

Supporting Information

Synthesis of Highly Twisted, Nonplanar Aromatic Macrocycles Enabled by Axially Chiral 4,5-Diphenylphenanthrene Building Block

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Table of Contents

1. General	S3
2. Preparation of the 4,5-diarylphenanthrene.....	S4
3. The optimization of quadruple Suzuki-Miyaura cross-coupling	S6
4. Screening the spacer	S7
5. The synthesis of twisted macrocycles.....	S8
6. The X-ray data	S13
7. The X-ray crystal structure	S14
7.1 The comparison of X-ray crystal structure and DFT calculated result of 3b ..	S14
7.2 The X-ray crystal structures of 3c	S15
8. Computational study	S16
8.1 Optimized structures	S16
8.2 Frontier molecular orbitals of macrocycles	S19
8.3 The calculation of strain energy.....	S24
8.4 The DFT calculation of racemization barrier of 3a , 3c , 3e and 3j	S25
8.5 The DFT calculation of racemization barrier of 1	S25
8.7 The rotation barrier and VT ^1H NMR spectrum of 3a	S27
8.8 The rotation barrier and VT ^1H NMR spectrum of 1	S28
8.9 TD-DFT vertical one-electron excitations	S29
8.10 Uncorrected and thermal-corrected energies of stationary points	S31
8.11 Cartesian coordinates of optimized structures	S33
9. Kinetic study of racemization barrier of 3c	S65
10. Photophysical properties.....	S68
11. Twisted intramolecular charge transfer (TICT) emission	S70
12. Circular dichroism spectra of 1c	S72
13. References.....	S72
14. NMR spectra of new compounds.....	S73

1. General

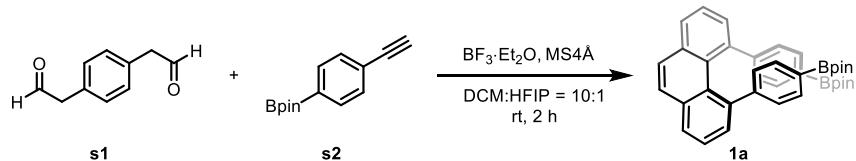
Unless otherwise noted, all reactants or reagents including dry solvents were obtained from commercial suppliers and used as received. Unless otherwise noted, all reactions were performed with dry solvents under an atmosphere of argon in dried glassware using standard vacuum-line techniques. All work-up and purification procedures were carried out with reagent-grade solvents in air.

Analytical thin-layer chromatography (TLC) was performed using E. Merck silica gel 60 F254 precoated plates (0.25 mm); detection with UV light or by dipping into a solution of KMnO₄ (1.5 g in 400 mL H₂O, 5 g NaHCO₃), followed by heating. Flash column chromatography was performed with E. Merck silica gel 60 (230-400 mesh). The developed chromatogram was analyzed by a UV lamp (254 nm). Medium pressure liquid chromatography (MPLC) was performed using Yamazen W-prep 2XY. Preparative thin-layer chromatography (PTLC) was performed using Wakogel B5-F silica-coated plates (0.75 mm) prepared in our laboratory. Preparative gel permeation chromatography (GPC) was performed with a JAI LC-9204 instrument equipped with JAIGEL-1H/JAIGEL-2H columns using chloroform as an eluent. Gas chromatography (GC) analysis was conducted on a Shimadzu GC-2010 instrument equipped with a HP-5 column (30 m · 0.25 mm, Hewlett-Packard) with dodecane as an internal standard.

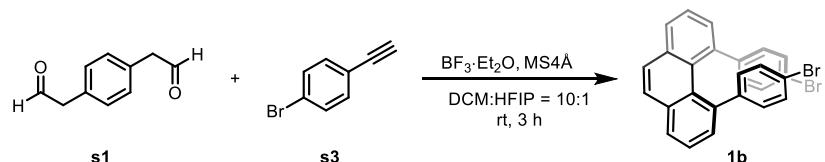
The high-resolution mass spectra (HRMS) were conducted on Thermo Fisher Scientific Exactive. Infrared spectra were recorded on a JASCO FTIR-6100 spectrometer. Nuclear magnetic resonance (NMR) spectra were recorded on a JEOLJNM-ECA-600 (¹H 600 MHz, ¹³C 150 MHz) spectrometer and a JEOL JNM-ECA-400 (¹H 400 MHz, ¹³C 100 MHz) spectrometer. Chemical shifts for ¹H NMR are expressed in parts per million (ppm) relative to tetramethylsilane (δ 0.00 ppm) or residual peak of acetone-*d*₆ (δ 2.05 ppm). Chemical shifts for ¹³C NMR are expressed in ppm relative to CDCl₃ (δ 77.16 ppm) or acetone-*d*₆ (δ 29.84 ppm). Data are reported as follows: chemical shift, multiplicity (s = singlet, d = doublet, dd = doublet of doublets, ddd = doublet of doublets of doublets, t = triplet, dt = doublet of triplets, td = triplet of doublets, q = quartet, p = quintet, m = multiplet, brs = broad singlet, brd = broad doublet), coupling constant (Hz), and integration.

2. Preparation of the 4,5-diarylphenanthrene building blocks

The reaction of diacetaldehyde compounds with terminal alkynes



Compared with our previous work,¹ we used cheaper and easier accessible $\text{BF}_3 \cdot \text{Et}_2\text{O}$ instead of $\text{B}(\text{C}_6\text{F}_5)_3$. A dry Schlenk tube equipped with a magnetic stir bar and a septum was charged with activated molecular sieve (1.1 g, 4 \AA , 1/16 in., pellets), diacetaldehyde compound **s1** (178 mg, 1.10 mmol) and alkyne **s2** (627 mg, 2.75 mmol) under air. DCM (25 mL) and hexafluoroisopropanol (HFIP) (2.5 mL) were then added under argon atmosphere. After that, $\text{BF}_3 \cdot \text{Et}_2\text{O}$ (0.27 mL, 2.2 mmol) was added dropwise at room temperature. After stirring at room temperature for 2 h, brine (20 mL) was added into the reaction. The resultant solution was extracted with DCM (3×10 mL). The combined organic layers were dried over anhydrous MgSO_4 , filtered and concentrated under vacuum. The residue was then purified by silica gel column chromatography with gradient elution of hexane/EtOAc (100:0 \rightarrow 90:10) to give **1a** (180 mg, 0.31 mmol, 28%) as a white solid. R_f (EtOAc/hexane = 1/10): 0.4; ^1H and ^{13}C NMR spectra are consistent with the previous report.¹



A dry Schlenk tube equipped with a magnetic stir bar and a septum was charged with activated molecular sieve (1.5 g, 4 \AA , 1/16 in., pellets), diacetaldehyde compound **s1** (243 mg, 1.50 mmol) and alkyne **s3** (679 mg, 3.75 mmol) under air. DCM (25 mL) and hexafluoroisopropanol (HFIP) (2.5 mL) were then added under argon atmosphere. After that, $\text{BF}_3 \cdot \text{Et}_2\text{O}$ (0.37 mL, 3.0 mmol) was added dropwise at room temperature. After stirring at room temperature for 3 h, brine (20 mL) was added into the reaction. The resultant solution was extracted with DCM (3×10 mL). The combined organic layers were dried over anhydrous MgSO_4 , filtered and concentrated under vacuum. The residue was then purified by silica gel column chromatography with gradient elution of hexane/DCM (100:0 \rightarrow 5:1) to give **1b** (180 mg, 0.61 mmol, 41%) as a white solid. R_f (DCM/hexane = 1/5): 0.4; ^1H and ^{13}C NMR spectra are consistent with the previous report.¹

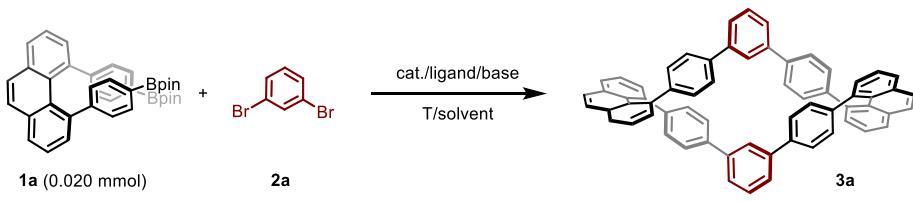


A dry Schlenk tube equipped with a magnetic stir bar and a septum was charged with activated molecular sieve (300 mg, 4 \AA , 1/16 in., pellets), diacetaldehyde compound **s1** (49 mg, 0.30 mmol) and $\text{B}(\text{C}_6\text{F}_5)_3$ (31 mg, 0.060 mmol) in a glovebox. DCM (7.5 mL) was then added under argon atmosphere. After that, alkyne **s4** (193 mg, 0.75 mmol) was added at room temperature. After stirring at room temperature for 15 h, the solvent was removed under vacuum. The residue was then purified by silica gel column chromatography with gradient elution of hexane/DCM (100:0 \rightarrow 5:1) to give **1c** directly (100 mg, 0.16 mmol, 52%) as a white solid. R_f (DCM/hexane = 1/5): 0.5; ^1H NMR (600 MHz, CDCl_3) δ 7.81 (d, J = 7.7 Hz, 2H), 7.75 (s, 2H), 7.73 (s, 2H), 7.55 (t, J = 7.5 Hz, 2H), 7.52 (d, J = 7.7 Hz, 2H), 7.49 (d, J = 7.9 Hz, 2H), 7.33 (t, J = 7.8 Hz, 2H), 7.23–7.15 (m, 6H), 6.74 (d, J = 7.3 Hz, 2H), 6.64 (d, J = 7.3 Hz, 2H). ^{13}C NMR (151 MHz, CDCl_3) δ 143.31, 143.27, 141.2, 137.0, 134.9, 130.5, 130.2, 130.0, 129.5, 128.9, 128.1, 127.9, 127.44, 127.37, 127.35, 126.9, 126.0, 125.5, 123.2. HRMS (APCI): Exact mass calculated for $\text{C}_{34}\text{H}_{35}$ ($[\text{M}]^+$): 638.0239, mass found: 638.02313.

3. The optimization of quadruple Suzuki-Miyaura cross-coupling

Optimized conditions based on our previous work²:

Table S1. The optimization of quadruple Suzuki-Miyaura cross-coupling.



1a:2a	Catalyst (mol%)	Ligand (mol%)	Base (equiv.)	T (°C)	Time (hour)	Dioxane ^a (μmol/mL)	3a ^b (%)
1:1	Pd(OAc) ₂ (20)	XPhos (20)	10 M NaOH (20)	80	21	2	30
1:1	Pd(OAc) ₂ (20)	XPhos (20)	10 M NaOH (20)	80	17	4	28
1:1	Pd(OAc) ₂ (20)	XPhos (20)	10 M NaOH (20)	60	17	2	20
1:1	Pd(OAc) ₂ (20)	XPhos (20)	10 M NaOH (20)	100	15	2	27
1:1	Pd(OAc) ₂ (20)	SPhos (20)	10 M NaOH (20)	80	16	2	14
1:1	Xphos Pd G3 (10)	–	4 M K ₃ PO ₄ (20)	80	5	2	4
1:1	Xphos Pd G2 (10)	–	4 M K ₃ PO ₄ (20)	80	5	2	n.d.
1:1	Sphos Pd G2 (10)	–	4 M K ₃ PO ₄ (20)	80	5	2	18
1:1	Sphos Pd G2 (10)	–	10 M NaOH (20)	80	16	2	15

^aThe concentration of **1a** in the solution of dioxane;

^bThe ¹H NMR yield of **3a**.

4. Screening the spacer

Our synthetic strategy using 1,3-dibromobenzene (specific angle $\approx 120^\circ$) as a keystone-like spacer is highly effective for locking the two building blocks to give the twisted 3D macrocycles. We also tested different dibromo-substituted aromatic compounds as the spacer for the twisted macrocycles. When **1a** was reacted with 1,4-dibromobenzene (**s5a**), 2,5-dibromothiophene (**s5b**), and 3,4-dibromothiophene (**s5c**), the corresponding macrocycles **s6a**, **s6b**, and **s6c** were not detected.

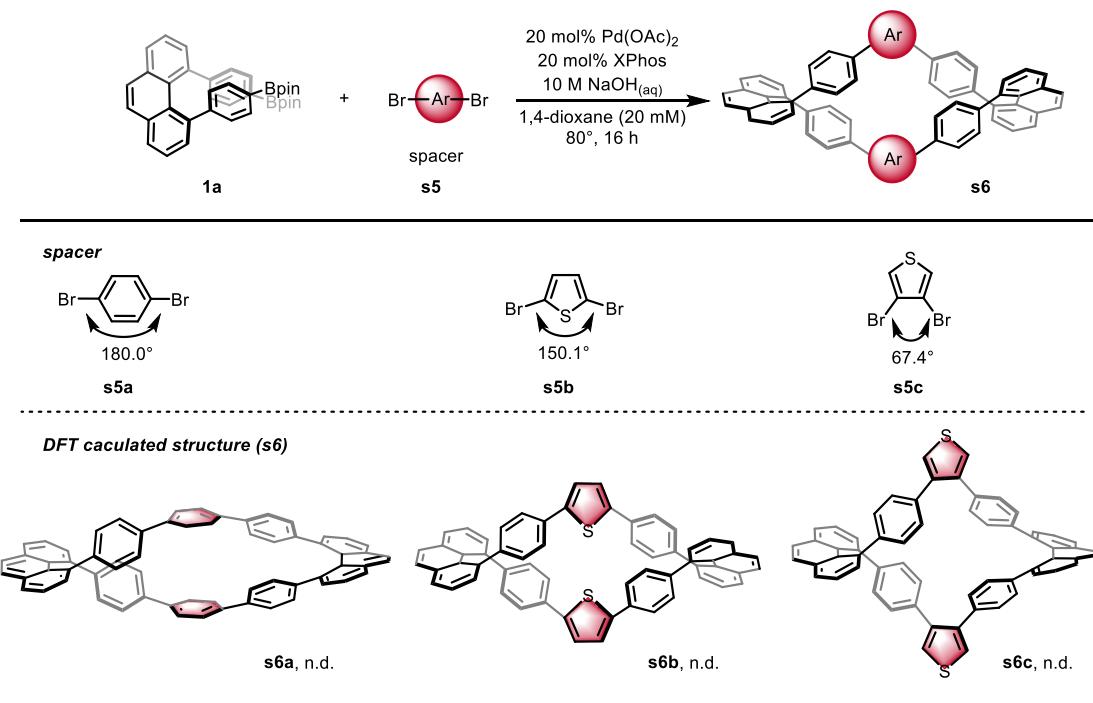
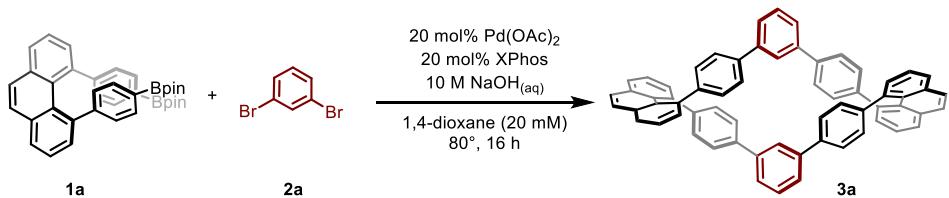


Figure S1: Screening the spacer.

5. The synthesis of twisted macrocycles

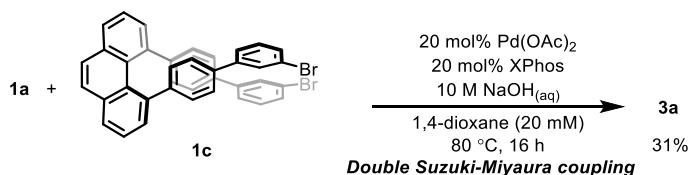
General procedure 1 (GP1):

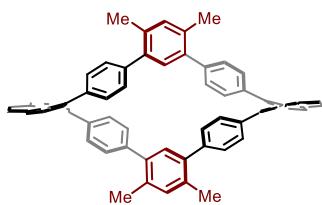


To a dry Schlenk tube containing a magnetic stirring bar were added **1a** (23.3 mg, 40 µmol), Pd(OAc)_2 (1.8 mg, 8.0 µmol), and XPhos (3.8 mg, 8.0 µmol), and the flask was evacuated and backfilled with argon three times. Then to this flask were added argon-bubbled 1,4-dioxane (20 mL), **2a** (100 µL, 48.1 µL of **2a** in 1.0 mL dioxane, 40 µmol), and 10 M NaOH(aq) (80 µL) under a stream of argon. After stirring at 80 °C for 15 h, the solvent was removed *via* rotary evaporation, the resulting oil was dissolved with DCM (30 mL), followed by washing with H_2O (30 mL), brine (20 mL), and finally placed over sodium sulfate. After removed the solvent, the residue was then purified by silica gel column chromatography with gradient elution of hexane/DCM (100:0 → 5:1) to give **3a** (4.6 mg, 5.7 µmol, 28%) as a white solid. ^1H NMR (600 MHz, CD_2Cl_2) δ 8.32 (t, $J = 1.6$ Hz, 2H), 7.86 (dd, $J = 7.7, 1.3$ Hz, 4H), 7.79 (s, 4H), 7.64 (dd, $J = 8.0, 2.0$ Hz, 4H), 7.61–7.56 (m, 8H), 7.53–7.48 (m, 2H), 7.38 (dd, $J = 8.0, 2.0$ Hz, 4H), 7.27 (dd, $J = 7.3, 1.3$ Hz, 4H), 6.85 (dd, $J = 8.0, 1.9$ Hz, 4H), 6.79 (dd, $J = 8.0, 2.0$ Hz, 4H). ^{13}C NMR (151 MHz, CD_2Cl_2) δ 143.5, 142.7, 141.7, 138.7, 135.5, 130.1, 130.0, 128.8, 128.5, 128.4, 128.2, 127.8, 127.3, 126.7, 126.2, 126.1 (one carbon overlap). HRMS (EI): Exact mass calculated for $\text{C}_{64}\text{H}_{40}$ ($[\text{M}]^+$): 808.3125, mass found: 808.3136; melting point: >300 °C.

General procedure 2 (GP2): Spacer incorporated substrate

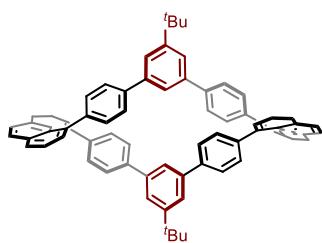
Spacer (*meta*-bromosubstituted benzene) incorporated 4,5-diarylphenanthrene (**1c**) was synthesized based on the configurational preorganization strategy,³ and then the reaction **1a** with **1c** gave the target product **3a** in comparable yield (31%) through double Suzuki-Miyaura coupling.



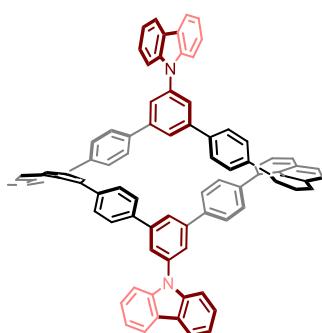


3b was prepared according to GP1 with **1a** (23.3 mg, 40 μ mol) and 1,5-dibromo-2,4-dimethylbenzene (**2b**) (10.6 mg, 40 μ mol). Then it was purified by chromatography on silica gel with gradient elution of hexane/DCM (100:0 \rightarrow 3:1) to give **3b** as a white solid. After being purified by a preparative GPC, 2.1 mg of **3b** was gained in

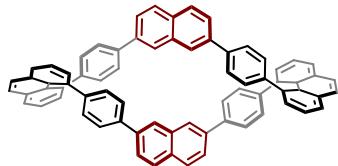
12% yield as a white solid. R_f (DCM/hexane = 1/2): 0.3. ^1H NMR (600 MHz, $\text{CDCl}_2\text{CDCl}_2$) δ 7.90 (s, 2H), 7.83 (d, J = 7.7 Hz, 4H), 7.77 (s, 4H), 7.58 (t, J = 7.5 Hz, 4H), 7.47 (dd, J = 8.1, 1.8 Hz, 4H), 7.32–7.28 (m, 4H), 7.27–7.21 (m, 4H), 6.95 (dd, J = 8.1, 1.9 Hz, 4H), 6.91 (dd, J = 8.1, 1.9 Hz, 4H), 2.37 (s, 12H). ^{13}C NMR (151 MHz, $\text{CDCl}_2\text{CDCl}_2$) δ 141.4, 141.1, 138.3, 137.5, 135.0, 134.6, 133.7, 129.5, 129.1, 129.0, 128.3, 127.5, 127.1, 127.0, 126.8, 126.7, 21.0. HRMS (EI): Exact mass calculated for $\text{C}_{68}\text{H}_{48}$ ([M] $^+$): 864.3751, mass found: 864.37513.



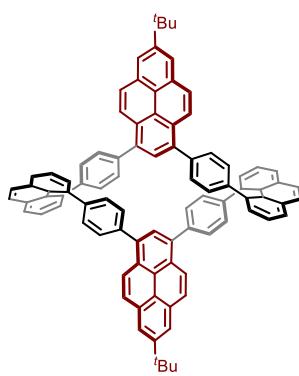
3c was prepared according to GP1 with **1a** (35.0 mg, 60 μ mol) and 1,3-dibromo-5-(*tert*-butyl)benzene (**2c**) (17.5 mg, 60 μ mol). Then it was purified by chromatography on silica gel with gradient elution of hexane/DCM (100:0 \rightarrow 4:1) to give **3c** (4.1 mg, 4.5 μ mol, 15%) as a white solid. R_f (DCM/hexane = 1/2): 0.5. ^1H NMR (600 MHz, CDCl_3) δ 8.17 (s, 2H), 7.83 (d, J = 7.7 Hz, 4H), 7.76 (s, 4H), 7.65–7.60 (m, 8H), 7.55 (t, J = 7.4 Hz, 4H), 7.40 (dd, J = 8.1, 1.8 Hz, 4H), 7.31–7.22 (m, 4H), 6.89 (dd, J = 8.0, 1.8 Hz, 4H), 6.79 (dd, J = 8.0, 1.7 Hz, 4H), 1.38 (s, 18H). ^{13}C NMR (151 MHz, CDCl_3) δ 152.8, 142.9, 142.0, 141.4, 138.6, 135.0, 129.7, 128.5, 128.10, 128.05, 127.9, 127.44, 127.37, 126.8, 126.27, 123.1, 35.2, 31.6. HRMS (EI): Exact mass calculated for $\text{C}_{72}\text{H}_{56}$ ([M] $^+$): 920.4377, mass found: 920.43820.



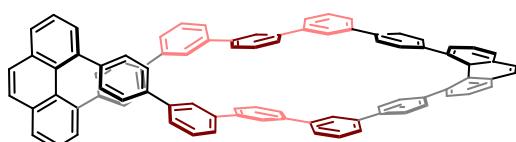
3d was prepared according to GP1 with **1a** (23.3 mg, 40 μ mol) and 9-(3,5-dibromophenyl)-9H-carbazole (**2d**) (16.0 mg, 40 μ mol). Purification by silica gel chromatography with gradient elution of hexane/DCM (100:0 \rightarrow 3:1) gave **3d** (5.2 mg, 4.6 μ mol, 23%) as a white solid. R_f (DCM/hexane = 2/5): 0.4; ^1H NMR (600 MHz, CD_2Cl_2) δ 8.46 (s, 2H), 8.14 (d, J = 7.7 Hz, 4H), 7.86 (d, J = 7.5 Hz, 4H), 7.85–7.81 (m, 8H), 7.78 (s, 4H), 7.63–7.56 (m, 8H), 7.45–7.40 (m, 8H), 7.31 (d, J = 7.4 Hz, 4H), 7.28 (t, J = 7.5 Hz, 4H), 6.93 (dd, J = 8.1, 1.8 Hz, 4H), 6.87 (dd, J = 8.0, 1.8 Hz, 4H). ^{13}C NMR (151 MHz, CD_2Cl_2) δ 144.6, 144.1, 141.5, 141.3, 139.6, 138.0, 135.6, 130.1, 128.9, 128.8, 128.6, 128.2, 128.1, 127.9, 127.3, 126.9, 126.6, 125.0, 124.5, 124.0, 120.8, 120.6, 110.4. HRMS (EI): Exact mass calculated for $\text{C}_{88}\text{H}_{54}\text{N}_2$ ([M] $^+$): 1138.4282, mass found: 1138.42715.



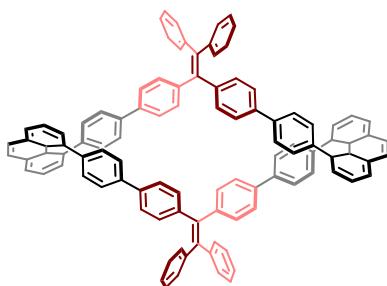
3e was prepared according to GP1 with **1a** (35.0 mg, 60 μ mol) and 2,7-dibromonaphthalene (**2e**) (17.2 mg, 60 μ mol). Purification by silica gel chromatography with gradient elution of hexane/DCM (100:0→3:1) gave **3e** (9.0 mg, 9.9 μ mol, 33%) as a white solid. R_f (DCM/hexane = 1/2): 0.4; 1 H NMR (600 MHz, CDCl₂/CDCl₂) δ 8.77 (s, 4H), 8.04 (d, J = 8.4 Hz, 4H), 7.86 (t, J = 8.6 Hz, 8H), 7.80 (s, 4H), 7.75 (d, J = 7.8 Hz, 4H), 7.59 (t, J = 7.5 Hz, 4H), 7.51 (d, J = 7.7 Hz, 4H), 7.29 (d, J = 7.2 Hz, 4H), 6.95 (d, J = 7.9 Hz, 4H), 6.79 (d, J = 7.9 Hz, 4H). 13 C NMR (151 MHz, CDCl₂/CDCl₂) δ 142.9, 140.7, 139.0, 137.2, 134.7, 134.1, 131.7, 129.7, 128.6, 128.2, 128.1, 127.6, 127.4, 127.3, 126.7, 125.7, 125.3, 125.2. HRMS (EI): Exact mass calculated for C₇₂H₄₄ ([M]⁺): 908.3438, mass found: 908.34491.



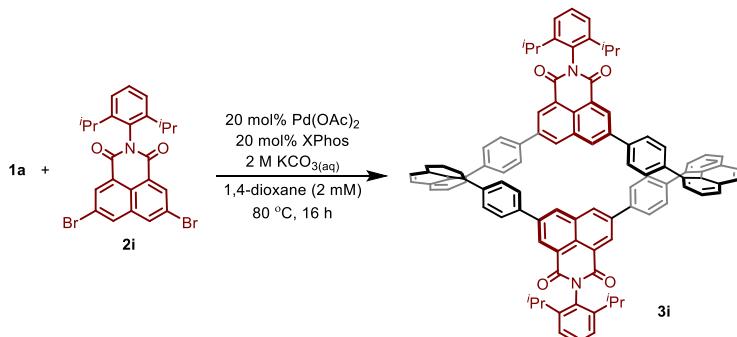
3f was prepared according to GP1 with **1a** (11.7 mg, 20 μ mol) and 1,3-dibromo-7-(*tert*-butyl)pyrene (**2f**) (8.3 mg, 20 μ mol). Then it was purified by chromatography on silica gel with gradient elution of hexane/DCM (100:0→3:1). After being purified by a preparative GPC, 0.9 mg of **3f** was gained in 8% yield as a white solid. R_f (DCM/hexane = 1/2): 0.5. 1 H NMR (600 MHz, CD₂Cl₂) δ 8.85 (s, 2H), 8.34 (d, J = 9.3 Hz, 4H), 8.17 (s, 4H), 8.00 (dd, J = 8.3, 1.8 Hz, 4H), 7.96 (d, J = 9.4 Hz, 4H), 7.88 (dd, J = 7.7, 1.2 Hz, 4H), 7.83 (s, 4H), 7.62–7.55 (m, 8H), 7.36 (dd, J = 7.3, 1.2 Hz, 4H), 7.16–7.06 (m, 8H), 1.55 (s, 18H). 13 C NMR (151 MHz, CD₂Cl₂) δ 150.1, 141.8, 143.2, 138.3, 137.0, 135.5, 131.8, 131.4, 130.6, 130.2, 128.6, 128.3, 128.0, 127.9, 127.8, 127.5, 127.1, 126.0, 123.9, 122.7, 35.6, 32.1. (aromatic 20C, 3 missing) HRMS (EI): Exact mass calculated for C₉₂H₆₄ ([M]⁺): 1168.5003, mass found: 1168.50117.



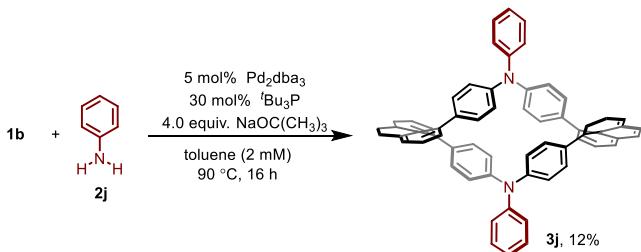
3g was prepared according to GP1 with **1a** (35.0 mg, 60 μ mol) and 3,3''-dibromo-1,1':3',1''-terphenyl (**2g**) (23.3 mg, 60 μ mol). Then it was purified by chromatography on silica gel with gradient elution of hexane/DCM (100:0→3:1). After being purified by a preparative GPC, 8.3 mg of **3g** was gained in 25% yield as a white solid. R_f (DCM/hexane = 1/4): 0.3. 1 H NMR (600 MHz, CDCl₂/CDCl₂) δ 8.15 (s, 1H), 8.11 (s, 2H), 8.03 (s, 1H), 7.98 (s, 2H), 7.85 (dd, J = 7.7, 3.0 Hz, 4H), 7.80–7.76 (m, 6H), 7.73–7.67 (m, 5H), 7.67–7.63 (m, 5H), 7.59 (t, J = 7.4 Hz, 4H), 7.52 (q, J = 7.4 Hz, 4H), 7.48 (d, J = 8.1 Hz, 2H), 7.40–7.36 (m, 4H), 7.34 (d, J = 8.0 Hz, 2H), 7.31–7.24 (m, 5H), 7.18 (t, J = 7.6 Hz, 1H), 6.84 (d, J = 8.2 Hz, 2H), 6.80 (d, J = 8.0 Hz, 2H), 6.75 (d, J = 8.3 Hz, 2H), 6.71 (d, J = 8.2 Hz, 2H). 13 C NMR (151 MHz, CDCl₂/CDCl₂) δ 142.46, 142.45, 141.6, 141.4, 141.1, 140.98, 140.95, 140.89, 140.87, 140.80, 137.7, 134.55, 134.53, 129.5, 129.4, 129.3, 129.2, 128.24, 128.19, 128.13, 127.9, 127.6, 127.35, 127.30, 127.12, 127.06, 126.6, 126.11, 126.04, 125.9, 125.8, 125.74, 125.66, 125.5, 125.4, 124.8. HRMS (EI): Exact mass calculated for C₈₈H₅₆ ([M]⁺): 1112.4377, mass found: 1112.43926.



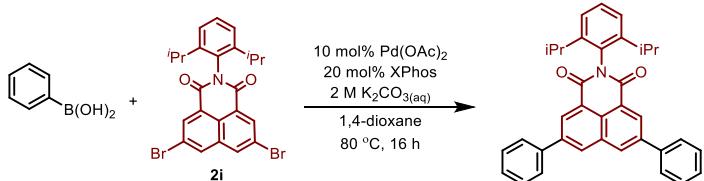
3h was prepared according to GP1 with **1a** (23.3 mg, 40 μ mol) and 4,4'-(2,2-diphenylethene-1,1-diyl) bis(bromobenzene) (**2h**) (19.6 mg, 40 μ mol). Then it was purified by chromatography on silica gel with gradient elution of hexane/DCM (100:0 \rightarrow 2:1). After being purified by a preparative GPC, 1.2 mg of **3h** was gained in 5% yield as a light-yellow solid. R_f (DCM/hexane = 1/2): 0.3. ^1H NMR (600 MHz, CDCl_3) δ 7.80 (dd, J = 7.7, 1.3 Hz, 4H), 7.72 (s, 4H), 7.55 (t, J = 7.5 Hz, 4H), 7.42 (d, J = 8.4 Hz, 8H), 7.23 (dd, J = 8.1, 1.9 Hz, 4H), 7.19 (dt, J = 8.0, 2.1 Hz, 8H), 7.16 (d, J = 8.4 Hz, 8H), 7.11–7.03 (m, 20H), 6.68 (dd, J = 8.1, 1.9 Hz, 4H), 6.61 (dd, J = 8.0, 1.8 Hz, 4H). ^{13}C NMR (151 MHz, CDCl_3) δ 143.6, 142.8, 142.7, 141.6, 141.1, 140.3, 138.4, 137.5, 134.8, 131.7, 131.4, 129.7, 128.3, 128.2, 127.92, 127.85, 127.3, 127.1, 126.8, 126.6, 126.1, 125.3. HRMS (EI): Exact mass calculated for $\text{C}_{104}\text{H}_{68} ([\text{M}]^+)$: 1316.5316, mass found: 1316.53189.



To a dry Schlenk tube containing a magnetic stirring bar were added **1a** (23.3 mg, 40 μ mol), **2i** (20.6 mg, 40 μ mol), $\text{Pd}(\text{OAc})_2$ (1.8 mg, 8.0 μ mol), and XPhos (3.8 mg, 8.0 μ mol), and the flask was evacuated and backfilled with argon three times. Then to this flask were added argon-bubbled 1,4-dioxane (20 mL), and 2 M K_2CO_3 (aq) (200 μ L) under a stream of argon. After stirring at 80 °C for 15 h, the solvent was removed *via* rotary evaporation, the resulting oil was dissolved with DCM (30 mL), followed by washing with H_2O (30 mL), brine (20 mL), and finally placed over sodium sulfate. After removing the solvent, it was purified by chromatography on silica gel with gradient elution of hexane/DCM/ethyl acetate (100:10:0 \rightarrow 100:10:20). After being further purified by a preparative GPC, 2.2 mg of **3i** was gained in 8% yield as a yellow solid. R_f (ethyl acetate/hexane = 1/5): 0.5. ^1H NMR (392 MHz, CD_2Cl_2) δ 9.15 (d, J = 1.7 Hz, 4H), 8.98 (d, J = 1.6 Hz, 4H), 7.91 (dd, J = 7.8, 1.4 Hz, 4H), 7.82 (s, 4H), 7.81 (dd, J = 8.2, 2.2 Hz, 4H), 7.69 (dd, J = 8.1, 2.0 Hz, 4H), 7.61 (t, J = 7.6 Hz, 4H), 7.50 (t, J = 7.7 Hz, 4H), 7.35 (d, J = 7.7 Hz, 4H), 7.30 (dd, J = 7.3, 1.3 Hz, 4H), 6.99 (dd, J = 8.2, 1.8 Hz, 4H), 6.86 (dd, J = 8.1, 1.9 Hz, 4H), 2.85–2.72 (m, 4H), 1.17 (d, J = 6.9 Hz, 12H), 1.13 (d, J = 6.8 Hz, 12H). ^{13}C NMR (151 MHz, CD_2Cl_2) δ 164.8, 146.7, 144.8, 141.3, 141.1, 136.4, 135.7, 133.9, 132.0, 131.4, 130.7, 130.5, 130.0, 129.1, 128.8, 128.7, 128.4, 128.0, 127.8, 127.4, 126.9, 124.6, 124.2, 29.7, 24.32, 24.27. HRMS (APCI): Exact mass calculated for $\text{C}_{100}\text{H}_{75}\text{N}_2\text{O}_4$ ($[\text{M}+\text{H}]^+$): 1367.5721, mass found: 1367.5708.



A catalyst consisting of tris(dibenzylideneacetone)dipalladium(0) (Pd_2dba_3) (0.9 mg, 1.0 μmol) and tris(*tert*-butyl)phosphine (1.2 mg, 6.0 μmol) dissolved in 5 mL toluene and performed by stirring for 15 min at room temperature. This catalyst was added to the solution of **1b** (9.8 mg, 20 μmol), aniline (50 μL , 36.6 μL of aniline in 1.0 mL toluene, 20 μmol), and sodium *tert*-butoxide (7.7 mg, 80 μmol) dissolved in 5 mL toluene. After stirring at 90 °C for 16 h, the solvent was removed *via* rotary evaporation, the resulting oil was dissolved with DCM (30 mL), followed by washing with H₂O (30 mL), brine (20 mL), and finally placed over sodium sulfate. After removed the solvent, the residue was then purified by silica gel column chromatography with gradient elution of hexane/DCM (100:0→5:1) to give **3j** (1.0 mg, 1.2 μmol , 12%) as a pale-yellow solid. R_f (DCM/hexane = 2/5): 0.6; ¹H NMR (600 MHz, CDCl₃) δ 7.75 (d, *J* = 7.7 Hz, 4H), 7.69 (s, 4H), 7.54 (t, *J* = 7.5 Hz, 4H), 7.32 (d, *J* = 7.5 Hz, 4H), 7.21 (dd, *J* = 8.3, 2.3 Hz, 4H), 7.09 (dd, *J* = 8.3, 2.3 Hz, 4H), 7.02 (t, *J* = 7.9 Hz, 4H), 6.91–6.83 (m, 8H), 6.76 (t, *J* = 7.4 Hz, 2H), 6.60 (dd, *J* = 8.4, 2.1 Hz, 4H). ¹³C NMR (151 MHz, CDCl₃) δ 147.4, 147.0, 141.4, 139.1, 134.8, 129.4, 128.91, 128.87, 127.9, 127.8, 127.2, 126.84, 126.79, 123.6, 122.1, 121.5. HRMS (EI): Exact mass calculated for C₆₄H₄₂N₂ ([M]⁺): 838.3343, mass found: 838.33417.



To a dry Schlenk tube containing a magnetic stirring bar were added **2i** (10.3 mg, 20 μmol), phenylboronic acid (6.1 mg, 50 μmol), Pd(OAc)₂(0.45 mg, 2.0 μmol), and XPhos (1.9 mg, 4.0 μmol), and the flask was evacuated and backfilled with argon three times. Then to this flask were added argon-bubbled 1,4-dioxane (2 mL), and 2 M K₂CO₃ (aq) (100 μL , 200 μmol) under a stream of argon. After stirring at 80 °C for 15 h, the solvent was removed *via* rotary evaporation, the resulting oil was dissolved with DCM (30 mL), followed by washing with H₂O (30 mL), brine (20 mL), and finally placed over sodium sulfate. After removed the solvent, it was purified by chromatography on silica gel with gradient elution of hexane/DCM/ethyl acetate (100:10:0→100:10:10) to give 3,6-diphenylnaphthalimide (9.0 mg, 18 μmol , 88%) as a yellow solid. R_f (DCM/hexane = 1/2): 0.2; ¹H NMR (600 MHz, CDCl₃) δ 8.91 (d, *J* = 1.7 Hz, 2H), 8.52 (d, *J* = 1.7 Hz, 2H), 7.83 (dd, *J* = 8.3, 1.2 Hz, 4H), 7.58–7.54 (m, 4H), 7.54–7.42 (m, 3H), 7.35 (d, *J* = 7.8 Hz, 3H), 2.80 (hept, *J* = 7.0 Hz, 3H), 1.19 (d, *J* = 6.9 Hz, 12H). ¹³C NMR (151 MHz, CDCl₃) δ 164.4, 145.9, 140.9, 139.4, 133.1, 131.8, 131.2, 131.1, 129.7, 129.4, 128.6, 127.7, 127.2, 124.2, 123.3, 29.3, 24.2.

6. The X-ray data

Details of the crystal data and a summary of the intensity data collection parameters for **3b** and **3c** are listed in Table S2. In each case, a suitable crystal was mounted with mineral oil on glass fiber and transferred to the goniometer of a Rigaku PILATUS diffractometer. Graphite-monochromated Mo K α radiation ($\lambda = 0.71075 \text{ \AA}$) was used. The structures were solved by direct methods with (SIR-97)⁴ or SHELXT and refined by full-matrix least-squares techniques against F^2 (SHELXL-2013/4)⁵ with Yadokari-XG program.⁶ The intensities were corrected for Lorentz and polarization effects. The non-hydrogen atoms were refined anisotropically. Hydrogen atoms were placed using AFIX instructions.

Table S2. Crystallographic data and structure refinement details for **3b** and **3c**.

	3b·CH₂Cl₂	3c·CH₂Cl₂
formula	C ₆₉ H ₅₀ Cl ₂	C ₇₃ H ₅₈ Cl ₂
fw	949.99	1006.09
T (K)	123(2)	123(2)
λ (Å)	0.71073	0.71073
cryst syst	Monoclinic	Orthorhombic
space group	<i>P</i> 2 ₁ / <i>c</i>	<i>P</i> 2 ₁ 2 ₁ 2 ₁
<i>a</i> (Å)	20.9151(4)	12.1203(4)
<i>b</i> (Å)	12.7570(2)	20.8051(8)
<i>c</i> (Å)	18.9773(3)	21.0967(7)
α (deg)	90	90
β (deg)	100.0900(18)	90
γ (deg)	90	90
<i>V</i> (Å ³)	4985.10(15)	5319.8(3)
<i>Z</i>	4	4
<i>D</i> _{calc} (g/cm ³)	1.266	1.256
μ (mm ⁻¹)	0.175	0.168
<i>F</i> (000)	1992	2120
cryst size (mm)	0.22 × 0.20 × 0.15	0.20 × 0.10 × 0.02
θ range (deg)	2.542 to 24.999	2.580 to 24.999
reflns collected	52758	30091
indep reflns/ <i>R</i> _{int}	8777/0.0252	9191/0.1039
params	663	710
GOF on <i>F</i> ²	1.031	1.036
<i>R</i> ₁ , <i>wR</i> ₂ [<i>I</i> >2σ(<i>I</i>)]	0.0508, 0.1408	0.0727, 0.1937
<i>R</i> ₁ , <i>wR</i> ₂ (all data)	0.0576, 0.1465	0.0821, 0.1991

7. The X-ray crystal structure

7.1 The comparison of X-ray crystal structure and DFT calculated result of **3b**

The structural analysis of **3b** was performed by comparing the structures of 4,5-diphenylphenanthrene (**1**)⁷ as the reference molecule. The geometric optimization of the structure of **3b** was carried out by DFT calculations at the M06-2X/6-31G(d), B3LYP/6-31G(d), B3LYP-D3/6-31G(d) and BMK/6-31G(d) level of theory respectively, and the M06-2X-calculated optimized structure reproduced the experimentally observed structure well. The averaged structural parameters of the experimentally observed and theoretically optimized structure of **3b** together with the corresponding values of 4,5-diphenylphenanthrene (**1**) are summarized in Table S3. The shortest carbon to carbon distances ($a \rightarrow f$) measure only 2.856 Å in **3b** and 2.866 Å in **1**, well within the van der Waals radius of the carbon atom (3.4 Å), which also shows the 4,5-diphenylphenanthrene fragments in **3b** are nearly undistorted with respect to **1**.

Table S3. The comparison of X-ray crystal structure and DFT calculated result of **3b**.

	3b					observed	
	observed	DFT calculation					
		M06-2X	B3LYP-D3	BMK	B3LYP		
distance: $a \rightarrow f$ (Å)	2.856, 2.864	2.867	2.911	2.951	3.013	2.866	
dihedral angle: $a-b-e-f$ (°)	60.1, 59.9	62.1	63.2	63.1	66.0	60.91	
dihedral angle: $b-c-d-e$ (°)	24.44, 26.35	27.27	27.6	27.5	28.84	26.83	
bent angle α (°)	114.6, 114.2	114.9	114.4	114.1	113.1	—	

Based on the DFT calculation of the structure, The sum of the interior angles of **3b** ($60.1+114.6+59.9+114.2 = 348.8$) are in good agreement with the Quadrilateral Sum Conjecture (360.0° , differ by 3.1%) as well.

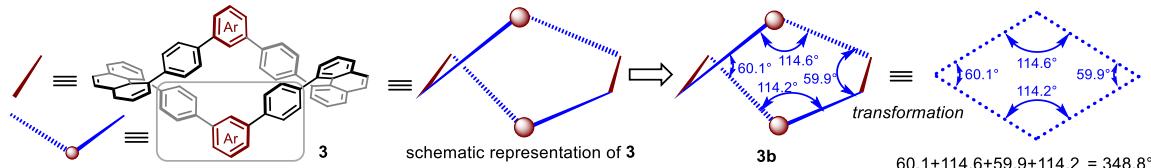
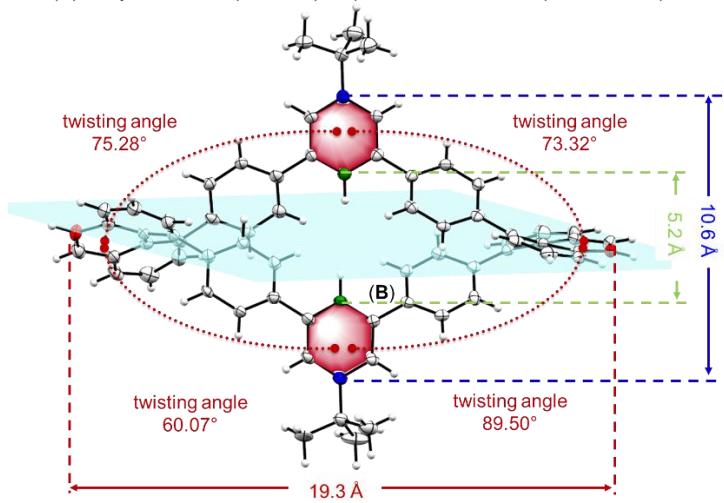


Figure S2: The structures of **3b**.

7.2 The X-ray crystal structures of **3c**

The structural analysis confirmed a highly twisted macrocycle shape for **3c** in the crystalline state. The distances between the farthest carbon atoms of **3c** are 10.6 Å and 19.3 Å. The distance across the cavity of this macrocycle is 5.2 Å with the two hydrogen atoms that are pointing toward the center of the cavity being perpendicular to the plane of phenanthrene backbone which shows that **3c** has small internal spaces. The four twisting angles between the plane of the spacer (red benzene ring) and the plane of the central benzene ring of phenanthrene subunit are 89.50°, 75.28°, 73.32°, and 60.07°, which exhibit macrocycle **3c** is a perpendicular π -system as a 3D structure. In the packing modes, homochiral **3c** also has a columnar structure formed through CH– π interaction in the a-b plane (Figure S3B). In the b-c plane, homochiral **3c** are also packed in an alternating fashion between layers.

(A) X-ray structure of (*P,P/M,M*)-**3c** (the shown structure represents *M,M*)



(B) Packing structure of (*P,P/M,M*)-**3c**
(the shown structure represents *M,M*; color: blue, cobalt, green, and pink)

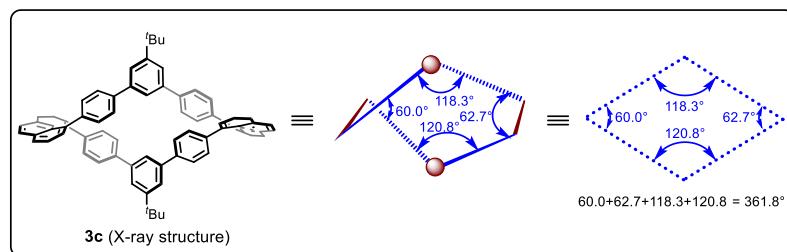
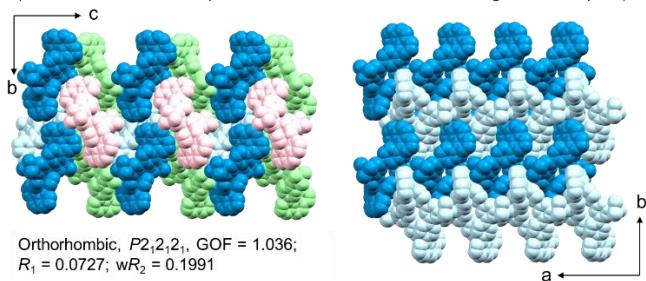


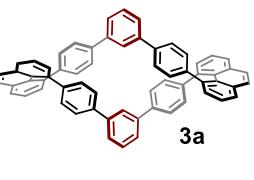
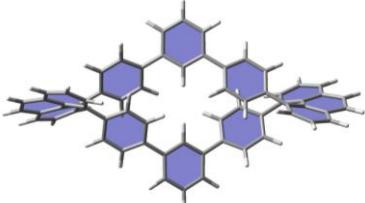
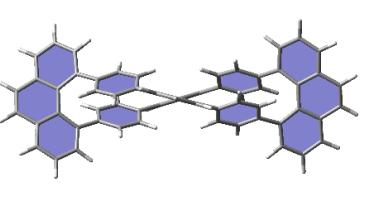
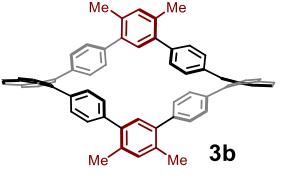
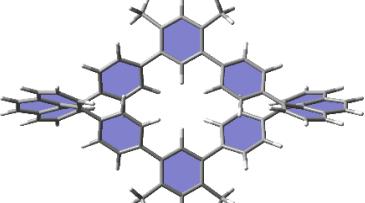
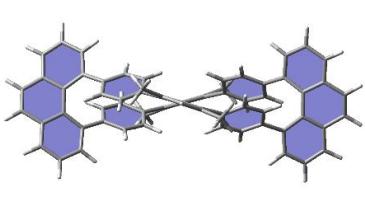
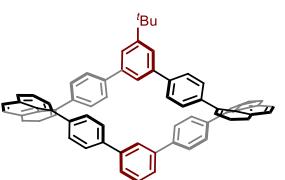
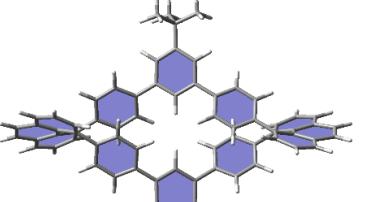
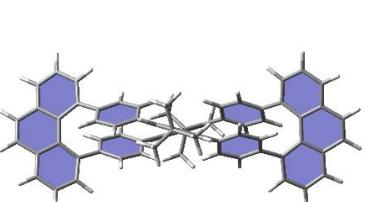
Figure S3: The X-ray crystal structures of **3c**.

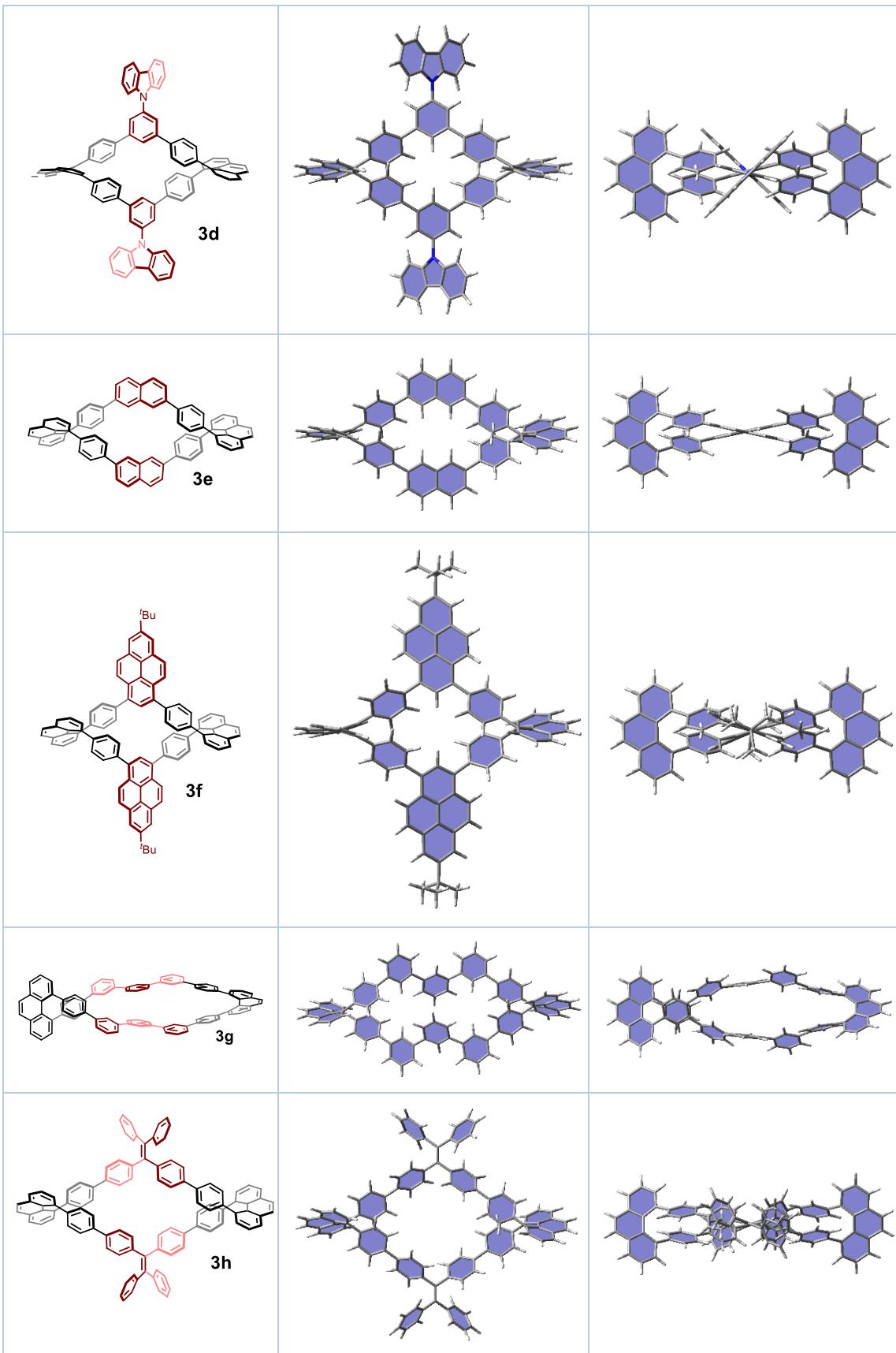
8. Computational study

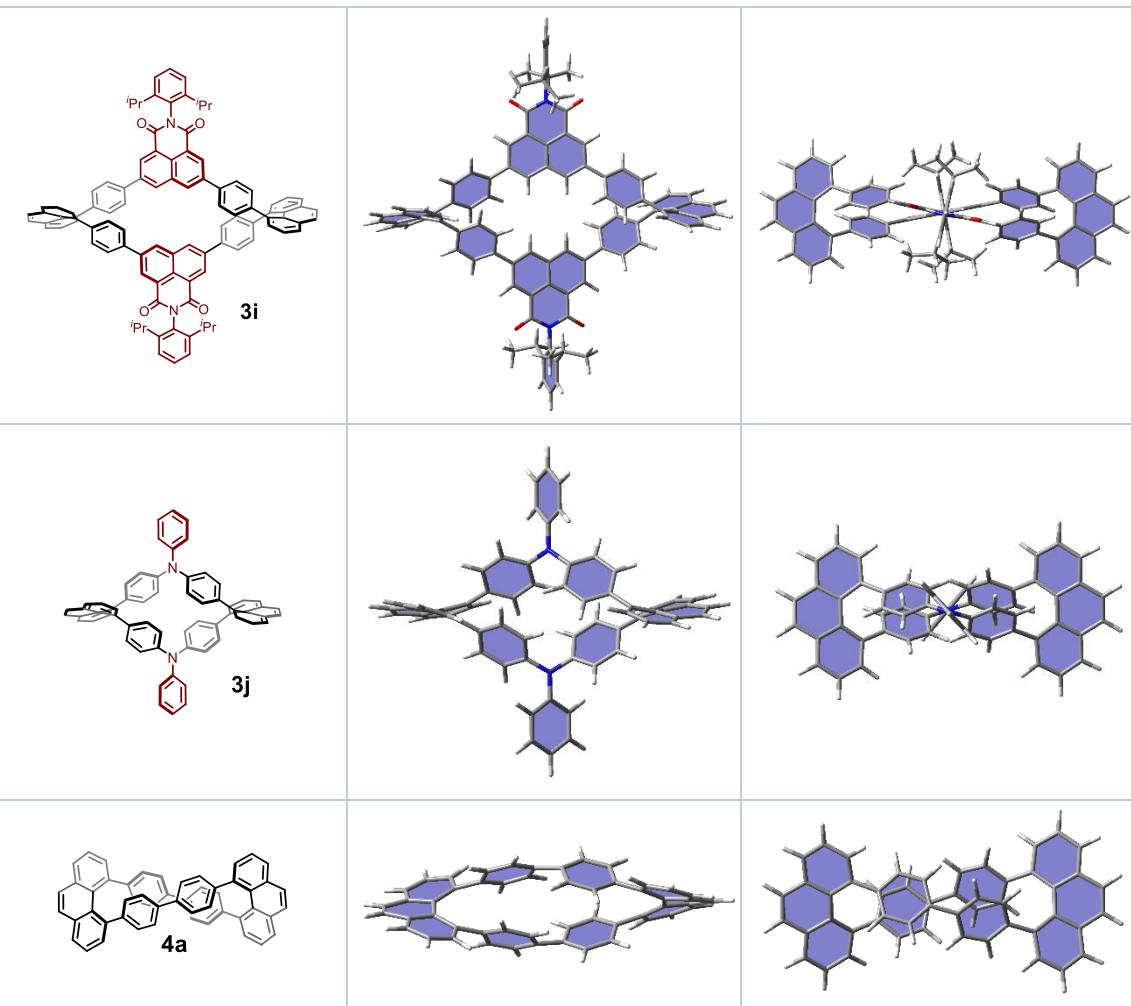
The Gaussian 09 program⁸ running on the SGI Altix4700 system was used for optimization (M062X/6-31G(d) and B3LYP/6-31G(d)). Structures were optimized without any symmetry assumptions. Zero-point energy, enthalpy, and Gibbs free energy at 298.15 K and 1 atm were estimated from the gas-phase studies. Harmonic vibration frequency calculation at the same level was performed to verify all stationary points as local minima (with no imaginary frequency) or transition states (with one imaginary frequency). IRC calculations were also performed to check transition states. Visualization of the results was performed by the use of GaussView 5.0.9 software.

8.1 Optimized structures.

Table S4. Optimized structures calculated by M06-2X/6-31G(d) (**3a**, **3b**, **3c**, **3j** and **4a**) or B3LYP/6-31G(d) (**3d**, **3e**, **3f**, **3g**, **3h**, **3i**) level of theory

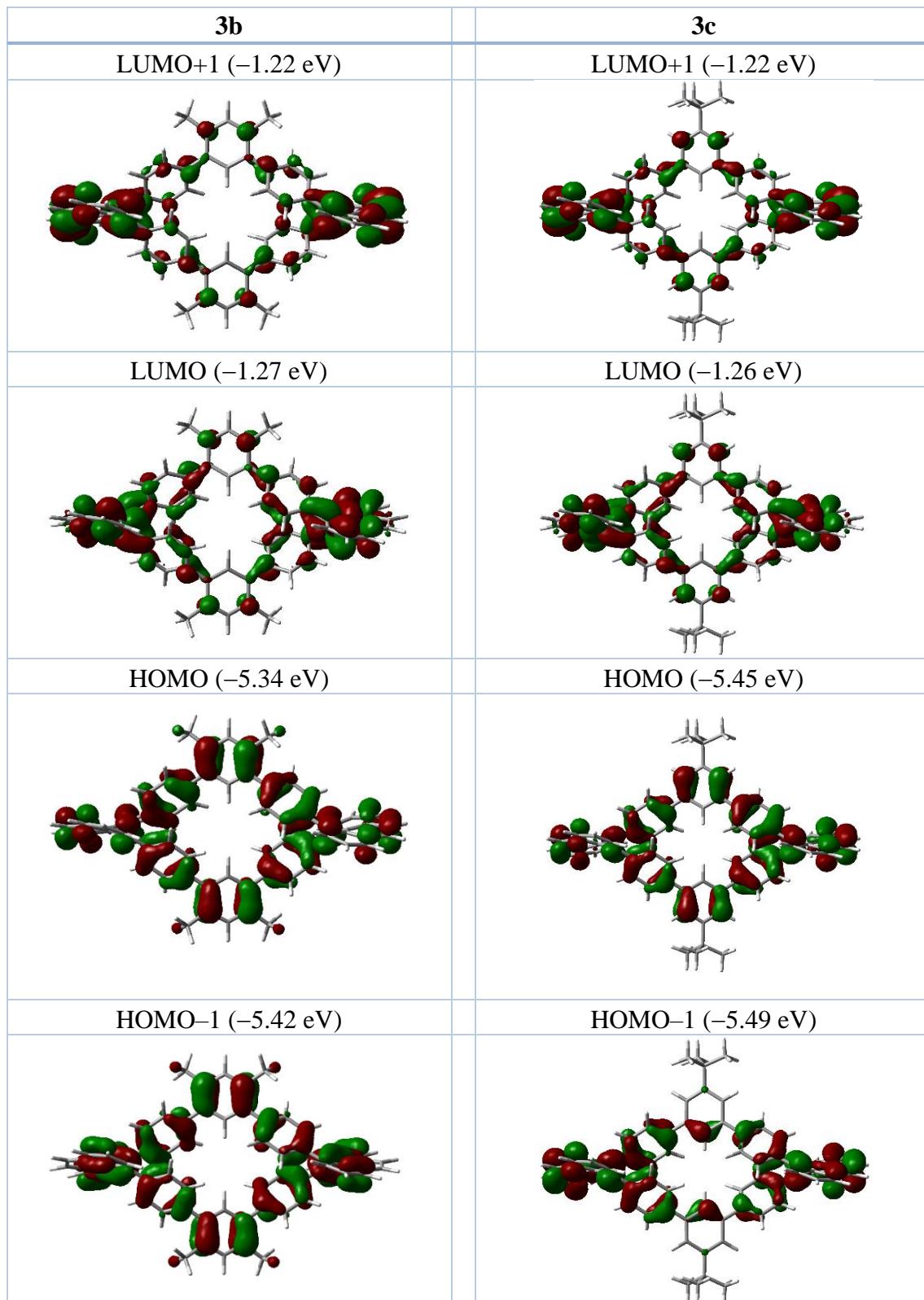
Compound	Top view	Side view
 3a		
 3b		
 3c		

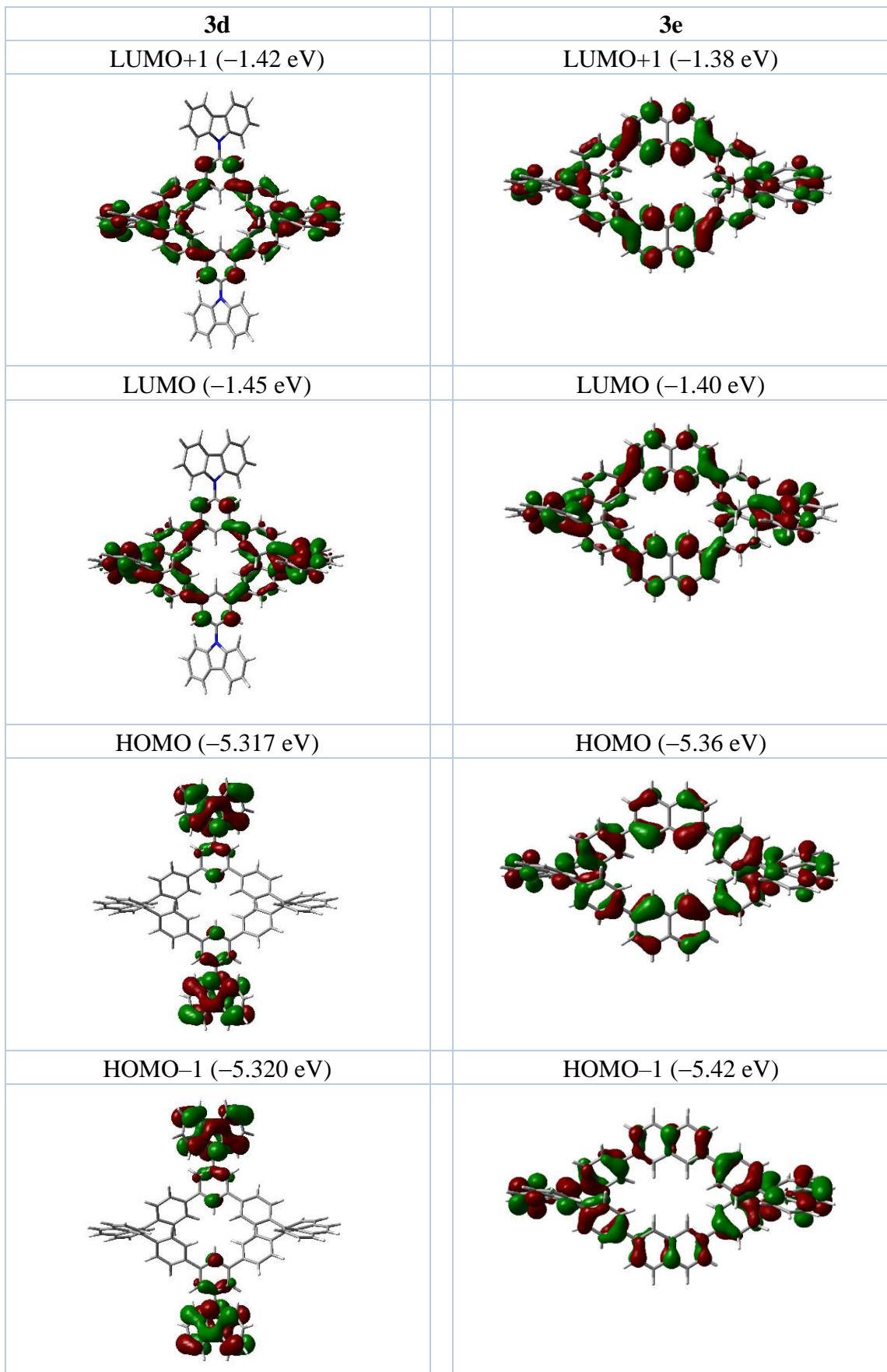


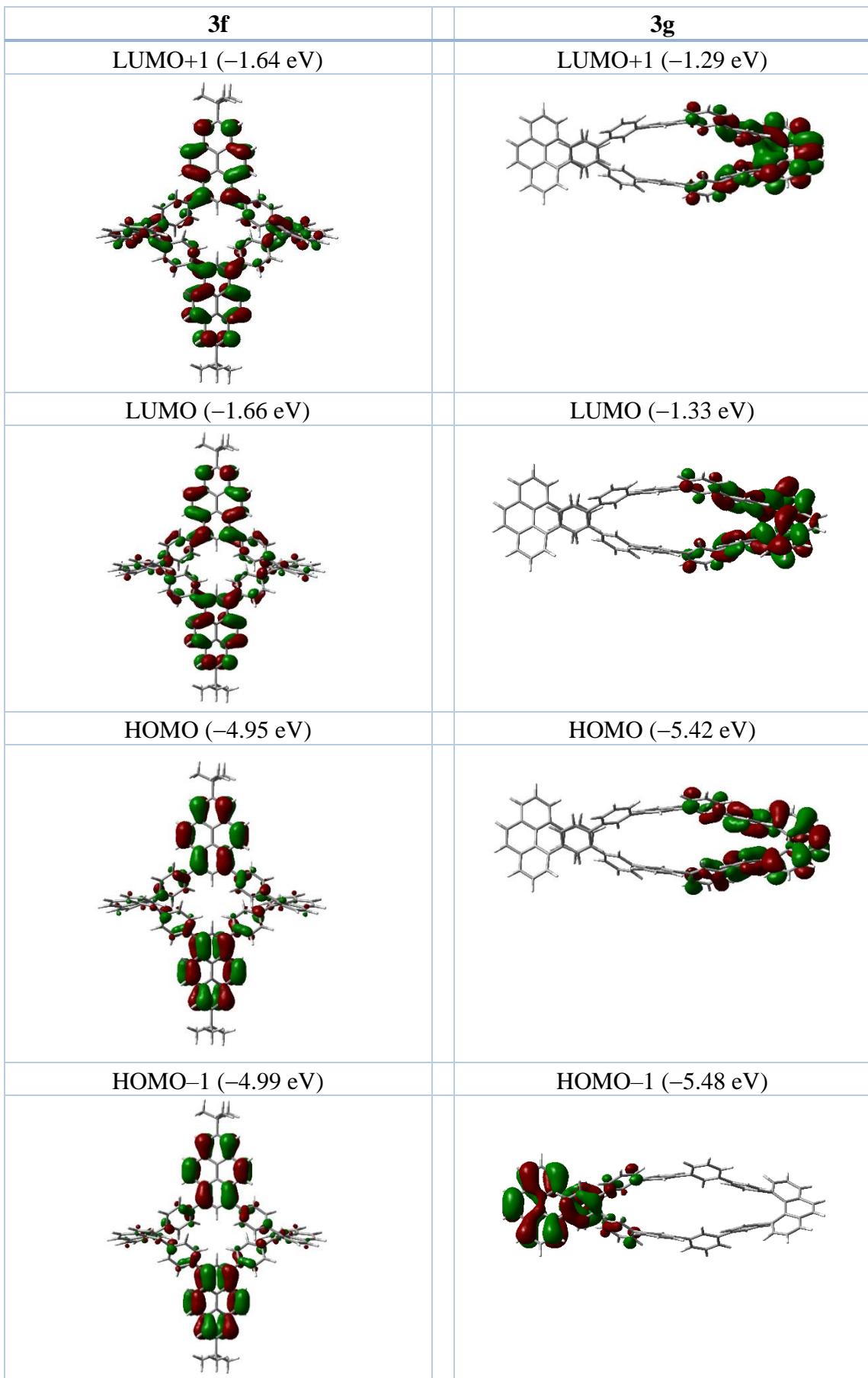


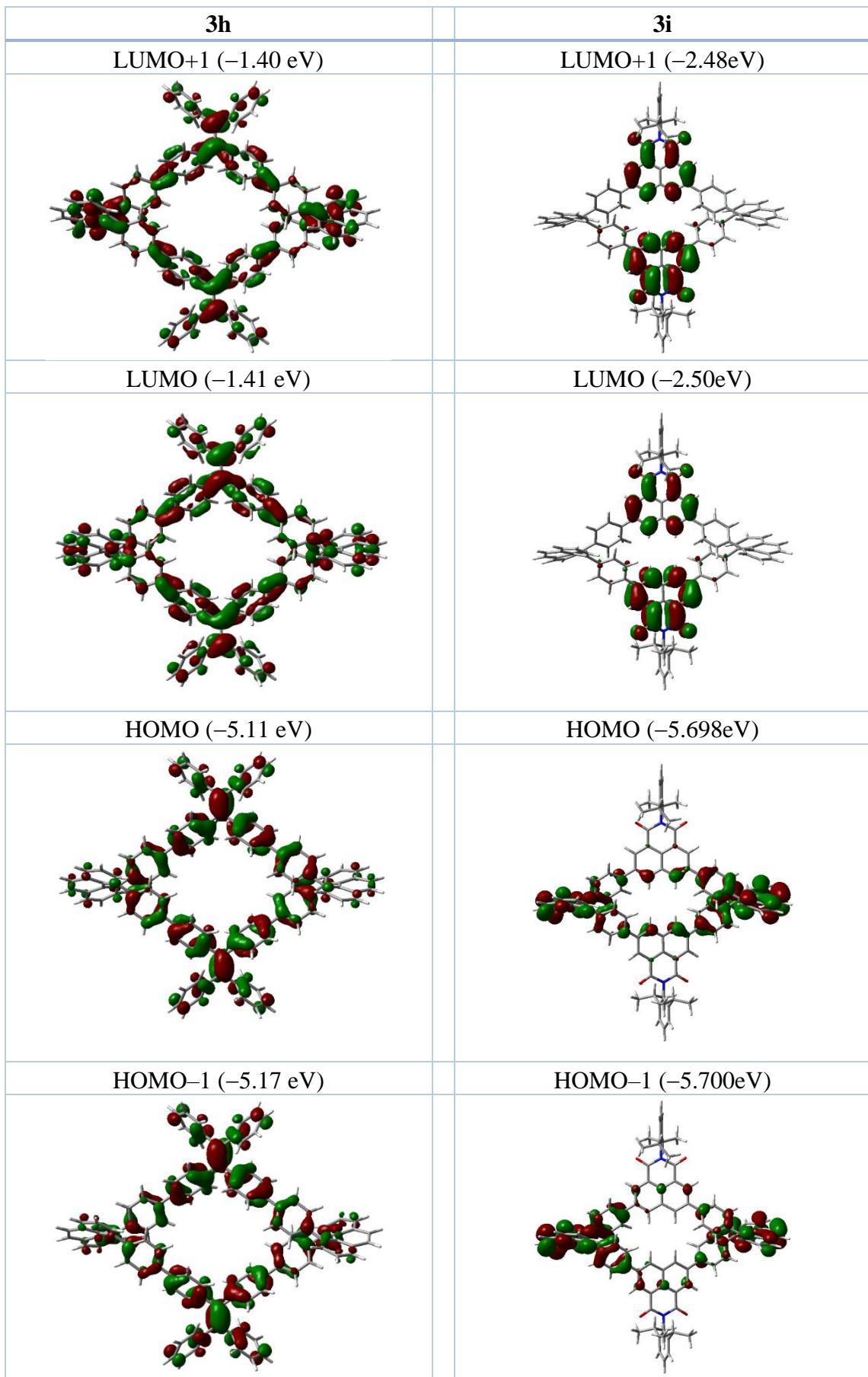
8.2 Frontier molecular orbitals of macrocycles

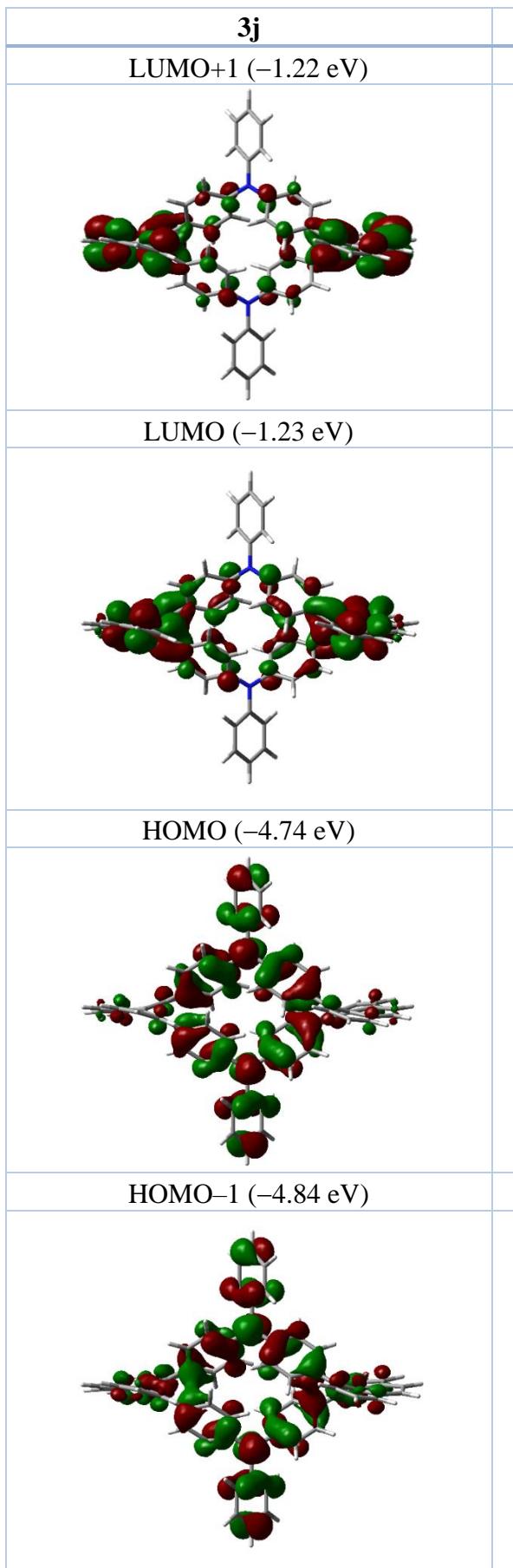
Table S5. Frontier molecular orbitals of macrocycles calculated by B3LYP/6-31G(d) level of theory (**3b**, **3c**, **3d**, **3e**, **3f**, **3g**, **3h**, **3i**, and **3j**)











8.3 The calculation of strain energy

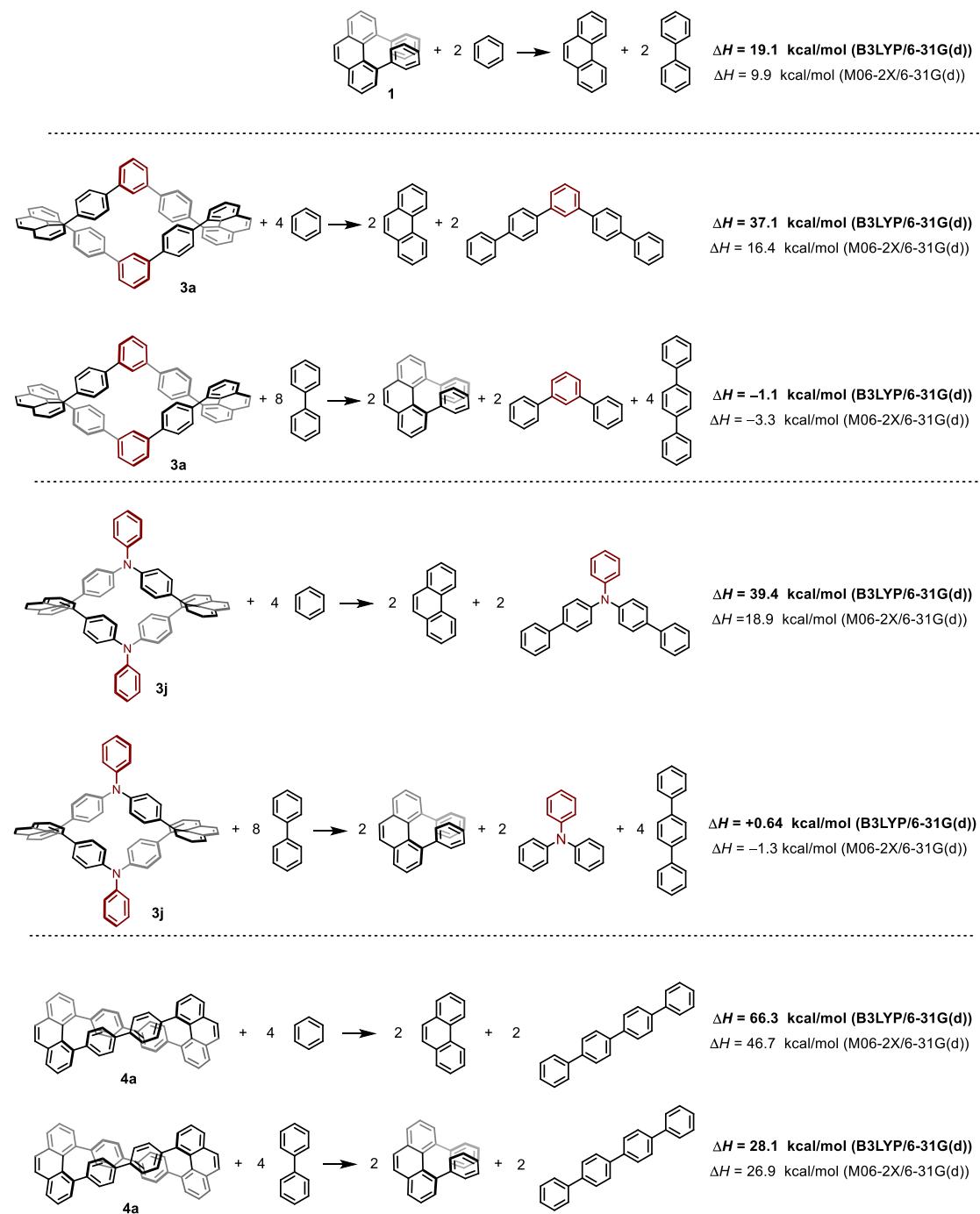
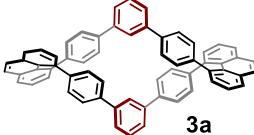
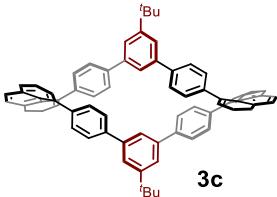


Figure S4. Homodesmotic reactions for the calculation of strain energies for **1**, **3a**, **3j** and **4a** calculated by M06-2X/6-31G(d) and B3LYP/6-31G(d) level of theory respectively.

8.4 The DFT calculation of racemization barrier 3a, 3c, 3e and 3j

We calculated the racemization barrier of **3a** and **3c** using M06-2X/6-31G(d) and B3LYP/6-31G(d) respectively. Compared with the experimental result of **3c**, the M06-2X functional was found to provide superior results for the racemization barrier.

Table S6. The comparison of racemization barrier between **3a** and **3c**

	M06-2X/6-31G(d)	B3LYP/6-31G(d)	Experimental result
	30.4 kcal/mol	28.2 kcal/mol	—
	30.1 kcal/mol	—	31.0 kcal/mol

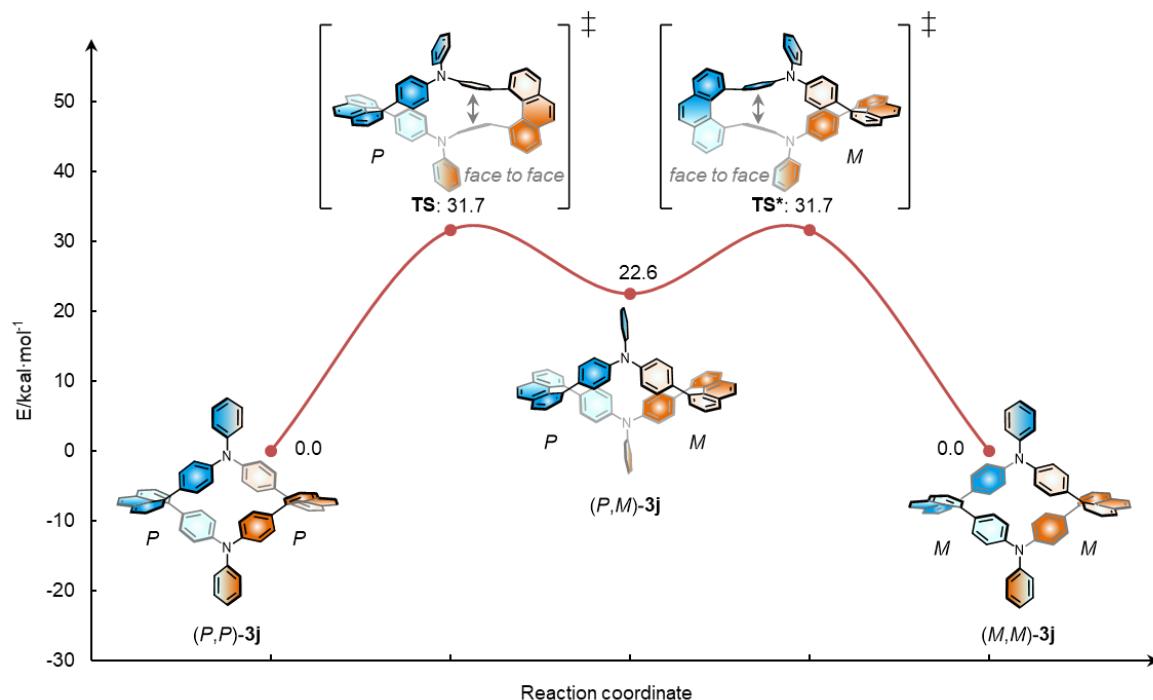


Figure S5. Racemization process between **(P,P)-3j** and **(M,M)-3j** and the relative Gibbs free energy calculated at the M06-2X/6-31G(d) level.

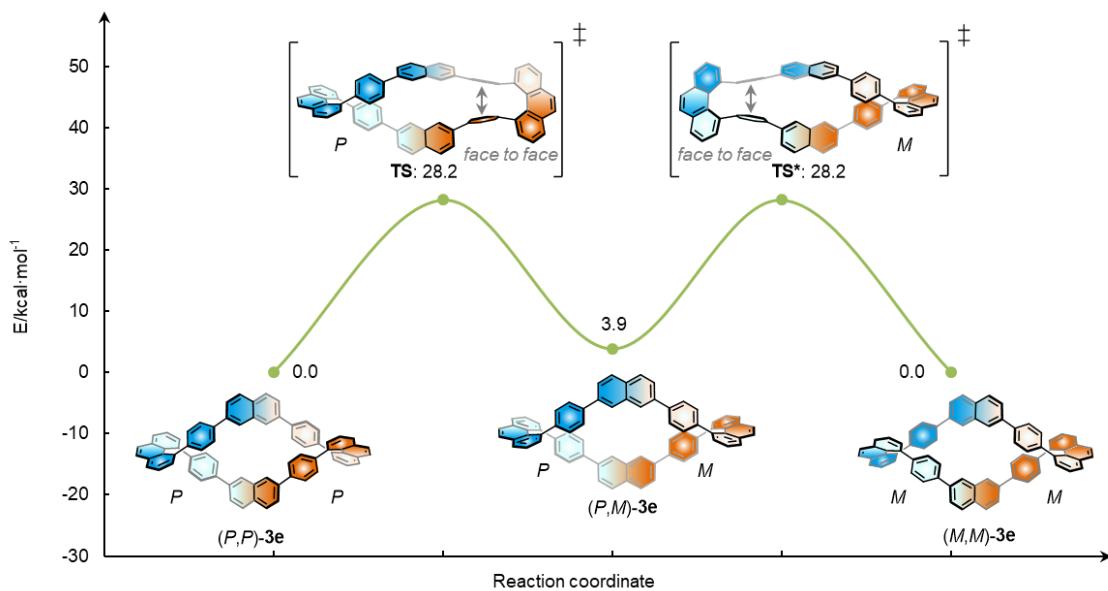


Figure S6. Racemization process between (P,P) -3e and (M,M) -3e and the relative Gibbs free energy calculated at the M06-2X/6-31G(d) level.

8.5 The DFT calculation of racemization barrier of 1

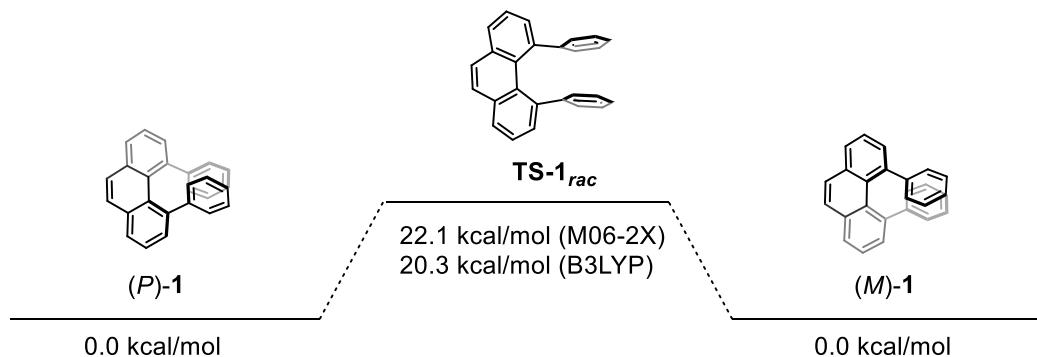


Figure S7. The DFT calculation of racemization barrier of 1

Table S7. The comparison of $\mathbf{TS-1}_{rac}$

	DFT calculation ($\mathbf{TS-1}_{rac}$)	
	M06-2X/6-31G(d)	B3LYP/6-31G(d)
distance: a→f (Å)	2.98	2.30
dihedral angle: a-b-e-f (°)	1.14	0.25
dihedral angle: b-c-d-e (°)	1.29	1.07

8.7 The rotation barrier and VT ^1H NMR spectrum of 3a

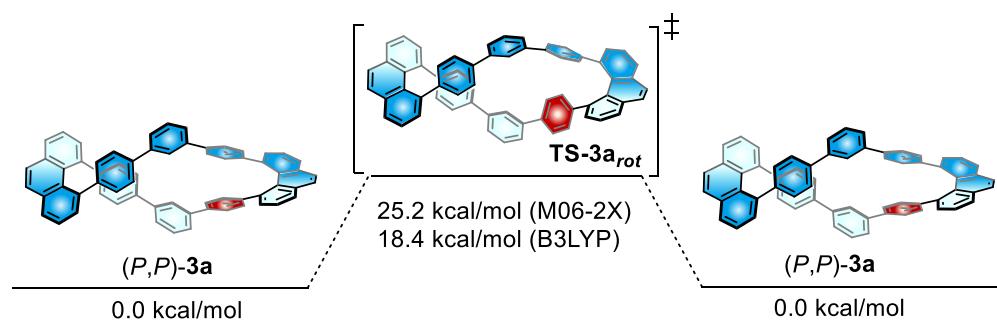


Figure S8. The rotation barrier of **3a**

Table S8. The comparison of **TS-3a**_{rot}

	DFT calculation (TS-3a_{rot})	
	M06-2X/6-31G(d)	B3LYP/6-31G(d)
distance: a→b (Å)	3.61	3.67
angle: A–B (°)	88.18	84.21

3a was studied by variable temperature ^1H NMR spectroscopy between 25 and 145 °C. The result shows that the signals of phenyl protons do not coalesce below 145 °C.

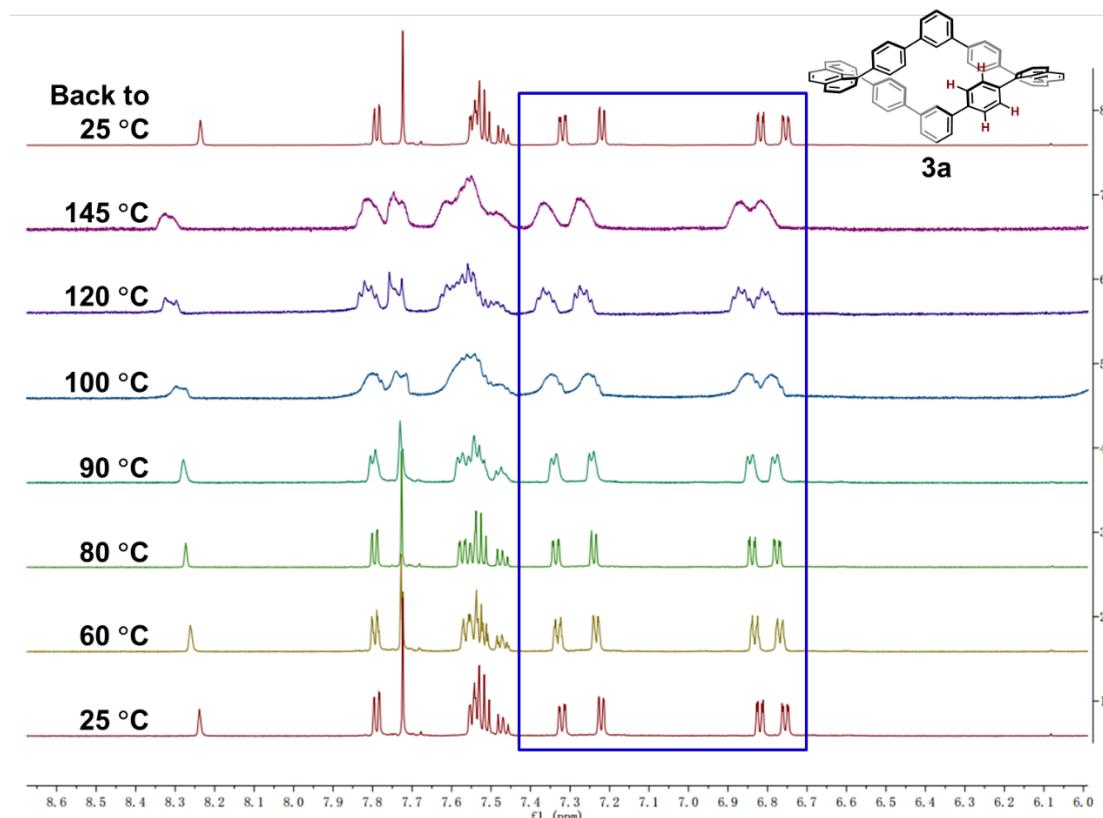


Figure S9. VT ^1H NMR spectrum of **3a** in 1,1,2,2-tetrachloroethane- d_2

8.8 The rotation barrier and VT ^1H NMR spectrum of **1**

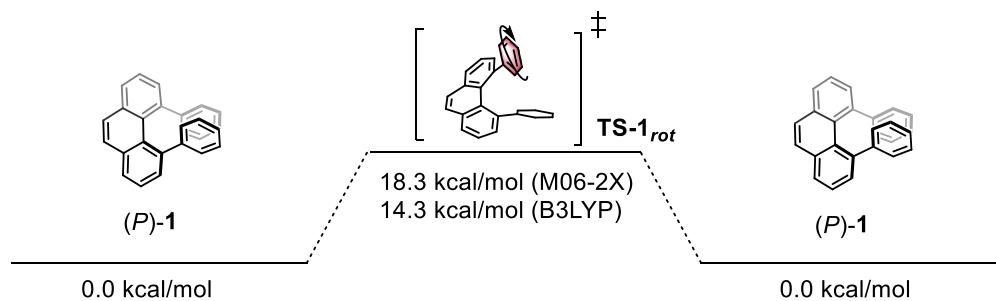


Figure S10. The rotation barrier of **1**

Table S9. The comparison of TS-1_{rot}

	DFT calculation (TS-1_{rot})	
	M06-2X/6-31G(d)	B3LYP/6-31G(d)
	distance: a→b (Å)	angle: A–B (°)
	3.61	3.68
	69.77	73.84

1 was studied by variable temperature ^1H NMR spectroscopy between 25 and 110 °C. VT ^1H NMR result shows that the broad peaks resulting from the phenyl coalesce at 50 °C, and the ^1H NMR signals recover to relatively broad peaks when the sample is cooled back to 25 °C.

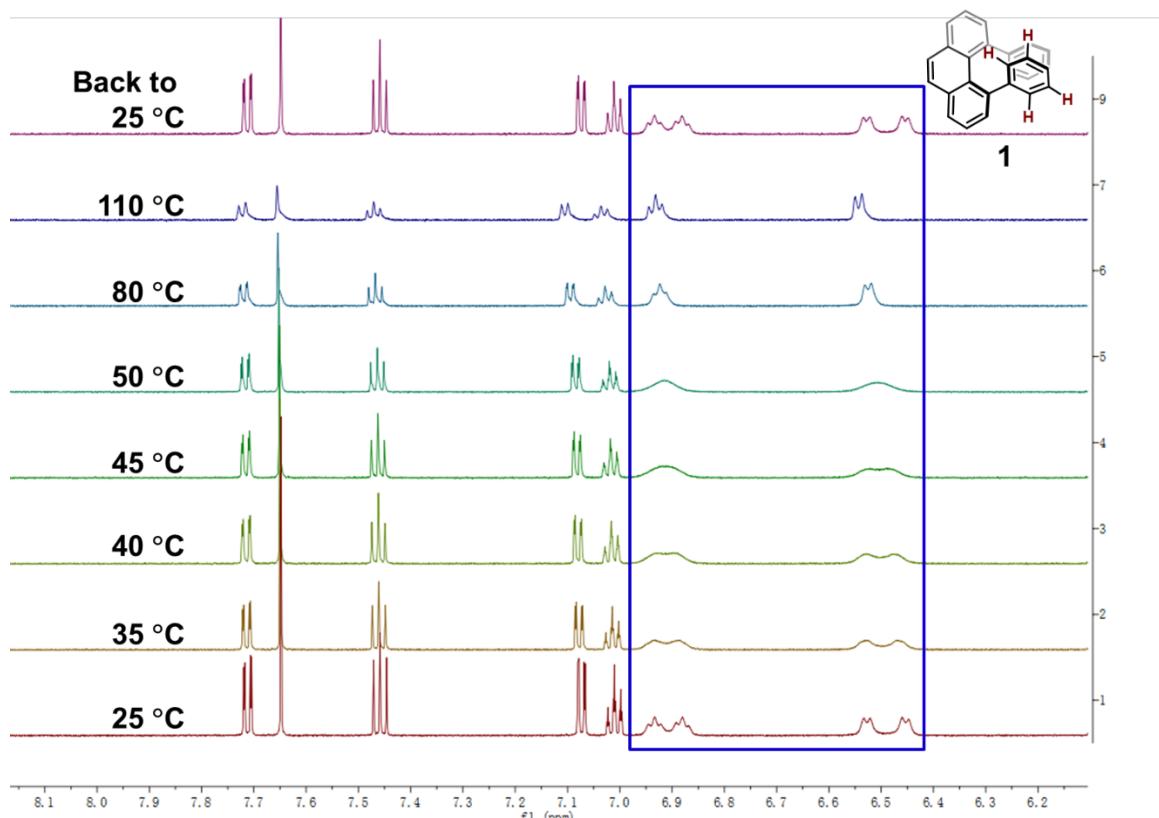


Figure S11. VT ^1H NMR spectrum of **1** in 1,1,2,2-tetrachloroethane- d_2

8.9 TD-DFT vertical one-electron excitations

Table S10. TD-DFT vertical one-electron excitations of **3c**.

TD-DFT at M06-2X/6-31G(d)				
	energy (eV)	Excitation [nm]	Oscillator strength (f)	Description
S₁	3.9972	310.18	0.1284	H–3→L+2; H–1→L; H→L+1
S₂	4.0020	309.81	0.0019	H–4→L; H–2→L+2; H–1→L+1; H→L
S₄	4.2125	294.33	0.1589	H–3→L+1; H–2→L
S₅	4.4692	277.42	2.2600	H–3→L+2
S₆	4.4986	275.60	0.2723	H–4→L+3; H→L+3
S₁₀	4.7978	258.42	0.3490	H→L+2
TD-DFT at B3LYP /6-31G(d)				
	energy (eV)	Excitation [nm]	Oscillator strength (f)	Description
S₁	3.5057	353.67	0.0302	H–3→L+3; H→L; H→L+2
S₂	3.5095	353.28	0.0472	H–2→L+3; H–1→L; H→L
S₄	3.6948	335.56	0.1343	H–2→L; H→L+1
S₆	3.8273	323.95	0.1355	H–3→L; H→L+3;
S₇	3.8689	320.46	1.0559	H–2→L+3; H→L; H→L+2
S₈	3.8726	320.16	0.0819	H–2→L+1; H→L
S₉	3.9032	317.64	0.2745	H–3→L+1; H–1→L; H→L+2
S₁₈	4.1386	299.58	0.1201	H–1→L+5; H→L+4;

Table S11. TD-DFT vertical one-electron excitations of **3f** at B3LYP /6-31G(d).

	energy (eV)	Excitation [nm]	Oscillator strength (f)	Description
S₁	3.0114	411.72	0.3612	H→L
S₃	3.0601	405.17	1.0442	H–1→L+1; H→L
S₆	3.3040	375.25	0.1257	H→L+2
S₁₁	3.4626	358.07	0.6273	H–3→L; H–1→L+3
S₁₉	3.6457	340.08	0.2463	H–7→L; H–6→L+1; H–3→L; H–1→L+6

Table S12. TD-DFT vertical one-electron excitations of **3i** at B3LYP /6-31G(d).

	energy (eV)	Excitation [nm]	Oscillator strength (f)	Description
S₁	2.8356	437.24	0.0038	H–1→L
S₂	2.8736	431.46	0.0008	H→L
S₃	2.8744	431.33	0.1709	H–1→L+1
S₅	2.9908	414.55	0.0761	H–3→L
S₁₇	3.5216	352.07	0.1453	H–3→L+5; H–1→L+4; H→L+2

Table S13. TD-DFT vertical one-electron excitations of **3j** at B3LYP/6-31G(d).

	energy (eV)	Excitation [nm]	Oscillator strength (f)	Description
S₁	3.0390	407.98	0.0068	H–1→L; H→L+1
S₂	3.0663	404.35	0.2066	H→L
S₅	3.1917	388.45	0.3686	H–1→L+1
S₇	3.2581	380.54	0.1179	H–1→L+3
S₁₀	3.6885	336.13	0.1965	H–3→L; H–2→L+3; H–1→L+4
S₁₅	3.8917	318.58	0.2149	H–2→L+1; H→L+5
S₁₆	3.9449	314.29	0.2614	H–4→L; H–2→L+1; H→L+5

8.10 Uncorrected and thermal-corrected energies of stationary points

Table S14. Uncorrected and thermal-corrected (298 K) energies of stationary points (Hartree) calculated by M06-2X/6-31G(d) or B3LYP/6-31G(d) level of theory.

Compound	E	E+ZPE	H	G
3a (B3LYP)	-2462.097701	-2462.143290	-2462.096757	-2462.220161
3b (B3LYP)	-2619.233750	-2619.285825	-2619.232806	-2619.369436
3c (B3LYP)	-2776.369854	-2776.426817	-2776.368909	-2776.516698
3d (B3LYP)	-3494.309674	-3494.374308	-3494.308730	-3494.476780
3e (B3LYP)	-2769.286780	-2769.337669	-2769.285835	-2769.420664
3f (B3LYP)	-3543.176120	-3543.245292	-3543.175176	-3543.349141
3g (B3LYP)	-3385.979380	-3386.043900	-3385.978435	-3386.146176
3h (B3LYP)	-4002.625860	-4002.704557	-4002.624916	-4002.826386
3i (B3LYP)	-4264.285372	-4264.370556	-4264.284428	-4264.496920
3j (B3LYP)	-2572.728675	-2572.776848	-2572.727731	-2572.858420
The calculation of strain energy				
1 (M06-2X)	-1000.833688	-1000.852107	-1000.832744	-1000.897627
3a (M06-2X)	-2461.115696	-2461.160517	-2461.114752	-2461.235774
3j (M06-2X)	-2571.711967	-2571.759499	-2571.711023	-2571.839499
4a (M06-2X)	-2571.711967	-2571.759499	-2571.711023	-2571.839499
The calculation of the racemization barrier				
3c (M06-2X)	-2775.231392	-2775.287411	-2775.230448	-2775.375304
TS-3c_{rac} (M06-2X)	-2775.184277	-2775.239720	-2775.183333	-2775.327416
(P,M)-3c (M06-2X)	-2775.222979	-2775.279036	-2775.222035	-2775.367202
TS-1_{rac} (M06-2X)	-1000.799152	-1000.816931	-1000.798207	-1000.862441
3e (M06-2X)	-2768.180056	-2768.230286	-2768.179112	-2768.312009
TS-3e_{rac} (M06-2X)	-2768.136578	-2768.186128	-2768.135634	-2768.267122
(P,M)-3e (M06-2X)	-2768.174228	-2768.224362	-2768.173284	-2768.305862
3j (M06-2X)	-2571.711967	-2571.759499	-2571.711023	-2571.839499
TS-3j_{rac} (M06-2X)	-2571.662111	-2571.708983	-2571.661167	-2571.789043
(P,M)-3j (M06-2X)	-2571.675552	-2571.722791	-2571.674608	-2571.803456

Compound	<i>E</i>	<i>E+ZPE</i>	<i>H</i>	<i>G</i>
The calculation of the rotation barrier				
TS-3a_{rot} (M06-2X)	-2461.075948	-2461.120380	-2461.075003	-2461.195553
TS-1_{rot} (M06-2X)	-1000.805452	-1000.823282	-1000.804507	-1000.868492

[a] E : electronic energy; ZPE : zero-point energy; H ($= E + ZPE + E_{\text{vib}} + E_{\text{rot}} + E_{\text{trans}} + RT$): sum of electronic and thermal enthalpies; G ($= H - TS$): sum of electronic and thermal free energies.

8.11 Cartesian coordinates of optimized structures

Table S15. Cartesian coordinates of optimized structures calculated by M06-2X/6-31G(d) (**1**, **TS-1_{rot}**, **3a**, **3b**, **3c**, (P,M)-**3c**, **3e**, (P,M)-**3e**, **3j**, (P,M)-**3j**, **TS-3a_{rot}**, **TS-3c_{rac}**, **TS-3e_{rac}**, **TS-3j_{rac}**, **4a**, **TS-1_{rac}**) or B3LYP/6-31G(d) (**3d**, **3e**, **3f**, **3g**, **3h**, **3i**, **3j**) level of theory.

1 (M06-2X/6-31G(d))						
C	-3.90981900	0.64951900	-0.18384300	C	3.33838600	-1.19448800
C	-3.90981800	-0.64952200	0.18384200	C	3.24871800	-0.36708400
C	-2.67721800	-1.38385800	0.27683800	C	1.99945300	0.08391500
C	-1.43827800	-0.73390100	0.02306900	C	0.85023400	-0.28516800
C	-1.43827900	0.73390000	-0.02307000	H	-4.83989900	1.18837300
C	-2.67722000	1.38385700	-0.27683800	H	-4.83989800	-1.18837700
C	-0.30403700	1.56718700	0.23020100	H	0.46857000	3.55290100
C	-0.39475000	2.93058600	-0.01935900	H	-1.61455500	4.60064300
C	-1.58357600	3.53266800	-0.45023100	H	-3.68565800	3.22543900
C	-2.72491300	2.77051400	-0.52653800	H	2.26715000	2.17107700
C	0.93236900	1.10421900	0.91830000	H	-0.12258400	-0.05873500
C	2.18949300	1.56038200	0.50948600	H	1.91799200	-0.71819400
C	0.85023200	0.28516600	2.05065200	H	4.14522600	0.07749200
C	1.99945100	-0.08391700	2.74111900	H	4.30736300	1.54339700
C	3.24871600	0.36708500	2.31834600	H	-3.68565500	-3.22544100
C	3.33838400	1.19449100	1.20233800	H	-1.61455100	-4.60064400
C	-2.72491000	-2.77051600	0.52653800	H	0.46857400	-3.55289900
C	-1.58357300	-3.53266900	0.45023200	H	2.26715200	-2.17107100
C	-0.39474700	-2.93058600	0.01936000	H	4.30736500	-1.54339100
C	-0.30403600	-1.56718700	-0.23020100	H	4.14522800	-0.07749100
C	2.18949500	-1.56037800	-0.50948400	H	1.91799300	0.71819000
C	0.93237100	-1.10421800	-0.91830000	H	-0.12258300	0.05873100
TS-1 _{rac} (M06-2X/6-31G(d))						
C	-4.12393100	0.66859700	-0.02550500	C	1.72289200	2.00260900
C	-4.12393100	-0.66859700	0.02550600	C	3.10584200	2.12587800
C	-2.89074800	-1.39544500	0.05286500	C	3.78266900	1.74011400
C	-1.60101700	-0.75190600	0.03086500	C	3.06617100	1.22780100
C	-1.60101700	0.75190700	-0.03086500	C	-3.06588600	-2.79258700
C	-2.89074800	1.39544500	-0.05286400	C	-1.99369100	-3.63926400
C	-0.49654800	1.68031700	-0.05654900	C	-0.73022500	-3.05890900
C	-0.73022400	3.05890900	-0.09792100	C	-0.49654900	-1.68031700
C	-1.99369000	3.63926500	-0.11926300	C	1.68050200	-1.11287800
C	-3.06588500	2.79258700	-0.09750300	C	0.99270400	-1.48767900
C	0.99270400	1.48767900	-0.06490900	C	3.06617100	-1.22780100
C	1.68050300	1.11287800	-1.21846100	C	3.78266900	-1.74011400

C	3.10584200	-2.12587800	-0.94931200	H	4.86264400	1.83570400	-0.26393200
C	1.72289300	-2.00260900	-1.01352200	H	3.58714600	0.92143500	-2.18493600
H	-5.05069300	1.23386500	-0.04655400	H	-4.08176000	-3.17632700	0.11342700
H	-5.05069400	-1.23386500	0.04655600	H	-2.11160700	-4.71713600	0.15690100
H	0.13843100	3.70699400	-0.13217200	H	0.13843100	-3.70699400	0.13217000
H	-2.11160700	4.71713600	-0.15690300	H	1.12334700	-0.73638000	2.07192000
H	-4.08175900	3.17632700	-0.11342700	H	3.58714500	-0.92143500	2.18493700
H	1.12334800	0.73638000	-2.07192000	H	4.86264400	-1.83570400	0.26393400
H	1.18722300	2.32605800	1.90219100	H	3.65285200	-2.52963300	-1.79628000
H	3.65285200	2.52963300	1.79628100	H	1.18722400	-2.32605800	-1.90219100

TS-1_{rot} (M06-2X/6-31G(d))

C	-3.66310700	0.00350000	-0.79022300	C	2.14766400	-3.56083600	-1.41385500
C	-3.63648900	-0.64588100	0.39476200	C	2.98933700	-2.68843900	-2.09739800
C	-2.38215900	-0.96405300	1.03148700	C	2.87662700	-1.32329400	-1.86374600
C	-1.16948800	-0.58132200	0.40001100	C	1.93781800	-0.82747900	-0.96169300
C	-1.25443400	0.50255400	-0.57698300	H	-4.59461300	0.15485400	-1.32843800
C	-2.47460700	0.65008500	-1.28729300	H	-4.54860900	-1.02255900	0.84961100
C	-0.27011900	1.52492100	-0.73365000	H	0.32347500	3.21796000	-1.89976200
C	-0.40140800	2.41702500	-1.79409100	H	-1.56472400	3.08693000	-3.48231800
C	-1.50197100	2.38352500	-2.65820000	H	-3.48703200	1.60901600	-2.92873100
C	-2.55885200	1.54884100	-2.36690200	H	2.23816400	2.54609000	-1.06367200
C	0.73492000	1.86239400	0.32130900	H	-0.53150300	1.30869200	1.97515500
C	1.96710500	2.44141200	-0.01575900	H	1.05563200	2.02475100	3.70819400
C	0.42597200	1.72635900	1.68092800	H	3.24491300	3.01762000	3.07755500
C	1.32202800	2.13873200	2.66190400	H	3.81573600	3.28542700	0.67157600
C	2.54598800	2.70005800	2.31018300	H	-3.29511900	-1.98667800	2.69468700
C	2.86422800	2.85157200	0.96330100	H	-1.12081100	-2.81339000	3.59568600
C	-2.35698600	-1.75192300	2.19901600	H	0.89229400	-2.63006100	2.16289900
C	-1.15943500	-2.23353200	2.67906200	H	0.54223900	-3.75165400	-0.00841400
C	-0.00827900	-2.08604600	1.89335900	H	2.20965500	-4.63121400	-1.58555100
C	0.00444700	-1.33226000	0.72297700	H	3.72141100	-3.06832000	-2.80336800
C	1.21266300	-3.06356800	-0.51440600	H	3.52949300	-0.62648900	-2.38119200
C	1.08588100	-1.68475400	-0.26185300	H	1.90533000	0.23348500	-0.78739300

3a (M06-2X/6-31G(d))

C	6.01483300	0.00854100	1.58889800	C	8.43991500	0.89920500	-2.67187300
C	6.11008200	-0.42424900	2.90563300	C	7.30133200	0.92961300	-3.44089000
C	7.30098800	-0.92960900	3.44115000	C	6.11037100	0.42425700	-2.90549300
C	8.43964600	-0.89921100	2.67224400	C	6.01499100	-0.00854100	-1.58877000
C	8.38788200	-0.46253700	1.33279100	C	7.14761000	0.12361900	-0.72430400
C	9.62055500	-0.27050400	0.61847900	C	7.14753800	-0.12362700	0.72454500
C	9.62061700	0.27048800	-0.61799100	C	4.77064800	0.73896000	1.22685600
C	8.38801600	0.46252700	-1.33242600	C	4.82925000	1.96511500	0.55478600

C	3.67010900	2.67310900	0.26912400	C	-1.16219300	4.33988200	-0.32536600
C	2.41359200	2.19123200	0.65749300	C	1.16219500	-4.33987600	-0.32536900
C	2.36115600	0.97957200	1.35525100	C	-1.16219200	-4.33987400	0.32486100
C	3.51885800	0.26597400	1.63354200	C	-0.00001100	-5.03027300	-0.00029600
C	1.17775800	2.94008100	0.32418800	H	5.24791900	-0.29903300	3.55349800
C	1.17780100	-2.94008200	-0.32452700	H	7.33506400	-1.26400600	4.47304300
C	2.41366300	-2.19123200	-0.65772500	H	9.40213000	-1.18316200	3.08906600
C	3.67014300	-2.67313000	-0.26926400	H	10.55034800	-0.50153700	1.13093500
C	4.82931100	-1.96513200	-0.55480800	H	10.55046200	0.50151900	-1.13035500
C	4.77076900	-0.73896200	-1.22685400	H	9.40244100	1.18315400	-3.08859800
C	3.51901700	-0.26595900	-1.63363700	H	7.33551300	1.26401400	-4.47277800
C	2.36128600	-0.97955600	-1.35545600	H	5.24827100	0.29904700	-3.55344300
C	-2.41366300	2.19123900	-0.65772400	H	5.79271600	2.35806000	0.24320200
C	-2.36128400	0.97956000	-1.35545100	H	3.73733600	3.60577000	-0.28409100
C	-3.51901400	0.26596300	-1.63363100	H	1.40204300	0.59164300	1.68936600
C	-4.77076800	0.73896700	-1.22685300	H	3.44968500	-0.69150900	2.14237600
C	-4.82931100	1.96514100	-0.55481300	H	3.73731300	-3.60581200	0.28392400
C	-3.67014300	2.67314000	-0.26926900	H	5.79275100	-2.35808900	-0.24315500
C	-6.01498800	0.00854400	-1.58876900	H	3.44989300	0.69153600	-2.14245600
C	-6.11036500	-0.42425500	-2.90549100	H	1.40219800	-0.59161200	-1.68962500
C	-7.30132400	-0.92961400	-3.44089100	H	-1.40219500	0.59161400	-1.68961500
C	-8.43990900	-0.89920600	-2.67187600	H	-3.44989000	-0.69153400	-2.14244500
C	-8.38801300	-0.46252800	-1.33242900	H	-5.79275000	2.35810100	-0.24316500
C	-9.62061600	-0.27049200	-0.61799600	H	-3.73731300	3.60582300	0.28391600
C	-9.62055600	0.27049700	0.61847500	H	-5.24826400	-0.29904500	-3.55343900
C	-8.38788600	0.46253100	1.33279000	H	-7.33550200	-1.26401500	-4.47277900
C	-8.43965300	0.89920000	2.67224400	H	-9.40243400	-1.18315800	-3.08860300
C	-7.30099600	0.92959700	3.44115200	H	-10.55045900	-0.50152600	-1.13036200
C	-6.11008900	0.42423900	2.90563600	H	-10.55035100	0.50152800	1.13093000
C	-6.01483700	-0.00854700	1.58890000	H	-9.40213800	1.18314900	3.08906600
C	-7.14754000	0.12362400	0.72454500	H	-7.33507500	1.26398900	4.47304600
C	-7.14760900	-0.12361900	-0.72430400	H	-5.24792700	0.29902100	3.55350200
C	-4.77065100	-0.73896300	1.22685500	H	-5.79271800	-2.35805800	0.24319200
C	-4.82925100	-1.96511400	0.55477900	H	-3.73733600	-3.60576600	-0.28410400
C	-3.67011000	-2.67310700	0.26911500	H	-1.40204600	-0.59164500	1.68936600
C	-2.41359400	-2.19123000	0.65748700	H	-3.44968900	0.69150300	2.14238300
C	-2.36115800	-0.97957300	1.35525000	H	-0.00005900	1.17306300	-0.00008300
C	-3.51886200	-0.26597800	1.63354400	H	0.00005700	-1.17305800	-0.00008700
C	-0.00003300	2.26049700	-0.00013200	H	2.05813600	4.88596500	0.60479700
C	-1.17780000	2.94008700	-0.32452400	H	0.00003400	6.11605300	-0.00035100
C	-1.17775900	-2.94007800	0.32418000	H	-2.05812500	4.88596200	-0.60534600
C	0.00003300	-2.26049200	-0.00013800	H	2.05812900	-4.88595500	-0.60534700
C	1.16219300	4.33987700	0.32487000	H	-2.05813500	-4.88596300	0.60478700
C	0.00001300	5.03027700	-0.00028900	H	-0.00003000	-6.11604900	-0.00035800

TS-3a_{rot} (M06-2X/6-31G(d))

C	-5.97216500	-0.16179700	-1.62025900	C	7.72397900	-0.29198100	-3.46782700
C	-6.09729700	-0.69713300	-2.89522200	C	6.54534000	-0.83664900	-2.95505400
C	-7.26551100	-1.34752900	-3.31462100	C	6.21184200	-0.76529600	-1.60347700
C	-8.35910800	-1.36249700	-2.48049200	C	7.08657300	-0.06742300	-0.70793700
C	-8.27358800	-0.82578500	-1.17962300	C	6.84824700	0.18906700	0.72623300
C	-9.46879100	-0.67912300	-0.39295400	C	5.03480900	-1.57549600	-1.17518700
C	-9.43518100	-0.03856200	0.79611300	C	4.98526900	-2.23237900	0.05904400
C	-8.18043000	0.31400500	1.40473400	C	3.82283600	-2.87062700	0.48112100
C	-8.16809400	0.86684700	2.70189700	C	2.67101000	-2.86899200	-0.31048400
C	-6.97943000	1.05595100	3.36680800	C	2.74499200	-2.29126500	-1.58194700
C	-5.79254300	0.58615000	2.78787500	C	3.91060000	-1.67599600	-2.01181800
C	-5.76263500	0.03617300	1.51326600	C	-0.21649400	2.81255500	-0.42168200
C	-6.96264300	0.01814200	0.73679700	C	0.90615300	3.60496000	-0.16549200
C	-7.03556300	-0.33858200	-0.68244600	C	1.38914100	-3.42076300	0.19484000
C	-4.80603600	0.72644800	-1.37023000	C	0.23762100	-2.62633500	0.18394300
C	-4.98539800	1.97951900	-0.77183100	C	-1.57529900	4.76208900	-0.75368700
C	-3.91045400	2.83421500	-0.57197000	C	-0.47139600	5.56397200	-0.47984600
C	-2.61980900	2.47664000	-0.97992400	C	0.76526300	4.99513300	-0.18634200
C	-2.45021500	1.23813300	-1.61120000	C	-1.03608700	-4.42169000	1.15181100
C	-3.52272900	0.37682200	-1.79955800	C	1.31461700	-4.72151700	0.70024700
C	-1.46120900	3.36670800	-0.72395200	C	0.10207700	-5.22020900	1.16531900
C	-0.98107500	-3.10680100	0.67185800	H	-5.29049300	-0.54017200	-3.60496500
C	-2.18723200	-2.24337700	0.74902500	H	-7.32742500	-1.75929200	-4.31687700
C	-3.45370900	-2.75619200	0.44222600	H	-9.31216800	-1.76030300	-2.81855200
C	-4.59918300	-1.99456500	0.62936700	H	-10.40717800	-1.02592300	-0.81695800
C	-4.51942300	-0.69032100	1.13275000	H	-10.34717000	0.15766800	1.35326700
C	-3.25232100	-0.16262200	1.40221100	H	-9.11583000	1.11565500	3.17169700
C	-2.10487100	-0.92363400	1.20783500	H	-6.96397700	1.48450700	4.36382400
C	2.19376400	2.93174900	0.12312100	H	-4.87991300	0.57963400	3.37623800
C	3.06033700	3.34785900	1.13896600	H	-5.97760300	2.27868800	-0.44722200
C	4.18567400	2.59783000	1.46252100	H	-4.06991700	3.78484200	-0.07073300
C	4.50085200	1.40213300	0.78861300	H	-1.46367100	0.94536300	-1.95960300
C	3.67551000	1.05247000	-0.27613500	H	-3.35828300	-0.59889100	-2.24935200
C	2.54795800	1.79191100	-0.59875900	H	-3.53983000	-3.77130900	0.06400200
C	5.62792300	0.59098900	1.36734200	H	-5.57286500	-2.42282800	0.40929500
C	5.53700000	0.44811500	2.75268300	H	-3.16542700	0.86092200	1.75797400
C	6.61764300	0.06516100	3.55337600	H	-1.13364400	-0.50377800	1.45725300
C	7.85825700	-0.02759800	2.96905300	H	2.82550900	4.23858300	1.71587900
C	7.99115800	0.08248000	1.57148000	H	4.82722400	2.92960700	2.27365600
C	9.31304800	0.22268000	1.01593900	H	3.86630000	0.16300800	-0.83905100
C	9.48038900	0.45608100	-0.30119800	H	1.92132700	1.46275800	-1.42374400
C	8.38189400	0.25207800	-1.20940000	H	4.59200500	0.69529500	3.22611000
C	8.65774000	0.20444700	-2.58785500	H	6.48988800	-0.05367800	4.62444300

H	8.75447400	-0.16428500	3.56802900	H	3.91356100	-1.17232700	-2.97414100
H	10.15481600	0.22879900	1.70280700	H	-0.12490600	1.73314800	-0.33716900
H	10.45971800	0.67106500	-0.71904500	H	0.30043300	-1.60863400	-0.19635200
H	9.64244100	0.50849200	-2.93209400	H	-2.52585800	5.21936500	-1.01268300
H	7.93591600	-0.35251200	-4.53038200	H	-0.57173200	6.64457500	-0.51463100
H	5.90032400	-1.39949200	-3.62131100	H	1.62955400	5.62673000	-0.00052600
H	5.85041400	-2.21391700	0.71406400	H	-1.97120300	-4.80181900	1.55282300
H	3.79130300	-3.33340600	1.46380600	H	2.20567300	-5.34306100	0.70658700
H	1.87091200	-2.31011400	-2.22724300	H	0.04572600	-6.23362600	1.55086300

3b (M06-2X/6-31G(d))

C	5.96483500	0.08148600	1.58263300	C	-6.05742900	-0.29231900	-2.91695100
C	6.05718900	-0.29284800	2.91717300	C	-7.24737700	-0.77468400	-3.47632600
C	7.24710600	-0.77527400	3.47656700	C	-8.38837100	-0.77814600	-2.71027100
C	8.38814300	-0.77868800	2.71057000	C	-8.33968100	-0.40113900	-1.35245900
C	8.33953900	-0.40152800	1.35279700	C	-9.57221500	-0.24163800	-0.63001200
C	9.57211200	-0.24192900	0.63043600	C	-9.57218500	0.24180700	0.63044800
C	9.57215800	0.24173200	-0.62994500	C	-8.33962100	0.40126000	1.35285600
C	8.33963200	0.40138800	-1.35237400	C	-8.38825700	0.77815100	2.71070200
C	8.38832800	0.77856700	-2.71013800	C	-7.24724500	0.77455700	3.47673000
C	7.24733400	0.77521900	-3.47619800	C	-6.05733300	0.29219100	2.91727800
C	6.05736400	0.29283800	-2.91687800	C	-5.96495000	-0.08190000	1.58267200
C	5.96491900	-0.08151900	-1.58235000	C	-7.10043800	0.09013500	0.72896500
C	7.10041100	0.09019700	-0.72859700	C	-7.10047000	-0.08999000	-0.72863400
C	7.10036600	-0.09029400	0.72894600	C	-4.72850700	-0.80674200	1.18496500
C	4.72840800	0.80638100	1.18498200	C	-4.80433100	-1.98563200	0.43599500
C	4.80429600	1.98535800	0.43615900	C	-3.66165800	-2.71629500	0.14448900
C	3.66166000	2.71609200	0.14469800	C	-2.40376000	-2.32368400	0.62105700
C	2.40373300	2.32345300	0.62115700	C	-2.33168800	-1.13925900	1.36445000
C	2.33159000	1.13894100	1.36440900	C	-3.47065600	-0.39150900	1.63484600
C	3.47052600	0.39111700	1.63475300	C	-1.18639000	-3.12308100	0.32608000
C	1.18642700	3.12295400	0.32621300	C	-1.17277100	-4.53133200	0.37082800
C	1.17299200	4.53120300	0.37088900	C	0.00003300	-5.18611600	-0.00041900
C	0.000028400	5.18612700	-0.00041900	C	1.17279500	-4.53118200	-0.37153200
C	-1.17255100	4.53132600	-0.37153800	C	1.18632700	-3.12294100	-0.32650100
C	-1.18626100	3.12309100	-0.32644600	C	-0.00005100	-2.45941900	-0.00014200
C	0.00001700	2.45942600	-0.00001600	C	2.40367900	-2.32343400	-0.62125300
C	-2.40368200	2.32371900	-0.62126000	C	3.66156400	-2.71613900	-0.14473100
C	-2.33165000	1.13897100	-1.36413900	C	4.80424100	-1.98541200	-0.43605000
C	-3.47067100	0.39123700	-1.63436100	C	4.72844100	-0.80637900	-1.18479400
C	-4.72853300	0.80680900	-1.18482400	C	3.47060000	-0.39103700	-1.63460600
C	-4.80432100	1.98605500	-0.43640600	C	2.33162200	-1.13884500	-1.36439200
C	-3.66160100	2.71670800	-0.14506100	C	2.34111400	5.37175900	0.83244300
C	-5.96500100	0.08193000	-1.58239100	C	-2.34048400	5.37198000	-0.83339500

C	-2.34073700	-5.37204500	0.83249400	H	-9.34950100	1.04344600	3.14243700
C	2.34083900	-5.37172000	-0.83331800	H	-7.27870600	1.06298800	4.52252800
H	5.19491000	-0.13720600	3.55817900	H	-5.19508000	0.13639100	3.55828100
H	7.27854500	-1.06390900	4.52231000	H	-5.76895000	-2.33047900	0.07564700
H	9.34938000	-1.04404900	3.14228000	H	-3.74680400	-3.60834100	-0.46736500
H	10.50207000	-0.44922500	1.15268600	H	-1.37112300	-0.80725200	1.75006800
H	10.50215400	0.44899300	-1.15214100	H	-3.38216500	0.54008400	2.18718900
H	9.34960100	1.04389300	-3.14179100	H	0.00007100	-6.27521500	-0.00051900
H	7.27884300	1.06387100	-4.52193300	H	-0.00008100	-1.37142000	-0.00001500
H	5.19511300	0.13724400	-3.55793400	H	3.74669500	-3.60832400	0.46692400
H	5.76894200	2.33022300	0.07589800	H	5.76885300	-2.33033600	-0.07575600
H	3.74685500	3.60823000	-0.46702000	H	3.38212600	0.54066800	-2.18676300
H	1.37099800	0.80691600	1.74994100	H	1.37106800	-0.80676400	-1.74997100
H	3.38198600	-0.54054600	2.18697000	H	2.95969100	4.84323300	1.56125000
H	0.00039600	6.27522700	-0.00059100	H	1.97369900	6.29197900	1.29489400
H	-0.00008400	1.37142600	0.00012100	H	2.99168300	5.66637500	0.00129800
H	-1.37106900	0.80667700	-1.74946900	H	-2.95914800	4.84335300	-1.56205700
H	-3.38221100	-0.54061500	-2.18627100	H	-2.99101800	5.66699400	-0.00236500
H	-5.76894800	2.33119700	-0.07636700	H	-1.97286200	6.29197700	-1.29612400
H	-3.74672300	3.60905300	0.46636300	H	-2.95937900	-4.84356800	1.56128100
H	-5.19519400	-0.13660800	-3.55799800	H	-2.99128200	-5.66684700	0.00139700
H	-7.27887600	-1.06321800	-4.52209400	H	-1.97314700	-6.29216300	1.29500800
H	-9.34963500	-1.04345500	-3.14195200	H	2.95945700	-4.84306200	-1.56199400
H	-10.50220300	-0.44883400	-1.15225000	H	2.99138800	-5.66661600	-0.00225600
H	-10.50215000	0.44899700	1.15273000	H	1.97333600	-6.29178500	-1.29600500

(P,M)-3c (M06-2X/6-31G(d))

C	-6.19116800	-0.19134100	1.57664400	C	-2.50165400	-2.18888400	0.55838700
C	-6.29511900	0.06975000	2.93868100	C	-2.51666200	-1.03590600	1.35354100
C	-7.48959600	0.49204400	3.53259200	C	-3.70073500	-0.37465400	1.63629200
C	-8.62574900	0.55384200	2.76244100	C	-1.22632800	-2.91696100	0.33622000
C	-8.56760100	0.29011800	1.37942100	C	-1.22636400	2.91693000	-0.33624200
C	-9.80026600	0.18876200	0.64776800	C	-2.50169800	2.18885700	-0.55836000
C	-9.80030100	-0.18871100	-0.64746500	C	-3.72623100	2.64645500	-0.05407700
C	-8.56767200	-0.29009400	-1.37917700	C	-4.91760200	1.99326900	-0.35015400
C	-8.62589100	-0.55381800	-2.76219400	C	-4.92409200	0.84298400	-1.14671200
C	-7.48977400	-0.49202800	-3.53240000	C	-3.70081500	0.37468700	-1.63631200
C	-6.29526500	-0.06974100	-2.93854800	C	-2.51673200	1.03593300	-1.35358900
C	-6.19124400	0.19134200	-1.57651500	C	-0.01046100	-2.23520900	0.36930100
C	-7.32447900	-0.03498700	-0.73382600	C	1.20962100	-2.91832100	0.33505300
C	-7.32444200	0.03499100	0.73400900	C	1.20957300	2.91826500	-0.33504900
C	-4.92403800	-0.84299200	1.14679400	C	-0.01051100	2.23515000	-0.36921000
C	-4.91757800	-1.99332700	0.35031000	C	-1.20912000	-4.30967000	0.17597200
C	-3.72621800	-2.64652100	0.05421100	C	-0.01251900	-5.01834900	0.07237500

C	1.18760800	-4.30528100	0.17670500	H	-7.52739200	-0.69109000	-4.59858700
C	-1.20915100	4.30966100	-0.17619100	H	-5.43310900	0.12765800	-3.56778100
C	1.18757300	4.30524800	-0.17690400	H	-5.85549500	-2.37807000	-0.04047700
C	-0.01254600	5.01834600	-0.07268500	H	-3.74997700	-3.52722800	-0.58160700
C	2.48430900	2.18913600	-0.55673400	H	-1.59124500	-0.66274700	1.78196400
C	2.49890900	1.03681700	-1.35256000	H	-3.67857000	0.53083600	2.23573400
C	3.68315500	0.37599200	-1.63607300	H	-3.74994500	3.52712700	0.58179200
C	4.90636800	0.84396000	-1.14613700	H	-5.85550100	2.37797300	0.04071300
C	4.89996600	1.99344100	-0.34829500	H	-3.67867800	-0.53076900	-2.23580700
C	3.70859300	2.64616500	-0.05154800	H	-1.59132100	0.66282000	-1.78206900
C	6.17354200	0.19262200	-1.57639200	H	-0.00998700	-1.15124700	0.43028000
C	6.27754600	-0.06733200	-2.93863800	H	-0.01005300	1.15117800	-0.43007000
C	7.47205500	-0.48912600	-3.53284300	H	-2.15392100	-4.84141600	0.17879000
C	8.60816800	-0.55151600	-2.76268600	H	2.13001900	-4.84624500	0.18121900
C	8.54996600	-0.28891400	-1.37945200	H	-2.15395600	4.84140000	-0.17910000
C	9.78261000	-0.18811200	-0.64769000	H	2.12999800	4.84618900	-0.18148200
C	9.78259700	0.18830100	0.64785100	H	1.57339100	0.66361000	-1.78072600
C	8.54994600	0.28902100	1.37961200	H	3.66105800	-0.52906300	-2.23616400
C	8.60813200	0.55160200	2.76285000	H	5.83786100	2.37752600	0.04317900
C	7.47202200	0.48913700	3.53300600	H	3.73161300	3.52594100	0.58567500
C	6.27753400	0.06729900	2.93879100	H	5.41539400	0.13057300	-3.56771800
C	6.17354700	-0.19263700	1.57654000	H	7.50965900	-0.68732800	-4.59918600
C	7.30677200	0.03439900	0.73402500	H	9.57359900	-0.77507100	-3.20843800
C	7.30677600	-0.03435500	-0.73387200	H	10.71213100	-0.35047000	-1.18627300
C	4.90639400	-0.84400500	1.14627300	H	10.71210700	0.35072500	1.18643300
C	4.90002300	-1.99350800	0.34846400	H	9.57355000	0.77520400	3.20860700
C	3.70866200	-2.64624500	0.05169500	H	7.50961600	0.68731800	4.59935300
C	2.48435400	-2.18920600	0.55681500	H	5.41538600	-0.13065200	3.56786200
C	2.49893000	-1.03687200	1.35262300	H	5.83793100	-2.37759900	-0.04297100
C	3.68316300	-0.37603900	1.63616400	H	3.73172000	-3.52603200	-0.58551100
C	0.03273400	6.54071200	0.09397000	H	1.57340800	-0.66365800	1.78077100
C	0.81253400	6.88567200	1.37398000	H	3.66104200	0.52902300	2.23624400
C	0.73917300	7.16855700	-1.11936000	H	1.83892600	6.50827000	1.33517700
C	-1.36683500	7.15397500	0.20553300	H	0.85838100	7.97236500	1.50693700
C	0.03274700	-6.54069200	-0.09448900	H	0.32616600	6.45111800	2.25340300
C	0.73938900	-7.16868800	1.11864400	H	1.76716200	6.80777000	-1.22043600
C	-1.36683500	-7.15395500	-0.20590300	H	0.20505600	6.92912500	-2.04449600
C	0.81233700	-6.88548500	-1.37467300	H	0.77390700	8.25869800	-1.01311300
H	-5.43293000	-0.12765000	3.56787000	H	-1.95566700	6.98554000	-0.70215500
H	-7.52716100	0.69110500	4.59878000	H	-1.91912000	6.74388200	1.05777800
H	-9.59115700	0.77778800	3.20805000	H	-1.28102000	8.23566900	0.35053300
H	-10.72976900	0.35160700	1.18623800	H	0.20540700	-6.92940100	2.04389500
H	-10.72983400	-0.35152600	-1.18589400	H	0.77413900	-8.25881300	1.01223900
H	-9.59132300	-0.77775000	-3.20775800	H	1.76738300	-6.80788300	1.21961300

H	-1.28103000	-8.23561300	-0.35117400	H	0.85814500	-7.97216000	-1.50779000
H	-1.95548000	-6.98574800	0.70194800	H	0.32583500	-6.45079900	-2.25395700
H	-1.91930600	-6.74367100	-1.05793600	H	1.83874300	-6.50810800	-1.33598400

3c (M06-2X/6-31G(d))

C	-7.14162100	-0.12093000	-0.72513900	C	1.16274800	-4.32885800	-0.33396300
C	-6.00916200	0.01455200	-1.58924900	C	1.17973600	-2.92706500	-0.32902000
C	-6.10503600	-0.41312000	-2.90773400	C	0.01045100	-2.24132700	-0.00395300
C	-7.29598700	-0.91629000	-3.44498200	C	-0.03116100	-6.57834900	-0.00241600
C	-8.43441500	-0.88899100	-2.67558700	C	-1.10040000	-7.06442800	-0.99529000
C	-8.38214300	-0.45755800	-1.33452800	C	-0.38730400	-7.06744900	1.41159500
C	-9.61482900	-0.26822100	-0.61946200	C	1.31178900	-7.19833400	-0.40134200
C	-9.61486100	0.26819300	0.61893700	C	2.41967800	2.18465900	0.66321000
C	-8.38221500	0.45749900	1.33408200	C	2.37080000	0.97165200	1.35914900
C	-8.43456800	0.88891500	2.67514100	C	3.52998800	0.26000500	1.63549000
C	-7.29619500	0.91618000	3.44461700	C	4.78059500	0.73605900	1.22869300
C	-6.10521400	0.41300500	2.90744200	C	4.83616600	1.96351900	0.55886200
C	-6.00925300	-0.01465300	1.58895800	C	3.67518000	2.66973400	0.27528600
C	-7.14165800	0.12085400	0.72477000	C	2.41971200	-2.18462400	-0.66307200
C	-4.76383000	0.74222600	-1.22541500	C	3.67526600	-2.66962500	-0.27522000
C	-3.51335600	0.26791900	-1.63462600	C	4.83620300	-1.96338500	-0.55893400
C	-2.35397100	0.97807600	-1.35509100	C	4.78053600	-0.73597800	-1.22885400
C	-2.40292100	2.18792500	-0.65390100	C	3.52988000	-0.25999600	-1.63557800
C	-3.65807500	2.67094800	-0.26253100	C	2.37074100	-0.97166300	-1.35908800
C	-4.81920900	1.96632100	-0.54935500	C	6.02584400	0.00653900	1.58896900
C	-4.76388000	-0.74232100	1.22523800	C	6.12178200	-0.42782300	2.90525100
C	-4.81917600	-1.96645600	0.54924400	C	7.31275700	-0.93375000	3.43985600
C	-3.65799700	-2.67106100	0.26253600	C	8.45115200	-0.90258800	2.67054600
C	-2.40289200	-2.18798800	0.65400100	C	8.39881600	-0.46432000	1.33171300
C	-2.35402500	-0.97811600	1.35515100	C	9.63145900	-0.27129600	0.61753300
C	-3.51345300	-0.26797800	1.63455300	C	9.63140900	0.27146100	-0.61809800
C	-1.16308800	2.92989800	-0.31846300	C	8.39871000	0.46447200	-1.33218400
C	0.01041600	2.24130800	0.00410600	C	8.45093300	0.90273800	-2.67102300
C	1.17965600	2.92707400	0.32927300	C	7.31247800	0.93387300	-3.44024500
C	1.16259300	4.32886400	0.33440300	C	6.12155500	0.42792100	-2.90554800
C	0.01192900	5.04715200	0.01220800	C	6.02573000	-0.00643100	-1.58925500
C	-1.14159300	4.32579000	-0.31555200	C	7.15820900	0.12470800	-0.72450900
C	-0.03144000	6.57832900	0.00313300	C	7.15826200	-0.12457200	0.72413400
C	-1.10083600	7.06421600	0.99593200	H	-5.24294200	-0.28556600	-3.55521100
C	-0.38742200	7.06760000	-1.41086100	H	-7.33036100	-1.24656100	-4.47820200
C	1.31142400	7.19833300	0.40232000	H	-9.39705900	-1.17127600	-3.09317900
C	-1.16301600	-2.92994400	0.31868800	H	-10.54460900	-0.49734900	-1.13280700
C	-1.14144800	-4.32583300	0.31596100	H	-10.54466900	0.49734800	1.13222100
C	0.01212100	-5.04717000	-0.01168900	H	-9.39723500	1.17121700	3.09267100

H	-7.33064000	1.24643600	4.47784000	H	-2.09503200	-6.69203700	-0.73172000
H	-5.24315700	0.28543900	3.55496500	H	-0.87002500	-6.72429500	-2.01011100
H	-3.44656800	-0.68839000	-2.14596200	H	-1.14169800	-8.15941000	-0.99954200
H	-1.39586900	0.58837500	-1.68995900	H	-1.36303800	-6.69289700	1.73526800
H	-3.72218300	3.60158000	0.29467800	H	0.36058300	-6.73197500	2.13737200
H	-5.78154800	2.35993400	-0.23501200	H	-0.42248000	-8.16247100	1.43390300
H	-5.78147600	-2.36011500	0.23484700	H	2.11028700	-6.90933900	0.29018000
H	-3.72202300	-3.60172500	-0.29462900	H	1.23075100	-8.28986300	-0.38045500
H	-1.39595600	-0.58839300	1.69009000	H	1.60746200	-6.90405400	-1.41383000
H	-3.44674500	0.68834300	2.14587400	H	1.41260800	0.58078400	1.69237600
H	0.01018100	1.15429000	0.00104400	H	3.46296200	-0.69867900	2.14235400
H	2.06847400	4.85110300	0.62231600	H	5.79864100	2.35876700	0.24696600
H	-2.04560100	4.85820200	-0.59989500	H	3.74004300	3.60349200	-0.27643900
H	-2.09540900	6.69178400	0.73219500	H	3.74021700	-3.60333400	0.27657800
H	-0.87056300	6.72398300	2.01074100	H	5.79871800	-2.35856600	-0.24706800
H	-1.14221300	8.15919400	1.00030500	H	3.46277100	0.69866200	-2.14248400
H	0.36056400	6.73223700	-2.13658700	H	1.41251500	-0.58084700	-1.69227400
H	-0.42262300	8.16262300	-1.43303400	H	5.25971400	-0.30351800	3.55340100
H	-1.36310600	6.69306400	-1.73470300	H	7.34719700	-1.26926100	4.47138900
H	2.11004800	6.90939900	-0.28908200	H	9.41381300	-1.18701400	3.08664900
H	1.60693400	6.90400900	1.41484200	H	10.56127700	-0.50305400	1.12963200
H	1.23035500	8.28986100	0.38147800	H	10.56118600	0.50322100	-1.13027200
H	-2.04543400	-4.85825300	0.60036300	H	9.41355800	1.18717500	-3.08720300
H	2.06865400	-4.85109000	-0.62180800	H	7.34682800	1.26938100	-4.47178200
H	0.01013700	-1.15430800	-0.00100800	H	5.25944200	0.30359100	-3.55363400

TS-3c_{rac} (M06-2X/6-31G(d))

C	-7.69598900	0.39676600	-0.61862900	C	-2.39414800	1.68387000	0.42974800
C	-6.60739500	1.23954800	-0.17904600	C	-3.28357300	1.55646100	1.50167100
C	-6.86944100	2.55737800	0.21959000	C	-4.61412700	1.23557600	1.28085500
C	-8.13349800	3.13430900	0.26668200	C	-5.16058200	-1.81056400	-0.78625300
C	-9.18816200	2.35508100	-0.11548500	C	-4.13953700	-1.99738200	-1.72581200
C	-8.98795300	1.03451200	-0.56071400	C	-2.82843200	-2.19729900	-1.33130400
C	-10.19507300	0.38857500	-0.98257400	C	-2.48377400	-2.20600100	0.02534600
C	-10.16303100	-0.83961000	-1.51405300	C	-3.49907000	-1.98270300	0.96244200
C	-8.92406200	-1.54740200	-1.62117100	C	-4.82048000	-1.80854600	0.56507100
C	-9.03988600	-2.81419700	-2.22597300	C	-1.07131800	2.34208900	0.65559200
C	-7.95052500	-3.62617300	-2.37975800	C	0.15664500	1.68951000	0.58587900
C	-6.73792400	-3.16290900	-1.88028700	C	1.34643300	2.40340300	0.80561000
C	-6.56974400	-1.91740400	-1.26731600	C	1.27826300	3.76847500	1.08364700
C	-7.67805100	-1.00941400	-1.14105900	C	0.05969400	4.44920100	1.16590400
C	-5.11740200	1.04851400	-0.01573400	C	-1.10388900	3.71320000	0.95314400
C	-4.21010400	1.08389200	-1.07395900	C	0.04955000	5.94551500	1.49080700
C	-2.86313600	1.37957800	-0.85095500	C	0.70141700	6.17197600	2.86528100

C	-1.37031700	6.51905500	1.53099200	H	-8.02390200	-4.60369900	-2.84471900
C	0.84713700	6.70400200	0.41674000	H	-5.87189500	-3.81315600	-1.93277200
C	-1.08852100	-2.49408900	0.43613100	H	-4.56735400	0.94391000	-2.09055700
C	-0.81765700	-3.16736600	1.63603400	H	-2.18731400	1.46545800	-1.69802700
C	0.48583000	-3.47641400	2.02099800	H	-2.93580300	1.76922600	2.50897700
C	1.52919600	-3.10424400	1.16581200	H	-5.30499600	1.20401100	2.11942700
C	1.29552900	-2.44008500	-0.04055400	H	-4.39487600	-2.01970400	-2.78179000
C	-0.02369300	-2.13585700	-0.38924300	H	-2.07036500	-2.39556200	-2.08271300
C	0.81527400	-4.18354900	3.33894800	H	-3.25371500	-1.94544300	2.01998400
C	1.57506000	-5.48793000	3.04564500	H	-5.59783000	-1.66803300	1.31172800
C	-0.44285500	-4.52956200	4.14151900	H	0.19165700	0.62286400	0.37094600
C	1.69658800	-3.25958300	4.19729400	H	2.20734700	4.30033200	1.27410800
C	2.66693300	1.72786700	0.76665100	H	-2.07559000	4.19341900	1.00133800
C	2.83291200	0.45996600	1.32884000	H	0.15081800	5.63901900	3.64724600
C	4.05767700	-0.18820200	1.26210900	H	1.73757300	5.82102700	2.88364400
C	5.16010400	0.39866200	0.63033400	H	0.70272400	7.23991200	3.11112300
C	5.00591600	1.68510300	0.10023900	H	-1.87814300	6.40584000	0.56745100
C	3.77903100	2.33512400	0.16731700	H	-1.32636600	7.58801600	1.76340600
C	2.43435300	-1.96356200	-0.86059800	H	-1.97881400	6.03381800	2.30133200
C	3.66848100	-2.62529500	-0.86909900	H	0.40195200	6.55659500	-0.57259600
C	4.79746700	-2.02558600	-1.41423300	H	1.88703400	6.36599700	0.37317500
C	4.71949700	-0.74598300	-1.97301900	H	0.85121500	7.77752100	0.63670900
C	3.46368600	-0.14044500	-2.07376800	H	-1.65348600	-3.47052800	2.25643400
C	2.34097300	-0.73648900	-1.52541200	H	2.55698500	-3.30419200	1.45765300
C	6.48028000	-0.29308000	0.65096800	H	-0.22160400	-1.60432200	-1.31544300
C	6.83892600	-0.82208000	1.88724500	H	0.96704200	-6.16087500	2.43246200
C	8.11306000	-1.33458900	2.14999600	H	2.51157400	-5.29898700	2.51215300
C	9.08067800	-1.21634800	1.18305600	H	1.81956600	-6.00125500	3.98232100
C	8.76743300	-0.67745300	-0.08055400	H	-1.10230300	-5.20447800	3.58582900
C	9.85277200	-0.40570300	-0.98263900	H	-1.01078300	-3.63183600	4.40764400
C	9.63131400	0.22496700	-2.15318300	H	-0.15673500	-5.03165600	5.07128600
C	8.29008900	0.44022900	-2.62056200	H	1.17677200	-2.32062600	4.41456200
C	8.11522100	0.96366400	-3.91712700	H	1.94132100	-3.74636400	5.14804600
C	6.86614000	1.02400100	-4.48600500	H	2.63704900	-3.01534800	3.69317300
C	5.78614100	0.47437100	-3.78848400	H	1.99057800	-0.03284600	1.80957300
C	5.91389000	-0.04067200	-2.50323500	H	4.15226500	-1.18899100	1.67499600
C	7.17394600	0.03883400	-1.83027300	H	5.85140600	2.17074300	-0.37949200
C	7.43024100	-0.32095200	-0.42296400	H	3.67067500	3.32022600	-0.27912200
H	-6.01985100	3.16663700	0.50532800	H	3.75220600	-3.60961700	-0.41635900
H	-8.26316500	4.16140400	0.59128100	H	5.75574900	-2.53624000	-1.37763000
H	-10.20333000	2.74077600	-0.10464200	H	3.38599100	0.85467800	-2.50186700
H	-11.12662800	0.93796600	-0.88612400	H	1.40390000	-0.18706000	-1.52402000
H	-11.06543600	-1.32817200	-1.86890800	H	6.11697300	-0.76991900	2.69580100
H	-10.02327400	-3.12726800	-2.56441900	H	8.34577200	-1.74429300	3.12763800

H	10.10878000	-1.50604800	1.38230900	H	8.99464700	1.28884200	-4.46630100
H	10.85953200	-0.65531200	-0.65937600	H	6.72597300	1.42226800	-5.48573500
H	10.45300100	0.51232800	-2.80323000	H	4.82289500	0.38767900	-4.28185000

3d (B3LYP/6-31G(d))

C	-0.19813200	-6.00963500	-1.58573300	C	-0.31835000	8.39051100	-1.37846600
C	0.10323000	-6.11017800	-2.94587900	C	-0.61833200	8.44023900	-2.75742400
C	0.56309500	-7.29862300	-3.52809900	C	-0.56306200	7.29864100	-3.52810700
C	0.61835600	-8.44022400	-2.75741900	C	-0.10319600	6.11019700	-2.94588700
C	0.31836200	-8.39050000	-1.37846400	C	0.19815600	6.00965000	-1.58574000
C	0.20333700	-9.61948400	-0.64639700	C	-0.03961600	7.14066100	-0.73393500
C	-0.20585900	-9.61944100	0.64638900	C	0.04147800	7.14066500	0.73397200
C	-0.32055400	-8.39044100	1.37848000	C	0.92171300	4.77248600	-1.17459500
C	-0.62054900	-8.44010900	2.75743600	C	2.11223400	4.83662500	-0.43124500
C	-0.56497300	-7.29853800	3.52813800	C	2.84917400	3.68850700	-0.15273500
C	-0.10479400	-6.11020600	2.94593600	C	2.43131400	2.42689900	-0.60822200
C	0.19658000	-6.00971800	1.58578900	C	1.25247000	2.36771900	-1.36886500
C	-0.04148800	-7.14065500	0.73397000	C	0.51625100	3.51362600	-1.64594500
C	0.03962500	-7.14065100	-0.73393300	C	3.19175600	1.19203100	-0.28875600
C	-0.92168400	-4.77247200	-1.17457700	C	4.59454300	1.17802900	-0.29045900
C	-2.11220800	-4.83661700	-0.43123200	C	5.28905000	-0.00070500	0.00002100
C	-2.84915100	-3.68850300	-0.15271600	C	4.59423100	-1.17925500	0.29049800
C	-2.43129100	-2.42689000	-0.60819000	C	3.19144000	-1.19288700	0.28879100
C	-1.25243900	-2.36770200	-1.36882000	C	2.51249700	-0.00033900	0.00001700
C	-0.51621700	-3.51360500	-1.64590600	C	2.43066900	-2.42755300	0.60825700
C	-3.19174400	-1.19202900	-0.28872600	C	2.84818600	-3.68927000	0.15275600
C	-4.59453100	-1.17803600	-0.29044600	C	2.11094600	-4.83719200	0.43127300
C	-5.28905000	0.00069200	0.00002700	C	0.92045400	-4.77274100	1.17464400
C	-4.59424300	1.17924800	0.29051200	C	0.51532900	-3.51377400	1.64599900
C	-3.19145200	1.19289000	0.28882100	C	1.25185000	-2.36806200	1.36891400
C	-2.51249600	0.00034500	0.00005600	N	-6.71091400	0.00087100	0.00001400
C	-2.43069200	2.42756200	0.60829000	C	-7.53000300	-0.83224600	0.77073100
C	-1.25188100	2.36808000	1.36895900	C	-8.88751400	-0.52976300	0.49222400
C	-0.51536400	3.51379500	1.64603800	C	-8.88737000	0.53190000	-0.49240500
C	-0.92048300	4.77275600	1.17466200	C	-7.52977800	0.83413100	-0.77079000
C	-2.11097200	4.83720000	0.43128600	C	-9.90015900	1.23217000	-1.15829900
C	-2.84820900	3.68927400	0.15277500	C	-9.55247500	2.20837800	-2.08737600
C	-0.19660500	6.00973400	1.58579600	C	-8.20193000	2.48521700	-2.36143900
C	0.10475900	6.11022600	2.94594500	C	-7.17443500	1.80388200	-1.71247100
C	0.56493800	7.29855800	3.52814700	C	-7.17492600	-1.80206400	1.71244500
C	0.62052300	8.44012600	2.75744100	C	-8.20260600	-2.48320800	2.36131900
C	0.32054000	8.39045200	1.37848200	C	-9.55307500	-2.20611600	2.08713400
C	0.20585300	9.61945200	0.64639000	C	-9.90049400	-1.22984300	1.15802700
C	-0.20333400	9.61949400	-0.64639800	N	6.71091400	-0.00089500	0.00002500

C	7.53000100	0.83222700	0.77074000	H	0.86470100	9.40131700	3.20292900
C	8.88751300	0.52973900	0.49224100	H	0.38310900	10.55166000	1.17675500
C	8.88737200	-0.53193000	-0.49238100	H	-0.38034500	10.55173900	-1.17678000
C	7.52978100	-0.83415900	-0.77077200	H	-0.86225800	9.40148700	-3.20292700
C	7.17492100	1.80205000	1.71244600	H	-0.79161300	7.33177800	-4.58965800
C	8.20260000	2.48319600	2.36132200	H	0.09677600	5.25519200	-3.58422800
C	9.55306900	2.20610000	2.08714500	H	2.46680000	5.79744100	-0.07138300
C	9.90049100	1.22982000	1.15804600	H	3.75572200	3.77113600	0.44108400
C	9.90016400	-1.23220500	-1.15826600	H	0.91623500	1.41260900	-1.76251200
C	9.55248200	-2.20841700	-2.08733900	H	-0.40271000	3.42961600	-2.21808200
C	8.20193800	-2.48525500	-2.36140900	H	5.15183800	2.07038900	-0.55598300
C	7.17444100	-1.80391500	-1.71244900	H	5.15128900	-2.07176300	0.55602600
H	-0.09673200	-5.25517000	-3.58421800	H	1.42735500	-0.00019500	0.00001900
H	0.79165500	-7.33175700	-4.58964800	H	3.75470500	-3.77213600	-0.44107400
H	0.86228200	-9.40147100	-3.20292400	H	2.46524900	-5.79810100	0.07140100
H	0.38035300	-10.55172800	-1.17677700	H	-0.40360300	-3.42952400	2.21814800
H	-0.38311900	-10.55164900	1.17675300	H	0.91587500	-1.41286300	1.76256900
H	-0.86472800	-9.40129900	3.20292600	H	-10.94495100	1.01213700	-0.95456800
H	-0.79353300	-7.33163000	4.58968800	H	-10.32982000	2.75915600	-2.60930200
H	0.09540300	-5.25526200	3.58428900	H	-7.95029800	3.24455200	-3.09700600
H	-2.46677700	-5.79743700	-0.07138400	H	-6.13411200	2.01535900	-1.93689900
H	-3.75570400	-3.77113900	0.44109300	H	-6.13466200	-2.01373400	1.93696700
H	-0.91620200	-1.41258700	-1.76245700	H	-7.95118300	-3.24259100	3.09690800
H	0.40274800	-3.42958900	-2.21803700	H	-10.33057000	-2.75674800	2.60899100
H	-5.15181700	-2.07040000	-0.55597800	H	-10.94522500	-1.00961300	0.95420300
H	-5.15131100	2.07175200	0.55603200	H	6.13465700	2.01372400	1.93696300
H	-1.42735500	0.00021000	0.00006900	H	7.95117400	3.24258300	3.09690600
H	-0.91590700	1.41288500	1.76262500	H	10.33056300	2.75673300	2.60900300
H	0.40356500	3.42955200	2.21819400	H	10.94522300	1.00958700	0.95422900
H	-2.46527200	5.79810500	0.07140000	H	10.94495400	-1.01217200	-0.95453000
H	-3.75472200	3.77213300	-0.44106400	H	10.32983000	-2.75919900	-2.60925800
H	-0.09544700	5.25528600	3.58429900	H	7.95030900	-3.24459300	-3.09697300
H	0.79348800	7.33165400	4.58969900	H	6.13412000	-2.01539100	-1.93688300

3e (B3LYP/6-31G(d))

C	7.26380500	0.11119400	1.59627900	C	8.55869900	0.74646800	-3.49583100
C	7.36890800	-0.25966300	2.93924800	C	7.36905800	0.25955800	-2.93943500
C	8.55854400	-0.74655200	3.49567000	C	7.26389300	-0.11116500	-1.59643400
C	9.69842600	-0.76090200	2.72100900	C	8.39419500	0.07921400	-0.73123100
C	9.64527000	-0.38995400	1.35967500	C	8.39416200	-0.07907400	0.73111800
C	10.87424100	-0.23728700	0.63491400	C	6.01836000	0.84382200	1.22858700
C	10.87426400	0.23749600	-0.63491900	C	6.06151500	2.06960500	0.54375900
C	9.64532400	0.39009700	-1.35974500	C	4.90253000	2.80758300	0.31504900
C	9.69853500	0.76095100	-2.72110400	C	3.64940800	2.35781700	0.76569200

C	3.61359300	1.14291100	1.47060900	C	-7.26380700	-0.11122800	1.59628200
C	4.76836700	0.40387700	1.69360700	C	-8.39416200	0.07905900	0.73112000
C	2.40121100	3.11409700	0.49899000	C	-8.39419400	-0.07919900	-0.73123300
C	2.38560300	4.54087200	0.48864700	C	-6.01836300	-0.84385400	1.22858600
C	1.22547800	5.24038000	0.24861200	C	-6.06151500	-2.06962700	0.54373900
C	-0.00010000	4.56728300	0.00013000	C	-4.90252900	-2.80760200	0.31502400
C	-0.00009400	3.13674400	0.00009700	C	-3.64940900	-2.35784300	0.76568000
C	1.21242800	2.44727800	0.25164400	C	-3.61359700	-1.14294900	1.47061800
C	0.00009700	-3.13674400	0.00007700	C	-4.76837200	-0.40391900	1.69362200
C	0.00010800	-4.56728300	0.00008600	C	-2.40120800	-3.11411500	0.49896900
C	1.22569000	-5.24037900	-0.24838100	H	6.51444400	-0.09558400	3.58824900
C	2.38580500	-4.54086700	-0.48845800	H	8.59347900	-1.02927500	4.54408800
C	2.40139000	-3.11409400	-0.49885000	H	10.66110700	-1.02640000	3.15090800
C	1.21261100	-2.44727300	-0.25150200	H	11.80634300	-0.44129200	1.15586600
C	3.64956800	-2.35780500	-0.76563000	H	11.80638500	0.44151000	-1.15583300
C	4.90268600	-2.80743400	-0.31484700	H	10.66122900	1.02645200	-3.15097300
C	6.06164700	-2.06944500	-0.54364700	H	8.59368100	1.02909900	-4.54427200
C	6.01845700	-0.84378900	-1.22869900	H	6.51463400	0.09538600	-3.58846700
C	4.76846400	-0.40397400	-1.69384000	H	7.01425000	2.45116200	0.18965100
C	3.61371600	-1.14302700	-1.47076200	H	4.97107900	3.74027600	-0.23854200
C	-1.21261100	2.44728200	-0.25149400	H	2.66834400	0.77908000	1.86272300
C	-2.38579700	4.54088400	-0.48841300	H	4.69888500	-0.54278200	2.22071100
C	-1.22568000	5.24038800	-0.24832600	H	3.30374900	5.08007900	0.70346200
C	-1.22546800	-5.24038900	0.24855600	H	1.23422100	6.32799900	0.25759400
C	-2.38559600	-4.54089000	0.48860100	H	1.20068100	1.36074500	0.22101300
C	-1.21242800	-2.44728700	0.25163500	H	1.23444000	-6.32799900	-0.25732800
C	-2.40138800	3.11411200	-0.49882900	H	3.30395900	-5.08006200	-0.70326500
C	-3.64956800	2.35783100	-0.76561900	H	1.20086400	-1.36073800	-0.22092400
C	-3.61372000	1.14306500	-1.47077200	H	4.97124600	-3.74003000	0.23890800
C	-4.76847000	0.40401500	-1.69385500	H	7.01438800	-2.45088100	-0.18941900
C	-6.01846000	0.84382200	-1.22869800	H	4.69896300	0.54259100	-2.22110900
C	-6.06164600	2.06946800	-0.54362800	H	2.66845800	-0.77931000	-1.86296000
C	-4.90268500	2.80745400	-0.31482300	H	-1.20086900	1.36074600	-0.22093400
C	-7.26389600	0.11119900	-1.59643700	H	-3.30395000	5.08008700	-0.70321000
C	-7.36906200	-0.25950100	-2.93944400	H	-1.23442500	6.32800800	-0.25725400
C	-8.55870300	-0.74640500	-3.49584500	H	-1.23420700	-6.32800900	0.25751900
C	-9.69853800	-0.76090200	-2.72111700	H	-3.30374000	-5.08010300	0.70340700
C	-9.64532400	-0.39007200	-1.35975200	H	-1.20068600	-1.36075300	0.22102200
C	-10.87426400	-0.23748500	-0.63492300	H	-2.66846400	0.77935500	-1.86298100
C	-10.87424100	0.23727600	0.63491800	H	-4.69897100	-0.54254100	-2.22114000
C	-9.64527000	0.38992900	1.35968200	H	-7.01438600	2.45089700	-0.18938800
C	-9.69842800	0.76085400	2.72102200	H	-4.97124100	3.74004000	0.23894800
C	-8.55854800	0.74648800	3.49568600	H	-6.51464100	-0.09531600	-3.58847400
C	-7.36891300	0.25960500	2.93925600	H	-8.59368600	-1.02901800	-4.54429100

H	-10.66123200	-1.02639700	-3.15098900	H	-6.51445000	0.09551300	3.58825700
H	-11.80638500	-0.44149000	-1.15584000	H	-7.01424800	-2.45117900	0.18962000
H	-11.80634300	0.44127300	1.15587400	H	-4.97107400	-3.74028600	-0.23858300
H	-10.66110900	1.02634500	3.15092400	H	-2.66835100	-0.77912500	1.86274200
H	-8.59348500	1.02919300	4.54410800	H	-4.69889300	0.54273200	2.22074100

3e (M06-2X/6-31G(d))

C	7.26902000	-0.06386300	1.58845800	C	3.60862900	-0.88221600	-1.43562900
C	7.36734000	-0.55145500	2.88615300	C	-1.21045100	2.20377100	-0.26061500
C	8.55924400	-1.07615700	3.39959900	C	-2.36719700	4.29707900	-0.53541400
C	9.69675400	-1.01191800	2.63134800	C	-1.21573200	4.99211400	-0.27699100
C	9.64276500	-0.51870000	1.31197200	C	-1.21529800	-4.99207800	0.27562800
C	10.87558600	-0.29614100	0.60718200	C	-2.36668300	-4.29698000	0.53422600
C	10.87582800	0.29677400	-0.60500500	C	-1.20975700	-2.20374400	0.25977300
C	9.64330800	0.51911300	-1.31039000	C	-2.38527400	2.87218700	-0.52760700
C	9.69785000	1.01227600	-2.62976300	C	-3.63856400	2.12838800	-0.79822200
C	8.56070000	1.07629300	-3.39856700	C	-3.60865600	0.88223000	-1.43566600
C	7.36862900	0.55143800	-2.88566600	C	-4.77538300	0.16678400	-1.65997900
C	7.26976700	0.06389700	-1.58799500	C	-6.01822000	0.67198300	-1.26362400
C	8.40183000	0.15547100	-0.71780500	C	-6.05563100	1.92902000	-0.65019800
C	8.40151400	-0.15523400	0.71880700	C	-4.88541100	2.63960900	-0.41569000
C	6.01750700	0.67187100	1.26354300	C	-7.26980000	-0.06386300	-1.58802200
C	6.05503800	1.92898200	0.65027500	C	-7.36869400	-0.55135200	-2.88571000
C	4.88485600	2.63951700	0.41542700	C	-8.56077800	-1.07618600	-3.39860300
C	3.63789000	2.12819200	0.79744800	C	-9.69791100	-1.01218900	-2.62977200
C	3.60785200	0.88192300	1.43467500	C	-9.64333900	-0.51906400	-1.31038500
C	4.77454400	0.16652400	1.65931900	C	-10.87584300	-0.29672200	-0.60497400
C	2.38466200	2.87203300	0.52663300	C	-10.87557100	0.29618400	0.60721800
C	2.36669900	4.29693400	0.53418000	C	-9.64273500	0.51872700	1.31198500
C	1.21530800	4.99203500	0.27561600	C	-9.69669600	1.01195700	2.63135800
C	-0.00024700	4.31403600	-0.00063300	C	-8.55917200	1.07620100	3.39958600
C	-0.00030900	2.89324100	-0.00050200	C	-7.36728100	0.55148800	2.88612400
C	1.20976300	2.20370100	0.25974700	C	-7.26898700	0.06387200	1.58843700
C	0.00031100	-2.89328100	-0.00050100	C	-8.40149700	0.15524200	0.71880100
C	0.00024900	-4.31407600	-0.00065000	C	-8.40184500	-0.15545300	-0.71781300
C	1.21572600	-4.99215100	-0.27705400	C	-6.01748400	-0.67188500	1.26353500
C	2.36718400	-4.29711300	-0.53550000	C	-6.05502400	-1.92902700	0.65032800
C	2.38526500	-2.87222100	-0.52765700	C	-4.88484600	-2.63957400	0.41549900
C	1.21044900	-2.20380800	-0.26062400	C	-3.63787600	-2.12823800	0.79749300
C	3.63855000	-2.12841600	-0.79827000	C	-3.60783000	-0.88194800	1.43467600
C	4.88540600	-2.63966800	-0.41580600	C	-4.77451800	-0.16653100	1.65929100
C	6.05562000	-1.92906500	-0.65029500	C	-2.38464900	-2.87207900	0.52667600
C	6.01819700	-0.67197700	-1.26361900	H	6.50563000	-0.45613500	3.53952400
C	4.77535100	-0.16675000	-1.65991200	H	8.59453800	-1.45329100	4.41660700

H	10.66020700	-1.31199100	3.03438800	H	-3.27939200	4.83416300	-0.77706600
H	11.80515800	-0.54863600	1.10980200	H	-1.21656800	6.07897900	-0.29287300
H	11.80559900	0.54942400	-1.10717900	H	-1.21624900	-6.07894600	0.29130800
H	10.66144900	1.31248600	-3.03235300	H	-3.27889700	-4.83405000	0.77583000
H	8.59642700	1.45337500	-4.41557900	H	-1.20075800	-1.11695000	0.22443800
H	6.50723500	0.45596300	-3.53943400	H	-2.66011500	0.46968800	-1.76830900
H	7.01045700	2.34719600	0.34662900	H	-4.72152800	-0.81419200	-2.12360300
H	4.93970500	3.59897900	-0.09128900	H	-7.01097200	2.34709800	-0.34612000
H	2.65924500	0.46925500	1.76696700	H	-4.94010400	3.59901700	0.09114900
H	4.72056400	-0.81452600	2.12277300	H	-6.50731100	-0.45586400	-3.53949100
H	3.27891600	4.83400300	0.77577300	H	-8.59653000	-1.45323400	-4.41562700
H	1.21625900	6.07890300	0.29130900	H	-10.66152100	-1.31237500	-3.03235300
H	1.20076000	1.11690800	0.22440700	H	-11.80562700	-0.54934700	-1.10713700
H	1.21656100	-6.07901500	-0.29295200	H	-11.80513100	0.54869300	1.10985400
H	3.27937400	-4.83419300	-0.77718300	H	-10.66014000	1.31204400	3.03441100
H	1.20161400	-1.11701800	-0.22508200	H	-8.59444400	1.45334800	4.41659000
H	4.94010800	-3.59911200	0.09096400	H	-6.50555900	0.45617000	3.53948000
H	7.01096800	-2.34717100	-0.34627500	H	-7.01044600	-2.34725100	0.34670600
H	4.72148400	0.81425900	-2.12346300	H	-4.93970000	-3.59905400	-0.09118200
H	2.66007900	-0.46964900	-1.76821700	H	-2.65921700	-0.46926700	1.76693800
H	-1.20161200	1.11698100	-0.22509000	H	-4.72053100	0.81454000	2.12269700

(P,M)-3e (M06-2X/6-31G(d))

C	-3.71346700	2.19811200	0.48451800	C	-6.13074800	-2.00012400	-0.30315000
C	-3.72151800	1.07090500	1.31594000	C	-4.94219100	-2.64559100	0.01864300
C	-4.90360000	0.41789900	1.62516200	C	-3.71348200	-2.19809300	-0.48448300
C	-6.13026200	0.86994700	1.12765500	C	-3.72152900	-1.07096100	-1.31600800
C	-6.13073500	2.00017000	0.30317100	C	-4.90360800	-0.41797500	-1.62528300
C	-4.94217600	2.64566100	-0.01856400	C	-2.44037900	-2.90419100	-0.19943300
C	-7.39524900	0.22514000	1.57301600	C	-2.44036400	2.90423900	0.19953700
C	-7.49867700	-0.00803200	2.93994900	C	-1.23725000	-2.23119900	-0.20887100
C	-8.69305700	-0.41904800	3.54213500	C	-0.00000500	-2.90962500	-0.07787800
C	-9.82903400	-0.49705800	2.77320000	C	-0.00000900	-4.31556500	0.12473300
C	-9.771108400	-0.26171400	1.38494800	C	-1.24649300	-4.98968900	0.19470100
C	-11.00376400	-0.17554800	0.65127500	C	-2.42433500	-4.31168700	0.02462500
C	-11.00376400	0.17554200	-0.65138700	C	-2.42432400	4.31175600	-0.02438700
C	-9.77108500	0.26169300	-1.38506400	C	-1.24648400	4.98977900	-0.19439300
C	-9.82903600	0.49700300	-2.77332200	C	0.00000200	4.31565300	-0.12448200
C	-8.69306200	0.41895200	-3.54225900	C	0.00001100	2.90969300	0.07799300
C	-7.49868600	0.00793700	-2.94006500	C	-1.23723200	2.23125000	0.20891600
C	-7.39525500	-0.22518700	-1.57312400	C	1.23724000	-2.23120100	-0.20889400
C	-8.52807100	0.01948300	-0.73468000	C	2.44036300	-2.90420400	-0.19947200
C	-8.52807000	-0.01949700	0.73456700	C	2.42431200	-4.31169800	0.02459700
C	-6.13027000	-0.86997400	-1.12773100	C	1.24647100	-4.98969600	0.19469500

C	1.24647900	4.98979800	-0.19437100	H	-11.93327100	-0.32741100	1.19291500
C	2.42432300	4.31178900	-0.02433100	H	-11.93327100	0.32740100	-1.19302800
C	2.44037800	2.90427400	0.19960100	H	-10.79433600	0.71223400	-3.22341600
C	1.23725900	2.23126300	0.20895000	H	-8.73068000	0.59639500	-4.61223500
C	7.39524100	-0.22519600	-1.57313200	H	-6.63682100	-0.20320700	-3.56526600
C	7.49866900	0.00791500	-2.94007600	H	-7.07163000	-2.37416700	0.09067300
C	8.69304400	0.41892500	-3.54227500	H	-4.97223800	-3.50805300	0.67854100
C	9.82902000	0.49697700	-2.77333900	H	-2.79222600	-0.71089600	-1.74715000
C	9.77107100	0.26167600	-1.38508100	H	-4.87694500	0.47018800	-2.24995600
C	11.00375600	0.17551100	-0.65141300	H	-1.21724600	-1.15353600	-0.35275500
C	11.00376200	-0.17557800	0.65124900	H	-1.25153200	-6.06619900	0.34511400
C	9.77108500	-0.26173300	1.38493200	H	-3.36200400	-4.85862300	0.01811100
C	9.82905000	-0.49706600	2.77318400	H	-3.36199600	4.85868800	-0.01782600
C	8.69308400	-0.41903100	3.54213400	H	-1.25152700	6.06630300	-0.34470200
C	7.49870400	-0.00800200	2.93995900	H	-1.21722400	1.15357300	0.35269600
C	7.39526100	0.22515500	1.57302400	H	1.21723700	-1.15354400	-0.35279600
C	8.52806800	-0.01950600	0.73456100	H	3.36197700	-4.85864400	0.01806800
C	8.52805800	0.01947700	-0.73469000	H	1.25151900	-6.06620500	0.34511600
C	6.13025700	-0.86998800	-1.12774600	H	1.25152200	6.06632100	-0.34468800
C	6.13073100	-2.00011600	-0.30313300	H	3.36198500	4.85873800	-0.01774300
C	4.94217800	-2.64559600	0.01865100	H	1.21726200	1.15359200	0.35274800
C	3.71347400	-2.19811600	-0.48450600	H	6.63680600	-0.20324000	-3.56527500
C	3.72152300	-1.07099600	-1.31604100	H	8.73066200	0.59635600	-4.61225200
C	4.90360100	-0.41800600	-1.62532000	H	10.79432000	0.71220100	-3.22343800
C	3.71349100	2.19816500	0.48457400	H	11.93325900	0.32736300	-1.19306100
C	4.94219300	2.64569200	-0.01854700	H	11.93327100	-0.32745300	1.19288200
C	6.13074700	2.00018300	0.30317400	H	10.79435300	-0.71231200	3.22326500
C	6.13027700	0.86998100	1.12768700	H	8.73071200	-0.59649100	4.61210600
C	4.90362400	0.41795800	1.62522900	H	6.63684900	0.20314300	3.56517500
C	3.72154400	1.07097300	1.31601100	H	7.07161200	-2.37412500	0.09073200
H	-2.79221600	0.71079600	1.74704800	H	4.97223100	-3.50803100	0.67858200
H	-4.87694000	-0.47031900	2.24975800	H	2.79221500	-0.71092600	-1.74716900
H	-7.07161600	2.37425800	-0.09061100	H	4.87693200	0.47015800	-2.24999100
H	-4.97222100	3.50818300	-0.67838400	H	4.97224300	3.50818700	-0.67840000
H	-6.63681000	0.20308500	3.56515400	H	7.07162600	2.37423100	-0.09065700
H	-8.73067200	-0.59652400	4.61210600	H	4.87695800	-0.47026000	2.24982500
H	-10.79433500	-0.71229400	3.22329100	H	2.79223700	0.71086600	1.74711000

TS-3e_{rac} (M06-2X/6-31G(d))

C	-7.18564500	-0.25584300	2.18854400	C	-10.91102000	-0.03830100	1.88924800
C	-7.06259900	0.09665900	3.52841300	C	-11.12652200	-0.52165900	0.64968400
C	-8.15050800	0.52747600	4.29352000	C	-10.04146200	-0.65291400	-0.28344900
C	-9.40130000	0.50891700	3.72574800	C	-10.35154200	-1.03480400	-1.60364900
C	-9.57183300	0.14791100	2.37448000	C	-9.38824600	-1.00865600	-2.58172300

C	-8.12335900	-0.50686700	-2.26099300	C	10.19087600	-2.90449900	1.63978600
C	-7.76777400	-0.13053000	-0.96894800	C	10.06629200	-1.54512800	1.29217000
C	-8.70997500	-0.31229000	0.09607600	C	11.28635200	-0.80476500	1.39499200
C	-8.45187200	-0.12461000	1.53582900	C	11.30817000	0.50310600	1.11022300
C	-5.97387900	-0.85959500	1.57648500	C	10.10562600	1.19380000	0.75053100
C	-6.01449200	-2.06348800	0.86607300	C	10.29007300	2.57778100	0.56893800
C	-4.86452100	-2.56916000	0.26981600	C	9.23421500	3.39459800	0.27987500
C	-3.64453500	-1.88871500	0.36669400	C	7.98539600	2.79631000	0.15523700
C	-3.59185600	-0.73996100	1.16380600	C	7.74084700	1.42313300	0.29133800
C	-4.73493700	-0.23769400	1.75999700	C	8.83114500	0.53248600	0.61881800
C	-2.47063500	-2.24878600	-0.46086900	C	8.82993100	-0.94845900	0.85888100
C	-2.66103000	-2.76534300	-1.77565000	C	6.26421400	1.23797000	0.03098500
C	-1.59814500	-2.98954800	-2.61048300	C	5.80446500	1.65995100	-1.22662100
C	-0.27201000	-2.71203500	-2.19091500	C	4.47330800	1.97935400	-1.44034400
C	-0.06614200	-2.21015700	-0.87709000	C	3.53727400	1.86708600	-0.40576000
C	-1.18483600	-1.99184500	-0.03559700	C	3.96852900	1.33794800	0.81326900
C	-0.23191100	2.57481100	-0.68389000	C	5.31661600	1.04518300	1.03515500
C	-0.19577300	3.99140400	-0.81229200	C	2.20281300	2.51559100	-0.56326100
C	-1.41528200	4.70787700	-0.91883800	H	-6.09469000	-0.02741900	4.00418300
C	-2.61590200	4.05304800	-0.91502600	H	-8.01314700	0.80028200	5.33485500
C	-2.67255600	2.63438100	-0.82095700	H	-10.28464300	0.74145700	4.31422400
C	-1.49409100	1.92319200	-0.70589400	H	-11.73437200	0.14623800	2.57359700
C	-3.98697300	1.95018600	-0.86225500	H	-12.12964200	-0.75149900	0.30148100
C	-5.10544000	2.47093900	-0.19710300	H	-11.37455800	-1.31959100	-1.83376300
C	-6.32182600	1.79699100	-0.19727500	H	-9.61891700	-1.29626500	-3.60242100
C	-6.45916500	0.57607700	-0.86792800	H	-7.40731200	-0.33883300	-3.05892100
C	-5.35133000	0.08034000	-1.56483700	H	-6.95962500	-2.58769000	0.75493900
C	-4.13762600	0.75041700	-1.56279200	H	-4.92079200	-3.49383100	-0.29844400
C	1.25444700	-1.93856900	-0.44178200	H	-2.66773200	-0.17368900	1.23750600
C	2.12239400	-2.64771100	-2.57457100	H	-4.68689100	0.70266700	2.30112800
C	0.85725700	-2.91429900	-3.02570100	H	-3.67234900	-2.94953900	-2.12664000
C	1.06023000	4.64729000	-0.84091300	H	-1.76082000	-3.36934400	-3.61586600
C	2.21992100	3.93177900	-0.73153000	H	-1.00833000	-1.61987800	0.97120500
C	0.99320300	1.85974600	-0.54317000	H	-1.37757000	5.78974300	-1.01756900
C	2.34448400	-2.15633500	-1.25604600	H	-3.54254000	4.60909800	-1.02403700
C	3.72037600	-1.94967600	-0.75006200	H	-1.52052300	0.83685600	-0.62529600
C	4.76969900	-1.56016100	-1.58951300	H	-5.01243000	3.40280800	0.35464700
C	6.07172200	-1.45702200	-1.11068300	H	-7.17242200	2.21270700	0.33615300
C	6.35594500	-1.70953000	0.22976600	H	-5.43591500	-0.86720600	-2.08949900
C	5.30225600	-2.07899700	1.07448000	H	-3.29098900	0.33225500	-2.10221300
C	4.01018000	-2.20084000	0.59639100	H	1.39573000	-1.53781700	0.55974100
C	7.74561600	-1.88604500	0.74468700	H	2.97738600	-2.84587700	-3.21371400
C	7.92103600	-3.22518300	1.10582400	H	0.70326100	-3.30271300	-4.02911500
C	9.12166300	-3.75387700	1.56791600	H	1.08545200	5.72859400	-0.94956300

H	3.18122800	4.43713700	-0.74718000	H	12.18387100	-1.33416900	1.70018700
H	0.96085900	0.77613000	-0.44693800	H	12.22636200	1.07920900	1.17282800
H	4.56661500	-1.33111800	-2.63192400	H	11.29318800	2.97752400	0.68446800
H	6.87727000	-1.17536400	-1.78388000	H	9.35110400	4.46618200	0.15685600
H	5.51700500	-2.30172300	2.11610500	H	7.13375800	3.43297400	-0.05453800
H	3.22235300	-2.53962100	1.26224900	H	6.52708900	1.80725300	-2.02507600
H	7.07261300	-3.88931100	0.98360000	H	4.15664100	2.37019300	-2.40380800
H	9.20285700	-4.80290300	1.83262100	H	3.25854700	1.24224300	1.63082500
H	11.16522700	-3.25818900	1.96406300	H	5.63966800	0.72302700	2.02134400

3f (B3LYP/6-31G(d))

C	-0.18013800	-5.90195800	-1.58279000	C	-2.92635600	3.62640200	0.08959600
C	0.10918300	-5.99811700	-2.94593800	C	-0.26721600	5.89861500	1.57620200
C	0.57935700	-7.18004200	-3.53387800	C	0.02076700	5.99898500	2.93933000
C	0.65430100	-8.32312200	-2.76702400	C	0.47354600	7.18769300	3.52725300
C	0.36666000	-8.27872900	-1.38508900	C	0.53159700	8.33176800	2.76041500
C	0.26884700	-9.50846600	-0.65168400	C	0.24454400	8.28317300	1.37849800
C	-0.12857700	-9.51139500	0.64510600	C	0.12859400	9.51133500	0.64510100
C	-0.24450000	-8.28323300	1.37850600	C	-0.26886300	9.50840600	-0.65168000
C	-0.53151700	-8.33183700	2.76043000	C	-0.36670300	8.27866800	-1.38508100
C	-0.473444000	-7.18776900	3.52727500	C	-0.65438100	8.32305200	-2.76701000
C	-0.02066200	-5.99906300	2.93934800	C	-0.57946200	7.17996500	-3.53385700
C	0.26729400	-5.89868700	1.57621600	C	-0.10928800	5.99803700	-2.94592100
C	0.02085300	-7.03288900	0.73050400	C	0.18006000	5.90188400	-1.58277700
C	0.08296100	-7.03242000	-0.73708300	C	-0.08299300	7.03236100	-0.73708000
C	-0.93015700	-4.68443300	-1.16098800	C	-0.02082000	7.03283000	0.73050000
C	-2.07952000	-4.78199600	-0.35917600	C	0.93006900	4.68436100	-1.16095400
C	-2.87217900	-3.66894700	-0.09599000	C	2.07943300	4.78194300	-0.35914600
C	-2.57090100	-2.40829500	-0.64316600	C	2.87210300	3.66890500	-0.09594700
C	-1.41377500	-2.31092000	-1.43463300	C	2.57083300	2.40824300	-0.64310400
C	-0.61097100	-3.41955800	-1.68214000	C	1.41369500	2.31084400	-1.43455200
C	-3.39983000	-1.20803800	-0.35458200	C	0.61087900	3.41947100	-1.68206900
C	-4.81910600	-1.20961000	-0.42234900	C	3.39979200	1.20800600	-0.35452400
C	-5.53260900	-0.04097900	-0.00215000	C	4.81906700	1.20961500	-0.42231400
C	-4.83607800	1.13834200	0.41731400	C	5.53260800	0.04100300	-0.00212700
C	-3.41817400	1.15812800	0.34867100	C	4.83611700	-1.13833700	0.41734800
C	-2.74992700	-0.02043200	-0.00318900	C	3.41821200	-1.15815900	0.34872800
C	-5.57749700	-2.31958400	-0.93379200	C	2.74992700	0.02038300	-0.00311700
C	-5.61112900	2.23785700	0.92976900	C	5.57741800	2.31961000	-0.93376900
C	-2.60666500	2.37034300	0.63685900	C	5.61120700	-2.23782900	0.92979200
C	-1.44804500	2.28989900	1.42806400	C	2.60673400	-2.37039400	0.63692100
C	-0.66156200	3.41017200	1.67550200	C	2.92643200	-3.62644300	0.08963900
C	-0.99934300	4.67024800	1.15442300	C	2.15014100	-4.75101000	0.35272000
C	-2.15005400	4.75095800	0.35268900	C	0.99943200	-4.67031900	1.15445800

C	0.66165500	-3.41025700	1.67557300	H	-3.79601800	3.72306400	-0.55345700
C	1.44812600	-2.28997300	1.42814500	H	-0.18629700	5.14509200	3.57658500
C	-6.96392300	-0.05168000	-0.00205800	H	0.69219500	7.21898000	4.59098800
C	-7.70245000	1.07358100	0.47058100	H	0.76707200	9.29301300	3.21053000
C	-6.97171500	2.20719000	0.95830700	H	0.29427600	10.44489200	1.17695100
C	-6.93928600	-2.30785900	-0.96137300	H	-0.44826600	10.43942100	-1.18353400
C	-7.68483500	-1.18555500	-0.47382500	H	-0.90395300	9.28073500	-3.21712300
C	-9.09087700	-1.17141500	-0.46792900	H	-0.79848300	7.20804800	-4.59760500
C	-9.82349900	-0.07530100	-0.00259000	H	0.11034100	5.14728700	-3.58317100
C	-9.10335000	1.03479100	0.46357600	H	2.36292500	5.74375900	0.05591400
C	6.93920700	2.30792300	-0.96137300	H	3.74026900	3.77838000	0.54705600
C	7.68479500	1.18564000	-0.47383800	H	1.14984400	1.35421300	-1.87724500
C	6.96392200	0.05174400	-0.00205900	H	-0.28478400	3.30119600	-2.28473800
C	7.70248800	-1.07349600	0.47056800	H	1.66422200	0.01200800	-0.00288800
C	6.97179300	-2.20712500	0.95830700	H	5.04252200	3.17661400	-1.32592800
C	9.09083800	1.17153800	-0.46796600	H	5.08815100	-3.10206600	1.32207400
C	9.82349800	0.07544500	-0.00263900	H	3.79608600	-3.72308600	-0.55342900
C	9.10338700	-1.03466700	0.46353900	H	2.44766800	-5.70853700	-0.06243400
C	-11.36362900	-0.04882900	0.01413500	H	-0.23576900	-3.30513800	2.27805600
C	-11.97997400	-1.35034100	-0.53295300	H	1.17012200	-1.33731700	1.87075400
C	-11.86755600	1.12531300	-0.85849000	H	-7.52853500	3.04961200	1.36211600
C	-11.85899100	0.14342500	1.46730600	H	-7.48426600	-3.15842500	-1.36427800
C	11.36362900	0.04901600	0.01406100	H	-9.60157000	-2.05268000	-0.84147000
C	11.85901700	-0.14325000	1.46722100	H	-9.63448400	1.90689400	0.83661200
C	11.97992900	1.35055500	-0.53301300	H	7.48415600	3.15850400	-1.36428700
C	11.86757700	-1.12509600	-0.85859200	H	7.52864300	-3.04953000	1.36210700
H	-0.11047200	-5.14737500	-3.58319000	H	9.60149900	2.05281800	-0.84151500
H	0.79835200	-7.20813100	-4.59763100	H	9.63455100	-1.90675500	0.83656700
H	0.90386900	-9.28080700	-3.21713600	H	-11.69214100	-1.53206100	-1.57467800
H	0.44823700	-10.43948100	-1.18354300	H	-11.68543600	-2.22280700	0.06128100
H	-0.29424600	-10.44495100	1.17696000	H	-13.07322100	-1.28243900	-0.49982500
H	-0.76698700	-9.29308400	3.21054400	H	-11.53740100	1.01109600	-1.89728400
H	-0.69206300	-7.21906200	4.59101500	H	-12.96389900	1.16225200	-0.85183100
H	0.18642800	-5.14517700	3.57660400	H	-11.49957000	2.09072200	-0.49586000
H	-2.36301500	-5.74380100	0.05590500	H	-11.52258700	-0.67971300	2.10794400
H	-3.74033600	-3.77840300	0.54702900	H	-11.49095300	1.07768900	1.90389600
H	-1.14991900	-1.35429800	-1.87734300	H	-12.95525300	0.17095000	1.49590500
H	0.28468800	-3.30129900	-2.28481700	H	11.52260300	0.67986900	2.10787800
H	-1.66422200	-0.01208600	-0.00297600	H	11.49100700	-1.07753000	1.90380100
H	-5.04263200	-3.17660200	-1.32596200	H	12.95528000	-0.17075100	1.49580300
H	-5.08804100	3.10208000	1.32203900	H	11.69205800	1.53229500	-1.57472400
H	-1.17004600	1.33723300	1.87065600	H	11.68539100	2.22300000	0.06125300
H	0.23586600	3.30503600	2.27797700	H	13.07317800	1.28267500	-0.49992100
H	-2.44757800	5.70849600	-0.06244400	H	11.53739900	-1.01087200	-1.89737900

H	12.96392000	-1.16200100	-0.85195300	H	11.49962700	-2.09052300	-0.49597200
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3g (B3LYP/6-31G(d))

C	-6.03346600	-2.32072600	-1.23087600	C	-4.90181700	-4.54902800	-1.53177400
C	-13.11431500	0.38328000	-0.55985700	C	-4.85346500	-3.21313000	-1.10080000
C	-13.11431400	-0.38328600	0.55986000	C	-3.67031500	-2.74612500	-0.51043800
C	-11.88535200	-0.70450200	1.22925900	C	3.85432800	5.56304600	0.08222000
C	-10.63954400	-0.24710500	0.69130400	C	2.58128500	5.03434900	-0.12096500
C	-10.63954500	0.24710400	-0.69130500	C	2.42351200	3.67998400	-0.45691200
C	-11.88535500	0.70449800	-1.22925900	C	3.57278400	2.88221000	-0.55724900
C	-9.50642600	0.24791700	-1.57224800	C	4.86683400	3.40160200	-0.38809500
C	-9.59387000	0.93255200	-2.78544800	C	4.98654600	4.76466100	-0.06370900
C	-10.77684500	1.55321400	-3.21075900	C	1.08019700	3.11708400	-0.75699800
C	-11.92459300	1.39018900	-2.46344100	C	-0.06551100	3.54958100	-0.07165000
C	-8.29916100	-0.60489400	-1.37900400	C	-1.34688300	3.07306800	-0.39098000
C	-7.01286100	-0.14019900	-1.69601900	C	-1.46407700	2.12055500	-1.41732700
C	-8.43179700	-1.95376400	-1.00886700	C	-0.33555500	1.66391700	-2.09303900
C	-7.32391200	-2.79166600	-0.93590100	C	0.92574900	2.15987800	-1.77382600
C	-5.90386700	-0.97802600	-1.61983500	C	-2.55601600	3.57634800	0.31368800
C	-11.92458700	-1.39019400	2.46344100	C	-2.63722300	4.90758600	0.75561900
C	-10.77683800	-1.55321900	3.21075700	C	-3.79731000	5.38217500	1.36495600
C	-9.59386400	-0.93255500	2.78544500	C	-4.90181700	4.54903100	1.53178000
C	-9.50642300	-0.24791800	1.57224600	C	-4.85346500	3.21313400	1.10080300
C	-7.01285900	0.14020000	1.69601400	C	-3.67031600	2.74613000	0.51043700
C	-8.29916000	0.60489500	1.37900300	C	13.24846900	0.16854800	0.65668300
C	-5.90386500	0.97802700	1.61983100	C	13.24847200	-0.16854100	-0.65667200
C	-6.03346600	2.32072900	1.23087700	C	12.01948200	-0.24314700	-1.39351000
C	-7.32391300	2.79166900	0.93590600	C	10.76940100	-0.00050000	-0.73457300
C	-8.43179600	1.95376700	1.00887000	C	10.76939800	0.00050100	0.73457400
C	3.85432200	-5.56305600	-0.08220900	C	12.01947600	0.24315200	1.39351600
C	2.58128100	-5.03435400	0.12097200	C	9.63659200	-0.28262900	1.57027500
C	2.42351200	-3.67998600	0.45691200	C	9.74001000	-0.05667900	2.94544700
C	3.57278700	-2.88221500	0.55724400	C	10.92810500	0.37067800	3.55222300
C	4.86683500	-3.40161200	0.38809300	C	12.06998700	0.46811500	2.78653300
C	4.98654300	-4.76467400	0.06371600	C	8.39873600	-0.98492300	1.12574600
C	1.08020000	-3.11708200	0.75699600	C	12.06999900	-0.46810800	-2.78652800
C	-0.06551000	-3.54957800	0.07164900	C	10.92812100	-0.37067000	-3.55222200
C	-1.34688100	-3.07306100	0.39097800	C	9.74002300	0.05668400	-2.94545000
C	-1.46407300	-2.12054400	1.41732200	C	9.63659800	0.28262900	-1.57027800
C	-0.33554900	-1.66390600	2.09303200	C	8.39873900	0.98492000	-1.12575100
C	0.92575400	-2.15987100	1.77382000	C	8.45103600	2.10969900	-0.28584900
C	-2.55601500	-3.57634200	-0.31368700	C	7.31177400	2.86294000	-0.01719700
C	-2.63722200	-4.90758100	-0.75561500	C	6.06781200	2.55005400	-0.59456500
C	-3.79731000	-5.38217200	-1.36494900	C	6.01825000	1.41484600	-1.42203600

C	7.14956700	0.64823500	-1.67190800	H	-3.84458200	-6.41443000	-1.70202600
C	8.45103700	-2.10970600	0.28584900	H	-5.79965900	-4.92602800	-2.01327100
C	7.31177700	-2.86295000	0.01719700	H	-3.62637400	-1.71305400	-0.17905600
C	6.06781300	-2.55006500	0.59456100	H	3.96795000	6.61693800	0.32267800
C	6.01824600	-1.41485300	1.42202600	H	1.71058900	5.68063200	-0.05998200
C	7.14956100	-0.64823800	1.67189700	H	3.44914400	1.82250400	-0.75451100
H	-14.04714500	0.70607200	-1.01547100	H	5.96947600	5.21310700	0.04049000
H	-14.04714200	-0.70608100	1.01547400	H	0.04751900	4.25021500	0.75042700
H	-8.73700100	0.91639200	-3.45222300	H	-2.44621700	1.76207600	-1.71008300
H	-10.80254800	2.08117900	-4.15996100	H	-0.44310100	0.93626700	-2.89294500
H	-12.88127900	1.75883600	-2.82537500	H	1.79253200	1.83182300	-2.33946100
H	-6.87645300	0.89978200	-1.97798100	H	-1.80238100	5.58208100	0.59015200
H	-9.41578700	-2.35056400	-0.77966500	H	-3.84458200	6.41443300	1.70203600
H	-7.45716800	-3.82436900	-0.62495600	H	-5.79965900	4.92602900	2.01327900
H	-4.92227300	-0.58872200	-1.87715400	H	-3.62637500	1.71306100	0.17905200
H	-12.88127200	-1.75884400	2.82537600	H	14.18060700	0.31615900	1.19625600
H	-10.80253900	-2.08118500	4.15995800	H	14.18061300	-0.31614900	-1.19624200
H	-8.73699500	-0.91639400	3.45221900	H	8.88730400	-0.29295000	3.57383500
H	-6.87644900	-0.89978200	1.97797200	H	10.96047300	0.54006400	4.62488400
H	-4.92227100	0.58872300	1.87714700	H	13.03142800	0.68693800	3.24454600
H	-7.45717000	3.82437400	0.62496500	H	13.03144200	-0.68692700	-3.24453700
H	-9.41578700	2.35056700	0.77967200	H	10.96049400	-0.54005300	-4.62488400
H	3.96794100	-6.61695000	-0.32266000	H	8.88731900	0.29295500	-3.57384100
H	1.71058300	-5.68063400	0.05999300	H	9.39868400	2.40886800	0.15067600
H	3.44915100	-1.82250700	0.75450200	H	7.39764900	3.71457200	0.65127000
H	5.96947100	-5.21312400	-0.04047800	H	5.08752100	1.13909700	-1.90752600
H	0.04751800	-4.25021600	-0.75042500	H	7.06317300	-0.22997900	-2.30457300
H	-2.44621100	-1.76206200	1.71007700	H	9.39868700	-2.40887600	-0.15067100
H	-0.44309200	-0.93625300	2.89293500	H	7.39765700	-3.71458400	-0.65126600
H	1.79253800	-1.83181600	2.33945400	H	5.08751500	-1.13910300	1.90751000
H	-1.80238100	-5.58207600	-0.59014700	H	7.06316400	0.22997800	2.30455800

3h (B3LYP/6-31G(d))

C	-8.24176600	-0.07823600	-1.58930000	C	-8.24154500	0.07847200	1.59017400
C	-8.32979800	-0.62583300	-2.87021600	C	-9.37502800	0.17059600	0.71471200
C	-9.51410600	-1.19223600	-3.36194700	C	-9.37513600	-0.17027100	-0.71368100
C	-10.66164900	-1.10979500	-2.60108100	C	-7.02846800	0.73731300	-1.30178200
C	-10.62151200	-0.56427700	-1.29895300	C	-7.14498800	2.04412600	-0.79902200
C	-11.85039400	-0.31840300	-0.59828400	C	-6.02610300	2.85142200	-0.62583800
C	-11.85029400	0.31888600	0.59965000	C	-4.73301900	2.39182100	-0.93696500
C	-10.62130300	0.56466300	1.30016200	C	-4.62394500	1.09094900	-1.45878200
C	-10.66123500	1.11013500	2.60231500	C	-5.74430200	0.28845900	-1.64622300
C	-9.51358900	1.19247100	3.36303700	C	-4.73298200	-2.39167400	0.93721800
C	-8.32937900	0.62601900	2.87112600	C	-6.02613000	-2.85123300	0.62629600

C	-7.14496300	-2.04390500	0.79967900	C	-1.17282000	7.83370800	-0.46029800
C	-7.02831900	-0.73711300	1.30245600	C	1.17323200	7.83371100	0.45913100
C	-5.74408500	-0.28830700	1.64671100	C	-1.79760800	7.58317700	-1.69360700
C	-4.62378200	-1.09082200	1.45906500	C	-2.87043100	8.36259600	-2.12424400
C	4.73297200	2.39166000	0.93715400	C	-3.34360400	9.40901900	-1.33041800
C	4.62375600	1.09079500	1.45896700	C	-2.72672300	9.67674200	-0.10646500
C	5.74405300	0.28827500	1.64663000	C	-1.64642800	8.90489600	0.31785500
C	7.02829900	0.73709000	1.30242500	C	1.79793200	7.58340800	1.69253100
C	7.14495700	2.04389200	0.79967600	C	2.87080300	8.36283100	2.12304400
C	6.02612900	2.85122400	0.62627800	C	3.34411100	9.40902700	1.32899800
C	8.24151900	-0.07849800	1.59016400	C	2.72732100	9.67651800	0.10494700
C	8.32933300	-0.62605900	2.87111100	C	1.64697900	8.90467100	-0.31925000
C	9.51353700	-1.19251600	3.36303300	C	-0.00013200	-5.66375800	-0.00033300
C	10.66119500	-1.11017600	2.60232700	C	-0.00017100	-7.02827200	-0.00051200
C	10.62128200	-0.56469200	1.30017900	C	-1.17321100	-7.83372900	0.45911700
C	11.85028000	-0.31891600	0.59967700	C	1.17283600	-7.83367200	-0.46032300
C	11.85039300	0.31838200	-0.59825200	C	-1.79790100	-7.58347800	1.69253200
C	10.62151800	0.56426600	-1.29893100	C	-2.87075600	-8.36293100	2.12302900
C	10.66166200	1.10979300	-2.60105500	C	-3.34405800	-9.40910600	1.32895200
C	9.51412100	1.19224700	-3.36192300	C	-2.72727600	-9.67654800	0.10488700
C	8.32980600	0.62585100	-2.87020000	C	-1.64694900	-8.90467000	-0.31929500
C	8.24176700	0.07824300	-1.58928900	C	1.79761100	-7.58310400	-1.69363100
C	9.37513700	0.17026200	-0.71366900	C	2.87044300	-8.36249800	-2.12429200
C	9.37501500	-0.17061500	0.71472000	C	3.34363800	-9.40893000	-1.33049200
C	7.02846400	-0.73729800	-1.30176800	C	2.72676900	-9.67668900	-0.10654000
C	7.14498100	-2.04411700	-0.79902400	C	1.64646600	-8.90486900	0.31780500
C	6.02609200	-2.85140700	-0.62583400	C	-1.22941400	-4.85260100	0.25172600
C	4.73300700	-2.39179300	-0.93693300	C	1.22922800	-4.85263600	-0.25216900
C	4.62393400	-1.09091200	-1.45873000	C	-1.22921300	-3.83962000	1.22572500
C	5.74429600	-0.28842800	-1.64617900	C	-2.36076400	-3.06756500	1.46388200
C	0.00017900	7.02828200	-0.00051200	C	-3.53593300	-3.23814200	0.70930300
C	0.00013100	5.66376900	-0.00035800	C	-3.52154000	-4.23283700	-0.28520500
C	-1.22923300	4.85265300	-0.25219800	C	-2.40074300	-5.02869700	-0.50155000
C	1.22941100	4.85260500	0.25168800	C	2.40044100	-5.02886300	0.50125100
C	-2.40043500	5.02886300	0.50124300	C	3.52130800	-4.23303400	0.28514000
C	-3.52130500	4.23303800	0.28513000	C	3.53588400	-3.23823400	-0.70925700
C	-3.53589500	3.23826200	-0.70928900	C	2.36082900	-3.06753300	-1.46398600
C	-2.36085200	3.06757900	-1.46404100	C	1.22921000	-3.83956400	-1.22607000
C	-1.22922900	3.83960500	-1.22612200	H	-7.47086900	-0.54017600	-3.52914200
C	1.22920400	3.83960100	1.22566400	H	-9.54091600	-1.61260300	-4.36346500
C	2.36075300	3.06753900	1.46380800	H	-11.61902100	-1.43459500	-3.00124600
C	3.53592700	3.23813400	0.70924100	H	-12.78331300	-0.58834300	-1.08693600
C	3.52153900	4.23285100	-0.28524400	H	-12.78312900	0.58889600	1.08842200
C	2.40074400	5.02871700	-0.50157800	H	-11.61853400	1.43498200	3.00261700

H	-9.54024400	1.61279300	4.36457800	H	2.33547200	2.33047000	2.26091800
H	-7.47036500	0.54029200	3.52993200	H	4.39180900	4.37062200	-0.92008100
H	-8.12795000	2.43926400	-0.56166500	H	2.42532200	5.79017800	-1.27542100
H	-6.16449700	3.86856400	-0.27114100	H	-1.43515300	6.77215000	-2.31725000
H	-3.64411800	0.67951000	-1.68135500	H	-3.33504400	8.15302400	-3.08426400
H	-5.61553600	-0.72519000	-2.01418900	H	-4.18117200	10.01505300	-1.66559500
H	-6.16460500	-3.86837200	0.27161900	H	-3.08394700	10.49182000	0.51775400
H	-8.12797400	-2.43899600	0.56244500	H	-1.16279900	9.12730200	1.26495500
H	-5.61523700	0.72531900	2.01470900	H	1.43537500	6.77254900	2.31633500
H	-3.64390100	-0.67942000	1.68147100	H	3.33534800	8.15344000	3.08313600
H	3.64386700	0.67939100	1.68133400	H	4.18171500	10.01506500	1.66407700
H	5.61519500	-0.72535900	2.01460200	H	3.08465300	10.49141600	-0.51944300
H	8.12797400	2.43898800	0.56248000	H	1.16342000	9.12689700	-1.26642800
H	6.16461600	3.86837100	0.27163100	H	-1.43535000	-6.77263600	2.31636100
H	7.47030900	-0.54033900	3.52990600	H	-3.33529400	-8.15358000	3.08313400
H	9.54017800	-1.61284800	4.36457000	H	-4.18165000	-10.01516800	1.66402000
H	11.61848700	-1.43503000	3.00263900	H	-3.08460200	-10.49143000	-0.51952700
H	12.78311000	-0.58893400	1.08845500	H	-1.16339500	-9.12685800	-1.26648500
H	12.78331700	0.58832100	-1.08689500	H	1.43514000	-6.77206800	-2.31725300
H	11.61903600	1.43459200	-3.00121300	H	3.33504600	-8.15289800	-3.08431100
H	9.54093600	1.61262300	-4.36343800	H	4.18121200	-10.01494500	-1.66568800
H	7.47087700	0.54020800	-3.52912900	H	3.08401000	-10.49177400	0.51765900
H	8.12794300	-2.43926700	-0.56168800	H	1.16284700	-9.12730200	1.26490300
H	6.16448500	-3.86855600	-0.27115600	H	-0.33296900	-3.67087800	1.81671900
H	3.64410800	-0.67946300	-1.68128300	H	-2.33548500	-2.33051400	2.26100800
H	5.61553000	0.72522600	-2.01412900	H	-4.39180700	-4.37059100	-0.92004900
H	-2.42485000	5.79036400	1.27505400	H	-2.42531700	-5.79013800	-1.27541300
H	-4.39147600	4.37091700	0.92007800	H	2.42486800	-5.79038200	1.27504300
H	-2.33572100	2.33045800	-2.26110500	H	4.39148900	-4.37093000	0.92007000
H	-0.33309300	3.67079400	-1.81726100	H	2.33568700	-2.33039500	-2.26103500
H	0.33295800	3.67084800	1.81665100	H	0.33306600	-3.67074000	-1.81719400

3i (B3LYP/6-31G(d))

C	-0.16821800	7.27707900	1.58743500	C	0.05323500	7.28291700	-1.60598500
C	0.19822300	7.38527000	2.93130300	C	-0.14852700	8.40992600	-0.73921800
C	0.66935700	8.58041500	3.48950400	C	0.00805800	8.41015000	0.72300700
C	0.67151100	9.72042200	2.71519600	C	-0.88518800	6.02237300	1.21970800
C	0.30334200	9.66417000	1.35317100	C	-2.11232200	6.04897200	0.53586800
C	0.13819000	10.89214100	0.62976000	C	-2.83579400	4.88065400	0.30854200
C	-0.33454100	10.88814800	-0.64079100	C	-2.36658800	3.63537200	0.75984400
C	-0.47189300	9.65829800	-1.36680500	C	-1.15142600	3.61434300	1.46412500
C	-0.84103300	9.70912200	-2.72877800	C	-0.42799200	4.77900400	1.68598000
C	-0.81307300	8.57109900	-3.50549900	C	-3.10377400	2.37548100	0.49299800
C	-0.31529500	7.38567200	-2.94971100	C	-4.52444600	2.33708000	0.48254600

C	-5.21001700	1.15950200	0.24646500	C	2.16158600	-6.03751500	0.53561900
C	-4.50550800	-0.04546000	0.00791500	C	2.88334100	-4.86999800	0.29893700
C	-3.08130200	-0.03040400	0.00345700	C	2.41729100	-3.62321300	0.74927800
C	-2.41457200	1.19452600	0.24749800	C	1.20763300	-3.59973000	1.46287100
C	3.12348400	0.03889400	-0.03109700	C	0.48603000	-4.76366800	1.69433200
C	4.54757800	0.05415000	-0.03822500	C	3.15173900	-2.36414000	0.47128600
C	5.22664300	1.27338900	-0.27590600	C	-6.69520900	1.16303200	0.25451400
C	4.51632400	2.43726000	-0.50743500	C	-6.67076600	-1.29981300	-0.22504200
C	3.09516800	2.44499600	-0.51899800	C	6.71119700	1.30757700	-0.28287700
C	2.43097500	1.24934000	-0.27514200	C	6.74062400	-1.14853100	0.20584600
C	2.33110300	3.68906800	-0.78445500	N	-7.32846600	-0.07518600	0.01681100
C	2.77268000	4.94349800	-0.33061600	N	7.37279100	0.07011100	-0.11578900
C	2.02380500	6.09604300	-0.55616300	O	-7.35358700	2.17272500	0.45293300
C	0.79783500	6.04373200	-1.24061200	O	-7.30900500	-2.32307300	-0.41962500
C	0.36837700	4.79153000	-1.70960600	O	7.34577400	2.34007500	-0.43206100
C	1.11714900	3.64265400	-1.48959400	O	7.39784100	-2.14698800	0.46065200
C	-2.39042200	-1.24108200	-0.24452400	C	-8.78133300	-0.09059400	0.02149700
C	-4.47718900	-2.42807700	-0.46587400	C	8.82781200	0.09638800	-0.10651200
C	-5.18596400	-1.26505000	-0.22612900	C	-9.46479000	0.13252000	-1.18646000
C	5.25514200	-1.14817400	0.20249600	C	-10.86390800	0.11263000	-1.15560500
C	4.57230800	-2.32439000	0.45348900	C	-11.55362900	-0.11990600	0.03046300
C	2.45956200	-1.18545400	0.22296000	C	-10.85148800	-0.33777300	1.21201600
C	-3.05613100	-2.43643500	-0.48502500	C	-9.45208400	-0.32813200	1.23381700
C	-2.29395400	-3.68073300	-0.75480500	C	9.54565500	-0.14802900	-1.29469600
C	-1.08526600	-3.63524400	-1.46897300	C	10.94437000	-0.08904100	-1.21903800
C	-0.33791800	-4.78438900	-1.69259900	C	11.60509400	0.19206600	-0.02793300
C	-0.76354600	-6.03580200	-1.21805000	C	10.86998300	0.42526700	1.12805000
C	-1.98447900	-6.08721900	-0.52459000	C	9.47132500	0.38429700	1.11244200
C	-2.73201500	-4.93446700	-0.29570000	C	-8.74038800	0.39013500	-2.50262000
C	-0.02137900	-7.27561300	-1.58627900	C	-9.06335100	1.79096700	-3.05650800
C	0.33687300	-7.38151500	-2.93252200	C	-9.03777500	-0.71561500	-3.53326000
C	0.83039800	-8.56828600	-3.48926300	C	-8.71401900	-0.57003500	2.54538900
C	0.86425900	-9.70448600	-2.71009600	C	-9.00616500	-1.97596400	3.10338600
C	0.50561200	-9.65042500	-1.34544200	C	-9.02587700	0.53134200	3.57647500
C	0.37377700	-10.87848900	-0.61537500	C	8.70712100	0.64744700	2.40618500
C	-0.08909700	-10.87934700	0.65881800	C	8.96320600	2.07326300	2.93072700
C	-0.24851000	-9.64960300	1.38051400	C	9.02497900	-0.42015500	3.47079800
C	-0.60599600	-9.70238800	2.74552400	C	8.95631900	-0.52656500	-2.65855500
C	-0.59764700	-8.56044200	3.51694600	C	8.65825100	-2.03842400	-2.74514900
C	-0.13073900	-7.36674100	2.95211500	C	7.76332900	0.30805100	-3.15965800
C	0.22519100	-7.26202500	1.60516800	H	0.04250100	6.52923000	3.58025600
C	0.04195700	-8.39719300	0.74497600	H	0.94955400	8.61825900	4.53835700
C	0.18714500	-8.40053600	-0.71840800	H	0.92530900	10.68569800	3.14606600
C	0.93959200	-6.00851800	1.22850800	H	0.33111000	11.82577800	1.15191800

H	-0.54848800	11.81829500	-1.16098300	H	-0.45627900	-4.70643600	2.23035500
H	-1.11642700	10.66934900	-3.15766300	H	-11.41957900	0.28164700	-2.07389000
H	-1.09385400	8.60485400	-4.55433700	H	-12.64053400	-0.13137800	0.03398200
H	-0.14027800	6.53470700	-3.60041900	H	-11.39750400	-0.51848700	2.13386600
H	-2.50751700	6.99628100	0.18277300	H	11.52284500	-0.27073700	-2.12163100
H	-3.77193500	4.93714100	-0.24038000	H	12.69098000	0.23222300	-0.00341000
H	-0.77553400	2.67521000	1.86014700	H	11.38616900	0.64619500	2.05814900
H	0.51839400	4.72349400	2.21495400	H	-7.66366300	0.36425400	-2.30840700
H	-5.10204400	3.23292300	0.68480600	H	-8.48886500	1.98259500	-3.97091800
H	-1.32834500	1.20433600	0.21756900	H	-10.12654500	1.88997500	-3.30533600
H	5.07454500	3.34604900	-0.70607800	H	-8.81477900	2.56521500	-2.32311600
H	1.34479800	1.23640400	-0.24473400	H	-8.77067700	-1.69983700	-3.13458000
H	3.70702500	5.01951200	0.21901400	H	-10.09984800	-0.73745300	-3.80461700
H	2.39786500	7.05114000	-0.20104300	H	-8.46335300	-0.54670900	-4.45215400
H	-0.57636600	4.71623000	-2.23907500	H	-7.63931600	-0.52365300	2.34393800
H	0.76228300	2.69621800	-1.88761600	H	-8.42232400	-2.15485500	4.01444200
H	-1.30405600	-1.22814300	-0.22126400	H	-10.06562600	-2.09525900	3.35909300
H	-5.03689300	-3.33612400	-0.66403200	H	-8.74718000	-2.74650500	2.36969100
H	5.15178000	-3.21778000	0.66114800	H	-10.08640900	0.53314800	3.85466100
H	1.37317700	-1.19673500	0.20024300	H	-8.44235800	0.37489400	4.49183900
H	-0.73354400	-2.68931900	-1.87102100	H	-8.78038000	1.51991400	3.17468400
H	0.60287100	-4.70987500	-2.22917900	H	7.63625500	0.57451700	2.19551900
H	-2.35563000	-7.04178100	-0.16500100	H	10.01562200	2.22003100	3.20069200
H	-3.66236300	-5.00960300	0.26079500	H	8.70091200	2.81787400	2.17227600
H	0.15685600	-6.53208300	-3.58387700	H	8.36103500	2.26382900	3.82741400
H	1.10315300	-8.60454600	-4.54013400	H	10.08092100	-0.39404400	3.76457600
H	1.13631300	-10.66573500	-3.13882500	H	8.42494500	-0.25005300	4.37296900
H	0.58361700	-11.80992600	-1.13493100	H	8.80368600	-1.42342200	3.09231400
H	-0.27802700	-11.81169800	1.18472100	H	9.77000400	-0.33346800	-3.37006800
H	-0.85651000	-10.66654500	3.18080100	H	8.32472100	-2.29993200	-3.75712900
H	-0.86961900	-8.59565100	4.56805400	H	9.55356500	-2.62722200	-2.51817900
H	0.03018900	-6.50908500	3.59766800	H	7.88205900	-2.34115300	-2.03719800
H	2.55402600	-6.98603200	0.18270000	H	7.64476100	0.15446500	-4.23879800
H	3.81534700	-4.92821100	-0.25680900	H	6.82074900	0.01232700	-2.68975300
H	0.83474900	-2.65915600	1.85833800	H	7.91432300	1.37697600	-2.98192200

3j (B3LYP/6-31G(d))

C	-4.70663700	-0.39453400	1.54646800	C	-7.08562300	-0.15931800	-1.40636500
C	-4.80431300	-0.25062600	2.93285400	C	-7.13209200	-0.29888500	-2.81048700
C	-5.98812300	0.14927600	3.56644600	C	-5.98839200	-0.14921600	-3.56608900
C	-7.13187700	0.29896500	2.81092900	C	-4.80452700	0.25066100	-2.93258500
C	-7.08551500	0.15939600	1.40680400	C	-4.70674600	0.39456500	-1.54620600
C	-8.31456900	0.13022900	0.66577400	C	-5.83719400	0.04691300	-0.73283400
C	-8.31462200	-0.13012800	-0.66524300	C	-5.83714000	-0.04685900	0.73318100

C	-3.48125500	-1.08385800	1.04984800	C	0.00010500	7.54586800	-0.00065800
C	-3.56044300	-2.17902700	0.17181200	C	0.75809300	6.83771900	0.93413600
C	-2.42941500	-2.91121400	-0.18101000	C	0.75476900	5.44452900	0.94494900
C	-1.17220900	-2.58396500	0.35168000	C	0.75466000	-5.44426700	-0.94570700
C	-1.08633700	-1.50383200	1.24118100	C	0.75795300	-6.83746100	-0.93530400
C	-2.21727600	-0.76833400	1.57453200	C	-0.00004900	-7.54586700	-0.00071800
N	-0.00001400	-3.31104200	-0.00006000	C	-0.75804400	-6.83774000	0.93408700
C	1.17220500	-2.58393300	-0.35170000	C	-0.75473600	-5.44455000	0.94491800
C	1.08639700	-1.50378700	-1.24118600	H	-3.95163300	-0.53178300	3.54318000
C	2.21736400	-0.76828600	-1.57444200	H	-6.01764300	0.25453400	4.64742100
C	3.48130300	-1.08383700	-1.04967600	H	-8.09097900	0.49392200	3.28442500
C	3.56042400	-2.17901800	-0.17164700	H	-9.24692900	0.24624200	1.21272500
C	2.42936300	-2.91120000	0.18108100	H	-9.24702400	-0.24612400	-1.21212500
C	4.70673300	-0.39453000	-1.54620500	H	-8.09123300	-0.49382300	-3.28391000
C	4.80451100	-0.25060800	-2.93258300	H	-6.01799400	-0.25447400	-4.64706200
C	5.98837600	0.14927400	-3.56608400	H	-3.95188600	0.53180300	-3.54297300
C	7.13207900	0.29893000	-2.81048300	H	-4.52345800	-2.46599000	-0.23906400
C	7.08561400	0.15934200	-1.40636300	H	-2.51884000	-3.75120000	-0.86315700
C	8.31461300	0.13013800	-0.66524100	H	-0.12140300	-1.24137500	1.66092700
C	8.31456100	-0.13023800	0.66577300	H	-2.11998000	0.07536100	2.25177700
C	7.08550600	-0.15941900	1.40680200	H	0.12149200	-1.24132300	-1.66099600
C	7.13186400	-0.29901000	2.81092600	H	2.12012600	0.07542400	-2.25167600
C	5.98810700	-0.14933400	3.56644100	H	4.52340900	-2.46599300	0.23928900
C	4.80429700	0.25057200	2.93285200	H	2.51872300	-3.75120400	0.86321700
C	4.70662400	0.39449700	1.54646700	H	3.95186800	-0.53173800	-3.54297400
C	5.83713200	0.04684400	0.73318100	H	6.01797700	0.25454700	-4.64705600
C	5.83718600	-0.04689700	-0.73283400	H	8.09122000	0.49387300	-3.28390600
C	3.48124300	1.08382200	1.04984300	H	9.24701600	0.24614200	-1.21212200
C	3.56044000	2.17899700	0.17181400	H	9.24692000	-0.24625900	1.21272200
C	2.42941800	2.91119300	-0.18100600	H	8.09096600	-0.49397100	3.28442100
C	1.17220800	2.58394800	0.35167800	H	6.01762500	-0.25460700	4.64741500
C	1.08632500	1.50380200	1.24116300	H	3.95161400	0.53171700	3.54318000
C	2.21725800	0.76829400	1.57451100	H	4.52345900	2.46596000	-0.23905200
N	0.00002000	3.31104300	-0.00005200	H	2.51885100	3.75118700	-0.86314100
C	-1.17220600	2.58395000	-0.35170300	H	0.12138800	1.24134800	1.66090300
C	-2.42936000	2.91122000	0.18108700	H	2.11995500	-0.07540700	2.25174800
C	-3.56042700	2.17904700	-0.17164300	H	-2.51871100	3.75121400	0.86323500
C	-3.48131500	1.08387300	-1.04968100	H	-4.52340700	2.46602100	0.23930400
C	-2.21738100	0.76832700	-1.57446400	H	-2.12015100	-0.07537700	-2.25170700
C	-1.08640900	1.50381700	-1.24120600	H	-0.12150700	1.24135200	-1.66102200
C	-0.00003600	-4.72837300	-0.00028700	H	-1.33455400	4.90344000	-1.68633400
C	0.00005900	4.72837300	-0.00026300	H	-1.34861600	7.37143500	-1.67529600
C	-0.75463200	5.44428800	-0.94567200	H	0.00012300	8.63207800	-0.00081100
C	-0.75790800	6.83748200	-0.93525100	H	1.34881500	7.37186100	1.67403400

H	1.33466600	4.90386900	1.68576800	H	-0.00005500	-8.63207700	-0.00088400
H	1.33457400	-4.90340200	-1.68636500	H	-1.34875700	-7.37189800	1.67398100
H	1.34866500	-7.37139800	-1.67535700	H	-1.33463700	-4.90390500	1.68574600

3j (M06-2X/6-31G(d))

C	-4.68516300	-0.28392900	1.55227600	C	5.82113800	-0.00153500	0.73314900
C	-4.77042000	-0.06923300	2.92248600	C	5.82118200	0.00148700	-0.73291900
C	-5.95503500	0.35336800	3.53878400	C	3.46205800	0.97780700	1.06563900
C	-7.10006800	0.45353800	2.78418400	C	3.55409000	2.08810800	0.21656600
C	-7.05801300	0.24021000	1.39153000	C	2.42505100	2.80864600	-0.15280400
C	-8.29060700	0.16728200	0.65439400	C	1.16755200	2.45287200	0.34733600
C	-8.29064500	-0.16722900	-0.65402300	C	1.06920300	1.35472000	1.20493900
C	-7.05809400	-0.24015900	-1.39123000	C	2.19722800	0.62297700	1.54666300
C	-7.10022900	-0.45348700	-2.78388200	N	-0.00000700	3.17737100	0.00000700
C	-5.95523900	-0.35331800	-3.53854800	C	-1.16757700	2.45286500	-0.34730400
C	-4.77058800	0.06928000	-2.92231700	C	-2.42505100	2.80865100	0.15288500
C	-4.68525300	0.28397400	-1.55211100	C	-3.55410900	2.08812500	-0.21644600
C	-5.82117700	-0.00149700	-0.73291900	C	-3.46211300	0.97782500	-1.06552600
C	-5.82113400	0.00154400	0.73314800	C	-2.19730600	0.62298700	-1.54660500
C	-3.46205000	-0.97778200	1.06562700	C	-1.06926400	1.35472500	-1.20492200
C	-3.55409000	-2.08808300	0.21655500	C	-0.00004100	-4.58882300	-0.00017100
C	-2.42505600	-2.80862700	-0.15281700	C	0.00002400	4.58882400	-0.00018100
C	-1.16755400	-2.45285900	0.34731900	C	-0.79607000	5.29984500	-0.90765800
C	-1.06919600	-1.35470200	1.20491500	C	-0.79839300	6.68962100	-0.89677200
C	-2.19721600	-0.62295200	1.54664000	C	0.00007100	7.39588300	-0.00052000
N	-0.00000100	-3.17737000	-0.00000700	C	0.79851100	6.68981100	0.89590700
C	1.16757500	-2.45287700	-0.34732100	C	0.79613900	5.30004000	0.90712900
C	1.06927200	-1.35474100	-1.20494500	C	0.79604600	-5.29986300	-0.90764000
C	2.19731900	-0.62301100	-1.54662600	C	0.79836100	-6.68963800	-0.89673200
C	3.46212200	-0.97785000	-1.06553900	C	-0.00010400	-7.39588200	-0.00046600
C	3.55411000	-2.08815000	-0.21645800	C	-0.79853600	-6.68979100	0.89595200
C	2.42504600	-2.80866900	0.15287100	C	-0.79615700	-5.30002000	0.90715200
C	4.68526400	-0.28399800	-1.55211600	H	-3.90893600	-0.30854000	3.53854100
C	4.77060200	-0.06931100	-2.92232200	H	-5.98092900	0.51644100	4.61146800
C	5.95525200	0.35328600	-3.53855300	H	-8.05793200	0.66992700	3.24941200
C	7.10023900	0.45346300	-2.78388400	H	-9.22085400	0.31233900	1.19679100
C	7.05810000	0.24014600	-1.39123100	H	-9.22092400	-0.31228300	-1.19636600
C	8.29065100	0.16722400	-0.65402300	H	-8.05812000	-0.66987300	-3.24905500
C	8.29061200	-0.16727700	0.65439600	H	-5.98119500	-0.51639000	-4.61123000
C	7.05801800	-0.24019800	1.39153200	H	-3.90914000	0.30858600	-3.53842200
C	7.10007600	-0.45351700	2.78418800	H	-4.52629100	-2.39044600	-0.16195300
C	5.95504500	-0.35334000	3.53878900	H	-2.51284800	-3.66628400	-0.81313400
C	4.77043100	0.06926200	2.92249100	H	-0.09198500	-1.08631900	1.59218000
C	4.68517200	0.28395200	1.55228000	H	-2.10025100	0.24718600	2.19205500

H	0.09208000	-1.08634900	-1.59225400	H	2.10026900	-0.24716000	2.19208000
H	2.10039900	0.24712700	-2.19204700	H	-2.51279400	3.66630300	0.81321500
H	4.52628900	-2.39052100	0.16210100	H	-4.52629200	2.39049200	0.16210600
H	2.51278300	-3.66632000	0.81320500	H	-2.10038000	-0.24715100	-2.19202400
H	3.90915600	-0.30862500	-3.53842800	H	-0.09207000	1.08633900	-1.59222800
H	5.98121100	0.51635100	-4.61123600	H	-1.40944200	4.75568100	-1.61856800
H	8.05813100	0.66984900	-3.24905600	H	-1.42259400	7.22310300	-1.60734400
H	9.22093000	0.31227500	-1.19636700	H	0.00008800	8.48085300	-0.00065000
H	9.22085900	-0.31233100	1.19679400	H	1.42272600	7.22344400	1.60635300
H	8.05794000	-0.66990500	3.24941500	H	1.40948700	4.75602500	1.61817500
H	5.98094100	-0.51640600	4.61147400	H	1.40942000	-4.75571300	-1.61856100
H	3.90894900	0.30857600	3.53854700	H	1.42255700	-7.22313500	-1.60729800
H	4.52628800	2.39047400	-0.16194900	H	-0.00012700	-8.48085200	-0.00058000
H	2.51283700	3.66630000	-0.81312600	H	-1.42275300	-7.22341000	1.60640800
H	0.09199500	1.08633300	1.59220900	H	-1.40949900	-4.75599100	1.61819200

TS-3j_{rac} (M06-2X/6-31G(d))

C	5.15302300	1.37729800	0.15710700	C	-5.30491000	0.04201500	-0.86492600
C	5.31895700	2.75448800	-0.04206000	C	-5.70288400	-0.26497200	-2.16205500
C	6.54463700	3.41165600	-0.04169700	C	-6.99394200	-0.70689900	-2.46908300
C	7.66070600	2.64908300	0.15659700	C	-7.93468900	-0.73950500	-1.46856000
C	7.55745500	1.26630700	0.39902900	C	-7.57895700	-0.42691900	-0.14150900
C	8.82025700	0.62817700	0.62624100	C	-8.62900700	-0.29280700	0.83093000
C	8.88231400	-0.66495200	0.96904500	C	-8.35681800	0.13462100	2.08074600
C	7.68277500	-1.43444500	1.09853800	C	-6.99737400	0.25583000	2.53074200
C	7.88530700	-2.75105200	1.55628500	C	-6.76440100	0.57077800	3.88396100
C	6.83169700	-3.60209000	1.74845600	C	-5.49185600	0.52838200	4.40186800
C	5.56363200	-3.12980200	1.42350200	C	-4.44957100	0.07336100	3.58773900
C	5.31378800	-1.84237400	0.94179500	C	-4.63520100	-0.24129400	2.24568200
C	6.38330300	-0.89674000	0.79676100	C	-5.91745100	-0.03254600	1.64769100
C	6.30479900	0.55429100	0.43730500	C	-6.22657900	-0.15389900	0.21332600
C	3.66969200	1.13288600	-0.04401800	C	-3.48567000	-0.89209700	1.56849200
C	3.18575900	1.32999800	-1.34581100	C	-3.61675100	-2.07854700	0.84147400
C	1.87525500	1.72718000	-1.57737400	C	-2.51948300	-2.67544100	0.23003700
C	1.00593900	1.93680000	-0.50490700	C	-1.25242500	-2.07849200	0.30356600
C	1.43714700	1.61063200	0.78292700	C	-1.10986300	-0.91709200	1.07484000
C	2.75683900	1.21505900	1.01003200	C	-2.20349200	-0.35184500	1.70313600
N	-0.21526300	2.65426000	-0.70676200	N	-0.15152800	-2.60145500	-0.40199900
C	-1.46831800	1.99401000	-0.72347400	C	1.17937800	-2.26143200	-0.05855400
C	-1.64672900	0.81943300	-1.45436700	C	1.59345000	-2.22670000	1.27765100
C	-2.88510800	0.19090600	-1.46357700	C	2.91738900	-1.95834000	1.58394200
C	-3.97346100	0.69966900	-0.75070000	C	3.86887300	-1.73633300	0.58183000
C	-3.79183400	1.89003400	-0.03527700	C	3.44641400	-1.76425500	-0.74638900
C	-2.55671000	2.52350700	-0.01577300	C	2.11469000	-1.99942300	-1.06518000

C	-0.11875100	4.02693200	-1.01477700	H	-2.42216000	3.44630600	0.54139100
C	-0.33742600	-3.47990600	-1.50532800	H	-4.99942300	-0.08882500	-2.96991900
C	-1.15128400	-3.11799100	-2.58100100	H	-7.26060800	-0.94267400	-3.49436600
C	-1.31440500	-3.98391800	-3.65699100	H	-8.97282600	-0.97639700	-1.68520500
C	-0.65156200	-5.20890500	-3.68010000	H	-9.65072900	-0.47149000	0.50742600
C	0.17366000	-5.56393800	-2.61527500	H	-9.15194600	0.32321200	2.79679500
C	0.32617800	-4.70927400	-1.52900500	H	-7.61524400	0.81871100	4.51273000
C	-1.11439700	4.67302900	-1.76330300	H	-5.30566600	0.76877700	5.44376100
C	-1.00371800	6.02618000	-2.05919900	H	-3.47164900	-0.10471200	4.02478900
C	0.09807000	6.76466100	-1.63516500	H	-4.59474400	-2.54296500	0.74786900
C	1.09263800	6.12334800	-0.90214700	H	-2.65048000	-3.59670100	-0.32762500
C	0.99077800	4.77311900	-0.58876000	H	-0.14814600	-0.42099300	1.12810800
H	4.42548700	3.34199900	-0.22371800	H	-2.07469200	0.57986300	2.24764300
H	6.59966800	4.48236100	-0.20745900	H	0.87782000	-2.43701600	2.06603000
H	8.65187600	3.09294100	0.14904900	H	3.23933400	-1.97124300	2.62188900
H	9.71810200	1.23234300	0.53776400	H	4.17244400	-1.61223400	-1.54088800
H	9.83062400	-1.15368100	1.17127000	H	1.79580200	-2.02163100	-2.10290800
H	8.90405300	-3.06646400	1.76211300	H	-1.64612900	-2.15272100	-2.56255700
H	6.97195200	-4.61438700	2.11289800	H	-1.95126100	-3.69281200	-4.48662600
H	4.71708100	-3.80254900	1.50857900	H	-0.77467400	-5.88052700	-4.52354800
H	3.88232800	1.27321000	-2.17805100	H	0.69437100	-6.51649000	-2.62410200
H	1.54343300	1.97764000	-2.58119200	H	0.96232600	-4.97927100	-0.69140500
H	0.76364200	1.77937300	1.61979100	H	-1.97089500	4.10867800	-2.11567400
H	3.10413800	1.07280300	2.02943200	H	-1.78708800	6.50303300	-2.64103500
H	-0.80412600	0.39009900	-1.99197600	H	0.18040900	7.81992800	-1.87307300
H	-3.01651900	-0.73623800	-2.01252500	H	1.95973600	6.67990900	-0.55849900
H	-4.62435600	2.31405500	0.51943900	H	1.76764900	4.29049000	-0.00468500

(P,M)-3j (M06-2X/6-31G(d))

C	5.18392300	0.36005400	-1.60647100	C	3.86699900	-1.75087600	-1.08140000
C	5.45148400	1.04150700	-2.79179900	C	2.66290200	-2.44274400	-1.01795400
C	6.64682200	1.72806900	-3.01860800	C	1.47566800	-1.87586100	-1.51616300
C	7.64827000	1.63704700	-2.08249200	C	1.60046000	-0.68806500	-2.25124700
C	7.43928400	0.92980800	-0.88337900	C	2.78502200	0.02956100	-2.23139600
C	8.58011200	0.66747300	-0.04870000	C	1.00820400	1.75418600	1.20398100
C	8.47677900	-0.15889800	1.01152100	C	2.22925900	2.45088500	1.16314500
C	7.18805800	-0.60529600	1.46404900	C	3.44684800	1.77582300	1.14218400
C	7.12130900	-1.37811900	2.64017000	C	3.50593400	0.38180600	1.22013800
C	5.90644500	-1.68758700	3.20247900	C	2.29045900	-0.30245000	1.24602300
C	4.75110800	-1.12086800	2.65355600	C	1.07372300	0.35216400	1.18412700
C	4.77403700	-0.34750900	1.49692700	N	0.21729900	-2.46948000	-1.26176400
C	6.00452100	-0.19275500	0.78648900	N	-0.21728000	2.46948600	1.26176500
C	6.16165000	0.38622300	-0.55838400	C	-1.47563700	1.87585900	1.51618100
C	3.93641300	-0.45276800	-1.59841700	C	-1.60043200	0.68806700	2.25127400

C	-2.78499900	-0.02954700	2.23143100	H	9.53920000	1.07913200	-0.35055800
C	-3.93638700	0.45279200	1.59845300	H	9.35058700	-0.44707900	1.58937700
C	-3.86696800	1.75089900	1.08143400	H	8.05037800	-1.70157400	3.10165400
C	-2.66286400	2.44275700	1.01798200	H	5.84464800	-2.28858600	4.10410800
C	-5.18389900	-0.36002600	1.60651100	H	3.80769000	-1.22268700	3.18121600
C	-5.45146000	-1.04146200	2.79184800	H	4.75678400	-2.21140300	-0.66200200
C	-6.64679700	-1.72802400	3.01866400	H	2.63938300	-3.40979500	-0.52780700
C	-7.64824300	-1.63701700	2.08254600	H	0.75395300	-0.29337500	-2.79645700
C	-7.43925700	-0.92979300	0.88342300	H	2.80314800	1.00560000	-2.70709500
C	-8.58008400	-0.66747200	0.04873900	H	2.23069200	3.53509500	1.16670700
C	-8.47675200	0.15888400	-1.01149400	H	4.36914700	2.35046200	1.12388300
C	-7.18803200	0.60528100	-1.46402500	H	2.29292700	-1.38635400	1.28847700
C	-7.12128600	1.37809100	-2.64015400	H	0.17813900	-0.24766100	1.11948900
C	-5.90642400	1.68756200	-3.20246400	H	-0.75392700	0.29337300	2.79648400
C	-4.75108400	1.12085600	-2.65353400	H	-2.80313600	-1.00558400	2.70713500
C	-4.77401000	0.34750900	-1.49689600	H	-4.75675000	2.21143400	0.66204000
C	-6.00449400	0.19275500	-0.78645800	H	-2.63933200	3.40980900	0.52783400
C	-6.16162400	-0.38620900	0.55842200	H	-4.72723000	-0.98118900	3.59708600
C	-3.50590300	-0.38179800	-1.22010600	H	-6.80313800	-2.25501100	3.95452500
C	-3.44681100	-1.77581500	-1.14215100	H	-8.62847400	-2.06759900	2.26809100
C	-2.22922000	-2.45087200	-1.16312300	H	-9.53917100	-1.07912700	0.35060400
C	-1.00817000	-1.75416800	-1.20397600	H	-9.35056000	0.44705400	-1.58935400
C	-1.07368900	-0.35214600	-1.18412000	H	-8.05035600	1.70153500	-3.10164300
C	-2.29042900	0.30246200	-1.24600400	H	-5.84462800	2.28855200	-4.10409900
C	0.21699300	-3.82118800	-0.79793800	H	-3.80766500	1.22267500	-3.18119300
C	-0.21704000	3.82117100	0.79787400	H	-4.36910800	-2.35045900	-1.12383700
C	0.11767100	4.10755800	-0.52660000	H	-2.23064200	-3.53508400	-1.16668000
C	0.09921800	5.42319200	-0.97770400	H	-0.17810700	0.24768200	-1.11949600
C	-0.26739400	6.45437300	-0.11459400	H	-2.29290000	1.38636700	-1.28846200
C	-0.60865300	6.16556100	1.20457700	H	0.40205000	3.29156000	-1.18595100
C	-0.57771300	4.85187200	1.66420300	H	0.36290300	5.64284300	-2.00757300
C	-0.11779500	-4.10762200	0.52650600	H	-0.28638000	7.47978300	-0.46968600
C	-0.09940600	-5.42327700	0.97755200	H	-0.89207100	6.96529000	1.88162300
C	0.26721100	-6.45443100	0.11441400	H	-0.83865200	4.60868500	2.68984900
C	0.60853300	-6.16557300	-1.20473200	H	-0.40217800	-3.29164400	1.18587900
C	0.57765700	-4.85186200	-1.66430100	H	-0.36314300	-5.64296500	2.00740000
H	4.72725500	0.98124600	-3.59703800	H	0.28614700	-7.47985800	0.46946100
H	6.80316300	2.25506800	-3.95446200	H	0.89195100	-6.96528100	-1.88180200
H	8.62850200	2.06762900	-2.26803500	H	0.83864800	-4.60864000	-2.68992500

4a (M06-2X/6-31G(d))

C	6.18286400	0.60670900	1.48312500	C	8.62676100	0.15517200	2.81927600
C	6.29756500	0.69118600	2.87413400	C	8.56659500	0.06817300	1.41168700
C	7.49052200	0.41675800	3.55330100	C	9.79562200	-0.01973700	0.67722000

C	9.79562600	0.01972300	-0.67718600	C	-9.79562200	-0.01973600	0.67721900
C	8.56660300	-0.06817800	-1.41166000	C	-8.56659500	0.06817600	1.41168600
C	8.62677600	-0.15517400	-2.81924900	C	-8.62676200	0.15517700	2.81927500
C	7.49053900	-0.41675100	-3.55328100	C	-7.49052400	0.41676300	3.55330100
C	6.29757800	-0.69117600	-2.87412100	C	-6.29756700	0.69119200	2.87413500
C	6.18287000	-0.60670300	-1.48311300	C	-6.18286500	0.60671600	1.48312600
C	7.31274000	-0.15783400	-0.71864600	C	-7.31273600	0.15783700	0.71866500
C	7.31273700	0.15783400	0.71866600	C	-7.31273900	-0.15783700	-0.71864600
C	4.91704500	1.16228000	0.92246000	C	-4.91704600	1.16229000	0.92246300
C	4.90688400	2.10660400	-0.11752900	C	-4.90688500	2.10661500	-0.11752400
C	3.72399900	2.72712800	-0.51634700	C	-3.72400000	2.72714000	-0.51634100
C	2.49951400	2.44875500	0.11630400	C	-2.49951500	2.44876500	0.11630900
C	2.51759800	1.50514900	1.15779900	C	-2.51760000	1.50516000	1.15780400
C	3.69148700	0.87414200	1.54404200	C	-3.69148900	0.87415300	1.54404700
C	1.23182900	3.13322300	-0.24821400	H	5.44466100	1.05120400	3.44031000
C	1.23182800	-3.13322600	0.24818900	H	7.52975800	0.48905100	4.63660600
C	2.49951400	-2.44875100	-0.11631400	H	9.59237100	0.04425000	3.30640300
C	3.72399300	-2.72712000	0.51634800	H	10.72734200	-0.04443200	1.23671300
C	4.90688000	-2.10659400	0.11753700	H	10.72734900	0.04441200	-1.23667400
C	4.91704600	-1.16227300	-0.92245400	H	9.59238900	-0.04425600	-3.30637000
C	3.69149200	-0.87413700	-1.54404500	H	7.52978000	-0.48904200	-4.63658600
C	2.51760200	-1.50514700	-1.15781000	H	5.44467500	-1.05119000	-3.44030200
C	-0.00000100	2.49476900	-0.03804700	H	5.83686000	2.36596900	-0.61440500
C	-1.23182900	3.13322900	-0.24821100	H	3.75606700	3.43952100	-1.33631000
C	-1.23182700	-3.13323100	0.24818700	H	1.60295800	1.27911700	1.69651800
C	-0.00000100	-2.49476300	0.03804400	H	3.65845900	0.13720700	2.34044400
C	1.21279600	4.44348900	-0.75556900	H	3.75605600	-3.43951300	1.33631200
C	0.00000400	5.07929300	-1.01832900	H	5.83685300	-2.36595500	0.61442100
C	-1.21279100	4.44349500	-0.75556700	H	3.65846800	-0.13720200	-2.34044800
C	1.21279600	-4.44350900	0.75550100	H	1.60296300	-1.27911700	-1.69653200
C	-1.21279100	-4.44351400	0.75549900	H	-0.00000300	1.46095000	0.28906900
C	0.00000400	-5.07932200	1.01824100	H	-0.00000300	-1.46093300	-0.28904300
C	-2.49951400	-2.44876100	-0.11631800	H	2.14460300	4.97991600	-0.90855500
C	-2.51760300	-1.50515700	-1.15781400	H	0.00000600	6.09800200	-1.39752800
C	-3.69149400	-0.87414800	-1.54404900	H	-2.14459600	4.97992600	-0.90855000
C	-4.91704700	-1.16228300	-0.92245600	H	2.14460400	-4.97993800	0.90846700
C	-4.90688100	-2.10660600	0.11753300	H	-2.14459700	-4.97994800	0.90846300
C	-3.72399400	-2.72713300	0.51634300	H	0.00000600	-6.09804300	1.39740500
C	-6.18287000	-0.60671000	-1.48311200	H	-1.60296400	-1.27912500	-1.69653500
C	-6.29757900	-0.69118400	-2.87412100	H	-3.65847000	-0.13721100	-2.34045000
C	-7.49054000	-0.41675800	-3.55328100	H	-5.83685300	-2.36596800	0.61441700
C	-8.62677600	-0.15518000	-2.81924900	H	-3.75605500	-3.43952600	1.33630700
C	-8.56660200	-0.06818200	-1.41166000	H	-5.44467700	-1.05119800	-3.44030200
C	-9.79562600	0.01972300	-0.67718700	H	-7.52978100	-0.48905000	-4.63658600

H	-9.59239000	-0.04426100	-3.30637000	H	-5.44466400	1.05121100	3.44031000
H	-10.72734800	0.04441000	-1.23667500	H	-5.83686100	2.36598000	-0.61440100
H	-10.72734100	-0.04442900	1.23671200	H	-3.75606800	3.43953400	-1.33630500
H	-9.59237300	0.04425400	3.30640100	H	-1.60296000	1.27912600	1.69652200
H	-7.52976000	0.48905700	4.63660600	H	-3.65846100	0.13721700	2.34044700

9. Kinetic study of racemization barrier of **3c**

HPLC analysis was conducted on a Shimadzu Prominence 2000 instrument equipped with a CHIRALPAK® IF-3 column (eluent: *n*-hexane/dichloromethane = 75:25, 1.0 mL·s⁻¹, 25 °C, Detector: PDA Ch2 315nm 4nm). (The chiral resolution of **3a** by chiral HPLC was failed.)

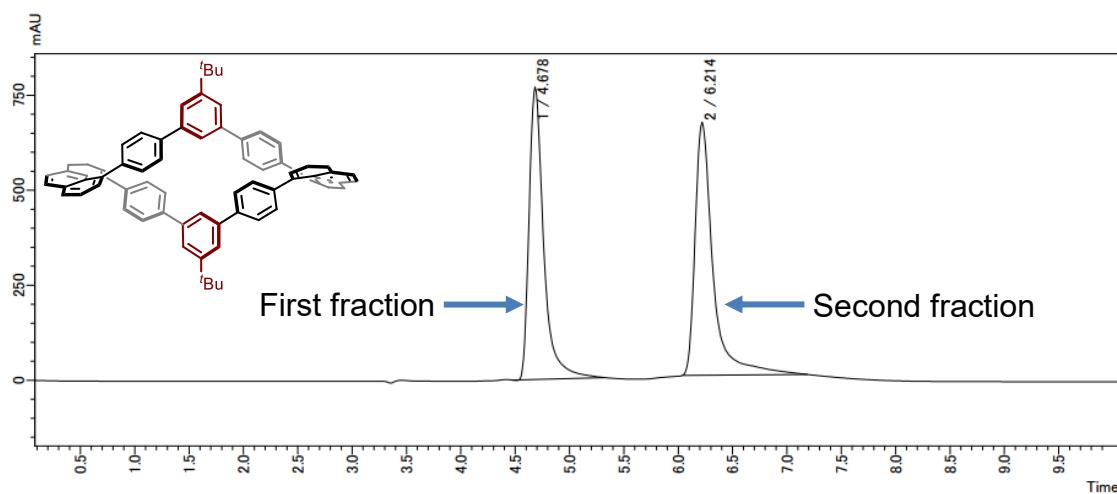


Figure S12. The HPLC analysis spectra

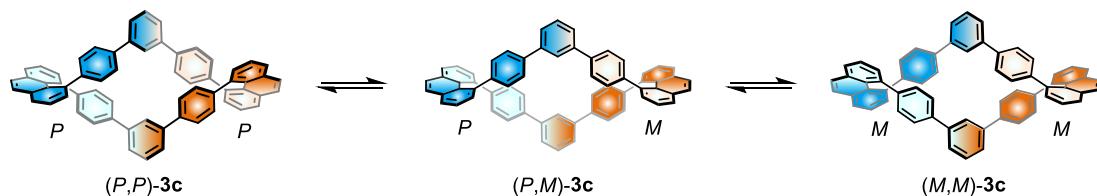
Table S16. Erosion in *e.r.* of **3c** in toluene.

* The *tert*-butyl groups are omitted for clarity.

	0 mins	90 mins	180 mins		
	97.6:2.4	97.3:2.7	94.7:5.3		
85 °C	0 mins	30 mins	60 mins	120 mins	180 mins
	97.6:2.4	95.1:4.9	88.9:11.1	81.0:19.0	73.6:26.4
100 °C	0 mins	45 mins	90 mins	135 mins	180 mins
	97.6:2.4	83.0:17.0	73.0:27.0	64.8:35.2	61.3:38.7
105 °C	0 mins	27 mins	53 mins	83 mins	114 mins
	97.6:2.4	78.6:21.4	68.7:31.3	61.2:38.8	56.8:43.2
111 °C	0 mins	27 mins	53 mins	83 mins	114 mins
	97.6:2.4	78.6:21.4	68.7:31.3	61.2:38.8	56.8:43.2

The activation barrier for racemization of **3c** was determined according to the literature method ($\Delta G^\ddagger = 31.0 \text{ kJ mol}^{-1}$ at 298 K and 1 atm).⁹

Table S17. Erosion in *e.r.* of **3c** over time in toluene.



* The *tert*-butyl groups are omitted for clarity.

Erosion in <i>e.r.</i> of 3c over time at 100 °C (373.15 K) in toluene					
Time/h	Time/s	% major ent.	% minor ent.	<i>ee</i>	$\ln([ee]_t/[ee]_0)$
0	0	97.6	2.4	95.2	0
0.5	1800	95.1	4.9	90.2	-0.05395
1.0	3600	88.9	11.1	77.8	-0.2018
2.0	7200	81.0	19.0	62.0	-0.4288
3.0	10800	73.6	26.4	47.2	-0.7016
Erosion in <i>e.r.</i> of 3c over time at 105 °C (378.15 K) in toluene					
Time/h	Time/s	% major ent.	% minor ent.	<i>ee</i>	$\ln([ee]_t/[ee]_0)$
0	0	97.6	2.4	95.2	0
45	2700	83.0	17.0	66.0	-0.366
90	5400	73.0	27.0	46.0	-0.727
135	8100	64.8	35.2	29.6	-1.17
180	10800	61.3	38.7	22.6	-1.44
Erosion in <i>e.r.</i> of 3c over time at 111 °C (384.15 K) in toluene					
Time/h	Time/s	% major ent.	% minor ent.	<i>ee</i>	$\ln([ee]_t/[ee]_0)$
0	0	97.6	2.4	95.2	0
27	1620	78.6	21.4	57.2	-0.509
53	3180	68.7	31.3	37.4	-0.934
83	4980	61.2	38.8	22.4	-1.45
114	6840	56.8	43.2	13.6	-1.95

To determine the chiral inversion barrier of **3c**, a kinetic study of the thermal racemization of **3c** was performed. The (*P,P*)-**3c** (95.2% *ee*) was obtained from HPLC, and the temperature-dependent decrease of the *ee* of **3c** in the toluene solution was monitored by HPLC. A reversible first-order rate constant k (s^{-1}) at various temperatures was estimated using Equation (1): $\ln([ee]_t/[ee]_0) = -2kt$, where $[ee]_0$ is the initial *ee* ratio of enantioenriched **3c** and $[ee]_t$ is the *ee* ratio at a certain time during the racemization.⁹

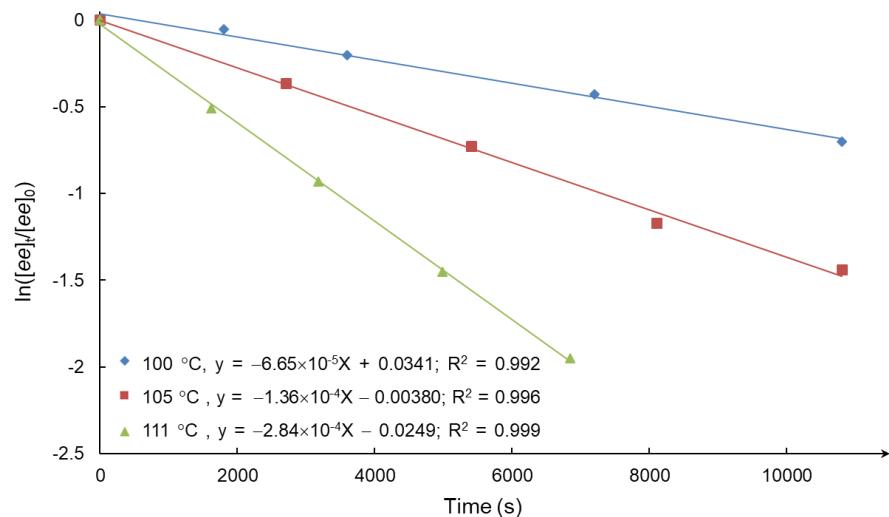


Figure S13. Temperature-dependent plots of the decreasing *ee* ratio of enantioenriched **3c** in toluene.

Using these data, an Eyring plot was constructed according to Equation (2): $\ln(k/T) = -\Delta H^\ddagger/RT + [\ln(k_B/h) + \Delta S^\ddagger/R]$, where R is the gas constant, T the measured temperature, ΔH^\ddagger the activation enthalpy, k_B the Boltzmann constant, h the Plank constant, and ΔS^\ddagger the activation entropy. This plot provided the following activation parameters: $\Delta H^\ddagger = 36.6 \text{ kcal}\cdot\text{mol}^{-1}$, $\Delta S^\ddagger = 18.7 \text{ cal}\cdot\text{mol}^{-1}$, and $\Delta G^\ddagger = 31.0 \text{ kcal}\cdot\text{mol}^{-1}$ at 298 K and 1 atm.

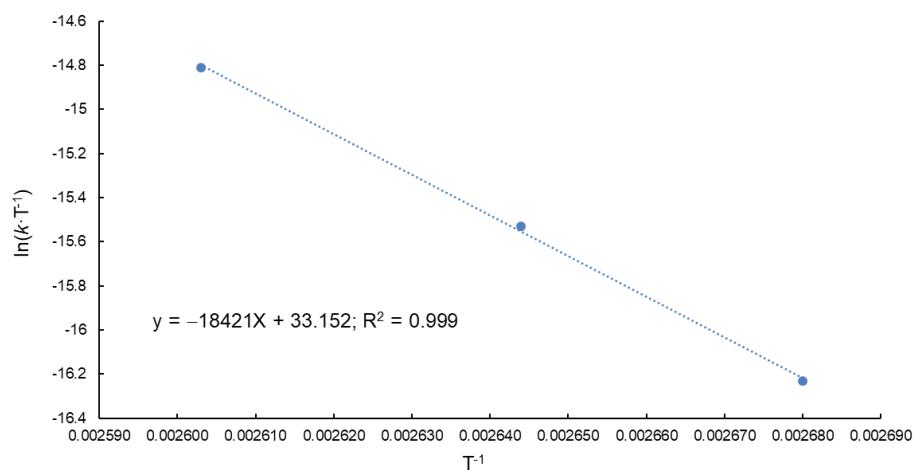


Figure S14. The Eyring plot for the determination of the racemization barrier.

Base on the Equation (2), the half-life of the racemization (in toluene at 85 °C) is obtained. $k_{\text{ent}} = 4.0 \times 10^{-6} \text{ s}^{-1}$; $t_{1/2}^{\text{rac}} = \ln(2)/(2k_{\text{ent}}) = 24 \text{ h}$.

10. Photophysical properties

UV/vis absorption spectra were recorded on a Shimadzu UV-3510 spectrometer with a resolution of 0.5 nm. Emission spectra were measured with an FP-6600 Hitachi spectrometer with a resolution of 0.2 nm. Circular dichroism spectra were measured with a JASCO FT/IR6100. Absolute fluorescence quantum yields were determined with a Hamamatsu C9920-02 calibrated integrating sphere system.

Table S18: Photophysical data for the macrocycles. The quantum yields (Φ_{fl}) were obtained by irradiation at 310 nm.

Compound	UV-vis		Fluorescence			
	λ_{max} (nm)	$\log \epsilon$	DCM solution		solid state	
			λ_{max} (nm)	Φ_{fl}	λ_{max} (nm)	Φ_{fl}
1	298	4.42	408	0.098	409	0.157
3a	308	5.02	397	0.118	—	0.155
3c	309	—	397	—	—	—
3d	306	5.11	396	0.131	420	0.166
3f	398	4.90	400	0.636	—	—
3g	307	4.86	408	0.089	416	0.074
3i	314	4.86	508	0.314	—	—
3j	353	4.44	466	0.412	445	0.140

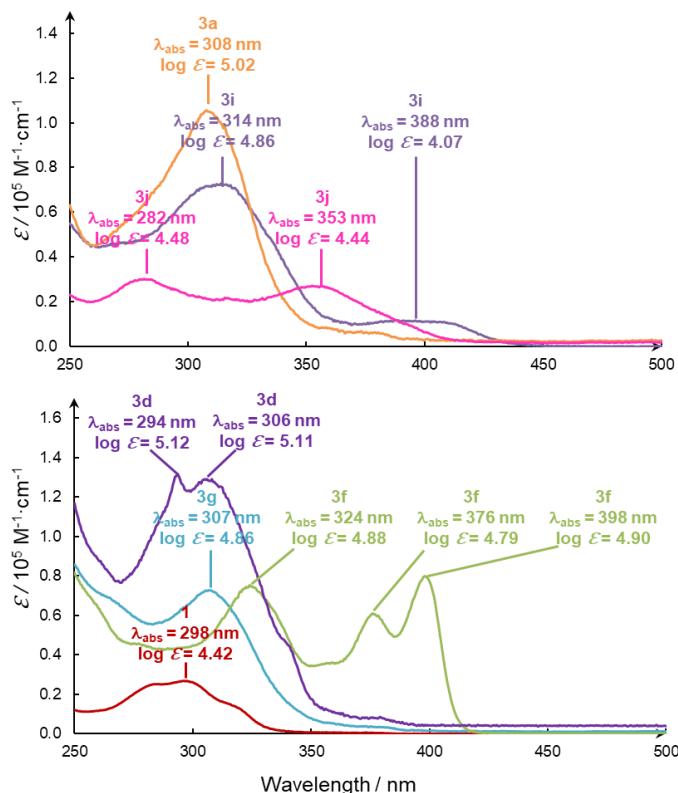


Figure S15. UV/vis absorption spectra of **1**, **3a**, **3d**, **3f**, **3g**, **3i**, and **3j** in CH_2Cl_2 .

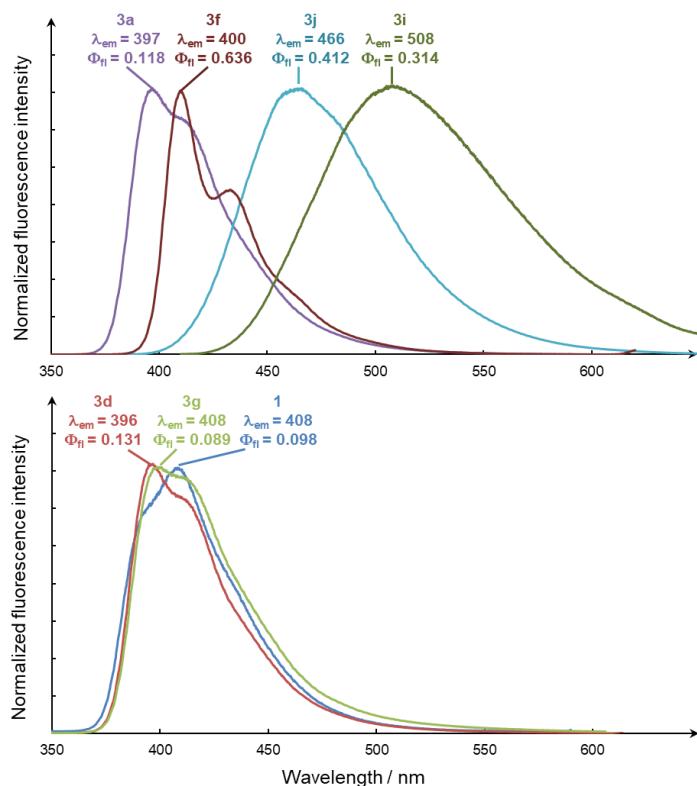


Figure S16. Fluorescence spectra of **1**, **3a**, **3d**, **3f**, **3g**, **3i**, and **3j** in CH_2Cl_2 . The fluorescence spectra were obtained by irradiation at 300 nm (**1**), 310 nm (**3a**, **3d**, **3f**, **3g**), 355 nm (**3j**) and 400 nm (**3i**).

11. Twisted intramolecular charge transfer (TICT) emission of **3j**

Table S19. UV-vis absorption and fluorescence spectra of **3j** in various solvents.

entry	solvent	UV-vis	Fluorescence		
		λ_{abs} (nm)	λ_{em} (nm)	Φ_{fl} (%)	excitation wavelength (nm)
1	<i>n</i> -Hexane	310	419	43.30	360
2	<i>c</i> -Hexane	—	421	48.25	360
3	C ₆ H ₆	—	445	54.45	360
4	C ₆ H ₅ Cl	—	466	35.54	400
5	H ₂ O	—	482	22.37	400
6	CHCl ₃	—	484	30.04	400
7	THF	310	484	35.35	400
8	DCM	314	508	31.4	400
9	CH ₃ (CH ₂) ₅ OH	—	531	18.41	400
10	DMA	—	542	26.17	400
11	DMF	—	551	19.53	400
12	EtOH	—	561	4.64	400
13	DMSO	314	563	14.22	400
14	HFIP	309	571	0.0	400
15	CH ₃ CN	—	572	3.76	400
16	MeOH	—	—	0.0	400

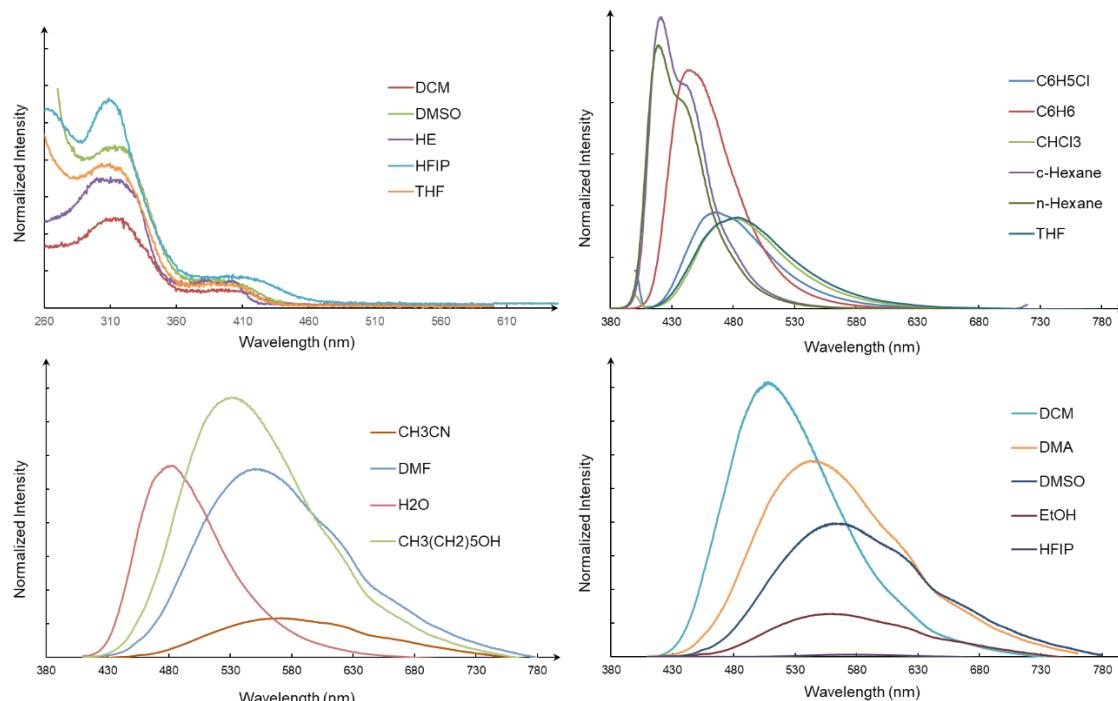


Figure S17. UV/vis absorption and fluorescence spectra of **3j** in various solvents.

Table S20. UV-vis absorption and fluorescence spectra of 3,6-diphenylnaphthalimide in various solvents.

entry	solvent	UV-vis	Fluorescence		
		λ_{abs} (nm)	λ_{em} (nm)	Φ_{fl} (%)	excitation wavelength (nm)
1	<i>n</i> -Hexane	359	393	7.36	350
2	DCM	365	408	23.55	350
3	EtOH	360	428	33.61	350
4	DMSO	—	433	0.18	350

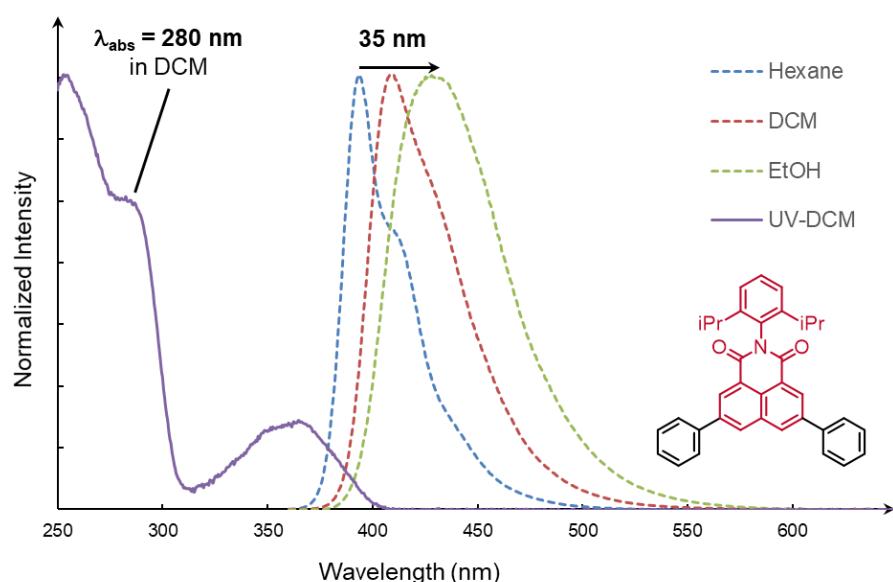


Figure S18. UV-vis absorption (in CH_2Cl_2 ; solid line) and fluorescence spectra of 3,6-diphenylnaphthalimide in various solvents (broken lines).

A twisted geometry between the donor and the acceptor promotes charge transfer causing strong solvatofluorochromism in fluorescence and large Stokes shifts.

Table S21. Solvatofluorochromism of the imides.

$\lambda_{\text{em}} (\Phi_{\text{fl}})$ in <i>n</i> -Hexane	419 (43.3)	393 (7.4)	406 (7.6)	427 (33)
$\lambda_{\text{em}} (\Phi_{\text{fl}})$ in DMF	551 (19.5)	433 (0.18) (in DMSO)	427 (74) ¹⁰	582 (13) ¹⁰

12. Circular dichroism spectra of **1c**

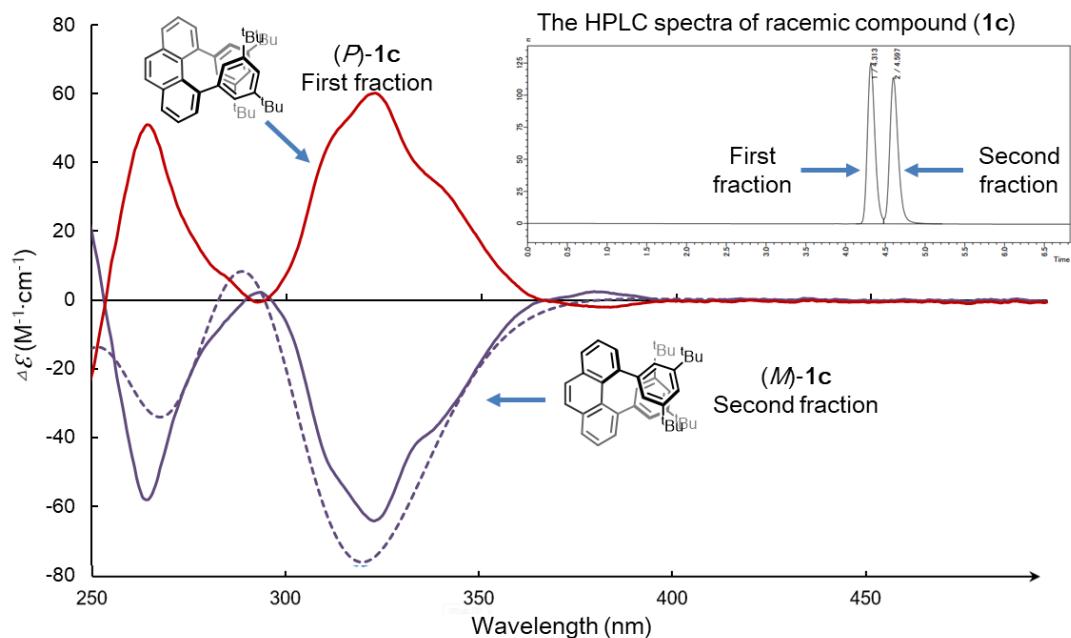


Figure S19. Circular dichroism spectra of *(P)*-**1c** (red line, the first fraction), *(M)*-**1c** (purple line, the second fraction). A simulated circular dichroism spectra of *(M)*-**1c** (purple dashed line) by M06-2X/6-31G(d).

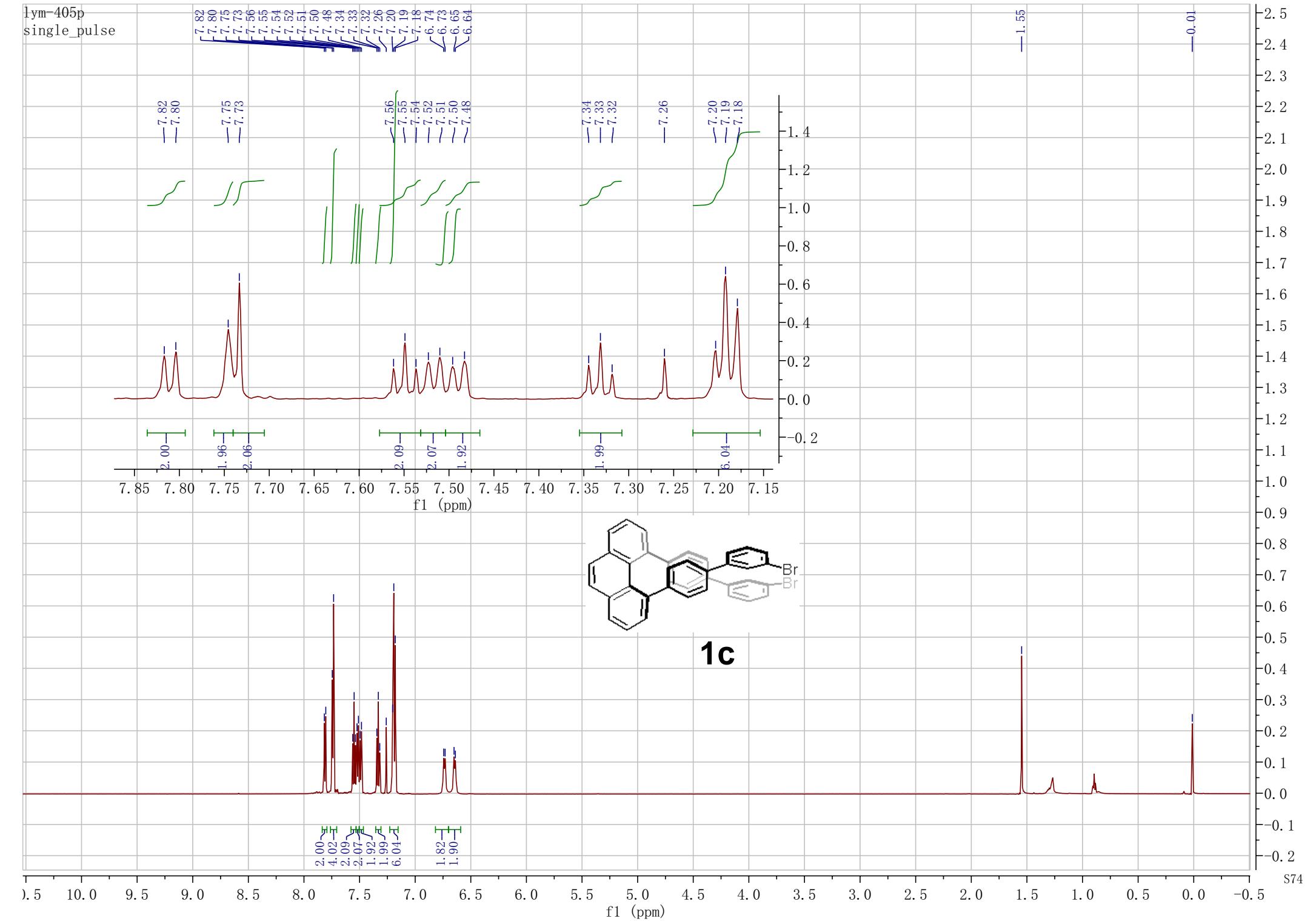
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14. NMR spectra of new compounds

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single pulse



lym-405p

single pulse decoupled gated NOE

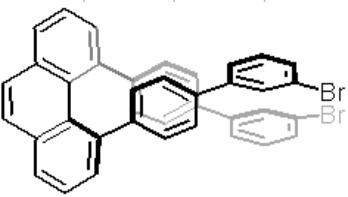
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143.31
143.27
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125.98
125.54
123.16
125.98
125.54

—123.16

2.0
1.5
1.0
0.5
0.0

77.37
77.16
76.95

**1c**

144 142 140 138 136 134 132 130 128 126 124

f1 (ppm)

210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0

f1 (ppm)

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7.5

7.0

6.5

6.0

5.5

5.0

4.5

4.0

3.5

3.0

2.5

2.0

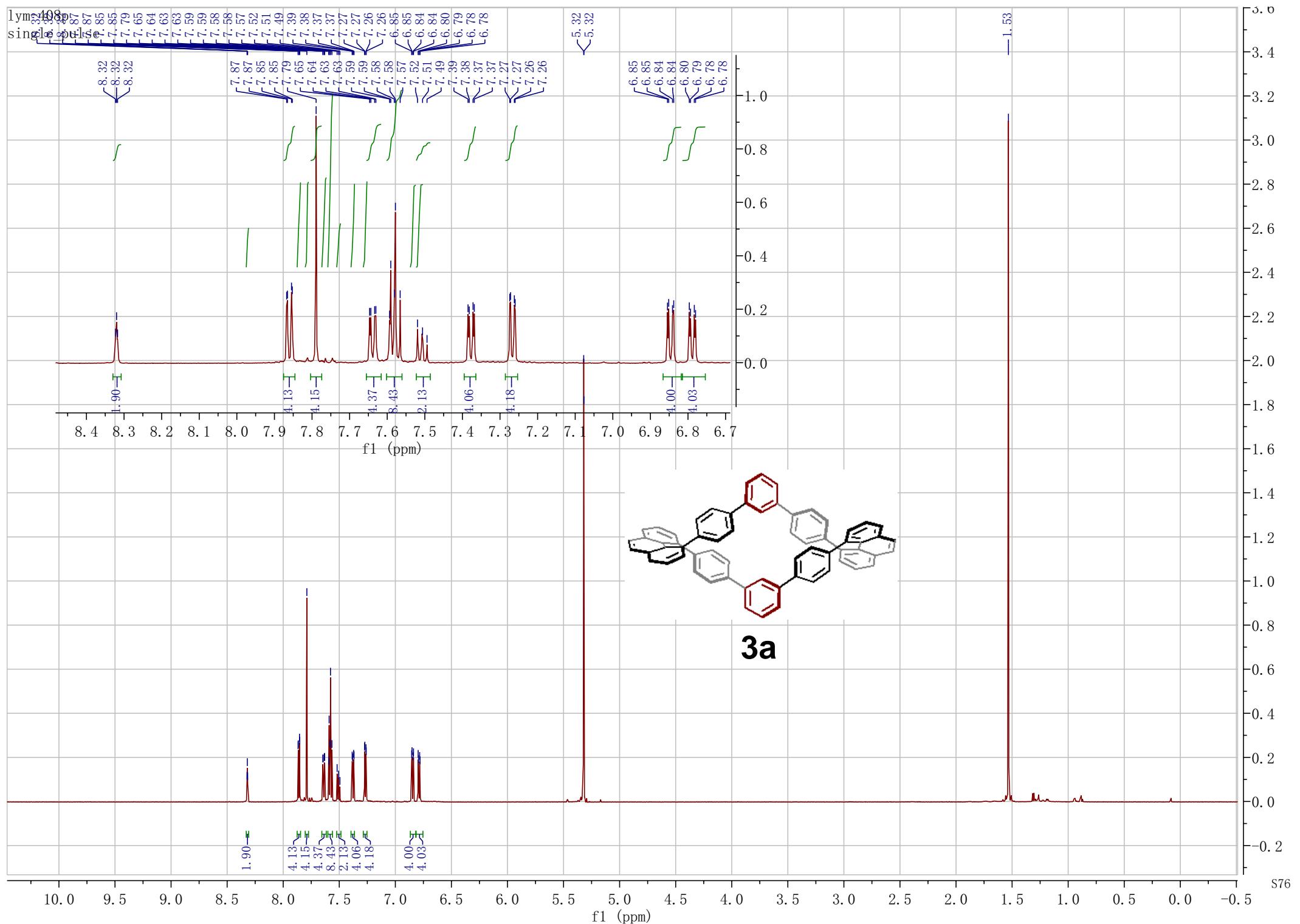
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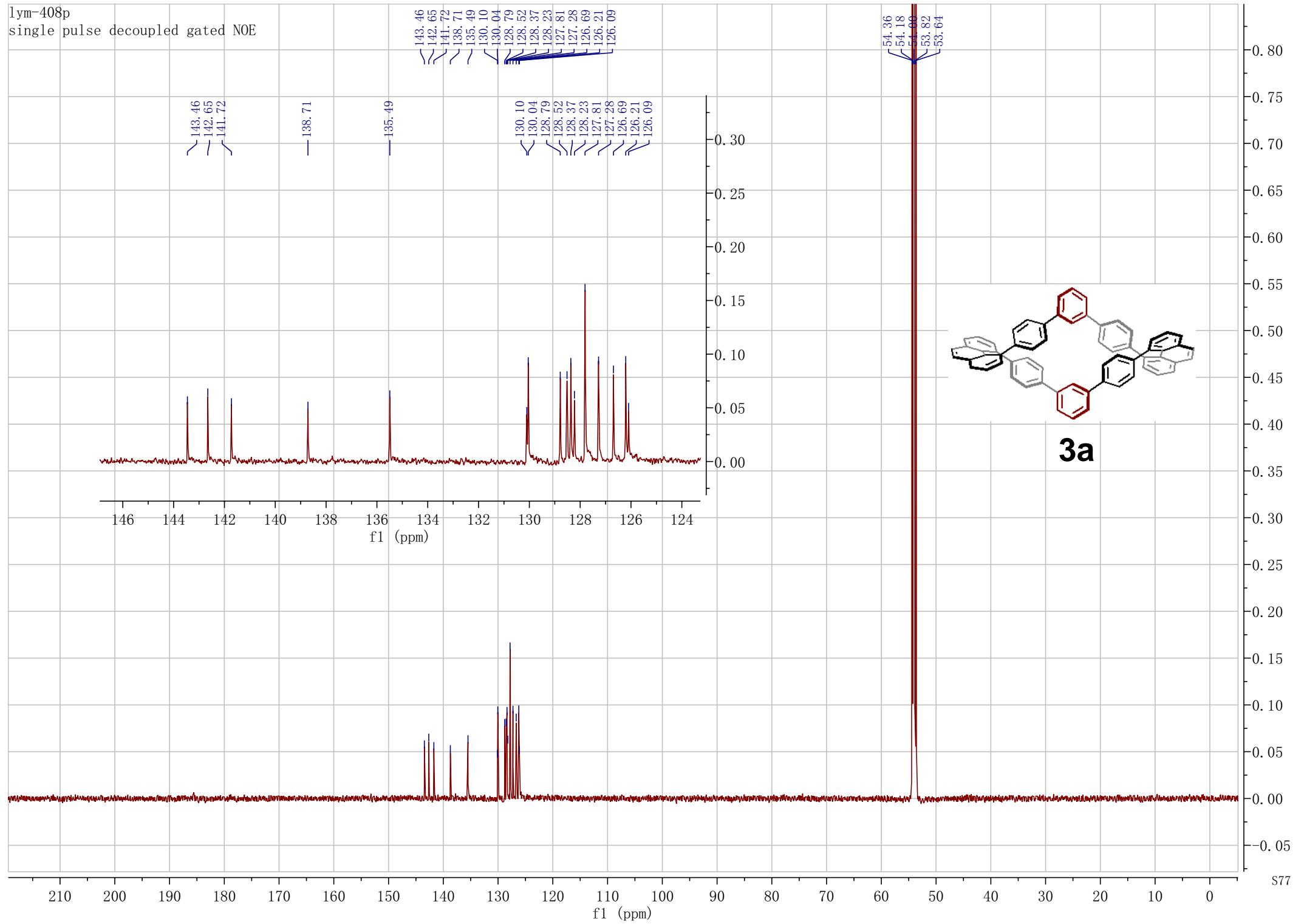
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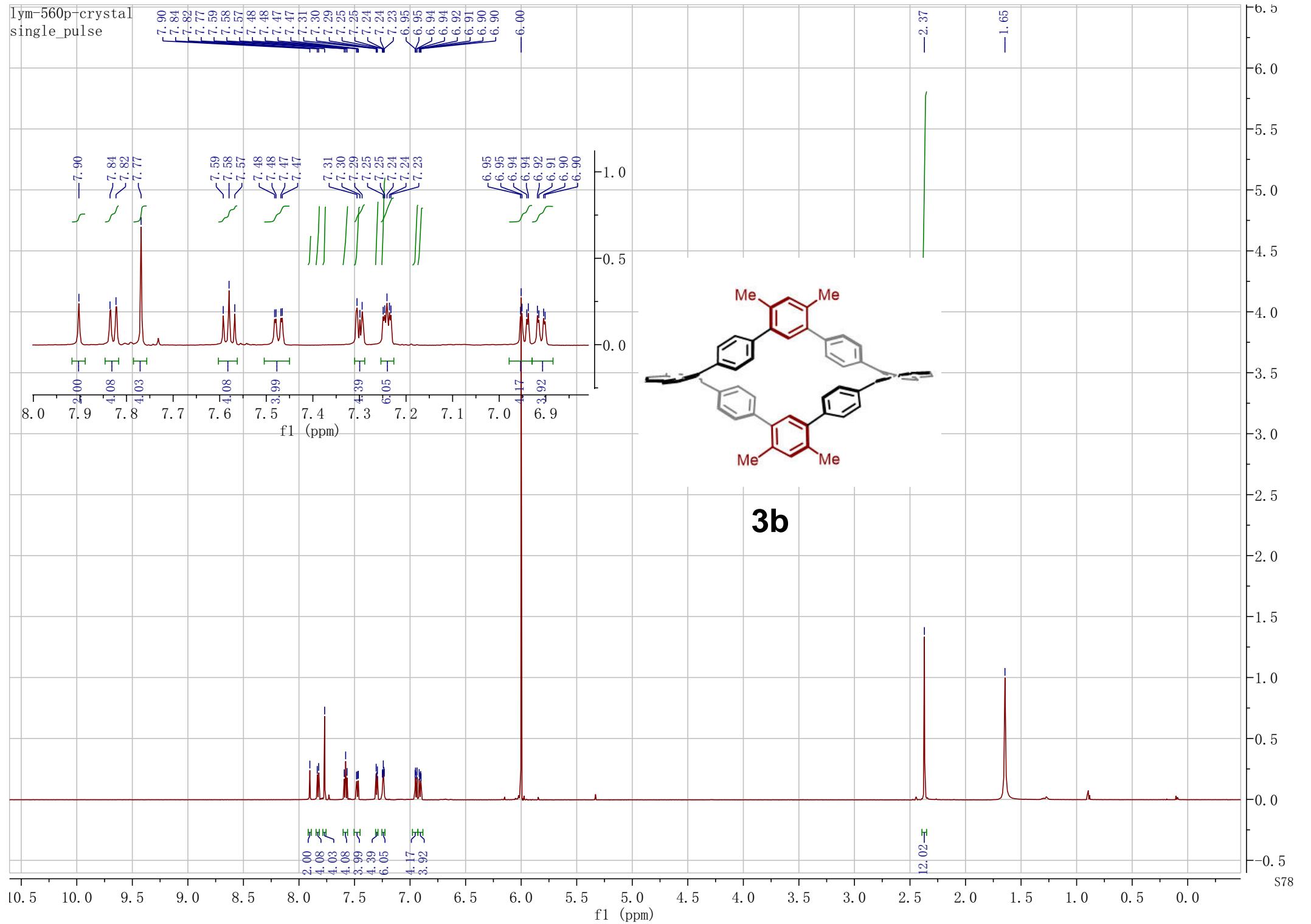
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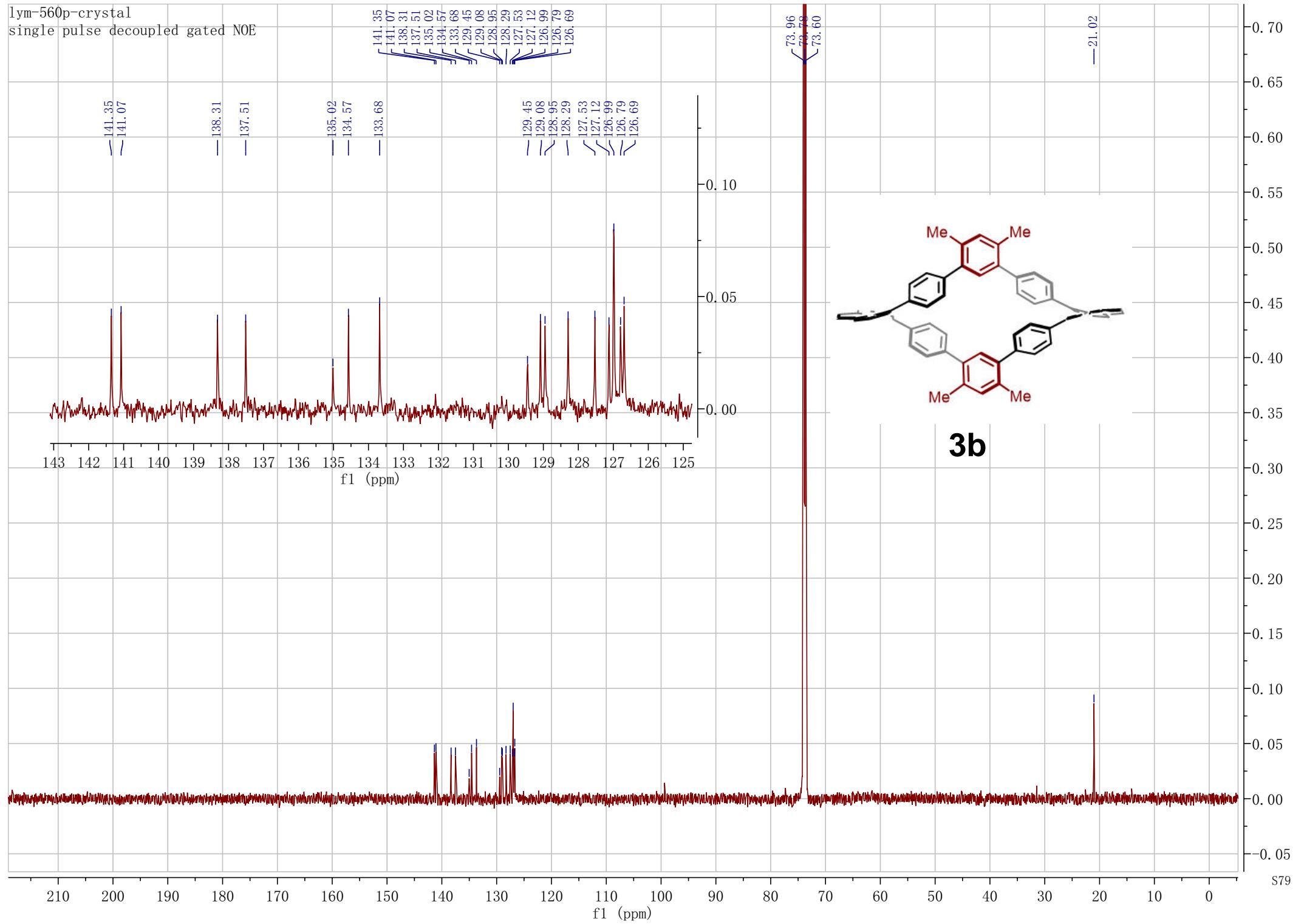
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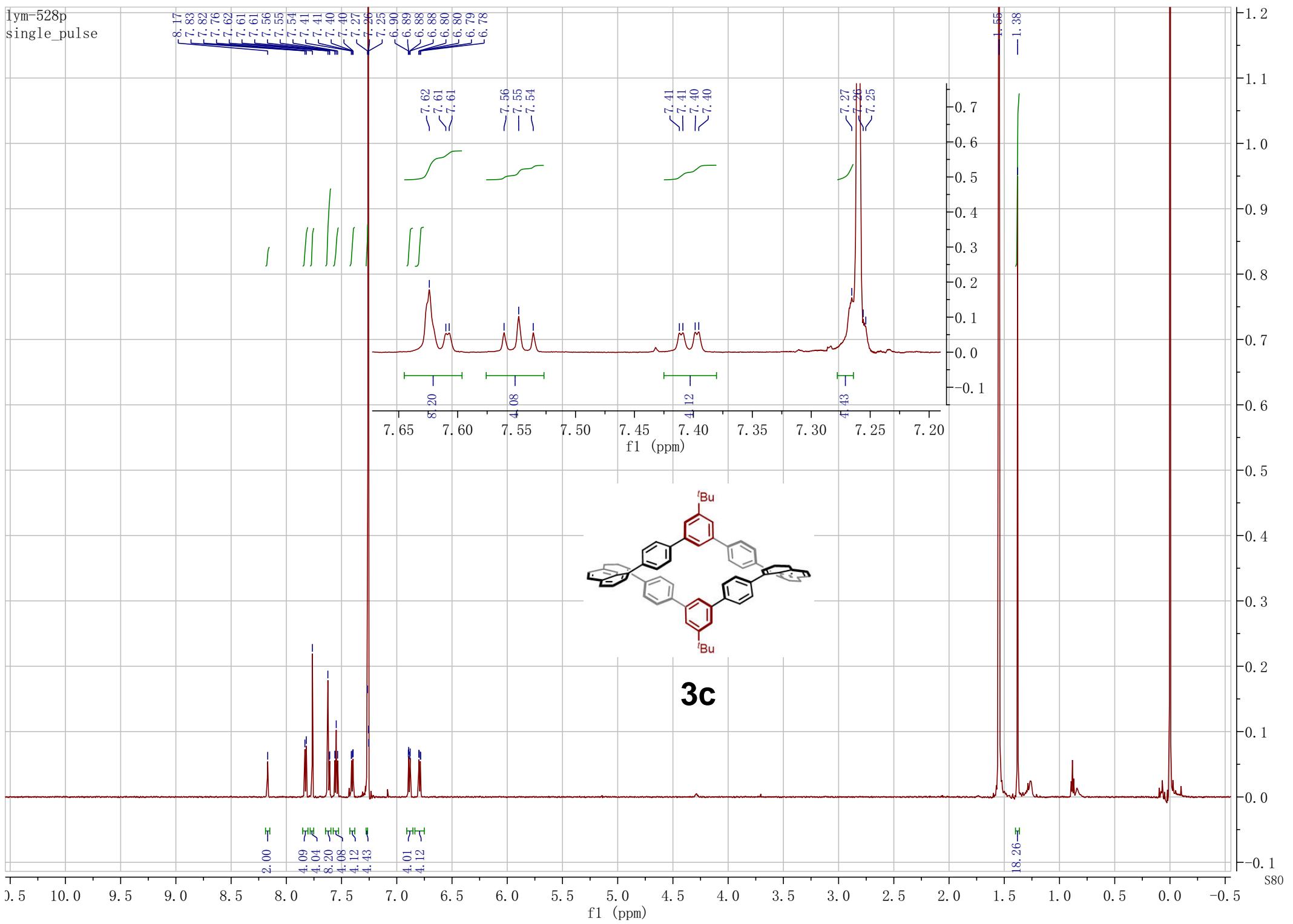


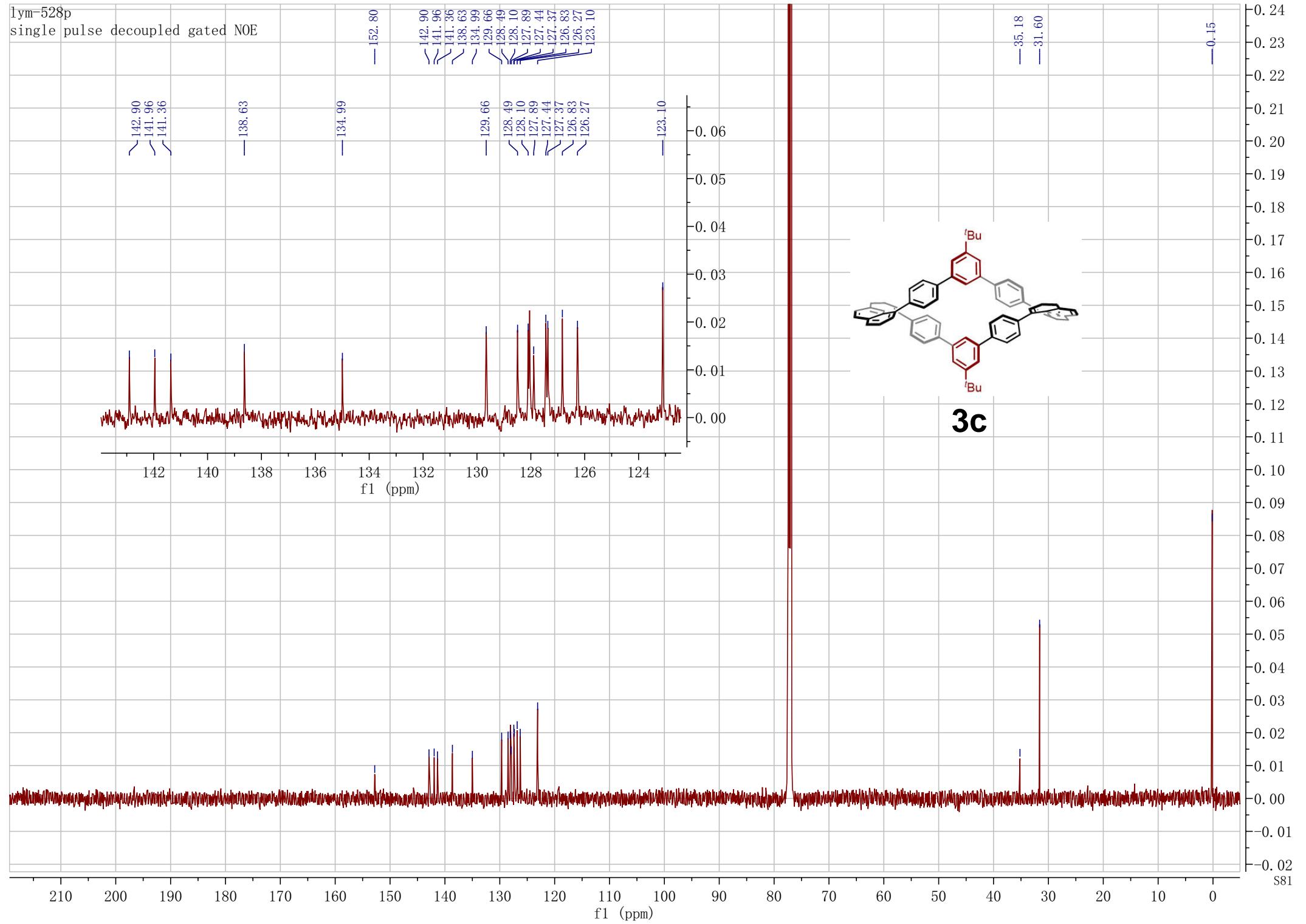
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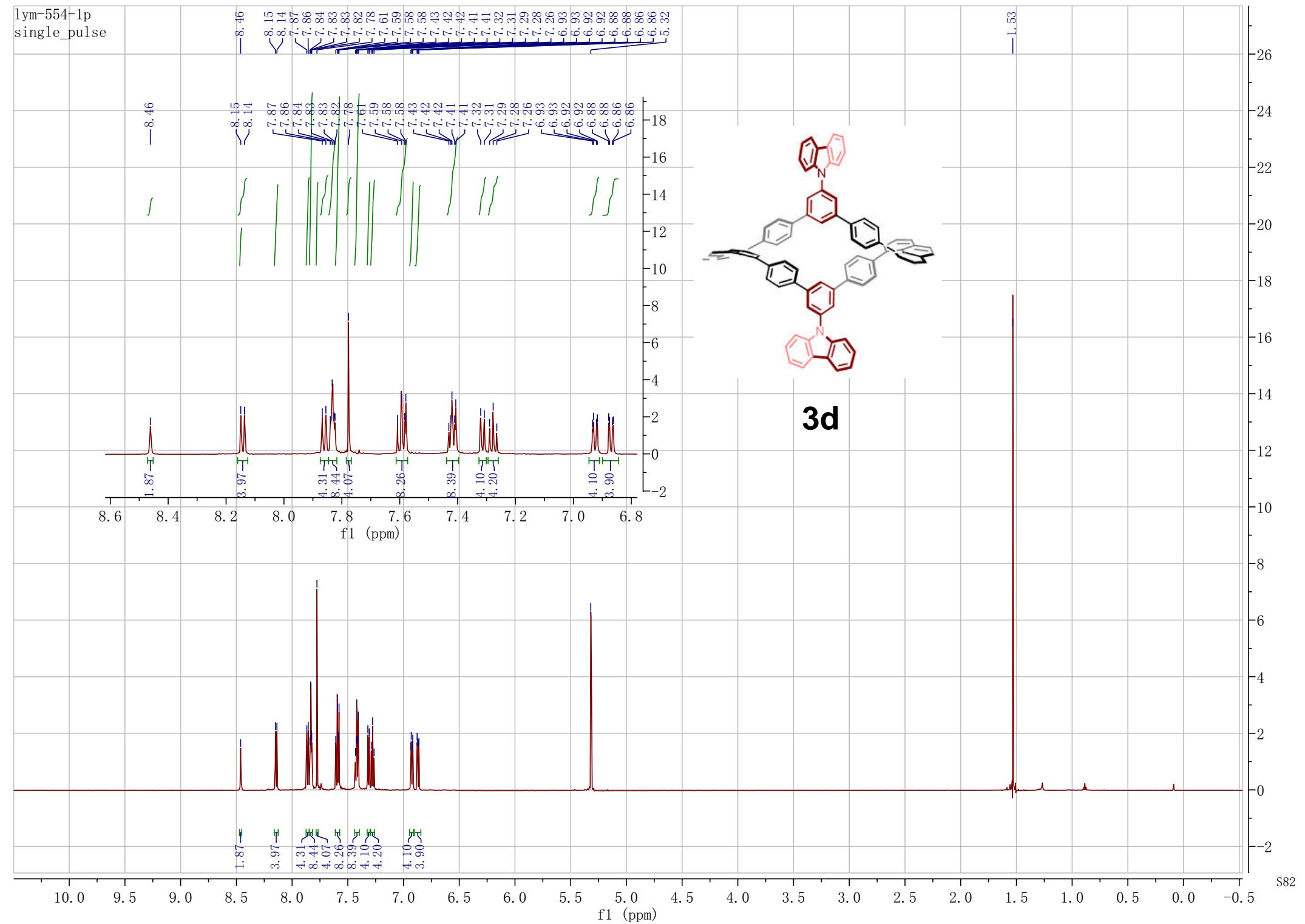


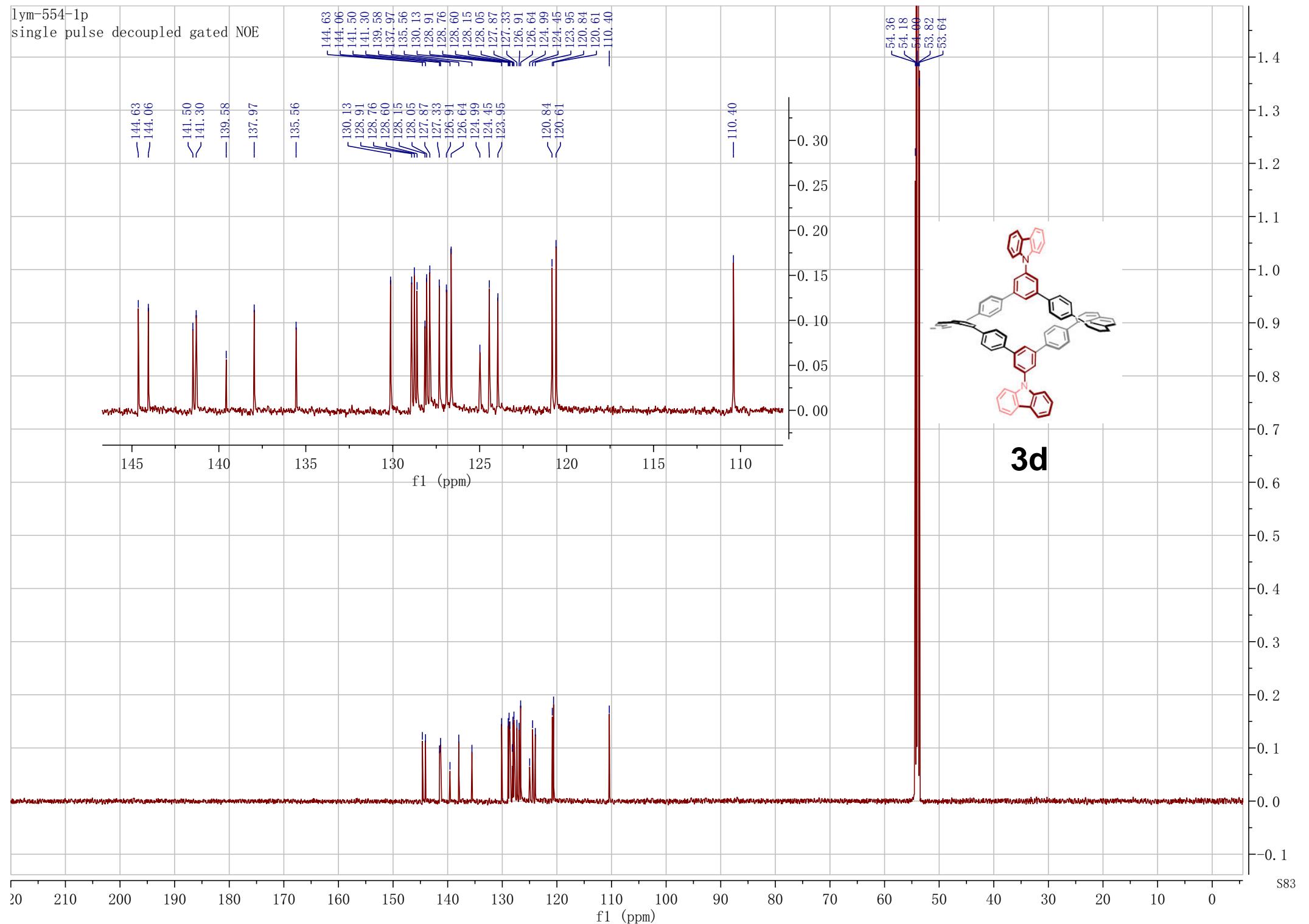
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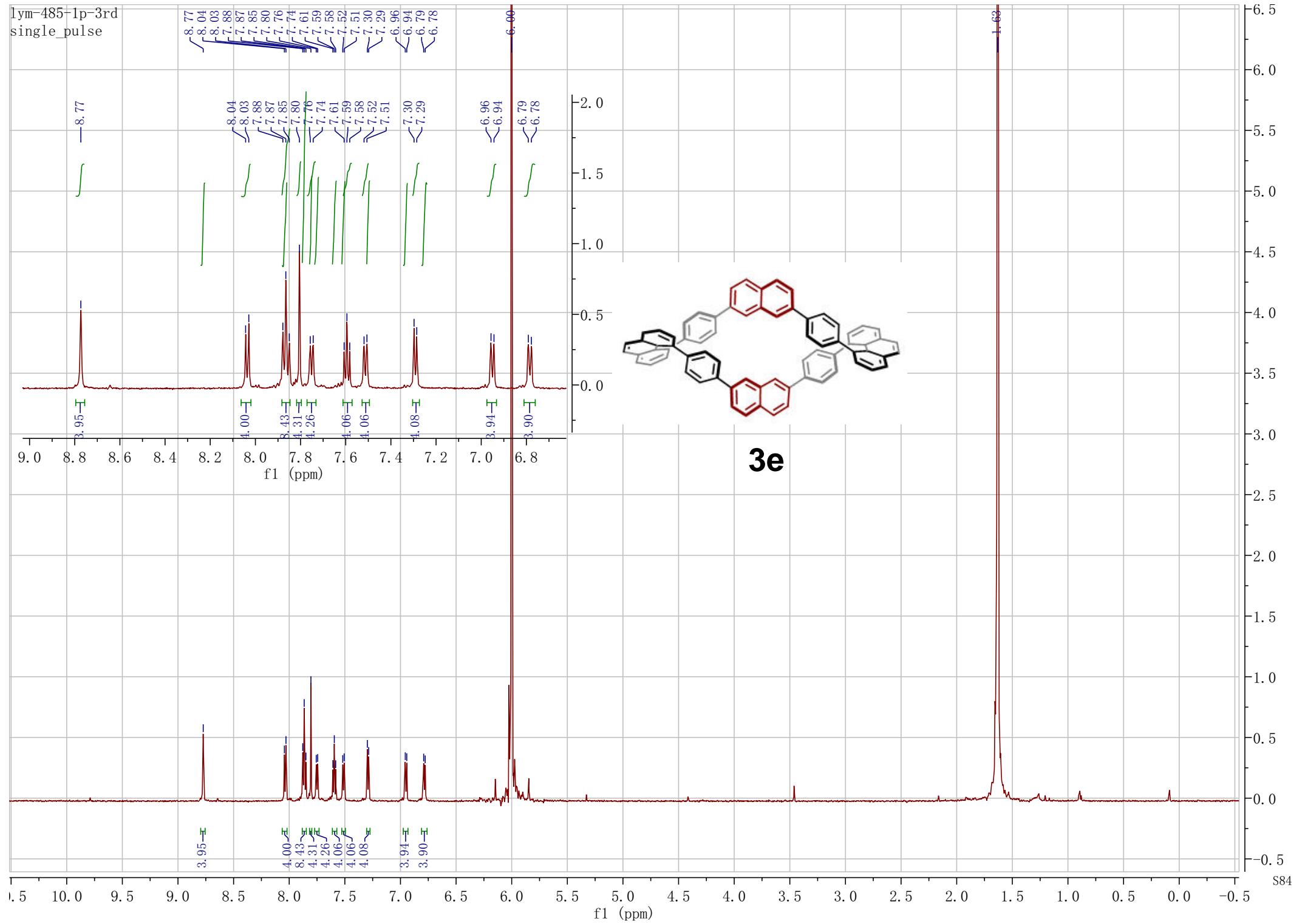




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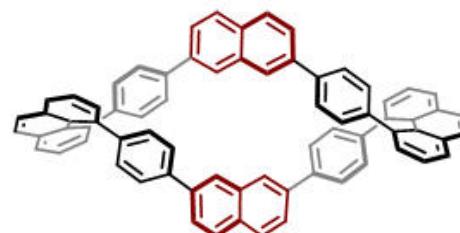
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129.71
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127.28
126.67
125.70
125.28
125.16

— 142.89
— 140.71
— 138.95
— 137.15
— 134.65
— 134.08
— 131.70

— 131.70
— 129.71
— 128.58
— 128.22
— 128.14
— 127.38
— 127.35
— 127.28
— 126.67
— 125.70
— 125.28
— 125.16

0.06
0.05
0.04
0.03
0.02
0.01
0.00

143 142 141 140 139 138 137 136 135 134 133 132 131 130 129 128 127 126 125
f1 (ppm)



3e

0.26

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0.22

0.20

0.18

0.16

0.14

0.12

0.10

0.08

0.06

0.04

0.02

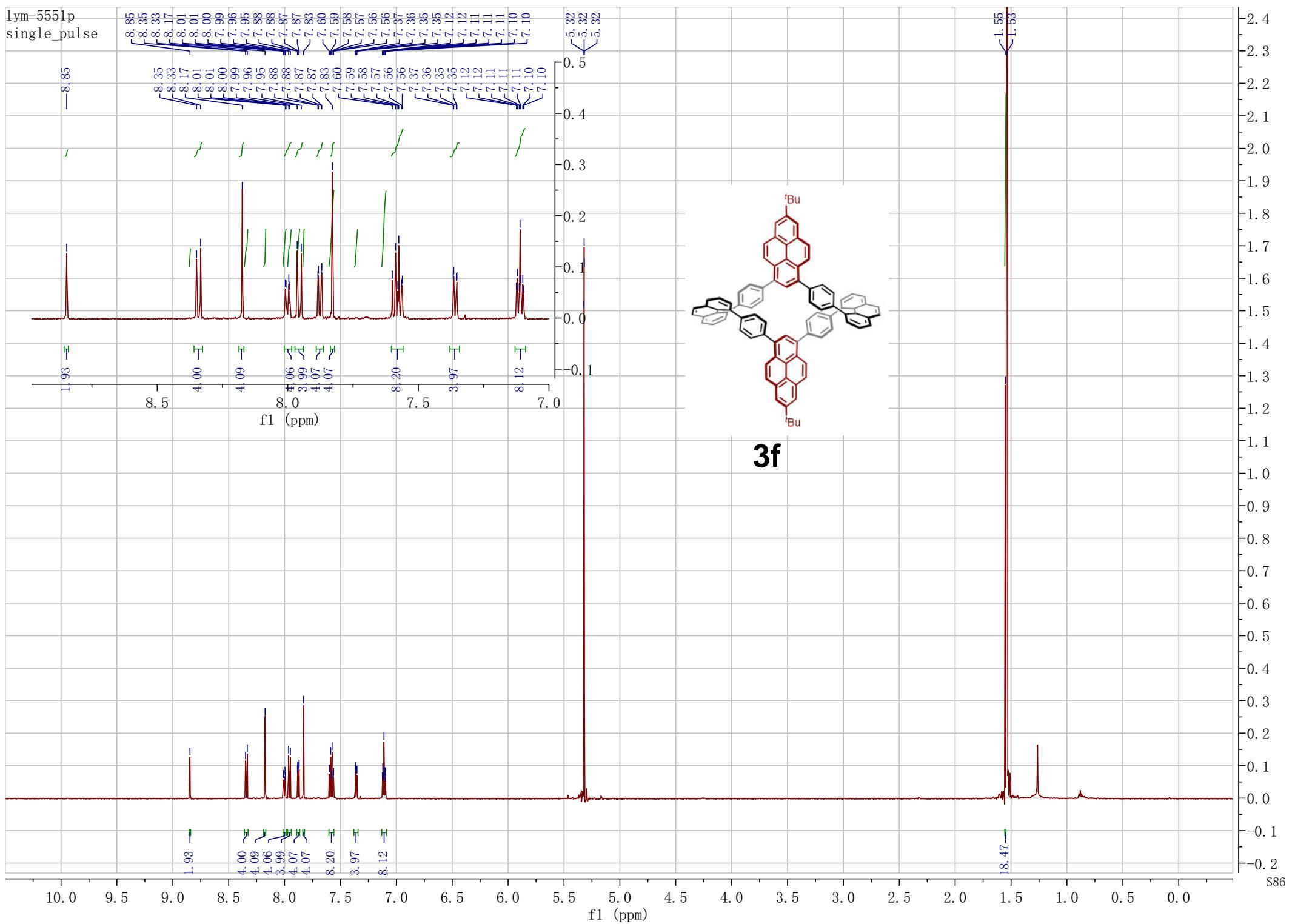
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S85

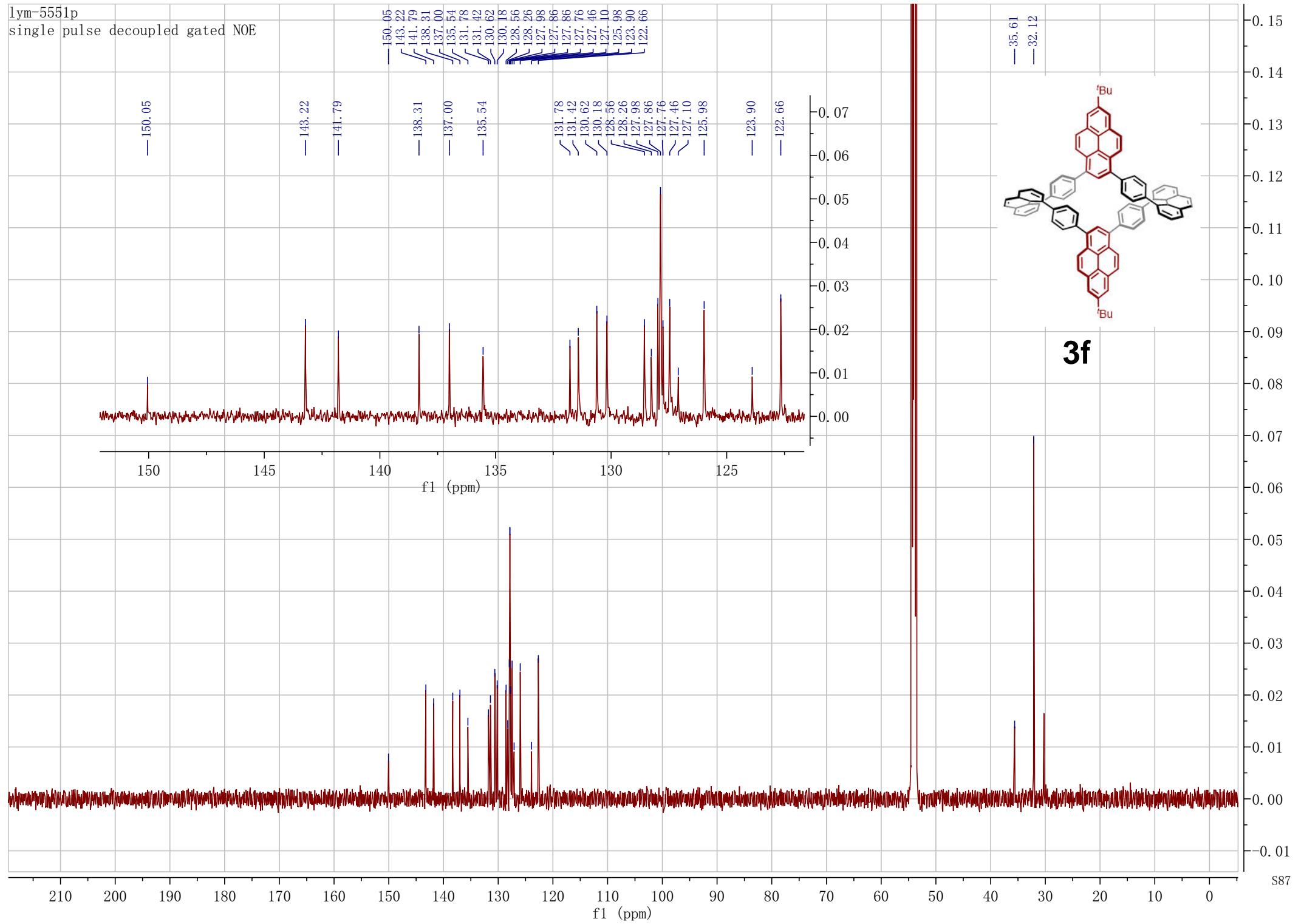
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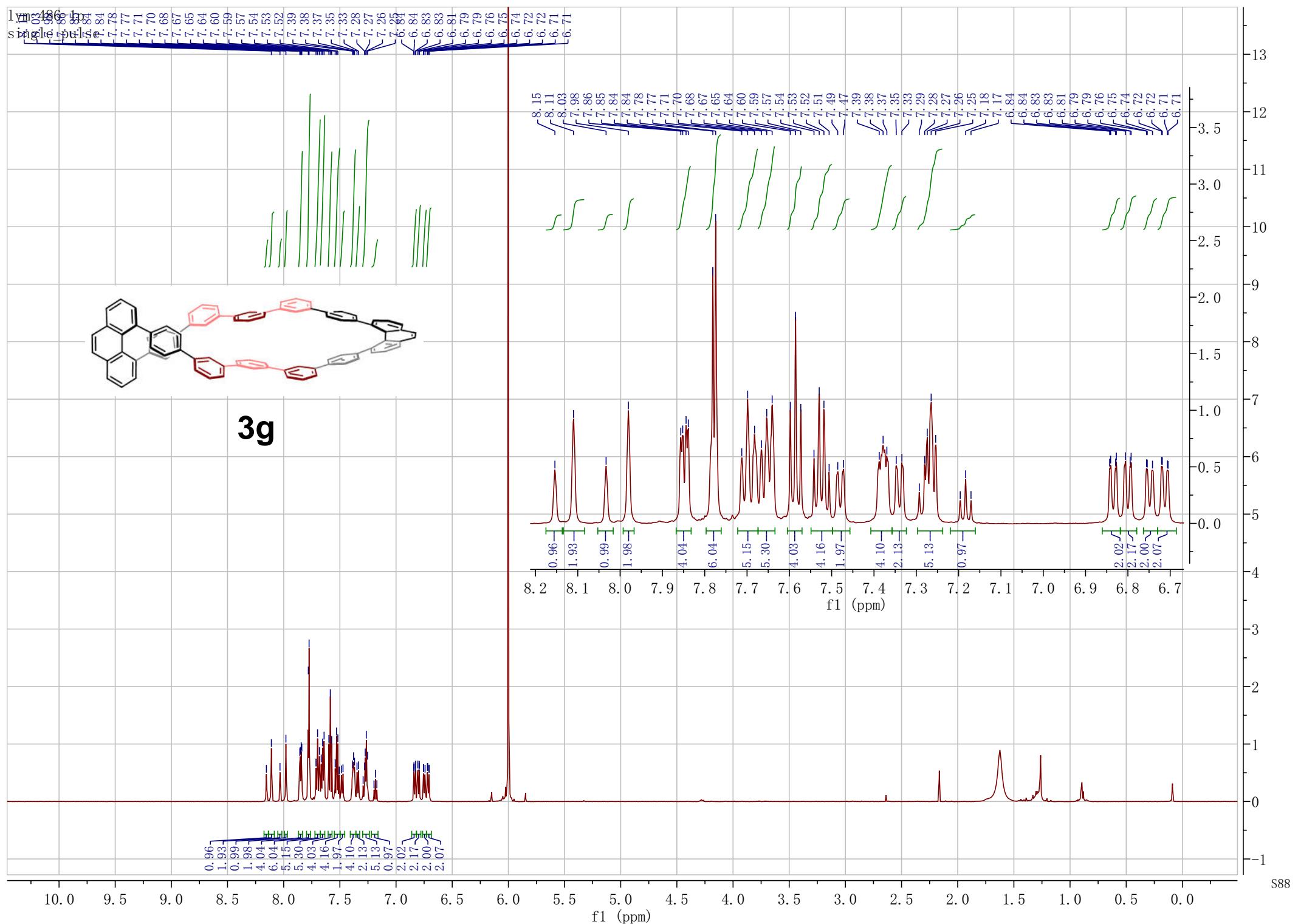
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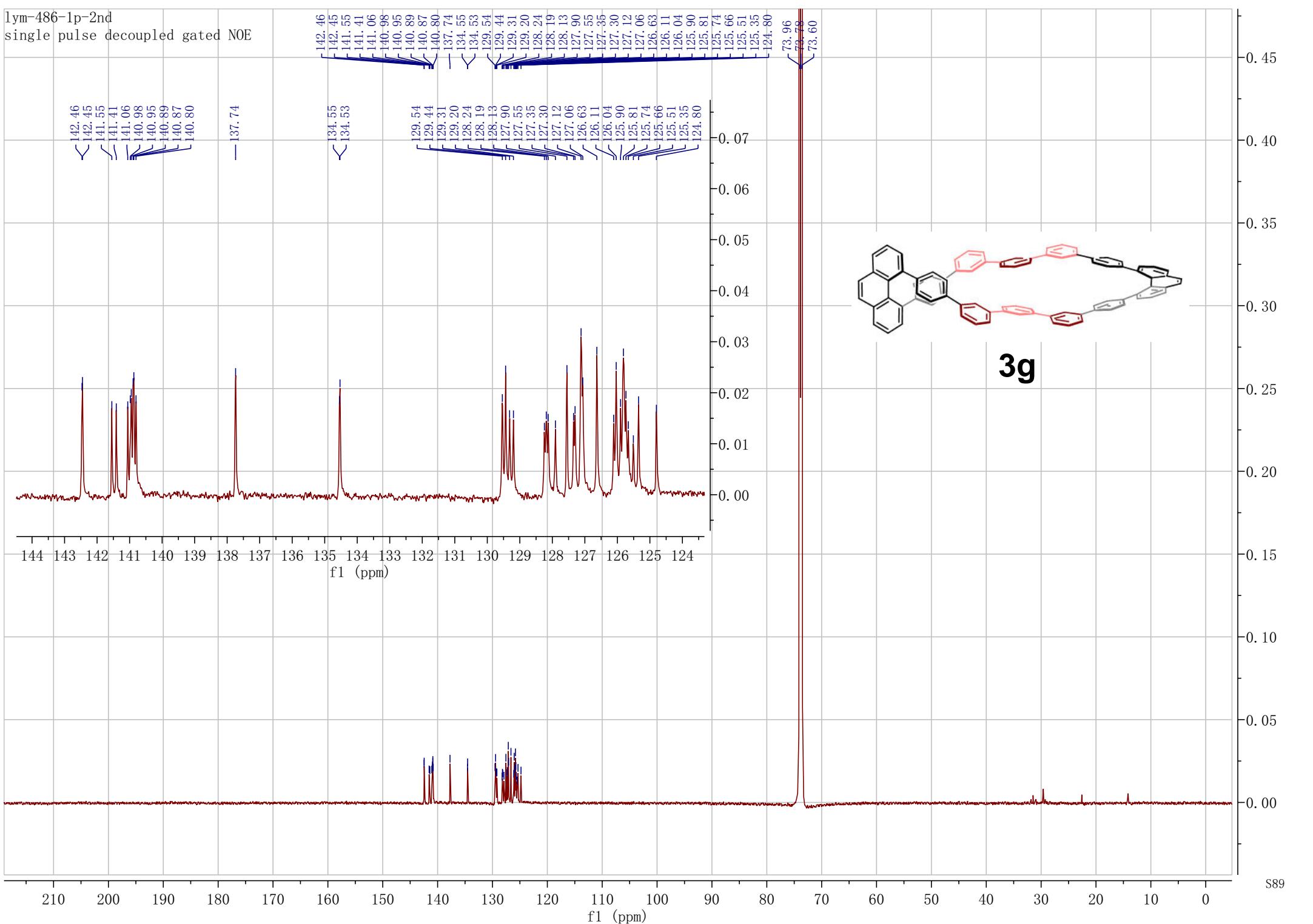


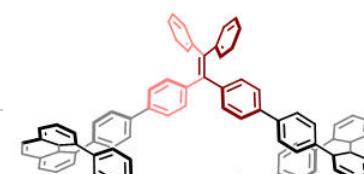
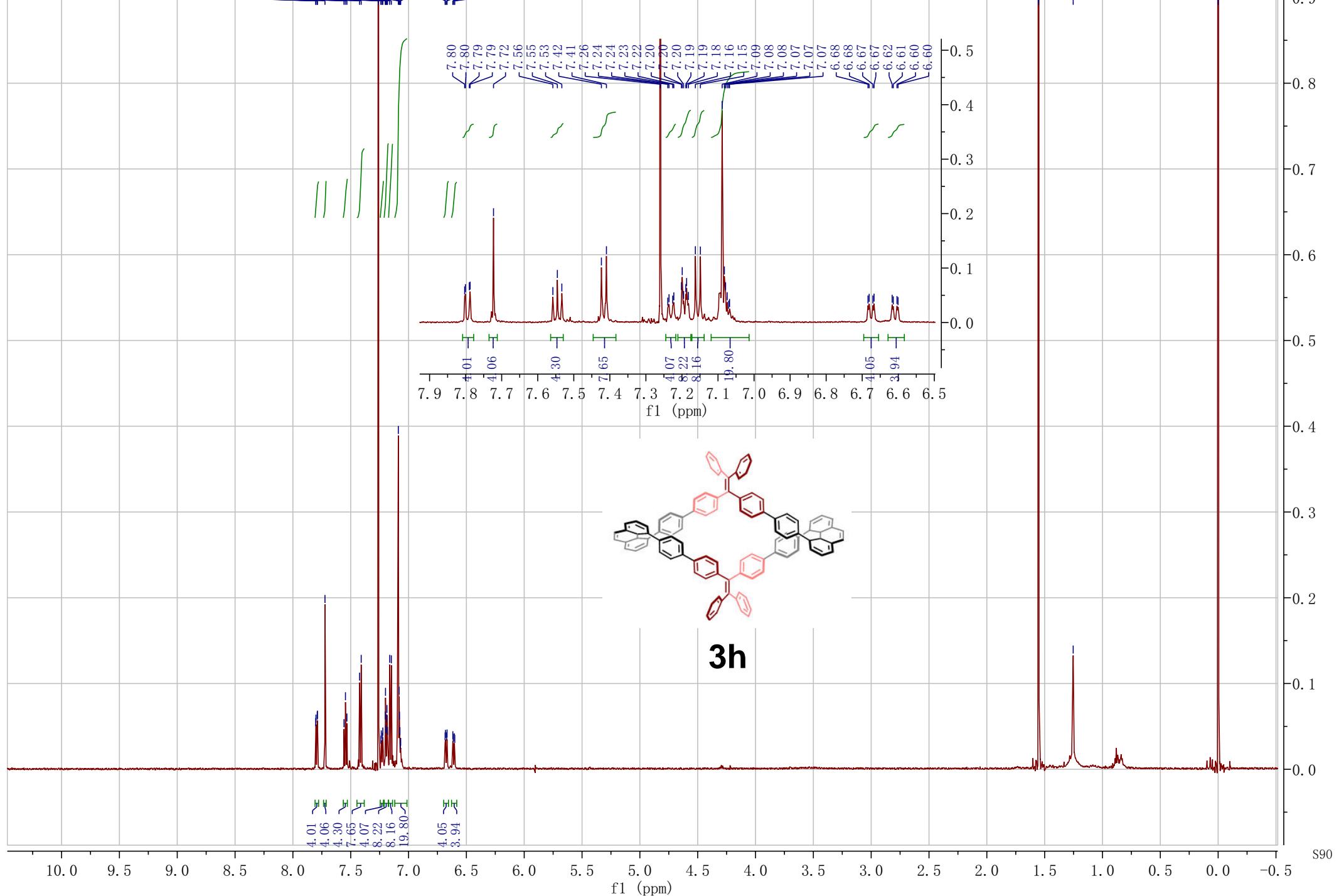
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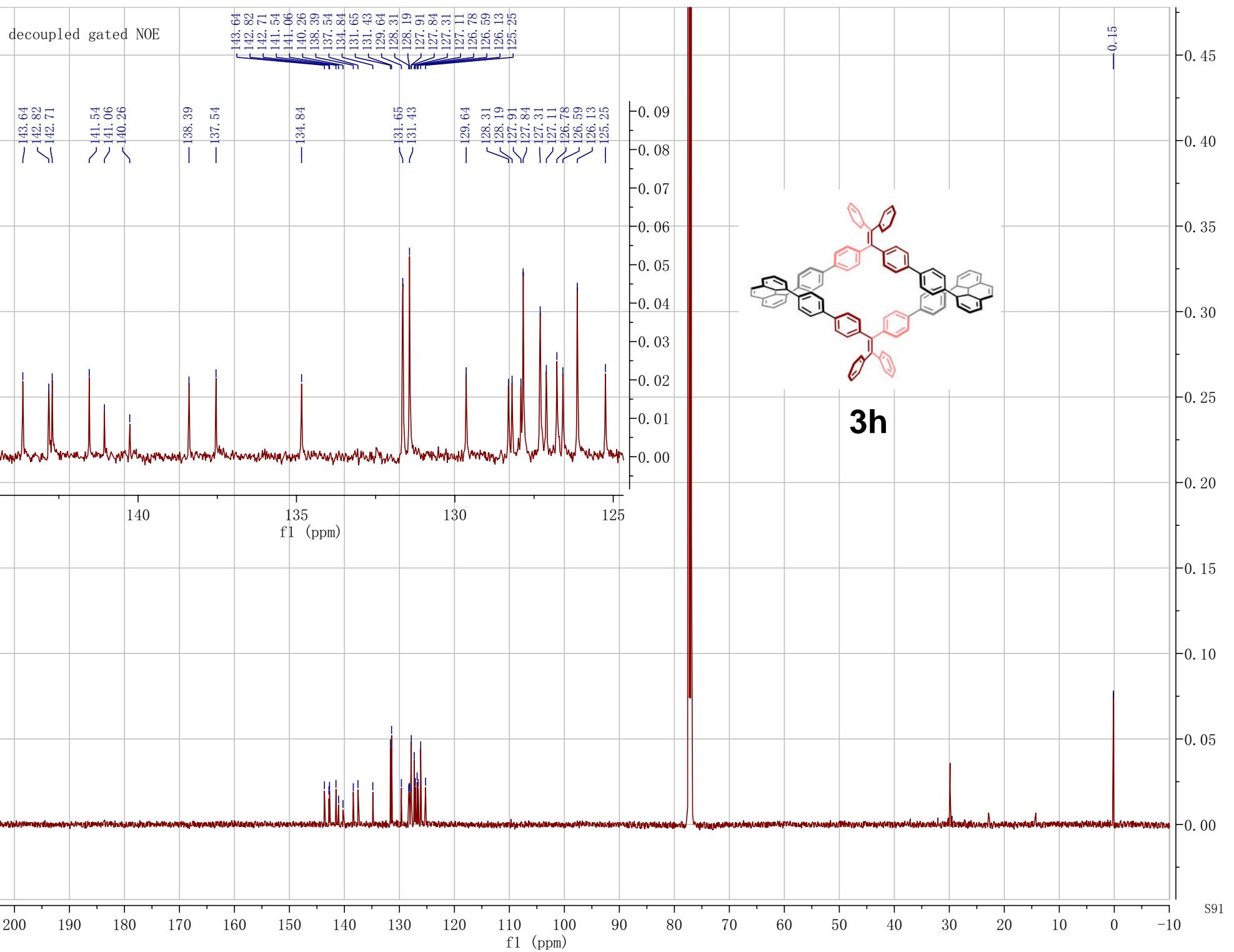
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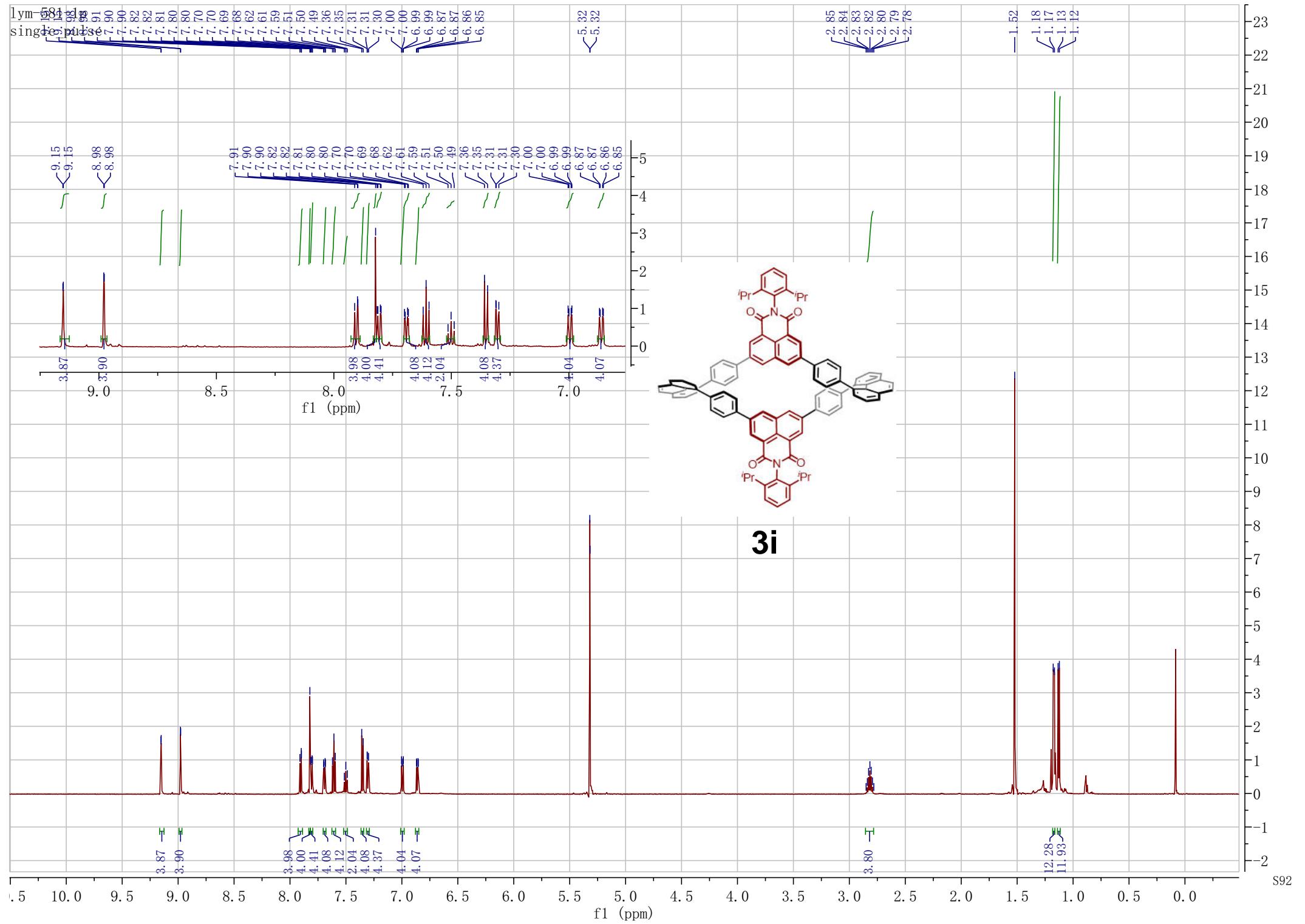




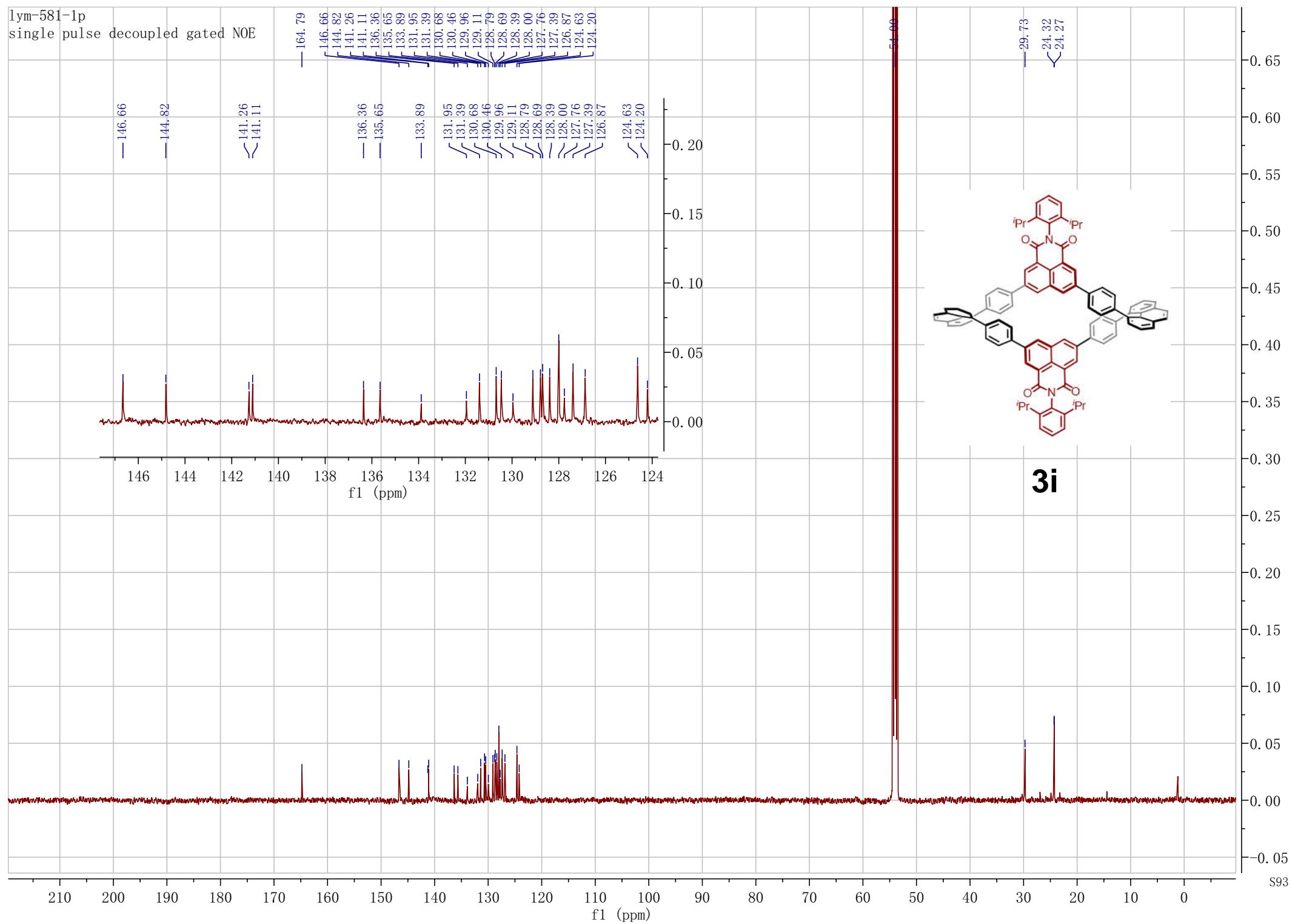
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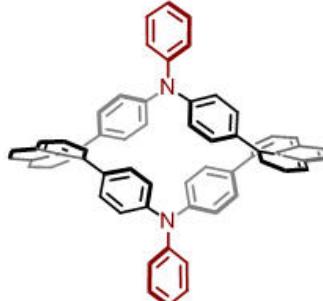




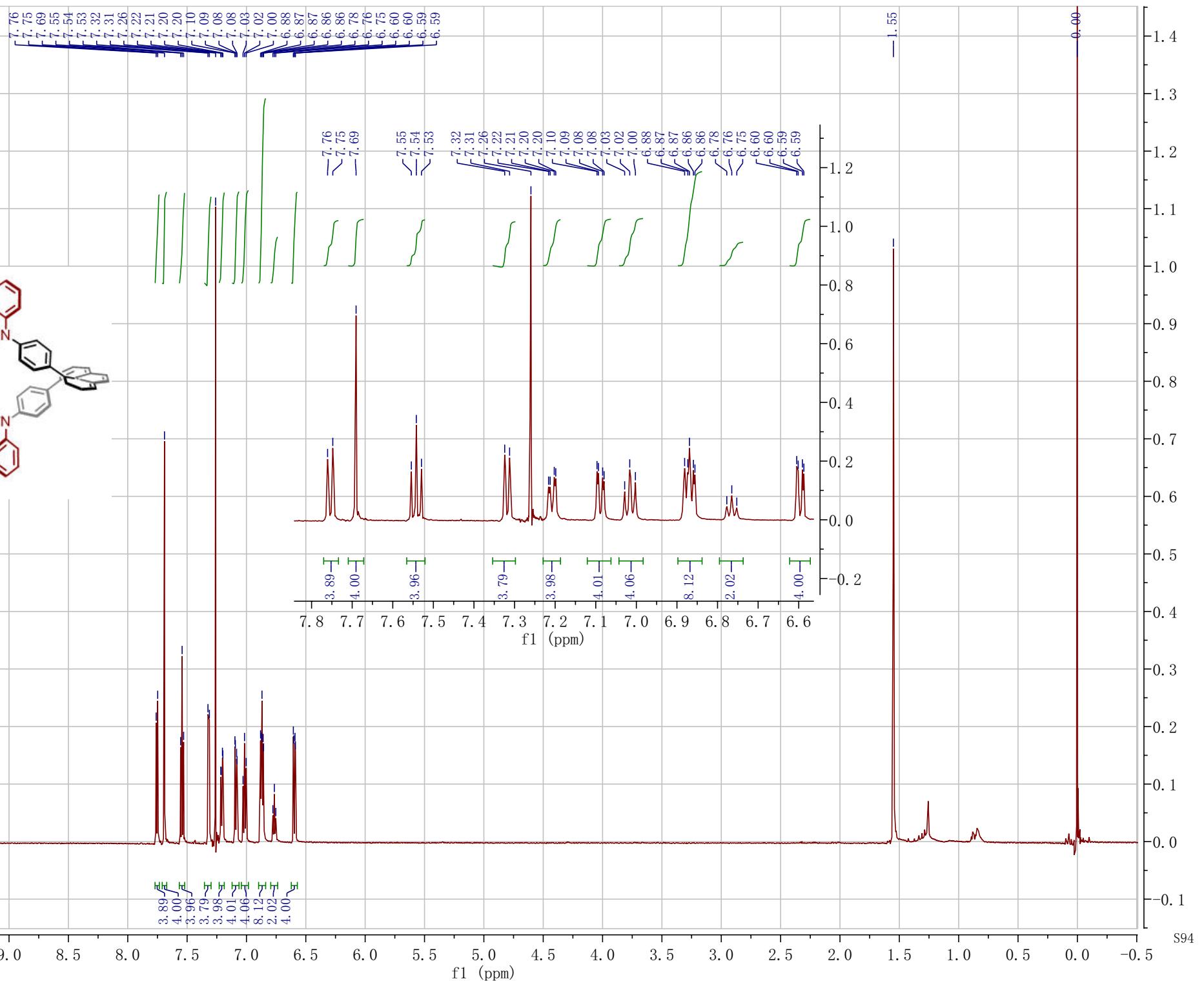
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lym-532p
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3j



lym-532p
single pulse decoupled gated NOE

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— 139.11

— 134.77

— 147.40

— 146.99

— 141.38

— 139.11

— 134.77

— 129.42

— 129.42

— 128.91

— 128.91

— 128.87

— 128.87

— 127.91

— 127.91

— 127.77

— 127.77

— 127.77

— 127.77

— 127.22

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— 126.83

— 126.83

— 126.79

— 126.79

— 123.55

— 123.55

— 122.05

— 122.05

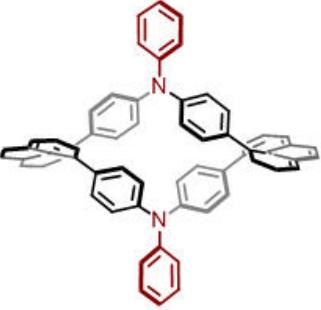
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— 121.45

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0.15
0.10
0.05
0.00

1.0
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0.0
-0.1



3j

210 200 190 180 170 160 150 140 130 120 110 100 f1 (ppm)

-0.1