

Supporting Information

for

Nickel-Catalyzed Skeletal Transformation of Tropone Derivatives via C–C Bond Activation: Catalyst-Controlled Access to Diverse Ring Systems

Takuya Kodama,^[a,b] Kanako Saito,^[a] Mamoru Tobisu*^[a,b]

*Department of Applied Chemistry, Graduate School of Engineering, Osaka University, Suita, Osaka 561-0871, Japan
Innovative Catalysis Science Division, Institute for Open and Transdisciplinary Research Initiatives (ICS-OTRI)*

tobisu@chem.eng.osaka-u.ac.jp

CONTENTS

I	General Information	S1
II	Materials	S1
III	Synthesis of Starting Materials	S2
IV	Optimization of Catalytic Decarbonylation Reaction	S5
V	Typical Procedure for Catalytic Decarbonylation Reaction	S6
VI	Typical Procedure for Catalytic Two-Carbon Ring Contraction Reaction	S9
VII	Nickel-Mediated Decarbonylation under Ambient Temperature	S12
VIII	Mechanistic Studies	S13
	a. Effect of CO Ligand	
	b. Stoichiometric Experiment	
	c. Ketene Elimination from Ketene Complex	
	d. Labelling Experiment	
	e. Role of Ni in the Cleavage of C–C bond in Nickel-Ketene Complex	
	f. Thermal Reaction of Phenylketene and Cyclopentadiene Derivatives	
	g. Retro [2+2] Reaction from Cyclobutanone Derivatives to Cyclopentadiene Derivatives	
	h. Thermal Reaction of Phenylketene and Ethanol	
IX	DFT Calculations	S24
	a. Distortion/Interaction Analysis.	
	b. Computed Energy Profiles	
X	Crystallographic Information	S28
XI	Cartesian Coordinates and Energies of Optimized Structures	S31
XII	Reference	S98
XIII	Copies of NMR spectra	S98

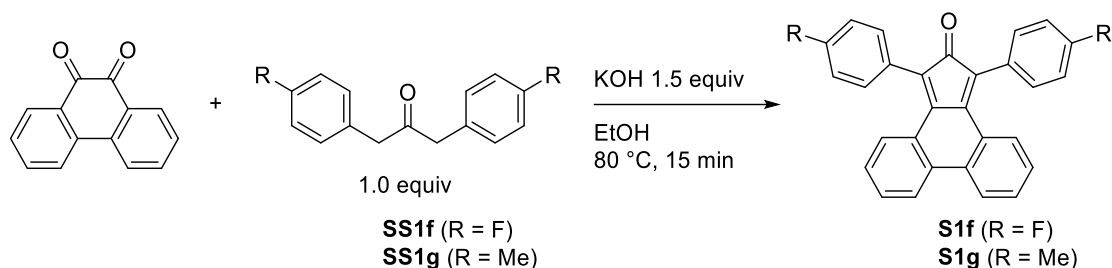
I. General Information

^1H NMR, ^{13}C NMR, ^{19}F NMR, ^{31}P NMR and ^2H NMR spectra were recorded on a JEOL ECS-400 spectrometer in CDCl_3 , $\text{THF-}d_8$, toluene- d_8 or $(\text{CD}_3)_2\text{CO}$. The chemical shifts in ^1H NMR spectra were recorded relative to CDCl_3 (δ 7.26), $\text{THF-}d_8$ (δ 3.58), toluene- d_8 (δ 2.08) or $(\text{CD}_3)_2\text{CO}$ (δ 2.05). The chemical shifts in ^{13}C NMR spectra were recorded relative to CDCl_3 (δ 77.16), $\text{THF-}d_8$ (δ 67.21), toluene- d_8 (δ 20.43) or $(\text{CD}_3)_2\text{CO}$ (δ 29.84). The chemical shifts in ^{19}F NMR spectra were recorded relative to benzotrifluoride (δ -65.64). The data is reported as follows: chemical shift (δ) in ppm, multiplicity (s = singlet, d = doublet, t = triplet, q = quartet, and m = multiplet), coupling constant (Hz), and integration. Infrared spectra (IR) were obtained using a JASCO FT/IR-4200 spectrometer. Absorption is reported in reciprocal centimeters (cm^{-1}) with the following relative intensities: s (strong), m (medium), or w (weak). High resolution mass spectra (HRMS) were obtained using JEOL-700 or JMS-T100LP spectrometer. Melting points were determined using a Yamato melting point apparatus. Column chromatography was performed with Biotage Isolera[®] equipped with Biotage SNAP Ultra Cartridge. Data collection for X-ray crystal analysis were performed on a Rigaku/XtaLAB Pro P200 Hybrid Photon Counting diffractometer (Cu-K α , λ = 1.54184 Å). The structures were solved with direct methods and refined with full-matrix least squares. All calculations were conducted using a Gaussian 09 suite program (G09 Rev D.01).¹ Optimization was performed at the M06-2X/6-31G(d,p)+LanL2DZ level of theory.² Harmonic vibration frequency analysis was conducted with the optimized structures at the same level of theory to verify all stationary points as local minima (with no imaginary frequency). Each reported minimum has zero imaginary frequency and each transition state (TS) structure has only one imaginary frequency.

II. Materials

Toluene (for Organic Synth.) was purchased from Wako Chemicals and used as received. $\text{Ni}(\text{cod})_2$ was purchased from Strem Chemicals and used as received. PCy_3 (Sigma-Aldrich), dcype (Sigma-Aldrich), $\text{IPr}\cdot\text{HCl}$ (TCI), $\text{IMes}\cdot\text{HCl}$ (TCI), $\text{ICy}\cdot\text{HBF}_4$ (TCI), Tropone (Sigma-Aldrich) and dibenzosuberone (TCI) were purchased from commercial suppliers and used as received. $\text{IMes}^{\text{Me}}\cdot\text{HCl}^3$ was prepared according to the literature procedures. 4,5-fused tropone derivatives **1a** [CAS:1154-38-7]⁴, **1c** [CAS:38558-34-8]⁵, **1e** [CAS:57969-70-7]⁶, **1h** [CAS:2707422-85-1]⁷, **1i** [CAS:2568057-82-7]⁸, were prepared according to the literature procedure.

III. Synthesis of Starting Materials



General procedure I. Synthesis of 2,5-diaryl-3,4-phenanthrene-fused cyclopentadienone **S1f**, **S1g**.

An ethanol solution of KOH (22 mmol, 1.5 equiv) was added to a mixture of 1,3-diarylacetone (15 mmol, 1.0 equiv) and phenanthrene-9,10-dione (15 mmol, 1.0 equiv) in ethanol (100 mL) at room temperature. The reaction mixture was stirred at 80 °C for 15 min. After cooling to 0 °C, the resulting solid was isolated on a filter and washed with cold ethanol.

1,3-Bis(4-fluorophenyl)-2H-cyclopenta[*l*]phenanthren-2-one (**S1f**).

green solid (42%). Mp 243–246 °C R_f 0.36 (SiO₂, hexane/CHCl₃ = 1/1 (v/v)).

¹H NMR (CDCl₃, 399.78 MHz) δ : 7.81 (dd, J = 8.2, 0.80 Hz, 2H), 7.51 (dd, J = 8.0, 1.1 Hz, 2H), 7.37 (qd, J = 5.6, 3.0 Hz, 4H), 7.32–7.28 (m, 2H), 7.13 (td, J = 9.0, 1.6 Hz, 4H), 6.99–6.95 (m, 2H).

¹³C{¹H} NMR (CDCl₃, 100.53 MHz) δ : 200.2, 162.8 (d, J^{C-F} = 248 Hz), 148.5, 133.7, 131.9 (d, J^{C-F} = 8.6 Hz), 131.8, 129.0, 128.5, 128.4, 128.1, 124.7, 122.2, 116.0 (d, J^{C-F} = 22 Hz).

¹⁹F NMR (CDCl₃, 376.17 MHz) δ : -116.1.

IR (KBr, cm⁻¹): 1686 s, 1597 m, 1583 w, 1577 w, 1507 s, 1482 w, 1448 m, 1347 m, 1305 m, 1225 s, 1155 m, 1105 w, 1100 w, 1097 w, 976 w, 853 w, 833 m, 825 w, 820 w, 764 m, 724 w, 569 w, 528 m.

HRMS (DART+TOF) m/z : [M+H]⁺ Calcd for C₂₉H₁₇OF₂ 419.1242; Found 419.1244.

1,3-Di-*p*-tolyl-2H-cyclopenta[*l*]phenanthren-2-one (**S1g**).

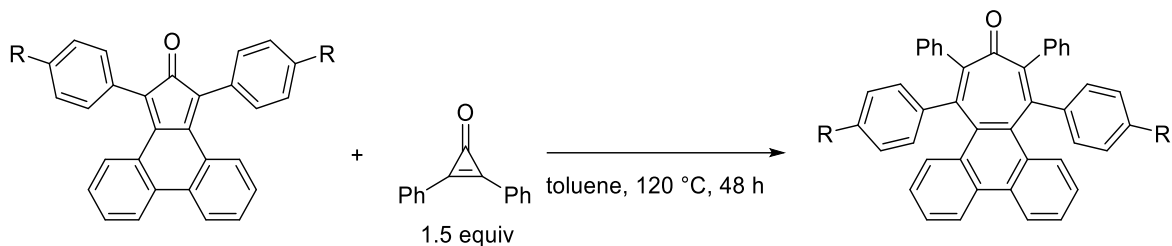
green solid (70%). Mp 242–248 °C R_f 0.36 (SiO₂, hexane/CHCl₃ = 1/1 (v/v)).

¹H NMR (CDCl₃, 399.78 MHz) δ : 7.80 (dd, J = 7.5 Hz, 1.5 Hz, 2H), 7.60 (dd, J = 8.0 Hz, 1.1 Hz, 2H), 7.30–7.22 (m, 10H), 6.95 (td, J = 7.6 Hz, 1.1 Hz, 2H), 2.40 (s, 6H).

¹³C{¹H} NMR (CDCl₃, 100.53 MHz) δ : 200.7, 147.9, 138.1, 133.7, 131.3, 130.0, 129.5, 129.3, 129.1, 128.9, 128.3, 124.5, 123.2, 21.6.

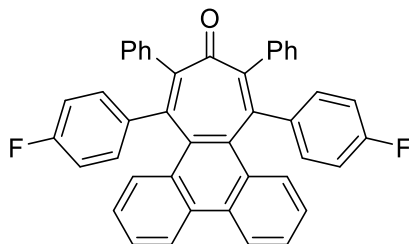
IR (KBr, cm⁻¹): 1695 s, 1594 m, 1509 m, 1447 m, 1347 m, 1302 m, 1182 m, 1106 m, 974 m, 838 w, 810 m, 768 m, 764 m, 756 s, 725 m, 653 w, 572 w, 524 m, 497 w, 446 w, 431 w, 415 m.

HRMS (DART+TOF) m/z : [M+H]⁺ Calcd for C₃₁H₂₃O 411.1743; Found 411.1747.



General procedure II. Synthesis of Tropone Derivatives 1f, 1g. A mixture of phencyclone **S1** (3.0 mmol, 1.0 equiv) and diphenylcyclopropanone (4.5 mmol, 1.5 equiv) in toluene (25 mL) was stirred at 120 °C under a nitrogen atmosphere for 48 h. The solvent was removed under reduced pressure and the resulting crude product was purified by silica gel column chromatography to give the desired product.

9,13-Bis(4-fluorophenyl)-10,12-diphenyl-11*H*-cyclohepta[*l*]phenanthren-11-one (1f).



Colorless solid (40%). Mp 271–272 °C R_f 0.40 (SiO₂, hexane/CH₂Cl₂ = 1/1 (v/v)).

¹H NMR (CDCl₃, 399.78 MHz) δ : 8.60 (d, J = 8.2 Hz, 2H), 7.85 (d, J = 7.8 Hz, 2H), 7.48 (t, J = 6.8 Hz, 2H), 7.22 (t, J = 7.1 Hz, 2H), 7.14 (dd, J = 7.6, 1.6 Hz, 4H), 7.00–7.06 (m, 10H), 6.82 (t, J = 8.7 Hz, 4H).

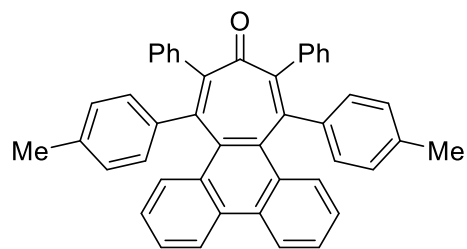
¹³C {¹H} NMR (CDCl₃, 100.53 MHz) δ : 199.4, 161.7 (d, J^{C-F} = 248 Hz), 146.2, 136.6, 135.5, 133.8, 133.3, 132.0 (d, J^{C-F} = 8.6 Hz), 131.1, 130.6, 129.6, 129.5, 128.2, 128.0, 127.0, 126.1, 122.5, 115.5 (d, J^{C-F} = 22.0 Hz)

¹⁹F NMR (CDCl₃, 376.17 MHz) δ : -116.9.

IR (KBr, cm⁻¹): 3076 m, 3052 m, 1708 s, 1601 s, 1506 s, 1496 m, 1491 s, 1440 s, 1263 m, 1232 s, 1159 s, 1099 m, 1076 m, 838 s, 828 m, 820 s, 799 m, 773 s, 751 s, 742 m, 731 s, 725 m, 719 s, 700 s, 554 s, 501 m.

HRMS (DART+TOF) m/z : [M+H]⁺ Calcd for C₄₃H₂₇OF₂ 597.2024; Found 597.2024.

10,12-Diphenyl-9,13-di-p-tolyl-11H-cyclohepta[*l*]phenanthren-11-one (1g).



Colorless solid (11%). Mp 244–247 °C R_f 0.14 (SiO₂, hexane/CHCl₃ = 7/13 (v/v)).

¹H NMR (CDCl₃, 399.78 MHz) δ : 8.59 (d, J = 8.2 Hz, 2H), 7.93 (d, J = 8.2 Hz, 2H), 7.47 (t, J = 7.8 Hz, 2H), 7.20 (t, J = 7.6 Hz, 2H), 7.16–7.14 (m, 4H), 7.04–6.97 (m, 10H), 6.92 (d, J = 8.2 Hz, 4H), 2.25 (s, 6H).

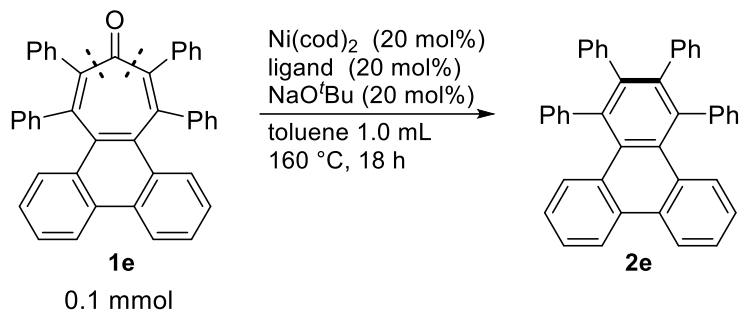
¹³C{¹H} NMR (CDCl₃, 100.53 MHz) δ : 200.2, 145.9, 137.6, 137.0, 135.7, 134.9, 133.9, 131.0, 130.7, 130.3, 129.9, 129.7, 129.0, 128.0, 127.6, 126.7, 125.9, 122.4, 21.4.

IR (KBr, cm⁻¹): 3022 w, 1739 m, 1732 m, 1720 s, 1509 m, 1591 m, 1443 m, 1264 m, 1240 m, 1075 m, 827 m, 811 m, 761 s, 752 m, 748 m, 732 m, 726 m, 722 m, 701 s, 697 s, 694 s, 564 m.

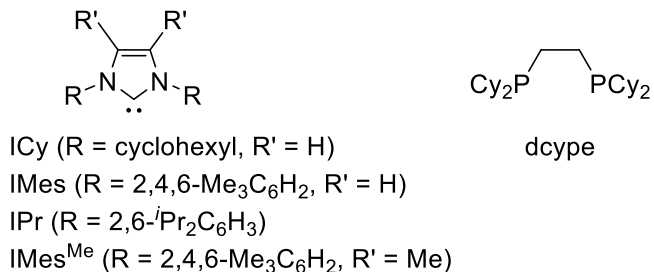
HRMS (DART+TOF) m/z : [M+H]⁺ Calcd for C₄₅H₃₃O 589.2526; Found 589.2529.

IV. Optimization of Catalytic Decarbonylation Reaction.

Table S1. Development of the Nickel-Mediated Decarbonylation of Tropone **1e**.^a

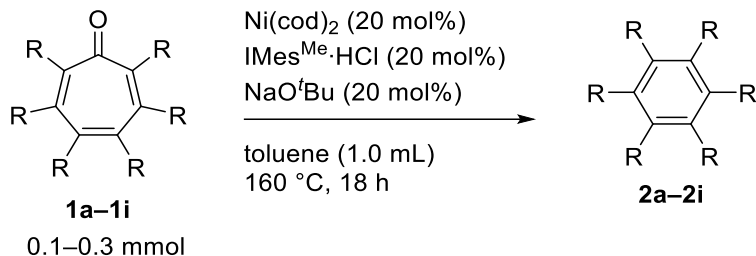


entry	ligand	Isolated yields (%)	
		2e	1e
1	IMes ^{Me} ·HCl	93(49) ^b	4(40) ^b
2 ^c	IMes ^{Me} ·HCl	59	30
3	ICy·HBF ₄	26	60
4	IMes·HCl	40	50
5	IPr·HCl	53	33
6	PCy ₃ (no NaO ^t Bu)	30	54
7 ^d	dcype (no NaO ^t Bu)	20	67



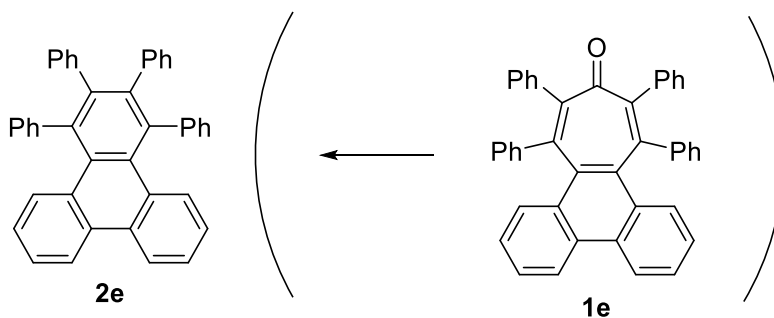
^aReaction condition : **1e** (0.10 mmol), Ni(cod)₂ (0.020 mmol), ligand (0.020 mmol), NaO^tBu (0.020 mmol), toluene (1.0 mL), 160 °C for 18 h. ^b**1e** (0.10 mmol), Ni(cod)₂ (0.010 mmol), NaO^tBu (0.010 mmol), ligand (0.010 mmol), toluene (1.0 mL), 160 °C for 18 h. ^c**1e** (0.10 mmol), Ni(cod)₂ (0.020 mmol), ligand (0.040 mmol), NaO^tBu (0.040 mmol), toluene (1.0 mL), 160 °C for 18 h. ^dNMR yields.

V. Typical Procedures for Catalytic Decarbonylation Reaction.



General procedure III. Decarbonylation of Tropone Derivatives 1e–1i. In a glovebox filled with nitrogen, $\text{Ni}(\text{cod})_2$ (5.5 mg, 0.020 mmol), $\text{IMes}^{\text{Me}}\cdot\text{HCl}$ (7.4 mg, 0.020 mmol), NaO^tBu (1.9 mg, 0.020 mmol) and toluene (0.5 mL) were added to a 10 mL pressure-proof vial with a Teflon-sealed screwcap, and stirred for 10 min at room temperature. **1e** (56 mg, 0.10 mmol) and toluene (0.5 mL) were then added, and the cap was applied to seal the vial. The vessel was heated at $160\text{ }^\circ\text{C}$ (aluminum heating block) for 18 h. The reaction mixture was cooled to room temperature, and the crude mixture was filtered through a pad of silica gel. The filtrate was then concentrated *in vacuo* to give a residue, which was purified by flash column chromatography over silica gel.

1,2,3,4-Tetraphenyltriphenylene (**2e**). [CAS: 36262-81-4]



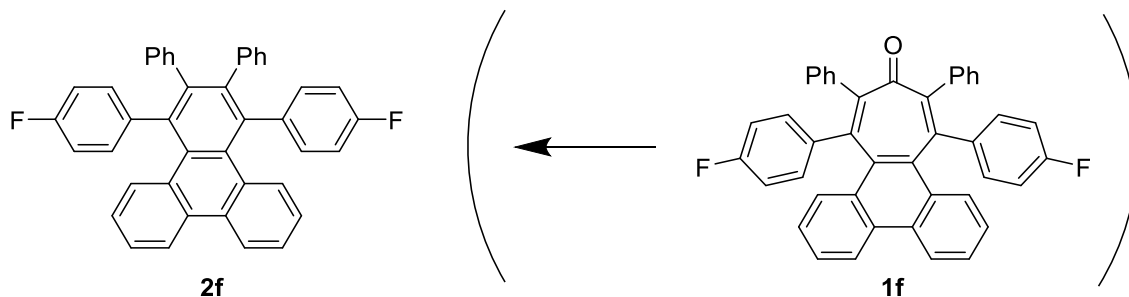
Colorless solid (50 mg, 93%). R_f 0.30 (SiO_2 , hexane/ CHCl_3 = 3/1 (v/v)).

^1H NMR (CDCl_3 , 399.78 MHz) δ : 8.43 (d, J = 8.2 Hz, 2H), 7.60 (d, J = 8.7 Hz, 2H), 7.43–7.39 (m, 2H), 7.14–7.00 (m, 12H), 6.95–6.83 (m, 6H), 6.74–6.70 (m, 4H).

$^{13}\text{C}\{^1\text{H}\}$ NMR (CDCl_3 , 100.53 MHz) δ : 142.9, 140.5, 140.4, 137.2, 132.2, 131.7 (2 peaks are overlapped), 131.3, 130.9, 130.1, 128.1, 126.7, 126.5, 126.3, 125.6, 125.4, 123.3.

HRMS (DART+TOF) m/z : $[\text{M}+\text{H}]^+$ Calcd for $\text{C}_{42}\text{H}_{29}$ 533.2264; Found 533.2260.

1,4-Bis(4-fluorophenyl)-2,3-diphenyltriphenylene (2f).



Colorless solid (59 mg, >99%). Mp 294–298 °C R_f 0.57 (SiO₂, hexane/CHCl₃ = 1/1 (v/v)).

¹H NMR (CDCl₃, 399.78 MHz) δ : 8.43 (d, J = 7.3 Hz, 2H), 7.55–7.53 (m, 2H), 7.44–7.40 (m, 2H), 7.09–7.04 (m, 2H), 7.02–6.96 (m, 4H), 6.94–6.89 (m, 6H), 6.82–6.77 (m, 4H), 6.68–6.66 (m, 4H).

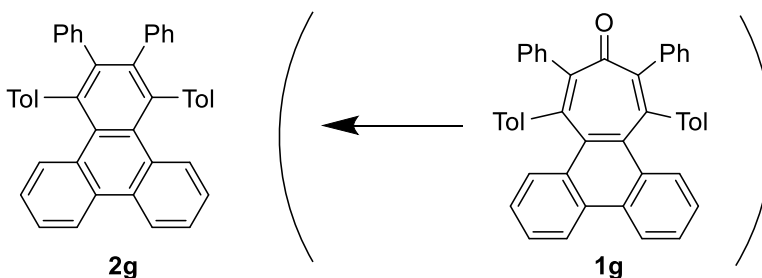
¹³C {¹H} NMR (CDCl₃, 100.53 MHz) δ : 161.2 (d, J^{C-F} = 247 Hz), 140.6, 140.2, 138.9, 138.8, 136.3, 133.7 (d, J^{C-F} = 7.6 Hz), 131.7, 131.6, 131.4, 130.6, 130.0, 127.0, 126.7, 125.8, 125.6, 123.5, 115.2 (d, J^{C-F} = 21.0 Hz).

¹⁹F NMR (CDCl₃, 376.17 MHz) δ : -118.5.

IR (KBr, cm⁻¹): 3053 w, 3026 w, 2926 w, 1601 s, 1509 s, 1440 m, 1392 m, 1224 s, 1157 m, 1143 w, 840 s, 821 m, 796 w, 760 m, 750 m, 728 m, 700 s, 560 m, 529 m.

HRMS (DART+TOF) m/z : [M+H]⁺ Calcd for C₄₂H₂₇F₂ 569.2075; Found 569.2052.

2,3-Diphenyl-1,4-di-*p*-tolyltriphenylene (2g).



Colorless solid (28 mg, 75%). Mp 314–320 °C R_f 0.37 (SiO₂, hexane/CHCl₃ = 1/1 (v/v)).

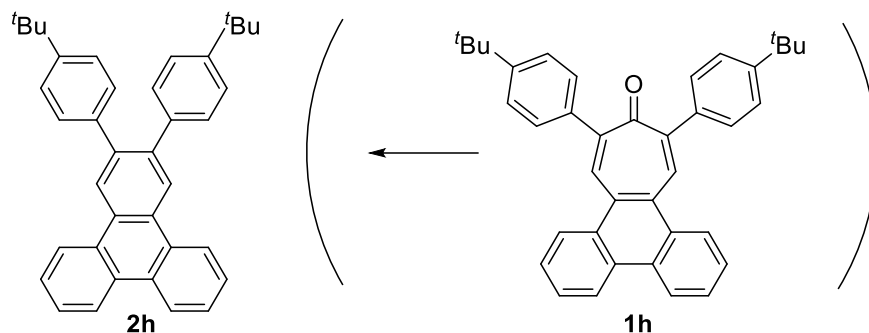
¹H NMR (CDCl₃, 399.78 MHz) δ : 8.41 (d, J = 7.3 Hz, 2H), 7.61 (dd, J = 8.7, 0.90 Hz, 2H), 7.41–7.37 (m, 2H), 7.05–7.00 (m, 2H), 6.94–6.87 (m, 14H), 6.71–6.69 (m, 4H), 2.26 (s, 6H).

¹³C {¹H} NMR (CDCl₃, 100.53 MHz) δ : 141.8, 141.6, 132.7, 131.2, 131.1, 130.7, 129.3, 128.8, 128.7, 127.9, 127.7, 127.2, 126.7, 126.5, 126.2, 126.1, 123.6, 24.3.

IR (KBr, cm⁻¹): 3080 w, 3073 w, 3060 m, 3039 w, 3022 m, 2919 w, 1717 w, 1511 m, 1493 m, 1440 m, 1110 w, 839 w, 827 m, 758 s, 748 m, 742 m, 736 w, 726 s, 700 s, 560 m.

HRMS (DART+TOF) m/z : [M+H]⁺ Calcd for C₄₄H₃₃ 561.2577; Found 561.2574.

2,3-Bis(4-(*tert*-butyl)phenyl)triphenylene (**2h**).



Colorless solid (3.0 mg, 6%). Mp 267–268 °C R_f 0.60 (SiO₂, hexane/CHCl₃ = 1/1 (v/v)).

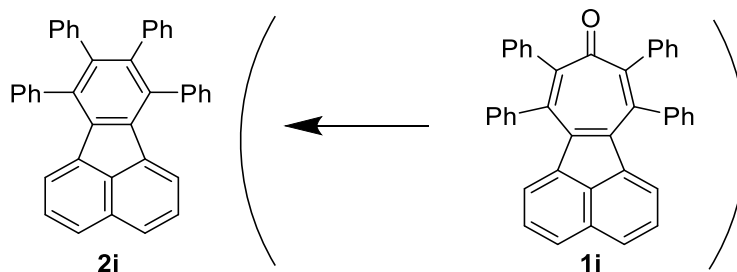
¹H NMR (CDCl₃, 399.78 MHz) δ : 8.69–8.65 (m, 6H), 7.68–7.58 (m, 4H), 7.31 (d, J = 8.2 Hz, 4H), 7.25 (d, J = 4.6 Hz, 4H), 1.29 (s, 18H).

¹³C {¹H} NMR (CDCl₃, 100.53 MHz) δ : 149.7, 139.9, 138.8, 130.1, 129.8 (two peaks are overlapped), 128.9, 127.4, 127.3, 125.6, 125.0, 123.6, 123.5, 34.6, 31.5.

IR (KBr, cm⁻¹): 2960 s, 2914 w, 2901 m, 2884 w, 2864 w, 1484 m, 1469 w, 1458 w, 1447 w, 1436 m, 1390 m, 1361 w, 1268 w, 1116 w, 891 w, 835 m, 755 s, 720 m, 624 w.

HRMS (DART+TOF) m/z : [M+H]⁺ Calcd for C₃₈H₃₇ 493.2890; Found 493.2888.

7,8,9,10-Tetraphenylfluoranthene (**2i**). [CAS: 13238-75-0]



Colorless solid (50 mg, 97%). Mp 325–326 °C R_f 0.50 (SiO₂, hexane/CHCl₃ = 3/1 (v/v)).

¹H NMR (CDCl₃, 399.78 MHz) δ : 7.73 (d, J = 8.2 Hz, 2H), 7.35–7.29 (m, 12H), 6.96–6.85 (m, 10H), 6.64 (d, J = 6.8 Hz, 2H).

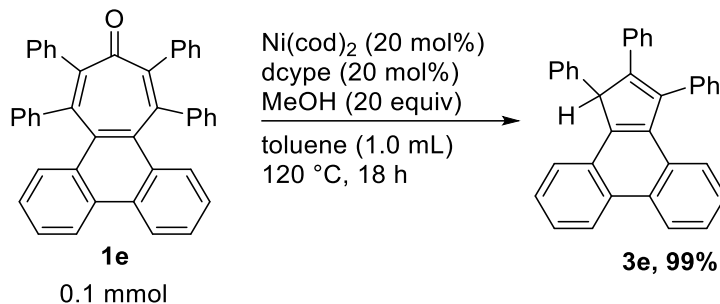
¹³C {¹H} NMR (CDCl₃, 100.53 MHz) δ : 140.7, 139.9, 139.8, 137.2, 136.6, 136.5, 133.3, 131.4, 130.2, 129.7, 128.2, 127.7, 127.0, 126.7, 126.6, 125.5, 123.3.

IR (KBr, cm⁻¹): 3057 w, 3039 w, 3028 w, 1600 w, 1496 w, 1440 w, 1436 w, 1428 m, 1421 m, 1417 w, 1375 w, 1070 w, 1039 w, 1028 w, 826 w, 774 m, 770 m, 765 m, 747 w, 741 w, 708 m, 706 m, 699 s, 578 w, 552 w.

HRMS (DART+TOF) m/z : [M+H]⁺ Calcd for C₄₀H₂₇ 507.2107; Found 507.2099.

VI. Typical Procedures for Catalytic Two-Carbon Ring Contraction Reaction.

1,2,3-Triphenyl-1*H*-cyclopenta[*l*]phenanthrene (**3e**).



In a glovebox filled with nitrogen, Ni(cod)₂ (5.8 mg, 0.021 mmol), dcype (8.9 mg, 0.020 mmol), MeOH (80 μ L), **1e** (60 mg, 0.11 mmol) and toluene (1.0 mL) were added to a 10 mL pressure-proof vial with a Teflon-sealed screwcap and the cap was closed. The contents of the vial were then stirred at 120 °C (aluminum heating block) for 18 h. The reaction mixture was cooled to room temperature, and the crude mixture was filtered through a pad of silica gel. The filtrate was then concentrated in vacuo to give a residue, which was purified by flash column chromatography over silica gel to give **3e** as a colorless solid (46 mg, >99%).

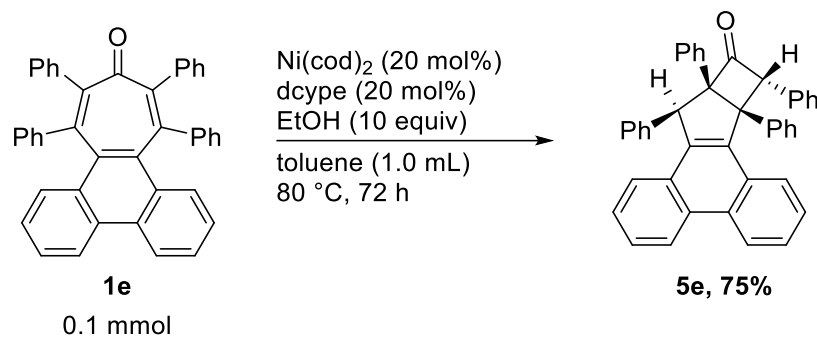
R_f 0.54 (SiO₂, hexane/CHCl₃ = 2/1 (v/v)).

¹H NMR ((CD₃)₂CO, 399.78 MHz) δ : 8.87 (d, *J* = 7.8 Hz, 1H), 8.80 (d, *J* = 8.7 Hz, 1H), 7.99–7.94 (m, 1H), 7.78 (d, *J* = 7.8 Hz, 1H), 7.62–7.37 (m, 7H), 7.30–7.18 (m, 6H), 7.12 (t, *J* = 7.6 Hz, 2H), 7.07–6.98 (m, 4H), 5.78 (s, 1H).

¹³C{¹H} NMR ((CD₃)₂CO, 100.53 MHz) δ : 151.4, 144.1, 141.8, 140.8, 139.5, 136.4, 132.3, 131.9, 130.4, 130.3, 130.1, 129.9, 129.4, 129.4, 129.3, 129.1, 128.5, 128.4, 127.5, 127.4, 127.4, 126.7, 126.6, 126.5, 125.7, 125.4, 124.4, 124.2, 58.6.

HRMS (DART+TOF) *m/z*: [M+H]⁺ Calcd for C₃₅H₂₅ 445.1951; Found 445.1944.

8c,9,10a,11-Tetraphenyl-8c,9,10a,11-tetrahydro-10*H*-cyclobuta[3,4]cyclopenta[1,2-*l*]phenanthren-10-one (**5e**).



In a glovebox filled with nitrogen, Ni(cod)_2 (5.6 mg, 0.020 mmol), dcype (9.2 mg, 0.020 mmol), EtOH (58 μL), **1e** (55 mg, 0.10 mmol) and toluene (1.0 mL) were added to a 10 mL pressure-proof vial with a Teflon-sealed screwcap and the cap was closed. The contents of the vial were then stirred at 80 °C (aluminum heating block) for 3 days. The reaction mixture was cooled to room temperature, and the crude mixture was filtered through a pad of silica gel. The filtrate was then concentrated in vacuo to give a residue, which was purified by flash column chromatography over silica gel to give **6e** as a colorless solid (42 mg, 75%).

Mp 236–237 °C R_f 0.22 (SiO₂, hexane/ CHCl_3 = 2/1 (v/v)).

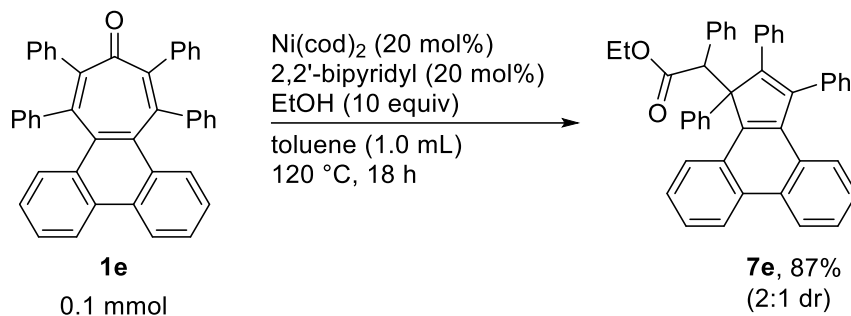
¹H NMR (CDCl_3 , 399.78 MHz) δ : 8.73 (d, J = 8.2 Hz, 1H), 8.59 (d, J = 8.7 Hz, 1H), 7.65 (t, J = 8.5 Hz, 2H), 7.48–7.43 (m, 2H), 7.30 (t, J = 8.0 Hz, 3H), 7.21 (t, J = 7.1 Hz, 1H), 7.14 (t, J = 7.6 Hz, 1H), 7.04–6.91 (m, 5H), 6.84 (t, J = 7.8 Hz, 2H), 6.80–6.72 (m, 4H), 6.67–6.60 (m, 3H), 6.52 (d, J = 8.2 Hz, 1H), 6.29 (m, 2H), 5.82 (s, 1H), 5.60 (s, 1H).

¹³C{¹H} NMR (CDCl_3 , 100.53 MHz) δ : 209.7, 140.6, 139.7, 139.3, 138.2, 133.0, 131.7, 131.1, 130.4, 129.8, 129.7, 129.5, 129.5, 129.3, 128.6, 128.5, 128.3, 128.0, 127.9, 127.8, 127.7, 127.5, 127.3, 126.9, 126.9, 126.8, 126.5, 125.7, 125.1, 123.2, 122.4, 85.0, 69.8, 66.6, 57.3.

IR (KBr, cm^{-1}): 3080 m, 3059 m, 3055 m, 3050 m, 3043 w, 3028 m, 1770 s, 1597 w, 1495 m, 1450 m, 1174 w, 1132 m, 1032 w, 777 m, 772 m, 755 s, 742 w, 734 m, 726 m, 724 m, 699 s, 556 m, 539 m, 510 w.
 HRMS (DART+TOF) m/z : $[\text{M}+\text{H}]^+$ Calcd for $\text{C}_{43}\text{H}_{31}\text{O}$ 563.2369; Found 563.2345.

The structure of **6e** was unambiguously determined by X-ray crystallography.

Ethyl 2-phenyl-2-(1,2,3-triphenyl-1H-cyclopenta[*l*]phenanthren-1-yl)acetate (7e).



In a glovebox filled with nitrogen, $\text{Ni}(\text{cod})_2$ (5.5 mg, 0.020 mmol), 2,2'-bipyridyl (3.2 mg, 0.020 mmol), EtOH (58 μL), **1e** (56 mg, 0.10 mmol) and toluene (1.0 mL) were added to a 10 mL pressure-proof vial with a Teflon-sealed screwcap and the cap was closed. The contents of the vial were then stirred at 120 °C (aluminum heating block) for 18 h. The reaction mixture was cooled to room temperature, and the crude mixture was filtered through a pad of silica gel. The filtrate was then concentrated in vacuo to give a residue, which was purified by flash column chromatography over silica gel to give **7e** as a colorless solid (53 mg, 87%).

Mp 243–247 °C R_f 0.26 (SiO₂, hexane/CHCl₃ = 1/1 (v/v)).

¹H NMR (CDCl₃, 399.78 MHz) major δ : 8.65 (dd, J = 8.6, 2.9 Hz, 2H), 7.60 (d, J = 8.2 Hz, 1H), 7.52–7.45 (m, 3H), 7.36–7.21 (m, 10H), 7.15 (t, J = 7.6 Hz, 1H), 7.04–6.88 (m, 8H), 6.80 (t, J = 7.8 Hz, 2H), 6.69 (d, J = 7.8 Hz, 2H), 5.41 (s, 1H), 3.78–3.70 (m, 1H), 3.63–3.55 (m, 1H), 0.96 (t, J = 7.1 Hz, 3H).

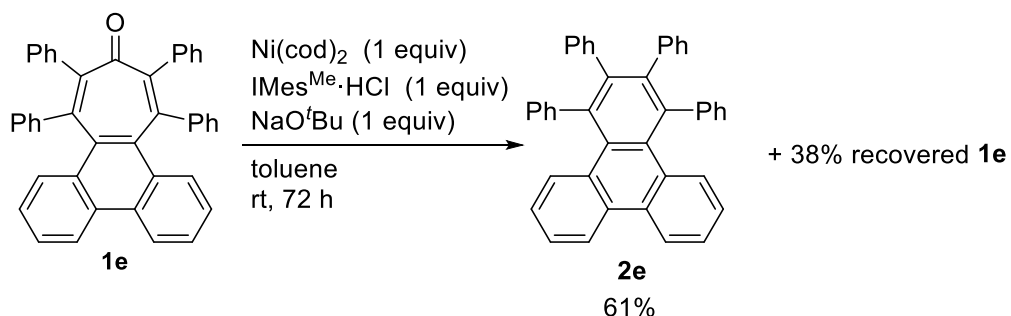
¹³C {¹H} NMR (CDCl₃, 100.53 MHz) δ : 171.3, 151.7, 145.5, 145.3, 139.8, 138.6, 138.2, 136.8, 134.5, 131.4, 130.8, 130.4, 130.1, 129.8, 129.5, 128.9, 128.4, 128.2, 127.9, 127.6, 127.4, 127.3, 127.1, 126.9, 126.8, 126.4, 126.0, 125.8, 125.7, 125.5, 125.2, 123.4, 123.2, 67.6, 60.9, 54.8, 13.8.

IR (KBr, cm⁻¹): 1733 s, 1493 m, 1487 m, 1483 m, 1453 m, 1449 w, 1441 m, 1369 m, 1192 m, 1146 s, 1112 m, 1045 w, 1031 m, 783 w, 756 s, 745 m, 738 m, 732 m, 722 s, 717 m, 710 s, 543 m.

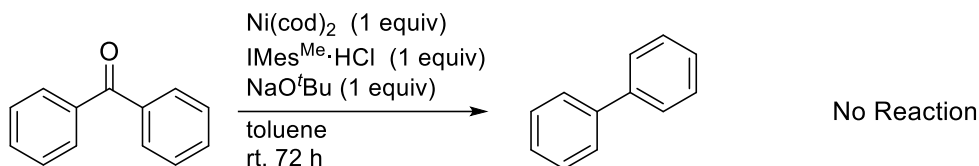
HRMS (DART+TOF) m/z : $[\text{M}+\text{H}]^+$ Calcd for C₄₅H₃₅O₂ 607.2632; Found 607.3633.

The structure of **5e** was unambiguously determined by X-ray crystallography.

VII. Nickel-Mediated Decarbonylation under Ambient Temperature.



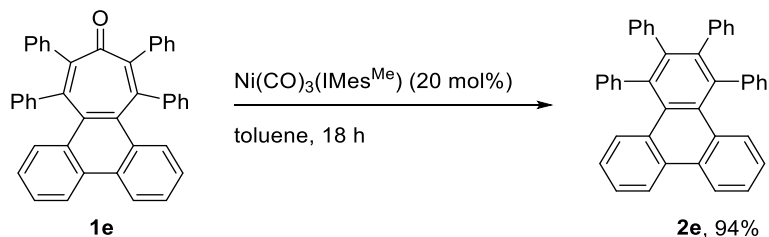
In a glovebox filled with nitrogen, Ni(cod)₂ (13 mg, 0.05 mmol), IMes^{Me}·HCl (19 mg, 0.050 mmol), NaO^tBu (5.2 mg, 0.050 mmol) and toluene (0.5 mL) were added to a 10 mL pressure-proof vial with a Teflon-sealed screwcap, and stirred for 10 min at room temperature. **1e** (27 mg, 0.05 mmol) and toluene (0.5 mL) were then added, and the cap was applied to seal the vial. The vessel was run at room temperature for 72 h. The crude mixture was filtered through a pad of silica gel. The filtrate was then concentrated *in vacuo* to give a residue, which was purified by flash column chromatography over silica gel to give **2e** in 61% yield.



In a glovebox filled with nitrogen, Ni(cod)₂ (13 mg, 0.050 mmol), IMes^{Me}·HCl (18 mg, 0.050 mmol), NaO^tBu (4.9 mg, 0.050 mmol) and toluene (0.5 mL) were added to a 10 mL pressure-proof vial with a Teflon-sealed screwcap, and stirred for 10 min at room temperature. Benzophenone (12 mg, 0.050 mmol) and toluene (0.5 mL) were then added, and the cap was applied to seal the vial. The vessel was heated at room temperatures for 72 h. The reaction mixture was cooled to room temperature, and the crude mixture was filtered through a pad of silica gel. It was confirmed by ¹H NMR that the reaction was not progressing.

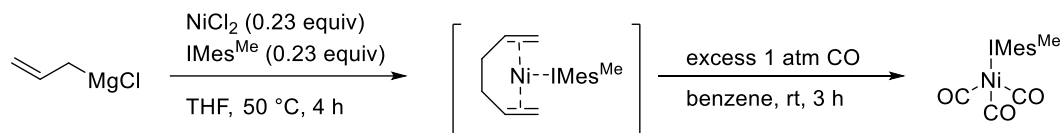
VIII. Mechanistic studies.

a. Effect of CO ligand.



$\text{Ni(CO)}_3(\text{IMes}^{\text{Me}})$ (10 mg, 0.020 mmol), **1e** (58 mg, 0.10 mmol) and toluene (1 mL) were added to a 10 mL-sample vial with a Teflon-sealed screwcap in a glovebox filled with nitrogen. The resulting mixture was stirred at room temperature for 3 min and the cap was closed. The contents of the vial were then stirred at 120 °C for 18 h. The contents were cooled to room temperature, and the crude mixture was filtered through a pad of silica gel. The filtrate was then concentrated *in vacuo* to give the decarbonylative product **2e** (94%).

$\text{Ni(CO)}_3(\text{IMes}^{\text{Me}})$



(Allyl)MgCl (7.4 mL, 0.7 M in THF, 5.2 mmol) was added to a stirred suspension of NiCl_2 (0.16 g, 1.2 mmol) and IMes^{Me} (0.40 g, 1.2 mmol) in 10 mL THF. The mixture was stirred at 50 °C for 4 h and the volatiles removed under reduced pressure. The resulting residue was extracted with pentane (3 x 6 mL) and filtered through celite. The pentane was removed under reduced pressure to give nickel-diene complex, which was used in the next step without further purification.

Excess 1 atm CO was added via a dual manifold Schlenk line to a solution of nickel-diene complex (0.14 g, 0.29 mmol) in 3 mL benzene at rt for 3 h and the volatiles were removed under vacuum to give $\text{Ni(CO)}_3(\text{IMes}^{\text{Me}})$ as colorless solid (0.13 g, 92%).

$^1\text{H NMR}$ (toluene- d_8 , 399.78 MHz) δ : 7.13 (s, 1H), 6.97 (s, 2H), 6.81 (s, 4H), 2.13 (s, 6H), 2.01 (s, 12H), 1.52 (s, 6H).

$^{13}\text{C}\{^1\text{H}\}$ NMR (CDCl_3 , 100.53 MHz) δ : 198.6, 190.5, 138.6, 136.3, 135.7, 129.5, 128.5, 21.1, 17.7, 9.2.

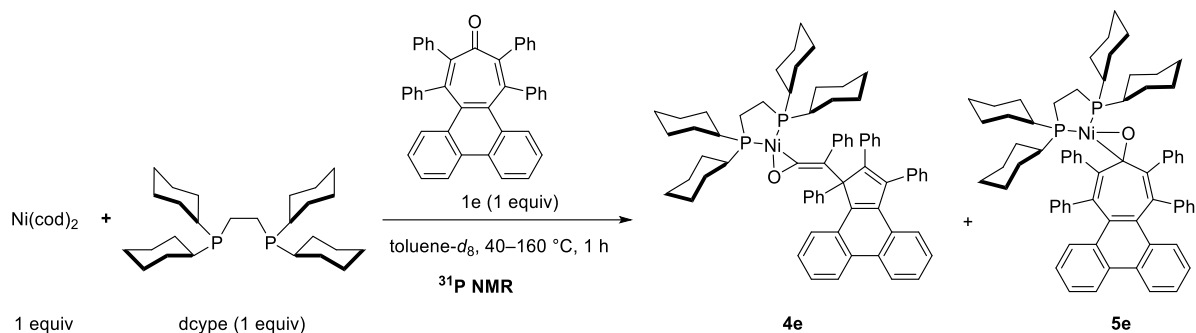
IR (KBr, cm^{-1}): 3385 m, 2975 m, 2920 s, 2858 m, 1702 s, 1663 s, 1609 s, 1541 m, 1488 s, 1439 s, 1387 s, 1302 m, 1255 w, 1035 w, 851 m, 750 w, 622 w, 567 m.

HRMS (FAB+TOF) m/z : $[\text{M}-\text{CO}+\text{H}]^+$ Calcd for $\text{C}_{24}\text{H}_{28}\text{N}_2\text{ONi}$ 418.1550; Found 418.1567.

HRMS (FAB+TOF) m/z : $[M-(CO)_2+H]^+$ Calcd for $C_{23}H_{28}N_2Ni$ 390.1600; Found 390.1616.

The structure of $Ni(CO)_3(IMes^{Me})$ was unambiguously determined by X-ray crystallography.

b. Stoichiometric experiment.



$Ni(cod)_2$ (19 mg, 0.070 mmol), dcype (30 mg, 0.070 mmol), **1e** (25 mg, 0.070 mmol) and $toluene-d_8$ (1.0 mL) were added to a 10 mL-sample vial with a Teflon-sealed screwcap in a glovebox filled with nitrogen. The resulting mixture was stirred at room temperature for 30 min and transferred to a NMR tube equipped with a screw cap. The cap was closed, and then it was taken out of the glovebox. The contents were then heated at $40\text{ }^\circ\text{C}$ for 1 h. The contents were cooled to room temperature, the reaction was monitored by ^{31}P NMR spectroscopy at room temperature. The same procedure was performed at 60, 80, 100, 120, 140 and $160\text{ }^\circ\text{C}$ (**Figure S1**).

During the course of the reaction, two new downfield peaks assignable to **5e** (**b**: $\delta = 62.5$ and 61.3 ppm, $J_{pp} = 50.2$ Hz) appeared at $60\text{ }^\circ\text{C}$ alongside the signal of the $Ni(cod)(dcype)$ (**a**: $\delta = 60.6$ ppm, s) on ^{31}P NMR. The signal of the $Ni(dcype)(CO)_2$ (**d**: $\delta = 64.0$ ppm) started to appear at $120\text{ }^\circ\text{C}$. Another two new downfield peaks assignable to the Ni-ketene complex (**4e**) (**c**: $\delta = 71.7$ and 55.1 ppm, $J_{pp} = 48.0$ Hz) appeared at $100\text{ }^\circ\text{C}$.

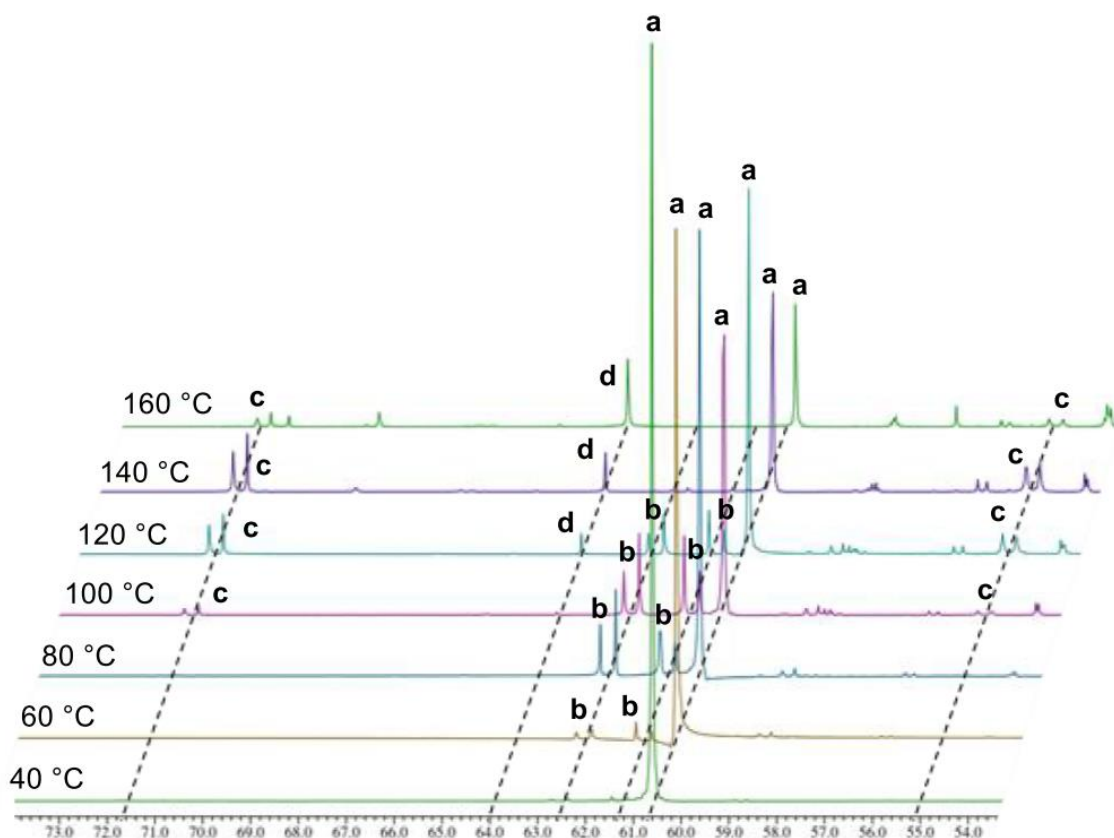
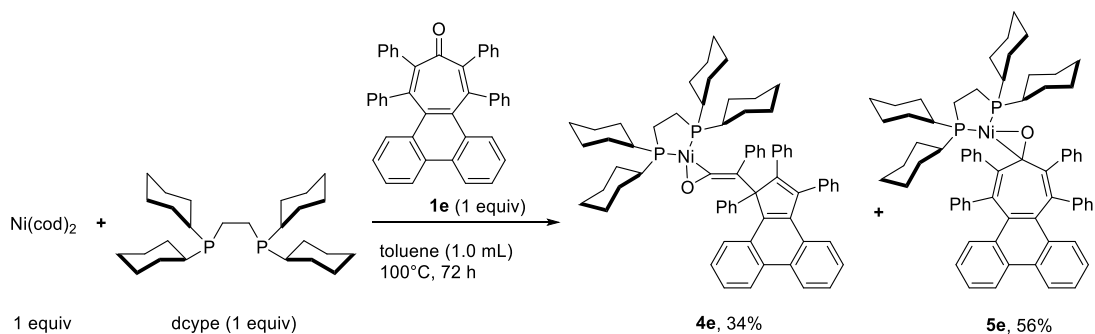


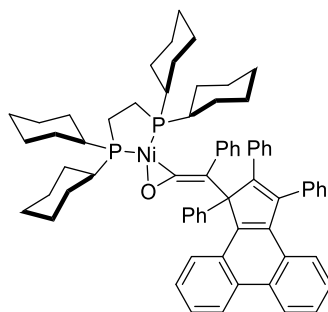
Fig. S1

Complex 4e and 5e.



$\text{Ni}(\text{cod})_2$ (28.1 mg, 0.1 mmol), dcype (45 mg, 0.1 mmol), **1e** (56 mg, 0.1 mmol) and toluene (1.0 mL) were added to a 10 mL-sample vial with a Teflon-sealed screwcap in a glovebox filled with nitrogen. The resulting mixture was stirred at room temperature for 30 min to give a homogeneous yellow solution, and the cap was closed. The contents of the vial were then heated at 100 °C for 72 h. Recrystallization from pentane gave orange crystal (**4e**, 34%) and red crystal (**5e**, 56%). They were collected by filtration and dried in a glovebox filled with nitrogen.

Complex **4e**.



Orange crystal. Decomposition temperature 208 °C.

^1H NMR (THF-*d*₈, 399.78 MHz) δ : 8.80 (d, *J* = 8.2 Hz, 1H), 8.72 (d, *J* = 8.2 Hz, 1H), 8.37 (d, *J* = 7.8 Hz, 1H), 7.48–7.40 (m, 3H), 7.28 (t, *J* = 7.1 Hz, 1H), 7.14–7.06 (m, 9H), 6.98–6.87 (m, 7H), 6.82 (d, *J* = 6.4 Hz, 2H), 6.73 (t, *J* = 7.1 Hz, 2H), 6.27 (d, *J* = 6.9 Hz, 2H), 1.56–0.87 (m, 48H).

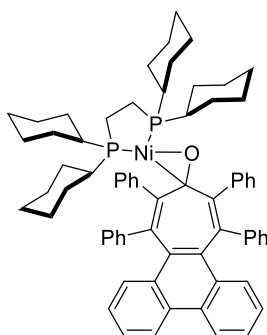
^{31}P NMR (CDCl₃, 161.83 MHz) δ : 70.2 (d, $J^{\text{P-P}}$ = 95.4 Hz), 54.2 (d, $J^{\text{P-P}}$ = 77.9 Hz).

IR (KBr, cm⁻¹): 3076 w, 3048 w, 3021 w, 2929 s, 2850 m, 1616 m, 1590 w, 1490 w, 1445 m, 1177 w, 1068 w, 1001 w, 850 w, 774 w, 756 m, 727 m, 704 m, 662 w, 654 w, 644 w, 582 w, 554 w.

HRMS (ESI+TOF) *m/z*: [M+MeOH]⁺ Calcd for C₇₀H₇₉O₂P₂Ni 1071.4903; Found 1071.4941.

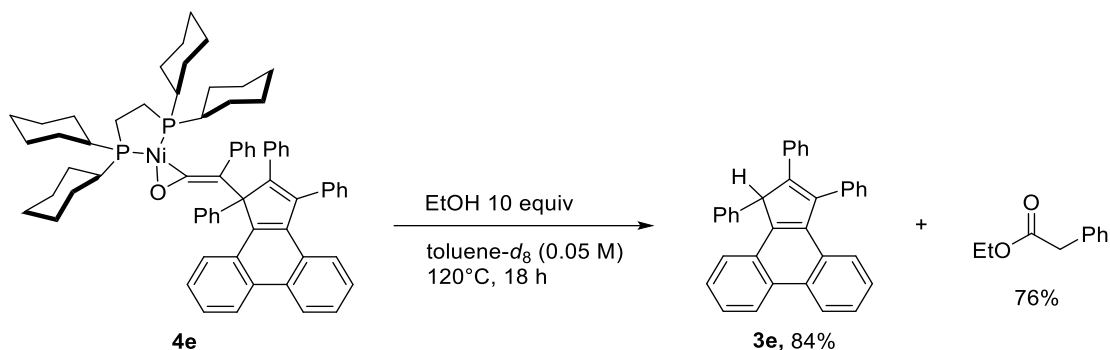
The structure of **4e** was unambiguously determined by X-ray crystallography.

Complex **5e**.



Obtained as a mixture with **1e**. Red crystal. The structure of **5e** was unambiguously determined by X-ray crystallography.

c. Ketene elimination from **4e**.



Complex **4e** (10 mg, 0.01 mmol), EtOH (6.0 μ L, 10 equiv) and toluene-*d*₈ (0.50 mL) were added to a 10 mL-sample vial with a Teflon-sealed screwcap in a glovebox filled with nitrogen. The resulting mixture was stirred at room temperature for 3 min and the cap was closed, and then it was taken out of the glovebox. The contents of the vial were then heated at 120 °C for 18 h. The contents were cooled to room temperature, the product yield was determined by ¹H NMR using 1,3,5-trimethoxybenzene as an internal standard (**3e**: 84%, corresponding ester: 76%).

After 18 h of heating, the peak indicating **4e** (**a**: δ = 8.76, 8.68 and 7.91 ppm) disappeared on ¹H NMR. New peaks (**b**: δ = 8.51, 7.90 and 5.18 ppm) appeared, and these peaks were consistent with the signal of **3e**. Two peaks (**c**: δ = 3.85 and 3.53 ppm) characteristic of the corresponding ester formed by the reaction of ketene and alcohol were also observed. The ratio of **3e** to ester was determined to be about 1:1 by ¹H NMR (**Figure S2**).

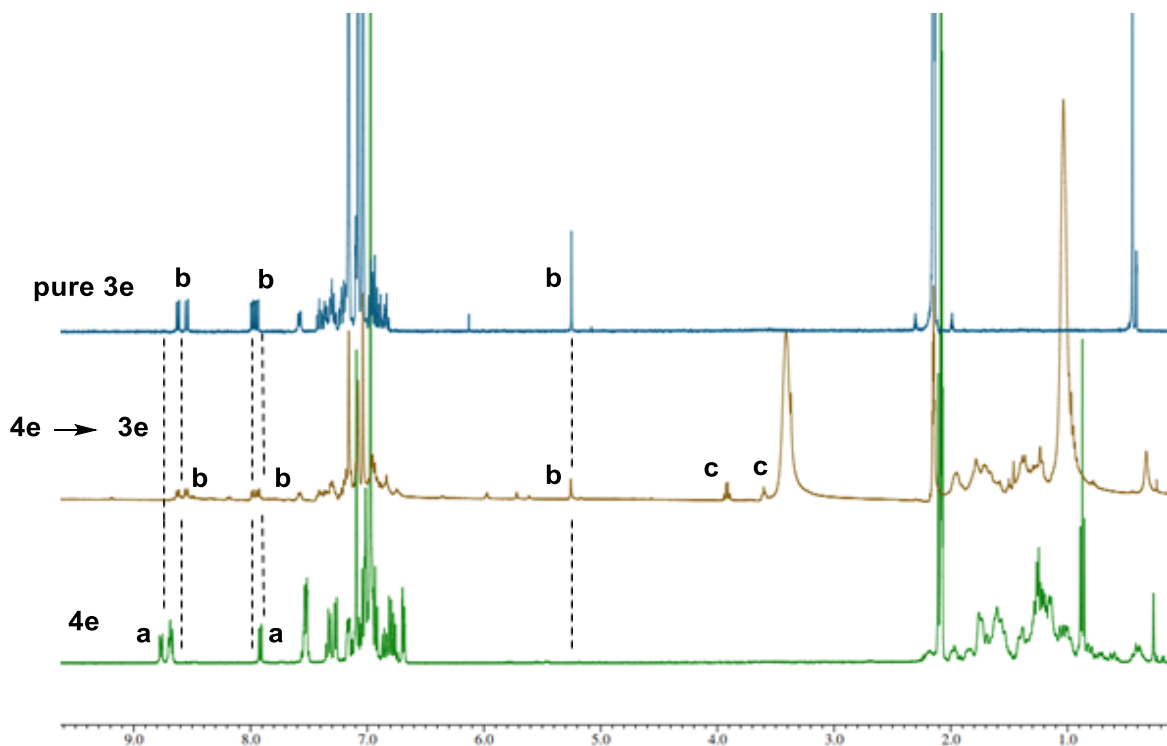
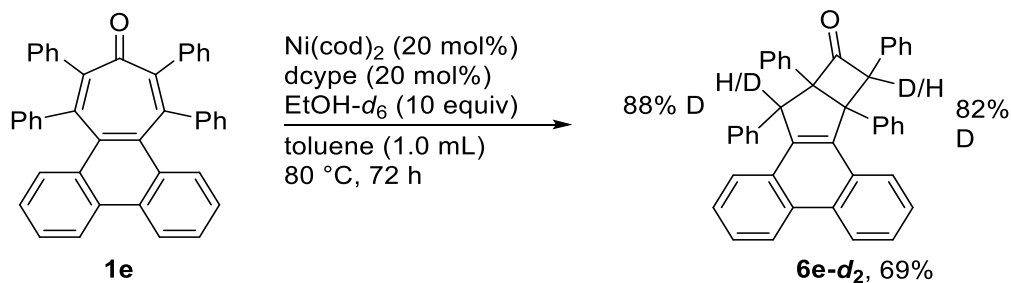


Fig. S2

d. Labelling experiment.

8c,9,10a,11-Tetraphenyl-8c,9,10a,11-tetrahydro-10*H*-cyclobuta[3,4]cyclopenta[1,2-*l*]phenanthren-10-one-9,11-*d*₂ (6e-*d*₂).



In a glovebox filled with nitrogen, Ni(cod)₂ (5.6 mg, 0.020 mmol), dcype (9.2 mg, 0.020 mmol), EtOH-*d*₆ (58 μL), **1e** (55 mg, 0.10 mmol) and toluene (1.0 mL) were added to a 10 mL pressure-proof vial with a Teflon-sealed screwcap and the cap was closed. The contents of the vial were then stirred at 80 °C (aluminum heating block) for 72 h. The reaction mixture was cooled to room temperature, and a colorless precipitate was formed. The solid obtained was filtered and washed hexane to give **5e-*d*₂**.

Colorless solid (39 mg, 69%). Mp 233–234 °C R_f 0.22 (SiO₂, hexane/CHCl₃ = 2/1 (v/v)).

¹H NMR (CDCl₃, 399.78 MHz) δ : 8.73 (d, J = 8.2 Hz, 1H), 8.59 (d, J = 8.2 Hz, 1H), 7.67–7.63 (m, 2H), 7.52–7.44 (m, 2H), 7.33–7.28 (m, 3H), 7.22 (t, J = 7.3 Hz, 1H), 7.14 (td, J = 7.6, 1.2 Hz, 1H), 7.05–6.91 (m, 5H), 6.85 (t, J = 7.8 Hz, 2H), 6.80–6.73 (m, 4H), 6.68–6.60 (m, 3H), 6.53 (d, J = 8.2 Hz, 1H), 6.29 (s, 2H), 5.83 (s, 0.2H), 5.61 (s, 0.1H).

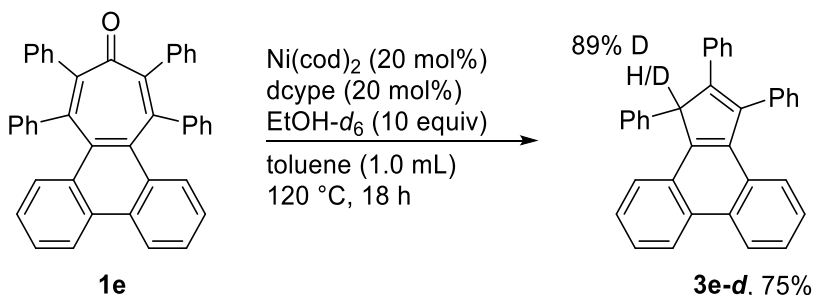
¹³C{¹H} NMR (CDCl₃, 100.53 MHz) δ : 209.7, 140.6, 139.6, 139.3, 138.2, 133.0 (two peaks are overlapped), 131.7, 131.1, 130.4, 129.8, 129.7, 129.5 (two peaks are overlapped), 129.3, 128.6, 128.5, 128.3, 128.0, 127.9, 127.7, 127.5, 127.3, 126.9 (three peaks are overlapped), 126.5, 125.7, 125.1, 123.2, 122.4, 84.9, 69.8, 66.5, 57.4.

²H NMR (CDCl₃, 399.78 MHz) δ : 5.82, 5.61.

IR (KBr, cm⁻¹): 3081 m, 3050 m, 3027 m, 1768 s, 1597 m, 1495 s, 1447 m, 1149 m, 1031 w, 922 w, 759 s, 730 s, 722 m, 699 s, 679 w, 618 w, 543 m, 533 m, 507 w.

HRMS (DART+TOF) m/z : [M+H]⁺ Calcd for C₄₃H₂₉OD₂ 565.2495; Found 565.2490.

1,2,3-Triphenyl-1*H*-cyclopenta[*l*]phenanthrene-1-*d* (**3e-d**).



In a glovebox filled with nitrogen, Ni(cod)₂ (5.8 mg, 0.021 mmol), dcype (8.9 mg, 0.020 mmol), EtOH-*d*₆ (80 μ L), **1e** (59.8 mg, 0.11 mmol) and toluene (1.0 mL) were added to a 10 mL pressure-proof vial with a Teflon-sealed screwcap and the cap was closed. The contents of the vial were then stirred at 120 °C (aluminum heating block) for 18 h. The reaction mixture was cooled to room temperature, and the crude mixture was filtered through a pad of silica gel. The filtrate was then concentrated in vacuo to give a residue, which was purified by flash column chromatography over silica gel to give **3e-d**.

Colorless solid (33 mg, 75%). Mp 205–213 °C R_f 0.54 (SiO₂, hexane/CHCl₃ = 2/1 (v/v)).

¹H NMR (CDCl₃, 399.78 MHz) δ : 8.77 (d, J = 8.2 Hz, 1H), 8.70 (d, J = 8.2 Hz, 1H), 7.88 (dd, J = 8.2, 0.9 Hz, 1H), 7.66 (d, J = 7.8 Hz, 1H), 7.63–7.50 (m, 4H), 7.45–7.36 (m, 3H), 7.29 (td, J = 7.7, 1.2 Hz, 2H), 7.20–7.13 (m, 4H), 7.11–7.01 (m, 6H), 5.48 (s, 0.1 H).

¹³C{¹H} NMR (CDCl₃, 100.53 MHz) δ : 150.2, 142.9, 141.4, 139.5, 139.0, 138.5, 135.6, 131.5, 130.9,

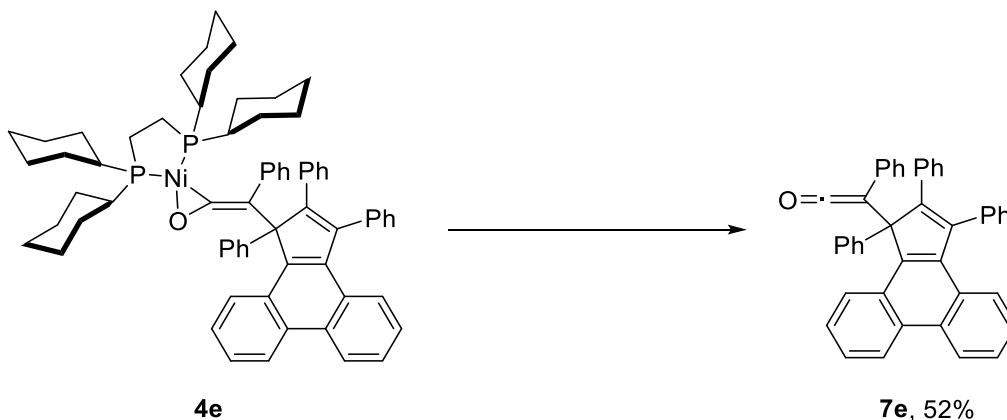
129.7, 129.5, 129.1, 128.8, 128.7, 128.6, 128.5, 128.3, 127.7, 127.6, 126.8 (two peaks are overlapped), 126.6, 126.0, 125.8, 125.6, 125.3, 124.5, 123.4 (two peaks are overlapped), 58.6.

^2H NMR (CDCl_3 , 399.78 MHz) δ : 5.49.

IR (KBr, cm^{-1}): 3078 w, 3057 w, 3023 w, 2924 w, 1599 w, 1492 m, 1442 m, 1239 w, 1215 w, 1157 w, 1075 w, 1028 w, 932 w, 909 w, 802 w, 787 w, 753 s, 725 s, 708 m, 698 s, 667 w, 615 w, 559 w, 536 w, 518 w.

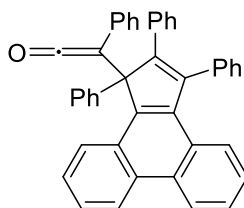
HRMS (DART+TOF) m/z : $[\text{M}+\text{H}]^+$ Calcd for $\text{C}_{35}\text{H}_{24}\text{D}$ 446.2014; Found 446.2014.

e. Role of Ni in the Cleavage of C–C bond in 7e.



Ni-ketene complex (**4e**) (15.2 mg, 0.01 mmol) was filtered through a pad of silica gel. The filtrate was then concentrated in vacuo to give **7e** (52%).

2-Phenyl-2-(1,2,3-triphenyl-1*H*-cyclopenta[*l*]phenanthren-1-yl)ethen-1-one (**7e**).



Yellow solid (4.1 mg, 52%). Mp 239–243 °C R_f 0.49 (SiO_2 , hexane/ CHCl_3 = 1/1 (v/v)).

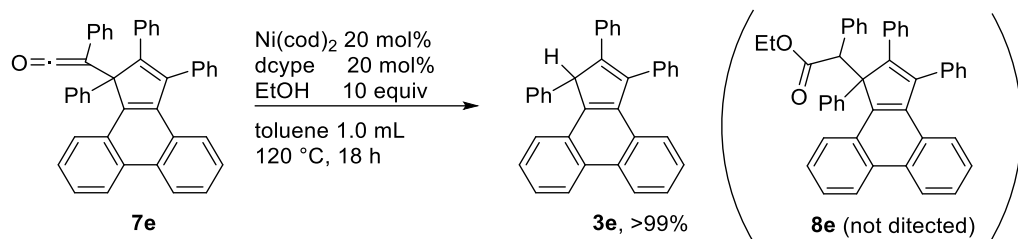
^1H NMR ($\text{THF}-d_8$, 399.78 MHz) δ : 8.86 (d, J = 10.4 Hz, 1H), 8.84 (d, J = 9.2 Hz, 1H), 7.96 (d, J = 8.2 Hz, 1H), 7.59–7.53 (m, 3H), 7.46 (dd, J = 8.0 Hz, 7.1 Hz, 1H), 7.33–7.09 (m, 11H), 7.07–6.91 (m, 8H), 6.67 (d, J = 8.2 Hz, 2H).

^{13}C NMR ($\text{THF}-d_8$, 100.53 MHz) δ : 202.2, 154.4, 144.2, 142.7, 139.8, 139.2, 138.7, 135.8, 132.7, 131.8, 131.5, 131.1, 130.7, 130.3, 129.3, 129.1, 129.0, 128.8, 128.7, 128.6, 128.5, 128.0, 127.7, 127.6, 127.0, 126.9, 126.6, 126.5, 126.4, 126.1, 126.0, 124.2, 124.1, 64.0, 46.7.

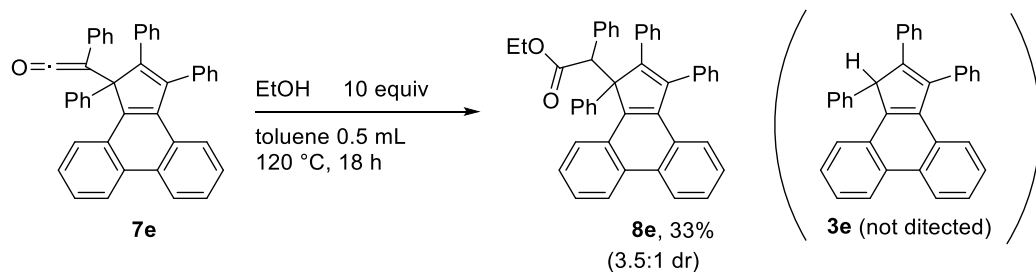
IR (KBr, cm^{-1}): 3898 w, 3851 w, 3646 w, 2093 s, 1595 w, 1557 w, 1538 w, 1505 w, 1494 w, 1443 w, 1029

w, 753 m, 725 w, 700 m, 559 w, 488 w, 480 w, 445 w, 435 w, 428 w, 416 m, 403 w.

HRMS (DART) Calcd for C₄₃H₂₉O ([M+H⁺]):561.2213. Found: 561.2210.

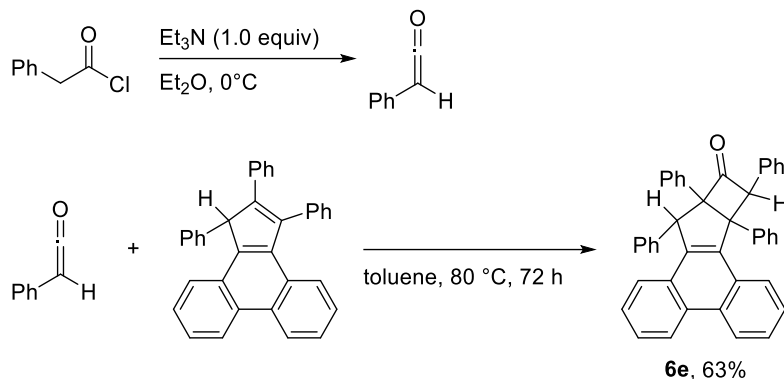


In a glovebox filled with nitrogen, Ni(cod)₂ (2.5 mg, 0.009 mmol), dcype (4.3 mg, 0.009 mmol), EtOH (30 μL, 10 equiv), **7e** (28.0 mg, 0.05 mmol) and toluene (0.5 mL) were added to a 10 mL pressure-proof vial with a Teflon-sealed screwcap and the cap was closed. The contents of the vial were then stirred at 120 °C (aluminum heating block) for 18 h. The reaction mixture was cooled to room temperature, and the crude mixture was filtered through a pad of silica gel. The filtrate was then concentrated in vacuo to give **3e** as a colorless solid (23 mg, >99%).



In a glovebox filled with nitrogen, **7e** (28 mg, 0.050 mmol), EtOH (30 μL, 10 equiv) and toluene (0.5 mL) were added to a 10 mL pressure-proof vial with a Teflon-sealed screwcap and the cap was closed. The contents of the vial were then stirred at 120 °C (aluminum heating block) for 18 h. Yield was determined by ¹H NMR spectroscopy using 1,3,5-trimethoxybenzene as an internal standard (33%).

f. Thermal conversion from **3e** to **6e**.

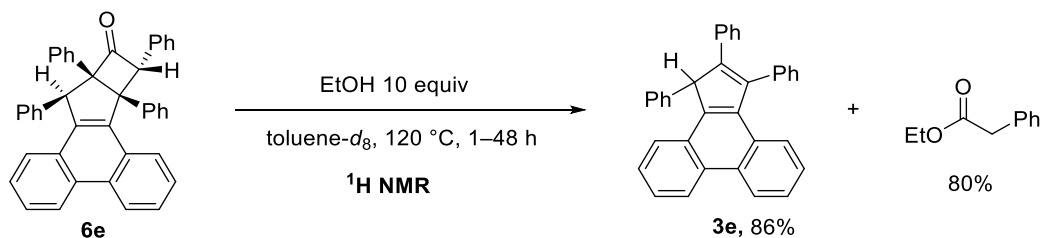


Phenylacetyl chloride (2.0 g, 13 mmol) was dissolved in diethyl ether (20 mL) and cooled to 0 °C. Freshly distilled triethylamine (1.8 mL, 1.0 equiv) was added dropwise over 30 min. When addition was complete the flask was stoppered and stored at 0 °C for overnight. The reaction mixture was warmed to rt and the salts were filtered and washed with diethyl ether until washings were colorless. The residue was concentrated to give phenylketene without further purification.

In a glovebox filled with nitrogen, phenylketene (5.9 mg, 0.05 mmol), **3e** (22 mg, 0.05 mmol) and toluene (0.5 mL) were added to a 10 mL pressure-proof vial with a Teflon-sealed screwcap and the cap was closed. The contents of the vial were then stirred at 80 °C (aluminum heating block) for 72 h. Yield was determined by ¹H NMR spectroscopy using 1,3,5-trimethoxybenzene as an internal standard (63%).

g. Retro [2+2] Reaction from cyclobutanone derivatives **6e** to cyclopentadiene derivatives **3e**.

NMR studies.



Cyclobutanone derivatives **6e** (57 mg, 0.1 mmol), EtOH (58 μL, 10 equiv) and toluene-*d*₈ (60 μL) were added to a NMR tube equipped with a screw cap. The cap was closed, and then it was taken out of the glovebox. The contents were then heated at 120 °C for 1 h. The contents were cooled to room temperature, the reaction was monitored by ¹H NMR spectroscopy at room temperature. The same procedure was performed at 120 °C for 6, 12, 18, 36, 48 h (**Figure S3**).

During the course of the reaction, new peaks (**b**: δ = 8.55, 8.48 and 5.18 ppm) appeared after 6 hours of heating alongside the signal of the **6e** (**a**: δ = 8.45, 8.35, 5.79 and 5.66 ppm) on ¹H NMR. These peaks were consistent with the signal of **3e**. Simultaneously, the characteristic peak of ester (**c**: δ = 3.84 ppm)

appeared. After 48 hours, the signal of cyclobutanone disappeared, and the peak of cyclopentadiene and ester were observed.

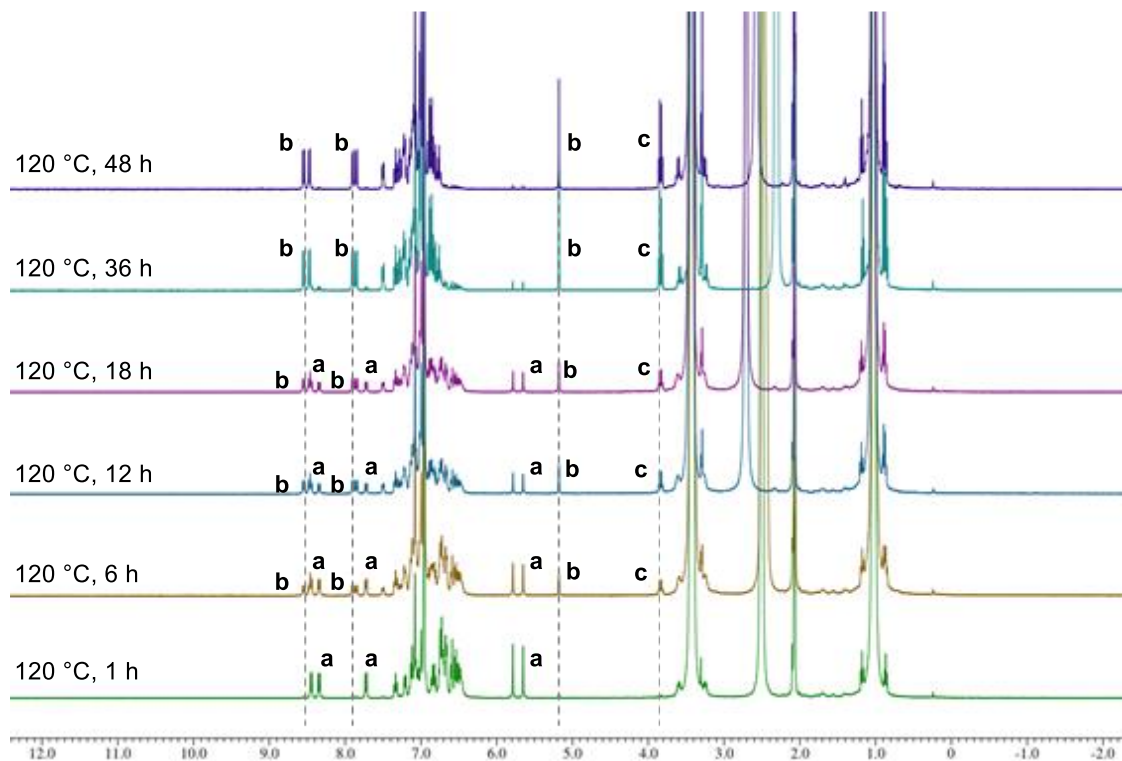
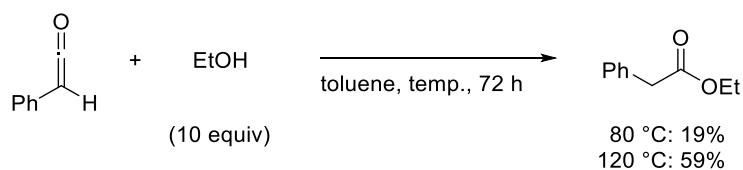


Fig. S3

h. Thermal Reaction of Ketene with Ethanol.



In a glovebox filled with nitrogen, phenyl ketene (11.5 mg, 0.05 mmol), EtOH (60 μ L) and toluene (0.5 mL) were added to a 10 mL pressure-proof vial with a Teflon-sealed screwcap and the cap was closed. The contents of the vial were then stirred at 80 $^\circ$ C or 120 $^\circ$ C (aluminum heating block) for 72 h. Yield was determined by ^1H NMR spectroscopy using 1,3,5-trimethoxybenzene as an internal standard.

IX. DFT Calculations.

All calculations were performed on actually used ligands (monodentate IMes^{Me} and bidentate dcype) and substrates (**1e** and **1c**) without simplification except for **1h**. For **1h**, α -phenyl analogue was used as a model for clarity.

a. Distortion/Interaction Analysis.

Table S2 Distortion/interaction analysis for **TS1**.

$\Delta E / \text{kcal mol}^{-1}$	TS1 (1c)	TS1 (1e)	TS1 (1h)
ΔE_{strain}	43.2	20.4	36.6
ΔE_{int}	17.5	10.3	15.4
$\Delta E = \Delta E_{\text{strain}} + \Delta E_{\text{int}}$	60.7	30.7	52.0

b. Computed energy profiles.

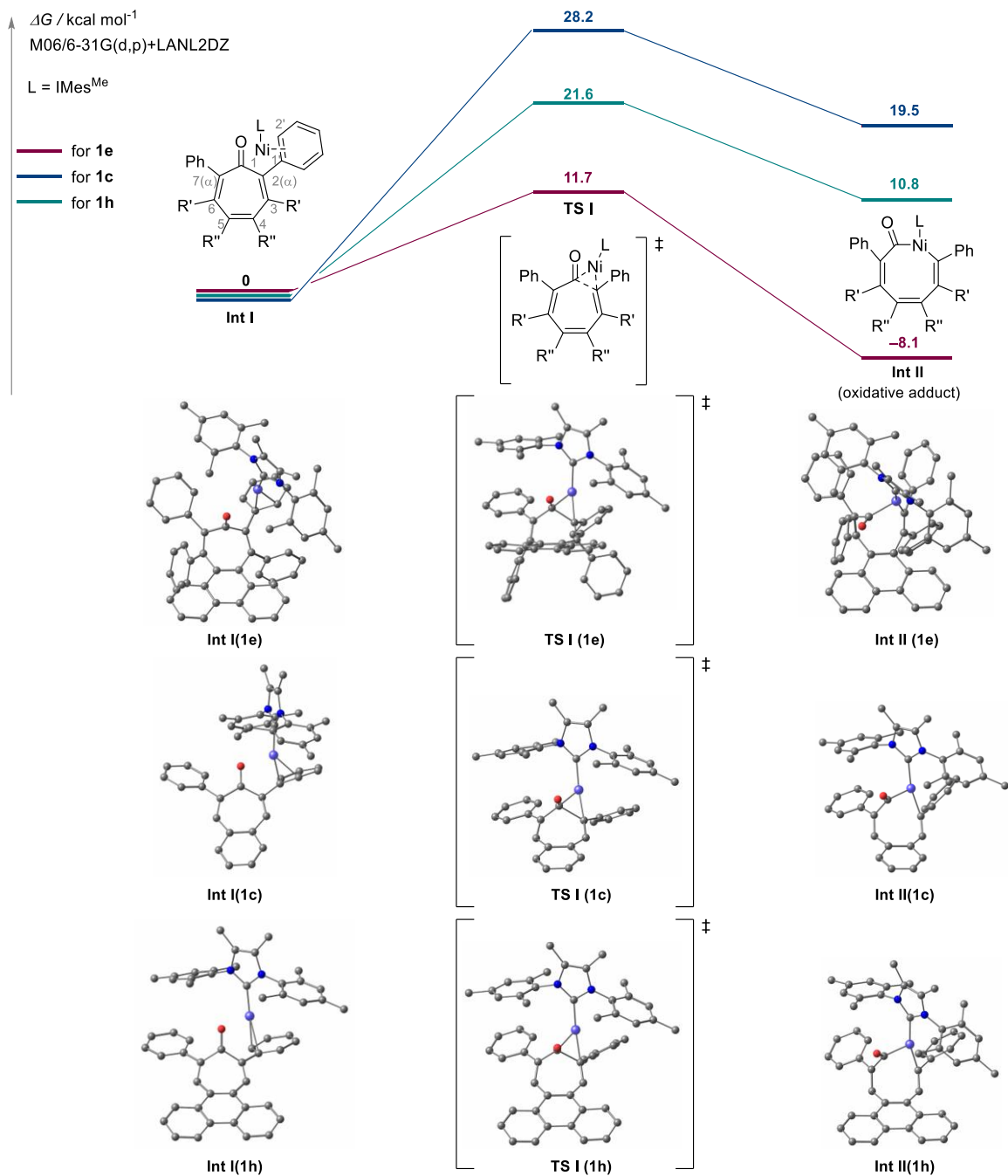


Fig. S4. Substrate dependence on oxidative addition of **1e** (red), **1c** (blue), and **1h** (green) to Ni-IMes^{Me} at the M06-2X/6-31G(d,p)-LanL2DZ level of theory. For **1h**, α -phenyl analogue was used as a model for clarity.

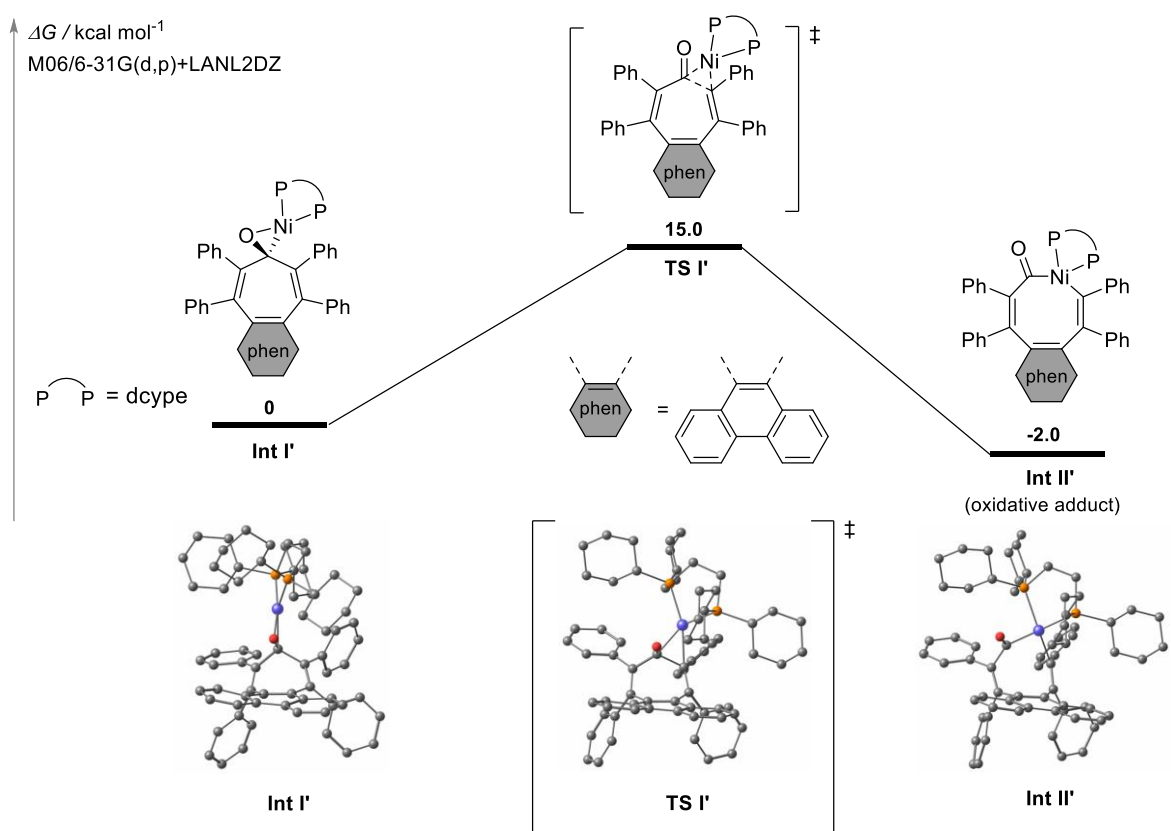


Fig. S5. Oxidative addition of **1e** to Ni-dcype at the at the M06-2X/6-31G(d,p)-Lanl2DZ level of theory.

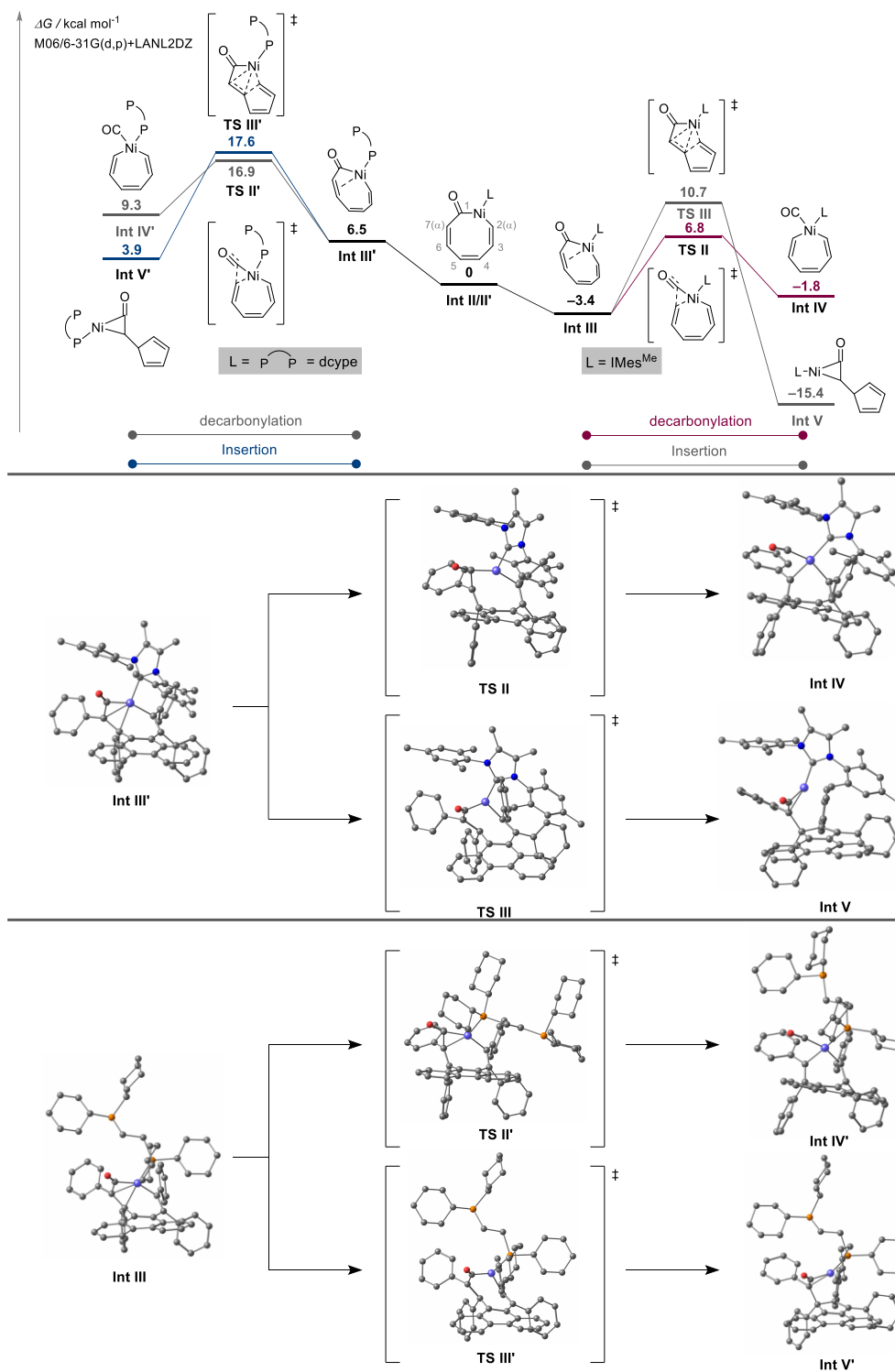
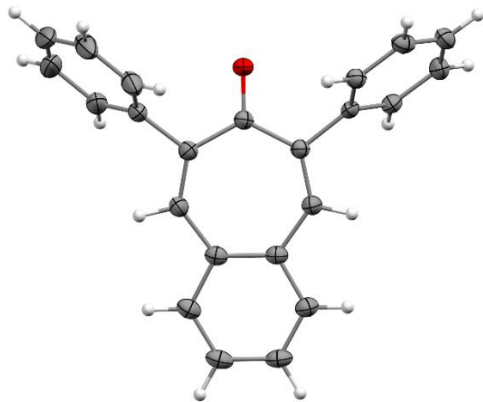


Fig. S6. Energy diagram for ligand-controlled selective ring contraction reactions of **1e** at the at the M06-2X/6-31G(d,p)-Lanl2DZ level of the theory.

X. Crystallographic Information.

View1



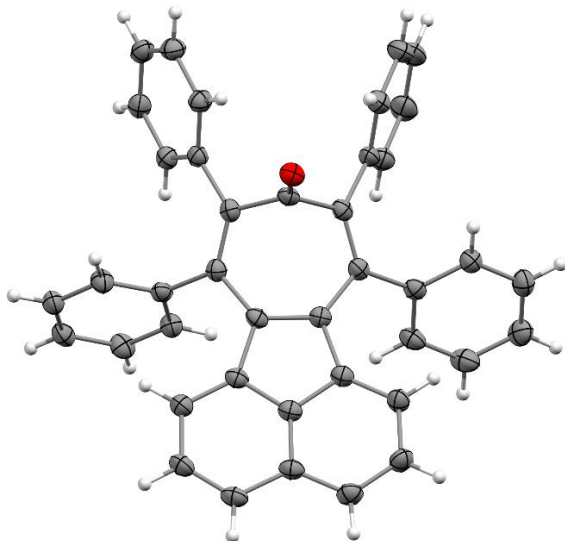
View2



Fig. S7. ORTEP drawing of **1c** with thermal ellipsoids set at the 50% probability level.^a

^aCrystal data for **1c**, triclinic, space group $P\bar{1}$ (no. 2), $a = 10.99710(10)$ Å, $b = 21.3867(2)$ Å, $c = 28.8610(2)$ Å, $\alpha = 76.1520(10)^\circ$, $\beta = 85.8840(10)^\circ$, $\gamma = 86.2040(10)^\circ$, $V = 6565.15(10)$ Å³, $T = 123$ K, $Z = 2$, $R1$ ($wR2$) = 0.0434 (0.1171) for 1729 parameters and 26553 unique reflections. GOF = 1.046. CCDC 2115589.

View1



View2

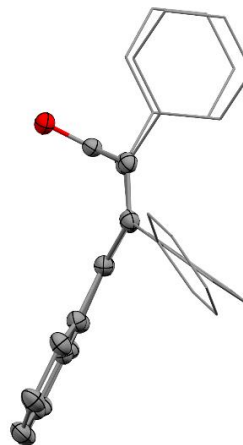


Fig. S8. ORTEP drawing of **1i** with thermal ellipsoids set at the 50% probability level.^a

^aCrystal data for **1i**, triclinic, space group $P\bar{1}$ (no. 2), $a = 10.4122(3)$ Å, $b = 11.1627(3)$ Å, $c = 14.3485(3)$ Å, $\alpha = 103.578(2)^\circ$, $\beta = 103.147(2)^\circ$, $\gamma = 112.391(3)^\circ$, $V = 1402.62(7)$ Å³, $T = 123$ K, $Z = 2$, $R1$ ($wR2$) = 0.0554 (0.1469) for 380 parameters and 5623 unique reflections. GOF = 1.059. CCDC 2115591.

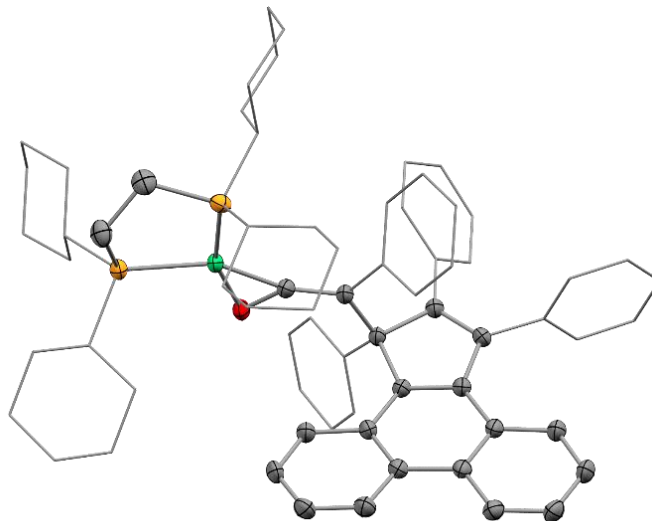


Fig. S9. ORTEP drawing of **4e** with thermal ellipsoids set at the 50% probability level.^a

^aCrystal data for **4e**, monoclinic, space group $P 2_1/c$ (no. 14), $a = 33.7405(2) \text{ \AA}$, $b = 13.53070(10) \text{ \AA}$, $c = 24.6084(2) \text{ \AA}$, $\alpha = \gamma = 90^\circ$ $\beta = 105.0390(10)^\circ$, $V = 10849.75(14) \text{ \AA}^3$, $T = 123 \text{ K}$, $Z = 4$, $R1$ ($wR2$) = 0.0531 (0.1423) for 1315 parameters and 21988 unique reflections. GOF = 1.383. CCDC 2115592.

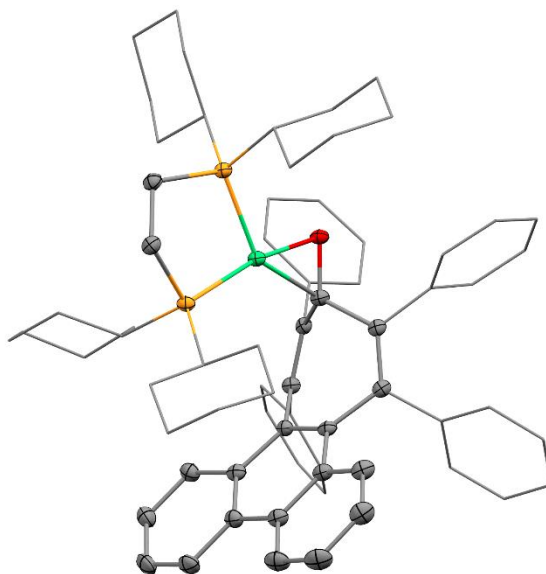


Fig. S10. ORTEP drawing of **5e** with thermal ellipsoids set at the 50% probability level.^a

^aCrystal data for **5e**, triclinic, space group $P \bar{1}$ (no. 2), $a = 10.9952(2) \text{ \AA}$, $b = 14.1370(2) \text{ \AA}$, $c = 21.6909(3) \text{ \AA}$, $\alpha = 104.7600(10)^\circ$, $\beta = 97.2130(10)^\circ$, $\gamma = 100.5840(10)^\circ$, $V = 3151.76(9) \text{ \AA}^3$, $T = 123 \text{ K}$, $Z = 2$, $R1$ ($wR2$) = 0.0728 (0.2025) for 748 parameters and 12709 unique reflections. GOF = 1.126. CCDC 2115590.

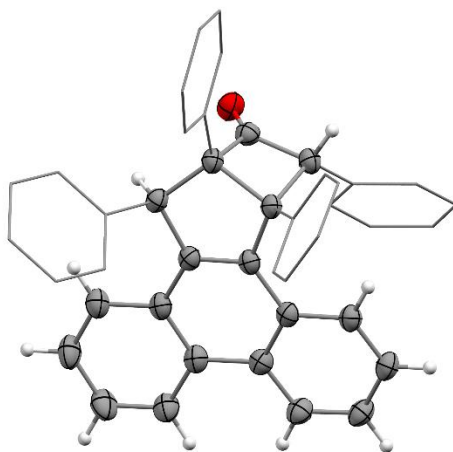


Fig. S11. ORTEP drawing of **6e** with thermal ellipsoids set at the 50% probability level.^a

^aCrystal data for **6e**, monoclinic, space group $P 2_1/n$ (no. 14), $a = 13.0907(5)$ Å, $b = 10.1466(3)$ Å, $c = 22.1188(7)$ Å, $\alpha = \gamma = 90^\circ$ $\beta = 94.055(3)^\circ$, $V = 2930.60(18)$ Å³, $T = 123$ K, $Z = 4$, $R1$ ($wR2$) = 0.0647 (0.1735) for 397 parameters and 5927 unique reflections. GOF = 1.050. CCDC 2115593.

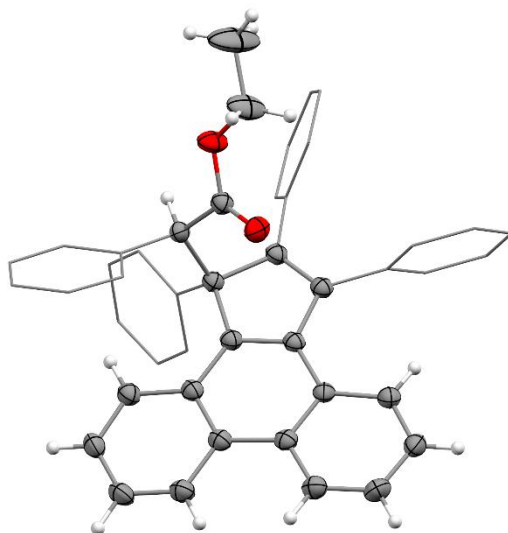


Fig. S12. ORTEP drawing of **8e** with thermal ellipsoids set at the 50% probability level.^a

^aCrystal data for **8e**, triclinic, space group $P \bar{1}$ (no. 2), $a = 10.26982(17)$ Å, $b = 12.9000(2)$ Å, $c = 13.4161(2)$ Å, $\alpha = 101.7874(13)^\circ$, $\beta = 98.9295(13)^\circ$, $\gamma = 108.9135(15)^\circ$, $V = 1598.20(5)$ Å³, $T = 123$ K, $Z = 2$, $R1$ ($wR2$) = 0.0529 (0.1489) for 425 parameters and 6464 unique reflections. GOF = 1.082. CCDC 2115594.

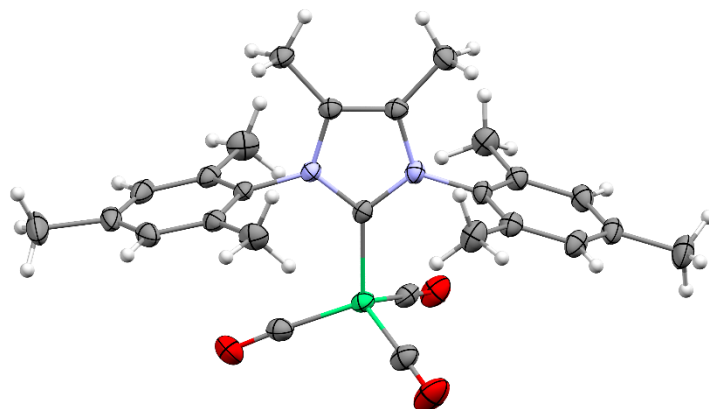
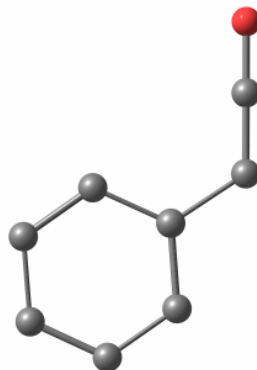


Fig. S13. ORTEP drawing of $\text{Ni}(\text{CO})_3(\text{IMes}^{\text{Me}})$ with thermal ellipsoids set at the 50% probability level.^a

^aCrystal data for $\text{Ni}(\text{CO})_3(\text{IMes}^{\text{Me}})$, monoclinic, space group $P 2_1/c$ (no. 14), $a = 19.0889(5)$ Å, $b = 15.9034(4)$ Å, $c = 18.9504(7)$ Å, $\alpha = \gamma = 90^\circ$ $\beta = 106.854(4)^\circ$, $V = 5505.8(3)$ Å³, $T = 123$ K, $Z = 4$, $R1$ ($wR2$) = 0.0365 (0.0991) for 657 parameters and 13240 unique reflections. GOF = 1.061. CCDC 2115595.

X. Cartesian Coordinates and Energies of Optimized Structures.

Phenylketene.

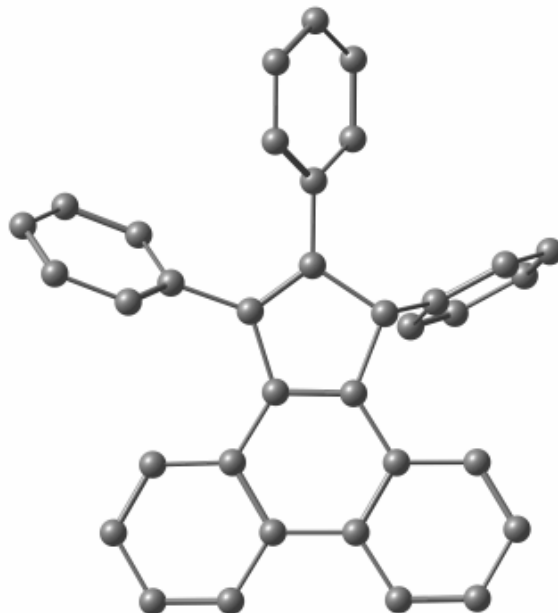


8	-3.47099900	0.56787300	-0.00002700
6	-2.53260600	-0.11982800	0.00001900
6	-1.46510400	-0.89730700	0.00001500
6	-0.08739400	-0.38625900	0.00000700
6	0.97543400	-1.29602900	-0.00000400
6	2.29164700	-0.84787300	-0.00001000
6	2.57149000	0.51516800	-0.00000600
6	1.51843000	1.42781700	0.00000400
6	0.20266500	0.98504300	0.00001100
1	-1.65886400	-1.96335600	0.00001000
1	0.76499300	-2.36162600	-0.00000700

1	3.10216400	-1.56997100	-0.00001900
1	3.59843600	0.86444400	-0.00001200
1	1.72251200	2.49390600	0.00000800
1	-0.60862300	1.70922200	0.00002000

Method: M06-2X/6-31G(d,p) Key word: opt freq pop=full
 imaginary frequencies: 0 Energy: -383.413497 Hartree

1,2,3-triphenyl-1*H*-cyclopenta[*l*]phenanthrene. (3e)

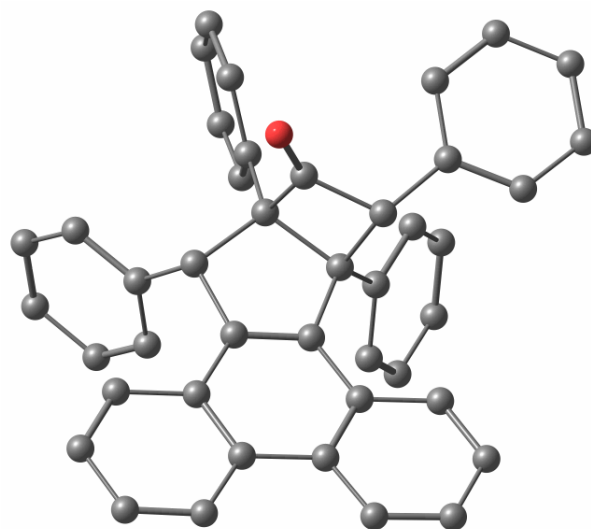


6	2.48500400	-0.90852500	-0.68350900
6	3.52128400	0.03882400	-0.48161200
6	3.19089000	1.37216400	0.01468800
6	1.83398900	1.74535500	0.22470100
6	0.80408000	0.78632900	-0.10718100
6	1.13353800	-0.48774600	-0.48086800
6	2.79947300	-2.21552600	-1.11704400
6	4.10352100	-2.58092900	-1.36127500
6	5.13406900	-1.64304300	-1.18344100
6	4.84591900	-0.36554300	-0.75295600
6	4.19662200	2.30832300	0.33753100
6	3.89264200	3.54386800	0.86573900
6	2.55659700	3.88956600	1.11356100
6	1.54907400	3.00403300	0.80022000
6	-0.67639700	0.90022200	-0.08809800
6	-1.21683100	-0.30998300	-0.36987500
6	-0.11286300	-1.32094500	-0.64096000
6	-2.65179500	-0.62656100	-0.54475800
6	-3.43208900	0.14700800	-1.41547700
6	-4.77937900	-0.13570400	-1.60459300
6	-5.37275300	-1.19840500	-0.92736600
6	-4.60941200	-1.97148400	-0.05768300
6	-3.25915100	-1.69181500	0.13374000
6	-1.46366200	2.14372800	0.08938100
6	-1.25648200	3.22700200	-0.77377400
6	-2.02016900	4.38194300	-0.65369400

6	-3.00239500	4.47014600	0.33108400
6	-3.21746400	3.39644900	1.19053500
6	-2.45449400	2.23838700	1.06957900
6	-0.16102700	-2.53443700	0.27135700
6	-0.52031800	-3.78760700	-0.22265200
6	-0.61992300	-4.88376600	0.63202900
6	-0.36046400	-4.73330500	1.99029200
6	0.00450400	-3.48322700	2.48956000
6	0.10533300	-2.39140100	1.63556200
1	1.99590900	-2.93254300	-1.25391300
1	4.33480600	-3.58723300	-1.69509500
1	6.16277900	-1.92277700	-1.38649300
1	5.66338600	0.33499600	-0.63127800
1	5.23893700	2.05317900	0.18914100
1	4.69053300	4.23872100	1.10727500
1	2.31451700	4.84835900	1.56051200
1	0.52292500	3.26831000	1.01906200
1	-0.21667100	-1.66537500	-1.68013000
1	-2.96881400	0.97572900	-1.94252500
1	-5.36702600	0.47438600	-2.28328200
1	-6.42495600	-1.42011500	-1.07505700
1	-5.06671700	-2.79618200	0.48005100
1	-2.67842800	-2.29139200	0.82659900
1	-0.48414100	3.15594100	-1.53531000
1	-1.84937700	5.21365800	-1.32984300
1	-3.59772100	5.37264000	0.42622800
1	-3.98249400	3.45964100	1.95788800
1	-2.62547100	1.39425000	1.73101100
1	-0.73790600	-3.90157000	-1.28180800
1	-0.90413000	-5.85318300	0.23492300
1	-0.43766100	-5.58504400	2.65829000
1	0.21247500	-3.36057300	3.54782200
1	0.38841600	-1.41420700	2.01949600

Method: M06-2X/6-31G(d,p) Key word: opt freq pop=full
imaginary frequencies: 0 Energy: -1347.258113 Hartree

8c,9,10a,11-Tetraphenyl-8c,9,10a,11-tetrahydro-10H-cyclobuta[3,4]cyclopenta[1,2-l]phenanthren-10-one. (5e)

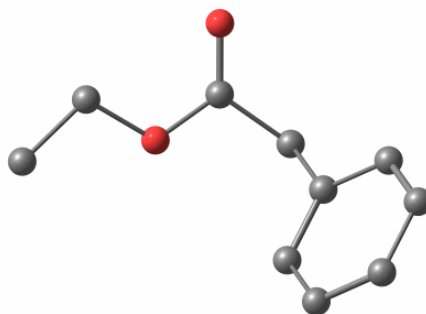


6	3.19777800	0.12964800	-0.75462400
6	3.88059200	-1.07246700	-0.44477000
6	3.12568300	-2.22022000	0.05357200
6	1.72536700	-2.10922700	0.25149800
6	1.07067300	-0.86331000	-0.06912400
6	1.77045900	0.18428500	-0.57639900
6	3.91490400	1.24355800	-1.23770600
6	5.27926600	1.17751800	-1.41699900
6	5.96275500	-0.01015400	-1.11492000
6	5.27706200	-1.10810100	-0.63853700
6	3.73954000	-3.45671900	0.34304100
6	3.01076100	-4.53229400	0.80557100
6	1.62733800	-4.41460200	1.00573200
6	0.99851200	-3.21890800	0.73387700
6	-0.42967700	-0.62508900	-0.03103500
6	-0.53029000	0.74036800	-0.85431900
6	0.89955400	1.36721500	-0.92586000
6	-1.03359800	-1.42291700	-1.27921700
6	-0.80456800	-0.14357200	-2.07856800
8	-0.77951600	0.08949100	-3.25636400
6	-1.63642300	1.73740100	-0.58536400
6	-1.85858000	2.24447100	0.70198400
6	-2.81850700	3.22567400	0.91901900
6	-3.56873000	3.72540900	-0.14306300
6	-3.34159100	3.24529500	-1.42761300
6	-2.37947900	2.26136400	-1.64763100
6	-1.06523700	-0.71391600	1.34074600
6	-2.45512500	-0.66036400	1.51295000
6	-3.01926200	-0.66516800	2.78457400
6	-2.21107200	-0.71608100	3.91612900
6	-0.82934700	-0.76022500	3.76266900
6	-0.26536400	-0.75968500	2.49007400
6	-2.44638400	-1.95111900	-1.26540600
6	-2.70415900	-3.17864000	-0.64816900
6	-3.99910200	-3.67754600	-0.56812900
6	-5.05867200	-2.95774600	-1.11521800
6	-4.80941400	-1.74660900	-1.75342300
6	-3.51162000	-1.24762200	-1.83270000
6	1.11251300	2.57712000	-0.03830500
6	0.83675600	3.85266300	-0.53655300

6	0.95515700	4.97411800	0.27699900
6	1.35586500	4.83311000	1.60345200
6	1.64035700	3.56694200	2.10656800
6	1.52064100	2.44557100	1.29012800
1	3.37823700	2.16239200	-1.45338300
1	5.82338800	2.04059200	-1.78626200
1	7.03762500	-0.06673400	-1.25347900
1	5.83534800	-2.00817800	-0.40987600
1	4.80632500	-3.57892500	0.19722200
1	3.51193800	-5.47161200	1.01537700
1	1.05546200	-5.25969200	1.37496500
1	-0.06718700	-3.11064400	0.90971900
1	1.05893700	1.67384300	-1.96913300
1	-0.36055400	-2.23082600	-1.58819200
1	-1.26654800	1.88246800	1.53577700
1	-2.97462000	3.60559000	1.92360300
1	-4.31790000	4.49169800	0.02941800
1	-3.90814300	3.63765000	-2.26635800
1	-2.18982200	1.91157500	-2.65806800
1	-3.10989700	-0.58379400	0.65367900
1	-4.09882200	-0.61855600	2.88634300
1	-2.65310600	-0.71693800	4.90746800
1	-0.18301100	-0.79579900	4.63396100
1	0.81486800	-0.80104600	2.39193900
1	-1.87793100	-3.74665000	-0.22860600
1	-4.18055700	-4.63029900	-0.08099500
1	-6.07075200	-3.34431200	-1.05283000
1	-5.62671600	-1.18580300	-2.19564100
1	-3.33316700	-0.30048700	-2.33237300
1	0.50400100	3.95913300	-1.56629900
1	0.73194000	5.95790800	-0.12365200
1	1.44777100	5.70674700	2.24095300
1	1.95752700	3.44997200	3.13810900
1	1.73950600	1.45823900	1.68795200

Method: M06-2X/6-31G(d,p) Key word: opt freq pop=full
 imaginary frequencies: 0 Energy: -1730.678737 Hartree

Ethyl 2-phenylacetate.

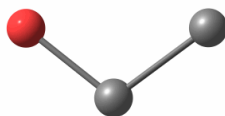


8	1.82606200	0.09331300	-0.32438000
6	1.26800900	-1.11716100	-0.15431100
6	0.05689900	-1.28718300	-1.04920200
8	1.67568100	-1.93505600	0.63108600
6	-1.10649000	-0.47438500	-0.51997100
6	-1.18591100	0.89684200	-0.77291000

6	-2.24013000	1.64723900	-0.26400400
6	-3.22583600	1.03567400	0.50764200
6	-3.14959700	-0.32897400	0.76843000
6	-2.09350200	-1.07917200	0.25809100
6	2.93117200	0.38756600	0.54275700
6	3.37294400	1.80197600	0.23963600
1	0.32034200	-0.95922200	-2.05881300
1	-0.18692800	-2.35021500	-1.06762400
1	-0.41001600	1.37319700	-1.36560800
1	-2.29391100	2.71142200	-0.47097200
1	-4.05015900	1.62085500	0.90248400
1	-3.91348700	-0.81269900	1.36889400
1	-2.03237900	-2.14426200	0.46431600
1	2.60511400	0.26915200	1.58031600
1	3.72568600	-0.34257900	0.36155300
1	4.21750600	2.07539200	0.87636300
1	3.68170500	1.89336500	-0.80419000
1	2.55723500	2.50499700	0.42268800

Method: M06-2X/6-31G(d,p) Key word: opt freq pop=full
 imaginary frequencies: 0 Energy: -538.369447 Hartree

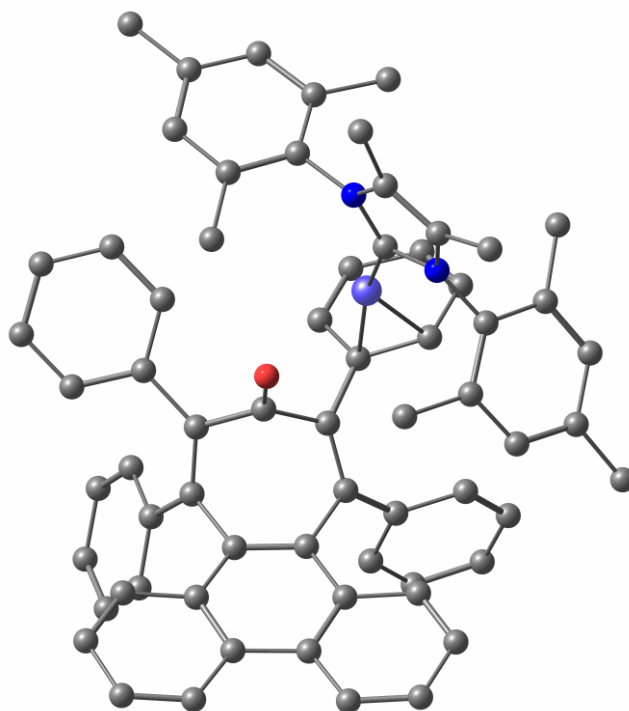
Ethanol.



6	-1.21576800	-0.22146900	0.00015000
6	0.08874500	0.54955200	-0.00013800
8	1.14007000	-0.39787900	-0.00031500
1	-2.07077400	0.45911300	-0.00019700
1	-1.27268200	-0.85933400	-0.88493900
1	-1.27277500	-0.85865000	0.88571800
1	0.14006900	1.19897700	0.88648200
1	0.13973800	1.19886300	-0.88687300
1	1.97799900	0.07555800	0.00225800

Method: M06-2X/6-31G(d,p) Key word: opt freq pop=full
 imaginary frequencies: 0 Energy: -154.907494 Hartree

Int I (1e).



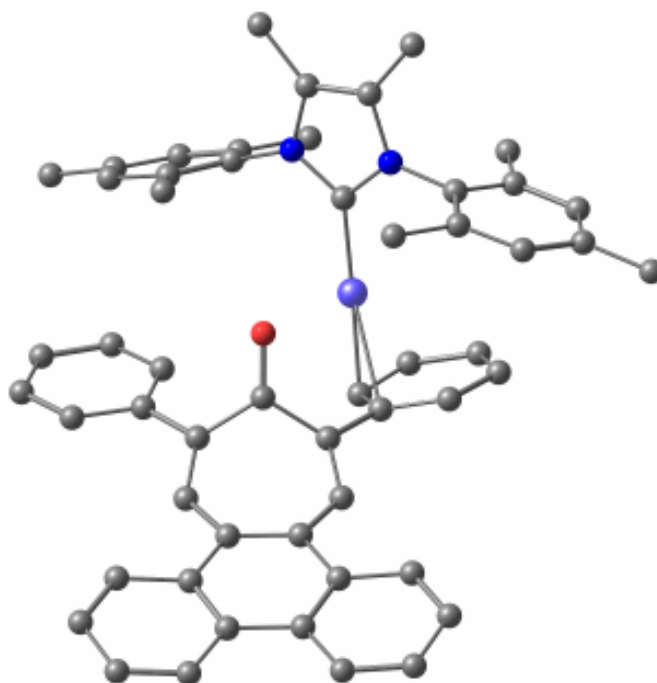
6	4.095832000	-0.823868000	1.908214000
6	4.629592000	0.273763000	2.629752000
6	4.290956000	1.622604000	2.222897000
6	3.412140000	1.810903000	1.127443000
6	2.958118000	0.677798000	0.348323000
6	3.319702000	-0.599165000	0.702436000
6	4.745769000	2.756952000	2.925131000
6	4.324854000	4.025783000	2.596731000
6	3.408608000	4.205960000	1.553191000
6	2.965056000	3.117656000	0.836683000
6	4.313374000	-2.128106000	2.406385000
6	5.073049000	-2.354507000	3.530543000
6	5.649593000	-1.273061000	4.207685000
6	5.419638000	0.010552000	3.767092000
6	2.029997000	0.909476000	-0.787187000
6	0.856646000	0.237882000	-0.765561000
28	-1.924599000	0.318133000	-0.751786000
6	0.629019000	-0.817377000	0.298463000
6	1.476612000	-2.039104000	0.091361000
6	2.821921000	-1.812299000	-0.022706000
8	-0.287693000	-0.758871000	1.099016000
6	0.755266000	-3.324706000	0.033318000
6	3.782812000	-2.628647000	-0.790610000
6	-0.226539000	0.287191000	-1.785994000
6	-0.402947000	-0.810133000	-2.683944000
6	-1.205467000	-0.711128000	-3.800841000
6	-1.882581000	0.492068000	-4.087031000
6	-1.780654000	1.558653000	-3.222886000
6	-0.998144000	1.473566000	-2.040962000
6	1.390156000	-4.513378000	0.429035000
6	0.708936000	-5.719543000	0.444519000
6	-0.633023000	-5.772363000	0.073392000
6	-1.284023000	-4.602925000	-0.299020000

6	-0.604744000	-3.390110000	-0.307236000
6	3.332135000	-3.463397000	-1.829590000
6	4.221235000	-4.146420000	-2.642635000
6	5.594557000	-4.005706000	-2.460020000
6	6.062133000	-3.156876000	-1.465017000
6	5.171388000	-2.472693000	-0.647422000
6	2.534344000	1.735488000	-1.915674000
6	1.863389000	2.828337000	-2.474352000
6	2.415512000	3.537547000	-3.534554000
6	3.649517000	3.171379000	-4.059851000
6	4.335461000	2.096191000	-3.504707000
6	3.788023000	1.394193000	-2.439233000
1	5.436198000	2.637931000	3.755083000
1	4.690791000	4.881447000	3.159004000
1	3.049493000	5.202795000	1.303557000
1	2.248502000	3.264639000	0.034208000
1	3.860318000	-2.970189000	1.890030000
1	5.218504000	-3.369237000	3.892483000
1	6.260206000	-1.442433000	5.091142000
1	5.850421000	0.836000000	4.326271000
1	0.163423000	-1.725442000	-2.509596000
1	-1.293591000	-1.559640000	-4.475190000
1	-2.486995000	0.572174000	-4.987780000
1	-2.293215000	2.495536000	-3.440310000
1	-0.799036000	2.381413000	-1.471185000
1	2.435220000	-4.483085000	0.730195000
1	1.225505000	-6.623455000	0.759129000
1	-1.168102000	-6.719366000	0.085644000
1	-2.335284000	-4.618925000	-0.580167000
1	-1.151158000	-2.487862000	-0.581790000
1	2.265555000	-3.564276000	-2.010593000
1	3.838051000	-4.781955000	-3.437425000
1	6.291732000	-4.540258000	-3.100602000
1	7.131135000	-3.017226000	-1.322603000
1	5.565141000	-1.802023000	0.110573000
1	0.913027000	3.147832000	-2.054665000
1	1.875421000	4.387460000	-3.946900000
1	4.079051000	3.725972000	-4.890758000
1	5.304460000	1.801819000	-3.901313000
1	4.329759000	0.555576000	-2.003084000
6	-3.295352000	0.699586000	0.467616000
6	-4.989694000	0.711125000	2.010699000
6	-6.120315000	0.134587000	2.776263000
1	-6.535079000	0.875968000	3.465739000
1	-6.928748000	-0.200629000	2.113836000
1	-5.810775000	-0.738068000	3.365417000
6	-4.423257000	1.945855000	2.028901000
6	-4.725444000	3.154613000	2.831906000
1	-5.584435000	2.976126000	3.485416000
1	-3.876693000	3.444676000	3.464876000
1	-4.958381000	4.017199000	2.194661000
6	-2.565913000	3.014055000	0.690833000
6	-2.136014000	4.809947000	-0.835930000
6	-0.505031000	4.219347000	0.818645000
1	-2.447843000	5.425583000	-1.680720000
1	0.470855000	4.371182000	1.283457000
6	-4.589375000	-1.371840000	0.675641000
6	-5.747406000	-2.890281000	-0.766596000
6	-4.377211000	-3.727344000	1.013138000
1	-6.402013000	-3.068725000	-1.620288000

1	-3.943159000	-4.567989000	1.557368000
6	-1.323678000	3.203527000	1.307107000
6	-0.849822000	2.297445000	2.398270000
1	0.049088000	2.699168000	2.877208000
1	-1.615376000	2.140171000	3.168125000
1	-0.610239000	1.306082000	1.988370000
6	-2.992398000	3.808899000	-0.376894000
6	-4.291367000	3.522352000	-1.063756000
1	-4.246165000	2.533485000	-1.542802000
1	-5.136748000	3.494935000	-0.364624000
1	-4.504672000	4.271393000	-1.832798000
6	-0.885775000	5.021734000	-0.258023000
6	0.053999000	6.063717000	-0.787489000
1	-0.402248000	6.648136000	-1.592904000
1	0.366622000	6.760447000	-0.000195000
1	0.969654000	5.603556000	-1.185868000
6	-4.025190000	-2.433181000	1.390440000
6	-3.014373000	-2.192332000	2.466893000
1	-2.062704000	-1.862924000	2.024881000
1	-3.323128000	-1.405361000	3.165394000
1	-2.823861000	-3.107909000	3.035700000
6	-5.432807000	-1.577294000	-0.420240000
6	-5.923068000	-0.419796000	-1.234379000
1	-5.084517000	0.030748000	-1.785262000
1	-6.679819000	-0.739126000	-1.957597000
1	-6.351755000	0.376971000	-0.612588000
6	-5.239661000	-3.974986000	-0.054575000
6	-5.608974000	-5.381895000	-0.419014000
1	-6.031422000	-5.439862000	-1.427384000
1	-4.738724000	-6.048452000	-0.377502000
1	-6.354989000	-5.790643000	0.274390000
7	-3.391908000	1.914083000	1.086868000
7	-4.281161000	-0.029187000	1.056003000

Method: M06-2X/6-31G(d,p) Key word: opt freq pop=full
imaginary frequencies: 0 Energy: -2899.943432 Hartree

Int I (phenyl analogue of 1h).



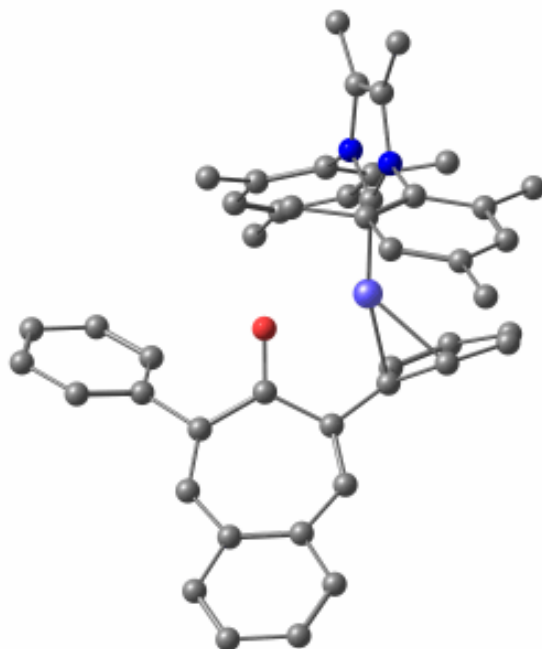
6	-5.727163000	-1.397503000	-0.455232000
6	-6.837184000	-0.516698000	-0.467293000
6	-6.641745000	0.882559000	-0.135299000
6	-5.345713000	1.341010000	0.201561000
6	-4.241307000	0.401605000	0.340134000
6	-4.424493000	-0.939803000	0.014996000
6	-7.696545000	1.814046000	-0.191411000
6	-7.490451000	3.156103000	0.036469000
6	-6.199964000	3.620604000	0.308314000
6	-5.154553000	2.728012000	0.384912000
6	-5.922188000	-2.715266000	-0.924223000
6	-7.159521000	-3.172401000	-1.319016000
6	-8.264653000	-2.317826000	-1.266973000
6	-8.094844000	-1.014022000	-0.859294000
6	-3.029597000	0.912791000	0.937338000
6	-1.741743000	0.507827000	0.818953000
28	1.764777000	0.461814000	1.132618000
6	-1.314656000	-0.632874000	-0.018396000
6	-2.057832000	-1.893285000	0.179012000
6	-3.413943000	-1.954798000	0.213618000
8	-0.318512000	-0.574794000	-0.726701000
6	-1.236349000	-3.115810000	0.318146000
6	-0.661310000	1.236347000	1.514615000
6	0.239294000	0.493343000	2.347193000
6	1.321133000	1.179310000	2.966637000
6	1.412319000	2.591410000	2.839666000
6	0.484377000	3.294092000	2.101053000
6	-0.540406000	2.614108000	1.417526000
6	-1.704861000	-4.361718000	-0.115244000
6	-0.958688000	-5.516129000	0.086002000
6	0.270743000	-5.449243000	0.732401000
6	0.758809000	-4.214473000	1.149696000
6	0.025710000	-3.058298000	0.927793000

1	-8.700808000	1.479133000	-0.431982000
1	-8.325093000	3.850601000	-0.016813000
1	-6.017040000	4.682508000	0.452192000
1	-4.156014000	3.115583000	0.563599000
1	-5.075093000	-3.389019000	-1.009330000
1	-7.269924000	-4.192587000	-1.678028000
1	-9.248057000	-2.670607000	-1.567272000
1	-8.959326000	-0.357054000	-0.855001000
1	-0.035949000	-0.517124000	2.657550000
1	1.927028000	0.676272000	3.719197000
1	2.222467000	3.119728000	3.340637000
1	0.576645000	4.373100000	1.994050000
1	-1.216714000	3.164698000	0.762912000
1	-2.654776000	-4.424599000	-0.643614000
1	-1.339113000	-6.470885000	-0.270033000
1	0.853602000	-6.353410000	0.897434000
1	1.728400000	-4.140257000	1.638712000
1	0.451225000	-2.099204000	1.224251000
6	3.021472000	0.475465000	-0.270581000
6	4.523616000	-0.021955000	-1.934400000
6	5.447702000	-0.886871000	-2.705903000
1	5.950808000	-0.308185000	-3.486272000
1	6.219118000	-1.328385000	-2.061832000
1	4.922238000	-1.720385000	-3.190170000
6	4.213630000	1.293328000	-2.055975000
6	4.669159000	2.330040000	-3.012385000
1	5.376714000	1.906944000	-3.731570000
1	3.828586000	2.756176000	-3.574652000
1	5.164014000	3.164991000	-2.499868000
6	2.750491000	2.871368000	-0.799596000
6	2.935080000	5.024746000	0.228593000
6	1.087831000	4.534936000	-1.218197000
1	3.466876000	5.717203000	0.882866000
1	0.161904000	4.842169000	-1.706787000
6	3.907923000	-1.836759000	-0.357206000
6	4.996783000	-3.399333000	1.092252000
6	3.449496000	-4.171553000	-0.567328000
1	5.687604000	-3.605641000	1.910615000
1	2.903647000	-4.988144000	-1.042567000
6	1.561860000	3.241211000	-1.433000000
6	0.804949000	2.264039000	-2.275265000
1	-0.021218000	2.755792000	-2.798841000
1	1.446130000	1.779148000	-3.022266000
1	0.394471000	1.456970000	-1.651074000
6	3.444184000	3.741622000	0.047076000
6	4.666279000	3.276304000	0.774605000
1	4.386639000	2.502538000	1.503365000
1	5.404743000	2.818870000	0.103605000
1	5.147597000	4.101110000	1.309304000
6	1.760212000	5.438692000	-0.398151000
6	1.206456000	6.811060000	-0.155418000
1	0.574453000	6.830827000	0.743052000
1	2.002910000	7.547601000	-0.002652000
1	0.586587000	7.148807000	-0.992771000
6	3.196684000	-2.866488000	-0.982399000
6	2.159824000	-2.569069000	-2.019849000
1	1.419036000	-1.856023000	-1.632626000
1	2.590825000	-2.124169000	-2.926984000
1	1.628553000	-3.483085000	-2.307216000
6	4.800715000	-2.078538000	0.691166000

6	5.498213000	-0.942979000	1.373099000
1	4.765918000	-0.308051000	1.891292000
1	6.227203000	-1.308326000	2.103019000
1	6.019977000	-0.292802000	0.657616000
6	4.342160000	-4.456950000	0.464522000
6	4.537611000	-5.870793000	0.923349000
1	5.432755000	-5.975104000	1.545100000
1	3.681464000	-6.211142000	1.522435000
1	4.627900000	-6.560667000	0.076608000
7	3.296702000	1.571364000	-1.038427000
7	3.780769000	-0.499840000	-0.847615000
1	-3.813138000	-2.953570000	0.376081000
1	-3.163784000	1.787278000	1.571348000

Method: M06-2X/6-31G(d,p) Key word: opt freq pop=full
 imaginary frequencies: 0 Energy: -2438.359604 Hartree

Int I (1c).



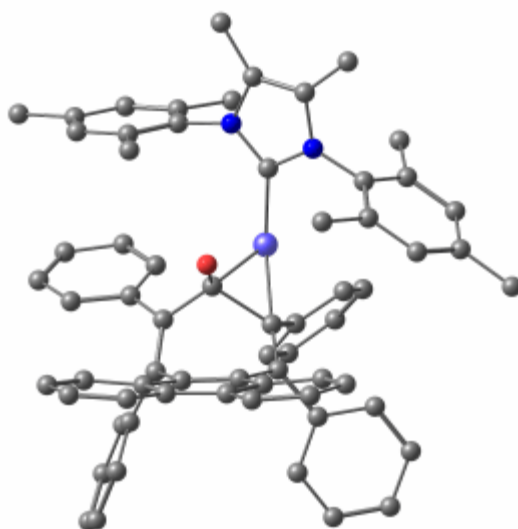
6	-5.841946000	2.705175000	-0.408761000
6	-6.123631000	3.988909000	0.008768000
6	-5.257664000	4.622132000	0.905286000
6	-4.139691000	3.955106000	1.358991000
6	-3.815270000	2.650677000	0.932622000
6	-4.693072000	2.008061000	0.018237000
6	-2.654891000	2.051612000	1.532341000
6	-1.963850000	0.915085000	1.245412000
28	0.544367000	0.207136000	0.641140000
6	-2.194816000	0.025053000	0.101155000
6	-3.514453000	-0.219437000	-0.490568000
6	-4.541240000	0.673015000	-0.498925000
8	-1.207119000	-0.573411000	-0.362010000
6	-3.673931000	-1.499736000	-1.226158000

6	-0.742394000	0.565675000	2.016169000
6	-0.672510000	-0.683804000	2.719634000
6	0.269083000	-0.903189000	3.696915000
6	1.211590000	0.098229000	4.034017000
6	1.249601000	1.264735000	3.309375000
6	0.339835000	1.490312000	2.238623000
6	-4.341322000	-1.542026000	-2.454832000
6	-4.547093000	-2.745105000	-3.120041000
6	-4.090210000	-3.934622000	-2.566612000
6	-3.411245000	-3.905843000	-1.351561000
6	-3.192253000	-2.703498000	-0.694548000
1	-1.414248000	-1.452574000	2.497593000
1	0.282890000	-1.857360000	4.221394000
1	1.915688000	-0.071786000	4.845850000
1	1.981778000	2.036366000	3.546145000
1	0.282870000	2.490147000	1.802516000
1	-4.681126000	-0.612744000	-2.908535000
1	-5.060741000	-2.749102000	-4.078635000
1	-4.253693000	-4.878605000	-3.080914000
1	-3.050775000	-4.832407000	-0.907047000
1	-2.632915000	-2.702430000	0.239461000
6	2.121337000	-0.218677000	-0.288121000
6	3.744905000	-1.554012000	-1.217657000
6	4.406640000	-2.837095000	-1.552834000
1	5.323124000	-2.660445000	-2.123825000
1	4.674858000	-3.402549000	-0.651027000
1	3.754368000	-3.485041000	-2.152661000
6	4.068212000	-0.267446000	-1.507310000
6	5.193580000	0.316449000	-2.275264000
1	5.834471000	-0.474325000	-2.676639000
1	4.834988000	0.921419000	-3.118243000
1	5.818735000	0.973313000	-1.656532000
6	2.992999000	1.947266000	-1.002310000
6	3.509629000	4.098851000	-0.099110000
6	2.192237000	3.916878000	-2.095457000
1	3.988144000	4.714378000	0.664133000
1	1.633170000	4.387357000	-2.905135000
6	1.825446000	-2.609721000	0.039780000
6	1.291181000	-4.047673000	1.875104000
6	0.035249000	-4.176945000	-0.162359000
1	1.473099000	-4.381526000	2.897647000
1	-0.771683000	-4.614717000	-0.751998000
6	2.264884000	2.525717000	-2.043372000
6	1.551230000	1.662292000	-3.037714000
1	1.100065000	2.264133000	-3.832531000
1	2.222463000	0.926544000	-3.499105000
1	0.756858000	1.086683000	-2.541731000
6	3.610280000	2.713473000	-0.009040000
6	4.313185000	2.048741000	1.133670000
1	3.601825000	1.452945000	1.723151000
1	5.092951000	1.354686000	0.794957000
1	4.777973000	2.787923000	1.793786000
6	2.808380000	4.716760000	-1.135746000
6	2.705021000	6.211595000	-1.194919000
1	2.012357000	6.593038000	-0.434190000
1	3.674859000	6.688329000	-1.011173000
1	2.340544000	6.551378000	-2.169801000
6	0.800923000	-3.164779000	-0.733844000
6	0.483016000	-2.639111000	-2.099265000
1	-0.076068000	-1.697411000	-2.007712000

1	1.386144000	-2.433217000	-2.686932000
1	-0.143775000	-3.346681000	-2.652447000
6	2.085752000	-3.032331000	1.345605000
6	3.140524000	-2.359111000	2.167700000
1	2.864727000	-1.310990000	2.350523000
1	3.256081000	-2.852998000	3.138263000
1	4.116501000	-2.351562000	1.665598000
6	0.258093000	-4.624163000	1.139590000
6	-0.603645000	-5.704563000	1.721814000
1	-0.427067000	-5.827760000	2.795242000
1	-1.669070000	-5.481411000	1.580650000
1	-0.415076000	-6.672969000	1.241271000
7	3.069111000	0.525150000	-0.927264000
7	2.559738000	-1.499511000	-0.479002000
1	-3.472932000	4.439119000	2.070405000
1	-5.466935000	5.631319000	1.251076000
1	-7.014452000	4.497461000	-0.350410000
1	-6.519290000	2.202777000	-1.097512000
1	-2.239928000	2.631074000	2.359728000
1	-5.425139000	0.334775000	-1.043532000

Method: M06-2X/6-31G(d,p) Key word: opt freq pop=full
 imaginary frequencies: 0 Energy: -2131.396949 Hartree

TS I (1e).



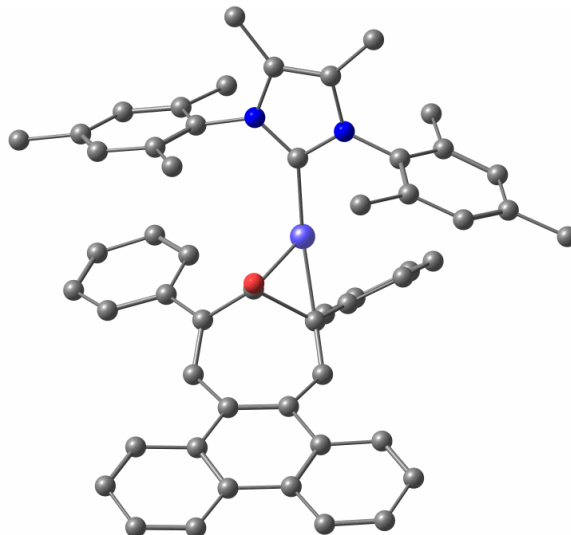
6	3.165364000	-1.670624000	2.060092000
6	3.865169000	-0.856356000	2.988003000
6	3.952551000	0.571145000	2.757552000
6	3.314216000	1.123467000	1.620291000
6	2.668820000	0.262635000	0.659341000
6	2.617544000	-1.097288000	0.849462000
6	4.598928000	1.444438000	3.655632000
6	4.586239000	2.808557000	3.469840000
6	3.906646000	3.357847000	2.374381000
6	3.284939000	2.527399000	1.470221000
6	2.993277000	-3.040401000	2.360936000

6	3.520659000	-3.602051000	3.500269000
6	4.246539000	-2.805464000	4.395021000
6	4.405059000	-1.462175000	4.140883000
6	2.012296000	0.860546000	-0.525002000
6	0.705035000	0.631476000	-0.801023000
28	-1.284017000	0.533150000	-0.639722000
6	0.052099000	-0.492169000	0.323986000
6	0.526334000	-1.847097000	-0.190501000
6	1.880090000	-2.008469000	-0.092596000
8	0.037813000	-0.262659000	1.534428000
6	-0.441227000	-2.810374000	-0.737617000
6	2.702505000	-2.902999000	-0.949584000
6	0.138810000	0.810868000	-2.168736000
6	0.410742000	-0.144902000	-3.172961000
6	-0.154302000	-0.031142000	-4.429658000
6	-1.009898000	1.033466000	-4.732591000
6	-1.269013000	1.997279000	-3.771733000
6	-0.696388000	1.900953000	-2.499401000
6	-0.326772000	-4.167741000	-0.398185000
6	-1.203864000	-5.110590000	-0.912675000
6	-2.232849000	-4.718598000	-1.765566000
6	-2.394112000	-3.371126000	-2.067077000
6	-1.514168000	-2.426098000	-1.554065000
6	2.211395000	-3.415899000	-2.164864000
6	3.013052000	-4.163818000	-3.013366000
6	4.342079000	-4.419349000	-2.690700000
6	4.859101000	-3.894928000	-1.513227000
6	4.057109000	-3.142921000	-0.663519000
6	2.892202000	1.538639000	-1.508640000
6	2.556133000	2.776933000	-2.068839000
6	3.386463000	3.376504000	-3.006719000
6	4.564237000	2.748568000	-3.401577000
6	4.911040000	1.521311000	-2.845994000
6	4.085949000	0.924419000	-1.900356000
1	5.112129000	1.042573000	4.524907000
1	5.091044000	3.457087000	4.181990000
1	3.871220000	4.436388000	2.235548000
1	2.754357000	2.957187000	0.623534000
1	2.428133000	-3.660527000	1.670384000
1	3.369232000	-4.659160000	3.705040000
1	4.671490000	-3.240865000	5.296350000
1	4.950812000	-0.857928000	4.860036000
1	1.091956000	-0.964196000	-2.944780000
1	0.076386000	-0.773913000	-5.190141000
1	-1.449450000	1.114725000	-5.723879000
1	-1.899877000	2.853958000	-4.004665000
1	-0.821758000	2.716092000	-1.788917000
1	0.479468000	-4.476882000	0.263708000
1	-1.083774000	-6.159057000	-0.647525000
1	-2.917100000	-5.458187000	-2.176957000
1	-3.214550000	-3.045971000	-2.704005000
1	-1.649452000	-1.372901000	-1.809979000
1	1.184886000	-3.217795000	-2.460634000
1	2.594858000	-4.540766000	-3.944125000
1	4.969256000	-5.006818000	-3.356902000
1	5.900754000	-4.064029000	-1.249639000
1	4.497146000	-2.732379000	0.240450000
1	1.640760000	3.272249000	-1.743008000
1	3.114653000	4.341805000	-3.429001000
1	5.213062000	3.217846000	-4.137521000

1	5.829617000	1.024699000	-3.150295000
1	4.350862000	-0.038976000	-1.464863000
6	-2.708316000	0.945025000	0.530424000
6	-4.400550000	1.032057000	2.067005000
6	-5.521520000	0.490293000	2.871069000
1	-5.960892000	1.275740000	3.492887000
1	-6.315047000	0.078913000	2.234334000
1	-5.193129000	-0.320298000	3.534399000
6	-3.864760000	2.276701000	1.993950000
6	-4.201293000	3.536858000	2.698259000
1	-5.064916000	3.390390000	3.353299000
1	-3.368501000	3.894072000	3.317341000
1	-4.444068000	4.341714000	1.993084000
6	-2.046064000	3.307049000	0.594932000
6	-1.720203000	5.070849000	-0.997171000
6	-0.041879000	4.608140000	0.650443000
1	-2.072001000	5.643190000	-1.856528000
1	0.932226000	4.822146000	1.095487000
6	-3.969499000	-1.141583000	0.920945000
6	-5.142102000	-2.801920000	-0.339751000
6	-3.792323000	-3.443867000	1.532619000
1	-5.794176000	-3.071044000	-1.172167000
1	-3.379554000	-4.221548000	2.176707000
6	-0.813580000	3.586406000	1.202280000
6	-0.319543000	2.799966000	2.373189000
1	0.594729000	3.243364000	2.781983000
1	-1.068555000	2.753052000	3.173763000
1	-0.097492000	1.760382000	2.089728000
6	-2.518571000	4.041736000	-0.497461000
6	-3.797260000	3.664898000	-1.180585000
1	-3.657544000	2.729727000	-1.742032000
1	-4.616533000	3.485576000	-0.473906000
1	-4.110657000	4.441531000	-1.885258000
6	-0.473374000	5.357922000	-0.444606000
6	0.389287000	6.451863000	-0.998115000
1	0.034849000	6.789494000	-1.977357000
1	0.402582000	7.324230000	-0.332781000
1	1.428535000	6.118854000	-1.108133000
6	-3.444431000	-2.117957000	1.775990000
6	-2.521693000	-1.754918000	2.895487000
1	-1.584696000	-1.328380000	2.511732000
1	-2.959962000	-1.000208000	3.561427000
1	-2.277407000	-2.635762000	3.496943000
6	-4.811099000	-1.462074000	-0.147351000
6	-5.301933000	-0.404161000	-1.087426000
1	-4.479492000	-0.035582000	-1.717491000
1	-6.084777000	-0.795379000	-1.744740000
1	-5.701685000	0.469555000	-0.556399000
6	-4.643162000	-3.803404000	0.488784000
6	-5.001058000	-5.241689000	0.268464000
1	-5.504243000	-5.387784000	-0.693685000
1	-4.103656000	-5.872969000	0.278639000
1	-5.669590000	-5.615069000	1.054266000
7	-2.832047000	2.200313000	1.054440000
7	-3.673827000	0.236624000	1.170282000

Method: M06-2X/6-31G(d,p) Key word: opt freq pop=full
imaginary frequencies: -186.2651 cm⁻¹ Energy: -2899.924784 Hartree

TS I (phenyl analogue of 1h).



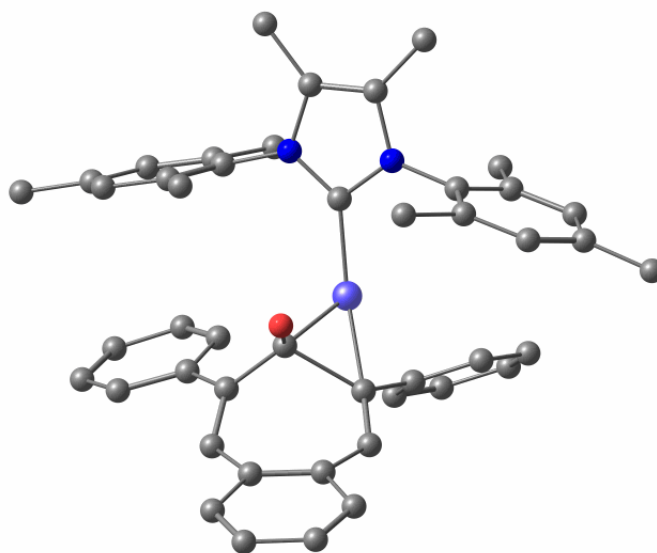
6	-4.633102000	-1.716126000	-0.456094000
6	-5.780128000	-0.928086000	-0.721435000
6	-5.729139000	0.500621000	-0.475676000
6	-4.537092000	1.070601000	0.034557000
6	-3.405072000	0.236632000	0.388404000
6	-3.448481000	-1.128246000	0.141910000
6	-6.814848000	1.351110000	-0.759179000
6	-6.734732000	2.713768000	-0.572514000
6	-5.543483000	3.282610000	-0.108087000
6	-4.468791000	2.472586000	0.183522000
6	-4.664267000	-3.085932000	-0.794940000
6	-5.792133000	-3.676096000	-1.319567000
6	-6.939578000	-2.905588000	-1.537033000
6	-6.922542000	-1.558168000	-1.251080000
6	-2.349034000	0.865102000	1.174905000
6	-1.014939000	0.670483000	1.186494000
28	0.847494000	0.464123000	0.569263000
6	-0.629747000	-0.539944000	-0.042116000
6	-1.071076000	-1.843615000	0.582795000
6	-2.408913000	-2.043328000	0.589953000
8	-0.954684000	-0.302537000	-1.206646000
6	-0.152021000	-2.826400000	1.181525000
6	-0.185928000	1.206367000	2.297580000
6	0.054032000	0.437392000	3.455464000
6	0.823790000	0.943011000	4.491304000
6	1.371647000	2.223438000	4.405396000
6	1.137172000	2.996729000	3.275467000
6	0.366298000	2.501144000	2.226398000
6	-0.471094000	-4.193377000	1.167741000
6	0.330994000	-5.124934000	1.810266000
6	1.486633000	-4.718878000	2.472731000
6	1.841912000	-3.375208000	2.455026000
6	1.039739000	-2.441837000	1.810012000
1	-7.741707000	0.933800000	-1.142761000
1	-7.590547000	3.343622000	-0.803409000
1	-5.461484000	4.360035000	0.014190000
1	-3.535493000	2.922288000	0.513109000
1	-3.766047000	-3.683894000	-0.662935000

1	-5.785271000	-4.733561000	-1.572701000
1	-7.837568000	-3.361586000	-1.947116000
1	-7.817148000	-0.975383000	-1.450704000
1	-0.383035000	-0.557576000	3.523036000
1	0.993453000	0.337641000	5.379035000
1	1.972776000	2.615319000	5.222386000
1	1.554109000	3.999818000	3.199092000
1	0.164427000	3.116875000	1.350455000
1	-1.357958000	-4.527330000	0.632179000
1	0.055403000	-6.177529000	1.788707000
1	2.114408000	-5.448087000	2.981155000
1	2.756315000	-3.045363000	2.945941000
1	1.339508000	-1.391107000	1.795969000
6	2.316169000	0.558169000	-0.620211000
6	3.977653000	0.272629000	-2.171037000
6	4.949473000	-0.500320000	-2.980551000
1	5.536247000	0.170266000	-3.614976000
1	5.646683000	-1.063290000	-2.347450000
1	4.449572000	-1.230160000	-3.629527000
6	3.689038000	1.597479000	-2.136835000
6	4.211137000	2.742285000	-2.919943000
1	4.959427000	2.402986000	-3.642034000
1	3.406471000	3.241337000	-3.474869000
1	4.677453000	3.503230000	-2.281854000
6	2.055625000	2.996788000	-0.875339000
6	2.016567000	5.044320000	0.359023000
6	0.307690000	4.578361000	-1.259105000
1	2.451084000	5.703648000	1.112044000
1	-0.603042000	4.870364000	-1.783098000
6	3.106993000	-1.753502000	-1.033408000
6	3.979736000	-3.687258000	0.064869000
6	2.339504000	-3.922172000	-1.667535000
1	4.630757000	-4.136693000	0.816888000
1	1.704908000	-4.556535000	-2.287202000
6	0.892459000	3.350651000	-1.568037000
6	0.285112000	2.429364000	-2.578530000
1	-0.473973000	2.949065000	-3.171190000
1	1.041226000	2.025553000	-3.264772000
1	-0.192161000	1.563795000	-2.092751000
6	2.629407000	3.820207000	0.097722000
6	3.828892000	3.371113000	0.874870000
1	3.591738000	2.472699000	1.461509000
1	4.676381000	3.109676000	0.229442000
1	4.159411000	4.151110000	1.568133000
6	0.858582000	5.439838000	-0.310343000
6	0.232382000	6.774468000	-0.037796000
1	0.448470000	7.121466000	0.978141000
1	0.612242000	7.537310000	-0.729423000
1	-0.855072000	6.739725000	-0.161991000
6	2.289430000	-2.539910000	-1.849564000
6	1.378244000	-1.930951000	-2.869368000
1	0.477741000	-1.512090000	-2.397976000
1	1.854956000	-1.105068000	-3.412414000
1	1.058417000	-2.681808000	-3.598701000
6	3.958204000	-2.303581000	-0.070038000
6	4.784197000	-1.419247000	0.813570000
1	4.142791000	-0.769487000	1.425452000
1	5.410606000	-2.013583000	1.486493000
1	5.439790000	-0.751522000	0.239288000
6	3.174012000	-4.510804000	-0.722213000

6	3.188242000	-5.995019000	-0.525365000
1	4.204489000	-6.372818000	-0.365270000
1	2.596581000	-6.268067000	0.358838000
1	2.758678000	-6.520688000	-1.384338000
7	2.682995000	1.748428000	-1.178805000
7	3.129763000	-0.338558000	-1.239176000
1	-2.772098000	-2.969039000	1.038376000
1	-2.724527000	1.543967000	1.947892000

Method: M06-2X/6-31G(d,p) Key word: opt freq pop=full
 imaginary frequencies: $-162.8271 \text{ cm}^{-1}$ Energy: $-2438.325062 \text{ Hartree}$

TS I (1c).



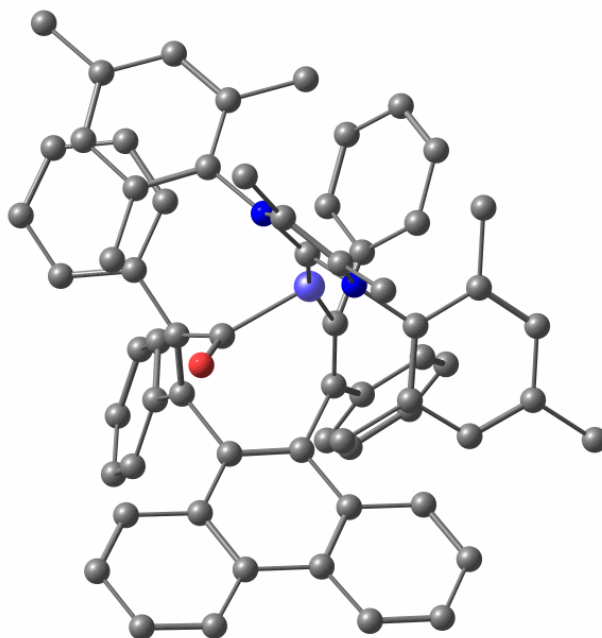
6	-0.774556000	5.515116000	-1.615087000
6	0.183597000	6.356544000	-2.150265000
6	1.529520000	6.127861000	-1.867379000
6	1.881758000	5.068752000	-1.050513000
6	0.932720000	4.172869000	-0.534726000
6	-0.436609000	4.400484000	-0.831868000
6	1.418409000	3.177456000	0.418774000
6	0.990013000	1.934368000	0.711498000
28	0.418907000	0.075369000	0.424746000
6	-0.335283000	1.537112000	-0.468892000
6	-1.550501000	2.300856000	0.002869000
6	-1.532499000	3.624079000	-0.268199000
8	-0.037185000	1.606566000	-1.660824000
6	-2.683475000	1.682555000	0.711671000
6	1.522986000	1.219841000	1.898139000
6	0.746063000	1.050215000	3.063877000
6	1.265636000	0.391987000	4.170264000
6	2.568840000	-0.102031000	4.151084000
6	3.348836000	0.064844000	3.011427000
6	2.835697000	0.709920000	1.892275000
6	-3.979041000	2.203927000	0.575253000
6	-5.036779000	1.703814000	1.320778000
6	-4.831862000	0.660560000	2.219812000

6	-3.563839000	0.103448000	2.333543000
6	-2.505547000	0.597552000	1.580370000
1	-0.259347000	1.467172000	3.092512000
1	0.652859000	0.277754000	5.061797000
1	2.973800000	-0.609655000	5.023344000
1	4.368588000	-0.316680000	2.982851000
1	3.442246000	0.832305000	0.995291000
1	-4.155661000	3.006752000	-0.137435000
1	-6.030157000	2.131382000	1.197713000
1	-5.660042000	0.269657000	2.807595000
1	-3.393007000	-0.730426000	3.012872000
1	-1.519170000	0.134759000	1.664495000
6	0.224054000	-1.609733000	-0.420000000
6	-0.348601000	-3.504044000	-1.575521000
6	-1.276969000	-4.499201000	-2.162921000
1	-0.715278000	-5.285570000	-2.675563000
1	-1.902209000	-4.975357000	-1.397085000
1	-1.958972000	-4.041098000	-2.889922000
6	1.005170000	-3.428558000	-1.580695000
6	2.043579000	-4.295013000	-2.185914000
1	1.583640000	-5.135151000	-2.714180000
1	2.658275000	-3.736859000	-2.903518000
1	2.726795000	-4.701254000	-1.429480000
6	2.671811000	-1.832396000	-0.650866000
6	4.685578000	-1.925736000	0.631130000
6	4.566371000	-0.546258000	-1.328013000
1	5.244544000	-2.303466000	1.489105000
1	5.033043000	0.156181000	-2.019096000
6	-2.193441000	-2.127866000	-0.662593000
6	-4.194816000	-2.509468000	0.583372000
6	-4.260229000	-1.222544000	-1.438695000
1	-4.702976000	-2.930518000	1.452336000
1	-4.823274000	-0.636857000	-2.166670000
6	3.246832000	-0.937919000	-1.558337000
6	2.459564000	-0.395034000	-2.710010000
1	3.110659000	0.139832000	-3.408146000
1	1.945592000	-1.192729000	-3.262468000
1	1.681091000	0.302871000	-2.363318000
6	3.364582000	-2.327566000	0.458013000
6	2.678161000	-3.187613000	1.473962000
1	1.958679000	-2.584740000	2.048725000
1	2.112661000	-4.011444000	1.020895000
1	3.398781000	-3.610035000	2.181498000
6	5.297493000	-1.027950000	-0.243781000
6	6.697227000	-0.559081000	0.016710000
1	6.717504000	0.167787000	0.839966000
1	7.352804000	-1.388223000	0.306103000
1	7.131421000	-0.071149000	-0.861640000
6	-2.889416000	-1.383857000	-1.622106000
6	-2.178065000	-0.768137000	-2.786340000
1	-1.481458000	0.017029000	-2.459593000
1	-1.580576000	-1.504921000	-3.338888000
1	-2.891356000	-0.318850000	-3.483816000
6	-2.820152000	-2.690630000	0.450208000
6	-2.022347000	-3.416973000	1.490061000
1	-1.289880000	-2.743769000	1.958402000
1	-2.671965000	-3.816580000	2.275277000
1	-1.446182000	-4.250041000	1.066661000
6	-4.928405000	-1.780767000	-0.349176000
6	-6.400656000	-1.564459000	-0.177485000

1	-6.787728000	-2.097583000	0.697239000
1	-6.620820000	-0.497783000	-0.042620000
1	-6.963476000	-1.900943000	-1.056485000
7	1.329495000	-2.271674000	-0.869012000
7	-0.801586000	-2.385638000	-0.863810000
1	2.928479000	4.908155000	-0.794424000
1	2.296331000	6.787219000	-2.267103000
1	-0.114023000	7.196908000	-2.772884000
1	-1.829733000	5.701780000	-1.811562000
1	2.235405000	3.551398000	1.047639000
1	-2.411627000	4.213093000	0.002779000

Method: M06-2X/6-31G(d,p) Key word: opt freq pop=full
 imaginary frequencies: $-173.6447 \text{ cm}^{-1}$ Energy: $-2131.351951 \text{ Hartree}$

Int II (1e).



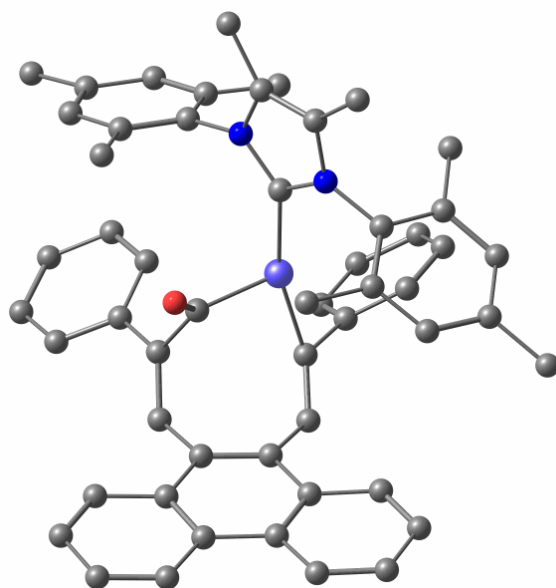
6	-2.512865000	-0.618771000	-2.707516000
6	-3.321807000	0.499746000	-3.032049000
6	-3.793326000	1.362531000	-1.966117000
6	-3.422858000	1.078369000	-0.625216000
6	-2.584179000	-0.061130000	-0.325358000
6	-2.166734000	-0.888363000	-1.334371000
6	-4.607083000	2.487469000	-2.213746000
6	-5.055618000	3.294265000	-1.190568000
6	-4.690518000	3.011330000	0.132196000
6	-3.877971000	1.933464000	0.402281000
6	-2.034833000	-1.445455000	-3.746245000
6	-2.351486000	-1.196001000	-5.061715000
6	-3.157250000	-0.096097000	-5.384631000
6	-3.625252000	0.732088000	-4.388318000
6	-2.125819000	-0.257533000	1.082655000
6	-0.832744000	-0.029830000	1.362725000
28	0.751017000	0.544920000	0.501272000

6	0.481741000	-0.412670000	-1.080992000
6	0.027948000	-1.838689000	-0.884083000
6	-1.299253000	-2.057761000	-0.987641000
8	0.683739000	0.036334000	-2.188853000
6	1.055954000	-2.836987000	-0.540439000
6	-2.012053000	-3.287838000	-0.574631000
6	-0.065947000	-0.110132000	2.590190000
6	0.288280000	-1.337430000	3.197350000
6	1.223495000	-1.377212000	4.213568000
6	1.843979000	-0.204535000	4.662871000
6	1.500930000	1.011759000	4.092192000
6	0.558358000	1.067756000	3.061924000
6	1.130481000	-4.039975000	-1.253831000
6	2.039688000	-5.023732000	-0.888978000
6	2.887143000	-4.824976000	0.197750000
6	2.849704000	-3.616950000	0.887354000
6	1.957936000	-2.620763000	0.508895000
6	-1.625684000	-4.006610000	0.564788000
6	-2.381719000	-5.076497000	1.022696000
6	-3.537644000	-5.460783000	0.349428000
6	-3.929648000	-4.763454000	-0.788194000
6	-3.179562000	-3.684870000	-1.240686000
6	-3.127328000	-0.696038000	2.085034000
6	-3.086722000	-0.265967000	3.417700000
6	-4.008437000	-0.733274000	4.345515000
6	-4.991703000	-1.641740000	3.964318000
6	-5.050280000	-2.068538000	2.641594000
6	-4.137852000	-1.590802000	1.710346000
1	-4.902472000	2.726727000	-3.231661000
1	-5.693048000	4.146955000	-1.413515000
1	-5.039539000	3.645799000	0.944487000
1	-3.579528000	1.728716000	1.427331000
1	-1.389346000	-2.282040000	-3.484941000
1	-1.970627000	-1.844909000	-5.846700000
1	-3.409385000	0.110330000	-6.422208000
1	-4.240942000	1.583035000	-4.666986000
1	-0.198578000	-2.247067000	2.846822000
1	1.476244000	-2.331102000	4.672668000
1	2.578664000	-0.248649000	5.463135000
1	1.960516000	1.933149000	4.447105000
1	0.244525000	2.028880000	2.648102000
1	0.447172000	-4.202393000	-2.085668000
1	2.075637000	-5.957245000	-1.446137000
1	3.577611000	-5.608775000	0.503873000
1	3.523291000	-3.441819000	1.724675000
1	1.936548000	-1.672964000	1.049440000
1	-0.731458000	-3.704143000	1.106721000
1	-2.072648000	-5.606257000	1.920865000
1	-4.131506000	-6.296259000	0.712679000
1	-4.830687000	-5.053602000	-1.324161000
1	-3.508732000	-3.130392000	-2.117626000
1	-2.327534000	0.453778000	3.719638000
1	-3.961737000	-0.380668000	5.373808000
1	-5.709841000	-2.010678000	4.693180000
1	-5.808622000	-2.782917000	2.327344000
1	-4.183828000	-1.939843000	0.679482000
6	2.222846000	1.553615000	-0.217359000
6	4.019891000	2.425843000	-1.315128000
6	5.376288000	2.409320000	-1.911573000
1	5.674411000	3.419740000	-2.206282000

1	6.118273000	2.031578000	-1.196611000
1	5.432034000	1.770022000	-2.801444000
6	3.111224000	3.425723000	-1.174511000
6	3.126683000	4.839978000	-1.617642000
1	4.090256000	5.088750000	-2.071673000
1	2.345663000	5.035637000	-2.363470000
1	2.953949000	5.533784000	-0.785732000
6	0.894819000	3.589720000	0.017134000
6	-0.093773000	4.789190000	1.839874000
6	-1.384306000	4.288752000	-0.117445000
1	-0.013733000	5.234270000	2.832506000
1	-2.328293000	4.329431000	-0.662489000
6	4.128349000	0.033288000	-0.599886000
6	5.469451000	-1.439531000	0.730329000
6	4.899706000	-2.037201000	-1.515065000
1	5.966680000	-1.671104000	1.673378000
1	4.933020000	-2.747802000	-2.342946000
6	-0.295376000	3.657362000	-0.716038000
6	-0.419666000	3.064804000	-2.083110000
1	-1.393484000	3.307894000	-2.520899000
1	0.366864000	3.425957000	-2.758436000
1	-0.319942000	1.973842000	-2.055535000
6	1.022138000	4.164779000	1.287752000
6	2.311544000	4.080071000	2.047737000
1	2.653986000	3.040162000	2.128536000
1	3.121404000	4.637890000	1.559347000
1	2.193761000	4.482631000	3.059174000
6	-1.309305000	4.842473000	1.158425000
6	-2.519865000	5.456001000	1.793155000
1	-2.250543000	6.246904000	2.501545000
1	-3.195316000	5.879876000	1.042002000
1	-3.090621000	4.699956000	2.348975000
6	4.188569000	-0.849675000	-1.683663000
6	3.515860000	-0.581540000	-2.995465000
1	2.693508000	-1.290527000	-3.151034000
1	3.073737000	0.415955000	-3.051407000
1	4.224277000	-0.709108000	-3.823013000
6	4.758570000	-0.248138000	0.619702000
6	4.648065000	0.682402000	1.787992000
1	3.660309000	0.591846000	2.265212000
1	5.404946000	0.449388000	2.543460000
1	4.766915000	1.733739000	1.494117000
6	5.547383000	-2.347605000	-0.323909000
6	6.289354000	-3.640801000	-0.179722000
1	6.676583000	-3.773046000	0.836223000
1	5.629208000	-4.488550000	-0.403689000
1	7.137528000	-3.699650000	-0.872491000
7	2.022280000	2.868025000	-0.501493000
7	3.447235000	1.287582000	-0.730170000

Method: M06-2X/6-31G(d,p) Key word: opt freq pop=full
imaginary frequencies: 0 Energy: -2899.956298 Hartree

Int II (phenyl analogue of 1h).



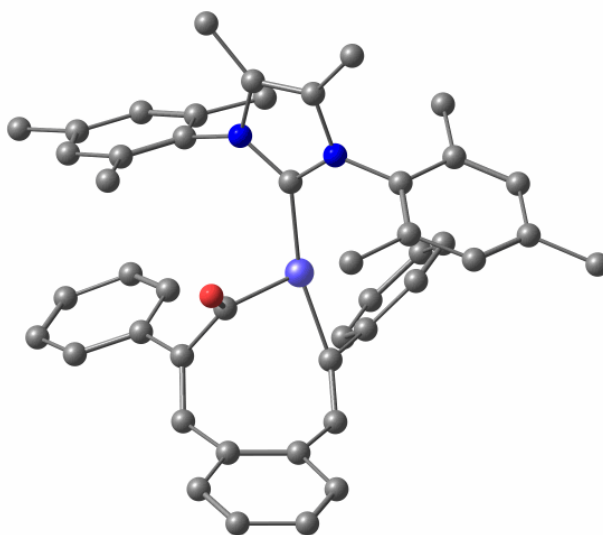
6	3.324026000	3.088180000	-0.443670000
6	4.625096000	2.600706000	-0.721931000
6	5.031989000	1.326316000	-0.163140000
6	4.129956000	0.615071000	0.669448000
6	2.828592000	1.165584000	0.994170000
6	2.436969000	2.359878000	0.432637000
6	6.290551000	0.754449000	-0.434578000
6	6.657197000	-0.468538000	0.082472000
6	5.758658000	-1.181571000	0.885739000
6	4.517830000	-0.650194000	1.162698000
6	2.907423000	4.299840000	-1.033328000
6	3.748397000	5.029723000	-1.842661000
6	5.043653000	4.561847000	-2.097806000
6	5.464712000	3.369233000	-1.551136000
6	2.023575000	0.444197000	1.994430000
6	0.770157000	0.000856000	1.856654000
28	-0.412194000	-0.402411000	0.473406000
6	-0.080642000	1.211653000	-0.358338000
6	-0.054613000	2.459112000	0.482510000
6	1.144896000	2.979424000	0.780119000
8	0.137467000	1.289471000	-1.550308000
6	-1.324248000	3.055276000	0.929108000
6	-0.013941000	-0.788133000	2.801200000
6	-0.955865000	-0.203445000	3.673426000
6	-1.789062000	-0.995320000	4.445820000
6	-1.727210000	-2.389161000	4.359466000
6	-0.815393000	-2.981699000	3.495852000
6	0.032970000	-2.192629000	2.720932000
6	-1.479862000	4.447480000	0.947833000
6	-2.645974000	5.027406000	1.426924000
6	-3.682524000	4.225892000	1.897060000
6	-3.548923000	2.841467000	1.861390000
6	-2.387762000	2.258064000	1.369734000
1	6.995940000	1.282161000	-1.070516000
1	7.638385000	-0.880519000	-0.141752000
1	6.038932000	-2.152221000	1.291365000
1	3.806814000	-1.221869000	1.756000000

1	1.892387000	4.646070000	-0.850512000
1	3.405311000	5.961302000	-2.286563000
1	5.715425000	5.132943000	-2.734391000
1	6.470569000	3.023277000	-1.773069000
1	-1.011675000	0.882873000	3.728807000
1	-2.497525000	-0.527103000	5.126113000
1	-2.385966000	-3.003568000	4.968668000
1	-0.749700000	-4.066872000	3.424836000
1	0.771718000	-2.648991000	2.061406000
1	-0.675280000	5.073494000	0.565568000
1	-2.747345000	6.110355000	1.431939000
1	-4.592395000	4.678200000	2.287125000
1	-4.357271000	2.204737000	2.216469000
1	-2.289247000	1.171178000	1.344570000
6	-1.362577000	-1.358138000	-0.914498000
6	-2.671915000	-2.125939000	-2.618620000
6	-3.880155000	-2.174276000	-3.475465000
1	-3.855904000	-3.055827000	-4.122604000
1	-4.792242000	-2.225881000	-2.867256000
1	-3.971884000	-1.289481000	-4.117462000
6	-1.571772000	-2.921485000	-2.567717000
6	-1.157997000	-4.077803000	-3.397719000
1	-1.902087000	-4.275049000	-4.174709000
1	-0.197061000	-3.893628000	-3.893851000
1	-1.039649000	-4.991675000	-2.802097000
6	0.398678000	-3.054292000	-1.007226000
6	1.396215000	-4.695859000	0.422479000
6	2.772411000	-3.129142000	-0.761511000
1	1.294109000	-5.526663000	1.122325000
1	3.758838000	-2.726251000	-0.994363000
6	-3.490774000	-0.184330000	-1.271538000
6	-5.312309000	0.512439000	0.111478000
6	-4.554432000	1.915340000	-1.676816000
1	-5.989736000	0.328332000	0.946770000
1	-4.625926000	2.843390000	-2.244980000
6	1.655127000	-2.543646000	-1.354329000
6	1.806964000	-1.420470000	-2.331290000
1	2.845949000	-1.077522000	-2.364120000
1	1.531010000	-1.740054000	-3.345826000
1	1.170784000	-0.562290000	-2.084880000
6	0.246258000	-4.128605000	-0.122941000
6	-1.114669000	-4.603561000	0.287271000
1	-1.633140000	-3.827192000	0.868868000
1	-1.755531000	-4.841394000	-0.570692000
1	-1.042533000	-5.498296000	0.913972000
6	2.665028000	-4.201174000	0.123152000
6	3.894375000	-4.816545000	0.719247000
1	3.679469000	-5.308092000	1.673881000
1	4.324044000	-5.573281000	0.050576000
1	4.669560000	-4.060241000	0.888373000
6	-3.578445000	0.986418000	-2.032614000
6	-2.671326000	1.236317000	-3.197763000
1	-1.656557000	0.873641000	-3.008934000
1	-3.039828000	0.738856000	-4.105747000
1	-2.612928000	2.306628000	-3.416995000
6	-4.343039000	-0.440597000	-0.192612000
6	-4.200325000	-1.686593000	0.628055000
1	-3.309604000	-1.634728000	1.272130000
1	-5.072617000	-1.831866000	1.272542000
1	-4.081257000	-2.580490000	0.001251000

6	-5.427975000	1.696908000	-0.613829000
6	-6.433807000	2.739032000	-0.232589000
1	-7.200678000	2.335521000	0.437123000
1	-5.938826000	3.569657000	0.289487000
1	-6.933750000	3.160877000	-1.111573000
7	-0.788994000	-2.433651000	-1.519041000
7	-2.512621000	-1.172991000	-1.606107000
1	1.180435000	3.903957000	1.363741000
1	2.556440000	0.222037000	2.928288000

Method: M06-2X/6-31G(d,p) Key word: opt freq pop=full
 imaginary frequencies: 0 Energy: -2438.342279 Hartree

Int II (1c).



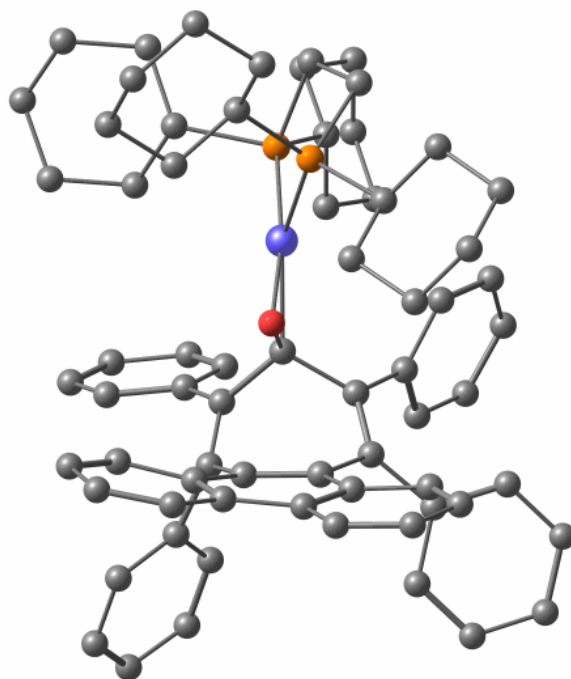
6	0.362666000	5.120572000	-1.794062000
6	1.558085000	5.716499000	-2.162321000
6	2.720146000	5.404451000	-1.460946000
6	2.661492000	4.507869000	-0.406978000
6	1.469341000	3.867460000	-0.035969000
6	0.294191000	4.184450000	-0.755356000
6	1.523659000	2.998660000	1.153888000
6	1.035970000	1.764925000	1.318210000
28	0.406602000	0.257157000	0.398945000
6	-0.412271000	1.350100000	-0.839534000
6	-1.388942000	2.370910000	-0.320882000
6	-1.027247000	3.662466000	-0.368811000
8	-0.168291000	1.297071000	-2.027452000
6	-2.688419000	1.960813000	0.243853000
6	1.063951000	0.906251000	2.491536000
6	0.092185000	1.015781000	3.514381000
6	0.004507000	0.063283000	4.512156000
6	0.868008000	-1.038730000	4.524733000
6	1.822428000	-1.170011000	3.528324000
6	1.919599000	-0.216340000	2.511793000
6	-3.852063000	2.657481000	-0.104517000
6	-5.065293000	2.371433000	0.508877000

6	-5.137701000	1.383519000	1.485867000
6	-3.995510000	0.658981000	1.812319000
6	-2.784319000	0.931230000	1.188265000
1	-0.587265000	1.866640000	3.491630000
1	-0.741329000	0.174087000	5.296773000
1	0.793646000	-1.780674000	5.316181000
1	2.516387000	-2.009451000	3.541163000
1	2.701134000	-0.297492000	1.757029000
1	-3.790994000	3.433549000	-0.865228000
1	-5.955584000	2.931096000	0.229654000
1	-6.081735000	1.171454000	1.984153000
1	-4.044468000	-0.126663000	2.564089000
1	-1.895189000	0.352853000	1.448195000
6	0.278307000	-1.388222000	-0.590597000
6	-0.296619000	-3.078647000	-2.017356000
6	-1.226472000	-3.980850000	-2.736316000
1	-0.667129000	-4.731522000	-3.302007000
1	-1.889360000	-4.507856000	-2.038267000
1	-1.868014000	-3.437694000	-3.440914000
6	1.058517000	-3.025780000	-1.985570000
6	2.089791000	-3.811546000	-2.704505000
1	1.618297000	-4.533781000	-3.377037000
1	2.737811000	-3.163963000	-3.308276000
1	2.742308000	-4.365923000	-2.017990000
6	2.721746000	-1.710410000	-0.665747000
6	4.552226000	-2.253468000	0.781312000
6	4.730561000	-0.423206000	-0.756081000
1	4.984254000	-2.873713000	1.567976000
1	5.306218000	0.396272000	-1.187218000
6	-2.130104000	-1.895983000	-0.826692000
6	-3.944612000	-2.435414000	0.638862000
6	-4.338451000	-1.139531000	-1.334873000
1	-4.316657000	-2.906071000	1.550062000
1	-5.018046000	-0.580868000	-1.980612000
6	3.439885000	-0.655524000	-1.235194000
6	2.851058000	0.221228000	-2.293197000
1	3.637116000	0.758109000	-2.832893000
1	2.250075000	-0.344184000	-3.014464000
1	2.166829000	0.960718000	-1.857177000
6	3.258234000	-2.520538000	0.344545000
6	2.438153000	-3.603768000	0.976312000
1	1.578454000	-3.171196000	1.508323000
1	2.032724000	-4.309553000	0.240194000
1	3.031949000	-4.171846000	1.699672000
6	5.300670000	-1.203761000	0.245722000
6	6.679528000	-0.912028000	0.756198000
1	7.219045000	-1.831866000	1.007306000
1	7.271228000	-0.359880000	0.018912000
1	6.641951000	-0.301426000	1.667020000
6	-2.989338000	-1.204156000	-1.684971000
6	-2.518496000	-0.532116000	-2.939153000
1	-2.659202000	0.553249000	-2.867954000
1	-1.454860000	-0.692106000	-3.132853000
1	-3.096754000	-0.879802000	-3.804165000
6	-2.587792000	-2.512667000	0.346329000
6	-1.637523000	-3.202312000	1.277805000
1	-1.020236000	-2.469245000	1.819269000
1	-2.179954000	-3.798205000	2.018224000
1	-0.943385000	-3.865109000	0.743485000
6	-4.834353000	-1.748683000	-0.187680000

6	-6.289415000	-1.652873000	0.156399000
1	-6.473989000	-1.939576000	1.197799000
1	-6.652942000	-0.627079000	0.020926000
1	-6.899958000	-2.304753000	-0.480931000
7	1.386457000	-1.991597000	-1.103398000
7	-0.748854000	-2.063659000	-1.164396000
1	3.562925000	4.278649000	0.160993000
1	3.666576000	5.868791000	-1.729327000
1	1.583604000	6.426217000	-2.985942000
1	-0.555520000	5.369752000	-2.324410000
1	2.100055000	3.434648000	1.980690000
1	-1.751531000	4.404445000	-0.020614000

Method: M06-2X/6-31G(d,p) Key word: opt freq pop=full
 imaginary frequencies: 0 Energy: -2131.365845 Hartree

Int I'.



6	3.274007000	0.692740000	2.265258000
6	4.241632000	1.673842000	1.945966000
6	4.704307000	1.776933000	0.577529000
6	4.106728000	0.961838000	-0.421532000
6	3.170136000	-0.086708000	-0.052047000
6	2.840465000	-0.260994000	1.273816000
6	5.672871000	2.726370000	0.195477000
6	6.017151000	2.920217000	-1.123201000
6	5.379380000	2.169835000	-2.117236000
6	4.447661000	1.218032000	-1.768641000
6	2.669257000	0.727048000	3.541081000
6	3.067796000	1.627837000	4.502834000
6	4.091057000	2.540226000	4.214190000
6	4.650411000	2.568159000	2.955806000

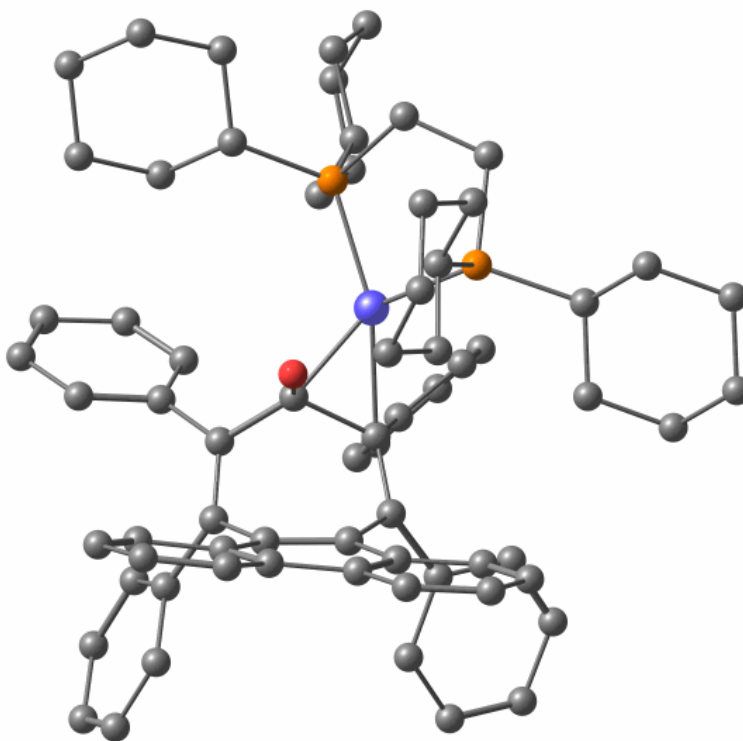
6	2.524507000	-0.906871000	-1.109996000
6	1.173794000	-1.078422000	-1.100459000
28	-1.250198000	0.529011000	-0.203794000
6	0.383571000	-0.538383000	0.086690000
6	0.700665000	-1.478168000	1.239254000
6	1.967429000	-1.380188000	1.715513000
8	0.462116000	0.755604000	0.316145000
15	-3.385546000	0.033004000	-0.530528000
15	-1.687838000	2.635069000	-0.777712000
6	-4.167060000	1.570982000	-1.285223000
6	-3.118388000	2.464772000	-1.943327000
6	-0.238678000	-2.508846000	1.719178000
6	2.641633000	-2.505739000	2.433654000
6	0.467277000	-1.867357000	-2.133948000
6	0.715435000	-3.228723000	-2.331927000
6	0.075105000	-3.928137000	-3.348924000
6	-0.810768000	-3.272056000	-4.197897000
6	-1.077937000	-1.919351000	-4.002331000
6	-0.459474000	-1.228625000	-2.966798000
6	-0.440780000	-2.682220000	3.094795000
6	-1.307070000	-3.657449000	3.573020000
6	-1.992024000	-4.482421000	2.685232000
6	-1.805204000	-4.315956000	1.316579000
6	-0.946690000	-3.333215000	0.838899000
6	2.619799000	-3.753325000	1.789642000
6	3.265371000	-4.857637000	2.327294000
6	3.963216000	-4.742144000	3.524535000
6	4.015001000	-3.509615000	4.164240000
6	3.369915000	-2.402131000	3.623900000
6	3.412697000	-1.600154000	-2.081046000
6	3.194524000	-1.615184000	-3.464347000
6	4.047553000	-2.311770000	-4.309813000
6	5.135531000	-3.009450000	-3.792798000
6	5.368102000	-2.996200000	-2.421963000
6	4.518511000	-2.293510000	-1.576103000
1	6.162260000	3.327940000	0.956362000
1	6.769291000	3.659931000	-1.387015000
1	5.616735000	2.333127000	-3.165928000
1	3.967386000	0.648635000	-2.556434000
1	1.848397000	0.041555000	3.741279000
1	2.580692000	1.639286000	5.475034000
1	4.421197000	3.249552000	4.969489000
1	5.401700000	3.321931000	2.737860000
1	-4.664119000	2.126968000	-0.478843000
1	-4.955362000	1.291026000	-1.996296000
1	-3.548335000	3.423725000	-2.264153000
1	-2.709098000	1.974323000	-2.841092000
1	1.438706000	-3.731856000	-1.690245000
1	0.281956000	-4.986639000	-3.489010000
1	-1.299641000	-3.814331000	-5.004461000
1	-1.777766000	-1.401931000	-4.656820000
1	-0.677204000	-0.173170000	-2.793300000
1	0.098452000	-2.041006000	3.790195000
1	-1.447480000	-3.773874000	4.645649000
1	-2.666967000	-5.249158000	3.058815000
1	-2.331437000	-4.955927000	0.609240000
1	-0.808043000	-3.212918000	-0.233197000
1	2.089694000	-3.840186000	0.841593000
1	3.227828000	-5.810349000	1.803740000
1	4.470360000	-5.604424000	3.951285000

1	4.564765000	-3.402823000	5.096910000
1	3.436465000	-1.450242000	4.142900000
1	2.348616000	-1.068680000	-3.878807000
1	3.862955000	-2.306164000	-5.381825000
1	5.801326000	-3.555871000	-4.456762000
1	6.216997000	-3.534412000	-2.006207000
1	4.699295000	-2.280776000	-0.501364000
6	-4.144826000	0.015459000	1.179950000
6	-5.635152000	0.307517000	1.373102000
6	-3.750182000	-1.241449000	1.955513000
1	-3.587436000	0.859649000	1.633573000
6	-5.945750000	0.483929000	2.858548000
1	-6.234884000	-0.528839000	0.986328000
1	-5.951766000	1.199289000	0.815637000
6	-4.076437000	-1.095990000	3.437310000
1	-4.296847000	-2.109746000	1.548392000
1	-2.682237000	-1.452260000	1.818163000
6	-5.544827000	-0.752221000	3.655779000
1	-7.012710000	0.703026000	2.996595000
1	-5.394723000	1.359116000	3.240419000
1	-3.806633000	-2.018312000	3.968481000
1	-3.445184000	-0.297525000	3.860754000
1	-5.754676000	-0.605668000	4.723144000
1	-6.165367000	-1.602904000	3.329627000
6	-4.149011000	-1.298002000	-1.601435000
6	-3.416219000	-2.631853000	-1.473419000
6	-5.658146000	-1.508009000	-1.472596000
1	-3.943894000	-0.905484000	-2.618303000
6	-3.931054000	-3.647933000	-2.485972000
1	-3.555654000	-3.026267000	-0.453783000
1	-2.338276000	-2.472250000	-1.602595000
6	-6.164820000	-2.507337000	-2.508888000
1	-5.870260000	-1.911592000	-0.470074000
1	-6.206968000	-0.558535000	-1.549434000
6	-5.438029000	-3.840532000	-2.376054000
1	-3.401305000	-4.602494000	-2.359631000
1	-3.684174000	-3.293229000	-3.500409000
1	-7.248915000	-2.643665000	-2.402382000
1	-5.998010000	-2.099037000	-3.518981000
1	-5.794774000	-4.551234000	-3.132598000
1	-5.677194000	-4.281978000	-1.394800000
6	-0.294449000	3.267463000	-1.829935000
6	-0.616269000	4.353626000	-2.858677000
6	0.939175000	3.635212000	-0.997411000
1	-0.030211000	2.345112000	-2.385563000
6	0.589657000	4.615209000	-3.757973000
1	-0.884462000	5.286713000	-2.340523000
1	-1.486877000	4.072585000	-3.467749000
6	2.131876000	3.902543000	-1.908072000
1	0.721093000	4.541482000	-0.406983000
1	1.173707000	2.825139000	-0.293701000
6	1.822144000	4.980529000	-2.938968000
1	0.354311000	5.406380000	-4.482040000
1	0.802870000	3.707238000	-4.345125000
1	3.015238000	4.168092000	-1.311953000
1	2.393445000	2.963858000	-2.424241000
1	2.684761000	5.144514000	-3.597685000
1	1.638359000	5.936944000	-2.421474000
6	-2.232955000	3.908068000	0.464434000
6	-1.425017000	3.757790000	1.759067000

6	-2.289445000	5.368777000	0.018181000
1	-3.268672000	3.585750000	0.693059000
6	-1.984037000	4.653127000	2.858574000
1	-0.373079000	4.023520000	1.567092000
1	-1.413247000	2.704508000	2.071378000
6	-2.851350000	6.255418000	1.126828000
1	-1.270497000	5.708402000	-0.228072000
1	-2.887306000	5.476379000	-0.897949000
6	-2.044615000	6.109184000	2.411861000
1	-1.381530000	4.553281000	3.770113000
1	-3.000872000	4.312543000	3.116828000
1	-2.871708000	7.302844000	0.799134000
1	-3.897762000	5.968859000	1.321465000
1	-2.468301000	6.739435000	3.204129000
1	-1.019718000	6.474426000	2.236376000

Method: M06-2X/6-31G(d,p) Key word: opt freq pop=full
 imaginary frequencies: 0 Energy: -3599.238937 Hartree

TS I'



6	-3.235723000	-1.525224000	-2.075811000
6	-4.027749000	-0.448339000	-2.550938000
6	-4.308480000	0.670900000	-1.675916000
6	-3.709863000	0.708691000	-0.392701000
6	-2.835727000	-0.362186000	0.029043000
6	-2.671050000	-1.484085000	-0.743319000
6	-5.128248000	1.749338000	-2.067572000
6	-5.337402000	2.833964000	-1.245429000
6	-4.737134000	2.875338000	0.019861000

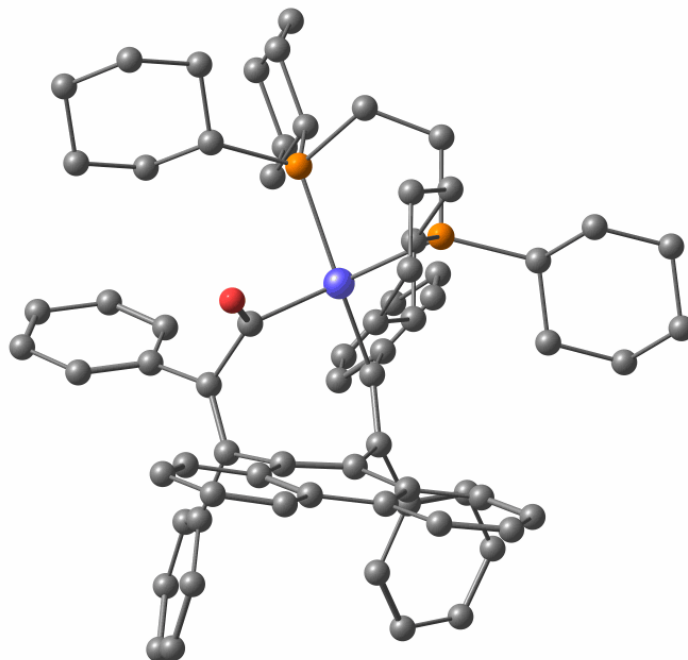
6	-3.943611000	1.829624000	0.433374000
6	-2.950339000	-2.592110000	-2.956602000
6	-3.426928000	-2.610652000	-4.246873000
6	-4.209330000	-1.547067000	-4.714244000
6	-4.495172000	-0.490562000	-3.879871000
6	-2.013781000	-0.186630000	1.254357000
6	-0.647198000	-0.183341000	1.139388000
28	1.070688000	0.645439000	0.166572000
6	-0.158756000	-0.792445000	-0.289484000
6	-0.408823000	-2.292130000	-0.292123000
6	-1.736951000	-2.594662000	-0.344069000
8	-0.326287000	-0.147039000	-1.349710000
15	3.193575000	0.630851000	-0.447362000
15	0.942949000	2.851461000	-0.081300000
6	3.539678000	2.411974000	-0.936685000
6	2.711637000	3.410663000	-0.134849000
6	0.706528000	-3.253933000	-0.307125000
6	-2.348486000	-3.892309000	0.038582000
6	0.177776000	-0.403544000	2.376844000
6	0.113526000	-1.649558000	3.015454000
6	0.843052000	-1.906925000	4.171297000
6	1.646060000	-0.917357000	4.727551000
6	1.698026000	0.336558000	4.125348000
6	0.969782000	0.592086000	2.968507000
6	0.777761000	-4.177737000	-1.360639000
6	1.815719000	-5.095613000	-1.434720000
6	2.808024000	-5.111896000	-0.457270000
6	2.759546000	-4.188725000	0.581279000
6	1.728877000	-3.257284000	0.648251000
6	-1.643840000	-4.867124000	0.767429000
6	-2.254944000	-6.040286000	1.183486000
6	-3.595528000	-6.281223000	0.899727000
6	-4.319811000	-5.318508000	0.208614000
6	-3.709114000	-4.142369000	-0.207647000
6	-2.737158000	-0.217691000	2.545612000
6	-2.378231000	0.567153000	3.651880000
6	-3.093515000	0.495158000	4.839326000
6	-4.181410000	-0.364876000	4.954506000
6	-4.552500000	-1.147255000	3.866173000
6	-3.845622000	-1.068037000	2.674004000
1	-5.612405000	1.734032000	-3.040115000
1	-5.971775000	3.652134000	-1.578027000
1	-4.898458000	3.727578000	0.677539000
1	-3.487822000	1.861751000	1.419001000
1	-2.336776000	-3.415370000	-2.601507000
1	-3.186292000	-3.444088000	-4.902328000
1	-4.581749000	-1.548117000	-5.735826000
1	-5.084585000	0.334751000	-4.269085000
1	3.279034000	2.490889000	-2.002696000
1	4.611920000	2.638600000	-0.859937000
1	2.836641000	4.430003000	-0.525891000
1	3.042650000	3.426984000	0.915580000
1	-0.537890000	-2.417249000	2.596786000
1	0.770172000	-2.883526000	4.644692000
1	2.216793000	-1.116104000	5.631836000
1	2.303196000	1.128187000	4.563360000
1	1.000586000	1.582878000	2.518061000
1	0.003326000	-4.162080000	-2.124785000
1	1.852170000	-5.801843000	-2.261229000
1	3.617682000	-5.835959000	-0.511493000

1	3.533524000	-4.183544000	1.347092000
1	1.702892000	-2.533601000	1.457360000
1	-0.601785000	-4.704245000	1.025680000
1	-1.676310000	-6.769952000	1.745486000
1	-4.071774000	-7.202471000	1.226593000
1	-5.373715000	-5.477135000	-0.008636000
1	-4.304170000	-3.401852000	-0.734494000
1	-1.534603000	1.249681000	3.576878000
1	-2.799717000	1.119240000	5.680323000
1	-4.739535000	-0.420760000	5.886185000
1	-5.400522000	-1.823840000	3.943502000
1	-4.139831000	-1.683271000	1.824647000
6	3.711259000	-0.234035000	-2.025530000
6	4.966160000	0.249087000	-2.758166000
6	3.737520000	-1.751709000	-1.859184000
1	2.838496000	0.003283000	-2.667209000
6	5.104427000	-0.449397000	-4.109311000
1	5.857497000	0.023076000	-2.154841000
1	4.952605000	1.337295000	-2.900241000
6	3.909110000	-2.458904000	-3.199097000
1	4.570808000	-2.032204000	-1.190985000
1	2.815816000	-2.091248000	-1.371477000
6	5.142597000	-1.963255000	-3.942682000
1	6.004840000	-0.092799000	-4.626752000
1	4.247887000	-0.175522000	-4.746407000
1	3.956795000	-3.544667000	-3.041886000
1	3.012225000	-2.272958000	-3.812202000
1	5.232195000	-2.457044000	-4.919027000
1	6.043815000	-2.237392000	-3.369644000
6	4.469498000	0.387506000	0.901353000
6	4.200063000	-0.873191000	1.724321000
6	5.951602000	0.466285000	0.534543000
1	4.238435000	1.250840000	1.559029000
6	5.072934000	-0.913889000	2.973078000
1	4.404078000	-1.761140000	1.101969000
1	3.137694000	-0.914642000	2.000353000
6	6.819809000	0.454199000	1.790170000
1	6.215696000	-0.408265000	-0.082186000
1	6.170011000	1.355885000	-0.072698000
6	6.552841000	-0.790508000	2.629349000
1	4.880913000	-1.837004000	3.537067000
1	4.778738000	-0.081340000	3.634202000
1	7.881727000	0.515231000	1.518174000
1	6.598172000	1.352478000	2.389112000
1	7.163466000	-0.778932000	3.541464000
1	6.864424000	-1.679525000	2.056878000
6	0.174886000	4.082431000	1.087947000
6	0.166280000	5.560374000	0.698643000
6	-1.225727000	3.641296000	1.514566000
1	0.832693000	3.979320000	1.975002000
6	-0.347981000	6.415004000	1.856698000
1	-0.496567000	5.698057000	-0.170970000
1	1.166145000	5.894520000	0.387908000
6	-1.732632000	4.478412000	2.680983000
1	-1.919222000	3.751996000	0.666052000
1	-1.227121000	2.570388000	1.757065000
6	-1.728495000	5.960205000	2.320574000
1	-0.370063000	7.473403000	1.566043000
1	0.359462000	6.338380000	2.698407000
1	-2.740652000	4.152442000	2.974767000

1	-1.083778000	4.309044000	3.557302000
1	-2.065358000	6.568756000	3.169579000
1	-2.454259000	6.127903000	1.507703000
6	0.309749000	3.105866000	-1.814652000
6	-1.205562000	2.893918000	-1.883691000
6	0.717621000	4.359918000	-2.585532000
1	0.758787000	2.232978000	-2.324769000
6	-1.664506000	2.781908000	-3.332166000
1	-1.722718000	3.745840000	-1.409471000
1	-1.481385000	1.987125000	-1.330381000
6	0.259793000	4.250826000	-4.039667000
1	0.256012000	5.247030000	-2.124710000
1	1.804744000	4.518973000	-2.547494000
6	-1.242489000	4.005736000	-4.137581000
1	-2.755286000	2.651036000	-3.367257000
1	-1.227298000	1.868343000	-3.767570000
1	0.540664000	5.155662000	-4.594964000
1	0.793755000	3.412557000	-4.516262000
1	-1.543265000	3.903442000	-5.188457000
1	-1.773273000	4.889991000	-3.746963000

Method: M06-2X/6-31G(d,p) Key word: opt freq pop=full
 imaginary frequencies: -94.807 cm^{-1} Energy: $-3599.215012 \text{ Hartree}$

Int II'



6	-2.534360000	1.350113000	2.500100000
6	-3.588241000	0.456597000	2.816983000
6	-4.176852000	-0.341627000	1.759907000
6	-3.651582000	-0.248235000	0.444088000
6	-2.540151000	0.634174000	0.158321000
6	-2.059579000	1.460569000	1.141465000
6	-5.231366000	-1.245627000	2.001079000

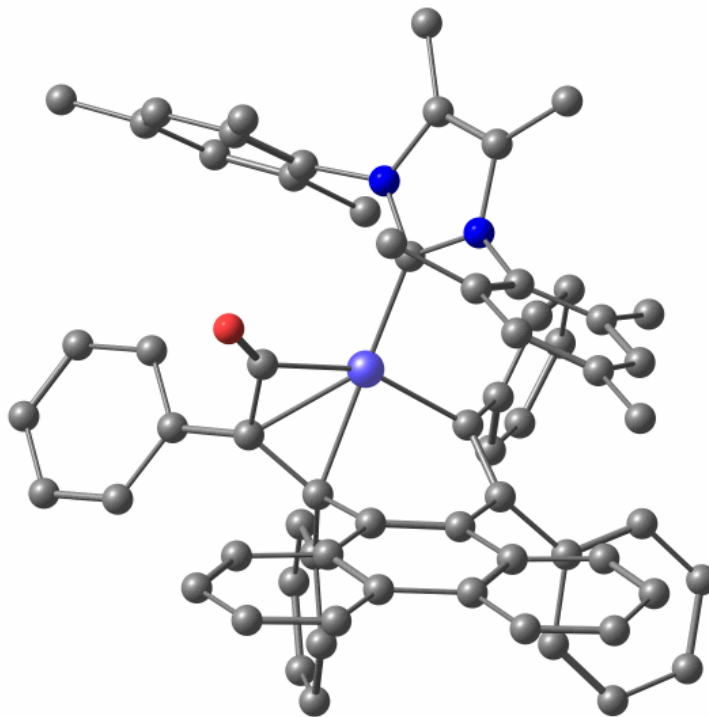
6	-5.757744000	-2.028250000	0.997288000
6	-5.254167000	-1.920593000	-0.305393000
6	-4.226007000	-1.044598000	-0.570062000
6	-1.940061000	2.103595000	3.535874000
6	-2.363757000	1.987451000	4.839425000
6	-3.410409000	1.110460000	5.153689000
6	-4.005444000	0.364777000	4.160473000
6	-1.899600000	0.626883000	-1.190264000
6	-0.629797000	0.173168000	-1.330339000
28	0.769096000	-0.577460000	-0.229066000
6	0.637033000	0.817886000	1.033163000
6	0.242948000	2.247667000	0.785050000
6	-1.071259000	2.534245000	0.800064000
8	0.741489000	0.393548000	2.173346000
15	2.918566000	-1.166943000	0.298476000
15	0.353088000	-2.828090000	-0.304987000
6	2.973111000	-3.015583000	0.538818000
6	1.988126000	-3.700475000	-0.398728000
6	1.366555000	3.190651000	0.616026000
6	-1.656112000	3.837578000	0.404543000
6	0.145041000	0.346475000	-2.571987000
6	0.401590000	1.644783000	-3.054720000
6	1.200028000	1.858382000	-4.169240000
6	1.765836000	0.781533000	-4.849004000
6	1.513291000	-0.510830000	-4.400388000
6	0.720125000	-0.726462000	-3.278184000
6	1.639967000	4.119332000	1.626271000
6	2.749995000	4.950979000	1.540363000
6	3.606837000	4.865756000	0.446119000
6	3.338793000	3.950633000	-0.566822000
6	2.229771000	3.116346000	-0.482170000
6	-1.093833000	4.600317000	-0.628758000
6	-1.707994000	5.760385000	-1.079031000
6	-2.899334000	6.193931000	-0.506021000
6	-3.466708000	5.453968000	0.525614000
6	-2.856787000	4.288095000	0.971602000
6	-2.721671000	1.162914000	-2.311086000
6	-2.708372000	0.595930000	-3.594307000
6	-3.486701000	1.119104000	-4.618620000
6	-4.303525000	2.222385000	-4.390221000
6	-4.339159000	2.788973000	-3.120724000
6	-3.567846000	2.259268000	-2.093963000
1	-5.644752000	-1.336712000	3.002089000
1	-6.568414000	-2.719098000	1.216910000
1	-5.671262000	-2.525310000	-1.108732000
1	-3.844857000	-0.957811000	-1.583476000
1	-1.117584000	2.769536000	3.285360000
1	-1.883317000	2.569144000	5.622386000
1	-3.752326000	1.013207000	6.181427000
1	-4.808417000	-0.315342000	4.431877000
1	2.699909000	-3.215084000	1.584674000
1	3.992989000	-3.397977000	0.401640000
1	1.909586000	-4.773652000	-0.179213000
1	2.320974000	-3.612361000	-1.444418000
1	-0.060932000	2.488347000	-2.542348000
1	1.374062000	2.874701000	-4.517278000
1	2.392239000	0.948712000	-5.722318000
1	1.934858000	-1.363023000	-4.931218000
1	0.515626000	-1.745785000	-2.955142000
1	0.970516000	4.176712000	2.483146000

1	2.948590000	5.668061000	2.333729000
1	4.476692000	5.515262000	0.382070000
1	3.996163000	3.882121000	-1.432558000
1	2.019708000	2.400684000	-1.274241000
1	-0.171745000	4.264547000	-1.097447000
1	-1.257817000	6.322016000	-1.894385000
1	-3.383494000	7.099467000	-0.864031000
1	-4.397528000	5.780554000	0.984062000
1	-3.325511000	3.711623000	1.765903000
1	-2.077723000	-0.269982000	-3.790661000
1	-3.457791000	0.656384000	-5.603050000
1	-4.910714000	2.632303000	-5.194142000
1	-4.968295000	3.654164000	-2.920677000
1	-3.607852000	2.715975000	-1.106116000
6	3.679345000	-0.520818000	1.868238000
6	4.788979000	-1.337749000	2.534947000
6	4.092143000	0.948496000	1.753814000
1	2.795412000	-0.548241000	2.531801000
6	5.105904000	-0.758701000	3.913476000
1	5.700365000	-1.317049000	1.918105000
1	4.503524000	-2.392815000	2.636299000
6	4.407477000	1.526040000	3.127967000
1	4.985466000	1.036090000	1.110720000
1	3.303246000	1.537847000	1.272499000
6	5.490171000	0.713875000	3.828112000
1	5.906605000	-1.339710000	4.389650000
1	4.217416000	-0.863421000	4.556301000
1	4.709518000	2.576815000	3.030777000
1	3.483388000	1.519044000	3.728837000
1	5.691406000	1.115744000	4.829390000
1	6.430511000	0.805214000	3.259667000
6	4.089649000	-0.974597000	-1.144029000
6	3.960536000	0.394779000	-1.811783000
6	5.556005000	-1.306697000	-0.859110000
1	3.699981000	-1.720920000	-1.863823000
6	4.825865000	0.491933000	-3.062475000
1	4.259332000	1.179015000	-1.097080000
1	2.907852000	0.579412000	-2.064547000
6	6.397323000	-1.219242000	-2.129648000
1	5.951365000	-0.584446000	-0.127513000
1	5.657147000	-2.300655000	-0.401561000
6	6.282003000	0.160890000	-2.764876000
1	4.726862000	1.493821000	-3.502812000
1	4.439396000	-0.212330000	-3.817908000
1	7.444392000	-1.458067000	-1.902630000
1	6.050506000	-1.979847000	-2.847893000
1	6.888026000	0.216150000	-3.678155000
1	6.692490000	0.911334000	-2.069397000
6	-0.681351000	-3.813869000	-1.499332000
6	-0.939297000	-5.289982000	-1.193667000
6	-1.996528000	-3.101470000	-1.804456000
1	-0.058382000	-3.775310000	-2.415624000
6	-1.662241000	-5.956801000	-2.363111000
1	-1.574206000	-5.365702000	-0.297235000
1	-0.005524000	-5.822658000	-0.965705000
6	-2.723127000	-3.757752000	-2.969839000
1	-2.640766000	-3.135872000	-0.911248000
1	-1.817250000	-2.036761000	-1.997377000
6	-2.965472000	-5.237463000	-2.696211000
1	-1.853047000	-7.013184000	-2.133712000

1	-1.004082000	-5.944021000	-3.247175000
1	-3.671599000	-3.236685000	-3.162099000
1	-2.115432000	-3.643433000	-3.883712000
1	-3.459738000	-5.717579000	-3.550372000
1	-3.655960000	-5.330270000	-1.841616000
6	-0.152844000	-3.122832000	1.468821000
6	-1.533991000	-2.547442000	1.782924000
6	0.005637000	-4.529411000	2.047045000
1	0.562262000	-2.463277000	1.996491000
6	-1.780031000	-2.539859000	3.288165000
1	-2.321896000	-3.143094000	1.288932000
1	-1.608568000	-1.528565000	1.381618000
6	-0.218649000	-4.498185000	3.557199000
1	-0.730813000	-5.208157000	1.591609000
1	0.997229000	-4.946818000	1.820735000
6	-1.590232000	-3.924086000	3.894794000
1	-2.790938000	-2.165296000	3.493920000
1	-1.084459000	-1.822517000	3.755030000
1	-0.104364000	-5.505995000	3.977703000
1	0.562487000	-3.873593000	4.021248000
1	-1.734539000	-3.891889000	4.982279000
1	-2.365022000	-4.600199000	3.496952000

Method: M06-2X/6-31G(d,p) Key word: opt freq pop=full
 imaginary frequencies: 0 Energy: -3599.248440 Hartree

Int III



6	-1.864844000	-1.198885000	-2.619767000
6	-3.173568000	-0.754204000	-2.954440000

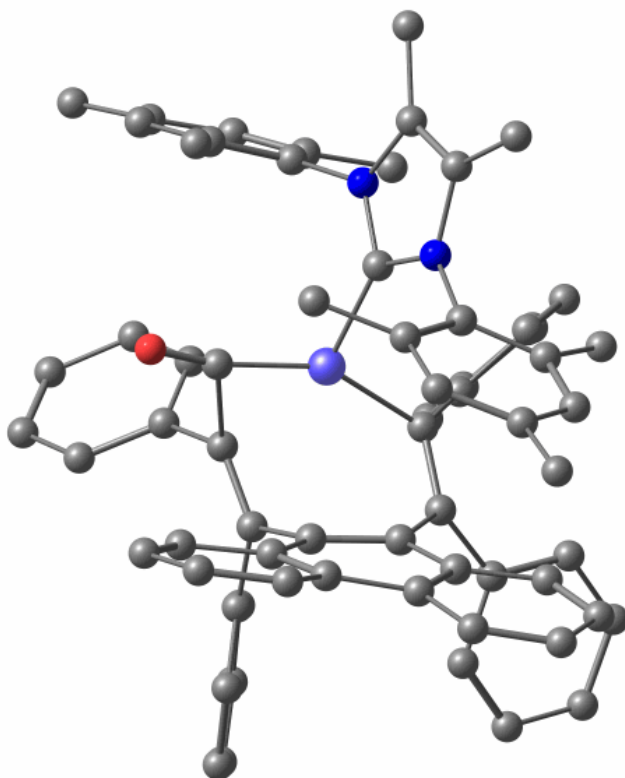
6	-4.039559000	-0.238055000	-1.915204000
6	-3.563088000	-0.160860000	-0.580540000
6	-2.247415000	-0.658913000	-0.243369000
6	-1.419465000	-1.141149000	-1.240806000
6	-5.358369000	0.182953000	-2.189697000
6	-6.174558000	0.691987000	-1.205895000
6	-5.682571000	0.834258000	0.097993000
6	-4.406130000	0.420137000	0.395713000
6	-1.069037000	-1.747042000	-3.654288000
6	-1.516674000	-1.825206000	-4.952711000
6	-2.792491000	-1.355667000	-5.282986000
6	-3.597786000	-0.836464000	-4.296418000
6	-1.762424000	-0.670578000	1.166870000
6	-0.469271000	-0.338907000	1.411863000
28	0.678039000	0.061011000	-0.164727000
6	1.236781000	-0.049252000	-1.978333000
6	1.084667000	-1.415006000	-1.559918000
6	-0.096359000	-1.735022000	-0.847714000
8	1.490349000	0.602115000	-2.950698000
6	2.289360000	-2.272019000	-1.657901000
6	-0.137467000	-3.029375000	-0.114119000
6	0.116894000	-0.461391000	2.755074000
6	0.177850000	-1.693648000	3.429185000
6	0.727893000	-1.791103000	4.700532000
6	1.198904000	-0.656704000	5.356052000
6	1.135314000	0.574023000	4.710131000
6	0.630512000	0.662962000	3.419012000
6	2.173381000	-3.545146000	-2.229084000
6	3.294242000	-4.349492000	-2.381628000
6	4.545971000	-3.899213000	-1.970545000
6	4.667605000	-2.633926000	-1.408332000
6	3.547735000	-1.825173000	-1.255826000
6	0.882351000	-3.409997000	0.765174000
6	0.861870000	-4.653080000	1.380528000
6	-0.182459000	-5.540879000	1.135064000
6	-1.201489000	-5.175657000	0.263532000
6	-1.176788000	-3.931392000	-0.357622000
6	-2.690139000	-1.215533000	2.201341000
6	-2.829441000	-0.655528000	3.478649000
6	-3.695616000	-1.205754000	4.414881000
6	-4.449866000	-2.332004000	4.101909000
6	-4.325359000	-2.900883000	2.839343000
6	-3.460429000	-2.347907000	1.903800000
1	-5.754470000	0.096310000	-3.196951000
1	-7.191077000	0.996052000	-1.446504000
1	-6.306933000	1.267383000	0.876529000
1	-4.043552000	0.527676000	1.412545000
1	-0.069757000	-2.105055000	-3.431473000
1	-0.870965000	-2.247566000	-5.718715000
1	-3.148784000	-1.402525000	-6.309156000
1	-4.586647000	-0.481266000	-4.570282000
1	-0.236489000	-2.576661000	2.947104000
1	0.766342000	-2.760613000	5.193399000
1	1.609941000	-0.731554000	6.360216000
1	1.504758000	1.470240000	5.206218000
1	0.636716000	1.621506000	2.900900000
1	1.194769000	-3.911654000	-2.535483000
1	3.187557000	-5.338197000	-2.822021000
1	5.420097000	-4.535760000	-2.085124000
1	5.635447000	-2.266949000	-1.069962000

1	3.638444000	-0.844552000	-0.796003000
1	1.690876000	-2.711191000	0.975583000
1	1.658529000	-4.922668000	2.070507000
1	-0.201032000	-6.512442000	1.623209000
1	-2.020445000	-5.862186000	0.061194000
1	-1.970468000	-3.652677000	-1.050093000
1	-2.249105000	0.224946000	3.747298000
1	-3.784136000	-0.745879000	5.397038000
1	-5.130170000	-2.760072000	4.834576000
1	-4.906934000	-3.782470000	2.577489000
1	-3.374129000	-2.800518000	0.916891000
6	1.210751000	1.848263000	0.215140000
6	2.473655000	3.620262000	0.920352000
6	3.707044000	4.317344000	1.358283000
1	3.466785000	5.323606000	1.712974000
1	4.200961000	3.782139000	2.178470000
1	4.442815000	4.411947000	0.549841000
6	1.195501000	4.054706000	0.811585000
6	0.602029000	5.396806000	1.024489000
1	1.382106000	6.121890000	1.272968000
1	0.088130000	5.749007000	0.121392000
1	-0.136739000	5.405798000	1.834847000
6	-0.923222000	3.124479000	-0.071927000
6	-3.258424000	3.444287000	0.351317000
6	-2.416470000	3.655881000	-1.872777000
1	-4.091569000	3.475073000	1.054420000
1	-2.578810000	3.866862000	-2.930289000
6	3.706325000	1.597203000	0.217681000
6	5.546434000	0.175158000	0.803308000
6	5.554037000	1.322132000	-1.291914000
1	6.016187000	-0.506800000	1.512893000
1	6.035017000	1.551040000	-2.243295000
6	-1.120122000	3.401223000	-1.433471000
6	0.025695000	3.489386000	-2.391550000
1	-0.301712000	3.922370000	-3.341526000
1	0.833527000	4.118418000	-1.993960000
1	0.462197000	2.507706000	-2.606478000
6	-1.982972000	3.165462000	0.840217000
6	-1.793510000	2.903385000	2.298798000
1	-0.933909000	3.437378000	2.721213000
1	-2.686222000	3.186566000	2.865497000
1	-1.612903000	1.834775000	2.457092000
6	-3.499982000	3.679508000	-0.998162000
6	-4.882704000	3.952922000	-1.503119000
1	-5.558637000	4.236778000	-0.689149000
1	-4.886449000	4.754843000	-2.250197000
1	-5.301585000	3.055217000	-1.976048000
6	4.325887000	1.910911000	-1.005974000
6	3.698955000	2.842997000	-1.995544000
1	2.765011000	2.423209000	-2.386629000
1	3.463754000	3.819718000	-1.553972000
1	4.370750000	3.010456000	-2.842274000
6	4.310781000	0.734084000	1.136696000
6	3.658897000	0.372153000	2.428535000
1	2.843118000	-0.348086000	2.272873000
1	4.376651000	-0.080361000	3.119649000
1	3.205790000	1.239080000	2.919672000
6	6.183777000	0.455047000	-0.399933000
6	7.517135000	-0.143506000	-0.732088000
1	7.764567000	-0.971869000	-0.059456000

1	7.538304000	-0.521312000	-1.761165000
1	8.319242000	0.600334000	-0.647716000
7	0.433747000	2.956523000	0.384946000
7	2.471730000	2.272755000	0.529440000

Method: M06-2X/6-31G(d,p) Key word: opt freq pop=full
 imaginary frequencies: 0 Energy: -2899.961724 Hartree

TS II



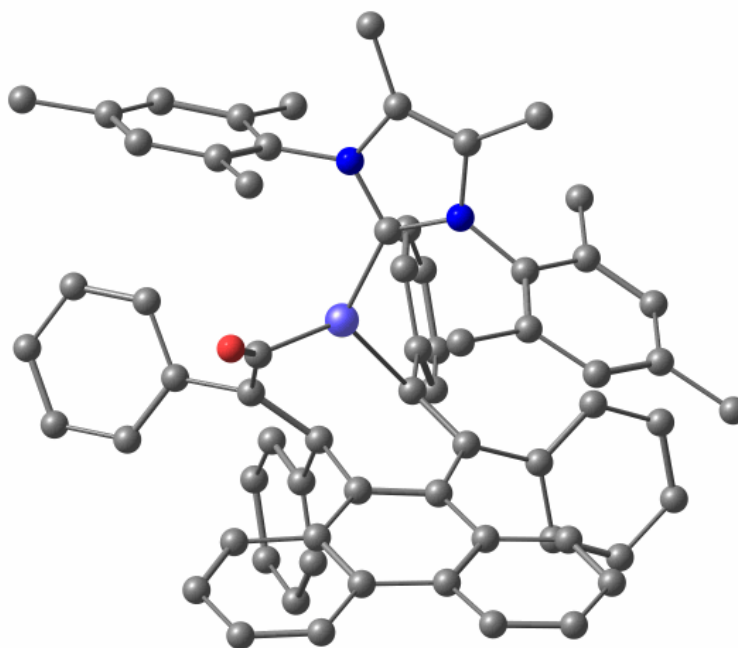
6	2.110103000	0.447428000	-2.436852000
6	3.332362000	-0.259591000	-2.316609000
6	4.002151000	-0.286255000	-1.033978000
6	3.319961000	0.182393000	0.119102000
6	2.016412000	0.802709000	-0.003488000
6	1.491125000	1.006470000	-1.260052000
6	5.326137000	-0.746751000	-0.898029000
6	5.954976000	-0.780381000	0.326804000
6	5.257301000	-0.391709000	1.476833000
6	3.964253000	0.069910000	1.371393000
6	1.502726000	0.555055000	-3.707671000
6	2.047203000	-0.061572000	-4.811654000
6	3.221244000	-0.815395000	-4.680653000
6	3.848515000	-0.905685000	-3.456730000
6	1.254904000	1.194438000	1.225906000
6	0.029304000	0.636576000	1.400456000
28	-0.736334000	-0.287082000	-0.173051000
6	-1.199393000	-0.276512000	-1.871167000

6	-0.953111000	1.362472000	-1.443249000
6	0.290801000	1.887757000	-1.419224000
8	-1.499059000	-0.561099000	-2.980742000
6	-2.229036000	2.077276000	-1.610834000
6	0.590152000	3.338609000	-1.425596000
6	-0.792553000	0.948963000	2.575441000
6	-1.431475000	2.191889000	2.696684000
6	-2.184687000	2.507649000	3.820640000
6	-2.316389000	1.590881000	4.860771000
6	-1.702046000	0.346610000	4.749029000
6	-0.969563000	0.021976000	3.613623000
6	-2.486659000	2.814527000	-2.772168000
6	-3.715039000	3.434655000	-2.953161000
6	-4.708126000	3.318650000	-1.982884000
6	-4.465734000	2.573841000	-0.833021000
6	-3.237682000	1.947777000	-0.651501000
6	-0.202078000	4.247408000	-0.712956000
6	0.147325000	5.589215000	-0.645325000
6	1.282986000	6.052667000	-1.301169000
6	2.072279000	5.162780000	-2.023516000
6	1.737418000	3.816256000	-2.074005000
6	1.879792000	2.220289000	2.107811000
6	1.799841000	2.183611000	3.507460000
6	2.372597000	3.182813000	4.284455000
6	3.043197000	4.246029000	3.687810000
6	3.146064000	4.289663000	2.301655000
6	2.581029000	3.285790000	1.526306000
6	-1.046773000	-2.034779000	0.404684000
6	-2.190218000	-3.892906000	1.068093000
6	-3.390290000	-4.692676000	1.411844000
6	-0.870332000	-4.200019000	1.088946000
6	-0.166754000	-5.464138000	1.411892000
6	1.223395000	-3.082189000	0.391486000
6	3.482250000	-3.246472000	1.165043000
6	2.974028000	-3.671090000	-1.132683000
6	-3.511156000	-1.964350000	0.188103000
6	-5.428320000	-0.575646000	0.540797000
6	-5.097157000	-1.627587000	-1.578885000
6	1.623871000	-3.411962000	-0.910852000
6	0.645821000	-3.497366000	-2.040859000
6	2.147168000	-2.952145000	1.433187000
6	1.733077000	-2.461895000	2.784060000
6	3.911339000	-3.631288000	-0.102529000
6	5.333139000	-4.034739000	-0.349725000
6	-3.935401000	-2.241682000	-1.123831000
6	-3.172647000	-3.157688000	-2.032840000
6	-4.267864000	-1.164672000	1.046726000
6	-3.882121000	-0.905745000	2.466740000
6	-5.844106000	-0.770569000	-0.770474000
6	-7.050315000	-0.068550000	-1.313058000
7	-0.183721000	-3.041880000	0.683506000
7	-2.281901000	-2.563675000	0.634574000
1	5.882729000	-1.047826000	-1.782383000
1	6.988880000	-1.112737000	0.396824000
1	5.737281000	-0.438000000	2.451864000
1	3.437566000	0.388983000	2.265771000
1	0.570192000	1.108476000	-3.800332000
1	1.555292000	0.022222000	-5.777520000
1	3.638635000	-1.329943000	-5.543002000
1	4.751673000	-1.505744000	-3.370846000

1	-1.288887000	2.925526000	1.904001000
1	-2.657586000	3.485146000	3.893554000
1	-2.893967000	1.843096000	5.746979000
1	-1.804325000	-0.384258000	5.549531000
1	-0.509553000	-0.962360000	3.524125000
1	-1.705819000	2.899874000	-3.527164000
1	-3.902283000	4.008542000	-3.857915000
1	-5.670833000	3.804830000	-2.125928000
1	-5.237453000	2.470930000	-0.071820000
1	-3.039948000	1.363522000	0.248869000
1	-1.087504000	3.890375000	-0.191984000
1	-0.468013000	6.274640000	-0.067763000
1	1.554772000	7.104167000	-1.246846000
1	2.961396000	5.515836000	-2.540642000
1	2.373924000	3.121524000	-2.618732000
1	1.285770000	1.356844000	3.992965000
1	2.295976000	3.125907000	5.368374000
1	3.486670000	5.029085000	4.298755000
1	3.667659000	5.111002000	1.813809000
1	2.673205000	3.331382000	0.441949000
1	-3.102355000	-5.707011000	1.702491000
1	-3.945965000	-4.249936000	2.247974000
1	-4.086485000	-4.767264000	0.567559000
1	-0.890601000	-6.247897000	1.653008000
1	0.437065000	-5.810383000	0.563271000
1	0.513548000	-5.359753000	2.265845000
1	4.208625000	-3.165381000	1.973754000
1	3.297173000	-3.925911000	-2.143258000
1	-6.020704000	0.059636000	1.201842000
1	-5.426620000	-1.823155000	-2.599858000
1	1.091515000	-4.007249000	-2.900471000
1	-0.267385000	-4.035855000	-1.756471000
1	0.335197000	-2.497576000	-2.373713000
1	1.494075000	-1.388917000	2.723048000
1	0.835848000	-2.967908000	3.162208000
1	2.538033000	-2.589253000	3.514564000
1	5.666593000	-3.735839000	-1.350647000
1	6.012567000	-3.580678000	0.379301000
1	5.448818000	-5.124331000	-0.280941000
1	-3.835155000	-3.565098000	-2.803241000
1	-2.367134000	-2.617352000	-2.546550000
1	-2.718567000	-3.998248000	-1.494640000
1	-3.125605000	-1.604931000	2.833392000
1	-3.462900000	0.101693000	2.583272000
1	-4.759526000	-0.966534000	3.121005000
1	-7.698876000	0.298026000	-0.510151000
1	-6.749015000	0.798645000	-1.916024000
1	-7.643762000	-0.722728000	-1.961556000

Method: M06-2X/6-31G(d,p) Key word: opt freq pop=full
imaginary frequencies: -105.5699 cm⁻¹ Energy: -2899.945426 Hartree

TS III



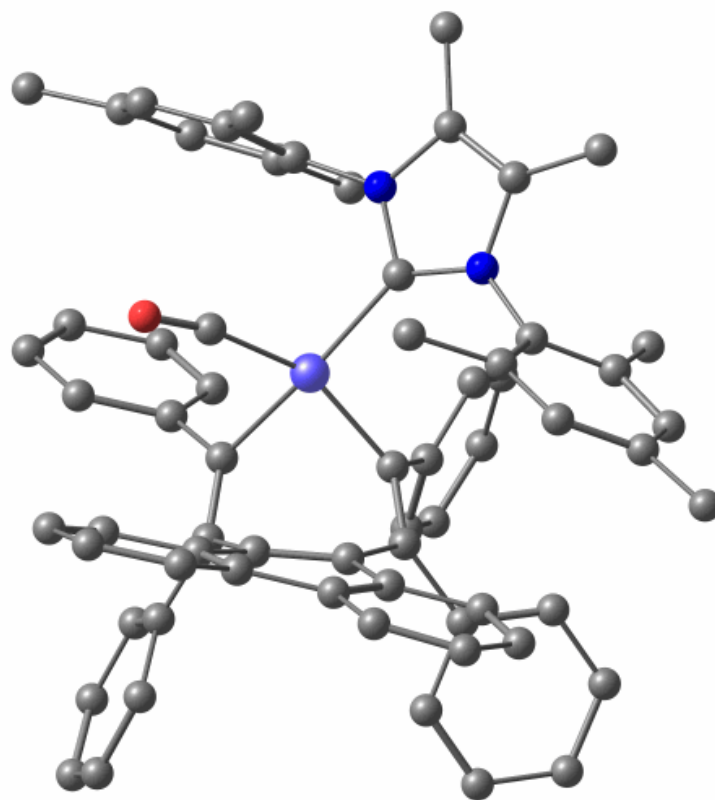
6	-1.094891000	-2.222452000	-2.403499000
6	-2.203640000	-2.024099000	-3.273417000
6	-3.329082000	-1.213842000	-2.843251000
6	-3.365273000	-0.694403000	-1.521322000
6	-2.237185000	-0.934939000	-0.649843000
6	-1.130331000	-1.628769000	-1.090351000
6	-4.405499000	-0.927171000	-3.707644000
6	-5.493051000	-0.191320000	-3.294574000
6	-5.535742000	0.307218000	-1.987841000
6	-4.483125000	0.074989000	-1.131261000
6	-0.037148000	-3.051256000	-2.843749000
6	-0.058486000	-3.655071000	-4.078836000
6	-1.144427000	-3.451540000	-4.937442000
6	-2.189813000	-2.652501000	-4.535057000
6	-2.074862000	-0.492226000	0.733922000
6	-0.774107000	-0.502574000	1.154515000
28	0.880613000	0.210623000	-0.016980000
6	1.620405000	-0.617829000	-1.505246000
6	1.345409000	-1.646598000	-0.561034000
6	-0.050532000	-1.773846000	-0.049382000
8	2.018342000	-0.378682000	-2.607602000
6	2.533095000	-2.459707000	-0.188864000
6	-0.224582000	-2.969603000	0.868410000
6	-0.386404000	-0.436415000	2.578941000
6	-0.994309000	-1.247799000	3.551868000
6	-0.583669000	-1.209235000	4.876168000
6	0.443941000	-0.355880000	5.271804000
6	1.058534000	0.455992000	4.326278000
6	0.650601000	0.407114000	2.996746000
6	2.537868000	-3.859306000	-0.293402000
6	3.684414000	-4.591006000	-0.013296000
6	4.860140000	-3.948437000	0.364474000
6	4.873408000	-2.562095000	0.461090000
6	3.723028000	-1.829548000	0.192500000
6	0.627702000	-3.175005000	1.960355000

6	0.484949000	-4.285739000	2.779715000
6	-0.519831000	-5.215590000	2.534834000
6	-1.377169000	-5.021434000	1.458832000
6	-1.229723000	-3.911789000	0.631705000
6	-3.221263000	-0.306381000	1.650871000
6	-3.326946000	0.805533000	2.489642000
6	-4.403174000	0.943220000	3.357778000
6	-5.384147000	-0.040960000	3.419592000
6	-5.277311000	-1.167799000	2.608267000
6	-4.209180000	-1.297181000	1.730882000
1	-4.385605000	-1.288430000	-4.731338000
1	-6.310488000	0.002698000	-3.985119000
1	-6.388983000	0.892474000	-1.650862000
1	-4.510209000	0.502474000	-0.134962000
1	0.823503000	-3.198313000	-2.202529000
1	0.773962000	-4.283905000	-4.384466000
1	-1.168083000	-3.923700000	-5.916684000
1	-3.030004000	-2.526062000	-5.210537000
1	-1.784717000	-1.934141000	3.252717000
1	-1.064660000	-1.858021000	5.604768000
1	0.764181000	-0.328585000	6.310851000
1	1.862217000	1.129487000	4.619924000
1	1.136409000	1.039211000	2.252589000
1	1.625691000	-4.385216000	-0.570106000
1	3.657149000	-5.675553000	-0.093408000
1	5.754787000	-4.526098000	0.585463000
1	5.780040000	-2.037962000	0.762787000
1	3.735387000	-0.745420000	0.284506000
1	1.413544000	-2.454569000	2.175756000
1	1.161539000	-4.416222000	3.621110000
1	-0.631268000	-6.086423000	3.176644000
1	-2.164455000	-5.742123000	1.249180000
1	-1.900817000	-3.787390000	-0.215018000
1	-2.557600000	1.571650000	2.444138000
1	-4.470755000	1.824829000	3.992734000
1	-6.225122000	0.065185000	4.100878000
1	-6.031768000	-1.949635000	2.658989000
1	-4.127542000	-2.176896000	1.093129000
6	1.181189000	2.095637000	-0.156512000
6	2.341012000	4.074567000	-0.317132000
6	3.545072000	4.940508000	-0.318439000
1	3.256997000	5.994733000	-0.361217000
1	4.139419000	4.790841000	0.591818000
1	4.208210000	4.735713000	-1.167825000
6	1.022447000	4.375870000	-0.391792000
6	0.327089000	5.667967000	-0.606450000
1	1.057225000	6.467716000	-0.760134000
1	-0.317759000	5.626412000	-1.493479000
1	-0.312415000	5.953431000	0.237993000
6	-1.089275000	3.119472000	-0.269346000
6	-3.141669000	3.640867000	0.833870000
6	-3.151903000	2.942205000	-1.459242000
1	-3.685321000	3.941424000	1.731732000
1	-3.697543000	2.692710000	-2.369993000
6	3.673786000	2.003489000	-0.295208000
6	5.625126000	1.026050000	0.687044000
6	5.432433000	1.180826000	-1.694385000
1	6.183087000	0.726029000	1.575608000
1	5.845845000	1.005846000	-2.688095000
6	-1.763932000	2.812884000	-1.452825000

6	-1.018981000	2.353696000	-2.668252000
1	-1.709313000	2.128445000	-3.486830000
1	-0.304284000	3.111654000	-3.019146000
1	-0.432413000	1.449041000	-2.456178000
6	-1.757292000	3.517759000	0.892897000
6	-1.008446000	3.776546000	2.165844000
1	-0.282460000	4.594425000	2.071129000
1	-1.698236000	4.032139000	2.977001000
1	-0.438830000	2.888097000	2.474724000
6	-3.853820000	3.364900000	-0.332296000
6	-5.346436000	3.495677000	-0.341162000
1	-5.810851000	2.727980000	0.294083000
1	-5.664087000	4.467391000	0.055063000
1	-5.756029000	3.390685000	-1.350715000
6	4.200216000	1.812801000	-1.583964000
6	3.466147000	2.291223000	-2.798785000
1	2.475853000	1.828665000	-2.864389000
1	3.330568000	3.380742000	-2.789445000
1	4.013803000	2.024758000	-3.707345000
6	4.378711000	1.636180000	0.851349000
6	3.823533000	1.824533000	2.228906000
1	3.330285000	0.902428000	2.568451000
1	4.622189000	2.046764000	2.944851000
1	3.078499000	2.627628000	2.277897000
6	6.157323000	0.773779000	-0.571873000
6	7.471322000	0.072606000	-0.736016000
1	7.974846000	-0.070436000	0.225986000
1	7.330022000	-0.916944000	-1.189314000
1	8.146746000	0.632624000	-1.393321000
7	0.338935000	3.159261000	-0.274198000
7	2.418528000	2.685193000	-0.185865000

Method: M06-2X/6-31G(d,p) Key word: opt freq pop=full
 imaginary frequencies: -197.3036 cm⁻¹ Energy: -2899.939208 Hartree

Int IV



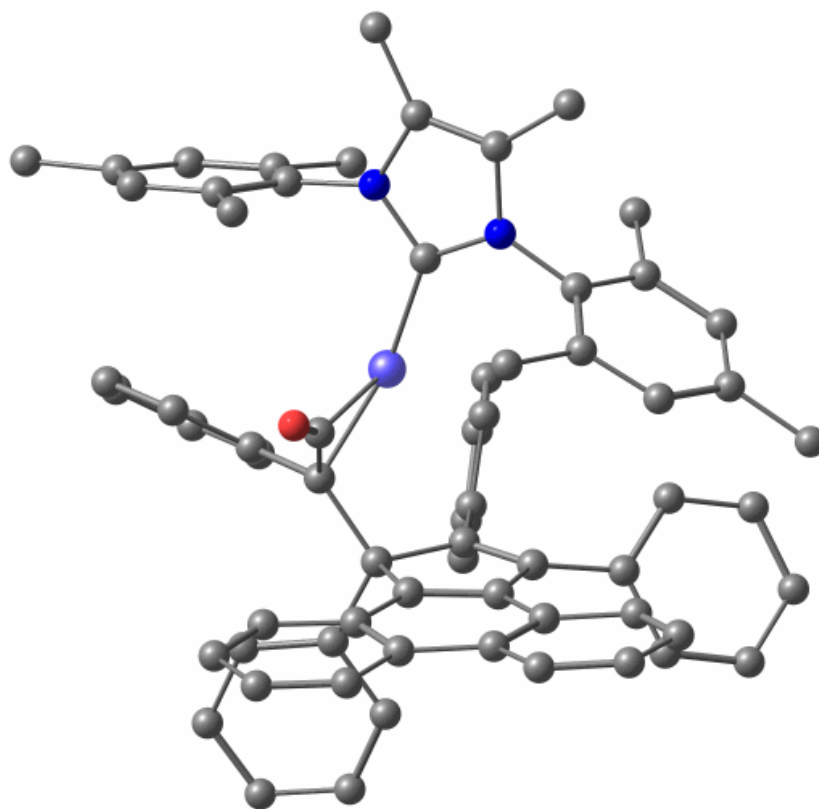
6	1.471946000	2.148543000	-2.378043000
6	2.546429000	1.580185000	-3.105296000
6	3.489979000	0.731279000	-2.407073000
6	3.220800000	0.347464000	-1.064878000
6	2.040357000	0.843809000	-0.380899000
6	1.274020000	1.816399000	-0.984259000
6	4.684927000	0.298606000	-3.015973000
6	5.613973000	-0.451660000	-2.329807000
6	5.351945000	-0.829311000	-1.008088000
6	4.167433000	-0.467948000	-0.406855000
6	0.573423000	3.006187000	-3.051806000
6	0.715373000	3.286815000	-4.390977000
6	1.769411000	2.711827000	-5.113138000
6	2.661550000	1.876049000	-4.478591000
6	1.673789000	0.382734000	0.987336000
6	0.402968000	-0.019118000	1.247595000
28	-0.851649000	-0.141355000	-0.231209000
6	-1.588562000	0.330264000	-1.816312000
6	-0.894788000	1.763657000	0.068012000
6	0.178767000	2.514743000	-0.243397000
8	-1.870944000	0.777649000	-2.835830000
6	-2.236182000	2.190063000	0.495002000
6	0.423047000	3.917203000	0.177054000
6	-0.111824000	-0.133394000	2.622489000
6	0.041015000	0.945033000	3.513334000
6	-0.494840000	0.902555000	4.792382000
6	-1.201956000	-0.218042000	5.223566000
6	-1.377348000	-1.287221000	4.352243000
6	-0.851317000	-1.236873000	3.064807000

6	-3.004275000	2.962190000	-0.394105000
6	-4.308772000	3.325497000	-0.087881000
6	-4.886774000	2.924680000	1.114240000
6	-4.142867000	2.151312000	1.999814000
6	-2.839430000	1.777970000	1.692696000
6	-0.358302000	4.537069000	1.167739000
6	-0.090910000	5.829642000	1.594612000
6	0.976457000	6.545927000	1.062176000
6	1.781265000	5.940674000	0.104903000
6	1.512453000	4.647692000	-0.326651000
6	2.692221000	0.576191000	2.054160000
6	2.976940000	-0.408781000	3.007425000
6	3.912697000	-0.184080000	4.008763000
6	4.590248000	1.029863000	4.075990000
6	4.328331000	2.012684000	3.126572000
6	3.394202000	1.785906000	2.123419000
6	-1.137426000	-2.081933000	-0.241510000
6	-2.393355000	-3.990754000	-0.396813000
6	-3.643069000	-4.779502000	-0.511531000
6	-1.095784000	-4.368295000	-0.294629000
6	-0.472159000	-5.712345000	-0.356553000
6	1.087626000	-3.237767000	-0.161117000
6	3.113913000	-3.983258000	0.871015000
6	3.131720000	-3.261720000	-1.408457000
6	-3.567578000	-1.811377000	-0.642478000
6	-5.407667000	-0.476289000	0.094268000
6	-4.995122000	-0.753081000	-2.246680000
6	1.772768000	-2.968992000	-1.354160000
6	1.079219000	-2.372662000	-2.539186000
6	1.747679000	-3.724122000	0.973103000
6	1.051394000	-3.979223000	2.276066000
6	3.814625000	-3.791659000	-0.315866000
6	5.263999000	-4.158338000	-0.413039000
6	-3.914360000	-1.591713000	-1.981417000
6	-3.159299000	-2.230242000	-3.108903000
6	-4.326656000	-1.292935000	0.412427000
6	-4.002844000	-1.588660000	1.841779000
6	-5.736676000	-0.167604000	-1.223830000
6	-6.855064000	0.783470000	-1.517519000
7	-0.347704000	-3.184655000	-0.173537000
7	-2.397826000	-2.595193000	-0.365956000
1	4.906400000	0.600851000	-4.036024000
1	6.546455000	-0.738487000	-2.811208000
1	6.077347000	-1.420752000	-0.453434000
1	3.966982000	-0.808252000	0.604053000
1	-0.254439000	3.434744000	-2.491623000
1	0.005036000	3.943447000	-4.887397000
1	1.881628000	2.917771000	-6.175132000
1	3.461024000	1.427205000	-5.061735000
1	0.577792000	1.829729000	3.172341000
1	-0.364161000	1.753323000	5.457548000
1	-1.620983000	-0.251961000	6.226576000
1	-1.944353000	-2.162472000	4.666494000
1	-1.028054000	-2.062144000	2.376022000
1	-2.554325000	3.274359000	-1.336070000
1	-4.875968000	3.933762000	-0.790458000
1	-5.908416000	3.211440000	1.355771000
1	-4.579763000	1.825823000	2.942886000
1	-2.267383000	1.183312000	2.401048000
1	-1.177449000	3.991043000	1.626939000

1	-0.717985000	6.275799000	2.363684000
1	1.186575000	7.557629000	1.401319000
1	2.632130000	6.475226000	-0.312189000
1	2.166148000	4.195448000	-1.068159000
1	2.460455000	-1.366309000	2.941857000
1	4.117639000	-0.963590000	4.739867000
1	5.323419000	1.205345000	4.859997000
1	4.853265000	2.964760000	3.168144000
1	3.183825000	2.560147000	1.384709000
1	-3.429228000	-5.849447000	-0.438728000
1	-4.348320000	-4.520341000	0.287784000
1	-4.160082000	-4.600519000	-1.463037000
1	-1.218799000	-6.456875000	-0.647533000
1	0.335499000	-5.734291000	-1.098668000
1	-0.038941000	-6.028259000	0.600422000
1	3.638127000	-4.370944000	1.745786000
1	3.676675000	-3.046849000	-2.328324000
1	-6.000641000	-0.052878000	0.905299000
1	-5.255356000	-0.542985000	-3.284457000
1	1.742654000	-2.353726000	-3.409140000
1	0.169663000	-2.927906000	-2.807121000
1	0.778224000	-1.335502000	-2.328304000
1	1.061287000	-3.083638000	2.912021000
1	-0.001405000	-4.252673000	2.149386000
1	1.550790000	-4.781116000	2.830049000
1	5.390375000	-5.240613000	-0.544332000
1	5.745228000	-3.662819000	-1.262863000
1	5.808807000	-3.879813000	0.496967000
1	-3.331212000	-1.688599000	-4.044134000
1	-2.078011000	-2.256159000	-2.929530000
1	-3.478633000	-3.269776000	-3.265840000
1	-3.614719000	-2.605711000	1.979654000
1	-3.235588000	-0.903435000	2.222622000
1	-4.891329000	-1.467764000	2.470293000
1	-7.748895000	0.547331000	-0.928635000
1	-6.558511000	1.808039000	-1.255267000
1	-7.130301000	0.774073000	-2.576886000

Method: M06-2X/6-31G(d,p) Key word: opt freq pop=full
imaginary frequencies: 0 Energy: -2899.959223 Hartree

Int V



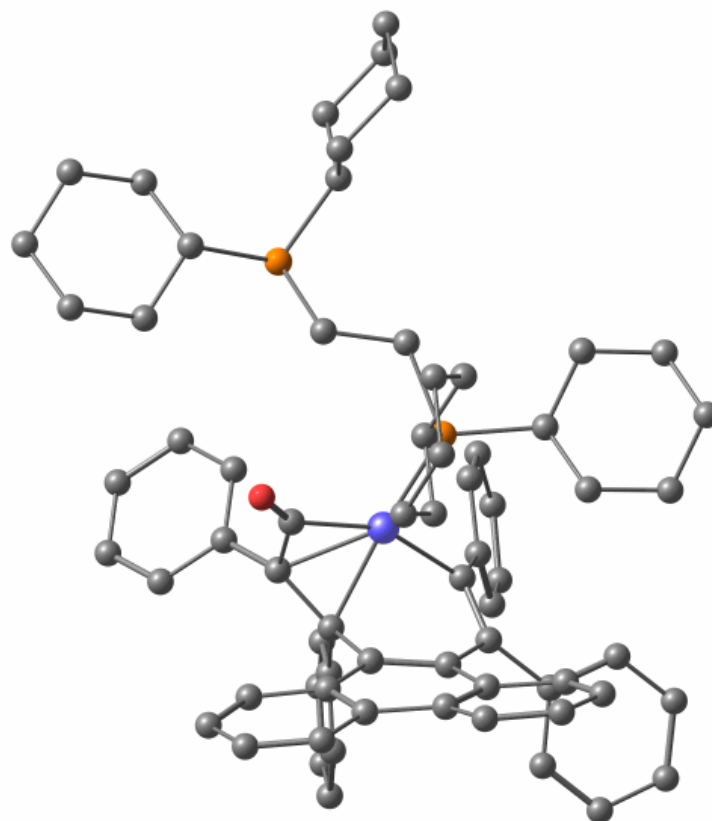
6	-1.783642000	-2.200656000	-2.260128000
6	-2.788811000	-1.775439000	-3.171567000
6	-3.717463000	-0.728955000	-2.783219000
6	-3.678284000	-0.189404000	-1.466075000
6	-2.686659000	-0.690726000	-0.551993000
6	-1.751576000	-1.610399000	-0.958977000
6	-4.662095000	-0.203945000	-3.688290000
6	-5.537620000	0.796198000	-3.327763000
6	-5.499022000	1.322626000	-2.030814000
6	-4.582151000	0.839360000	-1.124001000
6	-0.861489000	-3.189588000	-2.667329000
6	-0.938849000	-3.765637000	-3.912361000
6	-1.943842000	-3.367639000	-4.804496000
6	-2.841502000	-2.390513000	-4.438674000
6	-2.429812000	-0.344670000	0.858419000
6	-1.322601000	-1.003103000	1.274597000
28	1.146338000	0.269946000	0.060913000
6	0.891694000	-0.832424000	-1.360890000
6	0.667909000	-1.613425000	-0.188724000
6	-0.796025000	-1.943165000	0.187206000
8	0.974351000	-0.740642000	-2.551752000
6	1.905027000	-2.218054000	0.379591000
6	-1.073365000	-3.405432000	0.603903000
6	-0.694494000	-0.873070000	2.603842000
6	-0.934813000	-1.787193000	3.633043000
6	-0.279364000	-1.664378000	4.854502000
6	0.622756000	-0.627707000	5.069373000
6	0.853409000	0.303033000	4.061011000

6	0.194777000	0.182366000	2.843447000
6	2.984013000	-2.505456000	-0.478759000
6	4.151338000	-3.086622000	-0.004518000
6	4.284564000	-3.408929000	1.342552000
6	3.228118000	-3.133822000	2.204974000
6	2.060518000	-2.544539000	1.737545000
6	-0.179568000	-4.455477000	0.393026000
6	-0.514793000	-5.763542000	0.736494000
6	-1.751572000	-6.053848000	1.293380000
6	-2.659724000	-5.019276000	1.497684000
6	-2.323221000	-3.717499000	1.155368000
6	-3.311968000	0.411805000	1.771546000
6	-2.868066000	1.523192000	2.489386000
6	-3.706566000	2.165199000	3.395492000
6	-5.001951000	1.704694000	3.602392000
6	-5.454913000	0.592247000	2.897349000
6	-4.616941000	-0.049055000	1.995450000
1	-4.699631000	-0.581536000	-4.705913000
1	-6.251608000	1.178609000	-4.053572000
1	-6.180835000	2.118976000	-1.738698000
1	-4.535999000	1.272024000	-0.129404000
1	-0.070378000	-3.484243000	-1.984609000
1	-0.218911000	-4.526282000	-4.204104000
1	-2.014924000	-3.826087000	-5.788094000
1	-3.611867000	-2.101732000	-5.148177000
1	-1.626959000	-2.609692000	3.464710000
1	-0.474690000	-2.387595000	5.642962000
1	1.135729000	-0.538460000	6.024084000
1	1.543877000	1.128900000	4.223084000
1	0.354995000	0.930801000	2.057238000
1	2.893330000	-2.278483000	-1.541009000
1	4.958361000	-3.301518000	-0.703606000
1	5.194933000	-3.875385000	1.713311000
1	3.305716000	-3.383486000	3.261525000
1	1.244411000	-2.361949000	2.429183000
1	0.797158000	-4.265277000	-0.041962000
1	0.207666000	-6.557859000	0.562925000
1	-2.010033000	-7.075582000	1.561425000
1	-3.639848000	-5.225279000	1.922365000
1	-3.047656000	-2.920750000	1.319119000
1	-1.859965000	1.895646000	2.322695000
1	-3.341850000	3.033933000	3.940646000
1	-5.656447000	2.207371000	4.310599000
1	-6.464300000	0.219087000	3.054775000
1	-4.974754000	-0.915421000	1.439231000
6	1.826203000	1.990789000	-0.326340000
6	3.314786000	3.588531000	-1.005491000
6	4.654544000	4.136191000	-1.323698000
1	4.587213000	5.201153000	-1.564038000
1	5.339140000	4.024125000	-0.472952000
1	5.120404000	3.625099000	-2.175734000
6	2.087377000	4.168469000	-0.972889000
6	1.640763000	5.537752000	-1.322271000
1	2.476586000	6.121658000	-1.718502000
1	0.853514000	5.513436000	-2.086224000
1	1.230559000	6.078459000	-0.459690000
6	-0.192188000	3.406419000	-0.298936000
6	-1.888417000	4.333703000	1.113254000
6	-2.475849000	3.357444000	-0.994118000
1	-2.181361000	4.819473000	2.045572000

1	-3.230063000	3.083825000	-1.731862000
6	4.163990000	1.275574000	-0.561852000
6	5.767199000	0.025499000	0.693978000
6	5.600900000	-0.270389000	-1.679089000
1	6.221797000	-0.239209000	1.649373000
1	5.925763000	-0.767457000	-2.594223000
6	-1.143293000	3.044335000	-1.258651000
6	-0.758322000	2.352177000	-2.529074000
1	-1.646293000	2.129828000	-3.130325000
1	-0.075601000	2.964981000	-3.133992000
1	-0.238614000	1.405042000	-2.336890000
6	-0.546119000	4.029930000	0.903414000
6	0.486714000	4.316747000	1.952755000
1	1.153031000	5.144862000	1.675838000
1	0.010428000	4.578964000	2.902976000
1	1.131261000	3.442350000	2.121007000
6	-2.867399000	4.002841000	0.176819000
6	-4.313849000	4.272646000	0.455865000
1	-4.749878000	3.455185000	1.050307000
1	-4.449876000	5.193677000	1.033775000
1	-4.893942000	4.358195000	-0.469270000
6	4.562789000	0.656872000	-1.750347000
6	3.871775000	0.956798000	-3.045002000
1	2.787988000	0.802322000	-2.957574000
1	4.025898000	1.995036000	-3.368426000
1	4.241666000	0.303273000	-3.840744000
6	4.735894000	0.959504000	0.674433000
6	4.227664000	1.578704000	1.940326000
1	3.261602000	1.134729000	2.222870000
1	4.926513000	1.412728000	2.765828000
1	4.064364000	2.659253000	1.833897000
6	6.222713000	-0.586057000	-0.473020000
6	7.365282000	-1.554819000	-0.426681000
1	7.314120000	-2.193151000	0.463160000
1	7.379481000	-2.202424000	-1.310225000
1	8.329285000	-1.031302000	-0.391090000
7	1.196837000	3.174610000	-0.551177000
7	3.127465000	2.260113000	-0.615024000

Method: M06-2X/6-31G(d,p) Key word: opt freq pop=full
imaginary frequencies: 0 Energy: -2899.980783 Hartree

Int III'



6	-2.607792000	1.372219000	2.636277000
6	-3.228217000	0.442044000	3.511208000
6	-3.753109000	-0.795457000	2.972266000
6	-3.784996000	-0.989352000	1.565583000
6	-3.172648000	-0.019551000	0.681853000
6	-2.516222000	1.078324000	1.222822000
6	-4.208370000	-1.834022000	3.810704000
6	-4.685781000	-3.019387000	3.299871000
6	-4.737921000	-3.206123000	1.912599000
6	-4.300602000	-2.210542000	1.070482000
6	-2.144129000	2.595032000	3.172998000
6	-2.257250000	2.882550000	4.513037000
6	-2.841971000	1.950639000	5.379548000
6	-3.319481000	0.759970000	4.880929000
6	-3.121601000	-0.217399000	-0.794036000
6	-1.932144000	0.039610000	-1.398114000
28	-0.489941000	0.396671000	-0.127506000
6	0.338136000	1.240310000	1.384016000
6	-0.371639000	2.269311000	0.664639000
6	-1.719076000	1.978763000	0.311532000
8	0.990257000	1.059836000	2.371412000
15	0.590967000	-1.525329000	-0.038802000
15	4.605647000	0.362064000	-0.789701000
6	2.344941000	-1.359016000	-0.621670000
6	3.168692000	-0.353599000	0.172209000
6	0.494224000	3.307921000	0.053369000
6	-2.473815000	2.873929000	-0.602939000
6	-1.704954000	0.279639000	-2.825123000

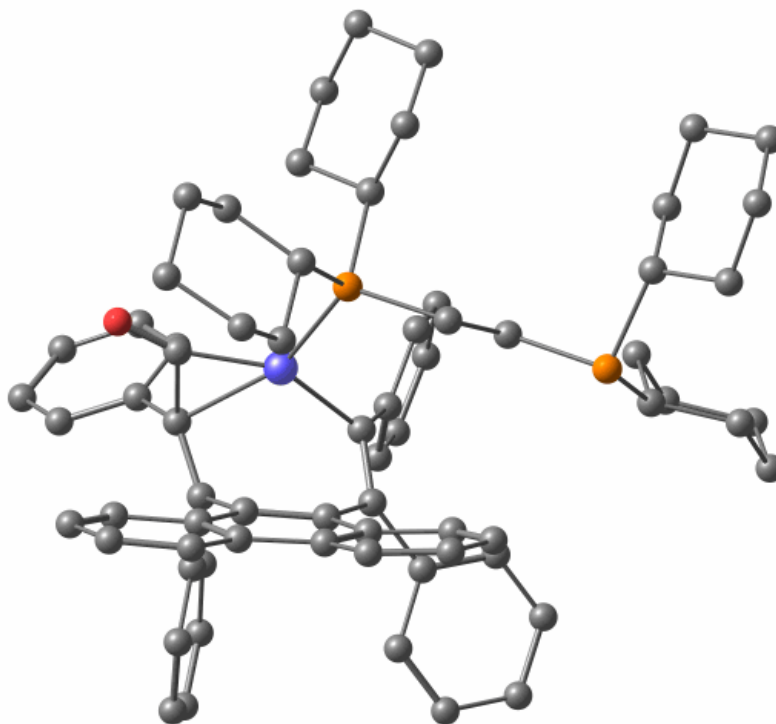
6	-2.665967000	0.885759000	-3.657246000
6	-2.369154000	1.222552000	-4.969788000
6	-1.107457000	0.965751000	-5.500665000
6	-0.134464000	0.384611000	-4.693992000
6	-0.429985000	0.063250000	-3.375550000
6	0.295813000	4.651949000	0.381660000
6	1.132280000	5.631638000	-0.137132000
6	2.185006000	5.283825000	-0.979298000
6	2.387519000	3.949362000	-1.314790000
6	1.543310000	2.968290000	-0.806537000
6	-1.946615000	3.351902000	-1.809018000
6	-2.684988000	4.209419000	-2.612987000
6	-3.964130000	4.605242000	-2.235477000
6	-4.498995000	4.139627000	-1.039598000
6	-3.759141000	3.285236000	-0.231231000
6	-4.378442000	-0.560832000	-1.502004000
6	-4.396378000	-1.529802000	-2.514175000
6	-5.570210000	-1.842568000	-3.184912000
6	-6.758762000	-1.195504000	-2.856040000
6	-6.758745000	-0.236407000	-1.848914000
6	-5.582622000	0.074268000	-1.175829000
1	-4.158825000	-1.714412000	4.889419000
1	-5.017819000	-3.806093000	3.973154000
1	-5.117059000	-4.137295000	1.497754000
1	-4.341747000	-2.373581000	-0.001670000
1	-1.695424000	3.326798000	2.507251000
1	-1.894995000	3.833726000	4.895050000
1	-2.932325000	2.170151000	6.440533000
1	-3.801192000	0.066124000	5.563955000
1	2.277523000	-1.059927000	-1.681464000
1	2.830976000	-2.344565000	-0.610925000
1	3.509684000	-0.796865000	1.121212000
1	2.546373000	0.505123000	0.447638000
1	-3.646351000	1.125756000	-3.249777000
1	-3.128980000	1.704261000	-5.581952000
1	-0.880119000	1.231976000	-6.530391000
1	0.862839000	0.198136000	-5.086480000
1	0.348078000	-0.343224000	-2.729545000
1	-0.530950000	4.927215000	1.034844000
1	0.961437000	6.674455000	0.119844000
1	2.839979000	6.053650000	-1.380053000
1	3.198962000	3.661037000	-1.979801000
1	1.674386000	1.927221000	-1.106457000
1	-0.963346000	3.023628000	-2.138903000
1	-2.261737000	4.551268000	-3.554888000
1	-4.542811000	5.270364000	-2.872180000
1	-5.496650000	4.442957000	-0.730232000
1	-4.179667000	2.929848000	0.708802000
1	-3.464929000	-2.033968000	-2.770896000
1	-5.559474000	-2.599700000	-3.965983000
1	-7.679813000	-1.441859000	-3.379075000
1	-7.681635000	0.275000000	-1.583657000
1	-5.587818000	0.827292000	-0.388705000
6	-0.074082000	-2.912150000	-1.099092000
6	0.882808000	-4.057316000	-1.447069000
6	-1.389087000	-3.449355000	-0.529757000
1	-0.321696000	-2.392029000	-2.042232000
6	0.212129000	-5.060295000	-2.384297000
1	1.197558000	-4.576958000	-0.529253000
1	1.795998000	-3.673496000	-1.920582000

6	-2.039578000	-4.447603000	-1.478669000
1	-1.199449000	-3.953169000	0.432120000
1	-2.070540000	-2.614913000	-0.323383000
6	-1.089886000	-5.593690000	-1.799934000
1	0.905085000	-5.882154000	-2.606042000
1	-0.001580000	-4.564064000	-3.344704000
1	-2.977315000	-4.819679000	-1.043189000
1	-2.312563000	-3.934147000	-2.415109000
1	-1.557280000	-6.305444000	-2.492171000
1	-0.870391000	-6.152662000	-0.875386000
6	0.768495000	-2.088397000	1.723133000
6	-0.538910000	-1.996693000	2.516865000
6	1.457505000	-3.432120000	1.960061000
1	1.420423000	-1.295209000	2.128817000
6	-0.278175000	-2.205839000	4.003214000
1	-1.260127000	-2.752414000	2.166591000
1	-1.012915000	-1.021315000	2.350100000
6	1.712975000	-3.641061000	3.451503000
1	0.815484000	-4.248029000	1.589231000
1	2.403420000	-3.495980000	1.401784000
6	0.421320000	-3.535772000	4.255985000
1	-1.227109000	-2.154125000	4.554806000
1	0.347901000	-1.379472000	4.376242000
1	2.195226000	-4.613232000	3.618049000
1	2.422558000	-2.874016000	3.801527000
1	0.626313000	-3.670803000	5.325701000
1	-0.252324000	-4.356976000	3.960362000
6	5.559796000	1.082549000	0.654986000
6	6.924525000	1.614919000	0.212782000
6	4.741882000	2.207108000	1.304293000
1	5.717957000	0.291215000	1.410026000
6	7.676062000	2.278037000	1.362239000
1	6.773984000	2.346353000	-0.599736000
1	7.537063000	0.806319000	-0.207234000
6	5.500159000	2.869394000	2.449894000
1	4.502603000	2.966766000	0.539341000
1	3.780025000	1.828757000	1.674626000
6	6.853656000	3.394784000	1.991079000
1	8.644422000	2.657256000	1.010361000
1	7.897370000	1.517918000	2.129263000
1	4.893757000	3.676785000	2.879388000
1	5.652056000	2.131871000	3.254602000
1	7.397229000	3.851230000	2.828400000
1	6.698734000	4.191957000	1.245889000
6	5.511913000	-1.224921000	-1.228483000
6	6.615763000	-1.008173000	-2.267146000
6	6.011589000	-2.087924000	-0.072496000
1	4.721022000	-1.796771000	-1.749450000
6	7.161258000	-2.341425000	-2.770611000
1	7.442784000	-0.432376000	-1.823102000
1	6.232650000	-0.403336000	-3.100312000
6	6.553787000	-3.421146000	-0.581477000
1	6.816177000	-1.556921000	0.462334000
1	5.211427000	-2.260182000	0.662253000
6	7.652481000	-3.207634000	-1.615902000
1	7.966109000	-2.174592000	-3.498173000
1	6.361040000	-2.876462000	-3.307721000
1	6.923537000	-4.028339000	0.255086000
1	5.728318000	-3.990736000	-1.040434000
1	8.025037000	-4.170781000	-1.987723000

1 8.507337000 -2.708624000 -1.130808000

Method: M06-2X/6-31G(d,p) Key word: opt freq pop=full
imaginary frequencies: 0 Energy: -3599.236983 Hartree

TS II'



6	-3.292685000	-0.944684000	-2.169842000
6	-2.661000000	-1.361048000	-3.369553000
6	-1.363943000	-0.812741000	-3.713585000
6	-0.767007000	0.157306000	-2.864482000
6	-1.437175000	0.596080000	-1.660113000
6	-2.651443000	0.032674000	-1.324876000
6	-0.638231000	-1.258618000	-4.837105000
6	0.626954000	-0.788272000	-5.111777000
6	1.222187000	0.157487000	-4.266534000
6	0.531826000	0.620702000	-3.170153000
6	-4.535945000	-1.511787000	-1.812263000
6	-5.133768000	-2.473142000	-2.594626000
6	-4.510219000	-2.890245000	-3.777698000
6	-3.306346000	-2.336664000	-4.155784000
6	-0.774646000	1.573435000	-0.731132000
6	-0.516136000	1.109571000	0.518180000
28	-1.236098000	-0.707952000	0.754367000
6	-2.660773000	-1.752322000	1.021511000
6	-3.256037000	-0.230491000	1.067745000
6	-3.351618000	0.494781000	-0.078107000
8	-3.334388000	-2.708445000	1.242020000
6	-3.838070000	0.111078000	2.377781000
6	-4.049775000	1.791740000	-0.206607000

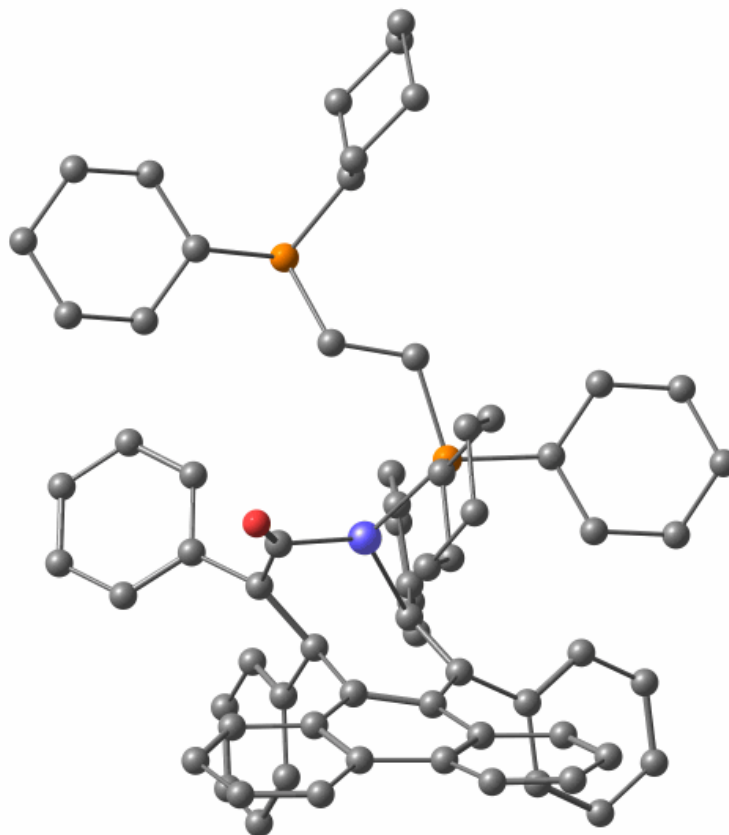
6	-0.106793000	1.931156000	1.663847000
6	-0.717215000	3.169243000	1.943018000
6	-0.409399000	3.881489000	3.093859000
6	0.531887000	3.396819000	3.998742000
6	1.152379000	2.178952000	3.741447000
6	0.821549000	1.453264000	2.603023000
6	-5.221875000	0.093074000	2.569351000
6	-5.760764000	0.414135000	3.808525000
6	-4.924692000	0.748083000	4.870227000
6	-3.544777000	0.751928000	4.690569000
6	-3.001733000	0.424003000	3.454054000
6	-4.023456000	2.757462000	0.807693000
6	-4.612067000	3.999752000	0.612707000
6	-5.264978000	4.290295000	-0.580932000
6	-5.316334000	3.332755000	-1.588493000
6	-4.699152000	2.102380000	-1.410164000
6	-0.504820000	2.931979000	-1.262216000
6	0.648005000	3.643381000	-0.899731000
6	0.906246000	4.905937000	-1.413859000
6	0.017111000	5.494132000	-2.310214000
6	-1.129954000	4.802154000	-2.682463000
6	-1.385193000	3.535594000	-2.168822000
1	-1.067415000	-2.007662000	-5.496729000
1	1.166010000	-1.161608000	-5.979236000
1	2.233030000	0.511795000	-4.452766000
1	1.004521000	1.342075000	-2.507490000
1	-5.018746000	-1.184254000	-0.893678000
1	-6.085360000	-2.904023000	-2.294197000
1	-4.976981000	-3.647182000	-4.403180000
1	-2.851375000	-2.671589000	-5.083577000
1	-1.446730000	3.567964000	1.239950000
1	-0.905497000	4.831459000	3.283472000
1	0.774904000	3.960908000	4.896119000
1	1.888771000	1.781542000	4.437861000
1	1.292101000	0.487894000	2.425691000
1	-5.869449000	-0.162247000	1.731173000
1	-6.839424000	0.404214000	3.946807000
1	-5.349705000	1.002682000	5.838259000
1	-2.884981000	1.017109000	5.513570000
1	-1.922308000	0.450849000	3.297270000
1	-3.504710000	2.547596000	1.739672000
1	-4.556539000	4.746843000	1.400837000
1	-5.728424000	5.263119000	-0.726928000
1	-5.825813000	3.549280000	-2.524384000
1	-4.719577000	1.368626000	-2.213760000
1	1.346442000	3.191667000	-0.195662000
1	1.811865000	5.433469000	-1.116499000
1	0.219517000	6.482181000	-2.716920000
1	-1.834607000	5.249474000	-3.380493000
1	-2.291164000	3.006466000	-2.463912000
15	3.886425000	0.329964000	-1.340144000
15	0.463727000	-2.053631000	0.485312000
6	2.532394000	-0.215732000	-0.180301000
6	1.831629000	-1.483494000	-0.635877000
1	1.797804000	0.600750000	-0.145412000
1	2.933638000	-0.328134000	0.837224000
1	2.537956000	-2.322528000	-0.740635000
1	1.388975000	-1.322311000	-1.629147000
6	4.161701000	2.065692000	-0.674995000
6	4.121061000	2.328471000	0.833204000

6	5.397547000	2.721486000	-1.293956000
1	3.283060000	2.579513000	-1.113759000
6	4.131289000	3.827557000	1.119525000
1	4.997983000	1.869920000	1.314583000
1	3.235340000	1.876277000	1.297727000
6	5.424359000	4.220204000	-1.005206000
1	6.306162000	2.258787000	-0.871978000
1	5.427796000	2.535416000	-2.377319000
6	5.347235000	4.499195000	0.492220000
1	4.102374000	4.002901000	2.203148000
1	3.208908000	4.277992000	0.714804000
1	6.326474000	4.675131000	-1.435089000
1	4.565432000	4.694021000	-1.508004000
1	5.334385000	5.580415000	0.681146000
1	6.258413000	4.109216000	0.975322000
6	5.284253000	-0.778071000	-0.745695000
6	6.452734000	-0.764251000	-1.736257000
6	5.806135000	-0.641743000	0.684150000
1	4.812674000	-1.778751000	-0.827708000
6	7.469129000	-1.854879000	-1.412201000
1	6.951163000	0.219032000	-1.695127000
1	6.076012000	-0.876018000	-2.761905000
6	6.803375000	-1.751244000	1.010498000
1	6.315669000	0.329165000	0.791560000
1	4.981881000	-0.641986000	1.411803000
6	7.966106000	-1.743944000	0.024473000
1	8.311035000	-1.814040000	-2.115468000
1	6.992481000	-2.838668000	-1.553081000
1	7.169489000	-1.643991000	2.040118000
1	6.289438000	-2.725813000	0.961285000
1	8.671220000	-2.553605000	0.252433000
1	8.525486000	-0.801328000	0.140301000
6	0.096963000	-3.712522000	-0.279532000
6	-0.692649000	-4.658471000	0.629734000
6	-0.643897000	-3.474597000	-1.599616000
1	1.075824000	-4.173947000	-0.506581000
6	-1.072276000	-5.946491000	-0.097957000
1	-1.609410000	-4.159303000	0.972189000
1	-0.108407000	-4.902459000	1.528396000
6	-1.015697000	-4.773109000	-2.301319000
1	-1.569860000	-2.916693000	-1.382918000
1	-0.049300000	-2.840236000	-2.272121000
6	-1.843395000	-5.657517000	-1.379948000
1	-1.659481000	-6.586481000	0.572726000
1	-0.158120000	-6.510301000	-0.348348000
1	-1.565503000	-4.540799000	-3.224524000
1	-0.100579000	-5.309212000	-2.601820000
1	-2.122260000	-6.592952000	-1.881669000
1	-2.782123000	-5.133978000	-1.132546000
6	1.342376000	-2.348370000	2.095462000
6	0.372082000	-2.508409000	3.267727000
6	2.408565000	-3.445270000	2.079740000
1	1.874490000	-1.394786000	2.258985000
6	1.128522000	-2.563515000	4.589656000
1	-0.220416000	-3.427152000	3.142877000
1	-0.350022000	-1.678469000	3.262907000
6	3.150432000	-3.487494000	3.413297000
1	1.938151000	-4.424864000	1.899602000
1	3.120393000	-3.283064000	1.255802000
6	2.183126000	-3.665539000	4.577538000

1	0.426493000	-2.707680000	5.420303000
1	1.619938000	-1.590632000	4.760375000
1	3.898462000	-4.290592000	3.402762000
1	3.706492000	-2.545143000	3.546455000
1	2.728985000	-3.688493000	5.529146000
1	1.680864000	-4.642051000	4.480881000

Method: M06-2X/6-31G(d,p) Key word: opt freq pop=full
 imaginary frequencies: -59.4549 cm^{-1} Energy: $-3599.224711 \text{ Hartree}$

TS III'



6	-2.672225000	1.156630000	2.621726000
6	-3.286824000	0.190916000	3.465121000
6	-3.785276000	-1.048981000	2.897474000
6	-3.831740000	-1.212050000	1.486880000
6	-3.261760000	-0.181394000	0.652067000
6	-2.606596000	0.898820000	1.207916000
6	-4.195353000	-2.124159000	3.711618000
6	-4.637665000	-3.312071000	3.173445000
6	-4.696617000	-3.467125000	1.783177000
6	-4.304492000	-2.435295000	0.960957000
6	-2.209550000	2.362444000	3.193103000
6	-2.335518000	2.611435000	4.539608000
6	-2.931455000	1.656406000	5.373200000
6	-3.396056000	0.474645000	4.840561000

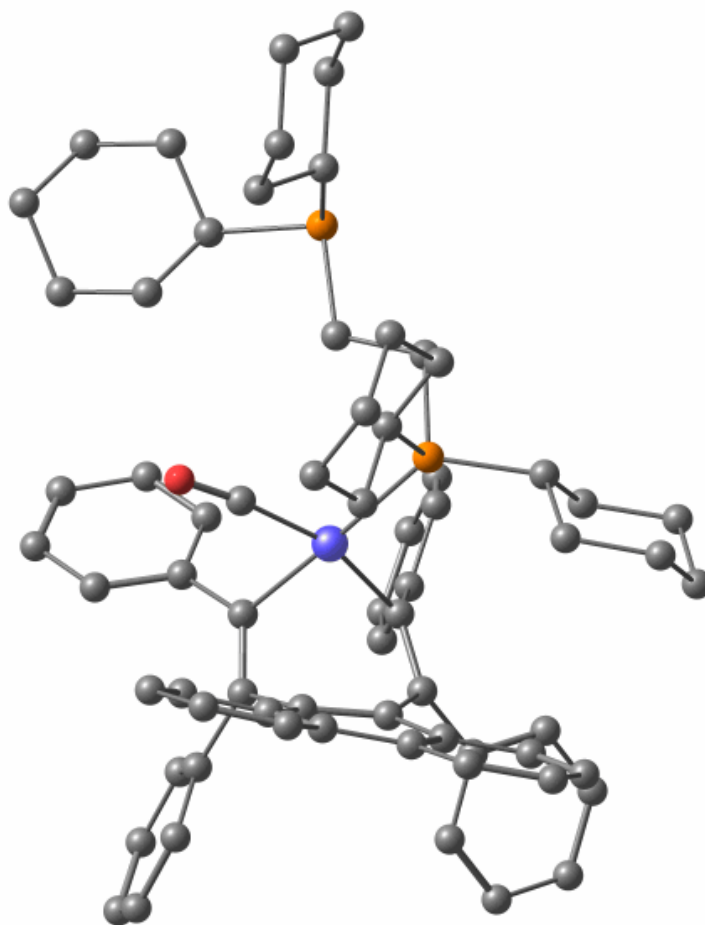
6	-3.142691000	-0.199723000	-0.806843000
6	-2.080924000	0.535750000	-1.245316000
28	-0.317978000	0.335964000	-0.165763000
6	0.293417000	1.203023000	1.379995000
6	-0.484136000	2.140543000	0.640346000
6	-1.865601000	1.753181000	0.207958000
8	0.940383000	1.012560000	2.368752000
15	0.632114000	-1.619047000	-0.171674000
15	4.633444000	0.299252000	-0.865893000
6	2.392389000	-1.446521000	-0.734759000
6	3.175714000	-0.410762000	0.061698000
6	0.295121000	3.328838000	0.195279000
6	-2.670837000	2.884080000	-0.400207000
6	-1.826386000	0.952491000	-2.630834000
6	-2.838522000	1.497187000	-3.437223000
6	-2.554352000	1.972417000	-4.708673000
6	-1.254139000	1.916988000	-5.205650000
6	-0.238133000	1.378607000	-4.423013000
6	-0.524981000	0.901775000	-3.149110000
6	-0.037251000	4.614395000	0.639836000
6	0.720108000	5.714938000	0.261202000
6	1.836124000	5.554108000	-0.556139000
6	2.185221000	4.282772000	-0.996366000
6	1.418863000	3.182688000	-0.625963000
6	-2.169996000	3.685647000	-1.433693000
6	-2.933525000	4.711041000	-1.975376000
6	-4.219498000	4.956088000	-1.507216000
6	-4.732657000	4.163641000	-0.487690000
6	-3.966476000	3.141268000	0.061293000
6	-4.154500000	-0.807748000	-1.692186000
6	-3.783443000	-1.585693000	-2.793500000
6	-4.745214000	-2.140993000	-3.627587000
6	-6.096515000	-1.914144000	-3.384456000
6	-6.478381000	-1.127978000	-2.301219000
6	-5.517420000	-0.582612000	-1.460043000
1	-4.132414000	-2.033688000	4.792570000
1	-4.931983000	-4.128020000	3.829116000
1	-5.040976000	-4.403034000	1.349127000
1	-4.340672000	-2.576905000	-0.114892000
1	-1.742511000	3.100648000	2.548484000
1	-1.973792000	3.549632000	4.952740000
1	-3.036476000	1.848850000	6.438145000
1	-3.882441000	-0.237640000	5.501049000
1	2.330312000	-1.154769000	-1.797603000
1	2.900794000	-2.420562000	-0.709109000
1	3.486161000	-0.822689000	1.035411000
1	2.525887000	0.445282000	0.286449000
1	-3.847984000	1.578243000	-3.035649000
1	-3.349981000	2.404442000	-5.311427000
1	-1.033621000	2.297399000	-6.200419000
1	0.780574000	1.334531000	-4.801148000
1	0.271748000	0.493630000	-2.521070000
1	-0.915737000	4.753231000	1.267634000
1	0.438466000	6.706040000	0.609672000
1	2.428041000	6.418038000	-0.849168000
1	3.052476000	4.137776000	-1.638235000
1	1.680821000	2.187814000	-0.989922000
1	-1.178746000	3.499428000	-1.838642000
1	-2.518266000	5.310710000	-2.782006000
1	-4.817132000	5.757872000	-1.934550000

1	-5.735208000	4.342439000	-0.105606000
1	-4.380700000	2.538988000	0.866815000
1	-2.724675000	-1.755857000	-2.984665000
1	-4.436464000	-2.754506000	-4.471363000
1	-6.849867000	-2.347768000	-4.037734000
1	-7.532181000	-0.939704000	-2.108875000
1	-5.816088000	0.027991000	-0.608836000
6	-0.011115000	-2.975188000	-1.288365000
6	0.928166000	-4.142117000	-1.606967000
6	-1.363903000	-3.483304000	-0.787658000
1	-0.192326000	-2.424607000	-2.233206000
6	0.274817000	-5.128369000	-2.572981000
1	1.191005000	-4.670139000	-0.677534000
1	1.869814000	-3.777340000	-2.037133000
6	-1.997795000	-4.472838000	-1.757060000
1	-1.226324000	-3.988295000	0.182108000
1	-2.033675000	-2.633116000	-0.599987000
6	-1.057428000	-5.637659000	-2.037170000
1	0.959002000	-5.962879000	-2.773690000
1	0.104525000	-4.625009000	-3.538632000
1	-2.958552000	-4.824026000	-1.354969000
1	-2.229320000	-3.962731000	-2.705946000
1	-1.512064000	-6.343267000	-2.744137000
1	-0.882580000	-6.197207000	-1.103608000
6	0.801603000	-2.225315000	1.580098000
6	-0.513948000	-2.195473000	2.365870000
6	1.542615000	-3.541322000	1.814325000
1	1.417765000	-1.411350000	2.003350000
6	-0.252264000	-2.397894000	3.853895000
1	-1.196651000	-2.985359000	2.011667000
1	-1.035439000	-1.243370000	2.200077000
6	1.807066000	-3.738910000	3.305773000
1	0.931683000	-4.382269000	1.446309000
1	2.489511000	-3.570129000	1.254104000
6	0.511079000	-3.692462000	4.108565000
1	-1.205445000	-2.394927000	4.401015000
1	0.329945000	-1.542969000	4.233299000
1	2.332399000	-4.688157000	3.474614000
1	2.480753000	-2.939813000	3.655231000
1	0.720648000	-3.815263000	5.178980000
1	-0.121645000	-4.546206000	3.814376000
6	5.483411000	1.155913000	0.573873000
6	6.861749000	1.682401000	0.167416000
6	4.597418000	2.304594000	1.069126000
1	5.611087000	0.438222000	1.404455000
6	7.518817000	2.491746000	1.281137000
1	6.750101000	2.314668000	-0.730520000
1	7.519046000	0.850335000	-0.119372000
6	5.266220000	3.111416000	2.176626000
1	4.372134000	2.975512000	0.222141000
1	3.631210000	1.924731000	1.426918000
6	6.625179000	3.637156000	1.735129000
1	8.495131000	2.866833000	0.946930000
1	7.716145000	1.826762000	2.137867000
1	4.608670000	3.935542000	2.481584000
1	5.396787000	2.471153000	3.064004000
1	7.104797000	4.203417000	2.544030000
1	6.486612000	4.340871000	0.898282000
6	5.639023000	-1.262348000	-1.154052000
6	6.747006000	-1.043431000	-2.188689000

6	6.171338000	-1.977788000	0.085685000
1	4.902067000	-1.933286000	-1.634115000
6	7.437819000	-2.355498000	-2.546679000
1	7.498020000	-0.341703000	-1.792773000
1	6.327976000	-0.566691000	-3.085246000
6	6.866242000	-3.285663000	-0.283711000
1	6.892377000	-1.324232000	0.603635000
1	5.357978000	-2.169013000	0.801198000
6	7.975892000	-3.051025000	-1.301398000
1	8.244315000	-2.177235000	-3.269769000
1	6.712954000	-3.019834000	-3.045013000
1	7.263701000	-3.772718000	0.616435000
1	6.123968000	-3.979304000	-0.711973000
1	8.461711000	-3.998701000	-1.567185000
1	8.754203000	-2.418092000	-0.844349000

Method: M06-2X/6-31G(d,p) Key word: opt freq pop=full
 imaginary frequencies: $-209.3214 \text{ cm}^{-1}$ Energy: $-3599.219381 \text{ Hartree}$

Int IV'



6	2.445711000	-0.426299000	-2.749750000
---	-------------	--------------	--------------

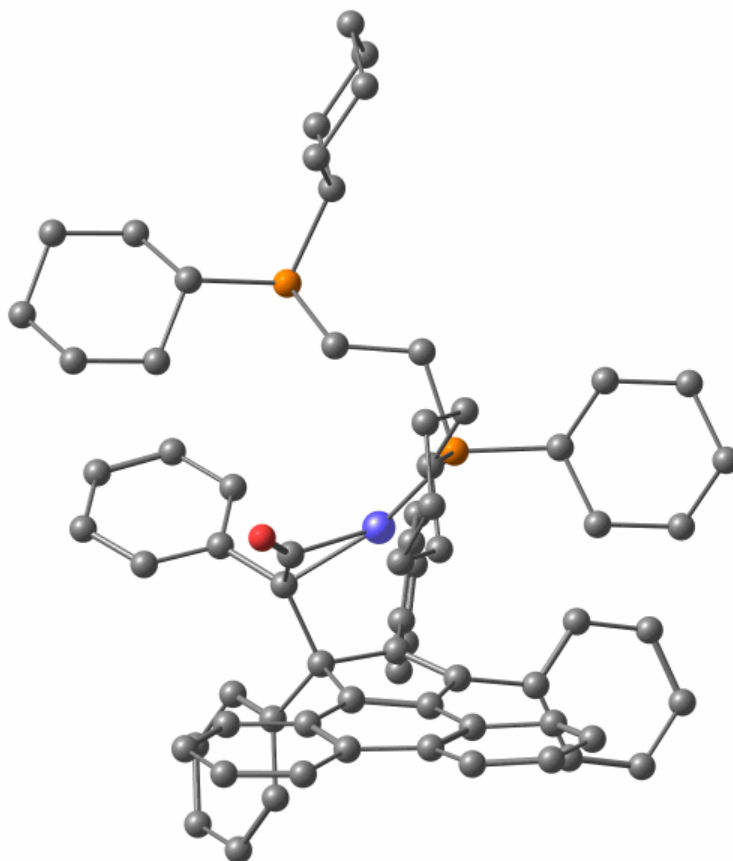
6	2.871657000	-1.770397000	-2.902150000
6	3.503972000	-2.440545000	-1.784077000
6	3.597929000	-1.773424000	-0.533031000
6	3.056070000	-0.439588000	-0.376103000
6	2.592626000	0.244920000	-1.478869000
6	4.002644000	-3.755134000	-1.888817000
6	4.590313000	-4.394052000	-0.820086000
6	4.700831000	-3.731280000	0.408852000
6	4.204059000	-2.454893000	0.547494000
6	1.786431000	0.208036000	-3.827323000
6	1.555485000	-0.448700000	-5.014635000
6	1.989786000	-1.771843000	-5.170998000
6	2.631886000	-2.413114000	-4.133930000
6	2.882873000	0.172777000	0.970739000
6	1.629587000	0.581425000	1.289202000
28	0.226184000	0.235943000	-0.011798000
6	-0.834831000	0.355477000	-1.459231000
6	0.964706000	1.876166000	-0.743166000
6	2.144050000	1.671008000	-1.362112000
8	-1.428827000	0.526680000	-2.427170000
6	0.139128000	3.088663000	-0.710689000
6	3.100735000	2.719623000	-1.787595000
6	1.307541000	1.478629000	2.408893000
6	2.043303000	2.662491000	2.587990000
6	1.672691000	3.597728000	3.543848000
6	0.564855000	3.373221000	4.357809000
6	-0.173077000	2.204574000	4.199485000
6	0.189112000	1.277406000	3.229012000
6	-0.042090000	3.835547000	-1.887245000
6	-0.890081000	4.933717000	-1.915703000
6	-1.585422000	5.313307000	-0.770781000
6	-1.438194000	4.568813000	0.395637000
6	-0.597051000	3.462727000	0.424005000
6	3.153144000	3.947028000	-1.106842000
6	4.082773000	4.917700000	-1.449191000
6	4.998731000	4.687372000	-2.471865000
6	4.977741000	3.468752000	-3.139735000
6	4.046391000	2.495239000	-2.798347000
6	4.079718000	0.377501000	1.819221000
6	4.060442000	0.137774000	3.200483000
6	5.200269000	0.323141000	3.971548000
6	6.387045000	0.748171000	3.380300000
6	6.422553000	0.982549000	2.009625000
6	5.283437000	0.793855000	1.236824000
1	3.940736000	-4.280213000	-2.838164000
1	4.975590000	-5.404347000	-0.936066000
1	5.171976000	-4.223244000	1.257520000
1	4.286879000	-1.954460000	1.507939000
1	1.436951000	1.230191000	-3.693961000
1	1.036283000	0.057562000	-5.824630000
1	1.814480000	-2.297441000	-6.106831000
1	2.943166000	-3.444522000	-4.276090000
1	2.900269000	2.844878000	1.941133000
1	2.250478000	4.513023000	3.651850000
1	0.275035000	4.107716000	5.105429000
1	-1.044301000	2.018735000	4.824302000
1	-0.417729000	0.386927000	3.078527000
1	0.499183000	3.539123000	-2.784897000
1	-1.009999000	5.496232000	-2.839089000
1	-2.249243000	6.174960000	-0.792193000

1	-1.986165000	4.846878000	1.294475000
1	-0.492014000	2.889226000	1.341951000
1	2.459947000	4.127360000	-0.287547000
1	4.101807000	5.857107000	-0.900962000
1	5.730878000	5.447066000	-2.735195000
1	5.695268000	3.268142000	-3.932410000
1	4.052567000	1.546730000	-3.330129000
1	3.135377000	-0.203104000	3.666261000
1	5.163965000	0.127619000	5.041150000
1	7.279914000	0.890381000	3.984541000
1	7.344578000	1.314022000	1.536912000
1	5.315792000	0.973448000	0.162459000
15	-4.611824000	0.376044000	1.715614000
15	-0.710080000	-1.699378000	0.780743000
6	-2.899194000	0.018619000	1.078411000
6	-2.254361000	-1.218040000	1.690583000
1	-2.279070000	0.902348000	1.291395000
1	-2.938617000	-0.069591000	-0.014868000
1	-2.937522000	-2.079895000	1.687727000
1	-2.000500000	-1.037319000	2.743577000
6	-4.959933000	1.976111000	0.775687000
6	-4.331426000	2.198151000	-0.604188000
6	-6.468131000	2.244266000	0.738508000
1	-4.512537000	2.730977000	1.451364000
6	-4.681908000	3.580467000	-1.151686000
1	-4.682445000	1.428139000	-1.309197000
1	-3.235910000	2.112925000	-0.559028000
6	-6.791173000	3.629350000	0.188847000
1	-6.947475000	1.494576000	0.086944000
1	-6.903771000	2.109869000	1.739641000
6	-6.185354000	3.812186000	-1.195989000
1	-4.227600000	3.712179000	-2.142740000
1	-4.218100000	4.341689000	-0.503339000
1	-7.878149000	3.781309000	0.164192000
1	-6.381956000	4.394156000	0.868293000
1	-6.411064000	4.811730000	-1.589343000
1	-6.646650000	3.090418000	-1.890449000
6	-5.538399000	-1.024319000	0.857926000
6	-6.971272000	-1.153590000	1.386672000
6	-5.511767000	-1.138495000	-0.666263000
1	-4.993384000	-1.905688000	1.251692000
6	-7.620766000	-2.451722000	0.918206000
1	-7.574561000	-0.304030000	1.029927000
1	-6.970520000	-1.092056000	2.483469000
6	-6.158437000	-2.444593000	-1.123497000
1	-6.064296000	-0.294048000	-1.110551000
1	-4.481629000	-1.073771000	-1.051576000
6	-7.584647000	-2.566998000	-0.600718000
1	-8.652914000	-2.515982000	1.286176000
1	-7.078736000	-3.304959000	1.357786000
1	-6.137843000	-2.516290000	-2.219388000
1	-5.560370000	-3.292354000	-0.745331000
1	-8.034467000	-3.512879000	-0.928585000
1	-8.196818000	-1.761593000	-1.038331000
6	0.032450000	-2.974204000	1.920600000
6	1.043533000	-3.878445000	1.212185000
6	0.683170000	-2.284756000	3.123574000
1	-0.810554000	-3.594835000	2.279702000
6	1.701247000	-4.860579000	2.176798000
1	1.819087000	-3.251362000	0.744078000

1	0.561243000	-4.438994000	0.401021000
6	1.314825000	-3.286958000	4.081495000
1	1.458821000	-1.598715000	2.745632000
1	-0.047418000	-1.665345000	3.661580000
6	2.340368000	-4.151082000	3.362196000
1	2.445679000	-5.457036000	1.633314000
1	0.940385000	-5.567719000	2.547242000
1	1.777228000	-2.752508000	4.921743000
1	0.530375000	-3.931099000	4.511799000
1	2.787498000	-4.878604000	4.051613000
1	3.161119000	-3.509139000	3.001480000
6	-1.414747000	-2.626639000	-0.678102000
6	-0.381512000	-2.857091000	-1.788301000
6	-2.199682000	-3.904791000	-0.381207000
1	-2.146367000	-1.896220000	-1.074101000
6	-1.050779000	-3.384156000	-3.051350000
1	0.379866000	-3.578192000	-1.452590000
1	0.166696000	-1.929365000	-2.007713000
6	-2.862061000	-4.425103000	-1.655487000
1	-1.525210000	-4.678184000	0.019292000
1	-2.966413000	-3.726215000	0.387642000
6	-1.840282000	-4.655737000	-2.762610000
1	-0.293152000	-3.556924000	-3.826468000
1	-1.729935000	-2.609729000	-3.445229000
1	-3.420762000	-5.345611000	-1.440901000
1	-3.603412000	-3.683403000	-1.998797000
1	-2.336829000	-5.019065000	-3.671154000
1	-1.142146000	-5.448930000	-2.448458000

Method: M06-2X/6-31G(d,p) Key word: opt freq pop=full
imaginary frequencies: 0 Energy: -3599.232579 Hartree

Int V'



6	2.799525000	-1.248780000	2.435204000
6	3.396355000	-0.252777000	3.255608000
6	3.886980000	0.975304000	2.653036000
6	3.873692000	1.134164000	1.237271000
6	3.323833000	0.069698000	0.438766000
6	2.740802000	-1.026082000	1.026851000
6	4.343777000	2.053348000	3.438648000
6	4.759600000	3.238940000	2.874048000
6	4.739202000	3.394051000	1.482760000
6	4.307173000	2.359106000	0.684052000
6	2.307462000	-2.432338000	3.025417000
6	2.392325000	-2.636294000	4.382106000
6	2.979520000	-1.657968000	5.196801000
6	3.469436000	-0.496344000	4.641541000
6	3.118355000	-0.012305000	-1.016510000
6	2.330451000	-1.085925000	-1.290660000
28	0.139276000	-0.005653000	-0.274673000
6	-0.013306000	-0.996316000	1.273011000
6	0.503812000	-1.861725000	0.280727000
6	2.036499000	-1.888907000	-0.007965000
8	-0.516717000	-0.828033000	2.345587000
15	-0.689939000	2.023563000	-0.090075000
15	-4.384465000	-0.219721000	-0.712639000
6	-2.490629000	1.895362000	-0.512350000
6	-3.140432000	0.754426000	0.271537000
6	-0.488692000	-2.942028000	-0.044226000
6	2.682826000	-3.266771000	-0.191435000

6	1.945479000	-1.516734000	-2.648983000
6	2.801894000	-2.320827000	-3.407843000
6	2.455186000	-2.701098000	-4.698561000
6	1.249534000	-2.282509000	-5.253106000
6	0.394090000	-1.471943000	-4.514600000
6	0.746098000	-1.089202000	-3.225420000
6	-0.669966000	-3.995239000	0.863210000
6	-1.591580000	-5.005405000	0.616954000
6	-2.368913000	-4.974952000	-0.538018000
6	-2.230912000	-3.916625000	-1.429859000
6	-1.305207000	-2.908079000	-1.179726000
6	2.090473000	-4.258278000	-0.982541000
6	2.746610000	-5.457023000	-1.238913000
6	4.018632000	-5.687656000	-0.729480000
6	4.630424000	-4.703330000	0.037264000
6	3.969972000	-3.509404000	0.302459000
6	3.746553000	0.830650000	-2.052990000
6	2.986974000	1.534386000	-2.990999000
6	3.605407000	2.290389000	-3.981374000
6	4.992315000	2.355736000	-4.048749000
6	5.759801000	1.650272000	-3.126103000
6	5.142734000	0.891769000	-2.140136000
1	4.350154000	1.965062000	4.521658000
1	5.094951000	4.053527000	3.511514000
1	5.056628000	4.330795000	1.030080000
1	4.281103000	2.499156000	-0.392519000
1	1.871565000	-3.191768000	2.381420000
1	2.010761000	-3.555284000	4.819951000
1	3.054846000	-1.816318000	6.269857000
1	3.932997000	0.235330000	5.297344000
1	-2.515584000	1.695334000	-1.596575000
1	-3.027237000	2.841209000	-0.350328000
1	-3.564982000	1.123667000	1.218592000
1	-2.371805000	0.017782000	0.542246000
1	3.745647000	-2.647106000	-2.972239000
1	3.131898000	-3.326840000	-5.275660000
1	0.980149000	-2.581841000	-6.263299000
1	-0.546075000	-1.131384000	-4.942499000
1	0.081822000	-0.437087000	-2.646430000
1	-0.079374000	-4.009529000	1.778509000
1	-1.710844000	-5.815077000	1.333786000
1	-3.091330000	-5.765149000	-0.731880000
1	-2.856979000	-3.861744000	-2.317731000
1	-1.213352000	-2.077249000	-1.874630000
1	1.114103000	-4.093099000	-1.428511000
1	2.257760000	-6.209532000	-1.853282000
1	4.531327000	-6.625068000	-0.932803000
1	5.628877000	-4.862208000	0.438605000
1	4.468607000	-2.752364000	0.903277000
1	1.900066000	1.487714000	-2.933733000
1	2.997296000	2.832217000	-4.702931000
1	5.475169000	2.950090000	-4.820654000
1	6.845403000	1.688568000	-3.177072000
1	5.741679000	0.342537000	-1.414777000
6	-0.086869000	3.448065000	-1.128687000
6	-0.927188000	4.725121000	-1.167027000
6	1.373385000	3.769975000	-0.807575000
1	-0.108629000	3.004909000	-2.145028000
6	-0.338334000	5.729499000	-2.155791000
1	-0.951110000	5.179120000	-0.164735000

1	-1.968415000	4.500559000	-1.434210000
6	1.953481000	4.769181000	-1.798880000
1	1.437788000	4.198406000	0.205780000
1	1.969277000	2.845974000	-0.787182000
6	1.119016000	6.043893000	-1.834422000
1	-0.940160000	6.647460000	-2.162557000
1	-0.400132000	5.308798000	-3.172642000
1	3.000698000	4.986743000	-1.545059000
1	1.970283000	4.314489000	-2.802570000
1	1.527133000	6.755469000	-2.563529000
1	1.172359000	6.538158000	-0.850754000
6	-0.700325000	2.448910000	1.720477000
6	0.689570000	2.367544000	2.356832000
6	-1.429241000	3.711066000	2.175908000
1	-1.255310000	1.576425000	2.111723000
6	0.580609000	2.379683000	3.876826000
1	1.310416000	3.220312000	2.036854000
1	1.203209000	1.459796000	2.014020000
6	-1.553030000	3.717033000	3.698491000
1	-0.859442000	4.601304000	1.862130000
1	-2.422466000	3.790120000	1.709083000
6	-0.183961000	3.606724000	4.362929000
1	1.586086000	2.351615000	4.321228000
1	0.066387000	1.461028000	4.200809000
1	-2.072413000	4.624127000	4.034594000
1	-2.178634000	2.863655000	4.006382000
1	-0.290762000	3.588634000	5.455222000
1	0.400271000	4.510324000	4.121835000
6	-5.089322000	-1.285388000	0.661781000
6	-6.128192000	-2.248405000	0.079233000
6	-3.971526000	-2.074645000	1.352917000
1	-5.576629000	-0.642893000	1.416471000
6	-6.668260000	-3.221379000	1.121473000
1	-5.651619000	-2.818932000	-0.736767000
1	-6.956525000	-1.689454000	-0.378610000
6	-4.519347000	-3.048476000	2.390403000
1	-3.414255000	-2.639698000	0.587838000
1	-3.247799000	-1.404405000	1.834527000
6	-5.536462000	-4.001348000	1.778017000
1	-7.396365000	-3.901987000	0.660665000
1	-7.213877000	-2.657016000	1.895336000
1	-3.688329000	-3.603713000	2.845325000
1	-5.000493000	-2.481448000	3.204432000
1	-5.929843000	-4.692527000	2.534983000
1	-5.032250000	-4.618720000	1.015808000
6	-5.675201000	1.123809000	-0.988287000
6	-6.729304000	0.727059000	-2.024958000
6	-6.342231000	1.718971000	0.249468000
1	-5.067323000	1.923370000	-1.453796000
6	-7.605422000	1.918958000	-2.398249000
1	-7.370836000	-0.069658000	-1.613379000
1	-6.244116000	0.303693000	-2.914968000
6	-7.216706000	2.914221000	-0.120490000
1	-6.973422000	0.951375000	0.727267000
1	-5.591393000	2.016036000	0.996670000
6	-8.259655000	2.531291000	-1.164811000
1	-8.367454000	1.619564000	-3.129651000
1	-6.981276000	2.681472000	-2.892197000
1	-7.700588000	3.325962000	0.774997000
1	-6.575471000	3.714553000	-0.525222000

1	-8.865246000	3.403814000	-1.442376000
1	-8.954423000	1.797162000	-0.724992000

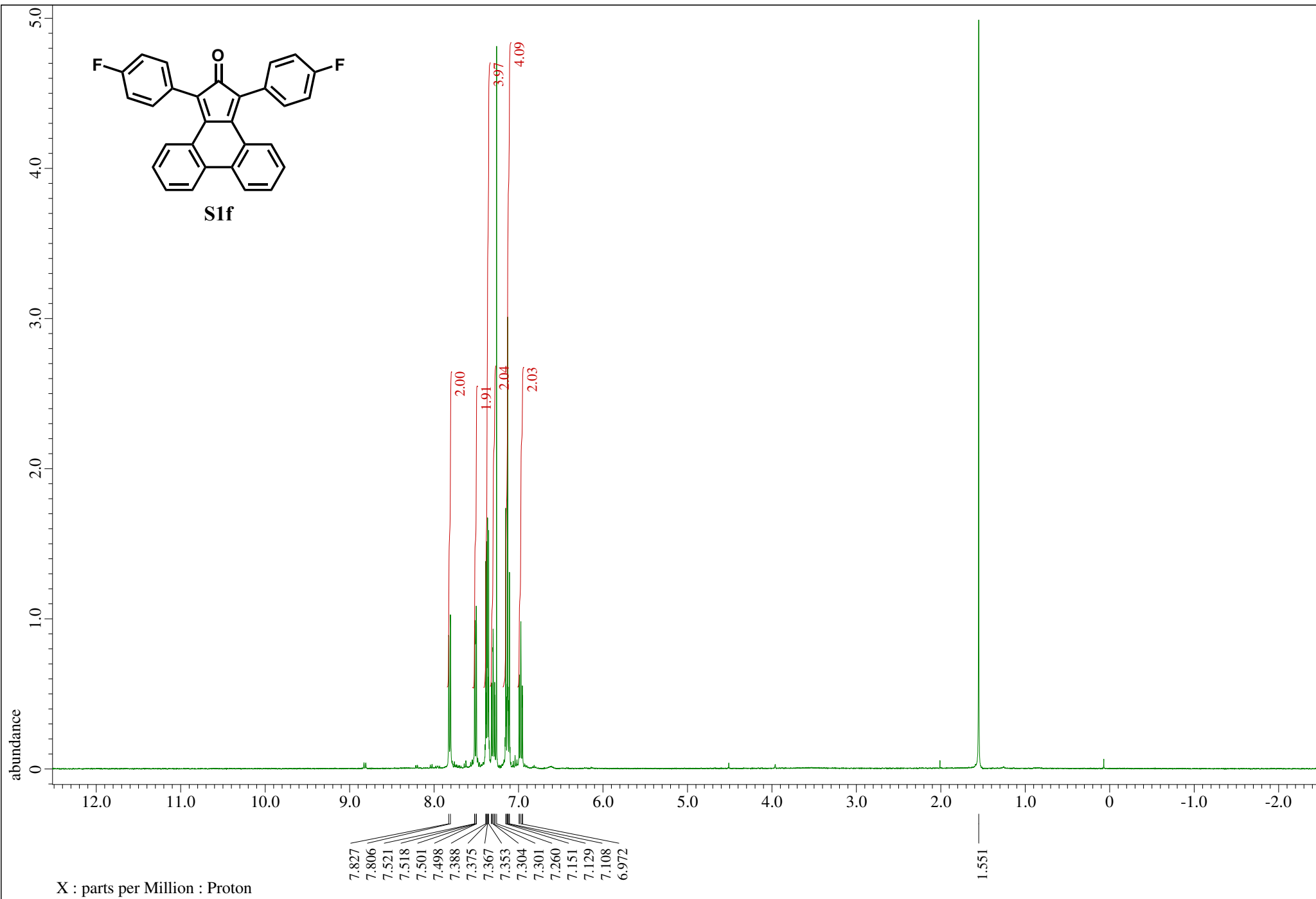
Method: M06-2X/6-31G(d,p) Key word: opt freq pop=full
imaginary frequencies: 0 Energy: -3599.241111 Hartree

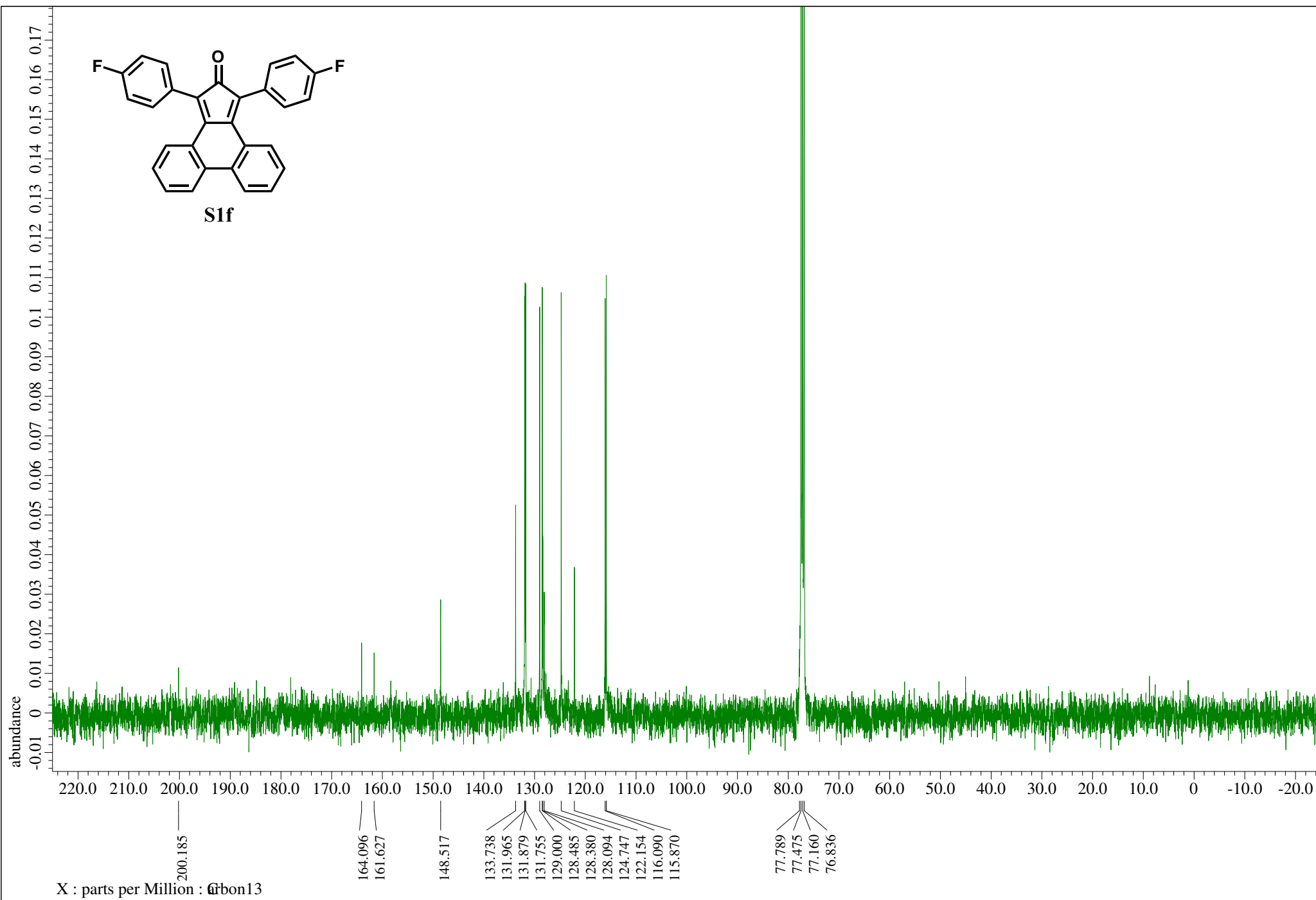
XI. Reference.

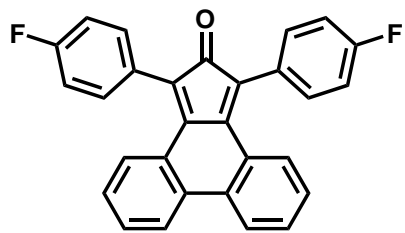
1. M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, T. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski and D. J. Fox, Gaussian, Inc., Wallingford CT, 2013.
2. Y. Zhao and D. G. Truhlar, *Theor. Chem. Acc.*, 2008, **120**, 215–241.
3. H. Kinuta, M. Tobisu and N. Chatani, *J. Am. Chem. Soc.*, 2015, **137**, 1593–1600.
4. R. M. Pike and R. R. Luongo, *J. Am. Chem. Soc.*, 1965, **87**, 1404–1405.
5. D. L. Crossley, C. D. Gabbutt, B. M. Heron, P. Kay and M. Mogstad, *Dyes Pigm.*, 2012, **96**, 62–68.
6. X. Yang, Q. Miao, *Synlett*, 2016, **27**, 2091–2094.
7. T. Kodama, Y. Kawashima, K. Uchida, Z. Deng and M. Tobisu, *J. Org. Chem.*, 2021, **86**, 13800–13807.
8. T. Kodama, Y. Kawashima, Z. Deng and Tobisu, M. *Inorg. Chem.*, 2021, **60**, 4332–4336.
9. K. Muto, J. Yamaguchi, A. Lei and K. Itami, *J. Am. Chem. Soc.*, 2013, **135**, 16384–16387.
10. K. Amaike, K. Muto, J. Yamaguchi and Itami, K., *J. Am. Chem. Soc.*, 2012, **134**, 13573–13576.

XII. Copies of NMR spectra.

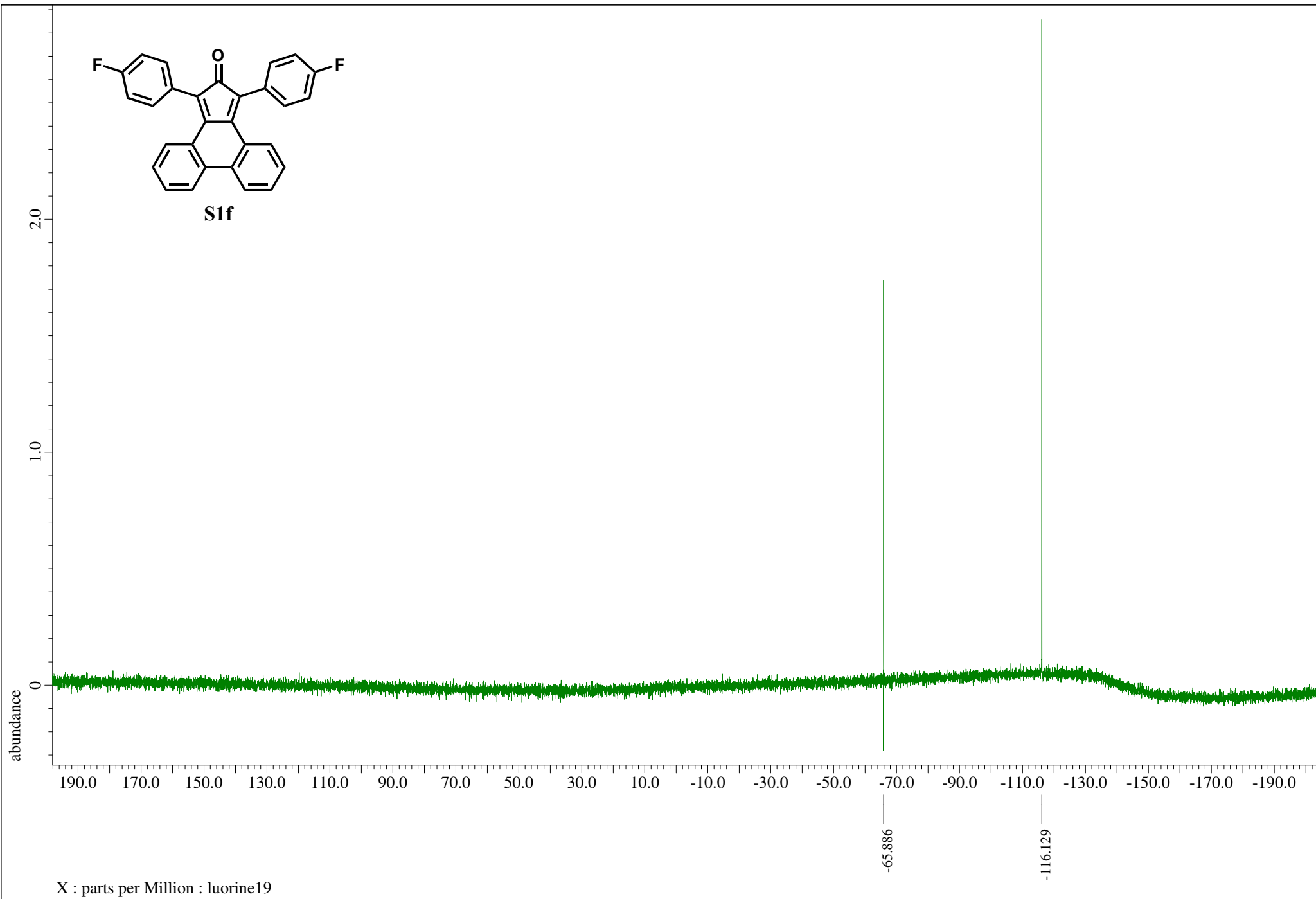
¹H NMR spectrum (400 MHz, CDCl₃) of **S1f**



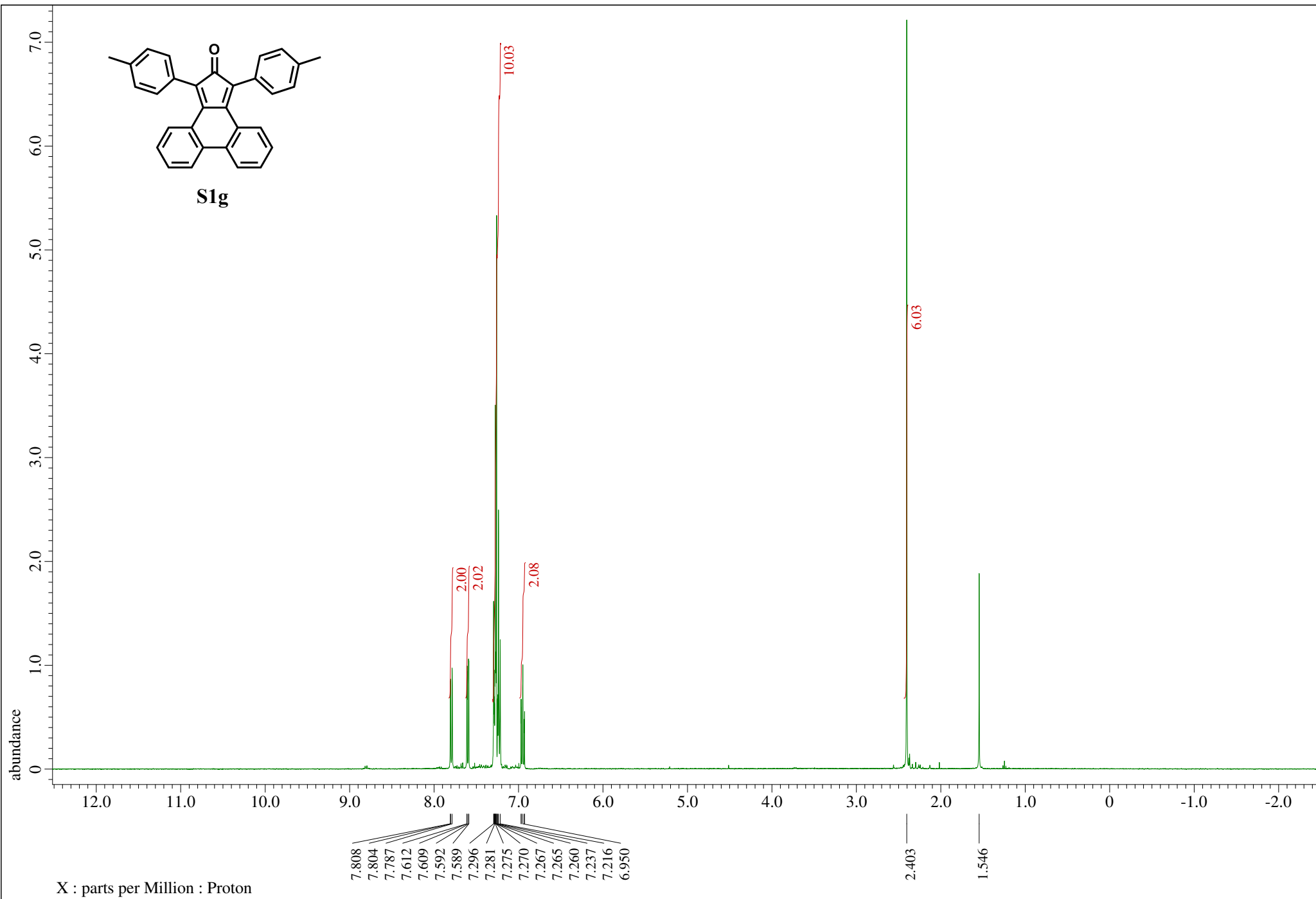


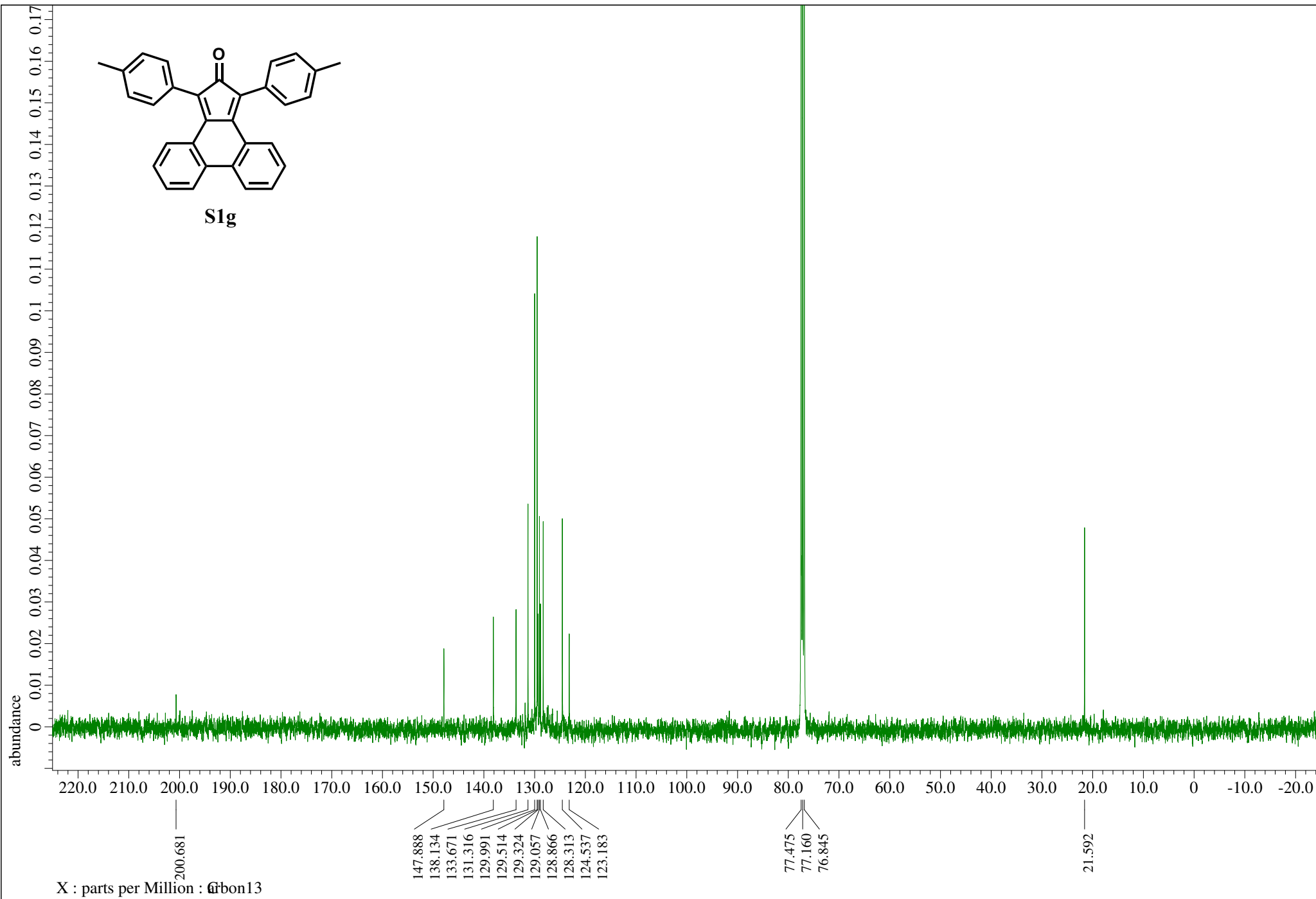


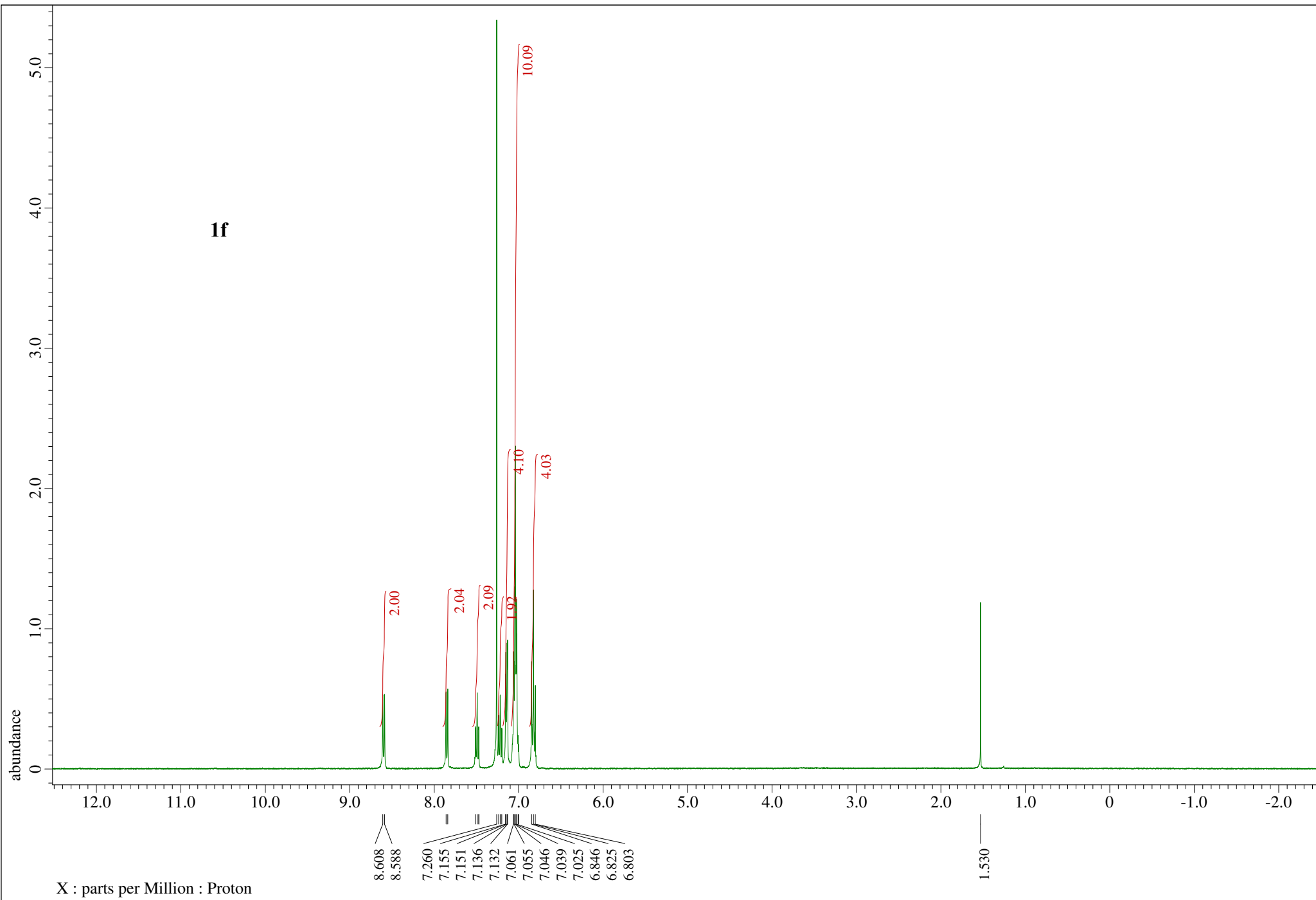
S1f

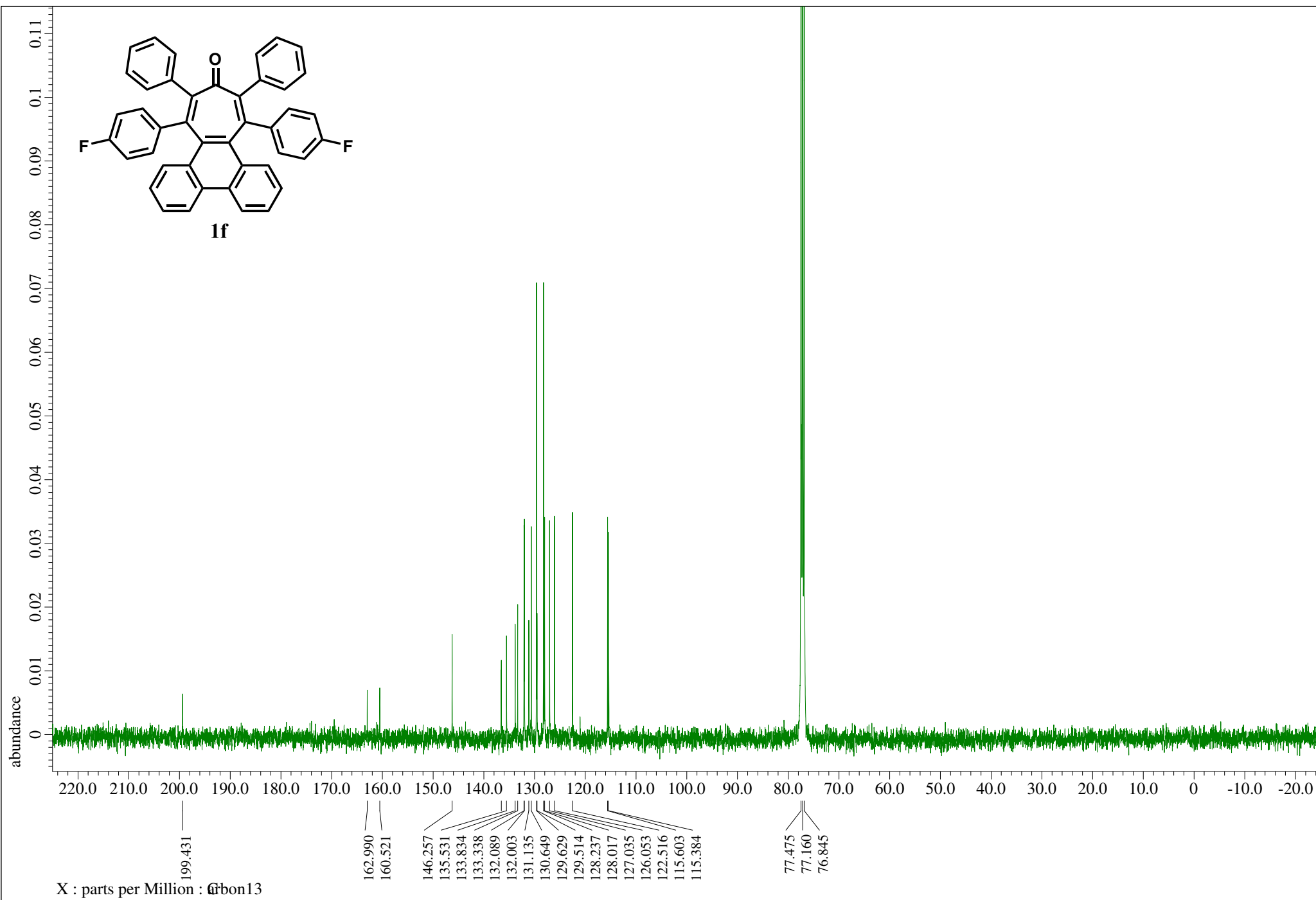


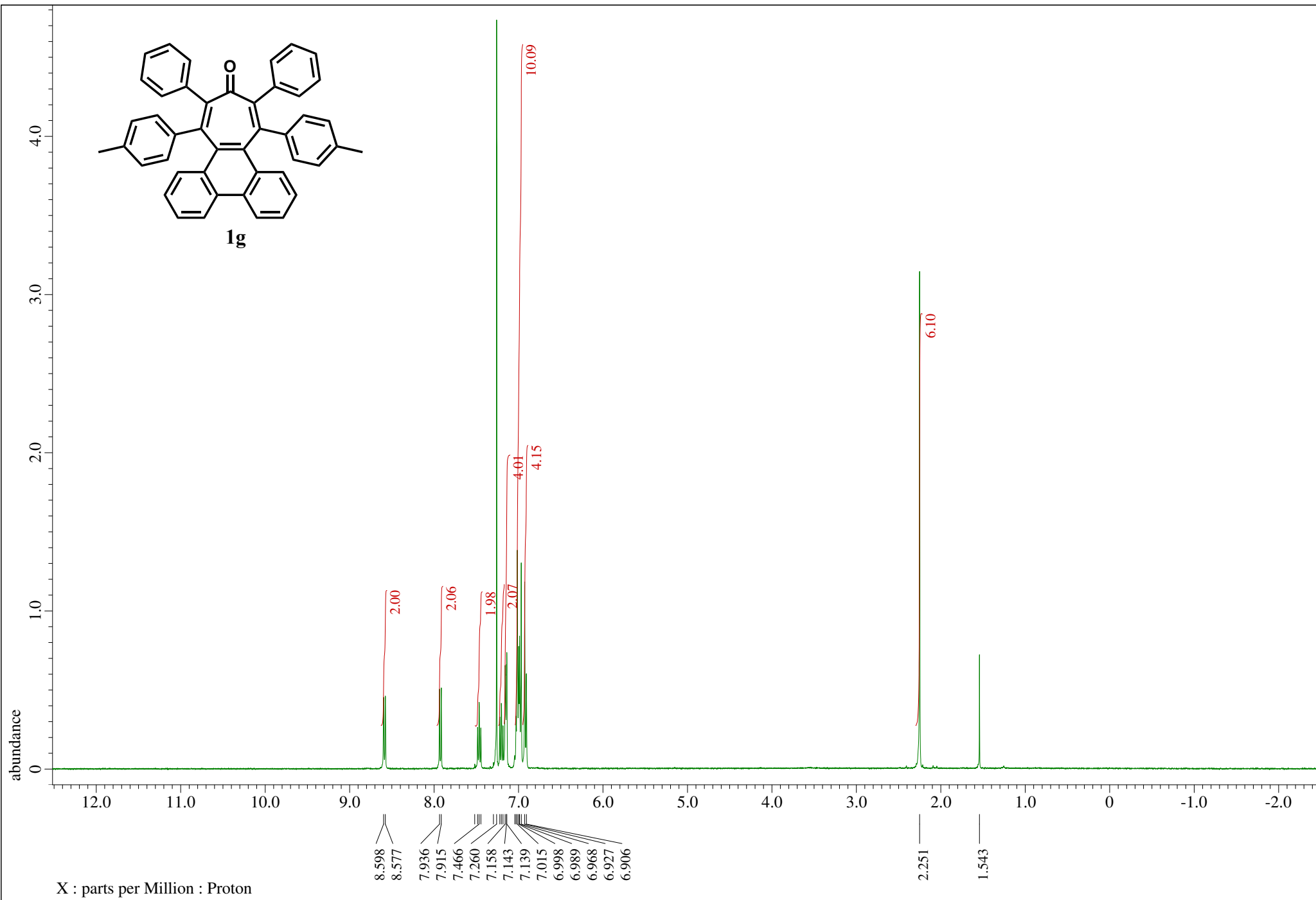
X : parts per Million : luorine19

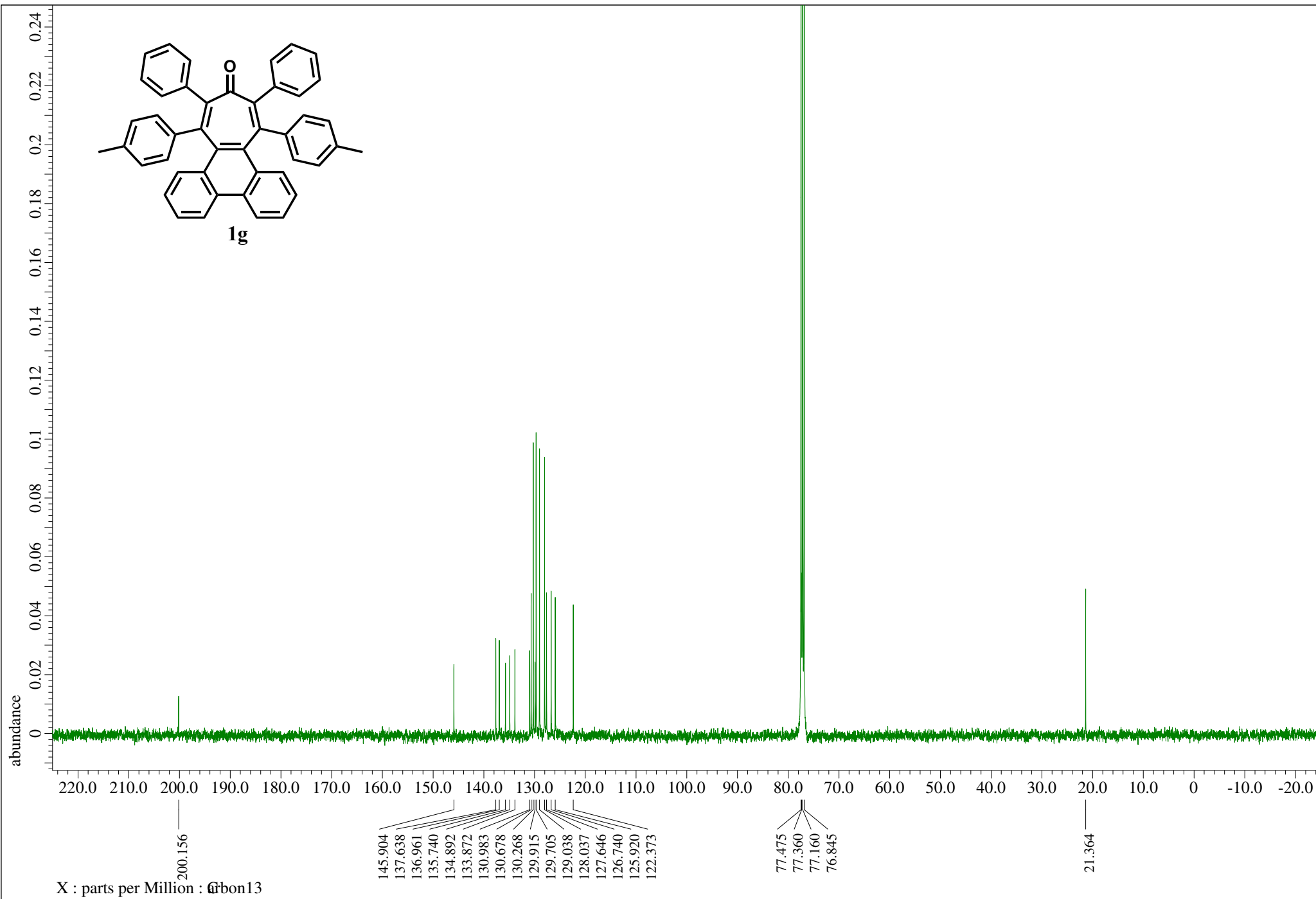


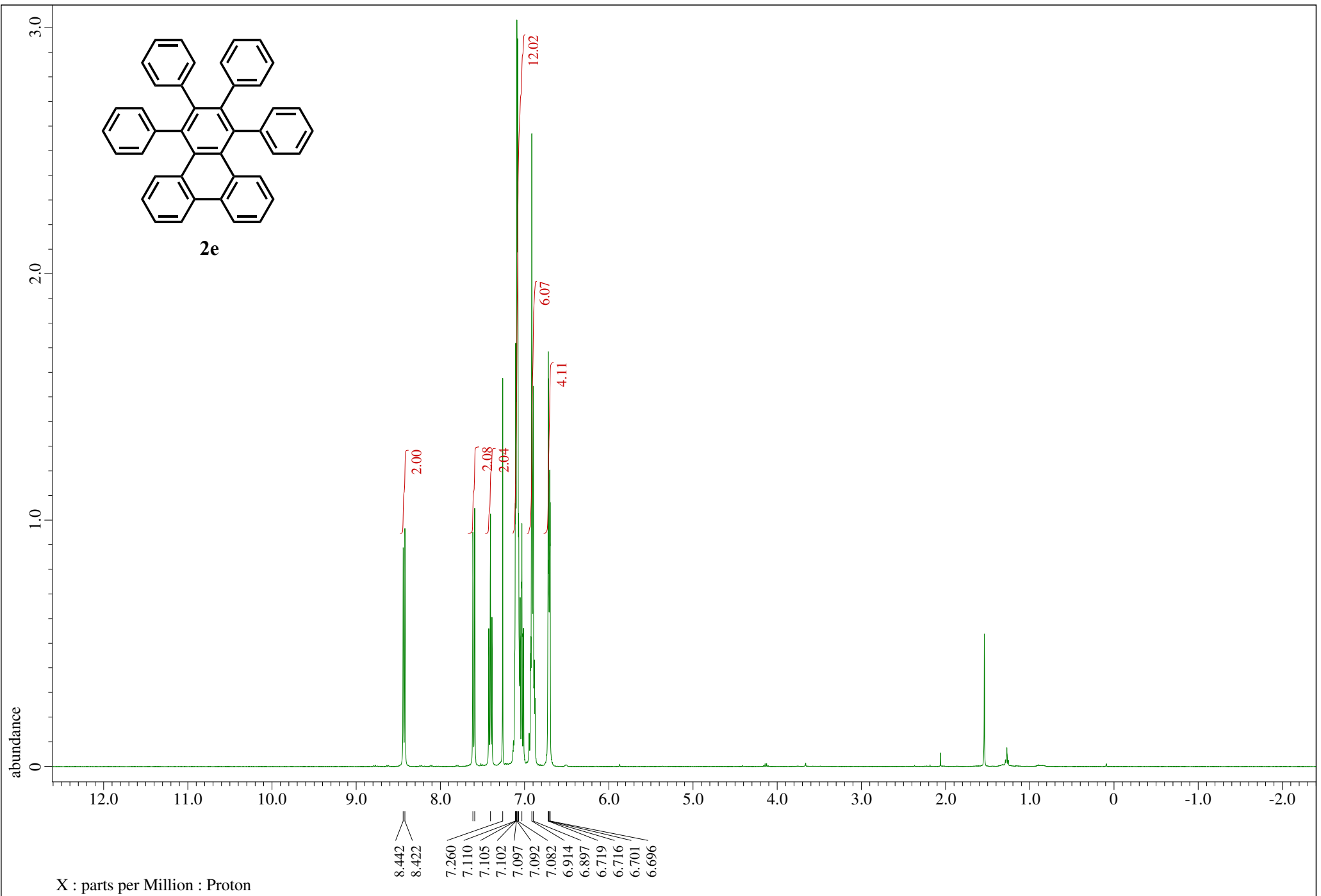


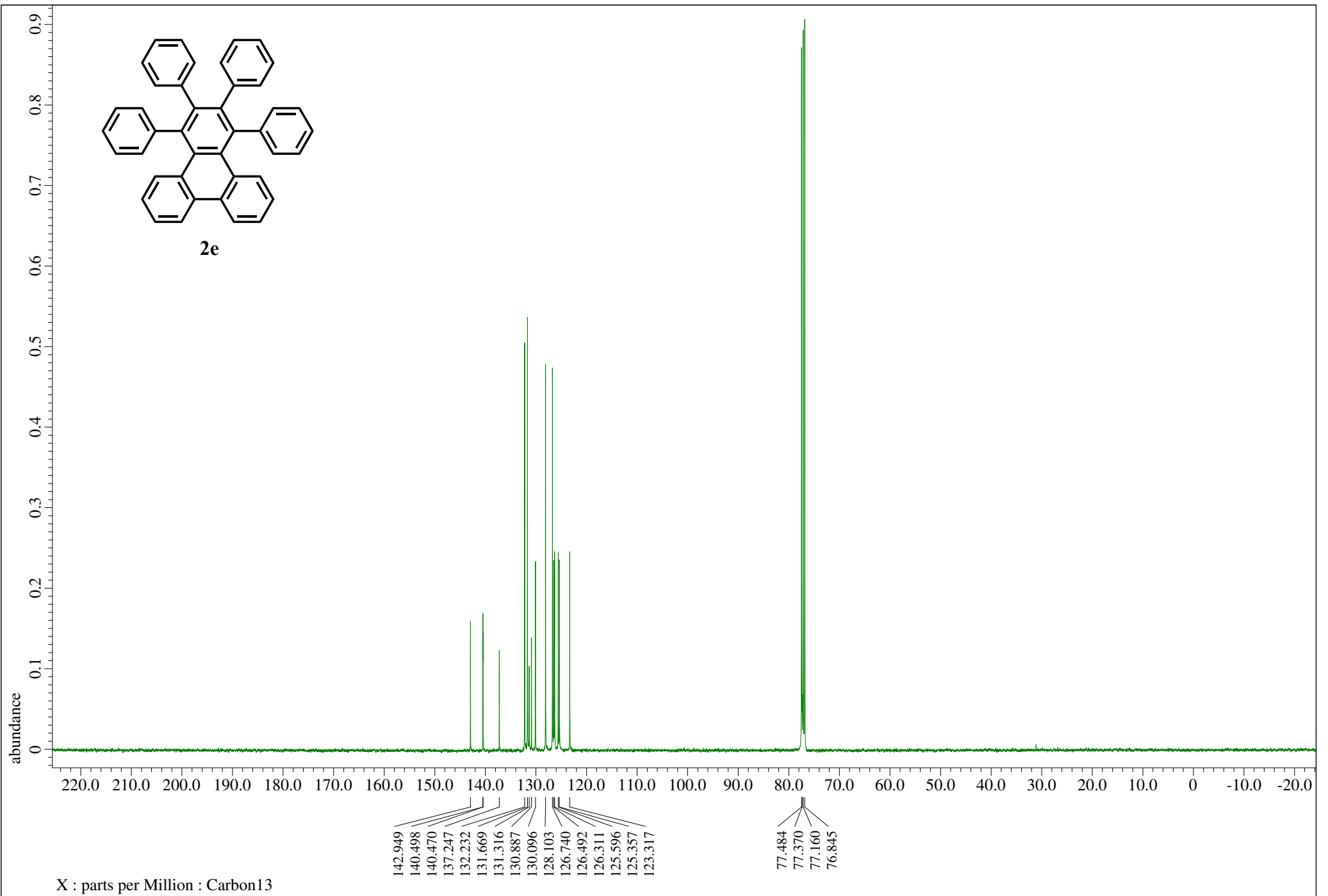


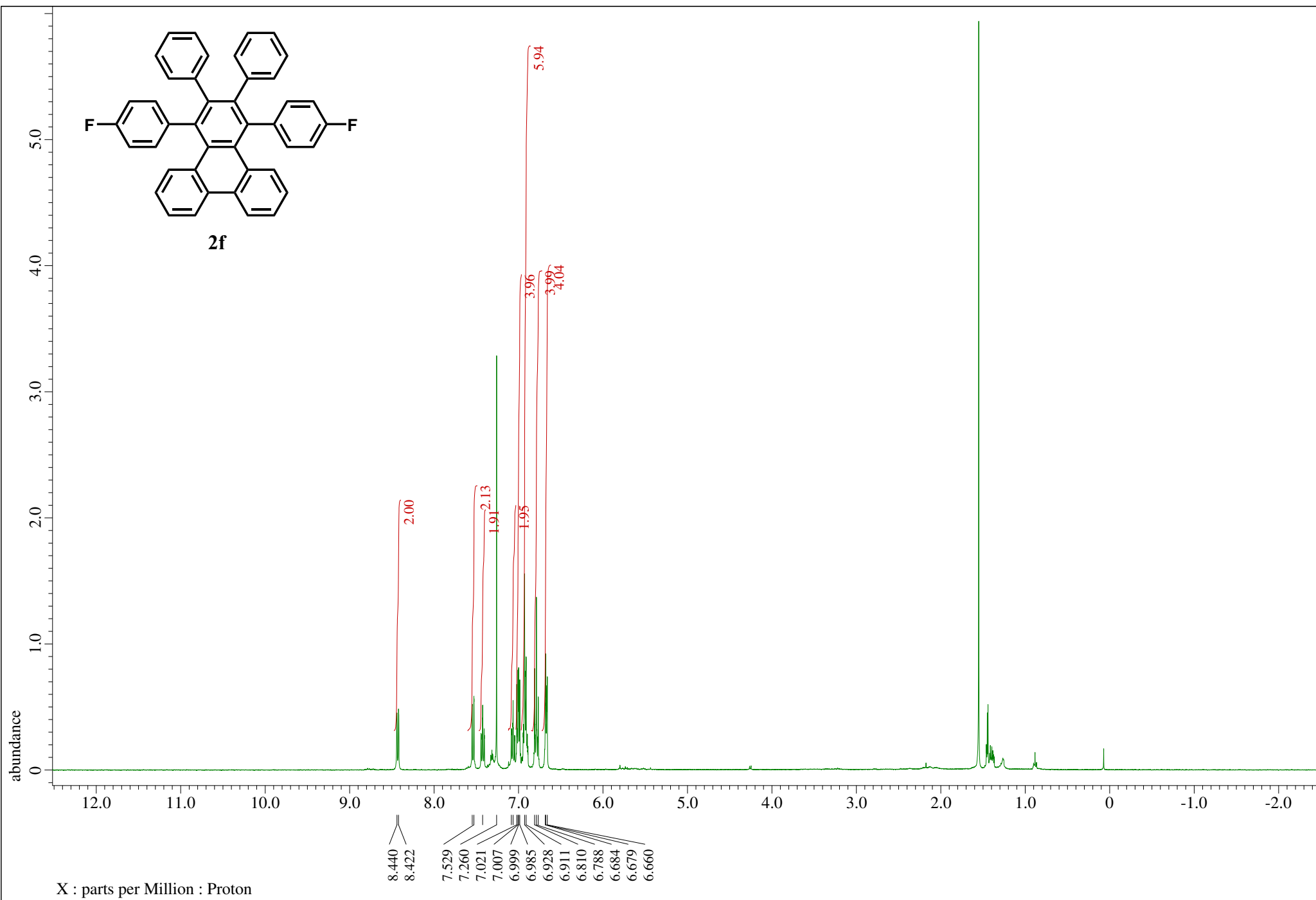


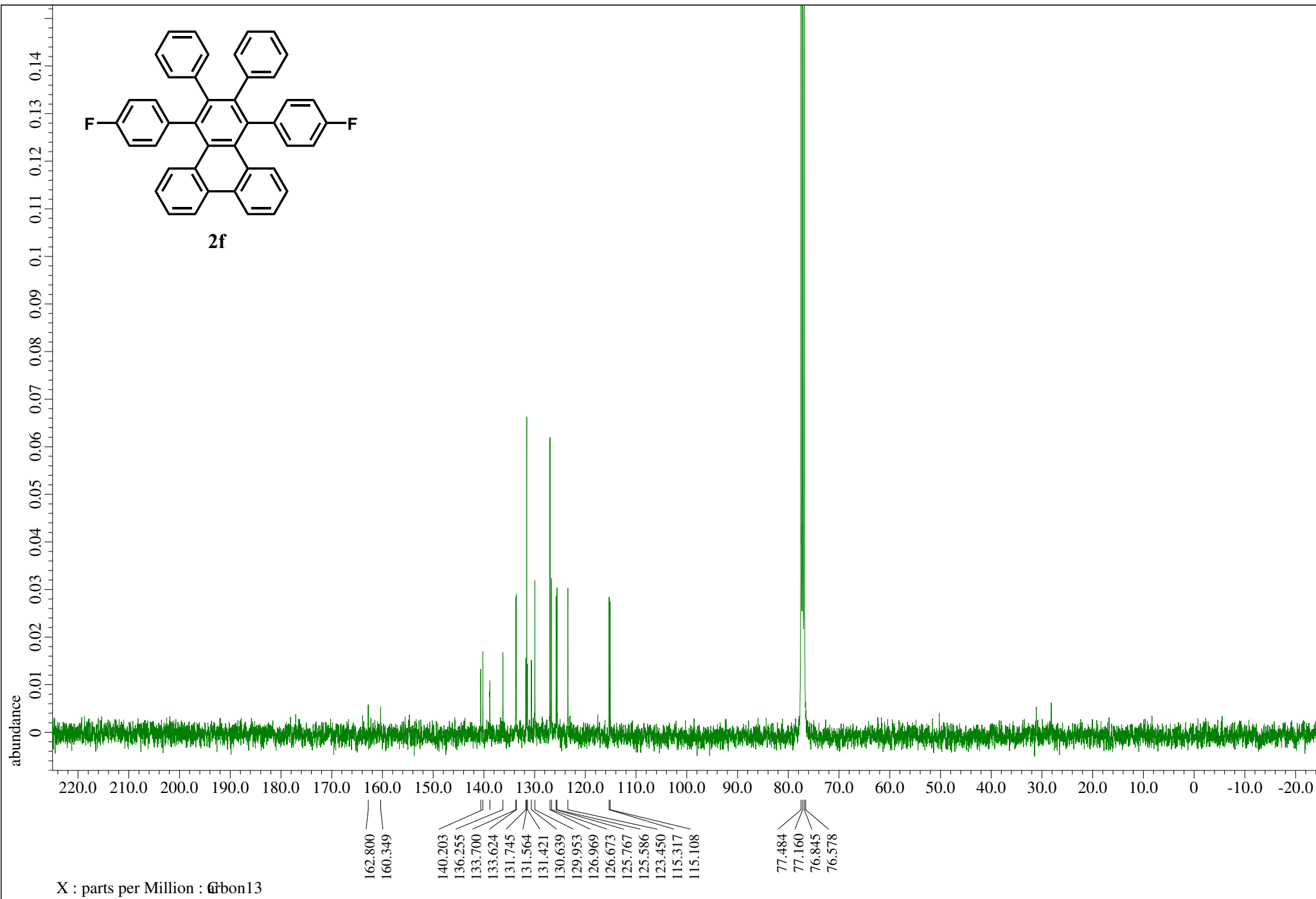


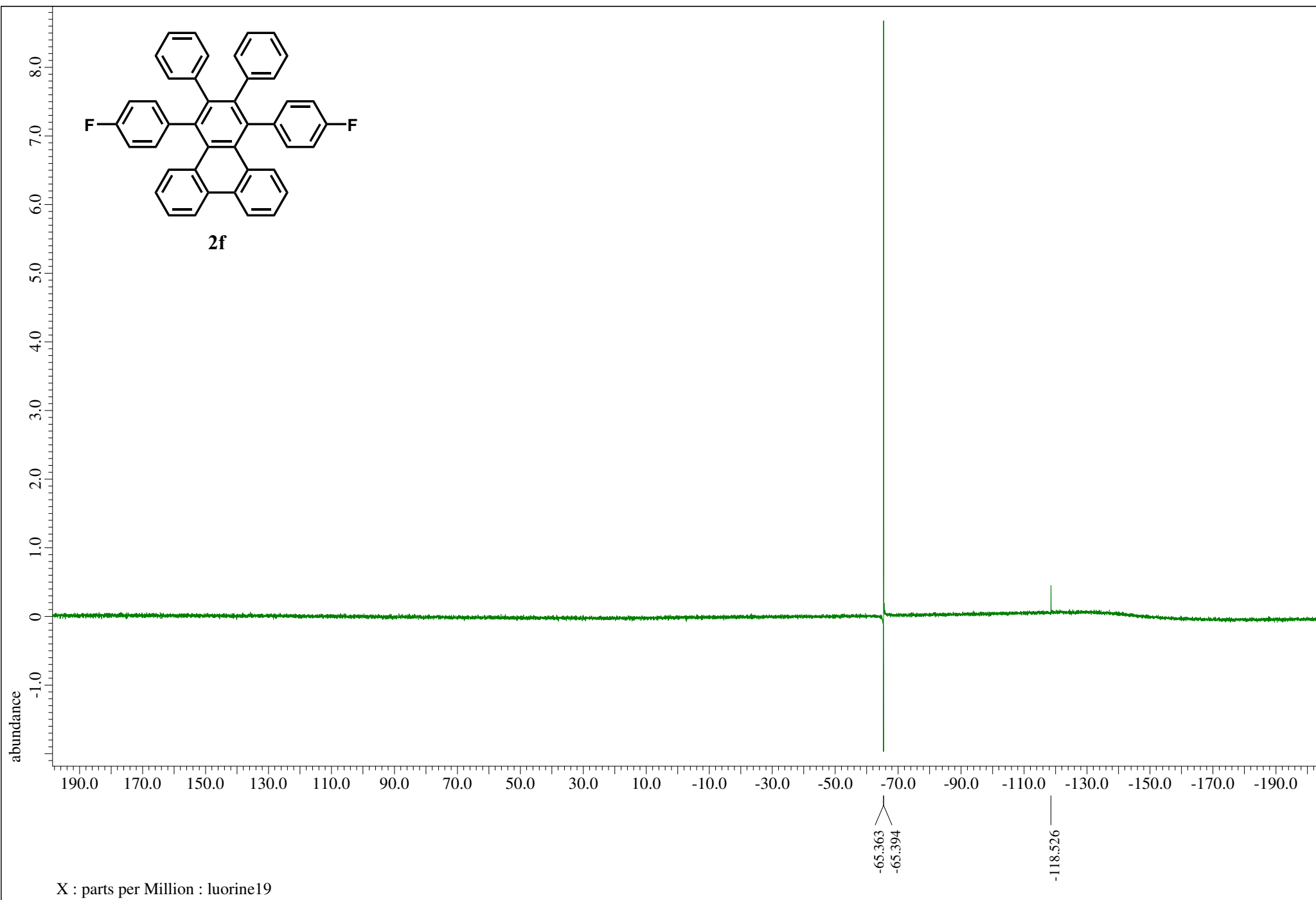


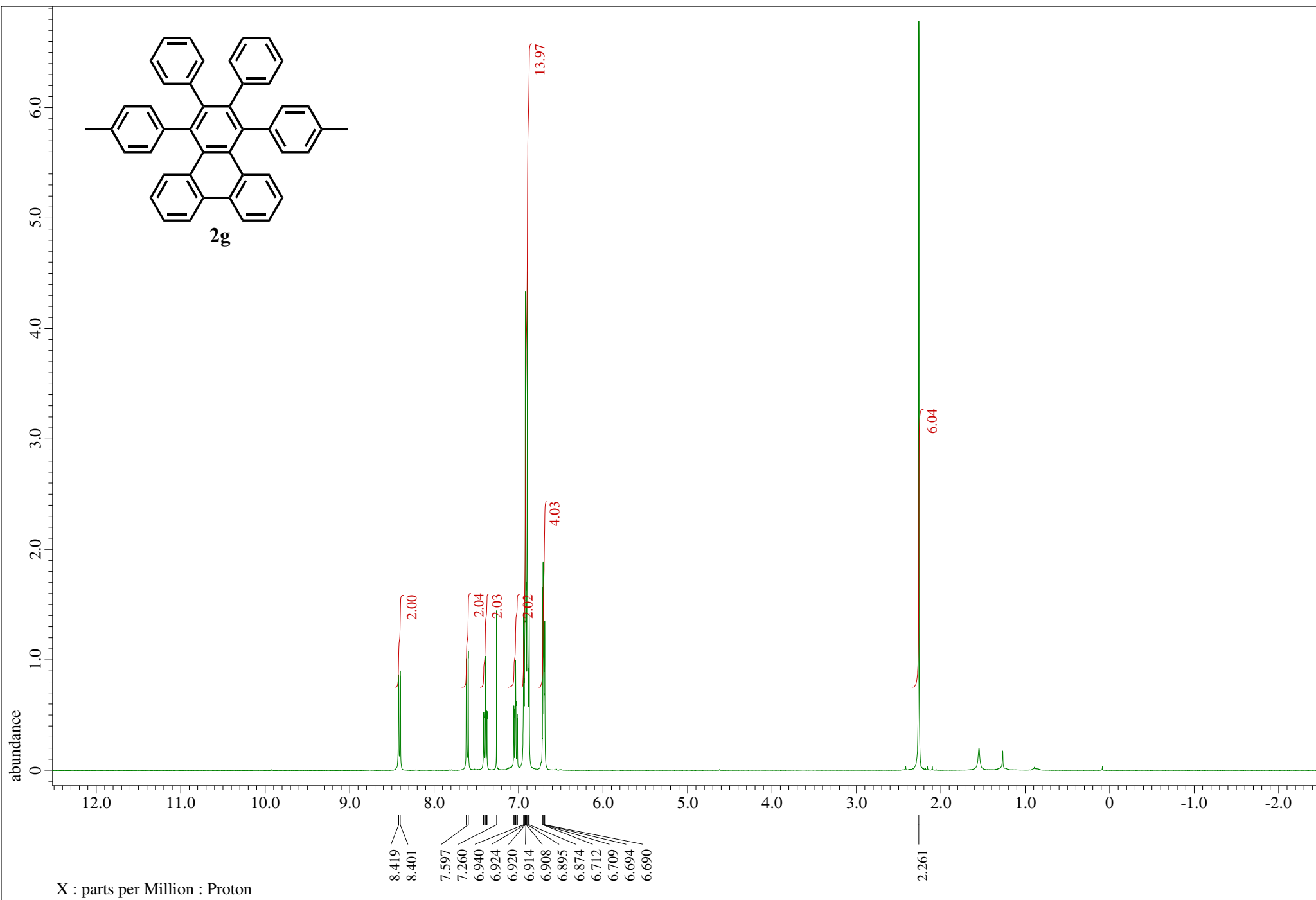


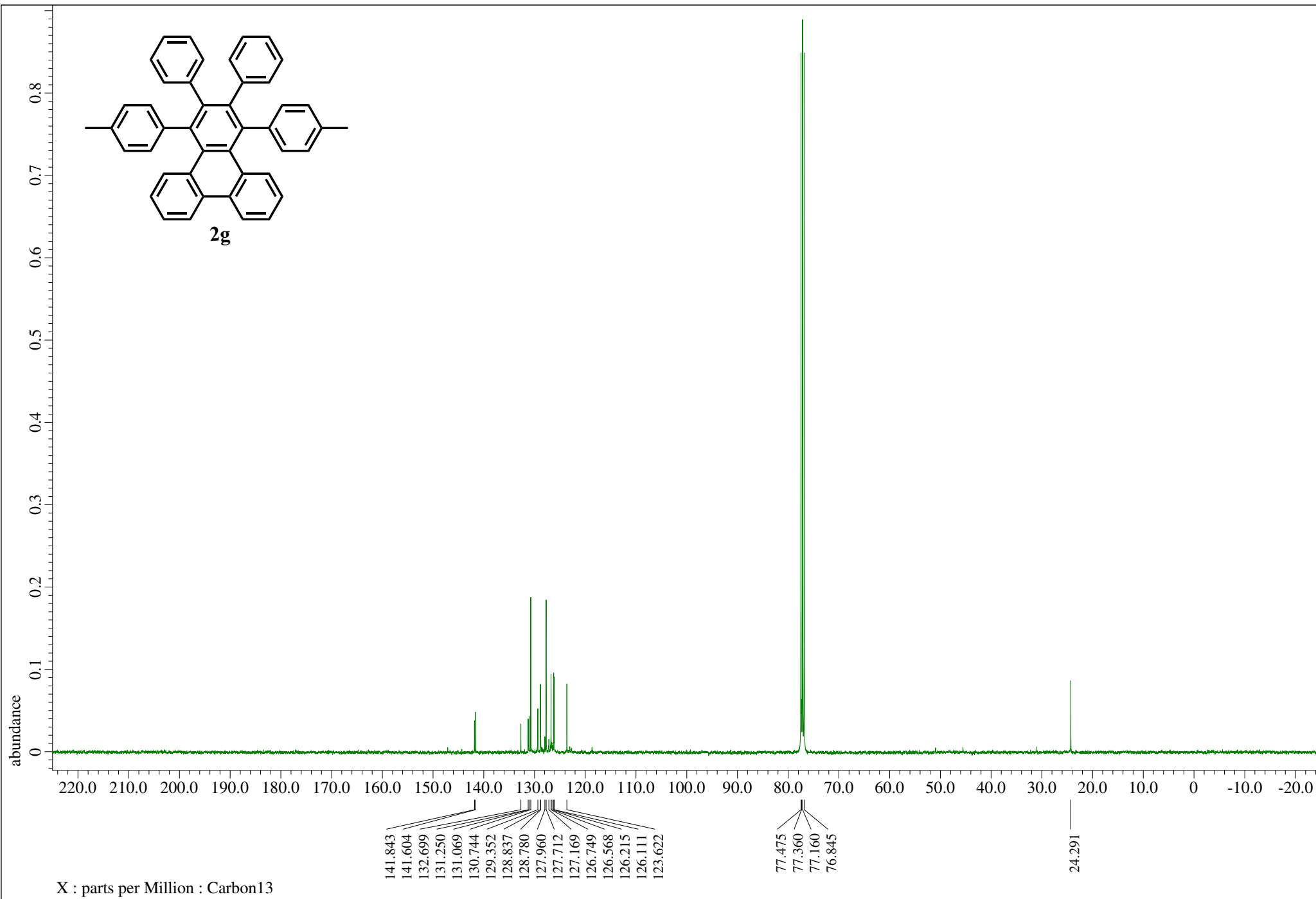


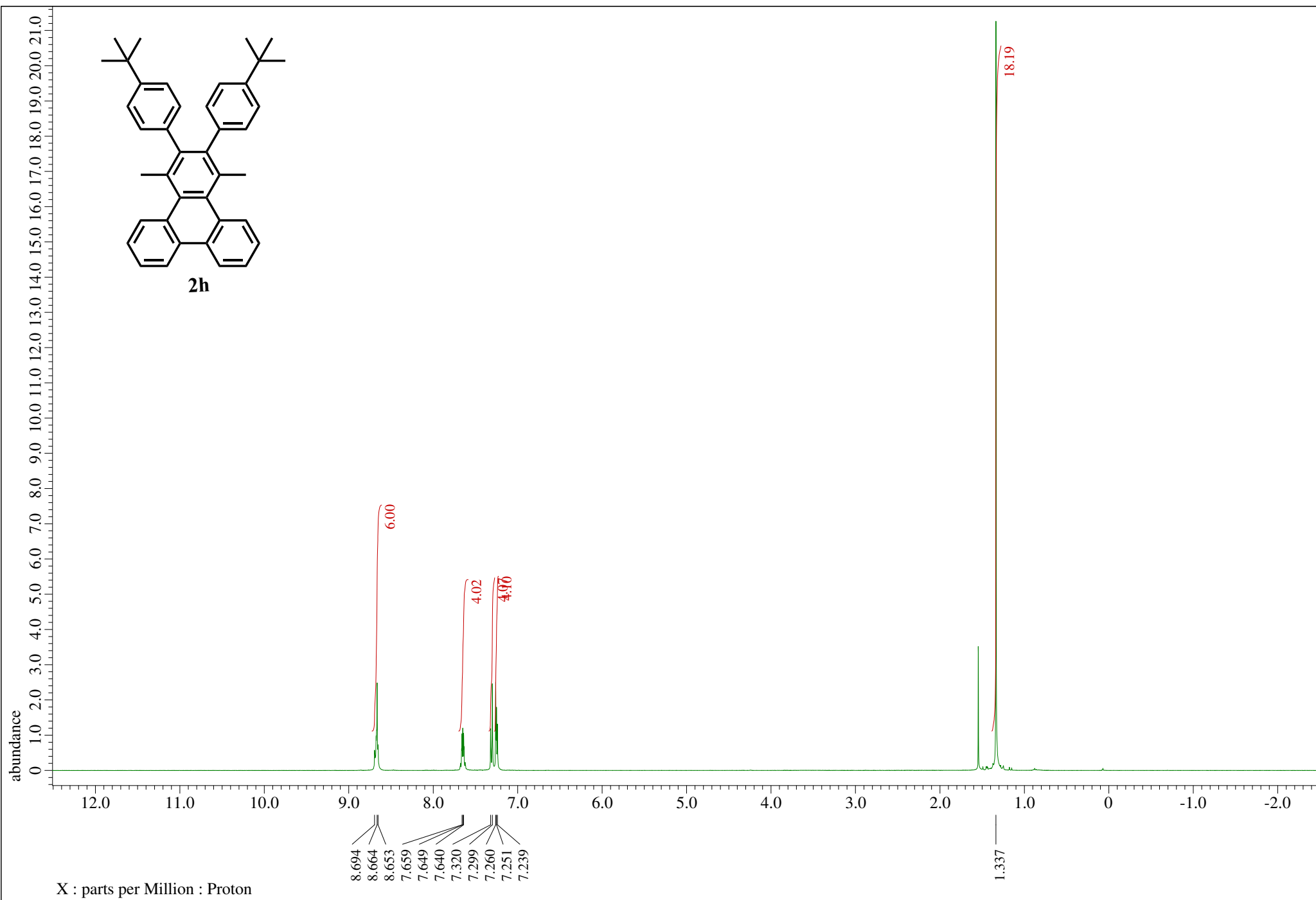


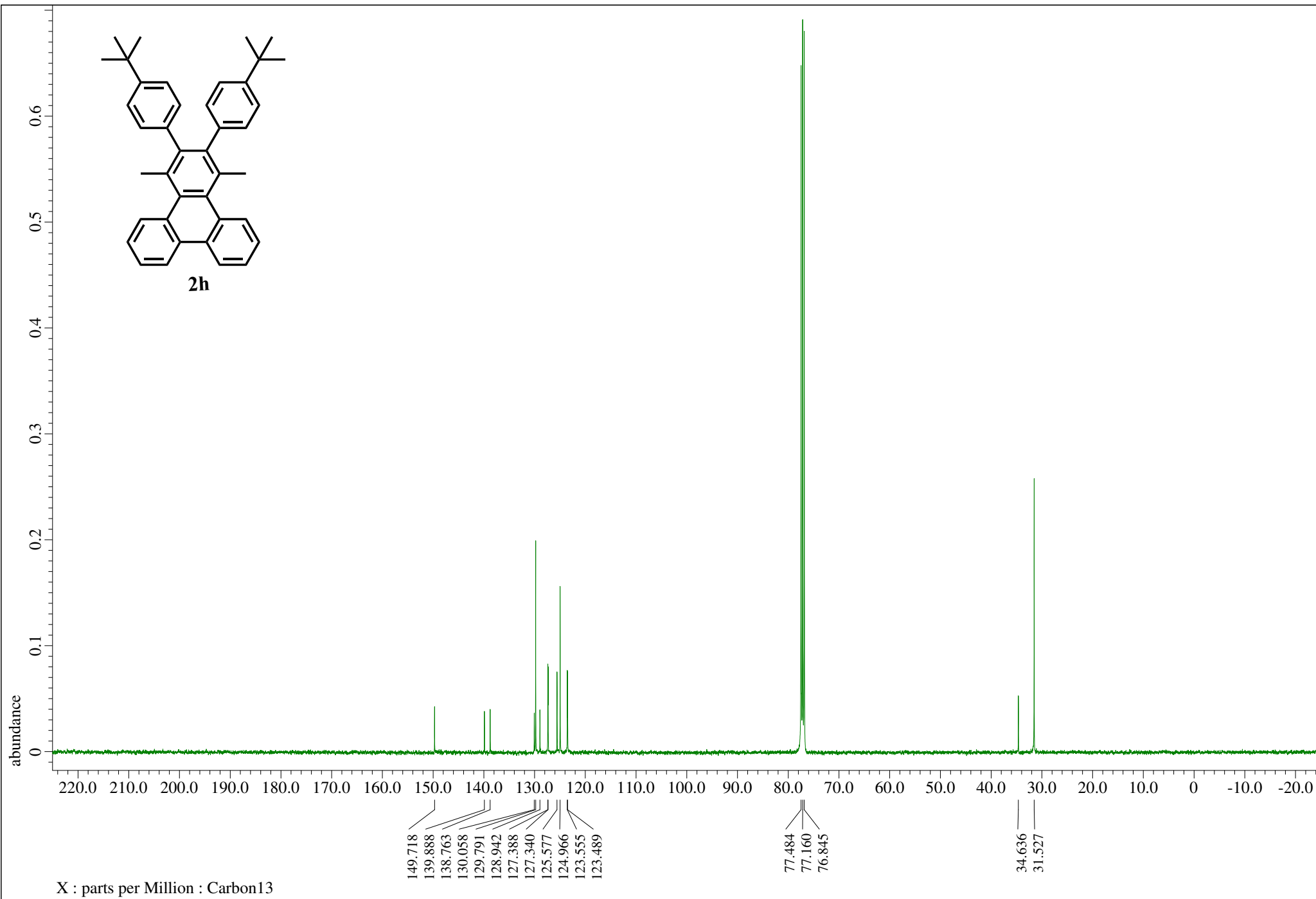


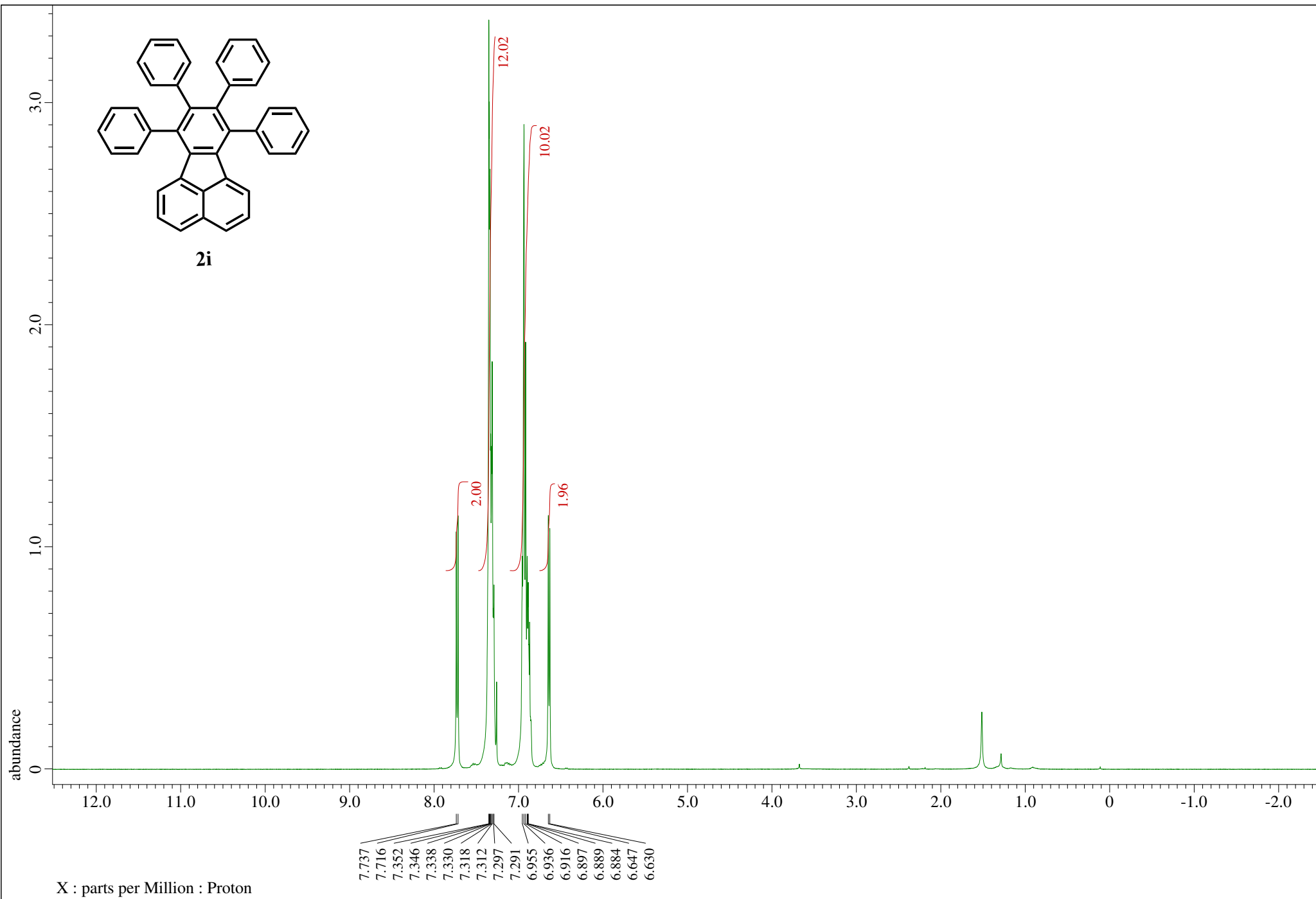


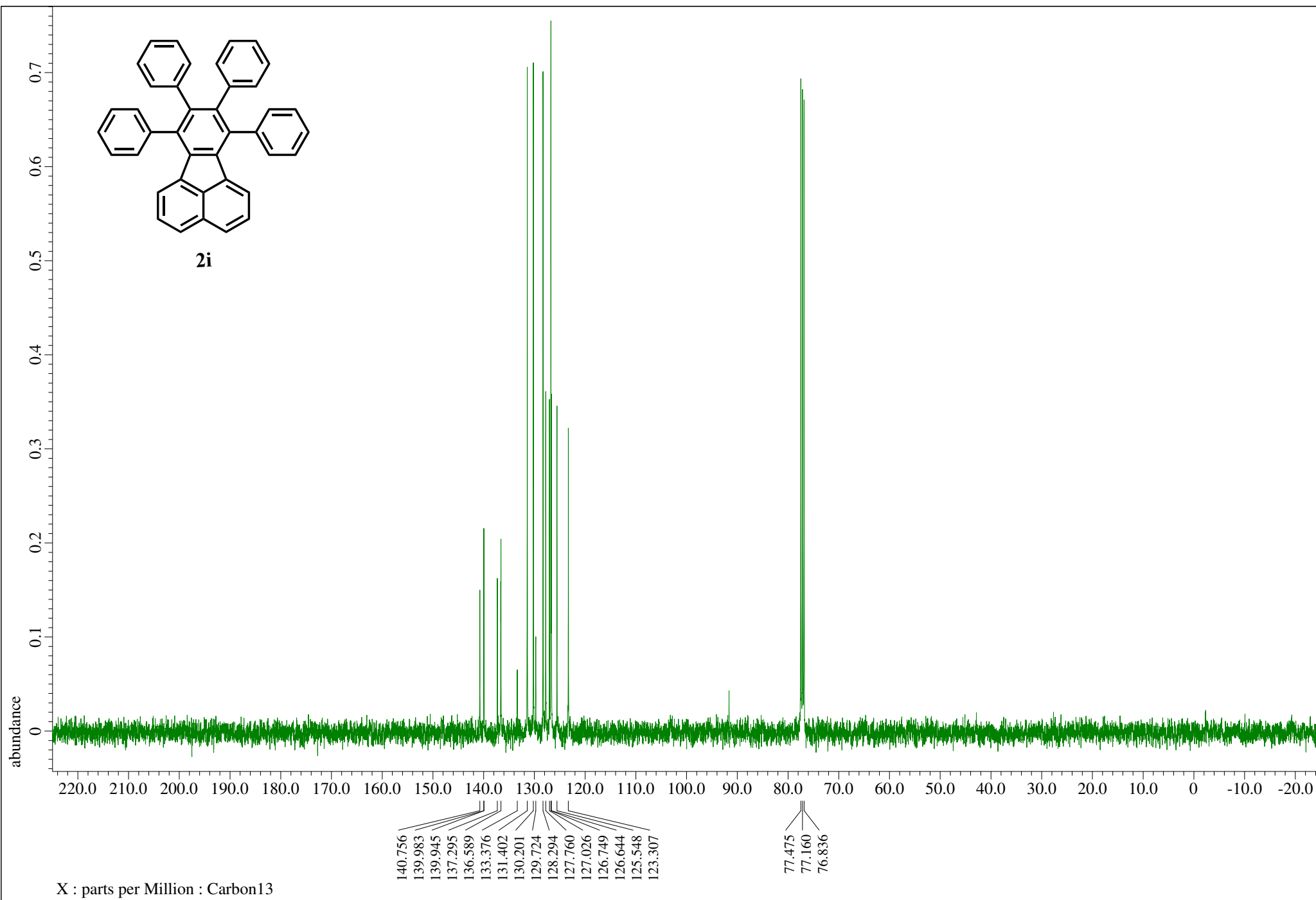


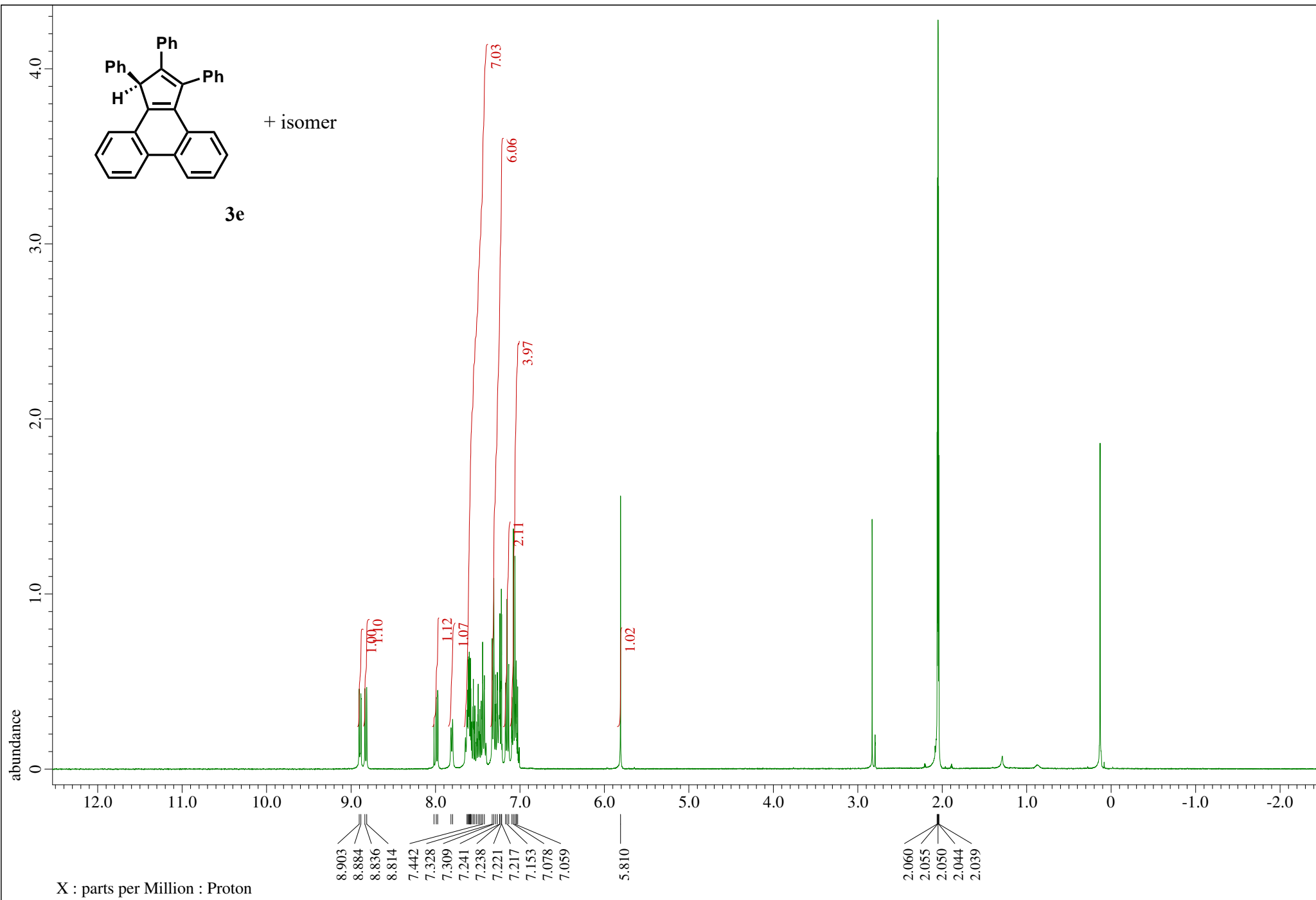


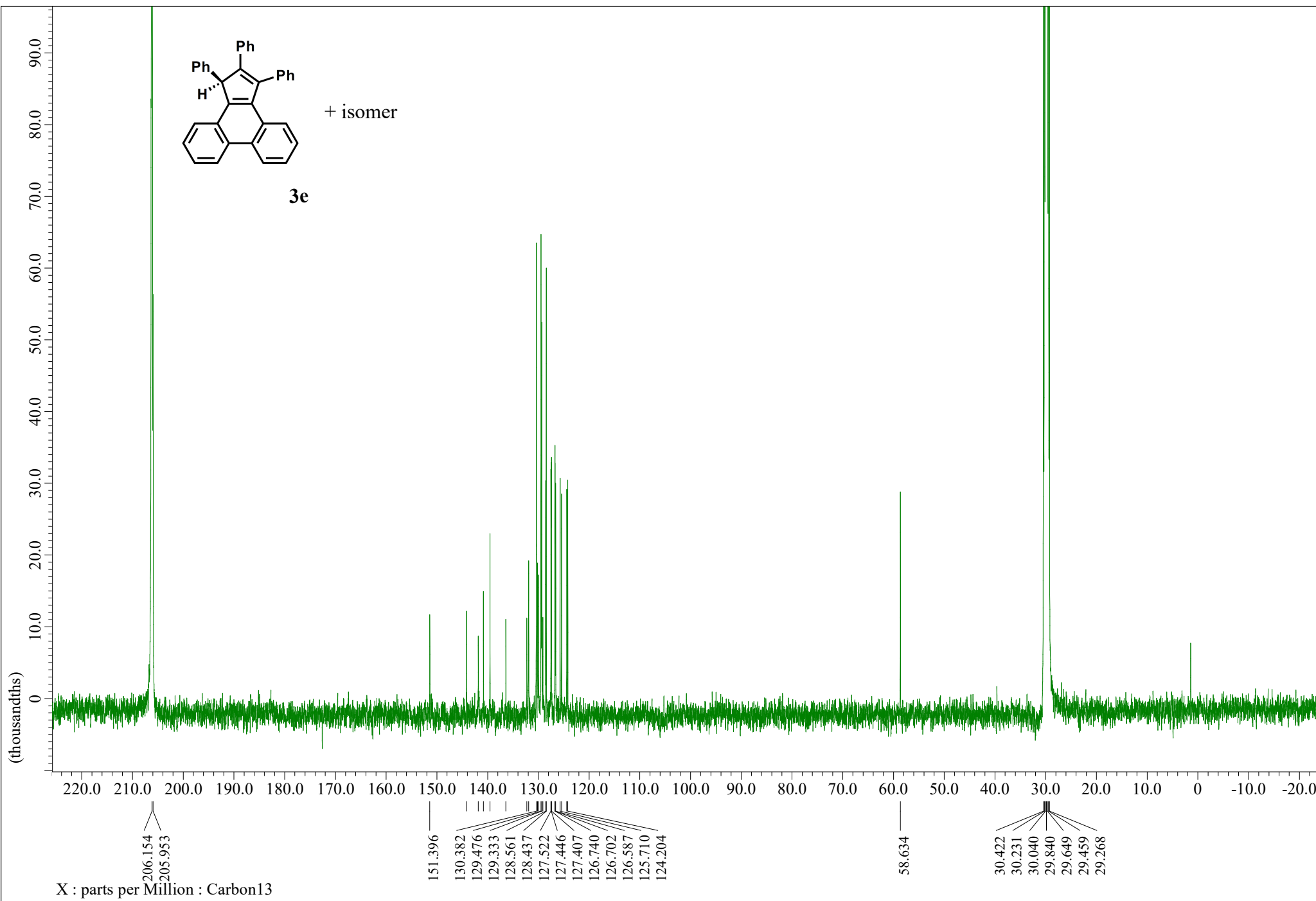


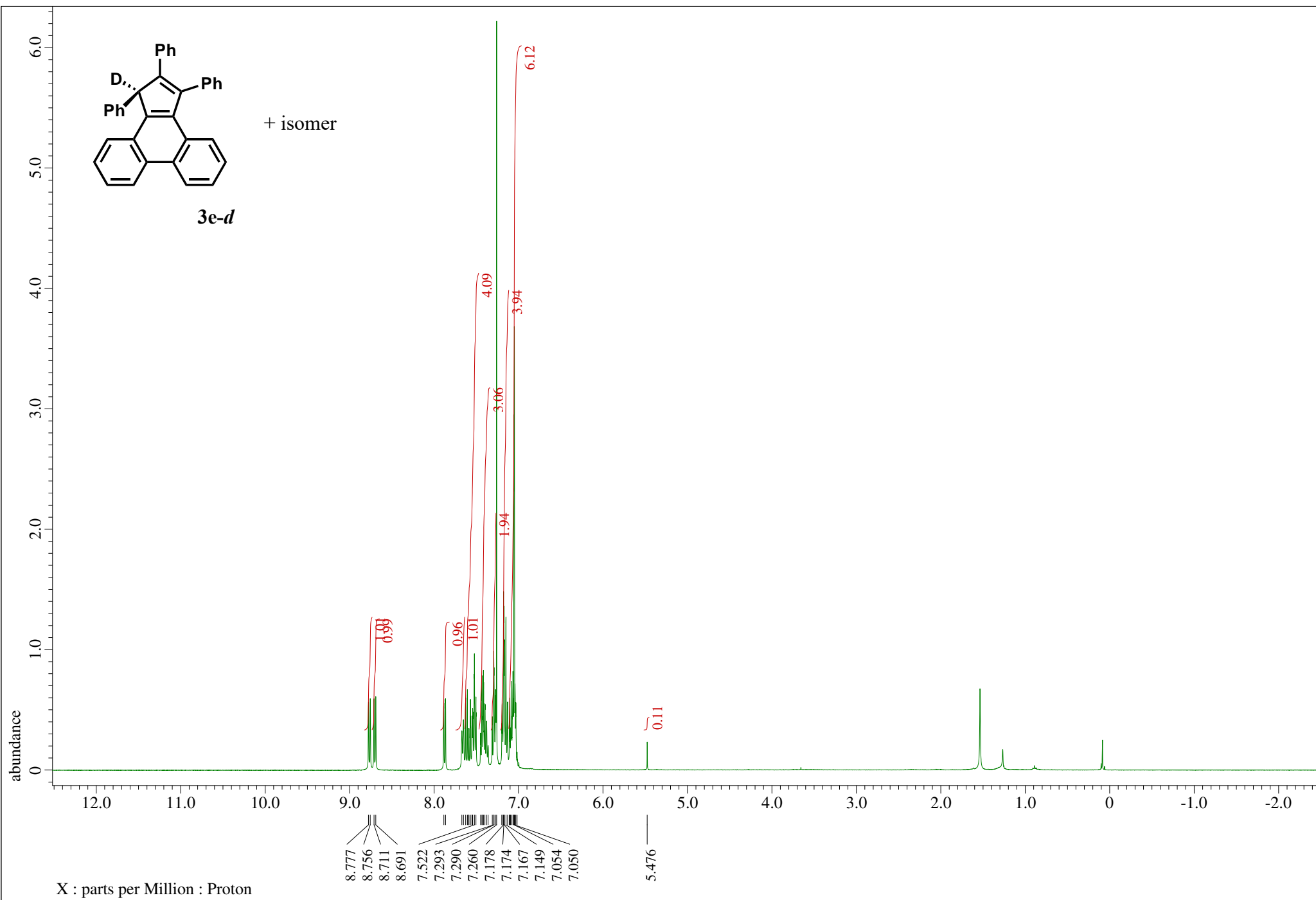


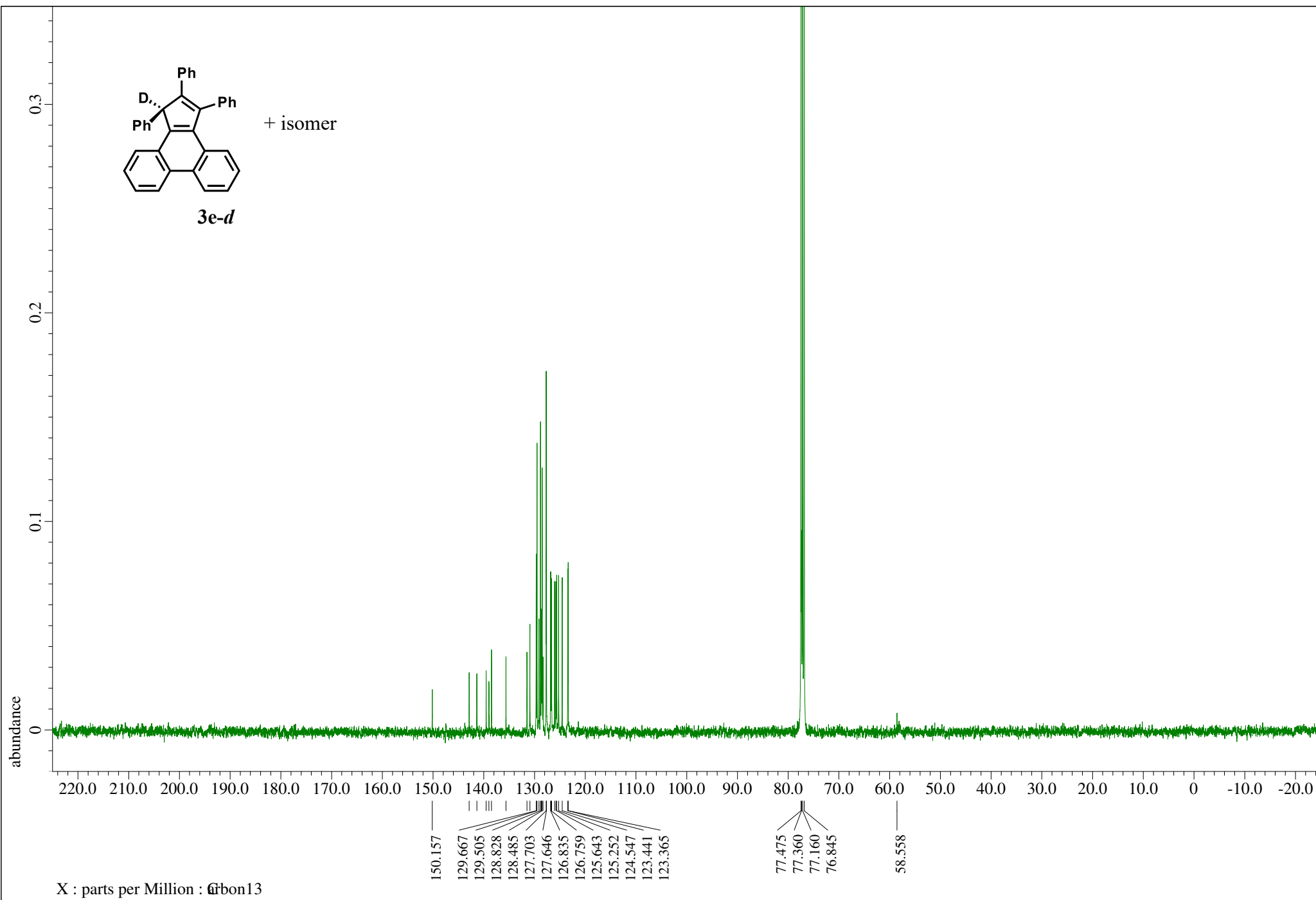


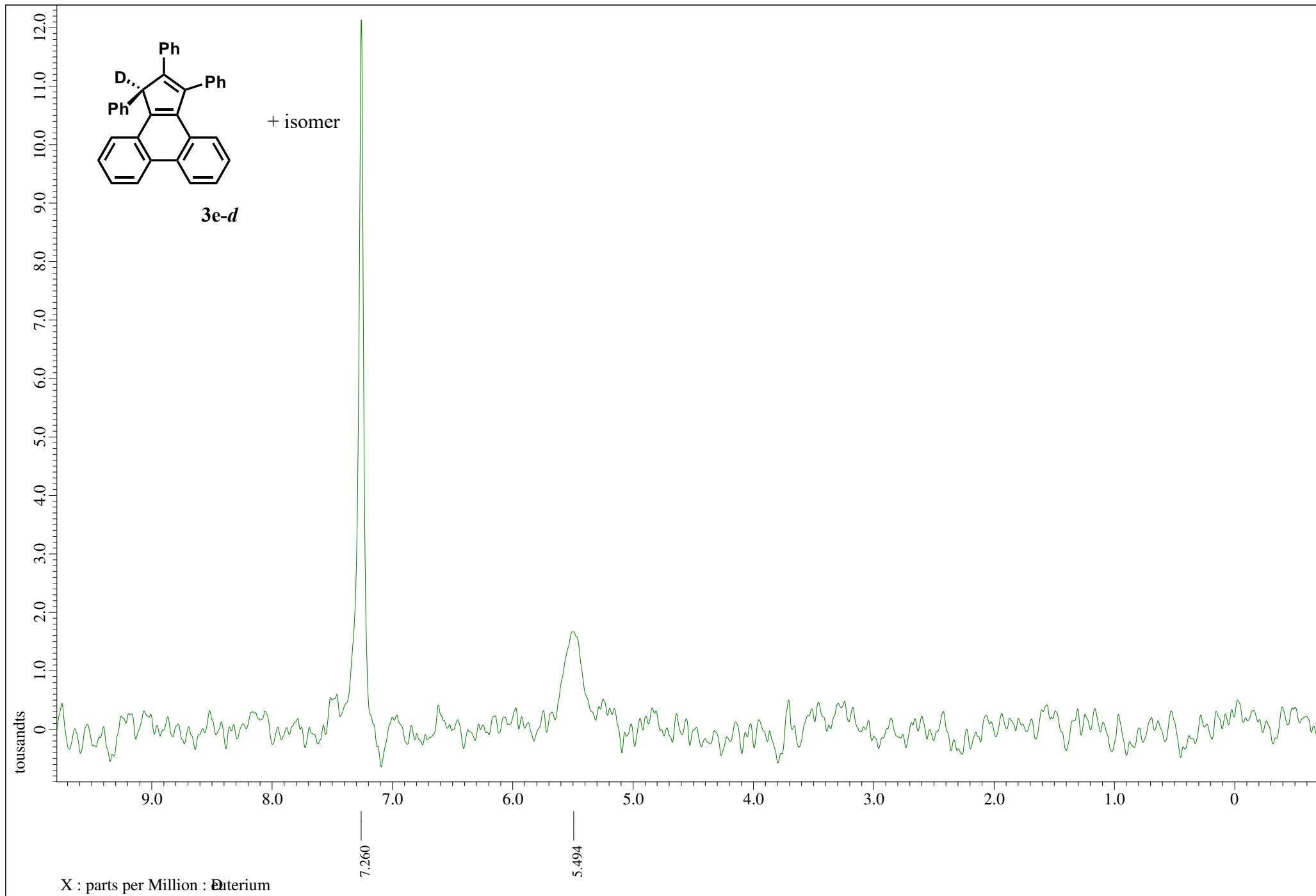


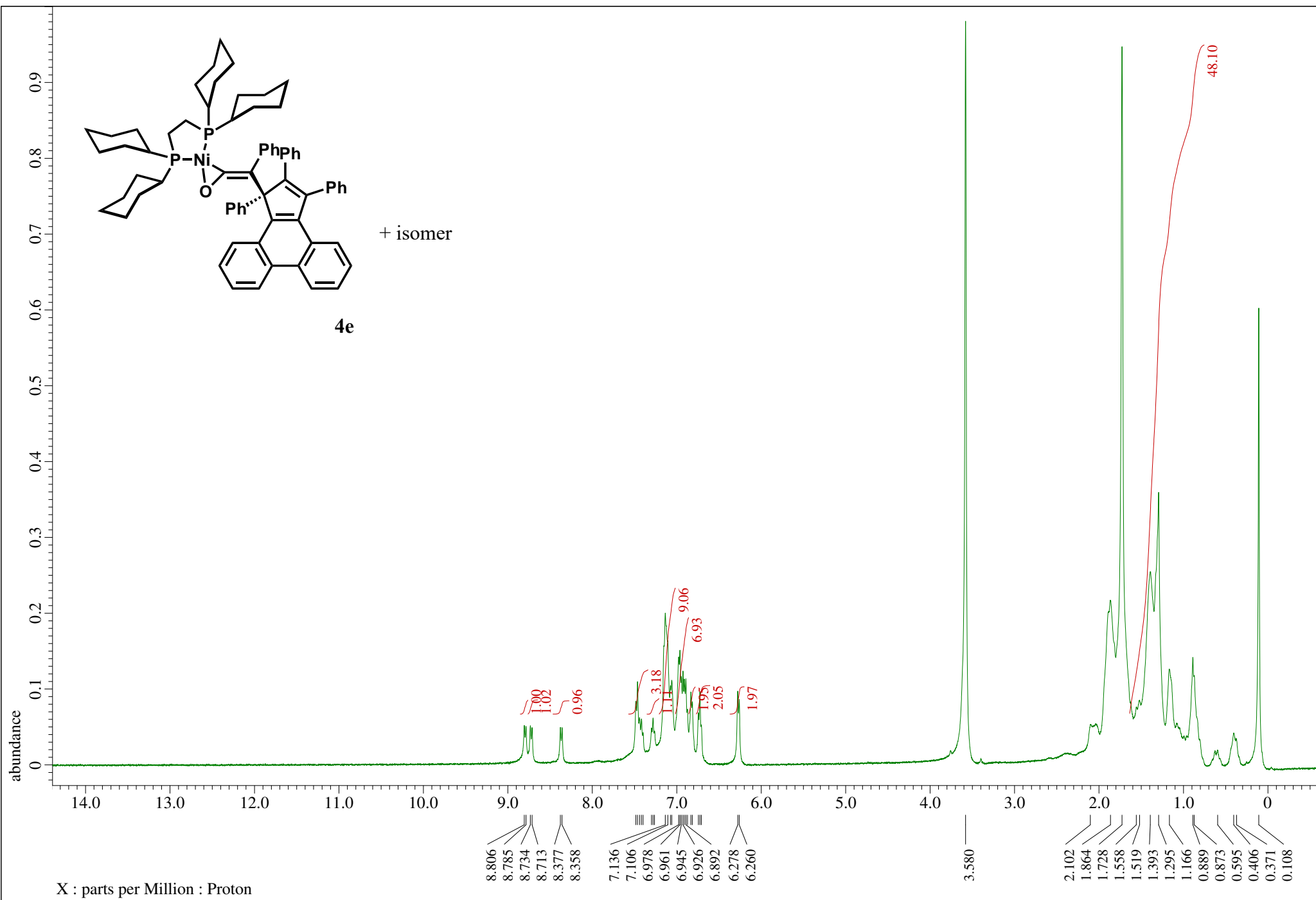


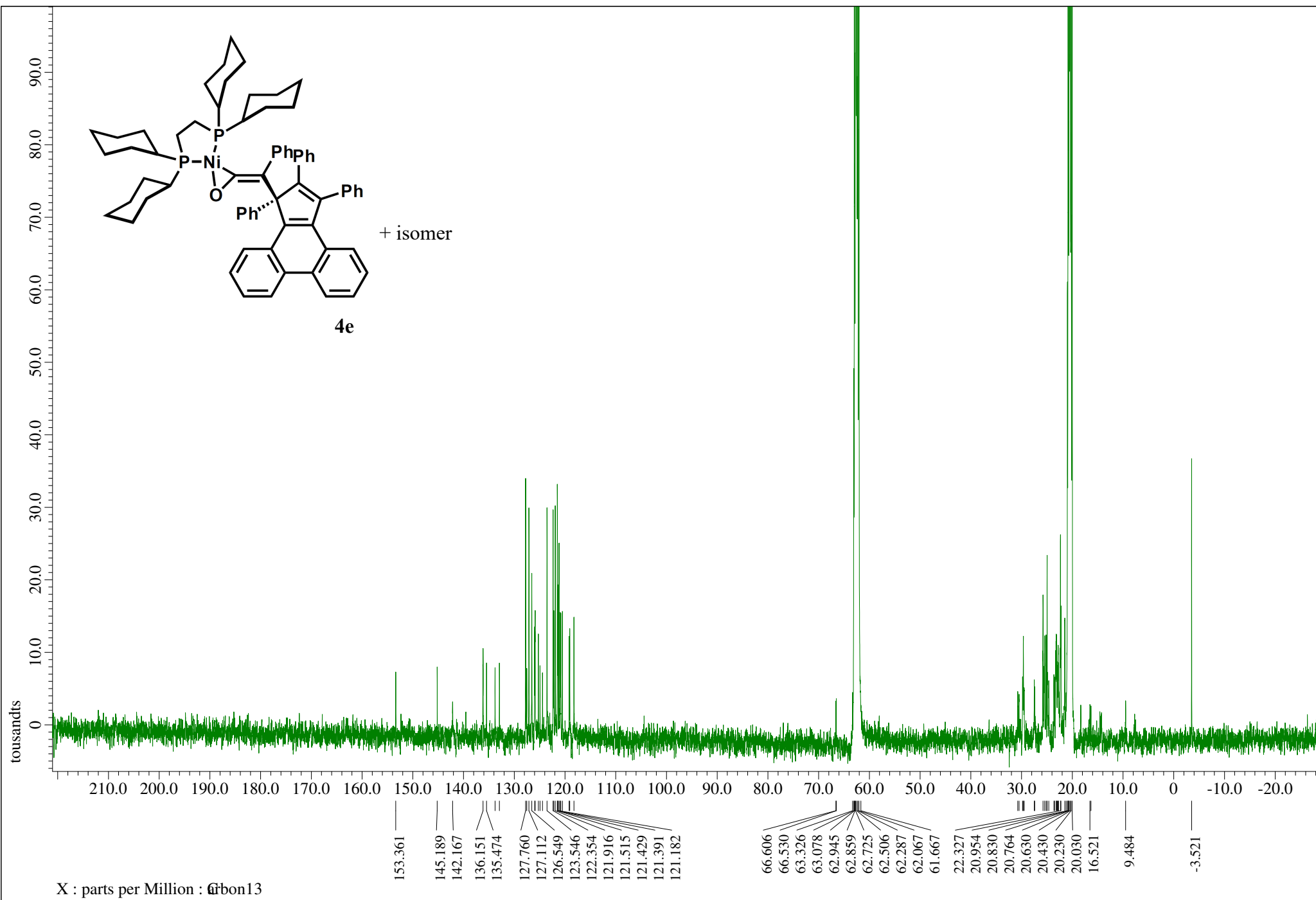


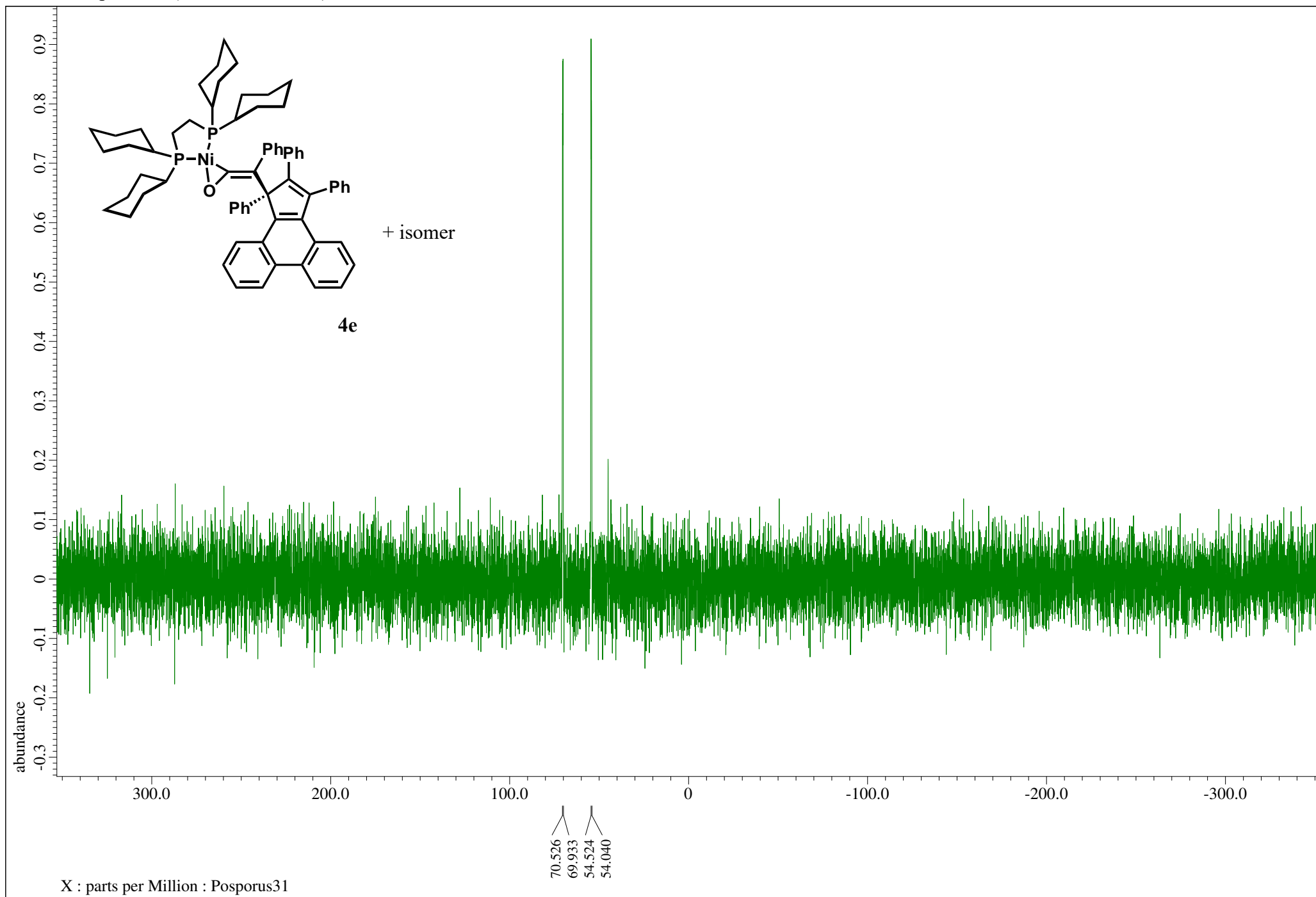




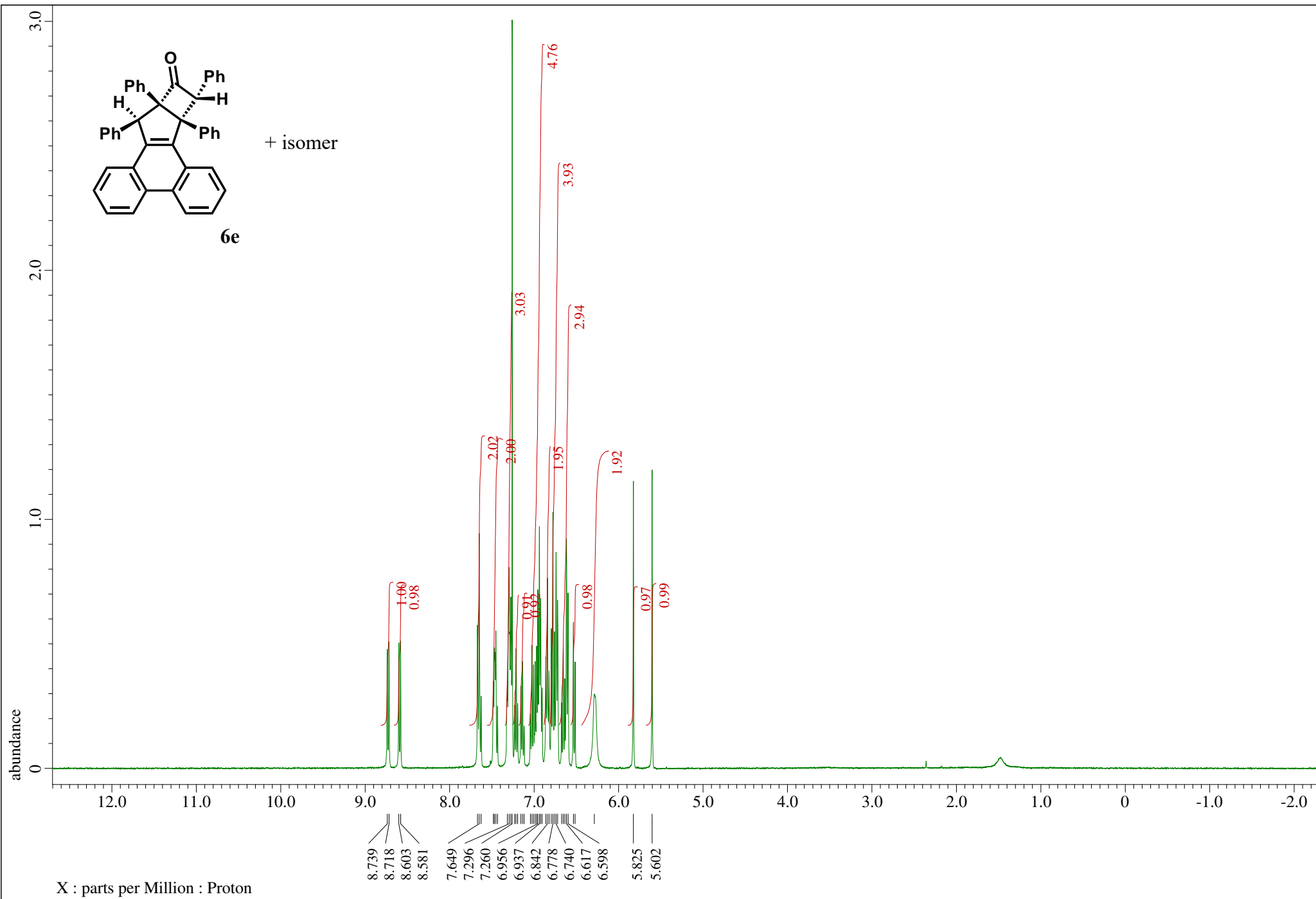


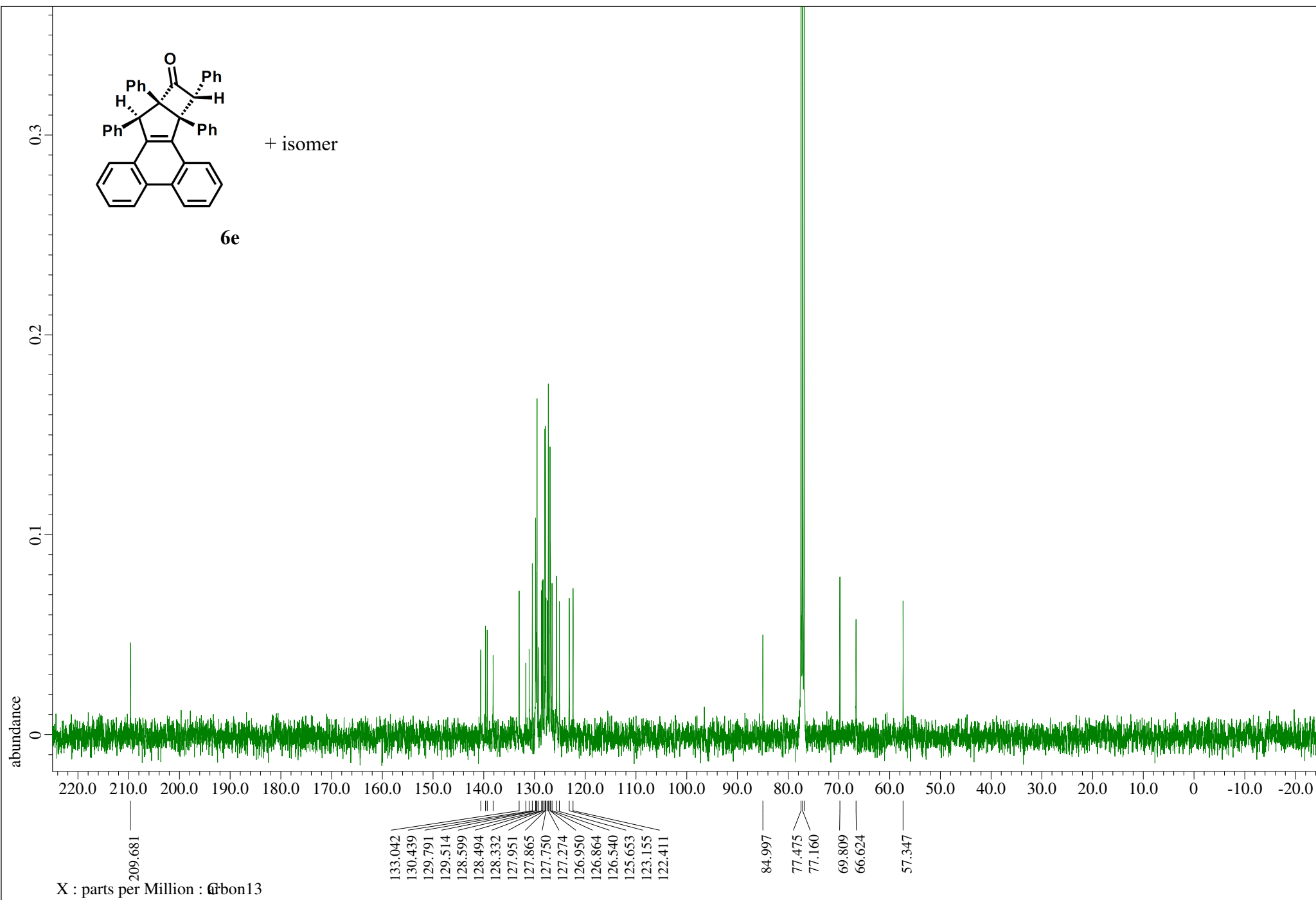






¹H NMR spectrum (400 MHz, CDCl₃) of **6e**





^1H NMR spectrum (400 MHz, CDCl_3) of **6e-d₂**

