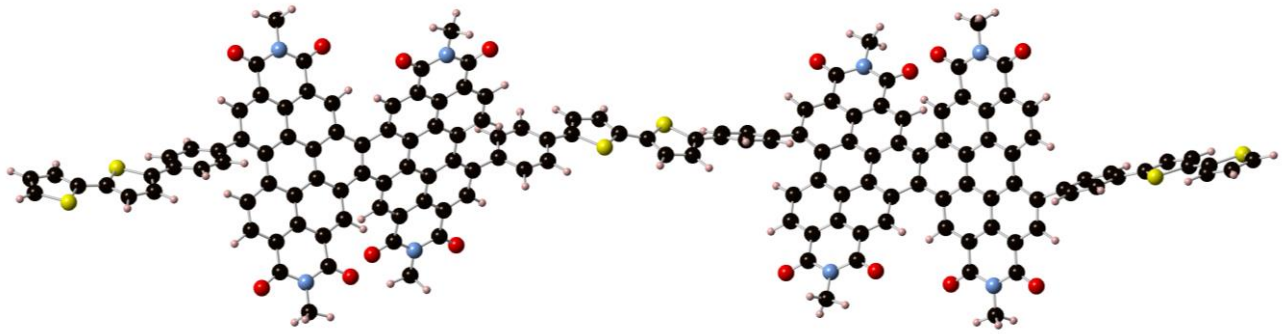
Compound *trans*-**cDBDB_Acyclic**

Structure



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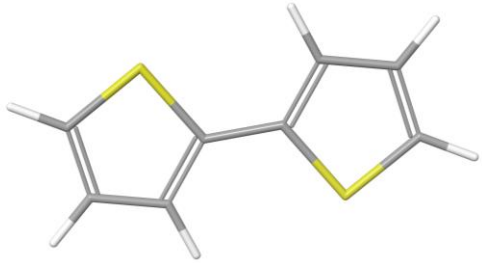
H	-9.018177	13.789513	-12.084250
H	-7.308564	13.595051	-11.580472
H	-8.065736	12.360398	-12.598531
H	10.102715	-7.400499	-5.887598
H	-13.826965	10.340060	-5.385539

Compound: **Bithiophene**

Structure

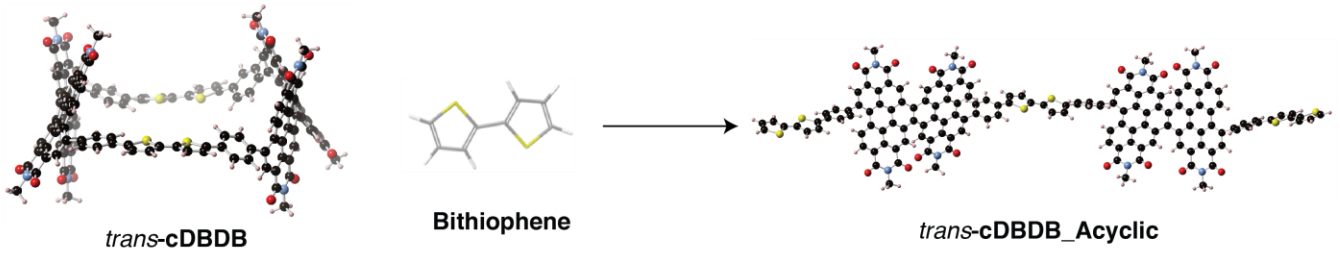


Energy: -1104.8268 hartrees

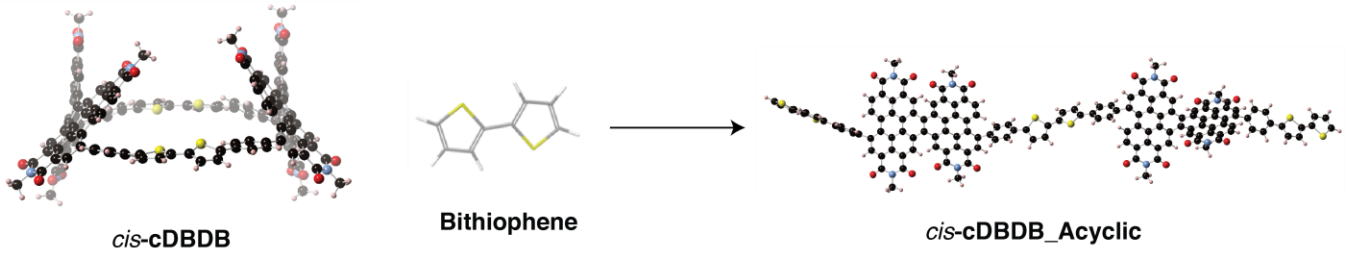
angstroms

atom	x	y	z
S1	-0.5229025548	2.1569531073	0.0161859979
C2	0.3530028893	0.6332102763	0.0062644825
C3	1.7098905419	0.8694103010	0.0122565205
C4	2.0501584230	2.2514544128	0.0246320264
C5	0.9547258678	3.0684516605	0.0281022419
C6	-0.3530028893	-0.6332102763	-0.0062644825
S7	0.5229025548	-2.1569531073	-0.0161859979
C8	-0.9547258678	-3.0684516605	-0.0281022419
C9	-2.0501584230	-2.2514544128	-0.0246320264
C10	-1.7098905419	-0.8694103010	-0.0122565205
H11	2.4448343075	0.0724557652	0.0078978216
H12	3.0698389079	2.6188720882	0.0306528745
H13	0.9193525791	4.1486289730	0.0368265795
H14	-0.9193525791	-4.1486289730	-0.0368265795
H15	-3.0698389079	-2.6188720882	-0.0306528745
H16	-2.4448343075	-0.0724557652	-0.0078978216

Homodesmotic calculations



trans-**cDBDB** + **Bithiophene** → *trans*-**cDBDB_Acyclic**



cis-**cDBDB** + **Bithiophene** → *cis*-**cDBDB_Acyclic**

Table of energies for the Homodesmotic Reaction (enthalpy)			
Compound	**Total energy (hartree)**	**Strain energy (hartrees)**	**Strain energy (kcal/mol)**
trans-**cDBDB**	-8915.8024	0.0296	18.575
trans-**cDBDB_Acyclic**	-10020.6588	-	-
Bithiophene	-1104.8268	-	-
cis-**cDBDB**	-8915.8154	0.0151	9.476
cis-**cDBDBB_Acyclic**	-10020.6573	-	-

VI. References

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