

Synthesis and photodimerization of 2- and 2,3-disubstituted anthracenes: influence of steric interaction and London dispersion on diastereoselectivity

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1. ^1H and $^{13}\text{C}\{^1\text{H}\}$ spectra

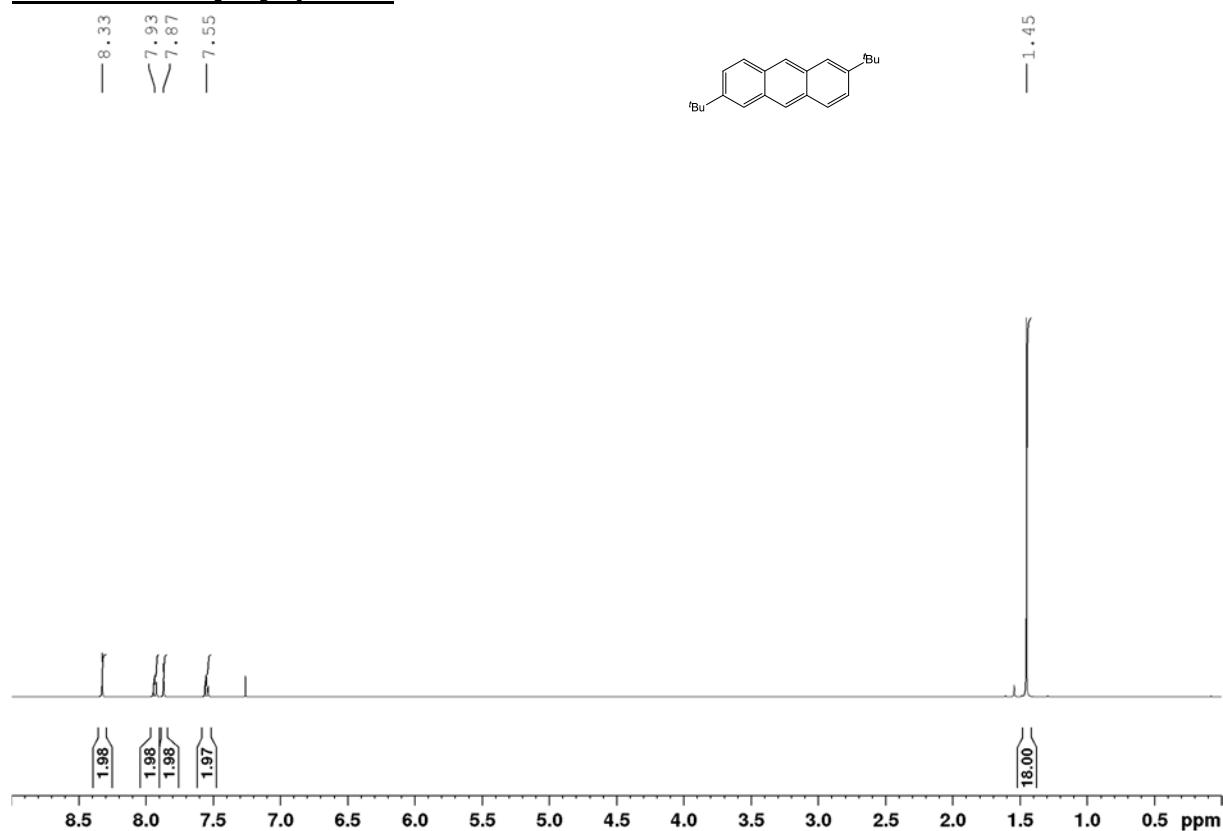


Figure S1. ^1H -NMR spectrum of **11** in CDCl_3

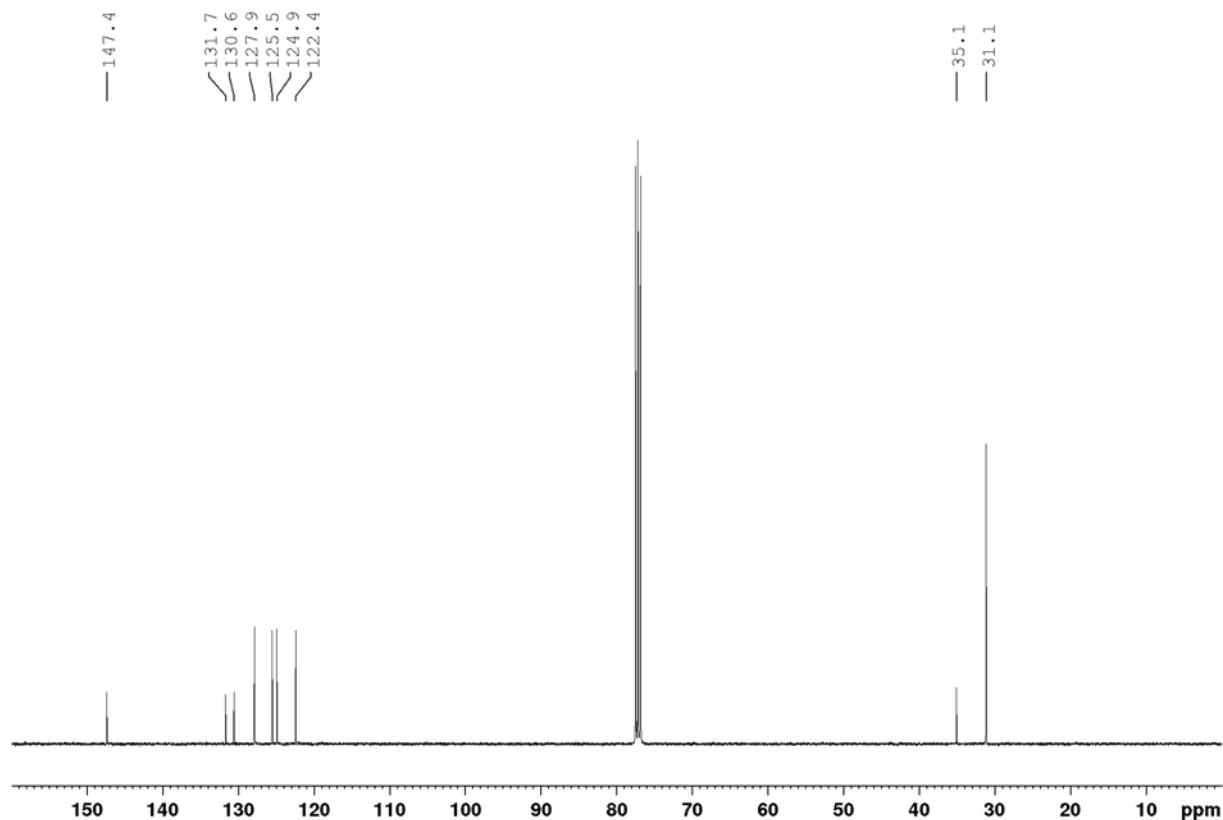


Figure S2. $^{13}\text{C}\{^1\text{H}\}$ -NMR spectrum of **11** in CDCl_3

Supporting Information (SI)

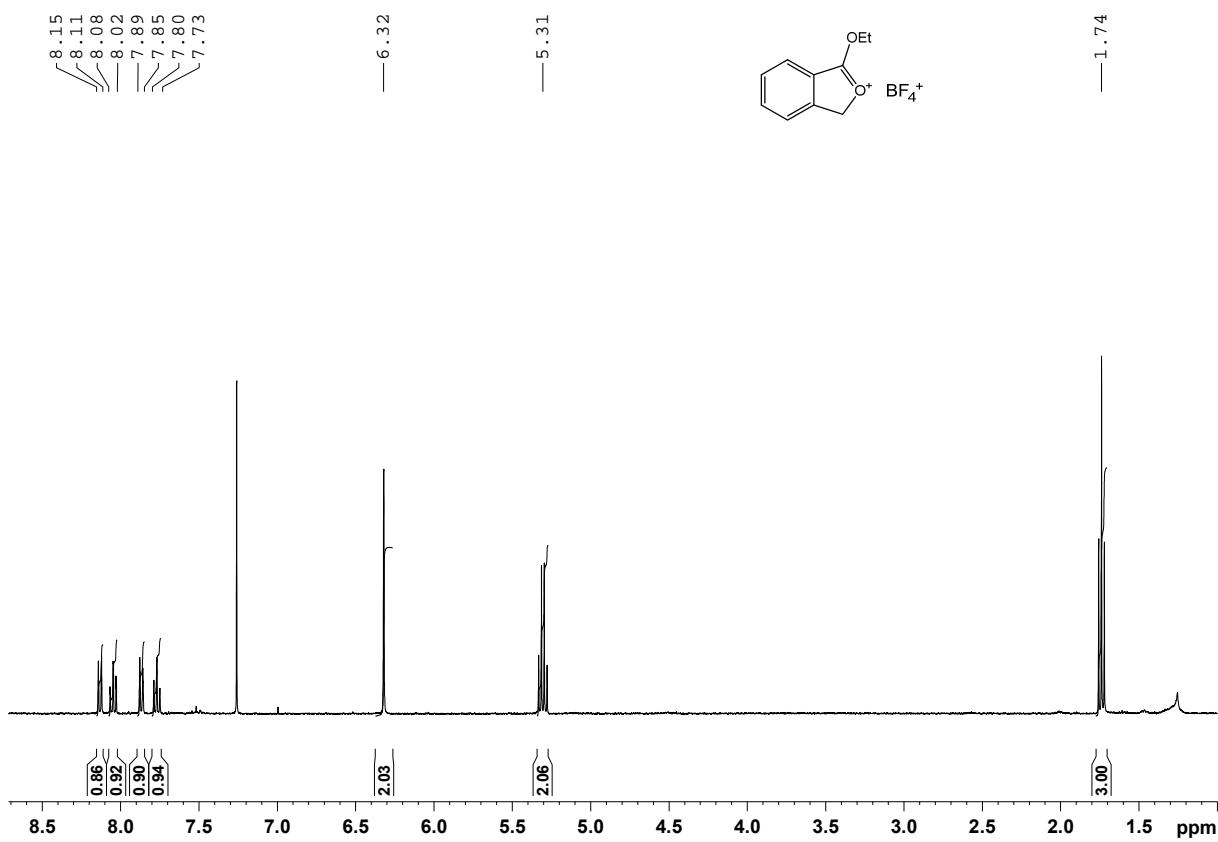


Figure S3. ¹H-NMR spectrum of **13** in CDCl₃

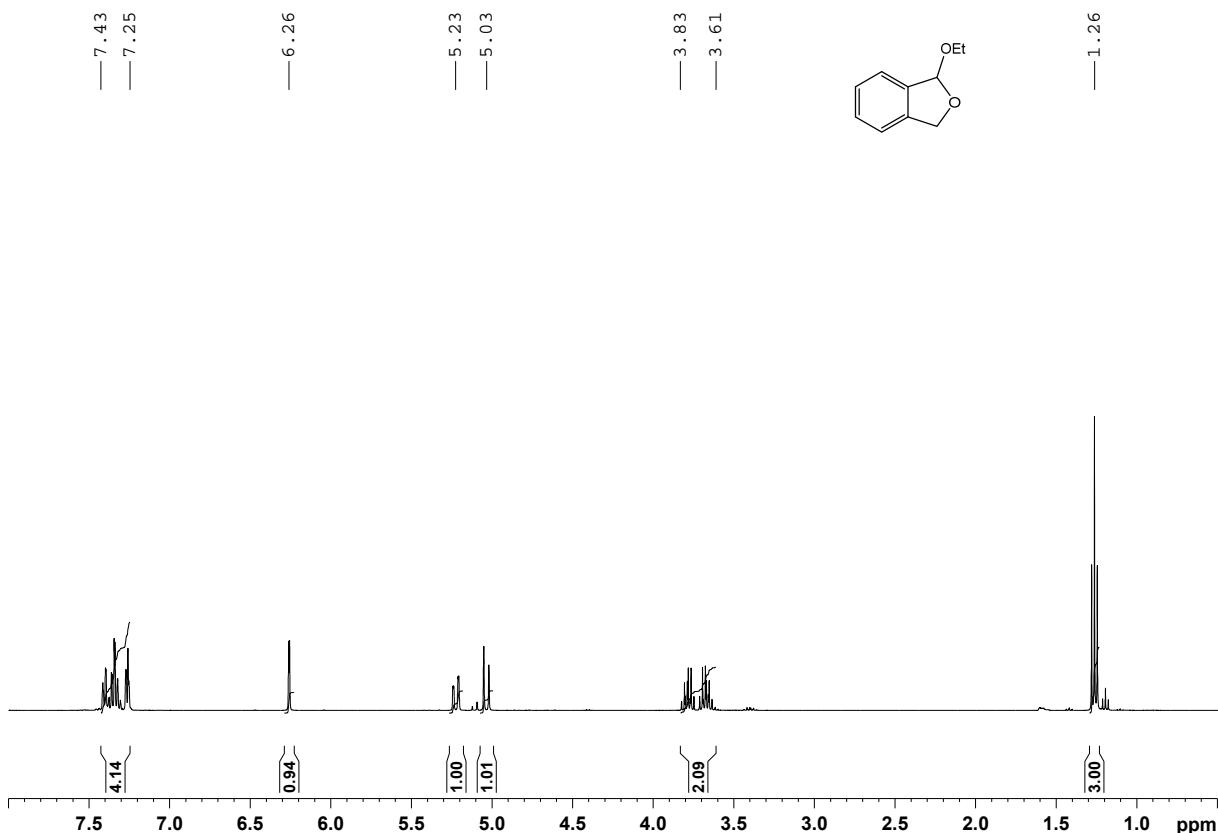


Figure S4. ¹H-NMR spectrum of **14** in CDCl₃

Supporting Information (SI)

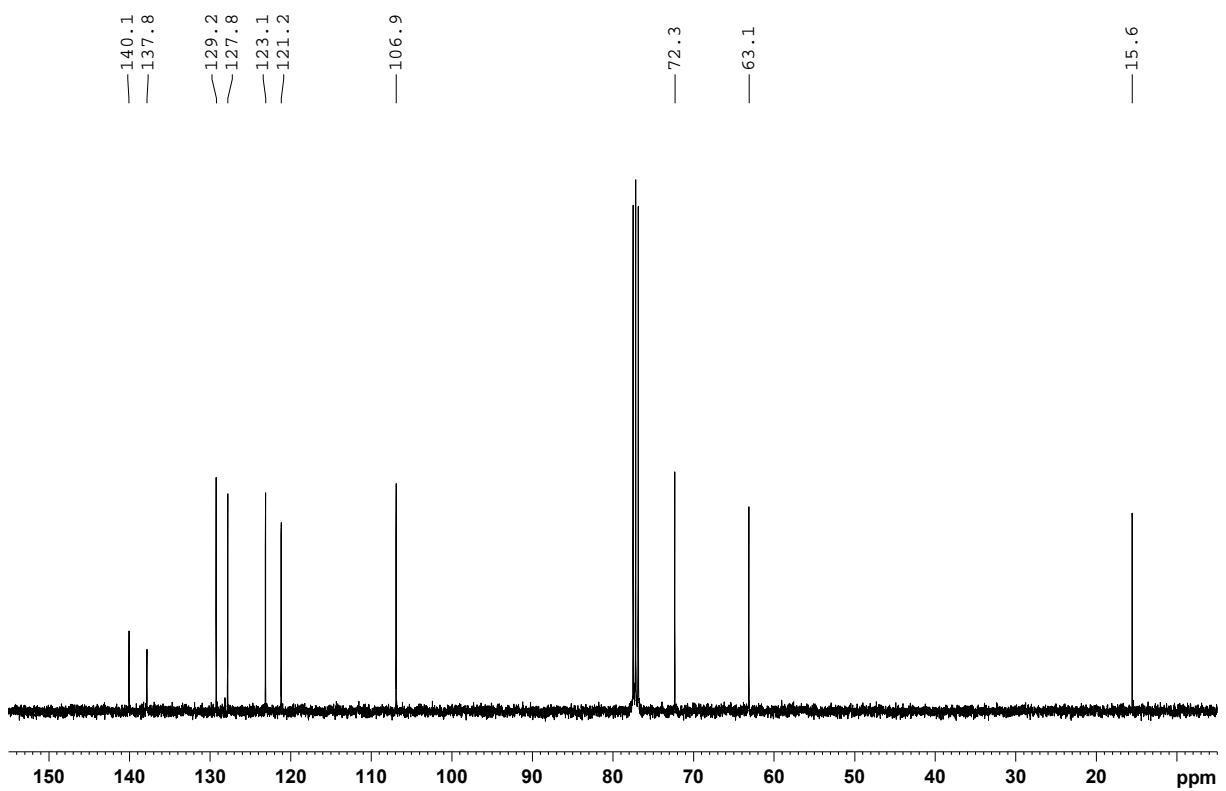


Figure S5. $^{13}\text{C}\{^1\text{H}\}$ -NMR spectrum of **14** in CDCl_3

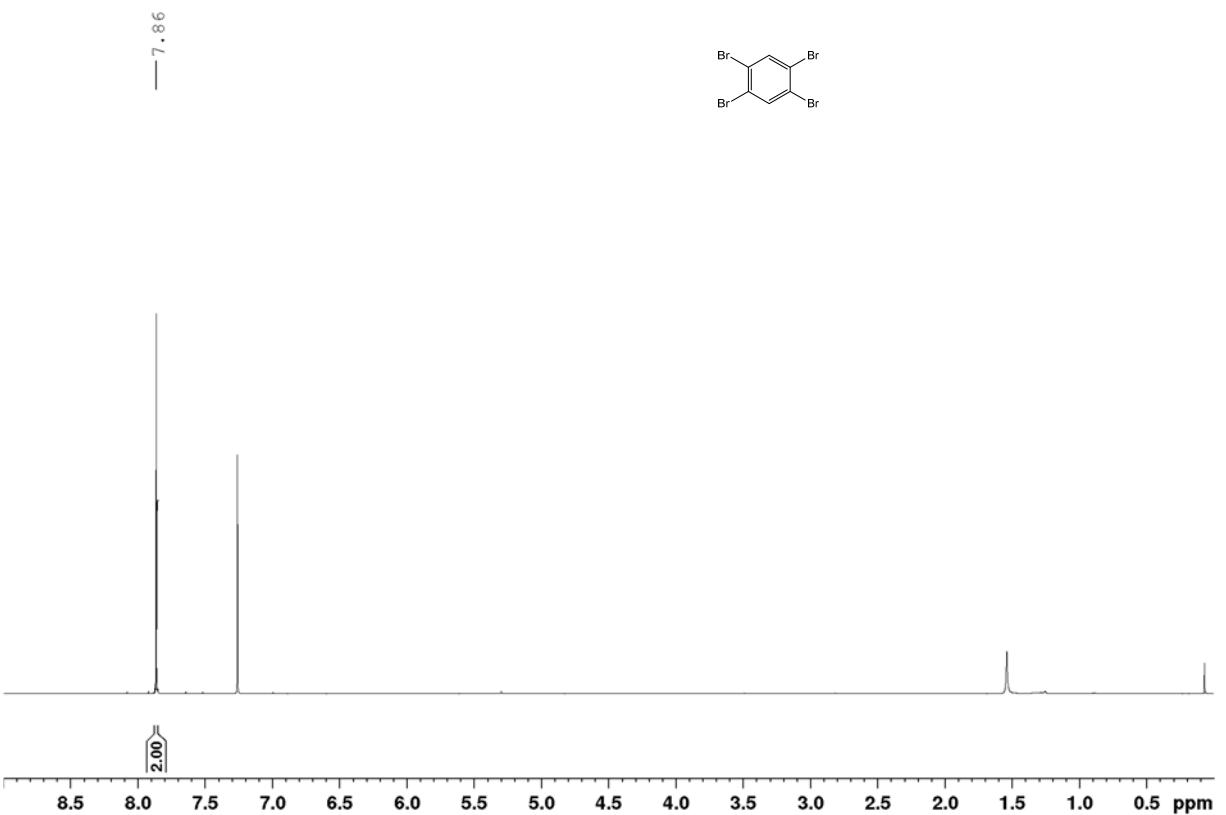


Figure S6. ^1H -NMR spectrum of **16** in CDCl_3

Supporting Information (SI)

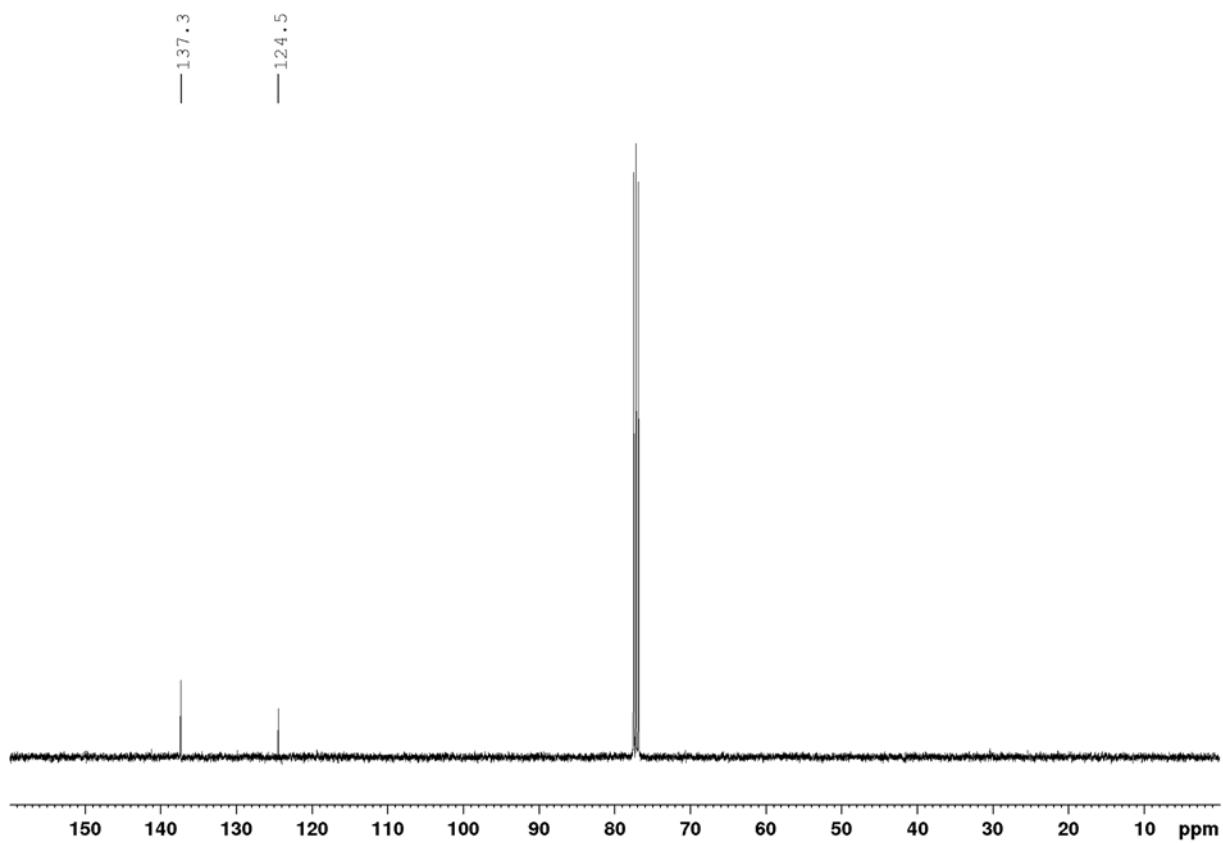


Figure S7. $^{13}\text{C}\{^1\text{H}\}$ -NMR spectrum of **16** in CDCl₃

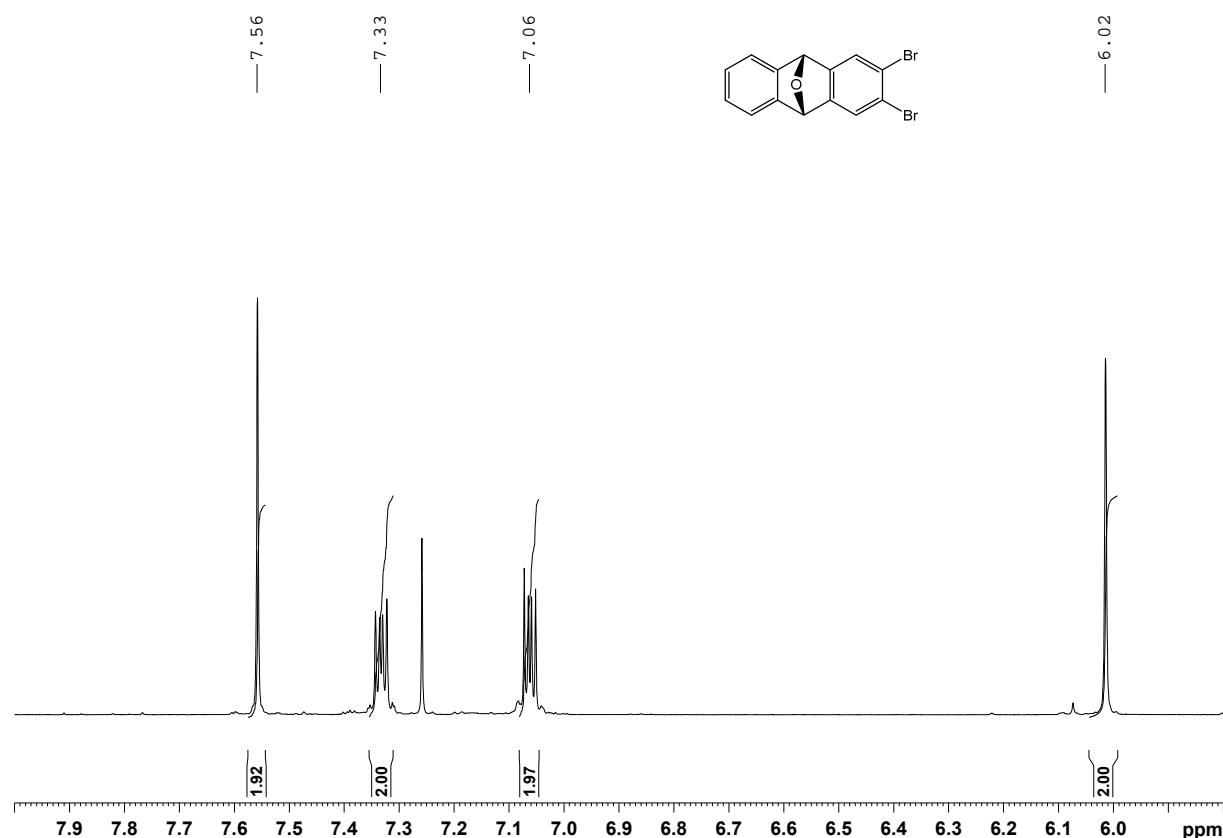


Figure S8. ^1H -NMR spectrum of **17** in CDCl₃

Supporting Information (SI)

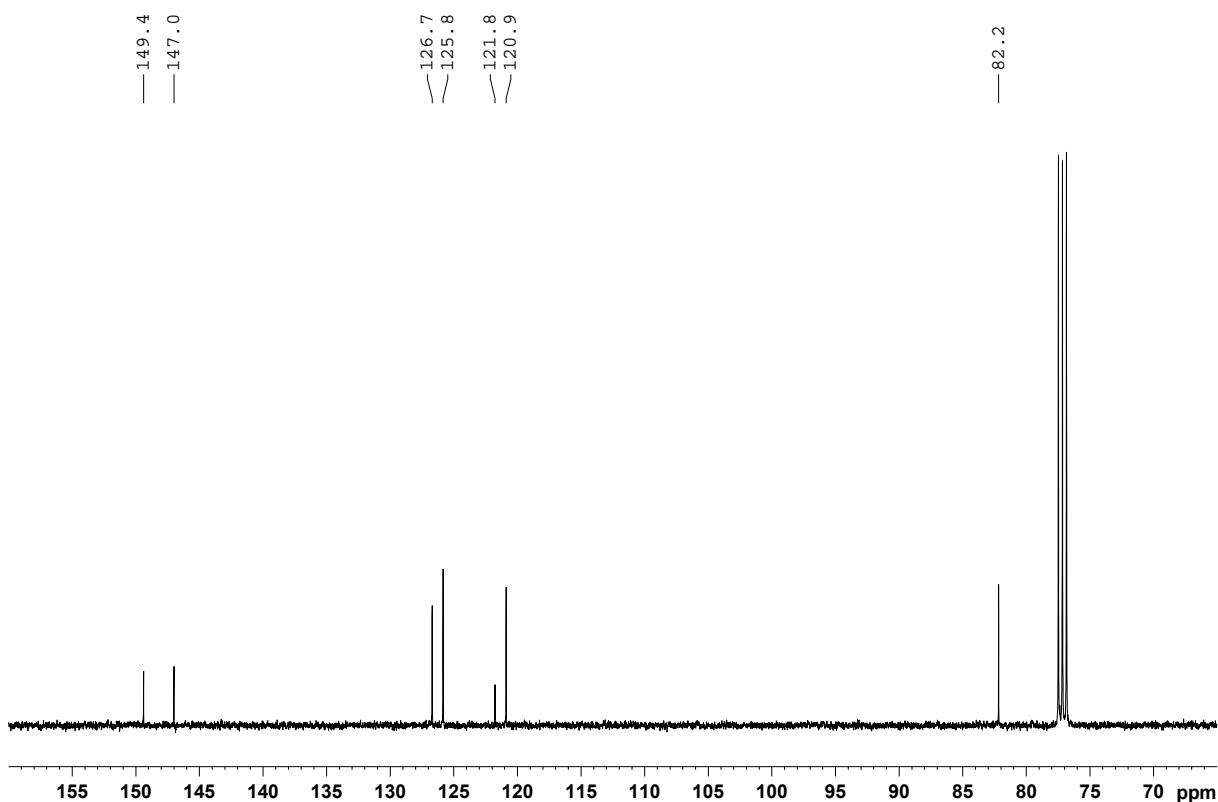


Figure S9. $^{13}\text{C}\{^1\text{H}\}$ -NMR spectrum of **17** in CDCl_3

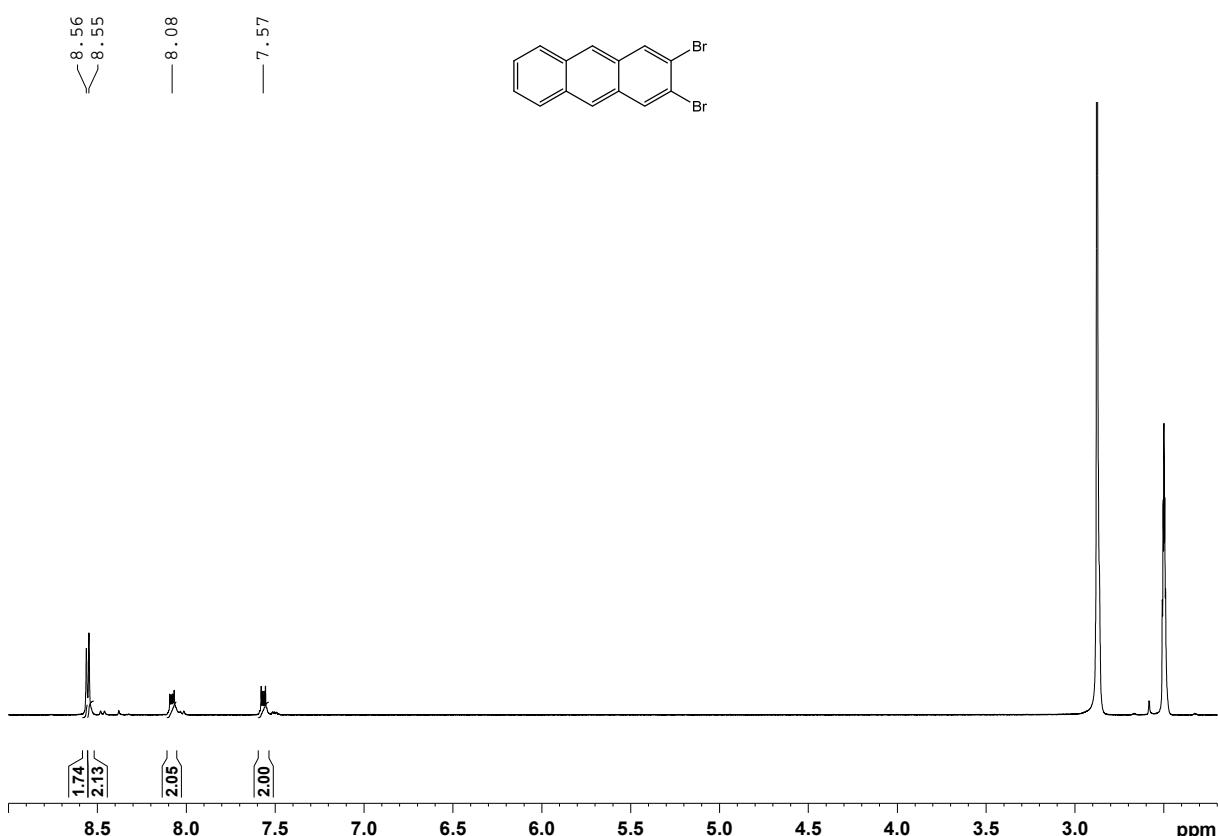


Figure S10. ^1H -NMR spectrum of **18** at 120°C in DMSO-d_6

Supporting Information (SI)

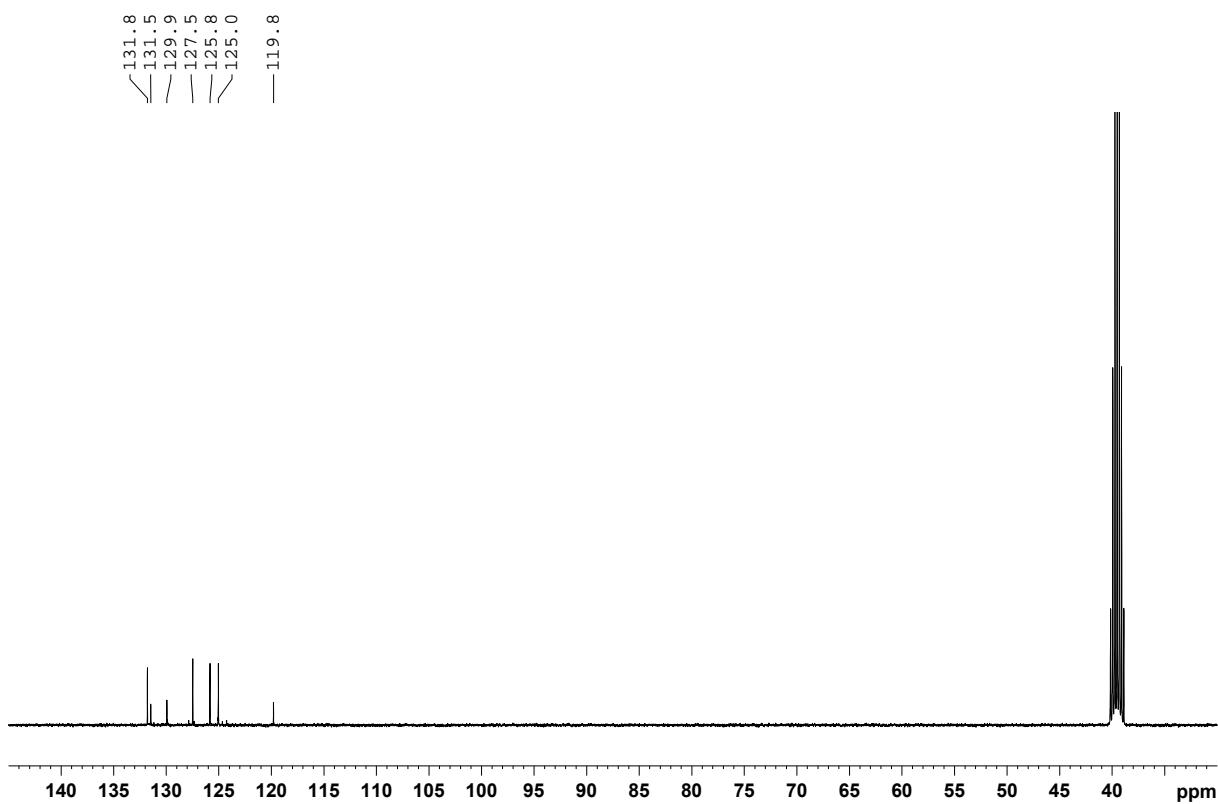


Figure S11. $^{13}\text{C}\{\text{H}\}$ -NMR spectrum of **18** at 120 °C in DMSO-d₆

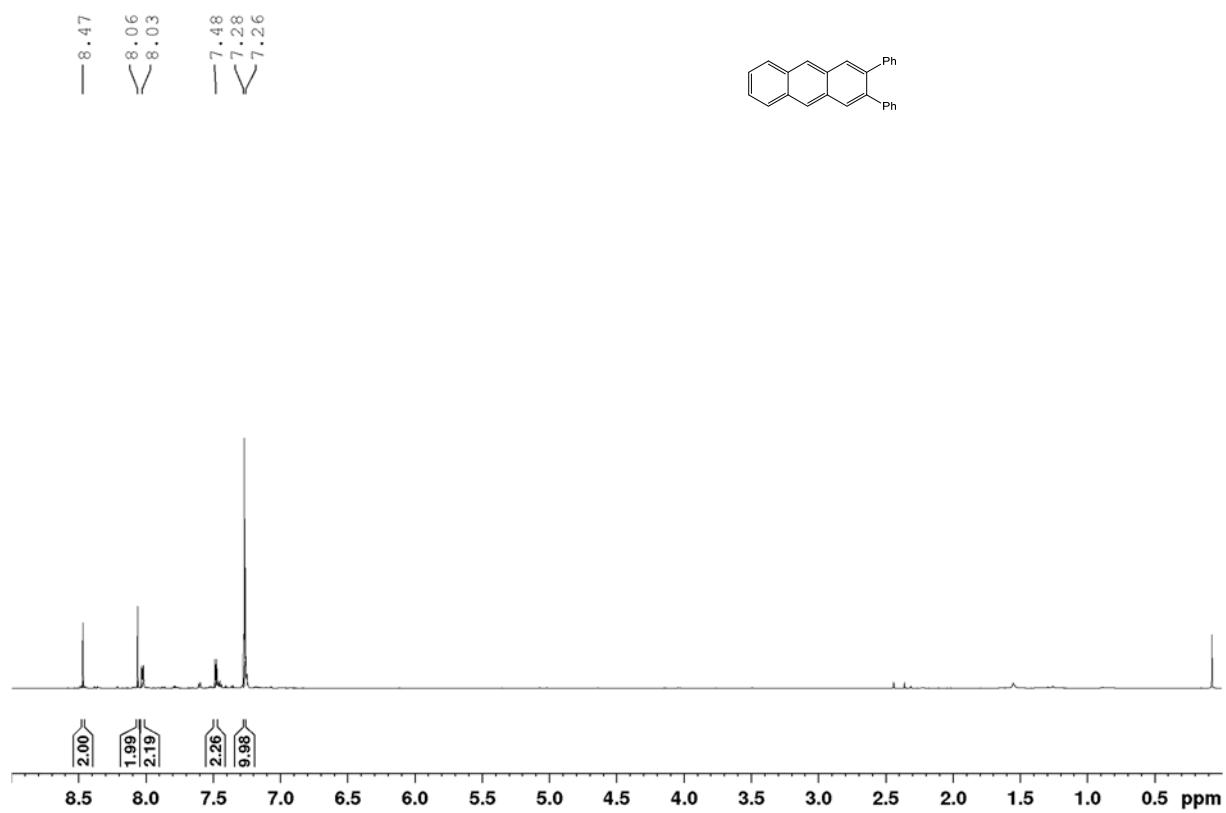


Figure S12. ^1H -NMR spectrum of **19** in CDCl₃

Supporting Information (SI)

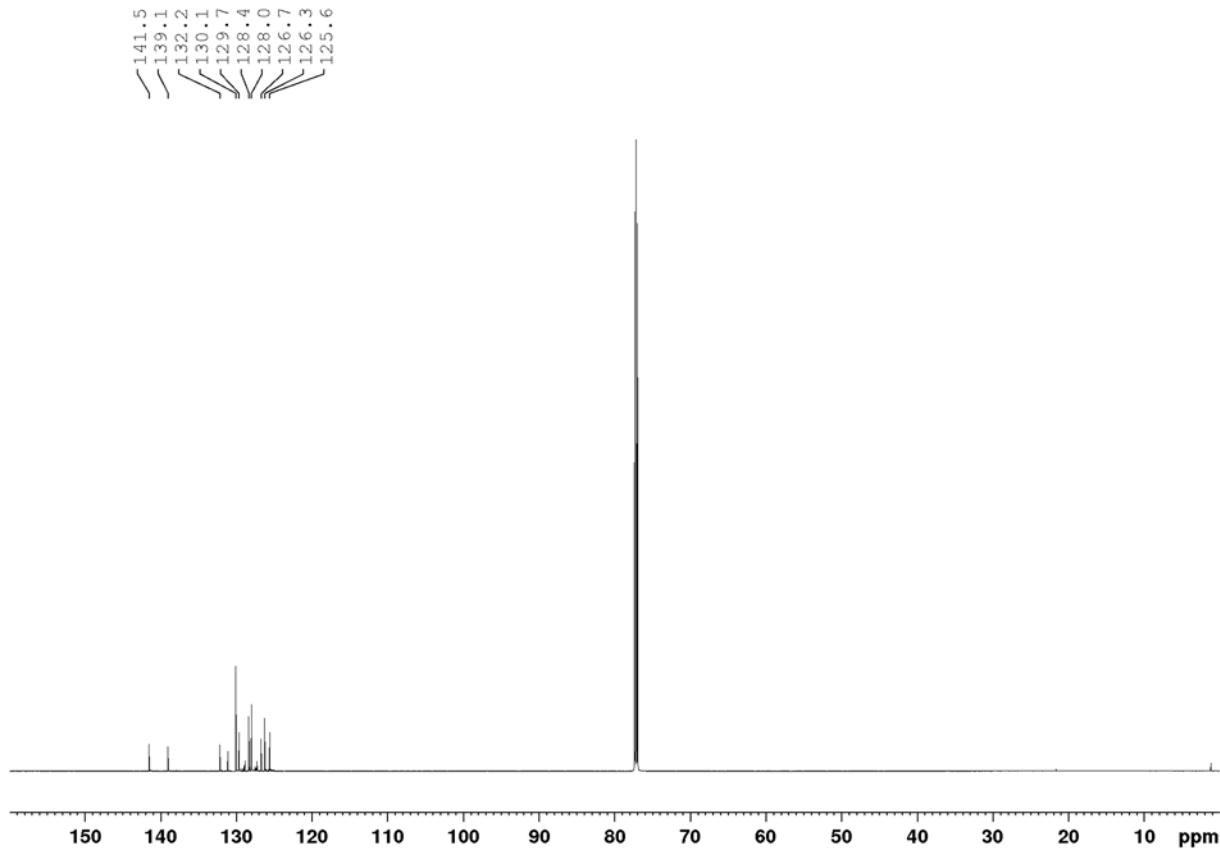


Figure S13. $^{13}\text{C}\{^1\text{H}\}$ -NMR spectrum of **19** in CDCl_3

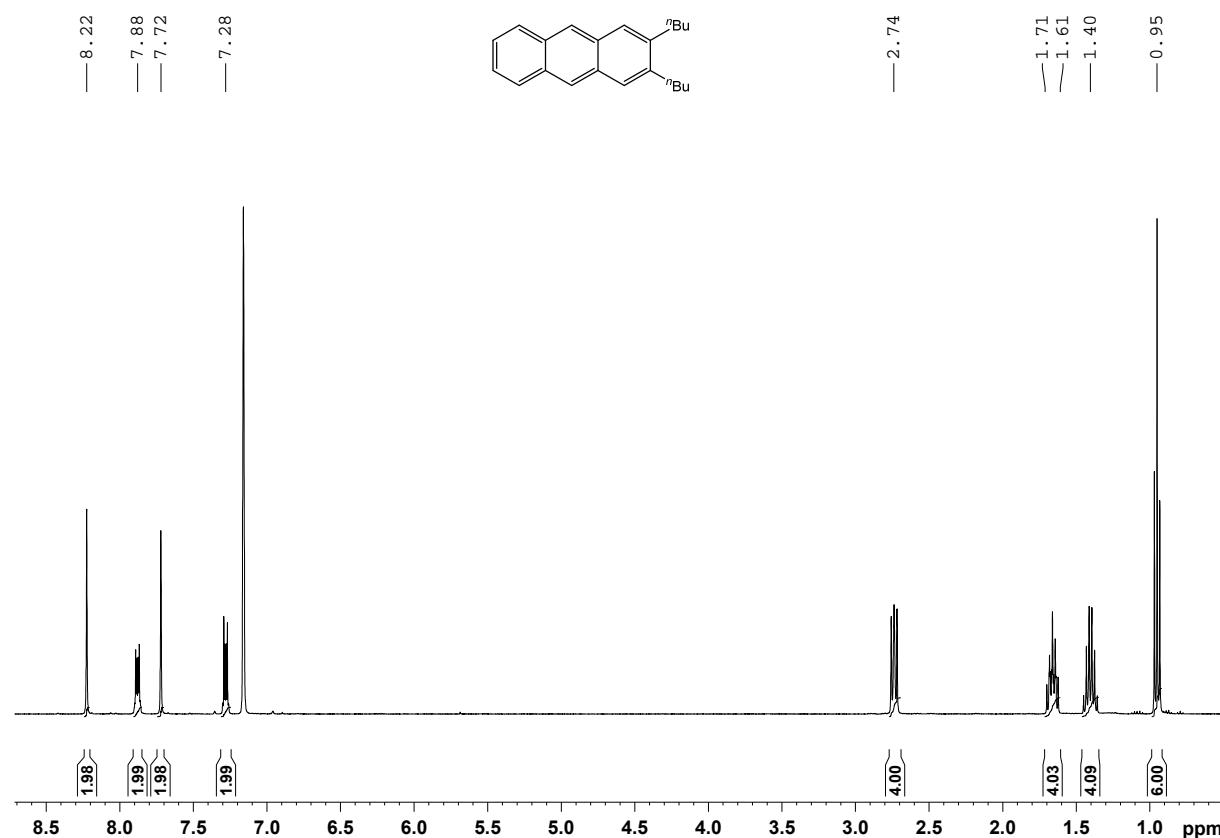


Figure S14. ^1H -NMR spectrum of **20** in C_6D_6

Supporting Information (SI)

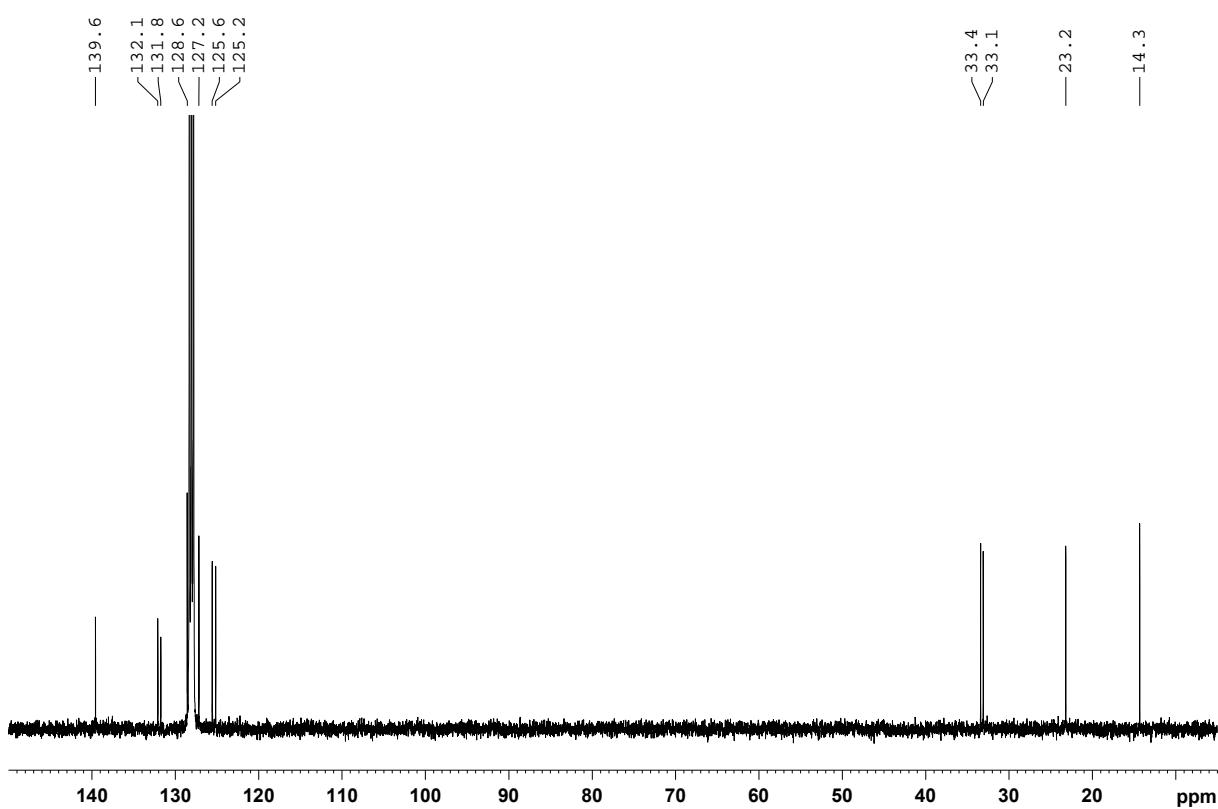


Figure S15. ¹³C{¹H}-NMR spectrum of **20** in C₆D₆

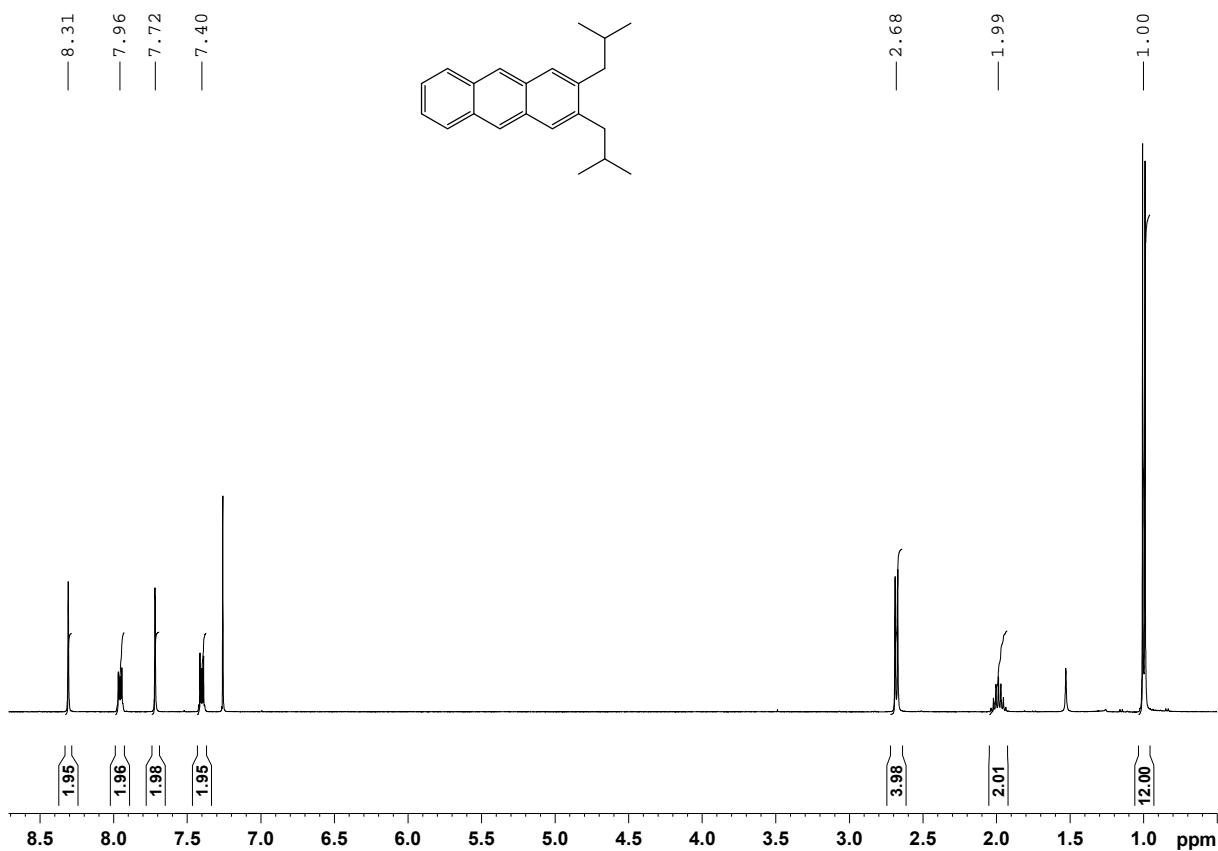


Figure S16. ¹H-NMR spectrum of **21** in CDCl₃

Supporting Information (SI)

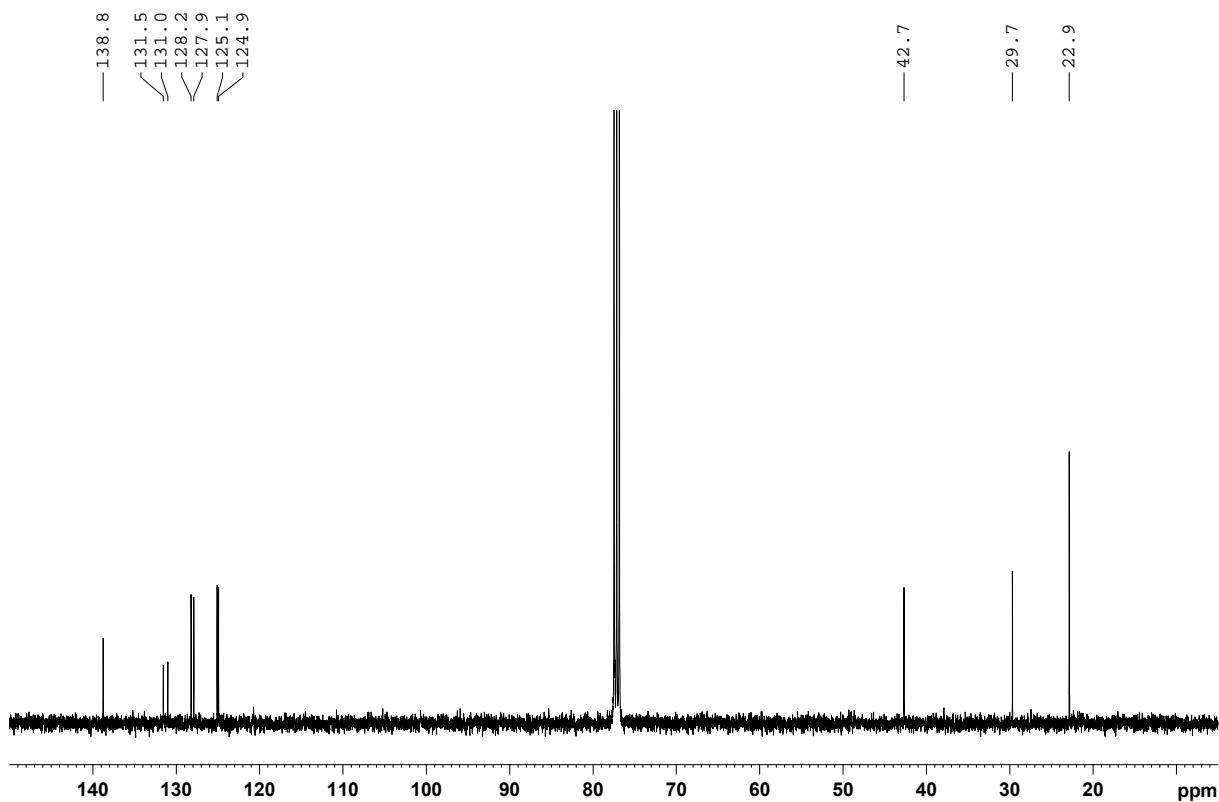


Figure S17. $^{13}\text{C}\{^1\text{H}\}$ -NMR spectrum of **21** in CDCl_3

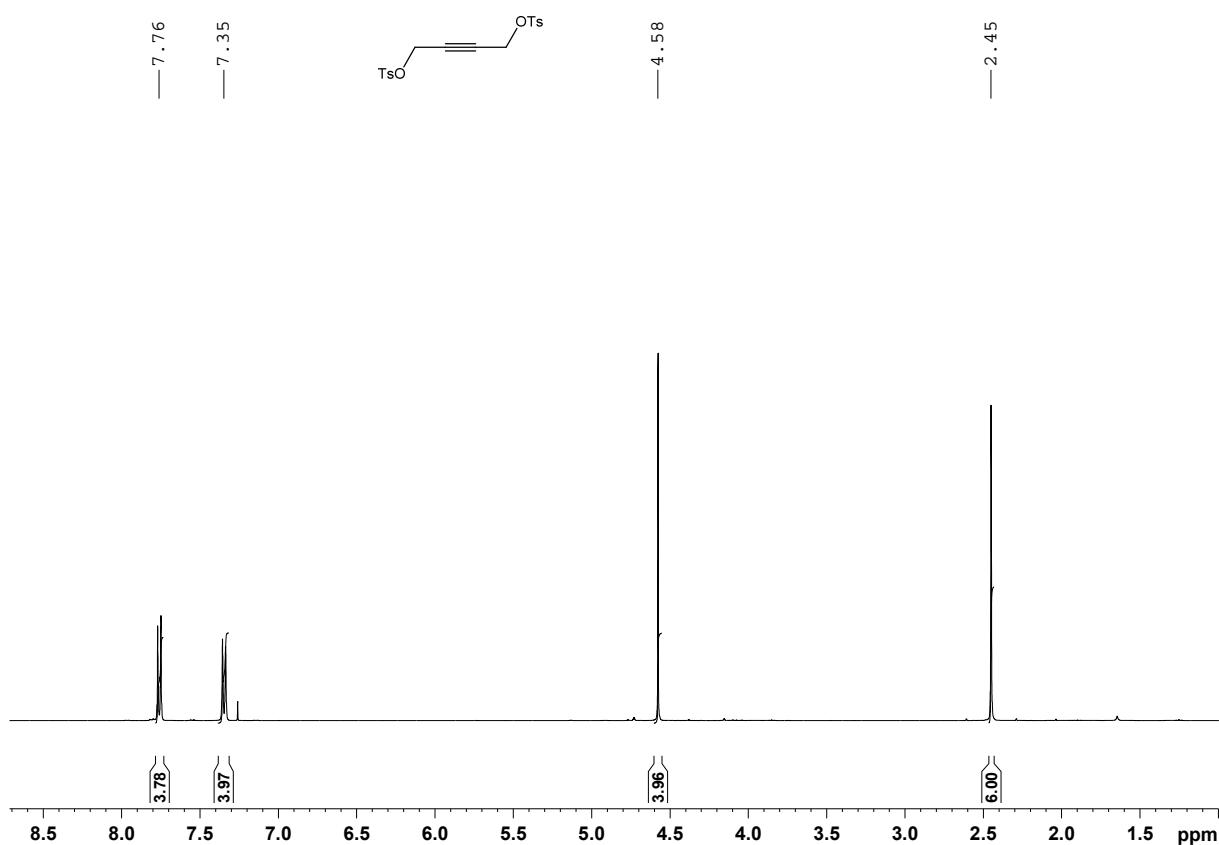


Figure S18. ^1H -NMR spectrum of **25** in CDCl_3

Supporting Information (SI)

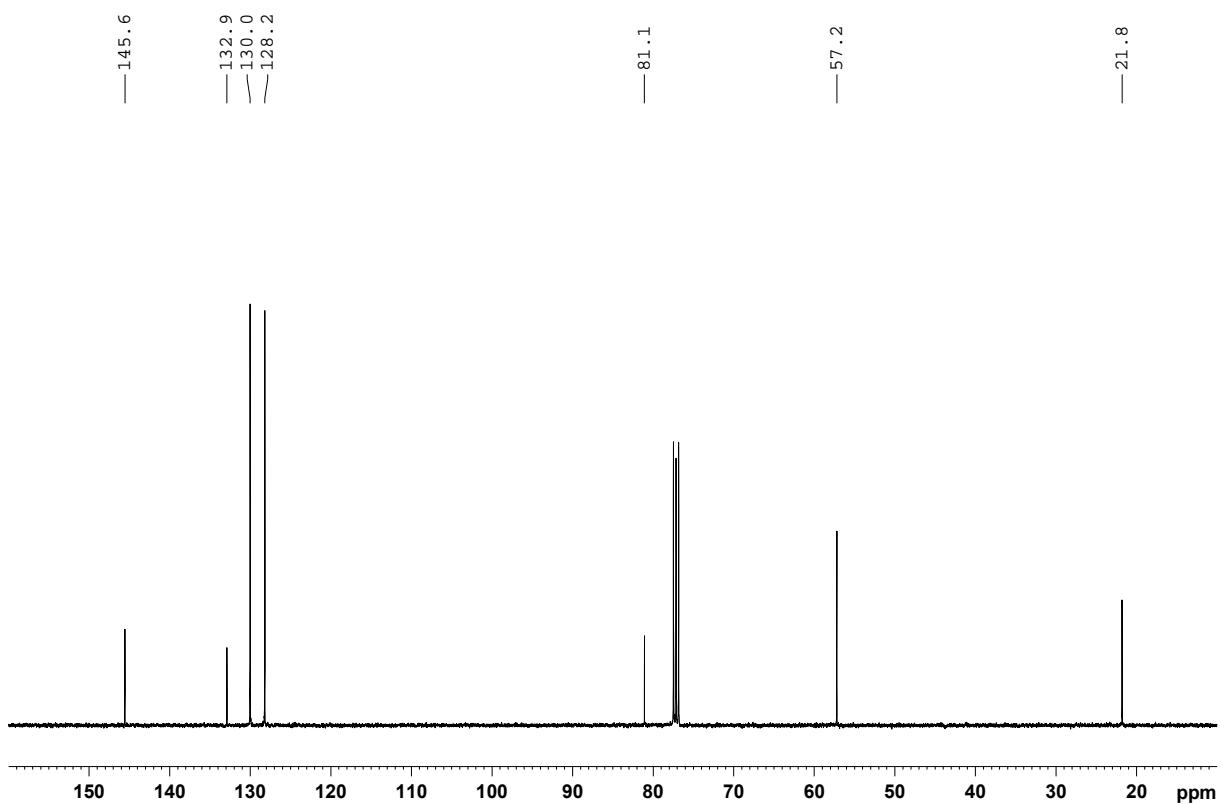


Figure S19. $^{13}\text{C}\{^1\text{H}\}$ -NMR spectrum of **25** in CDCl_3

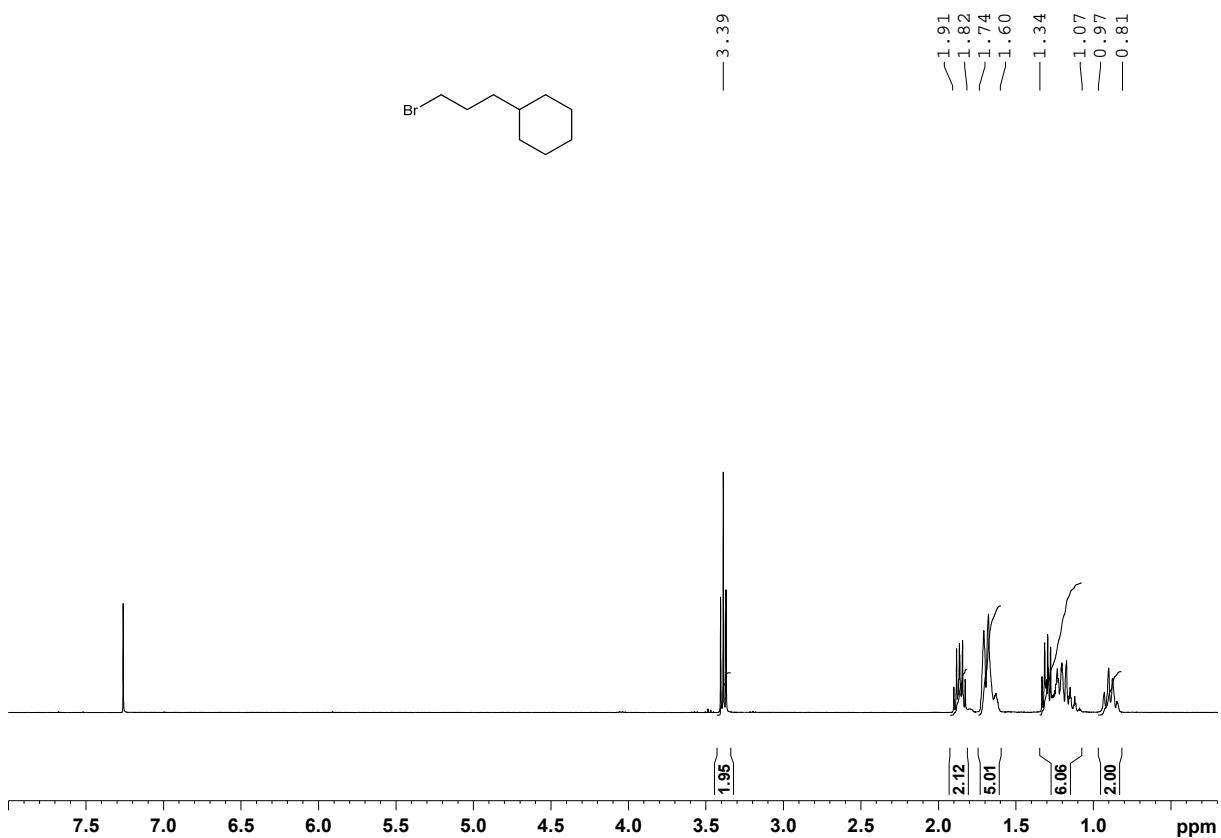


Figure S20. ^1H -NMR spectrum of **26** in CDCl_3

Supporting Information (SI)

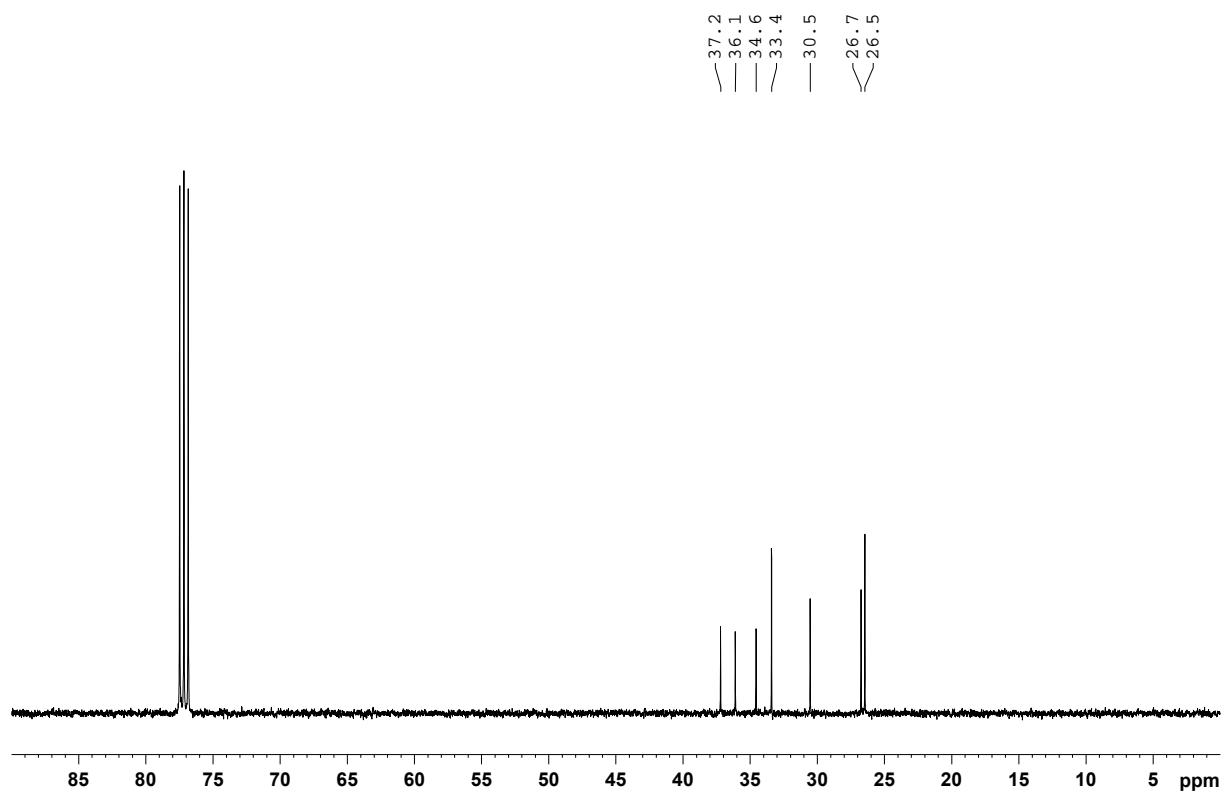


Figure S21. $^{13}\text{C}\{\text{H}\}$ -NMR spectrum of **26** in CDCl_3

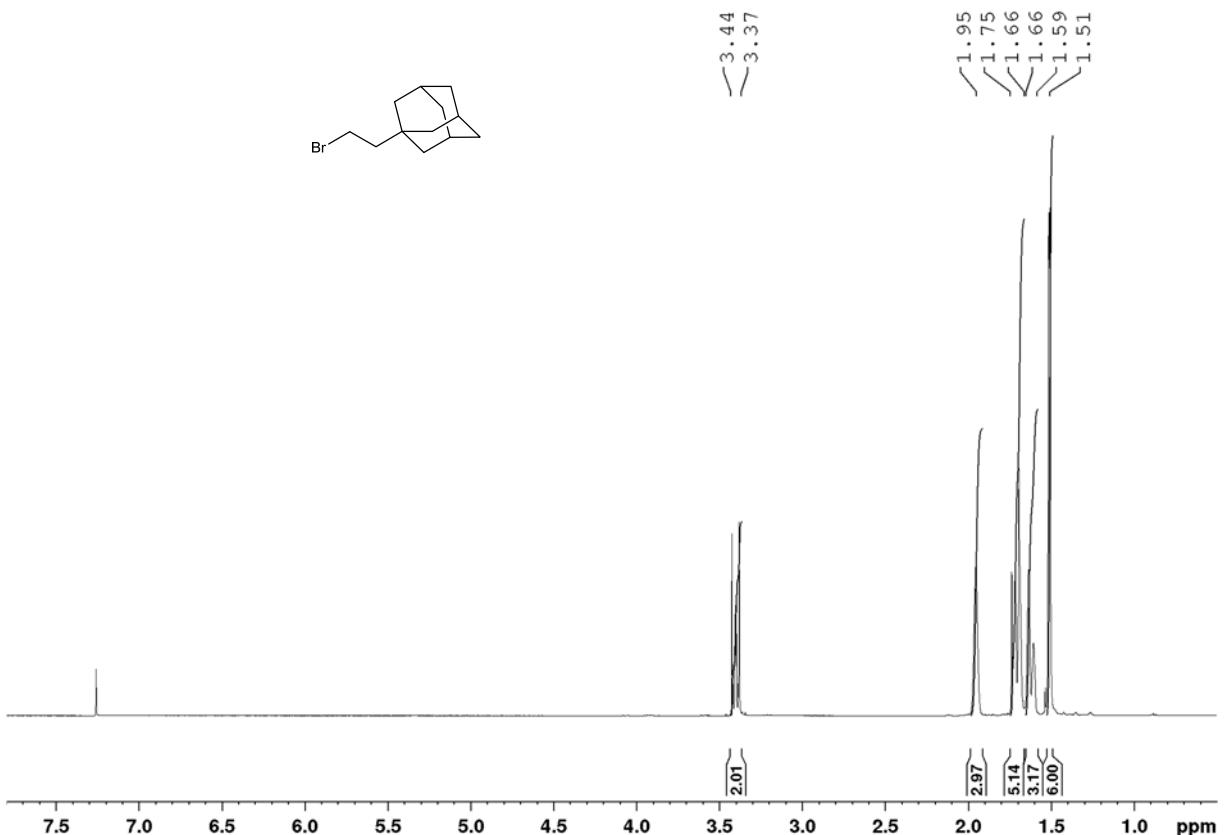


Figure S22. ^1H -NMR spectrum of **27** in CDCl_3

Supporting Information (SI)

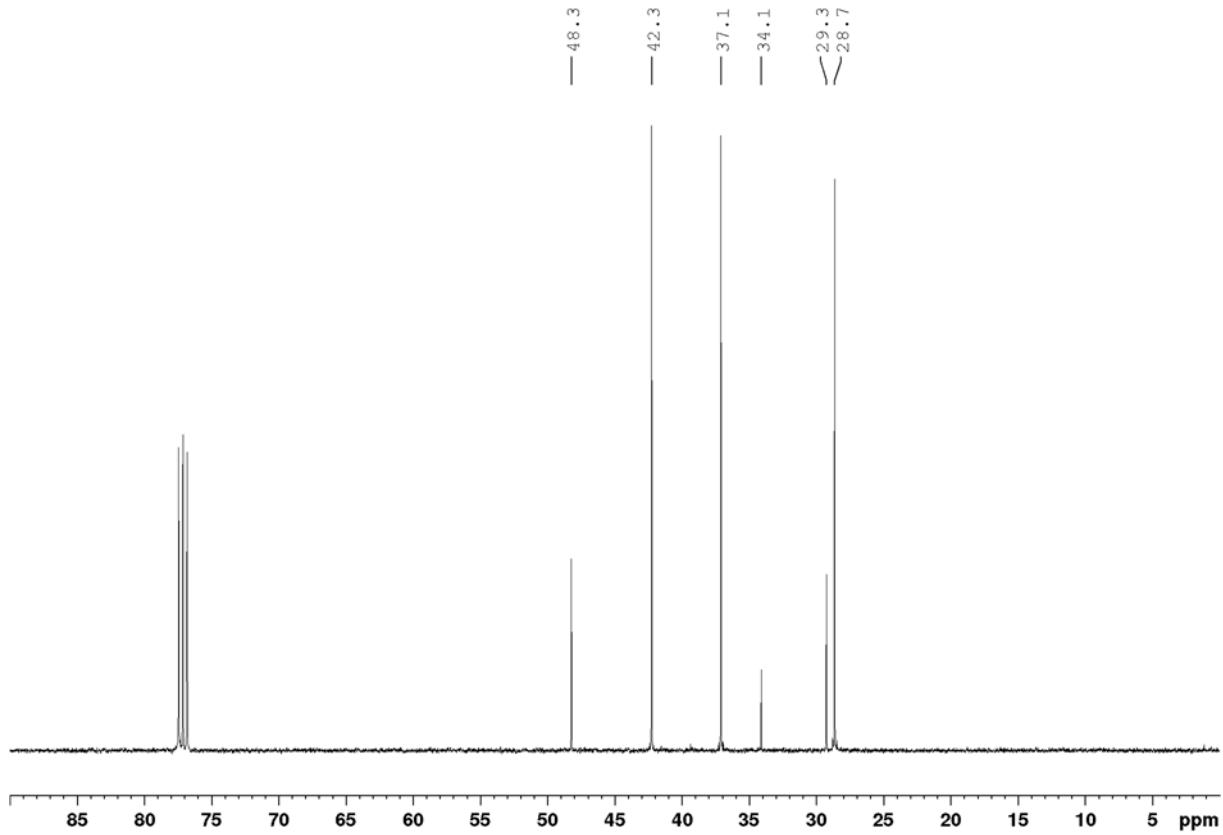


Figure S23. $^{13}\text{C}\{^1\text{H}\}$ -NMR spectrum of **27** in CDCl_3

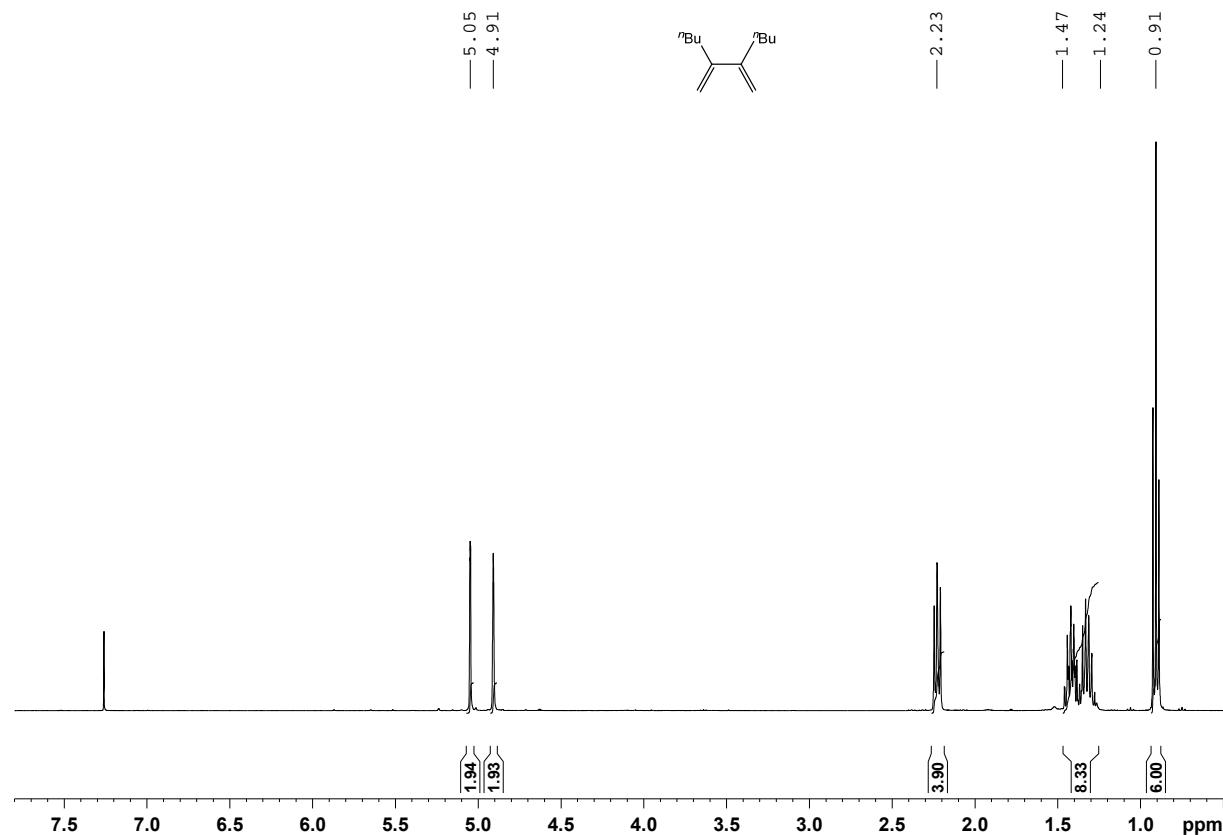


Figure S24. ^1H -NMR spectrum of **28a** in CDCl_3

Supporting Information (SI)

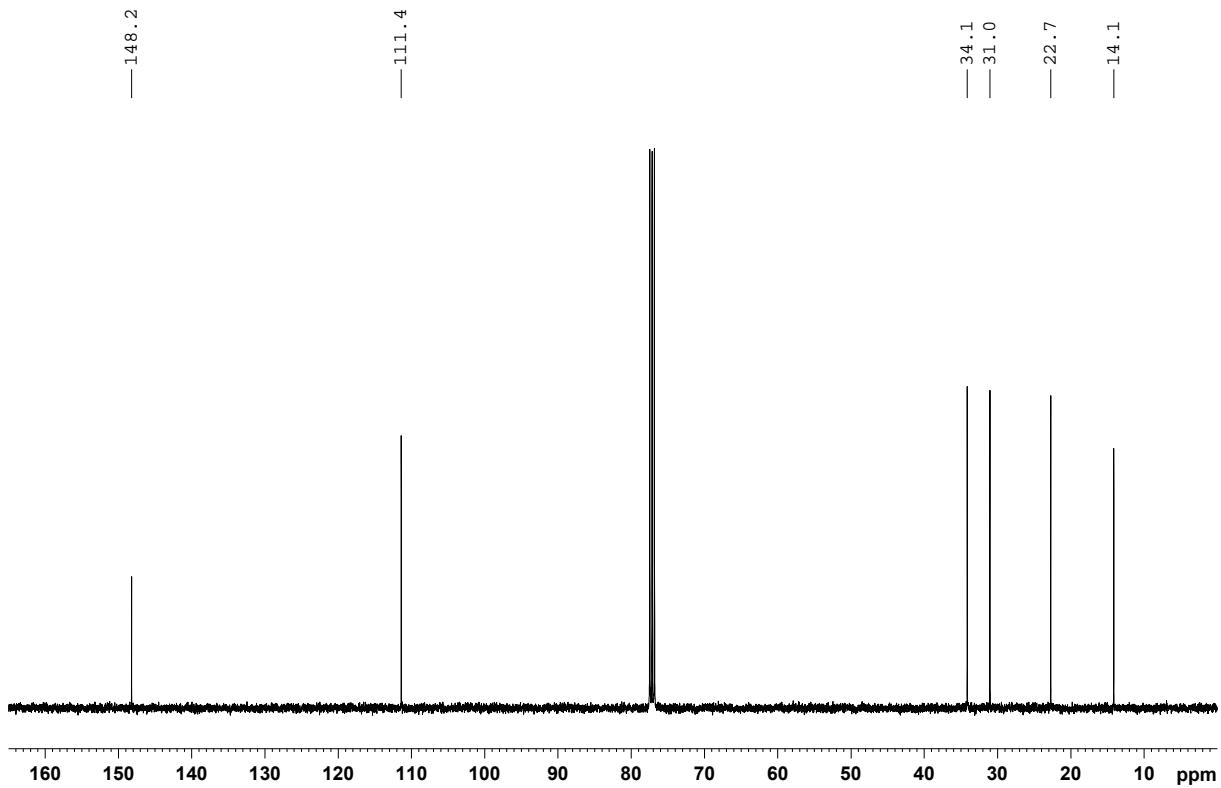


Figure S25. $^{13}\text{C}\{\text{H}\}$ -NMR spectrum of **28a** in CDCl_3

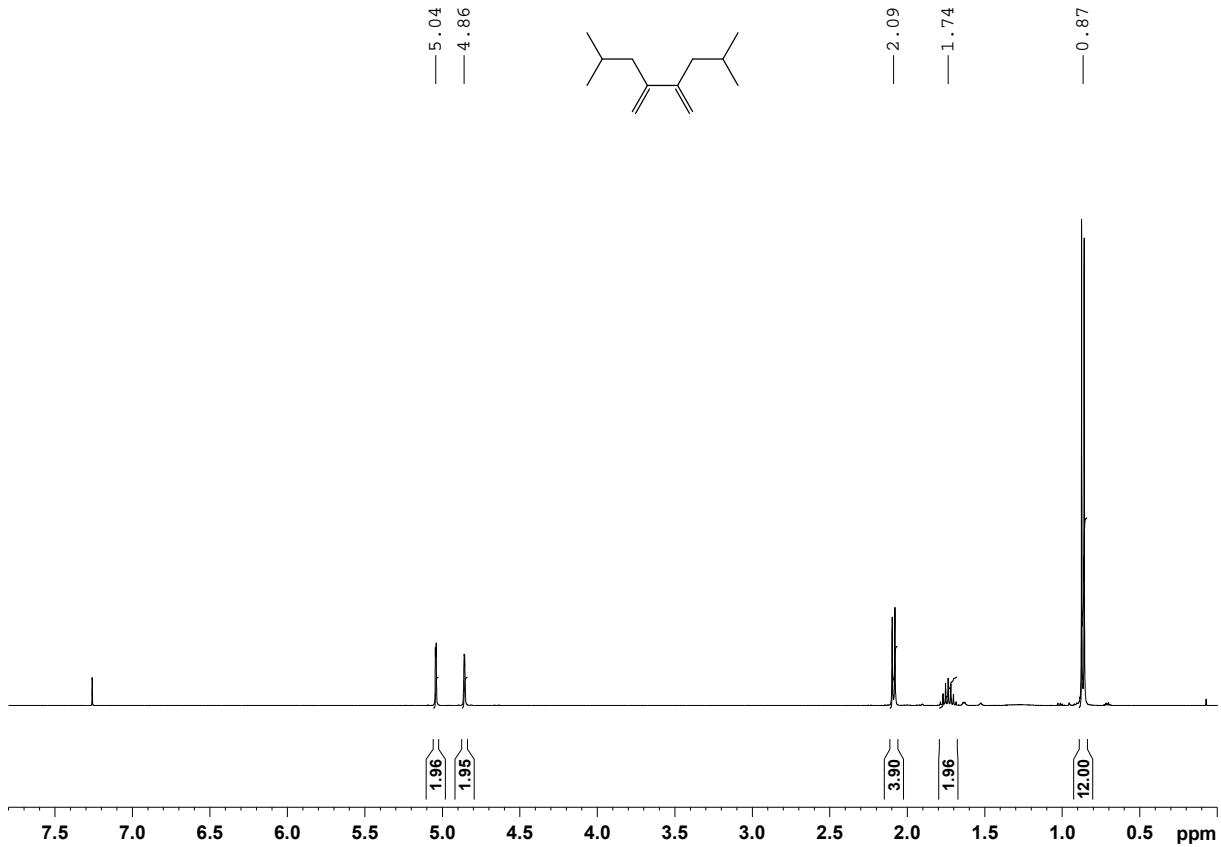


Figure S26. ^1H -NMR spectrum of **28b** in CDCl_3

Supporting Information (SI)

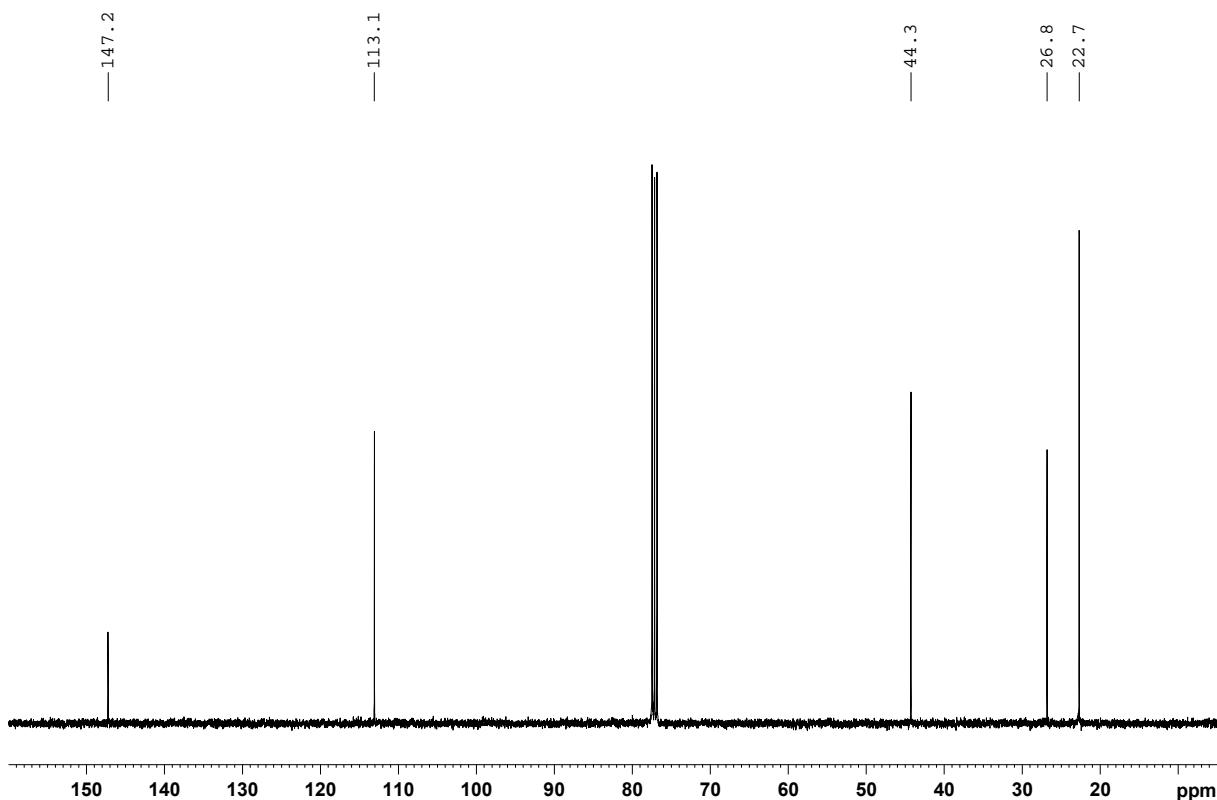


Figure S27. $^{13}\text{C}\{^1\text{H}\}$ -NMR spectrum of **28b** in CDCl_3

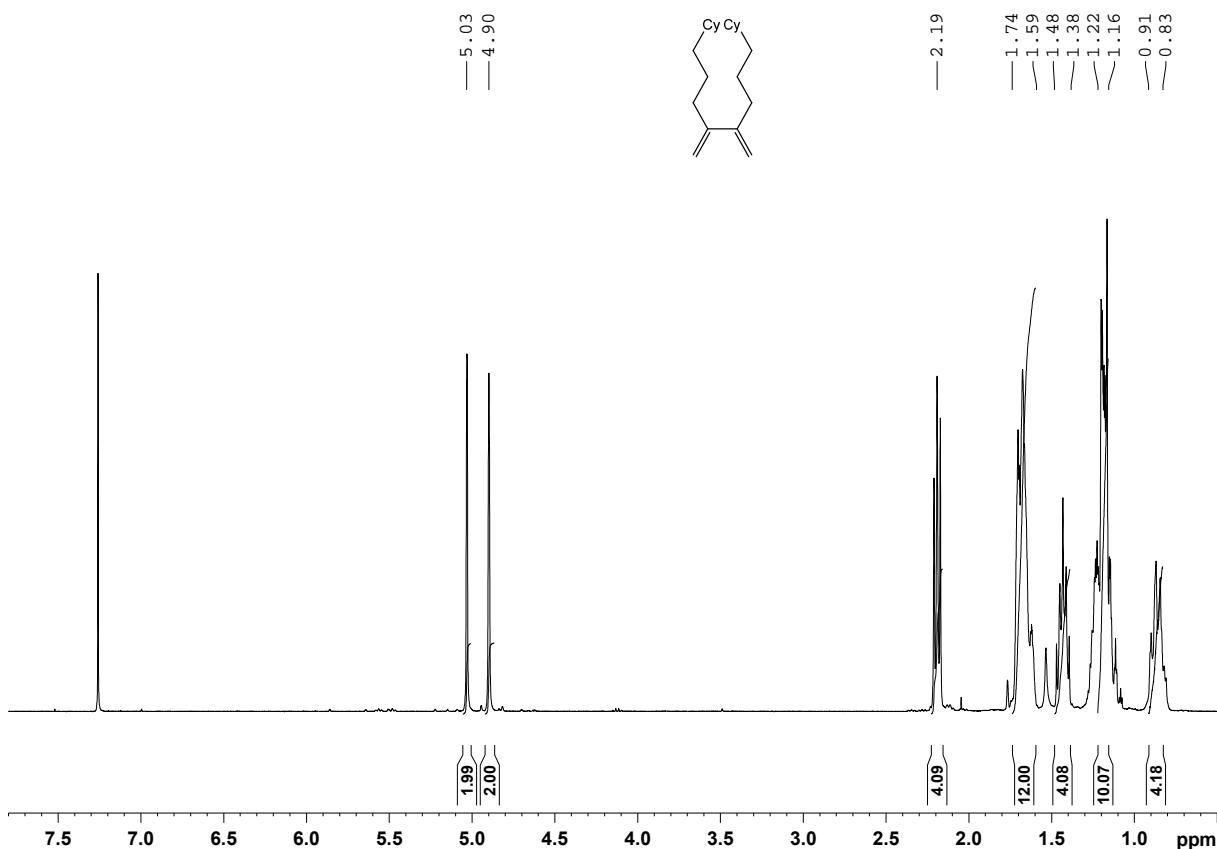


Figure S28. ^1H -NMR spectrum of **28c** in CDCl_3

Supporting Information (SI)

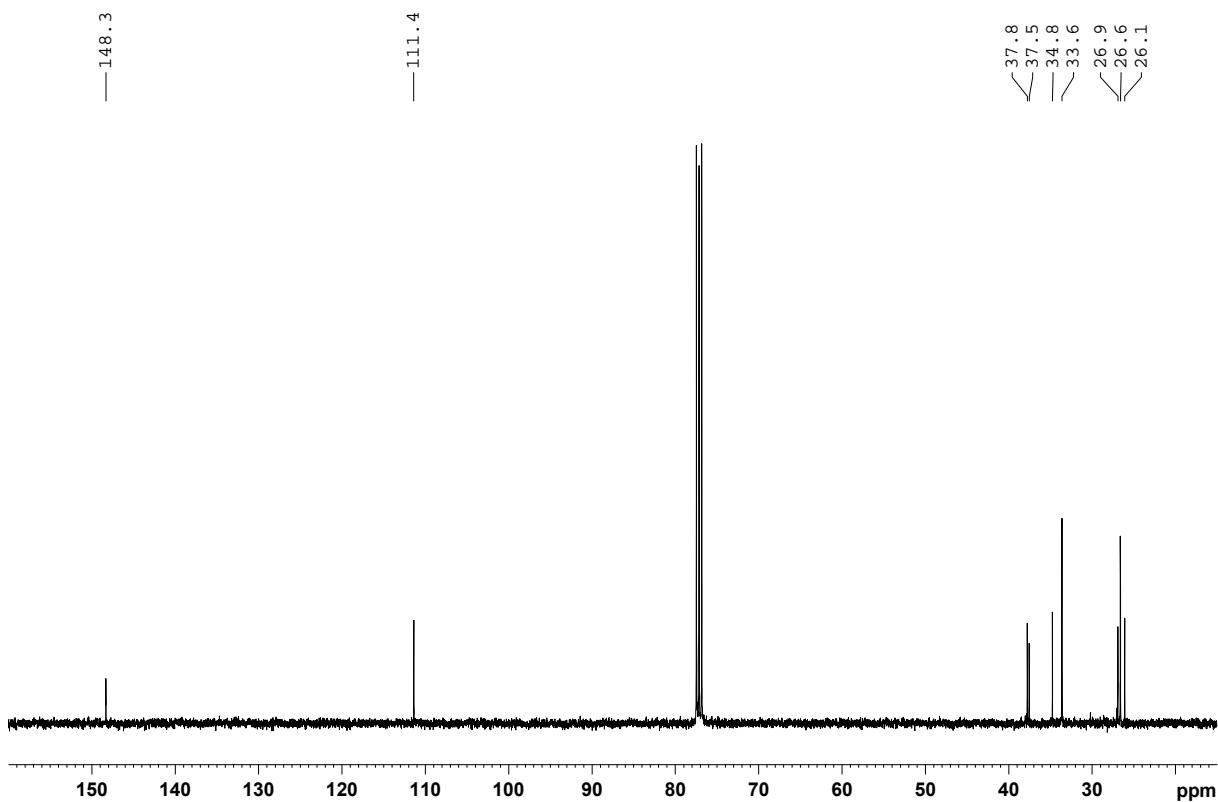


Figure S29. $^{13}\text{C}\{^1\text{H}\}$ -NMR spectrum of **28c** in CDCl_3

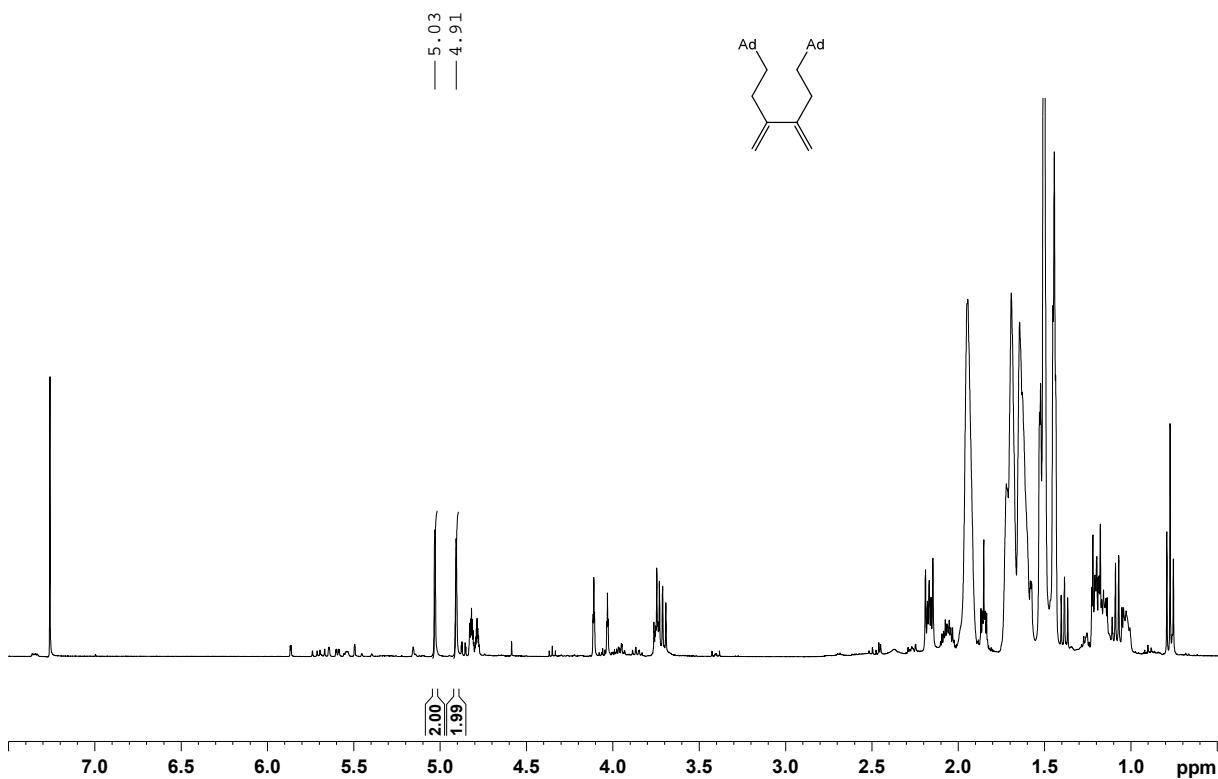


Figure S30. ^1H -NMR spectrum of **28d** in CDCl_3

Supporting Information (SI)

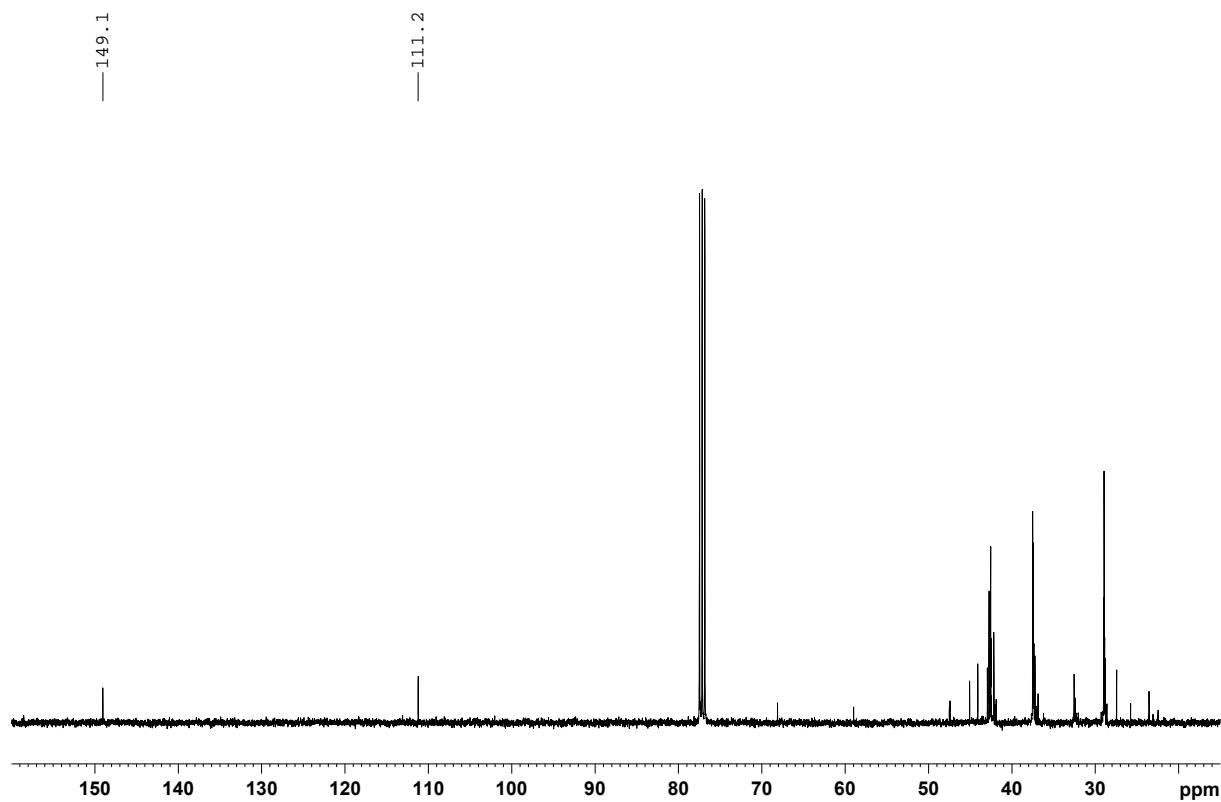


Figure S31. $^{13}\text{C}\{^1\text{H}\}$ -NMR spectrum of **28d** in CDCl_3

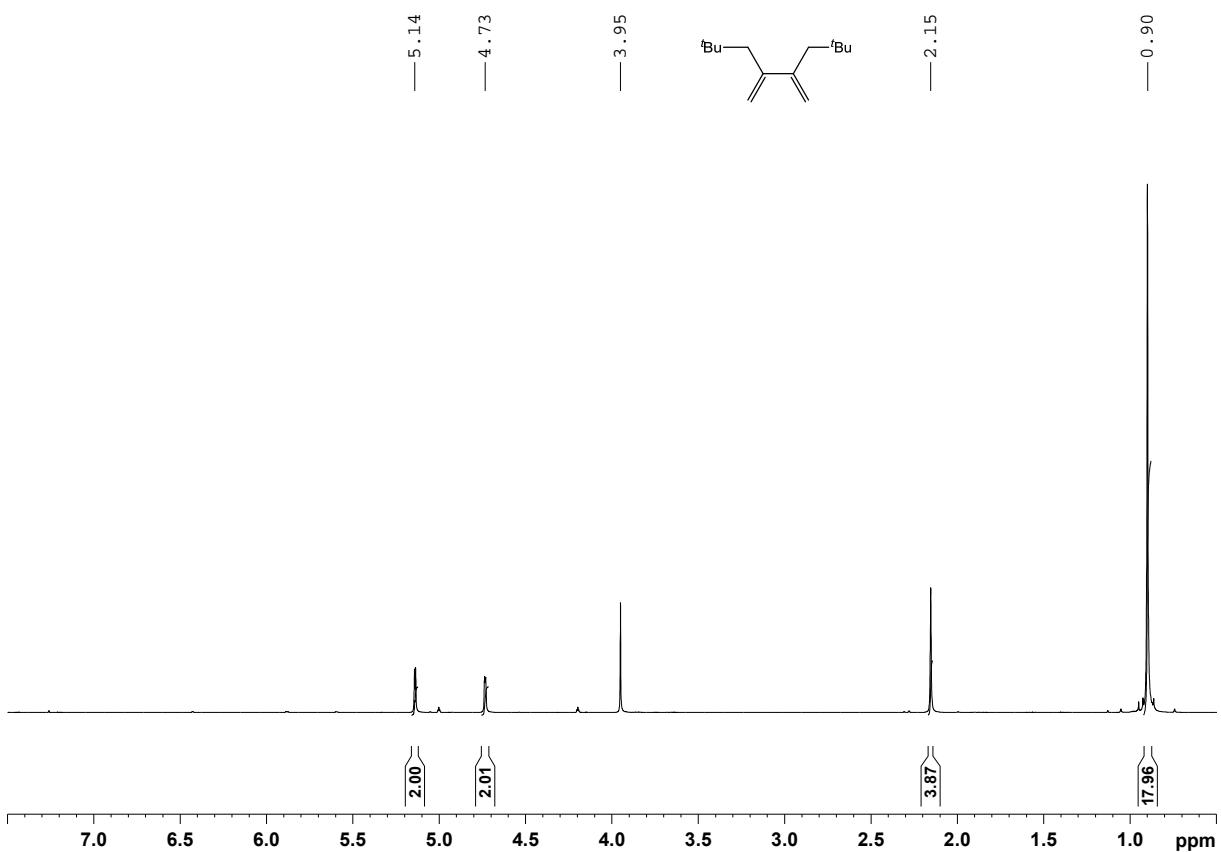


Figure S32. ^1H -NMR spectrum of **28e** in CDCl_3

Supporting Information (SI)

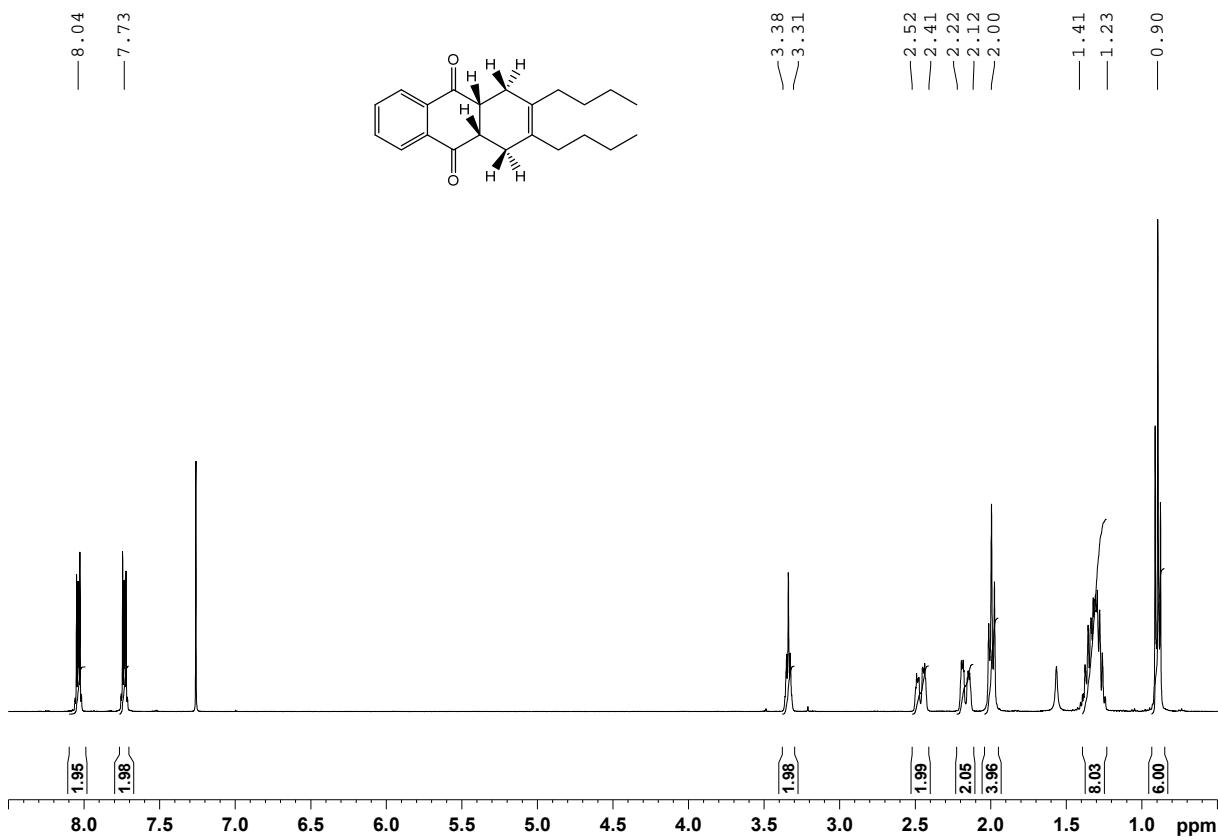


Figure S33. ^1H -NMR spectrum of **30a** in CDCl_3

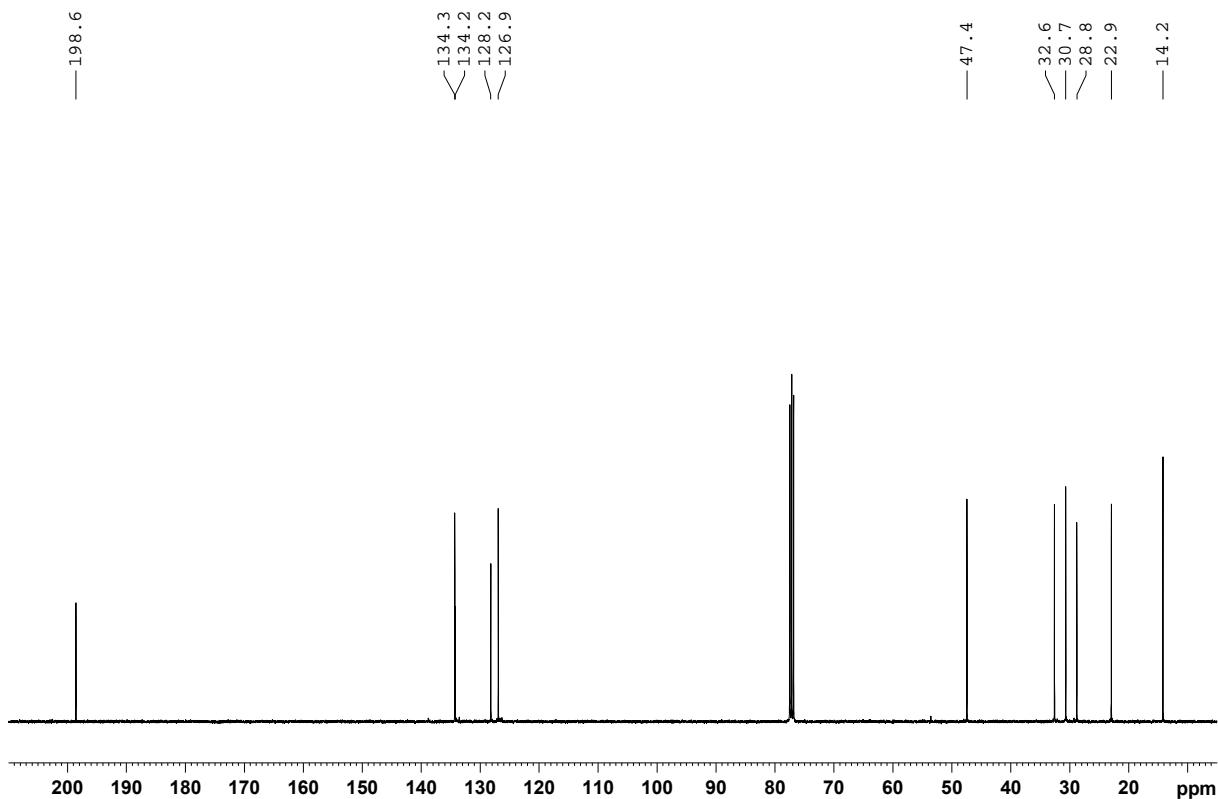


Figure S34. $^{13}\text{C}\{^1\text{H}\}$ -NMR spectrum of **30a** in CDCl_3

Supporting Information (SI)

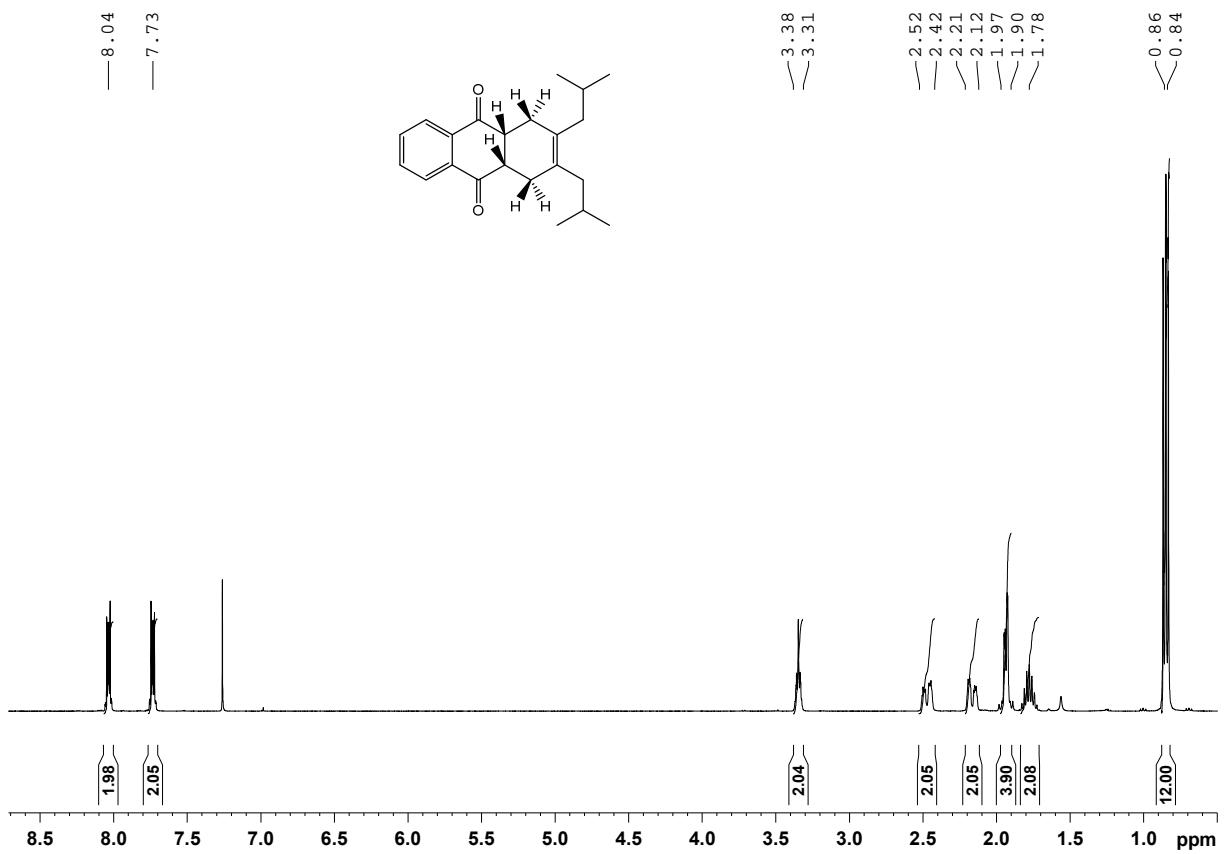


Figure S35. ^1H -NMR spectrum of **30b** in CDCl_3

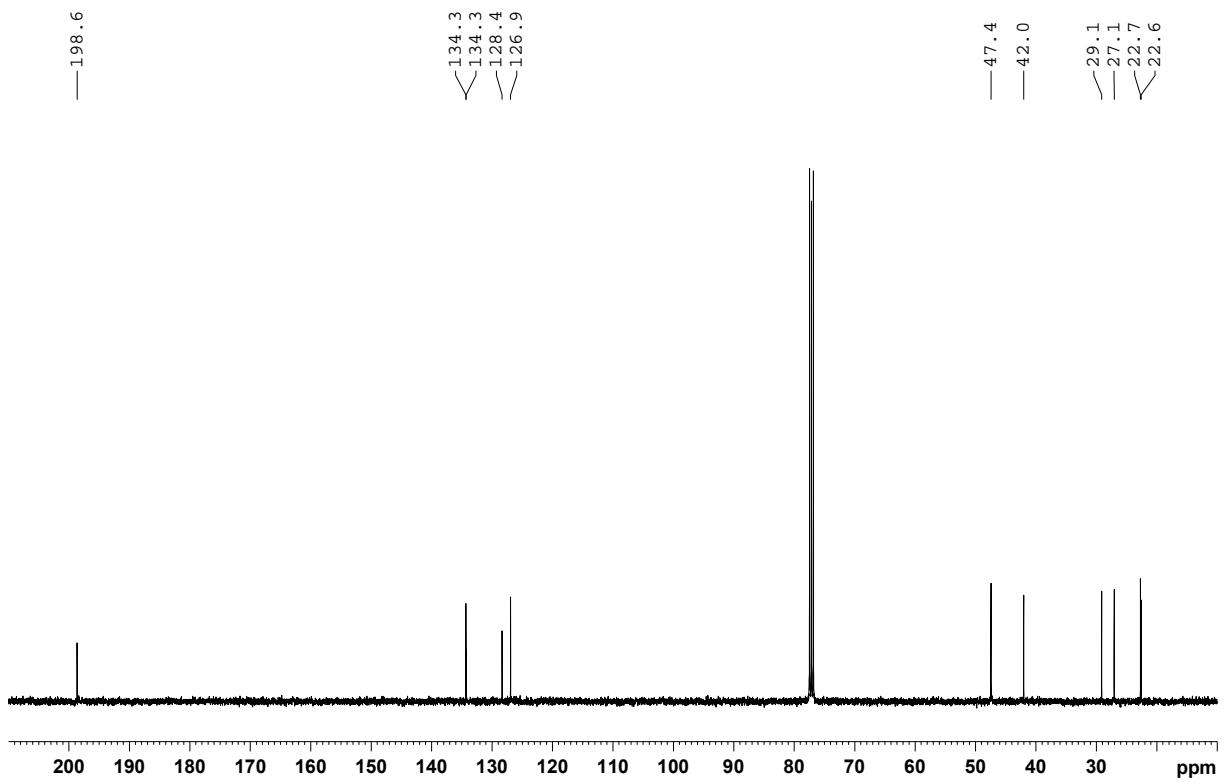


Figure S36. $^{13}\text{C}\{^1\text{H}\}$ -NMR spectrum of **30b** in CDCl_3

Supporting Information (SI)

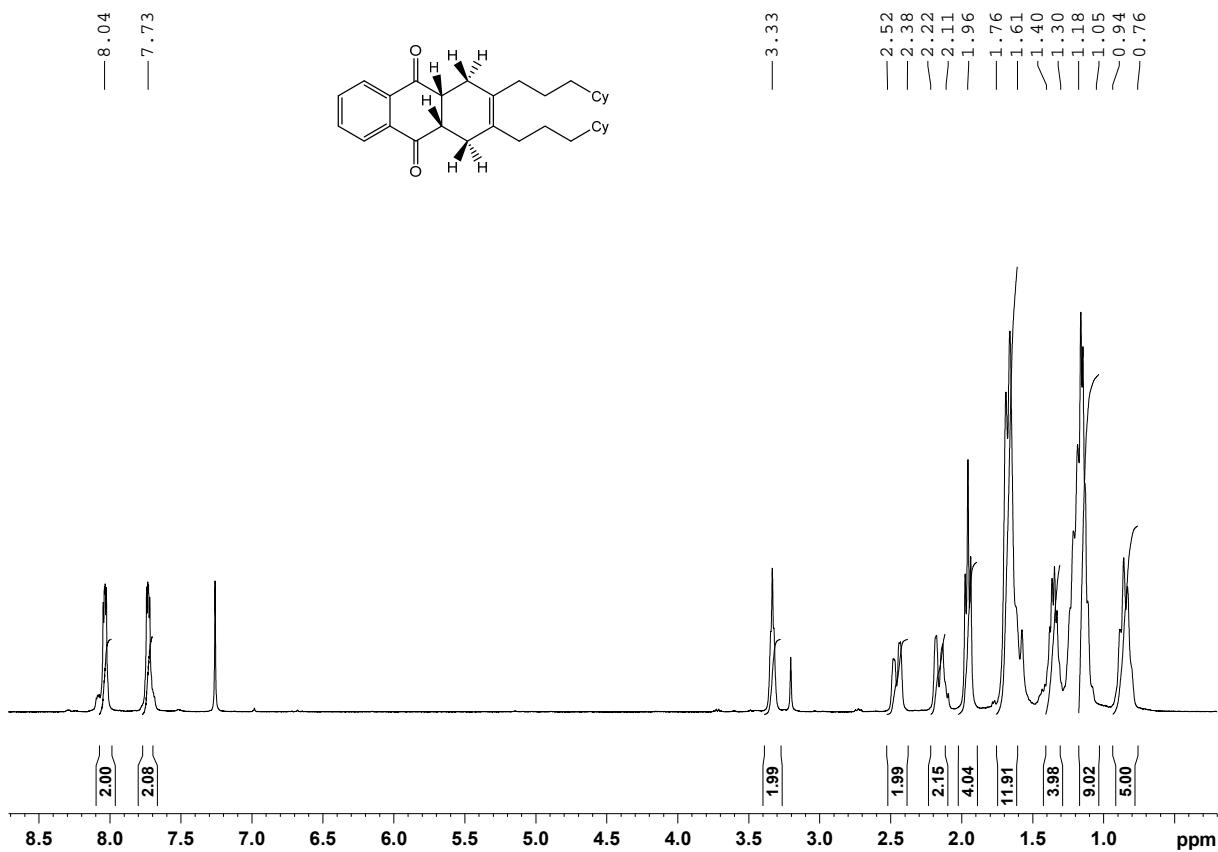


Figure S37. ^1H -NMR spectrum of **30c** in CDCl_3

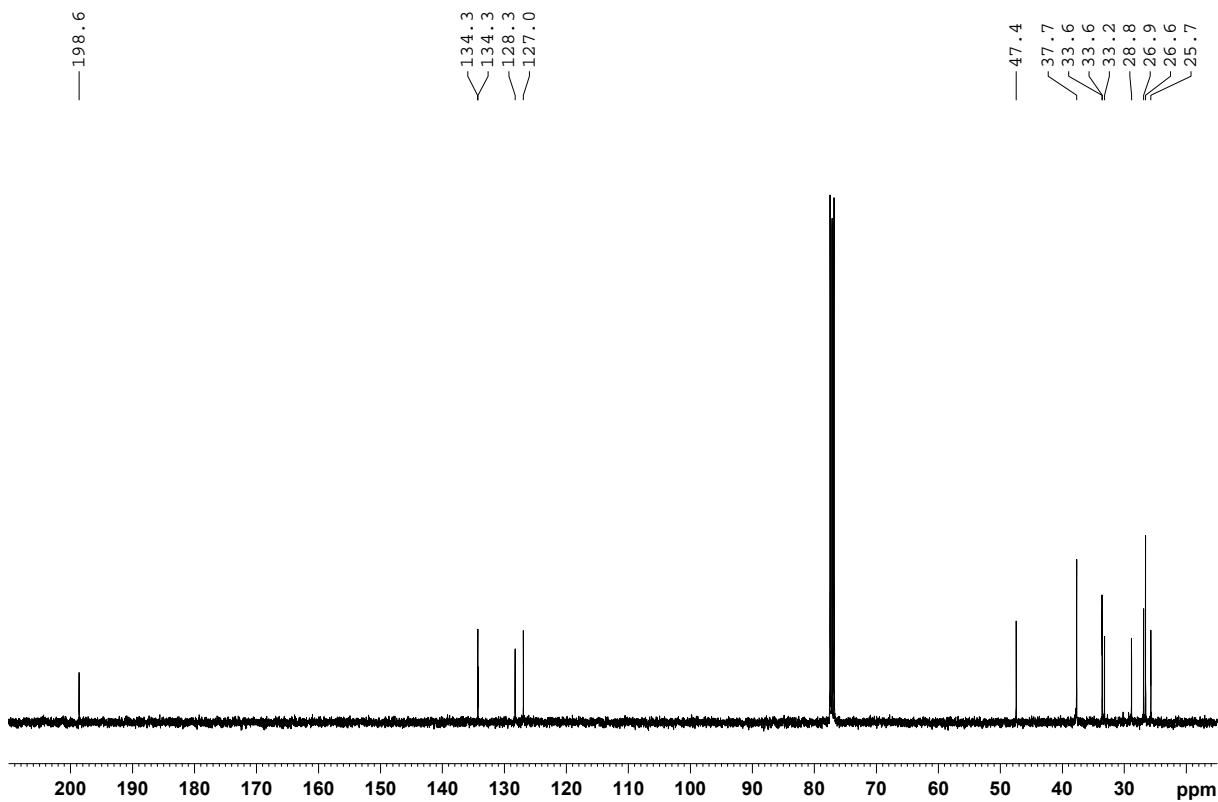


Figure S38. $^{13}\text{C}\{{}^1\text{H}\}$ -NMR spectrum of **30c** in CDCl_3

Supporting Information (SI)

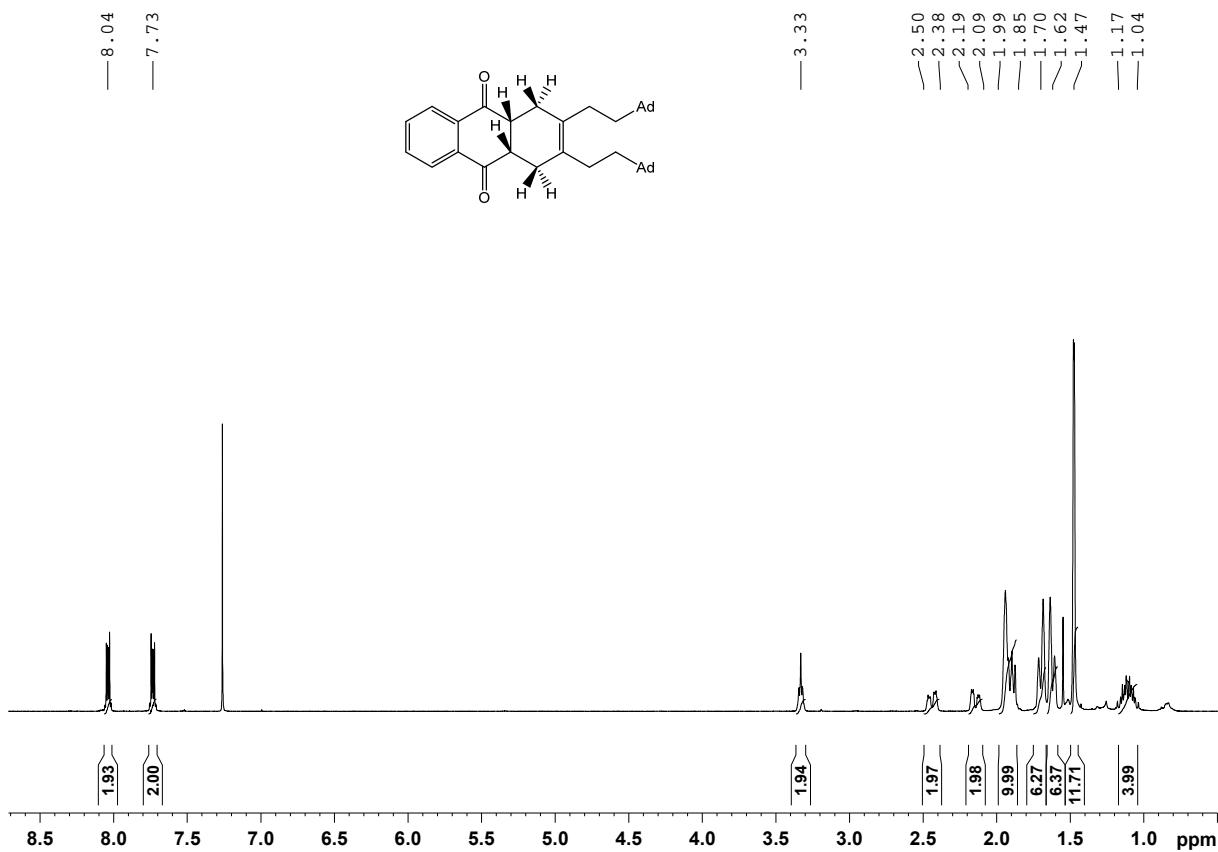


Figure S39. ¹H-spectrum of **30d** in CDCl₃

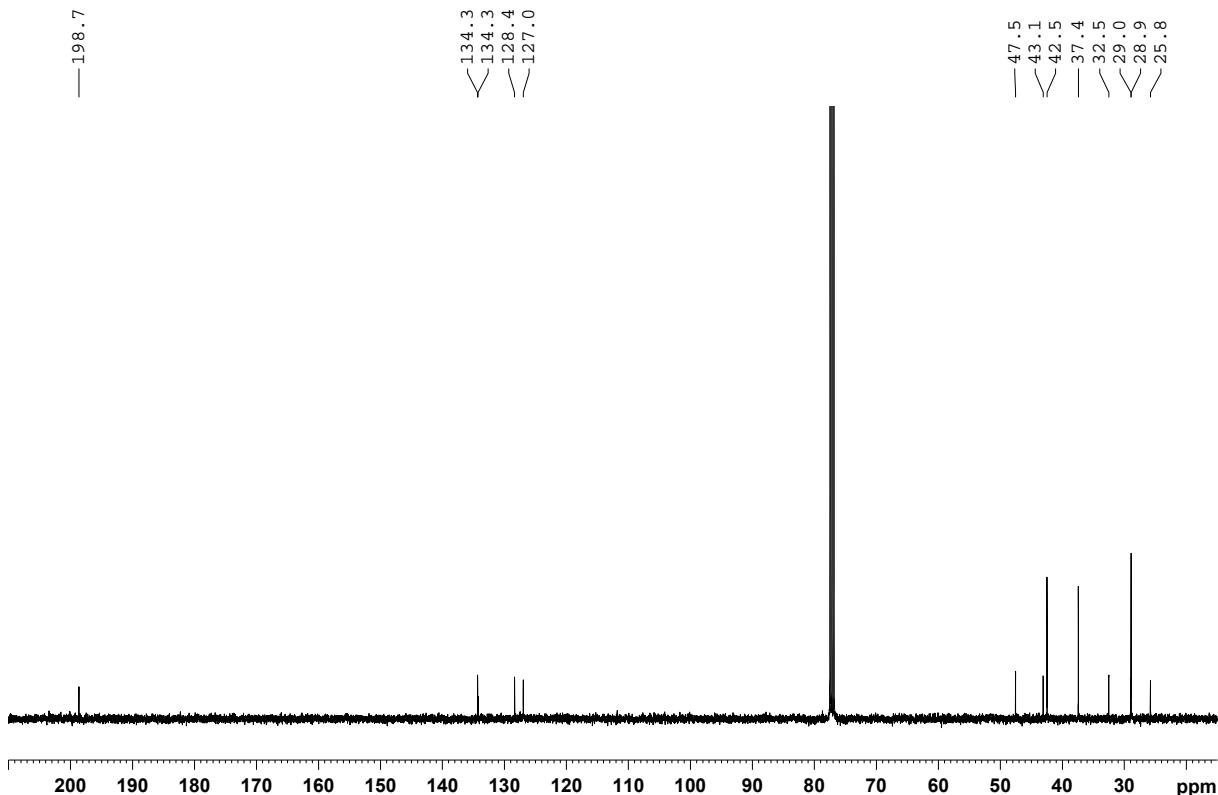


Figure S40. ¹³C{¹H}-spectrum of **30d** in CDCl₃

Supporting Information (SI)

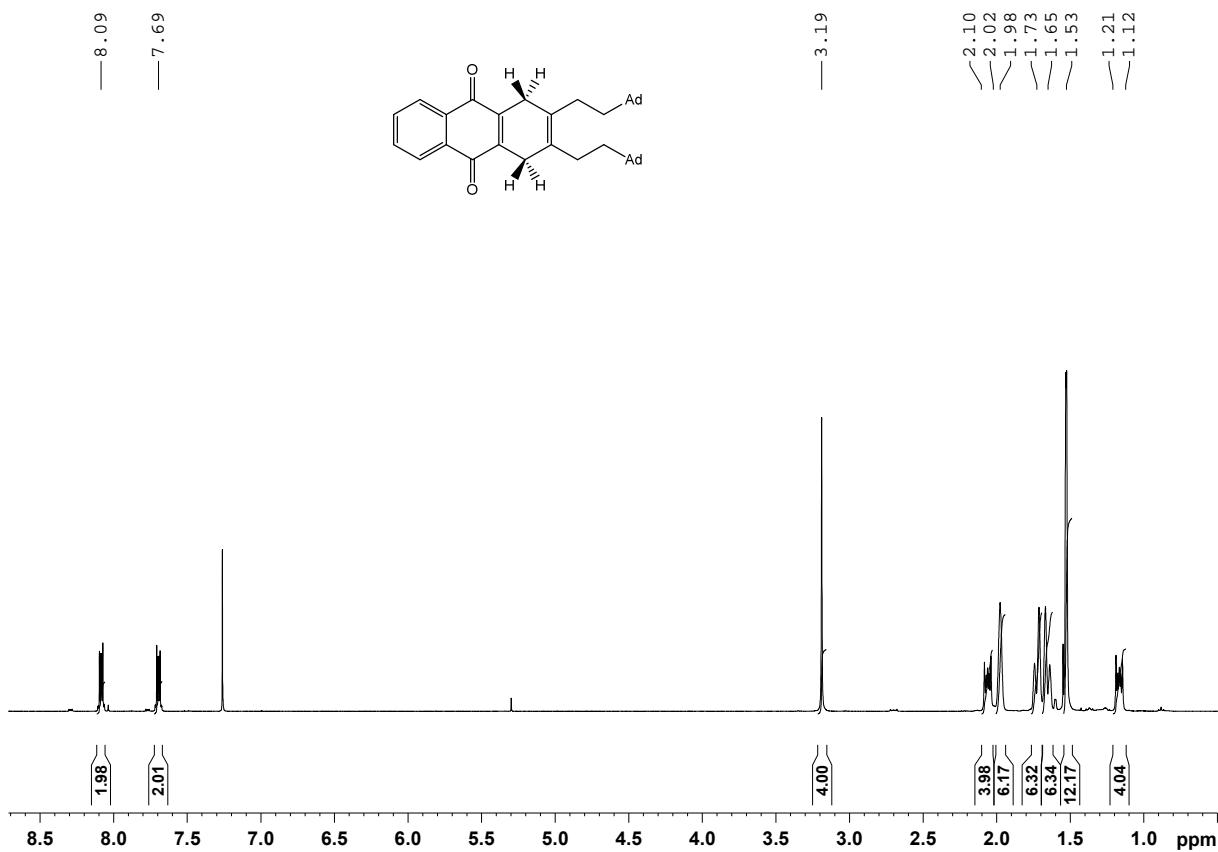


Figure S41. ^1H -spectrum of **30d-2H** in CDCl_3

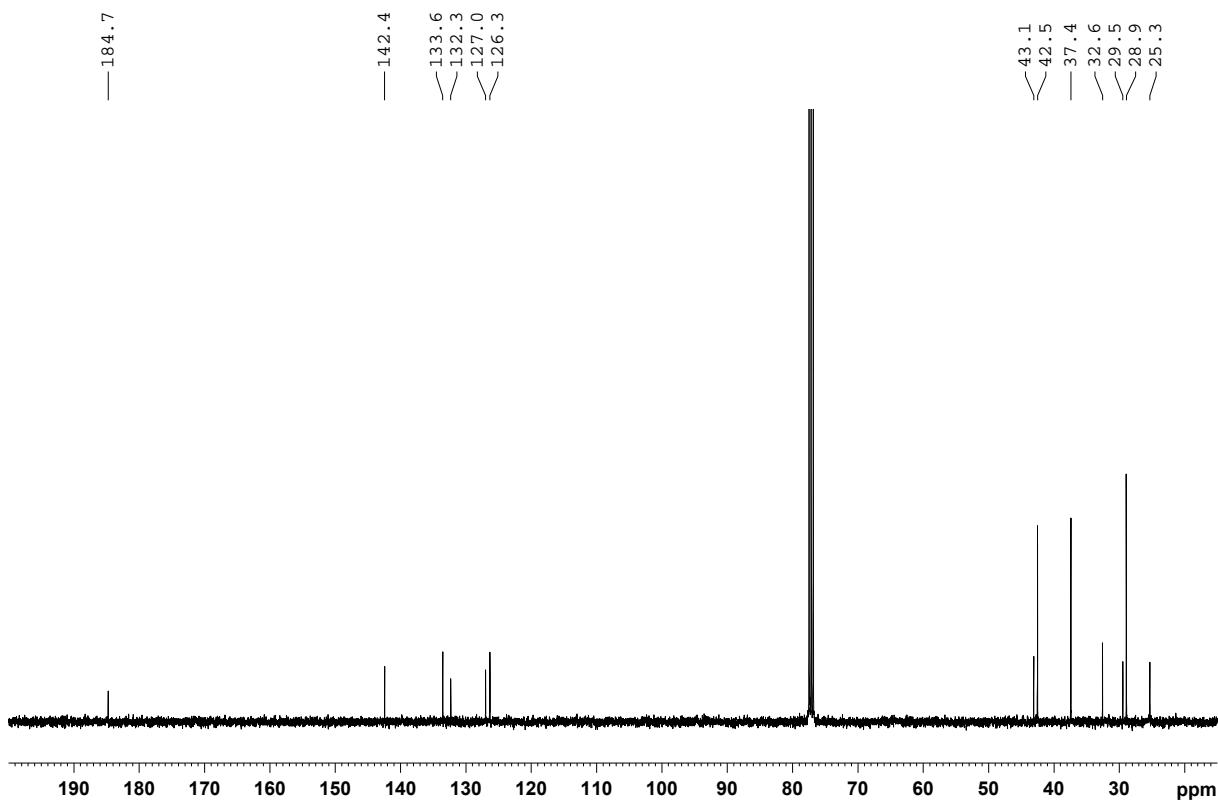


Figure S42. $^{13}\text{C}\{^1\text{H}\}$ -spectrum of **30d-2H** in CDCl_3

Supporting Information (SI)

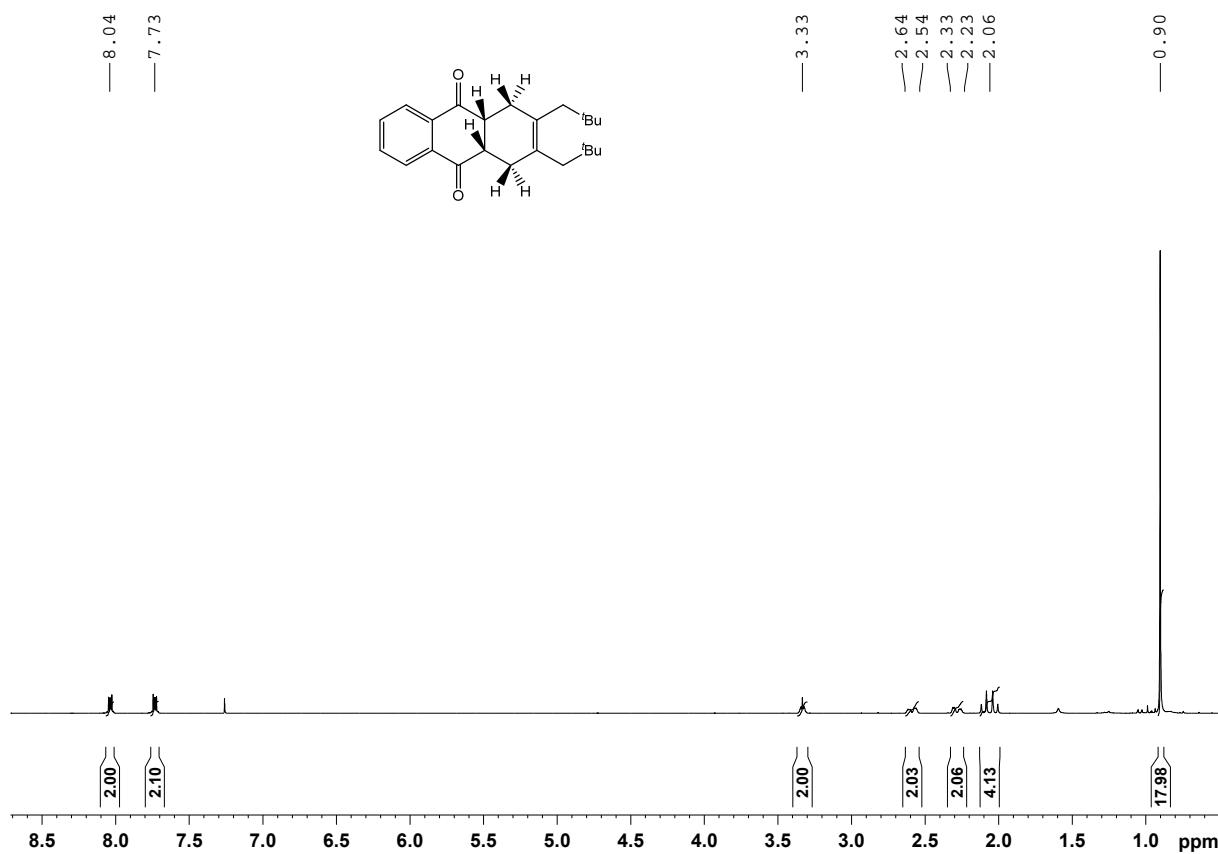


Figure S43. ^1H -NMR spectrum of **30e** in CDCl_3

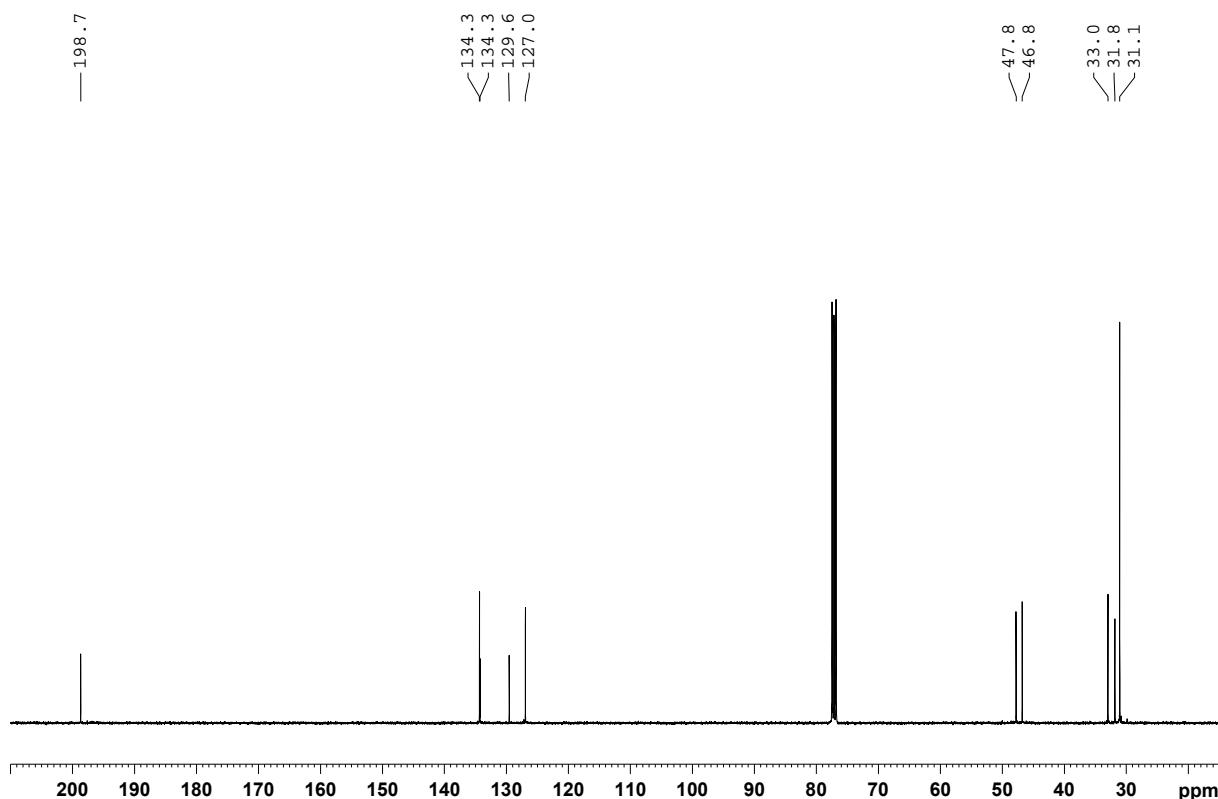


Figure S44. $^{13}\text{C}\{{}^1\text{H}\}$ -NMR spectrum of **30e** in CDCl_3

Supporting Information (SI)

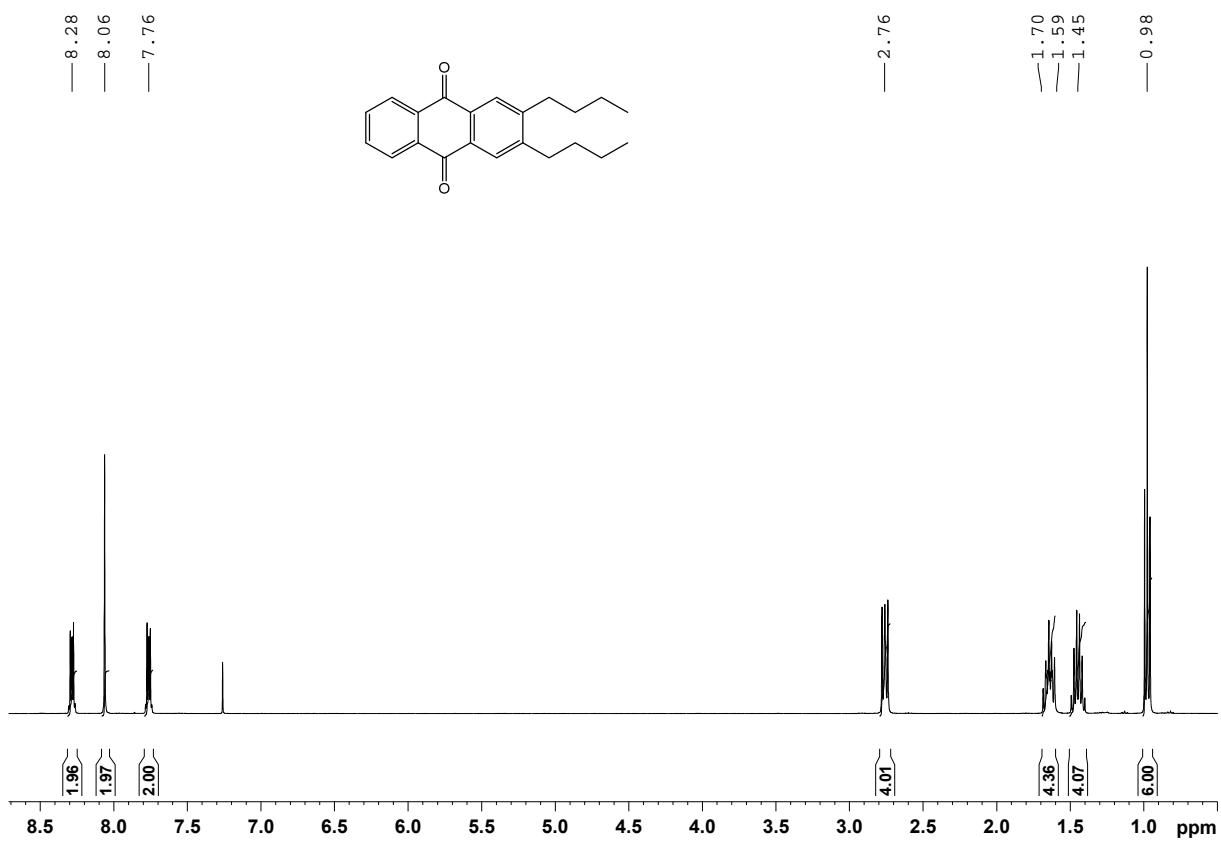


Figure S45. ¹H-NMR spectrum of 31a in CDCl₃

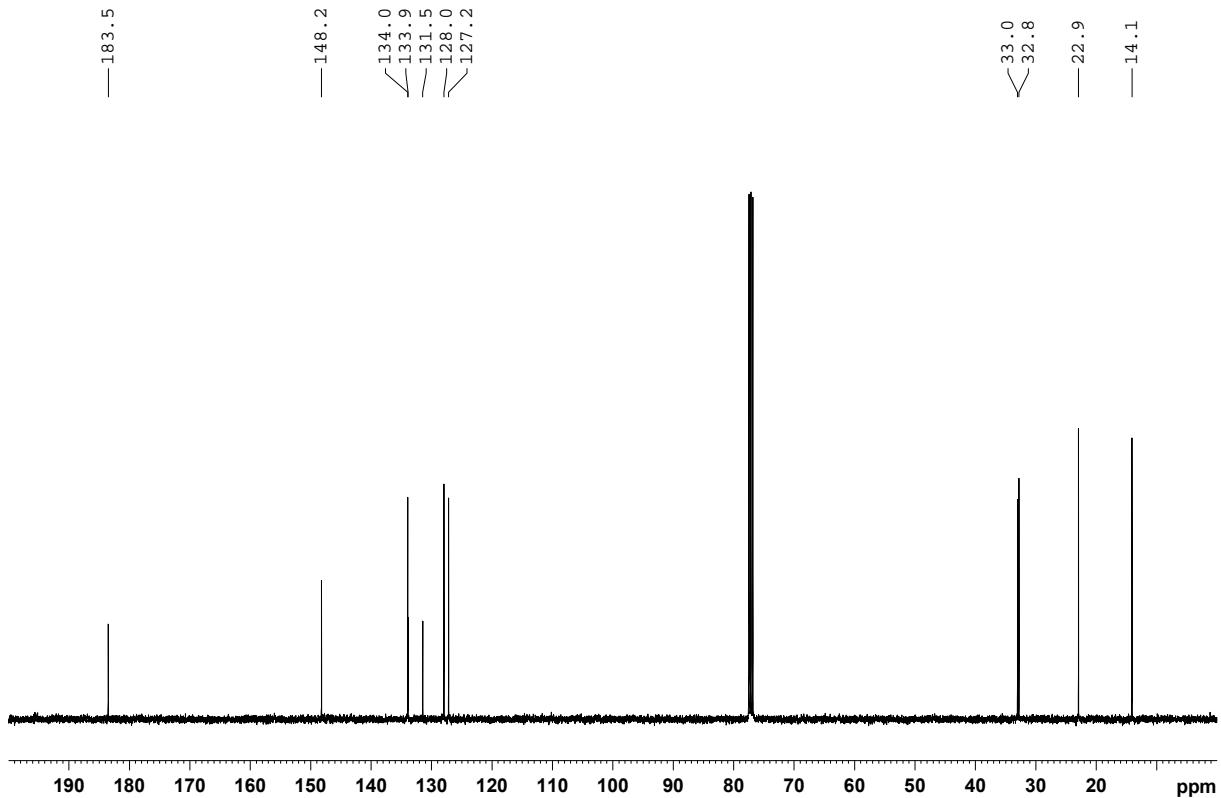


Figure S46. ¹³C{¹H}-NMR spectrum of 31a in CDCl₃

Supporting Information (SI)

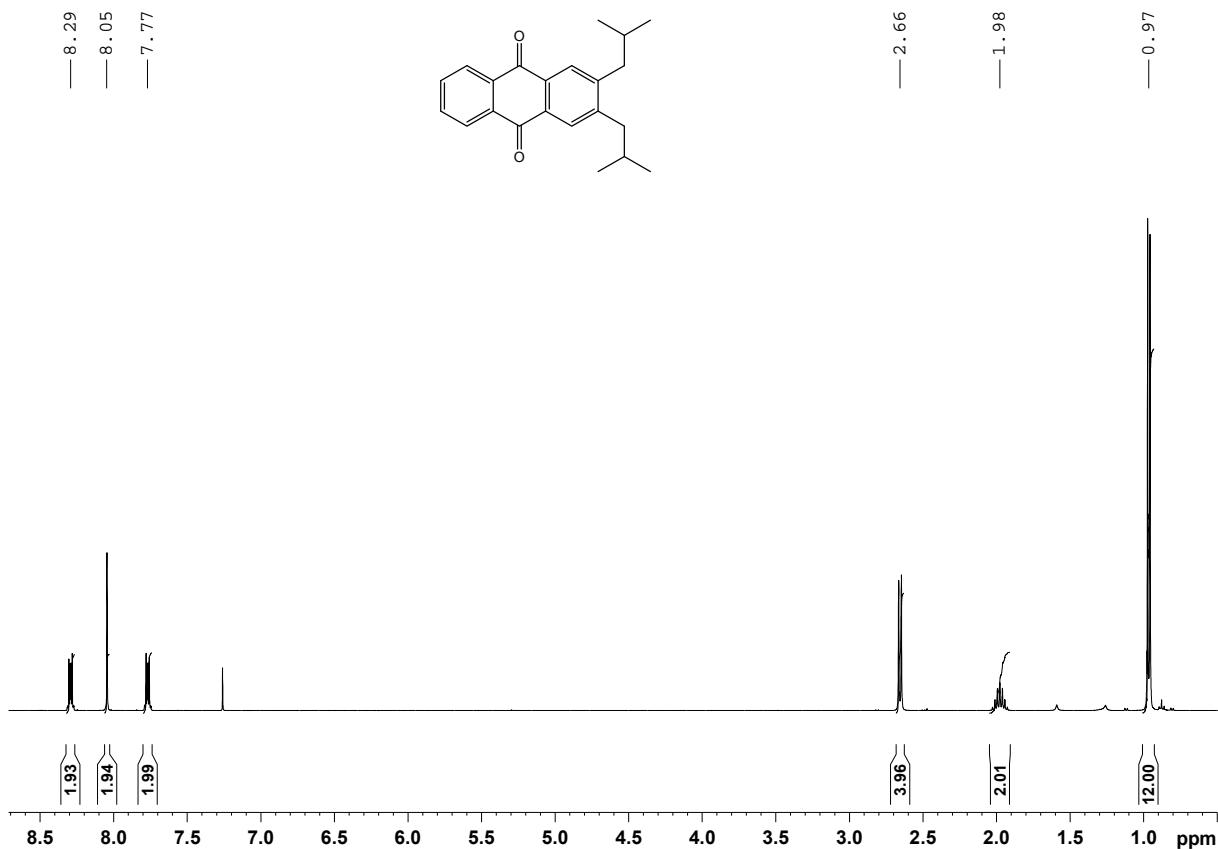


Figure S47. ¹H-NMR spectrum of **31b** in CDCl₃

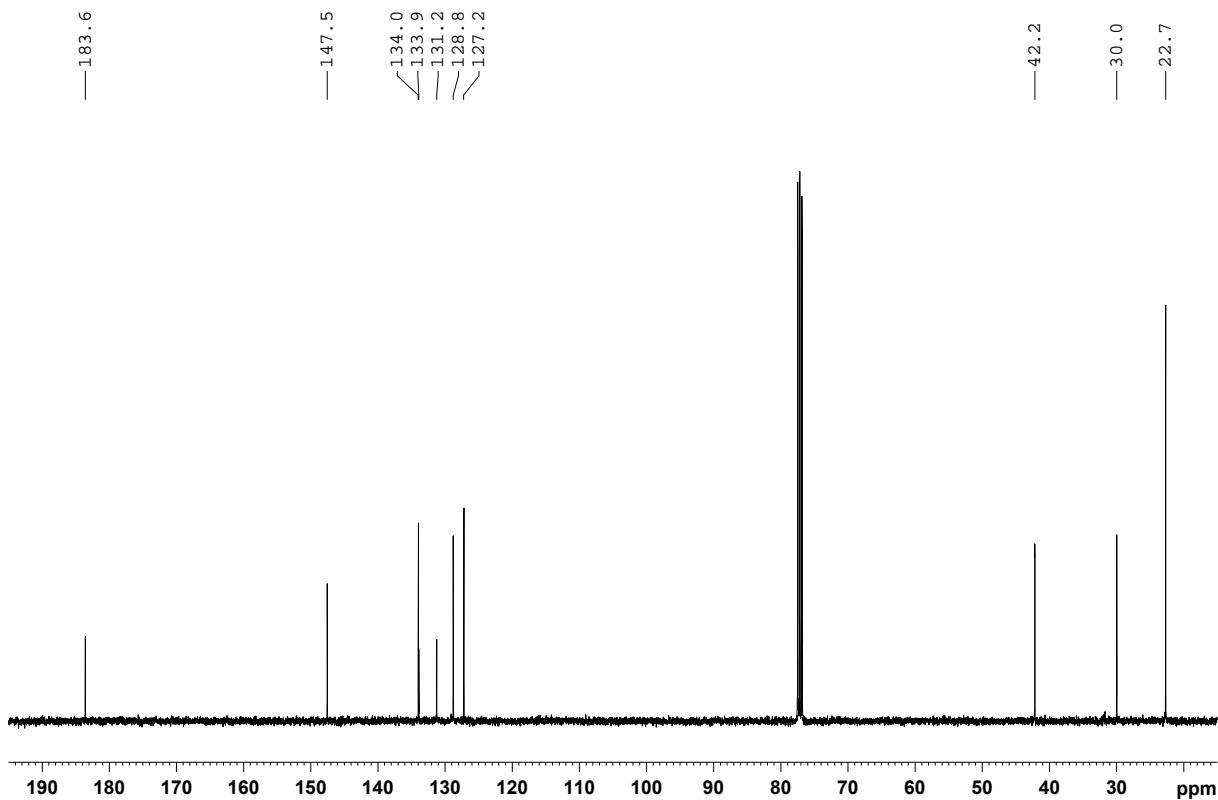


Figure S48. ¹³C{¹H}-NMR spectrum of **31b** in CDCl₃

Supporting Information (SI)

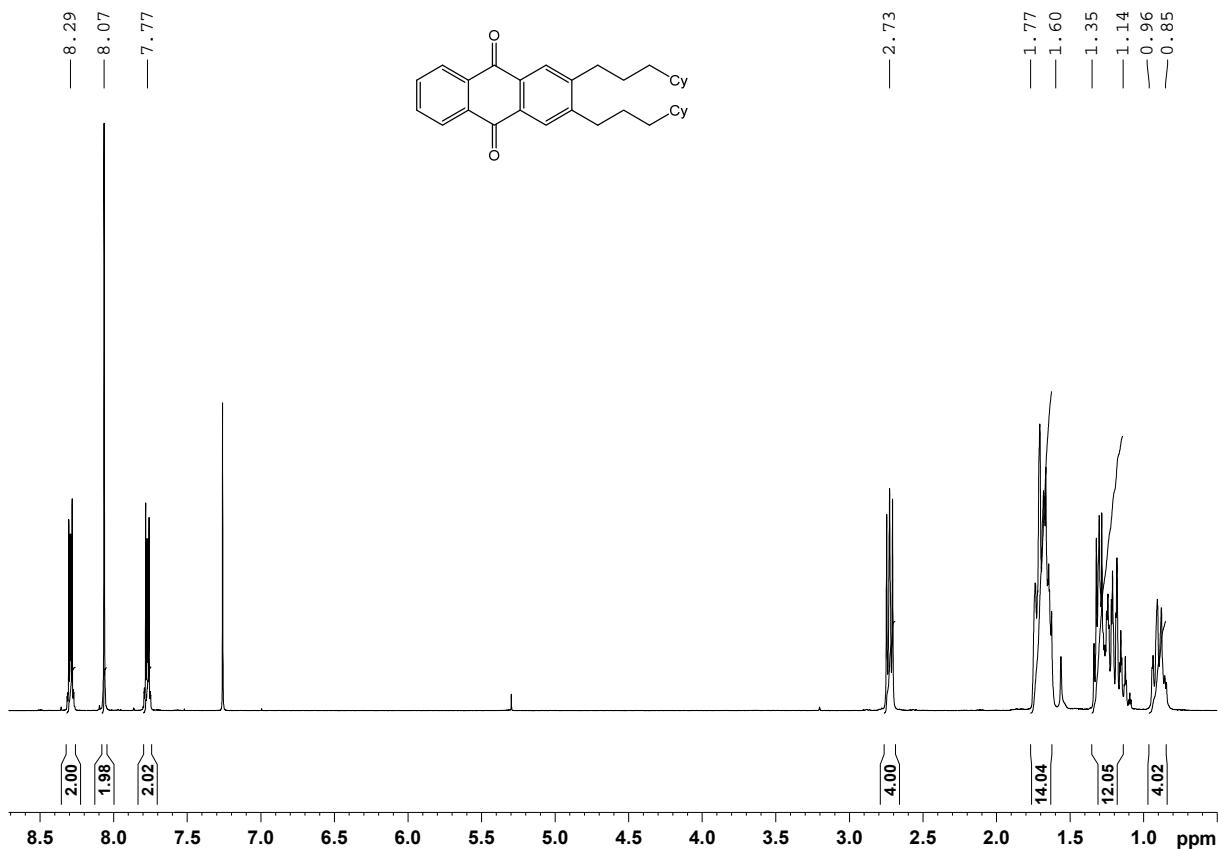


Figure S49. ^1H -NMR spectrum of **31c** in CDCl_3

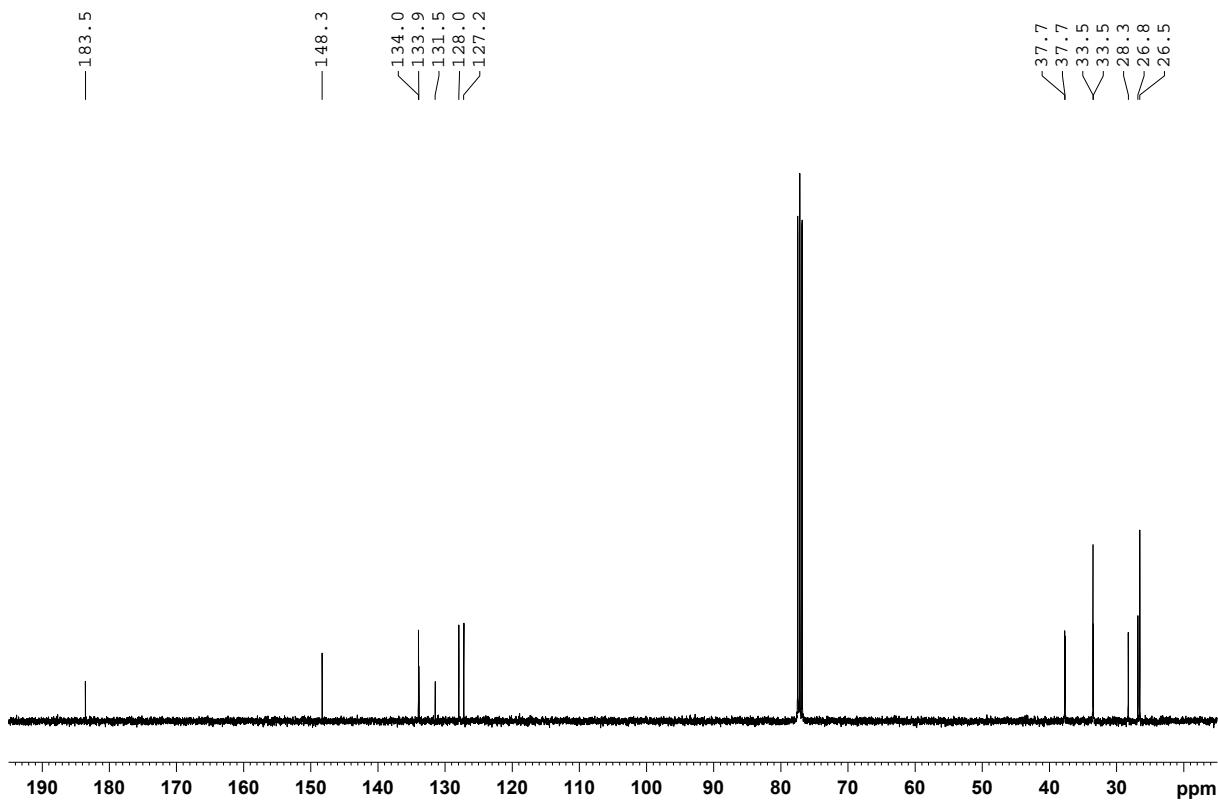


Figure S50. $^{13}\text{C}\{^1\text{H}\}$ -NMR spectrum of **31c** in CDCl_3

Supporting Information (SI)

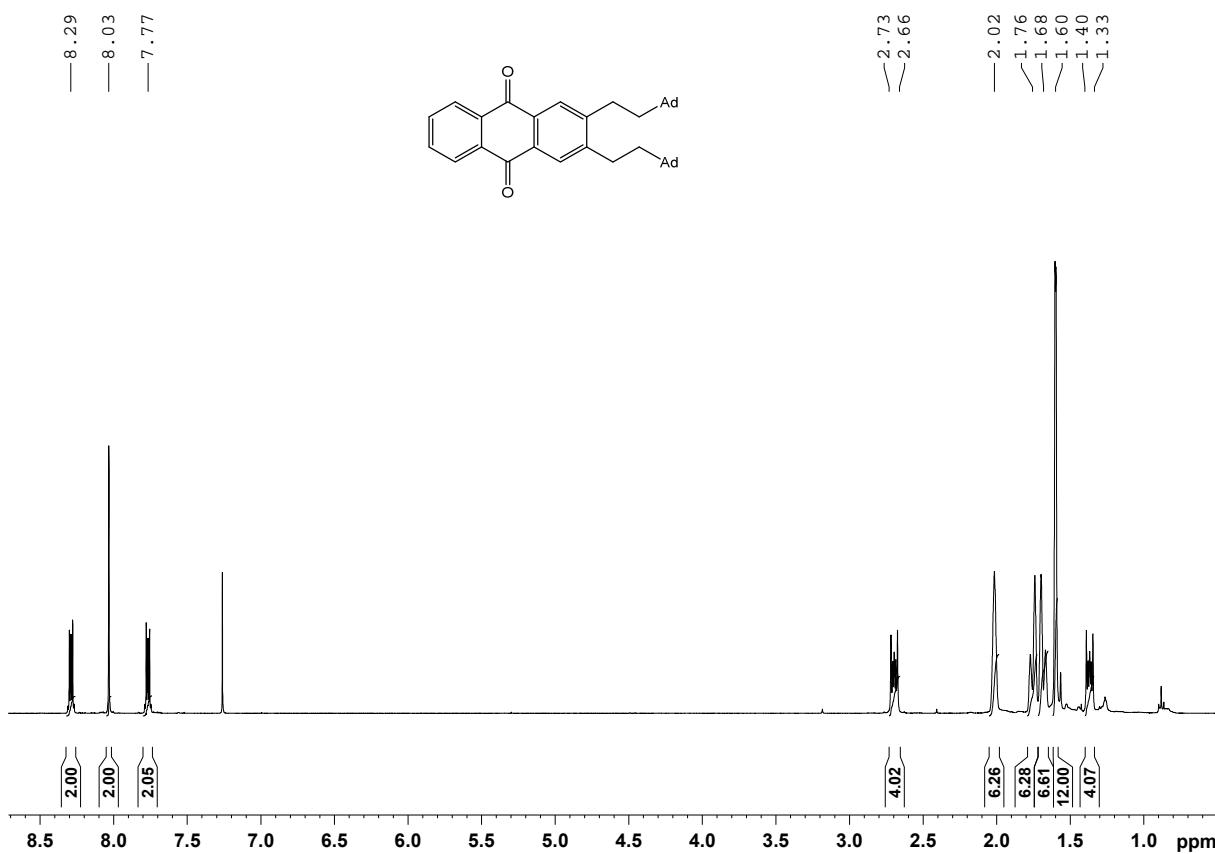


Figure S51. ^1H -spectrum of **31d** in CDCl_3

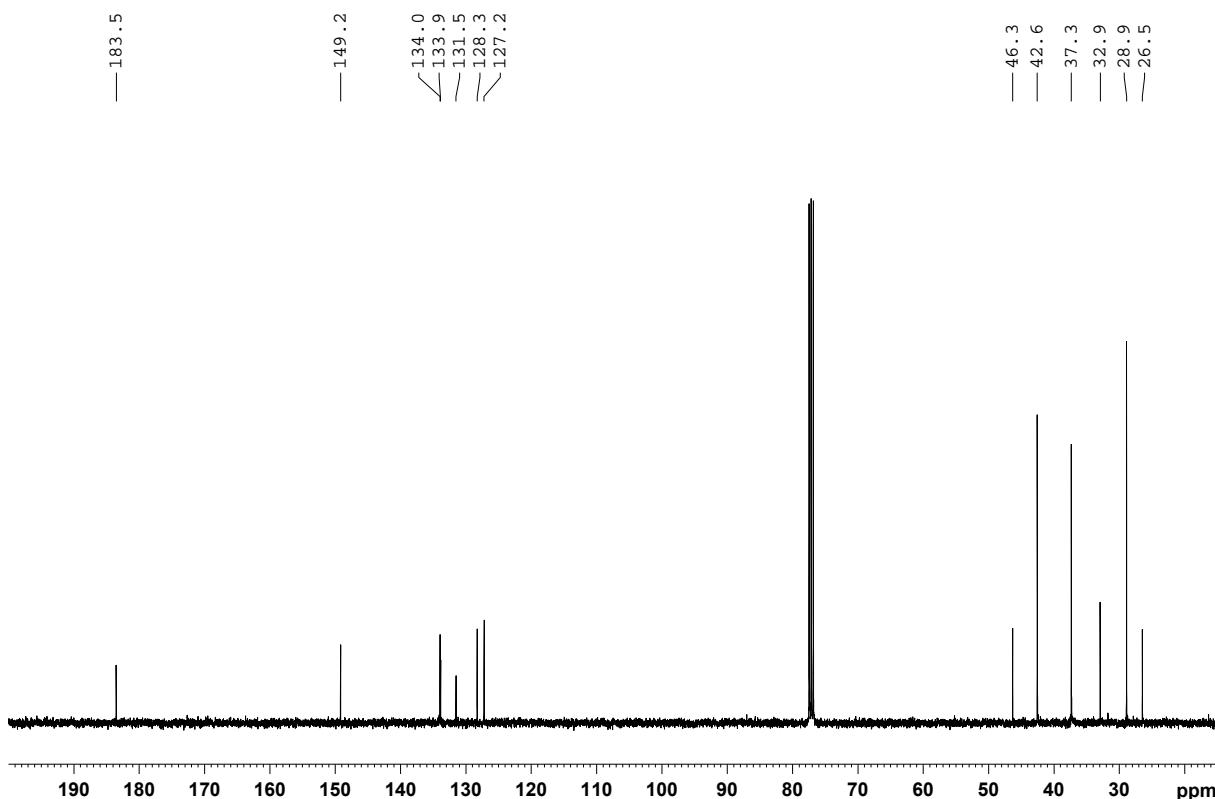


Figure S52. $^{13}\text{C}\{^1\text{H}\}$ -spectrum of **31d** in CDCl_3

Supporting Information (SI)

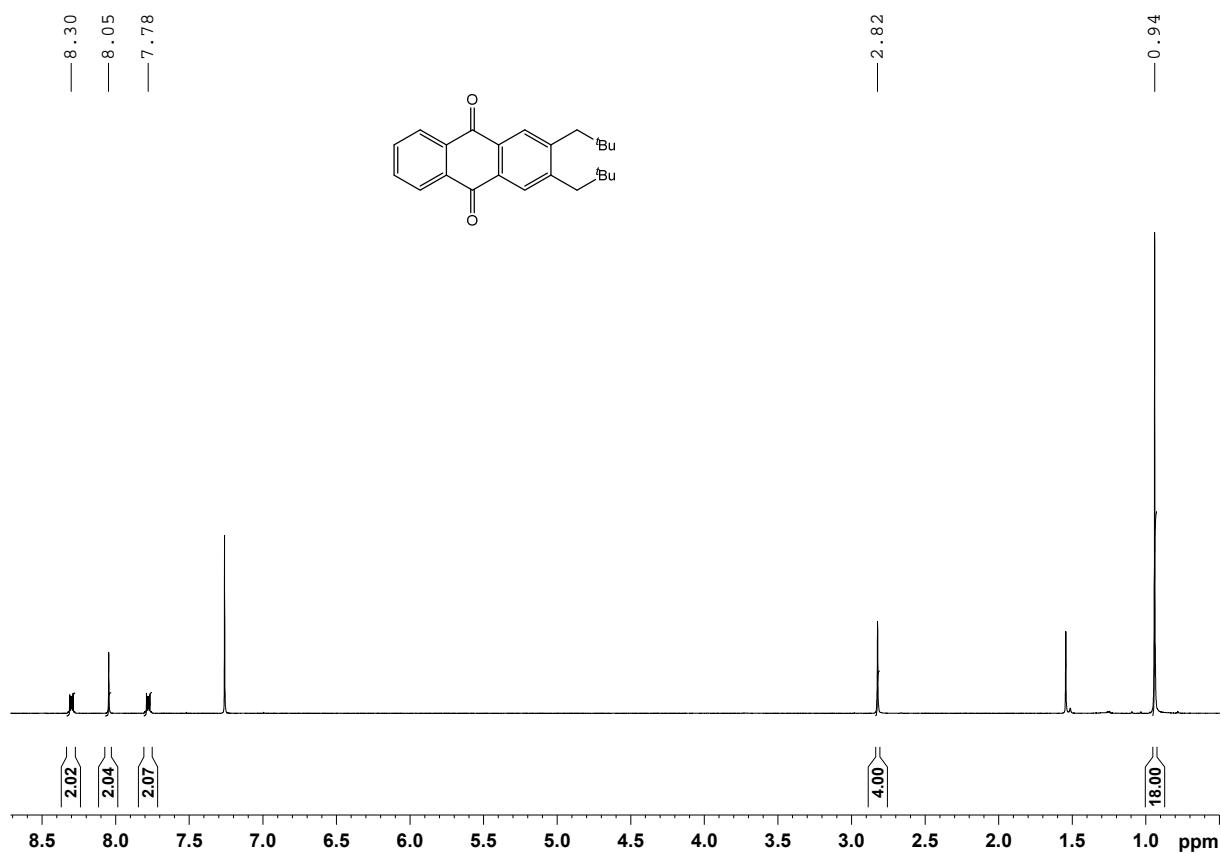


Figure S53. ^1H -NMR spectrum of **31e** in CDCl_3

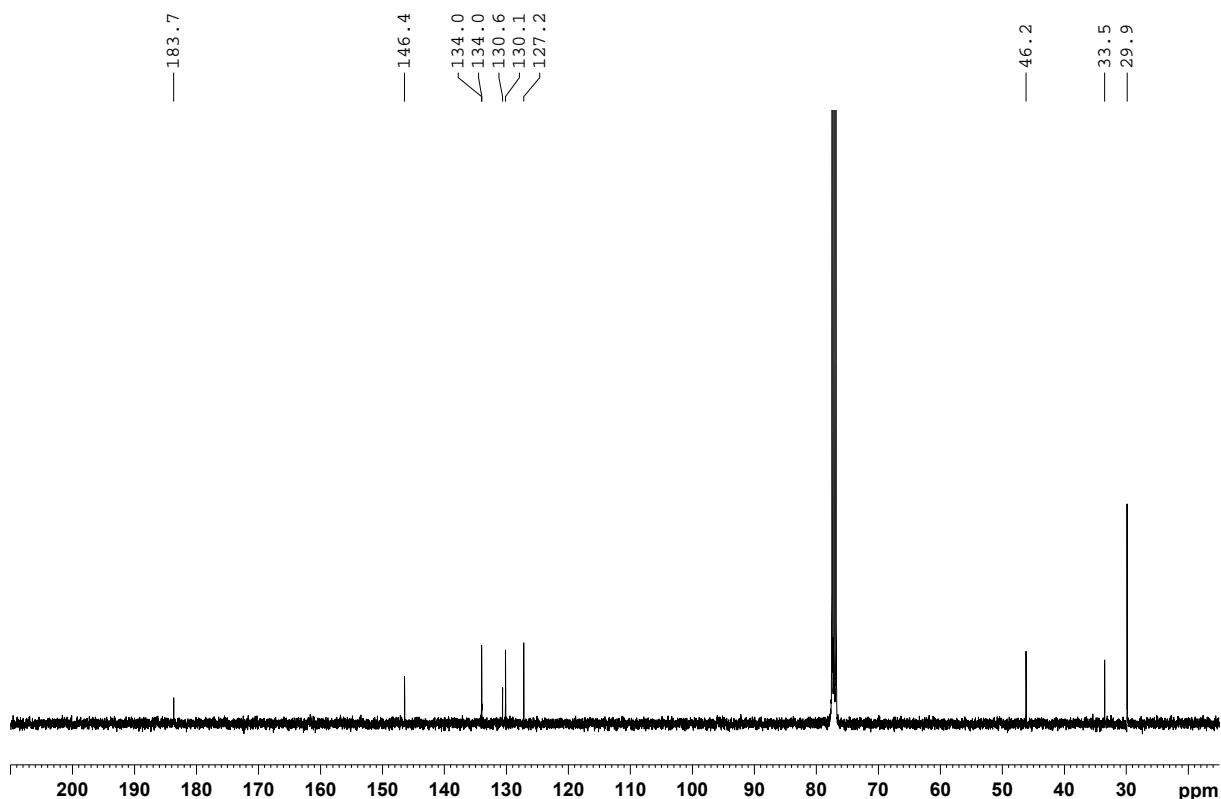
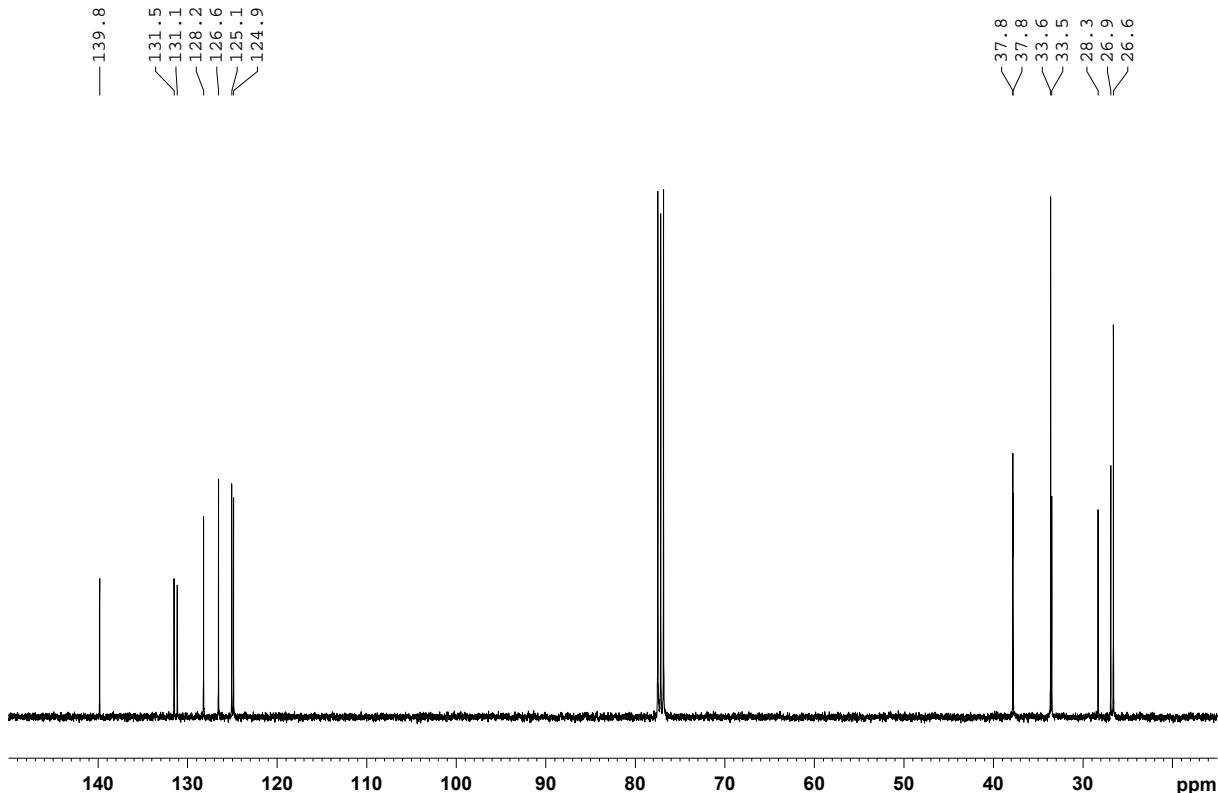
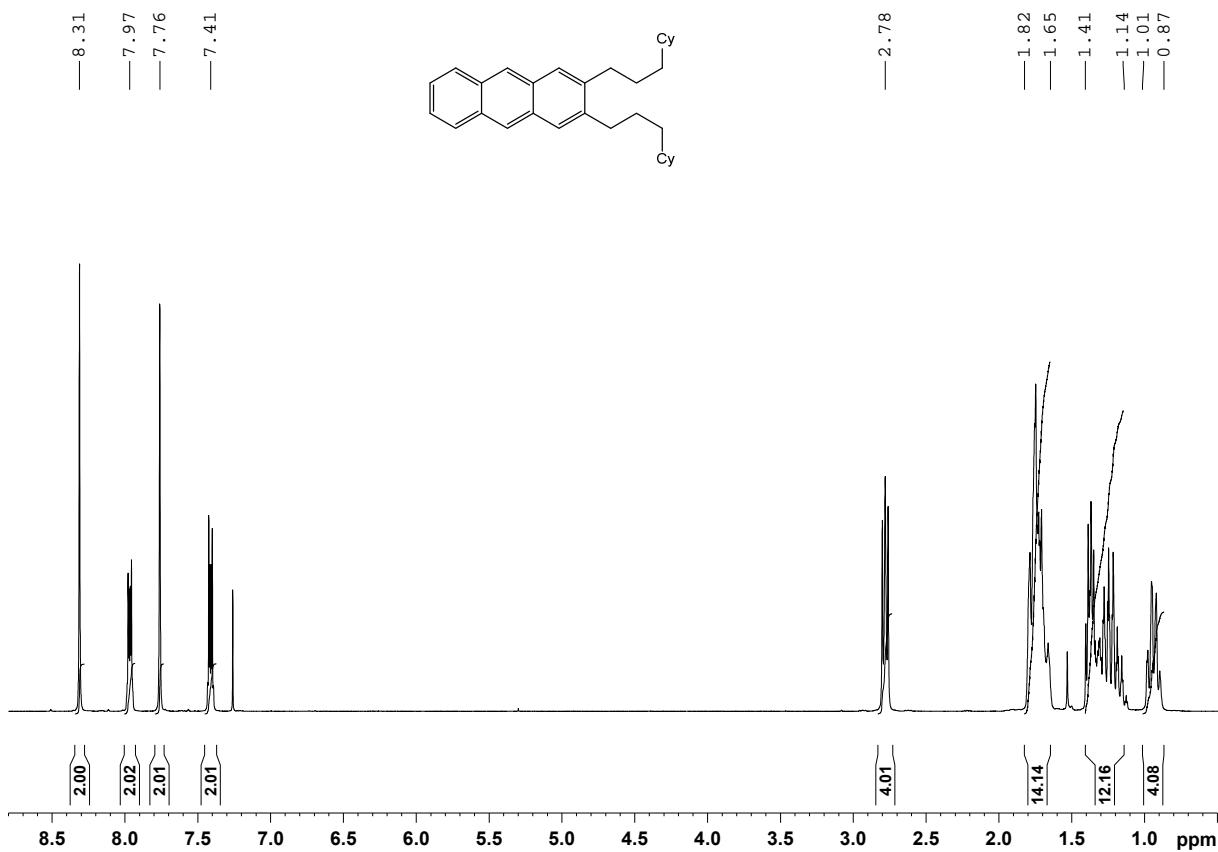


Figure S54. $^{13}\text{C}\{^1\text{H}\}$ -NMR spectrum of **31e** in CDCl_3

Supporting Information (SI)



Supporting Information (SI)

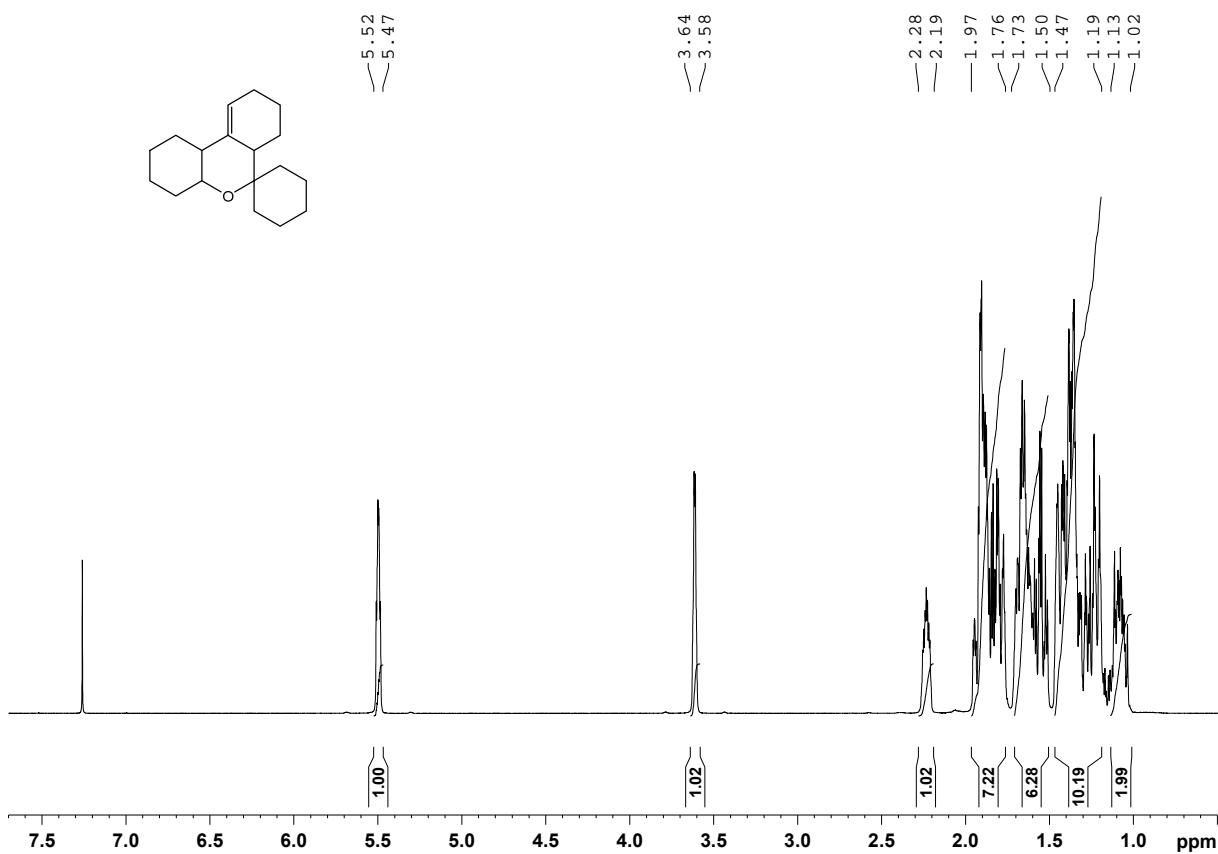


Figure S57. ^1H -NMR spectrum of **33** in CDCl_3

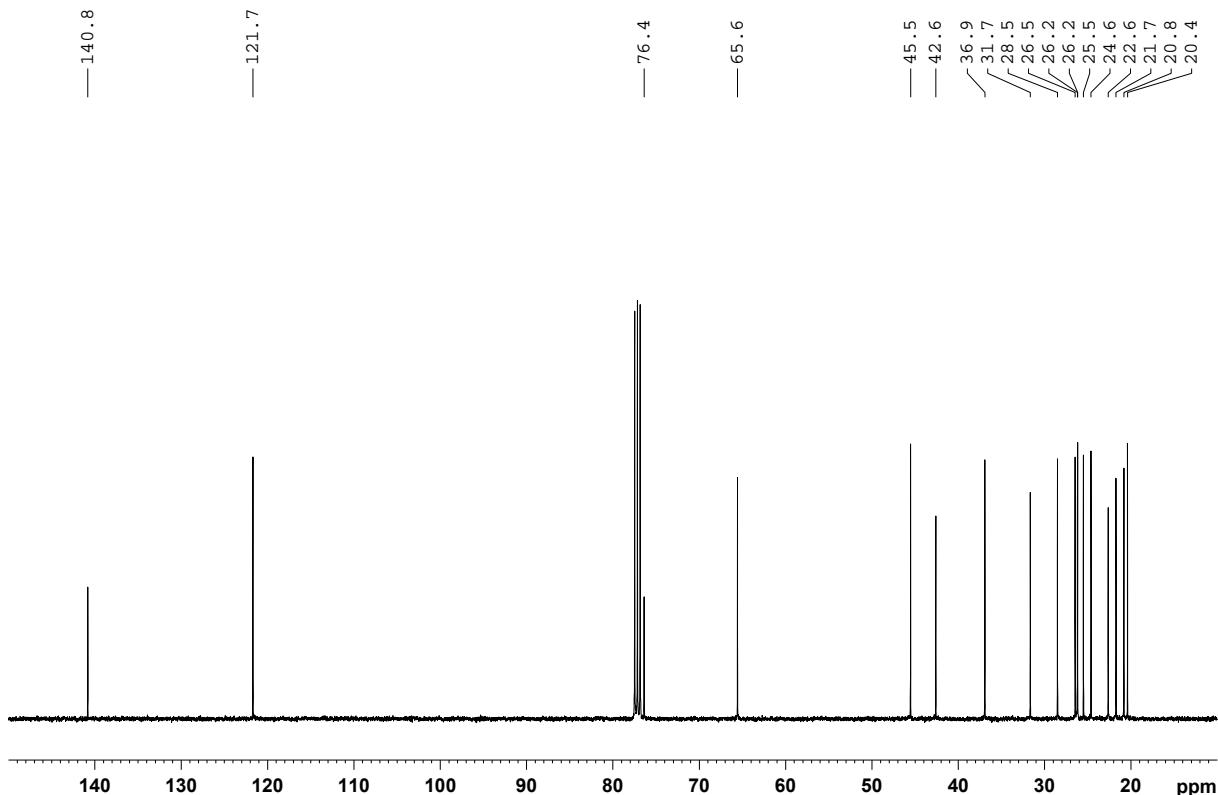


Figure S58. $^{13}\text{C}\{^1\text{H}\}$ -NMR spectrum of **33** in CDCl_3

Supporting Information (SI)

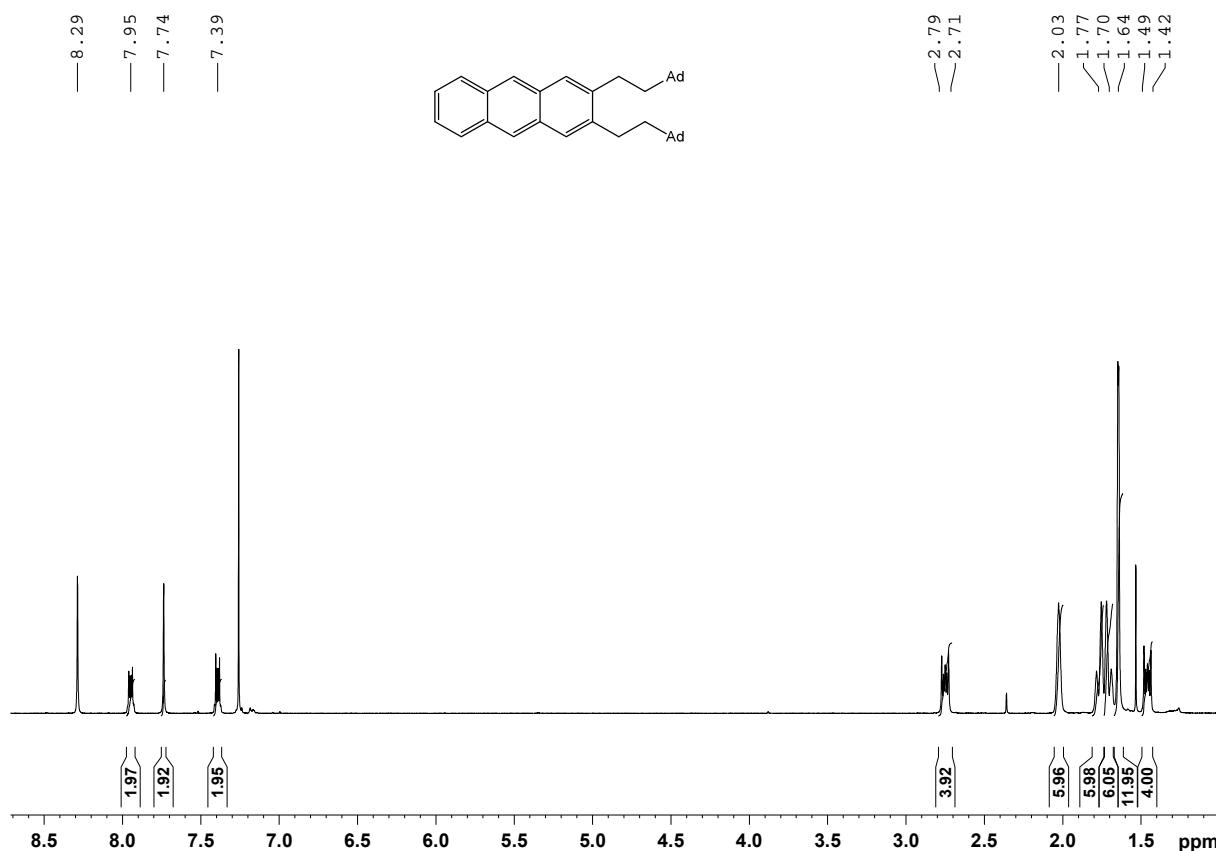


Figure S59. ¹H-NMR spectrum of **35** in CDCl₃

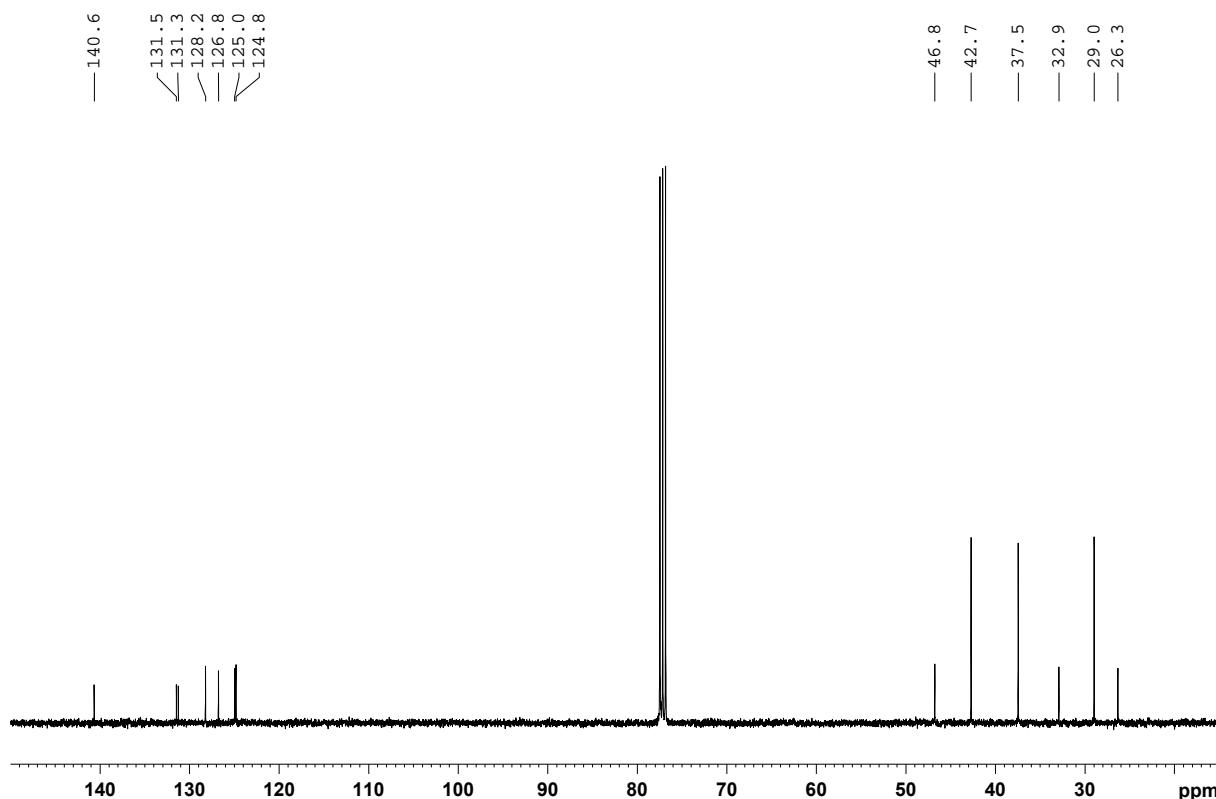


Figure S60. ¹³C{¹H}-NMR spectrum of **35** in CDCl₃

Supporting Information (SI)

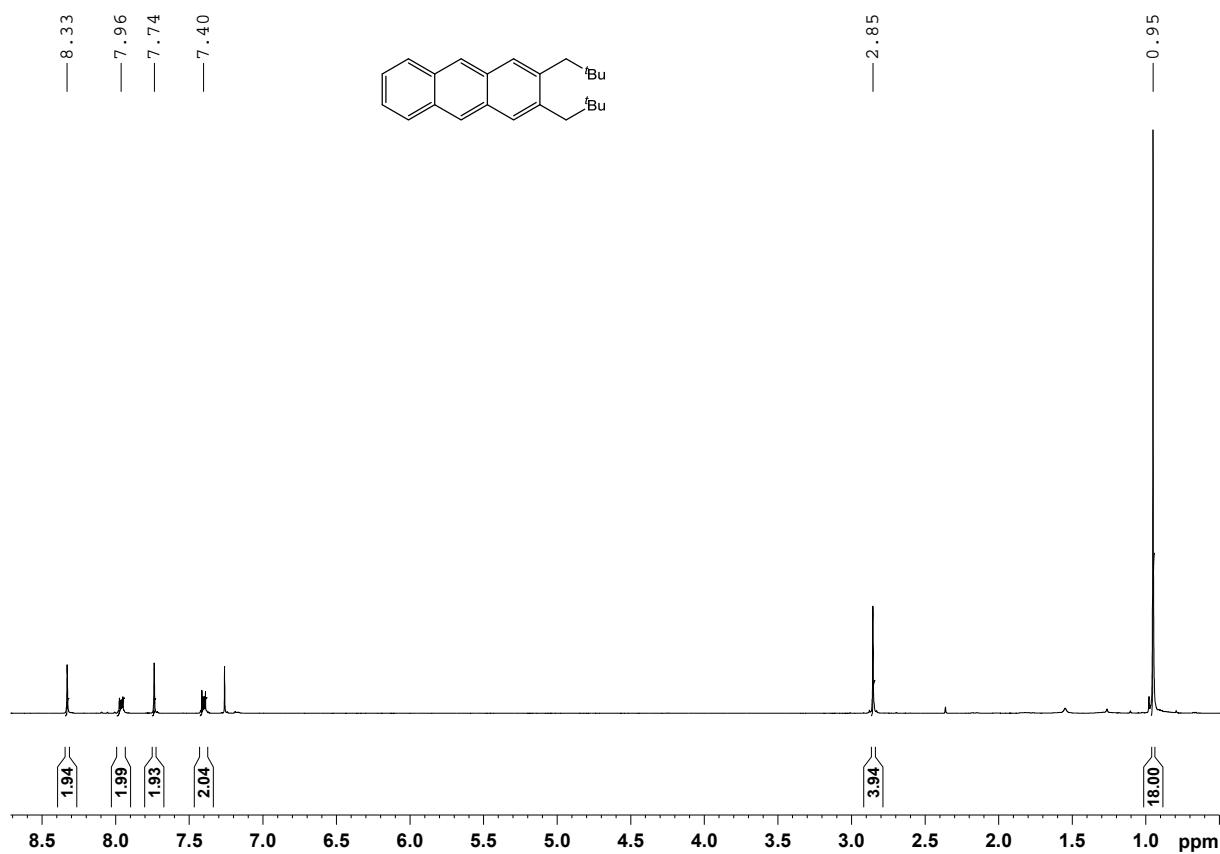


Figure S61. ^1H -NMR spectrum of **36** in CDCl_3

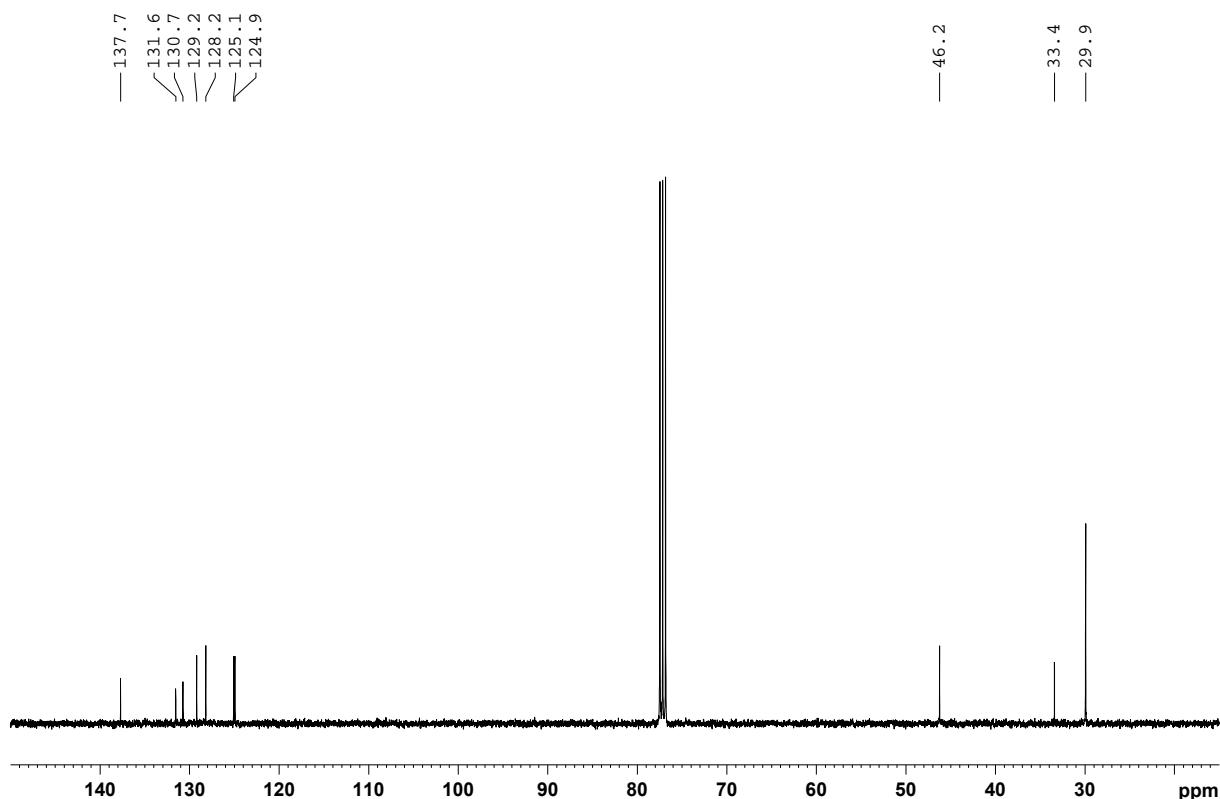


Figure S62. $^{13}\text{C}\{\text{H}\}$ -NMR spectrum of **36** in CDCl_3

Supporting Information (SI)

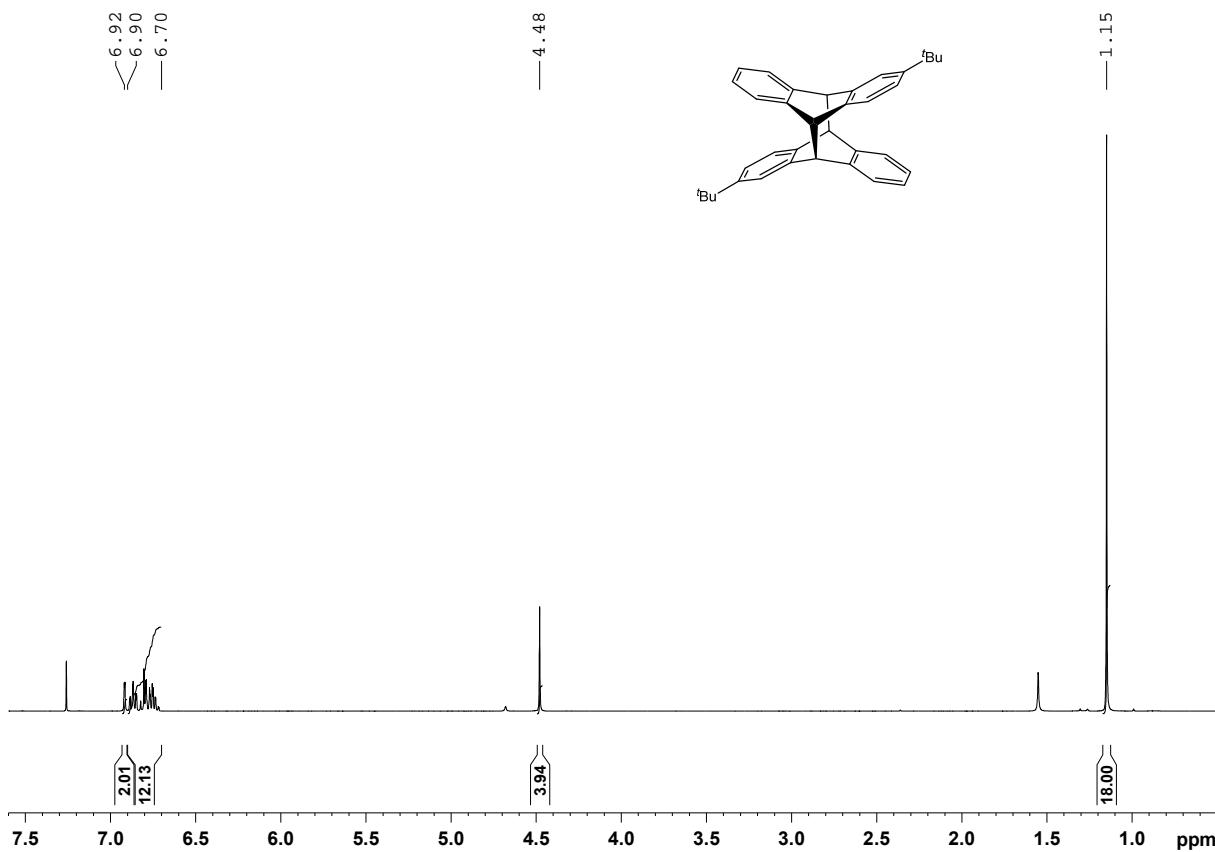


Figure S63. ^1H -NMR spectrum of **37a** in CDCl_3

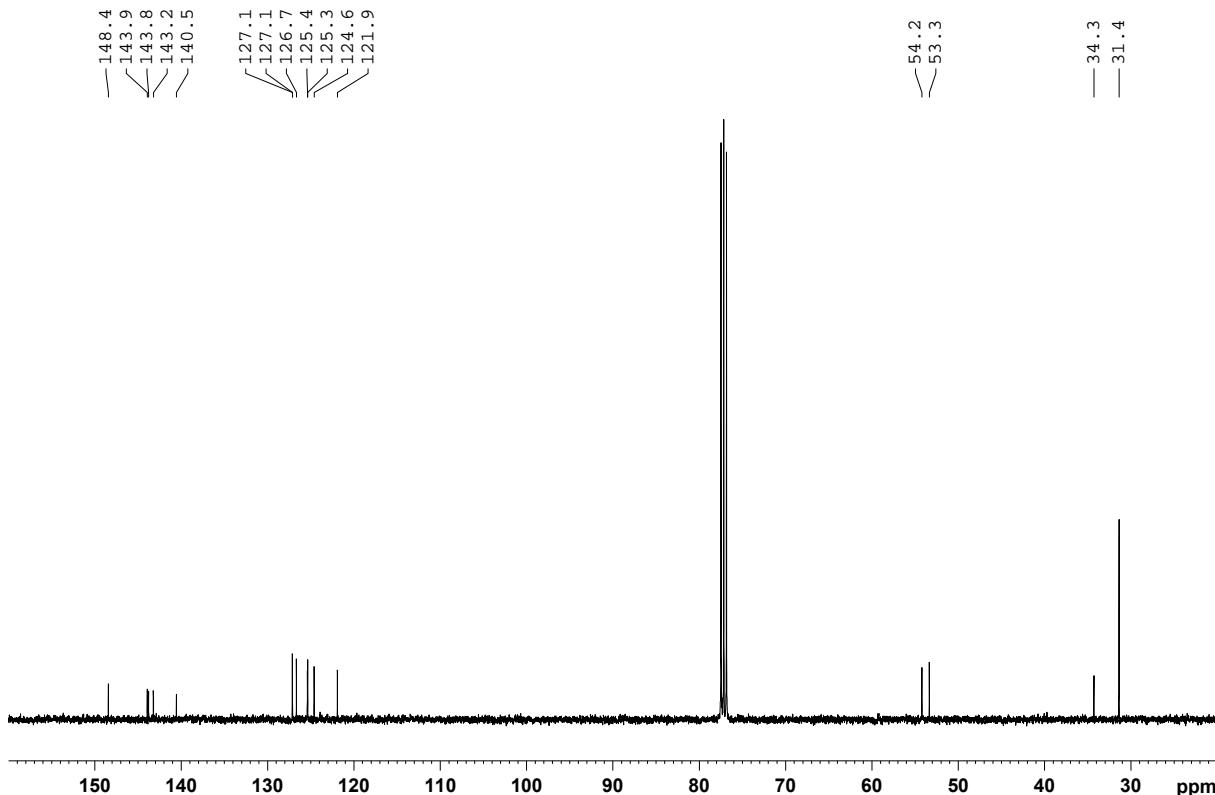


Figure S64. $^{13}\text{C}\{^1\text{H}\}$ -NMR spectrum of **37a** in CDCl_3

Supporting Information (SI)

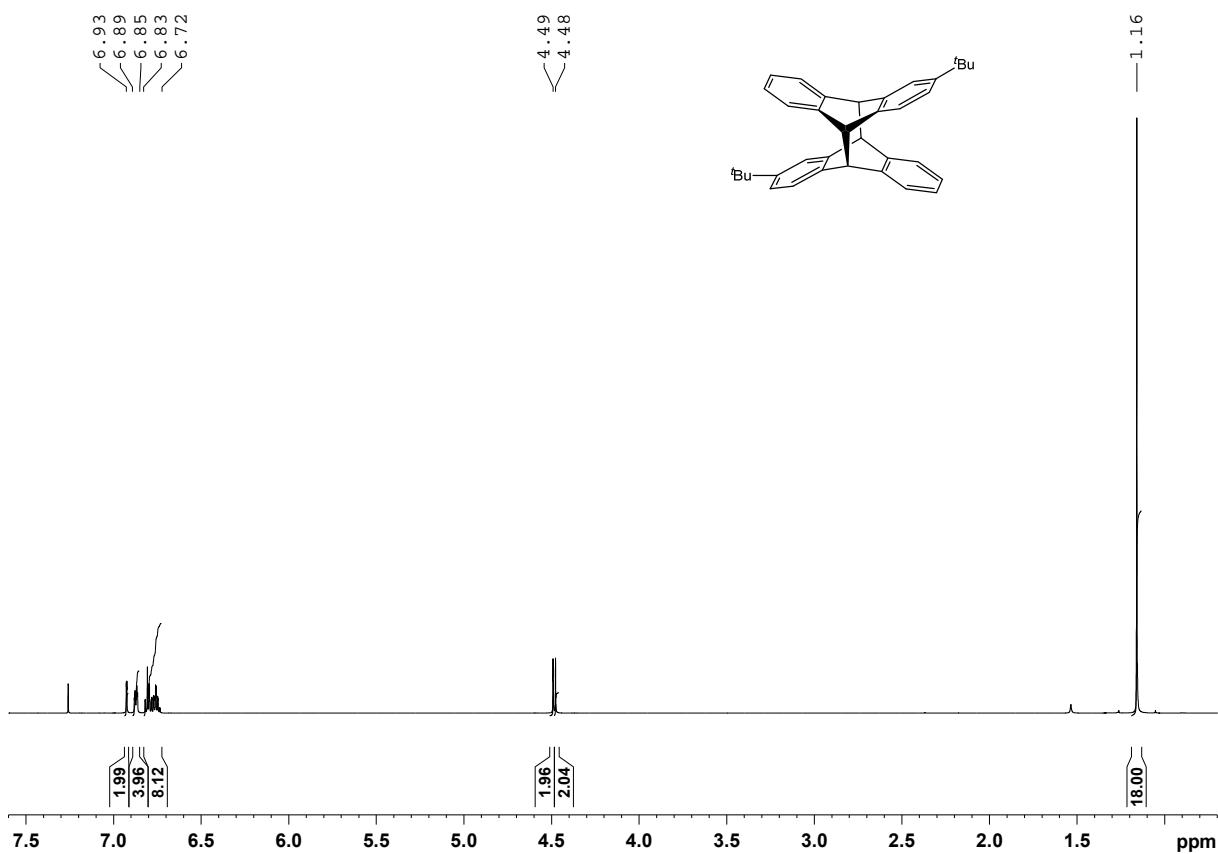


Figure S65. ^1H -NMR spectrum of **37b** in CDCl_3

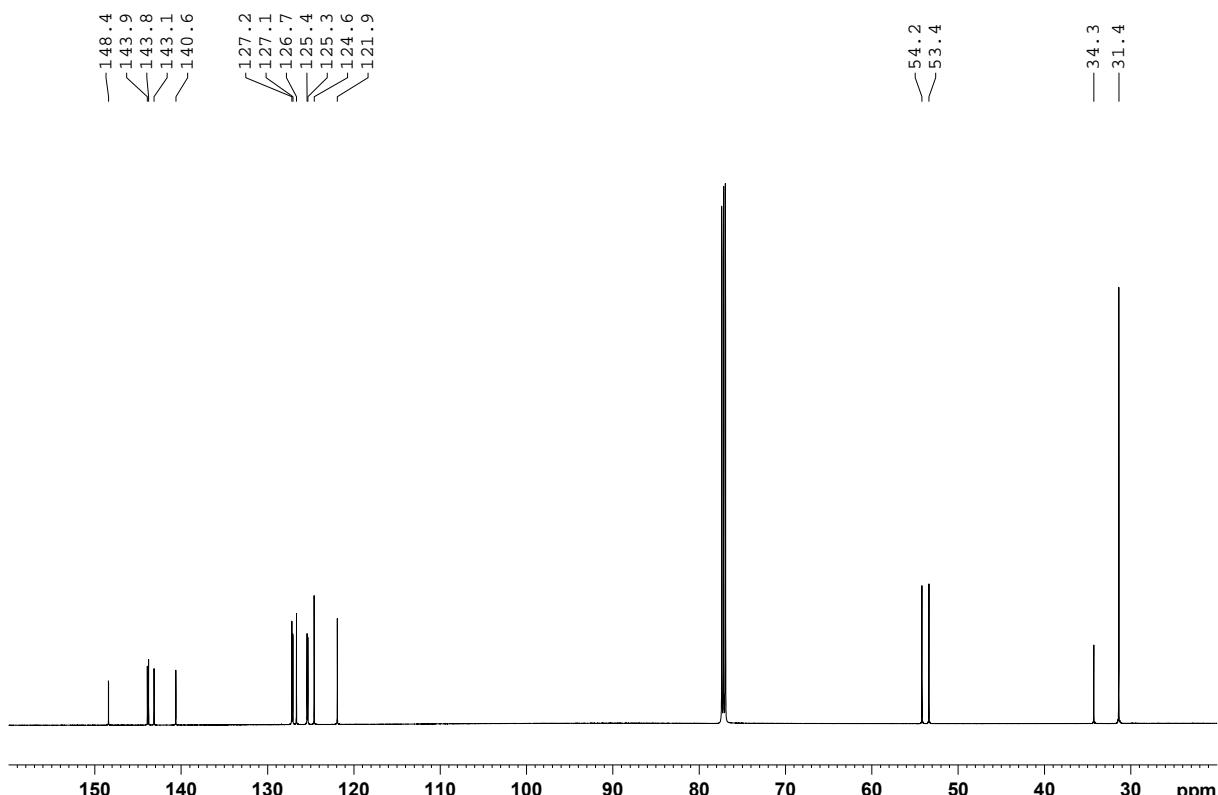


Figure S66. $^{13}\text{C}\{\text{H}\}$ -NMR spectrum of **37b** in CDCl_3

Supporting Information (SI)

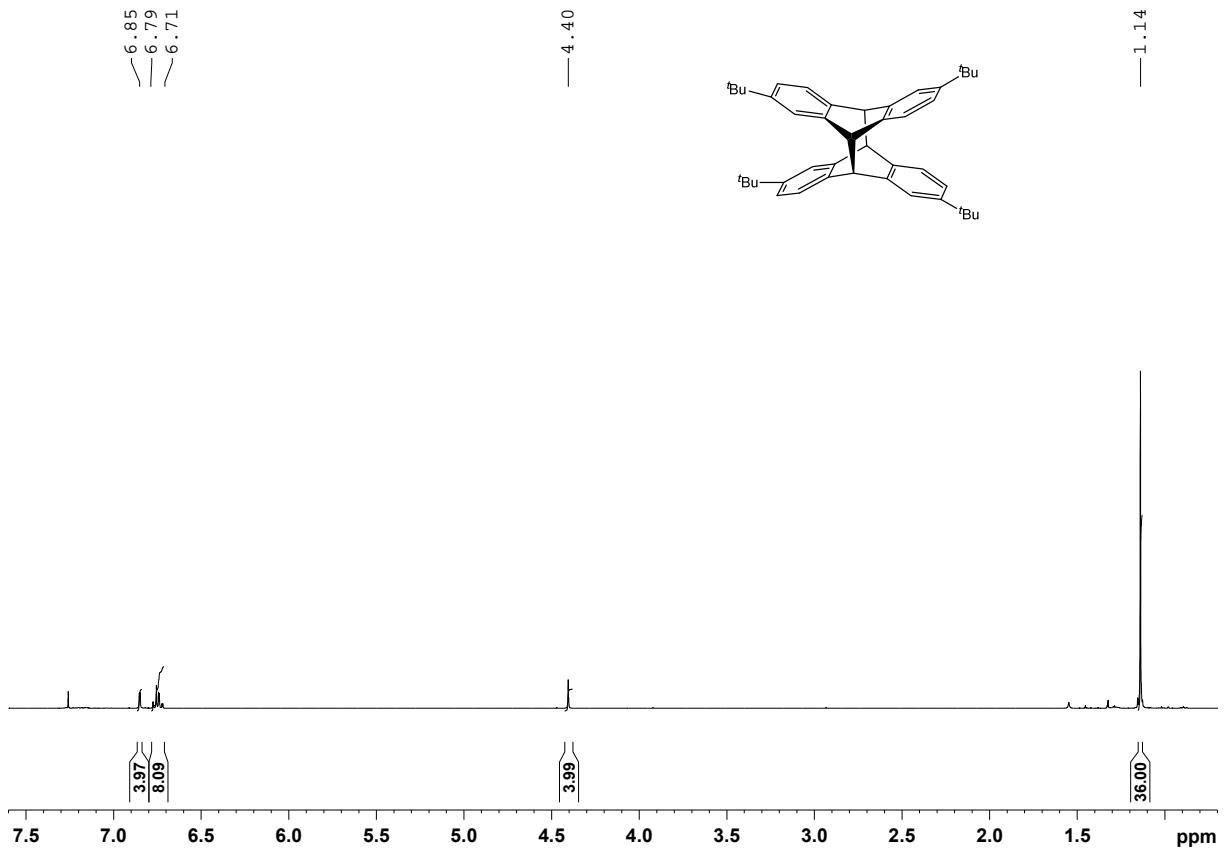


Figure S67. ^1H -NMR of **38a** in CDCl_3

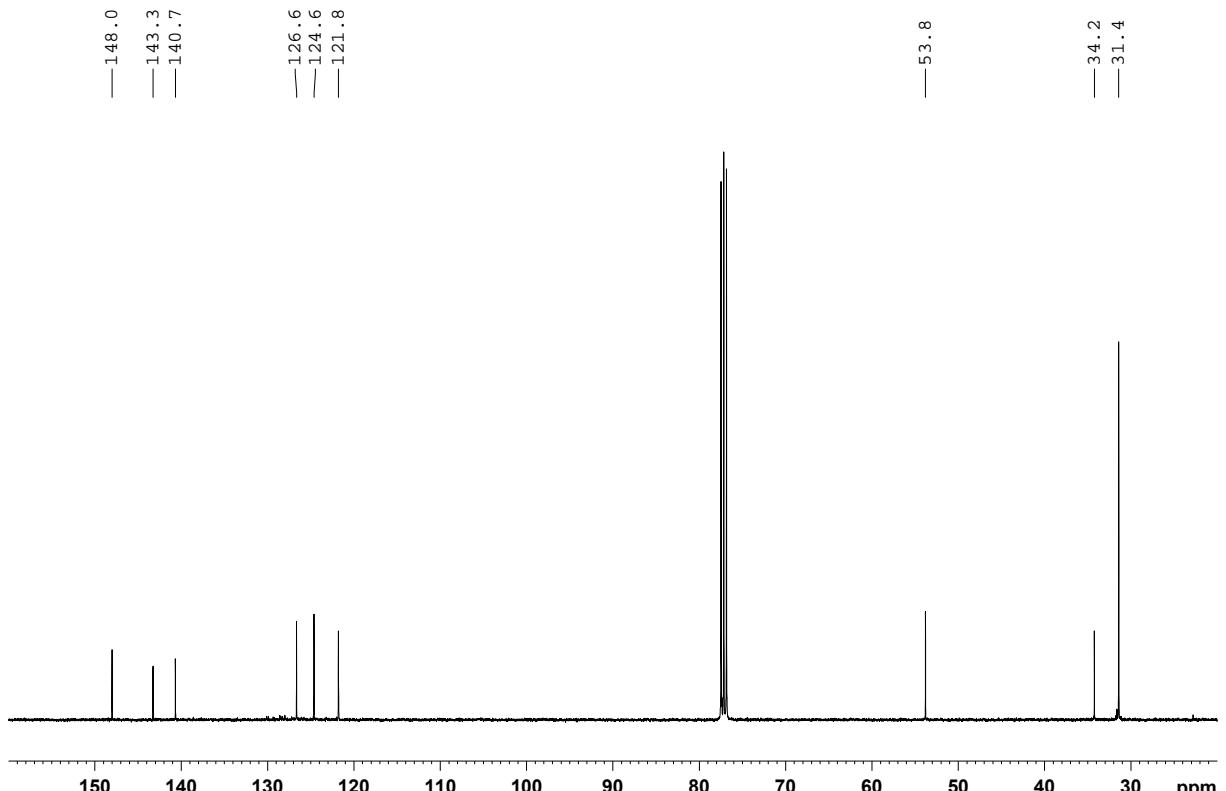


Figure S68. $^{13}\text{C}\{\text{H}\}$ -NMR of **38a** in CDCl_3

Supporting Information (SI)

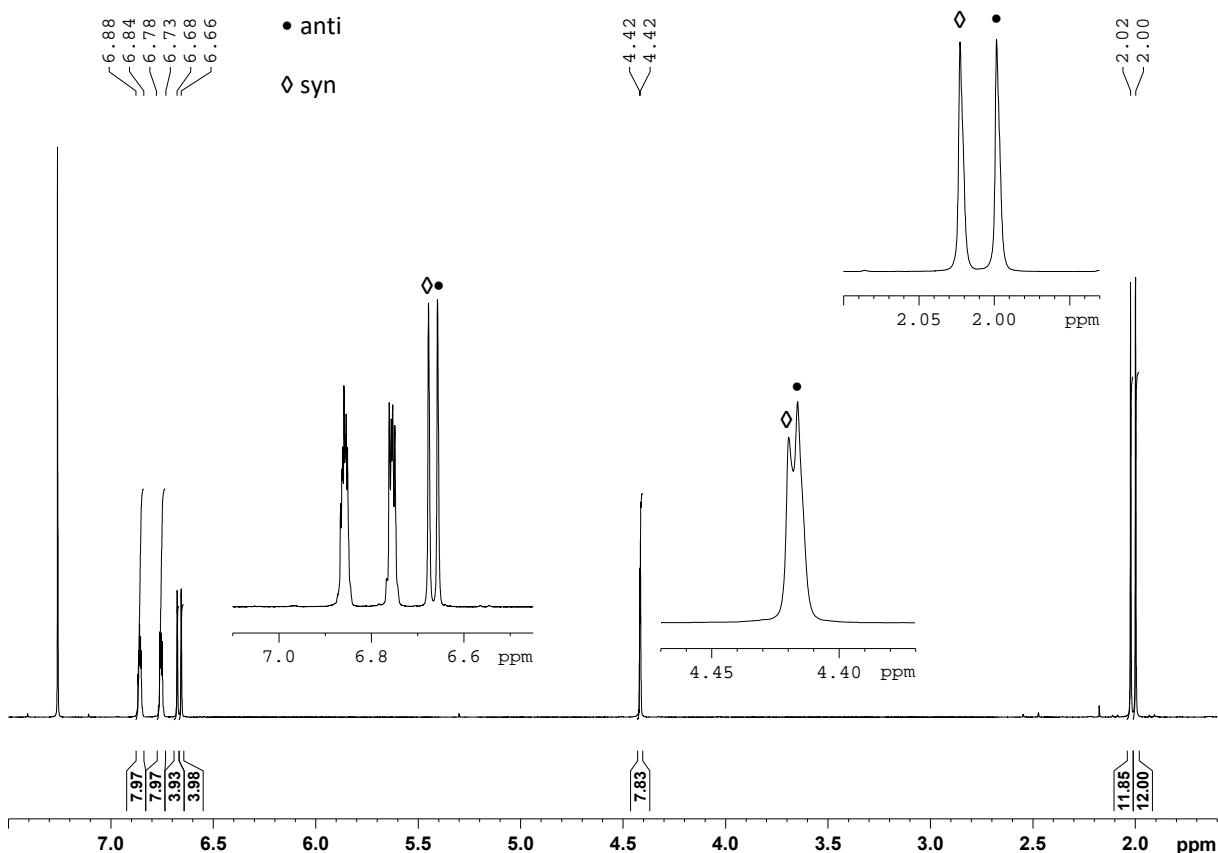


Figure S69. ^1H -NMR spectrum of the *anti/syn* mixture of **39a/b** in CDCl_3

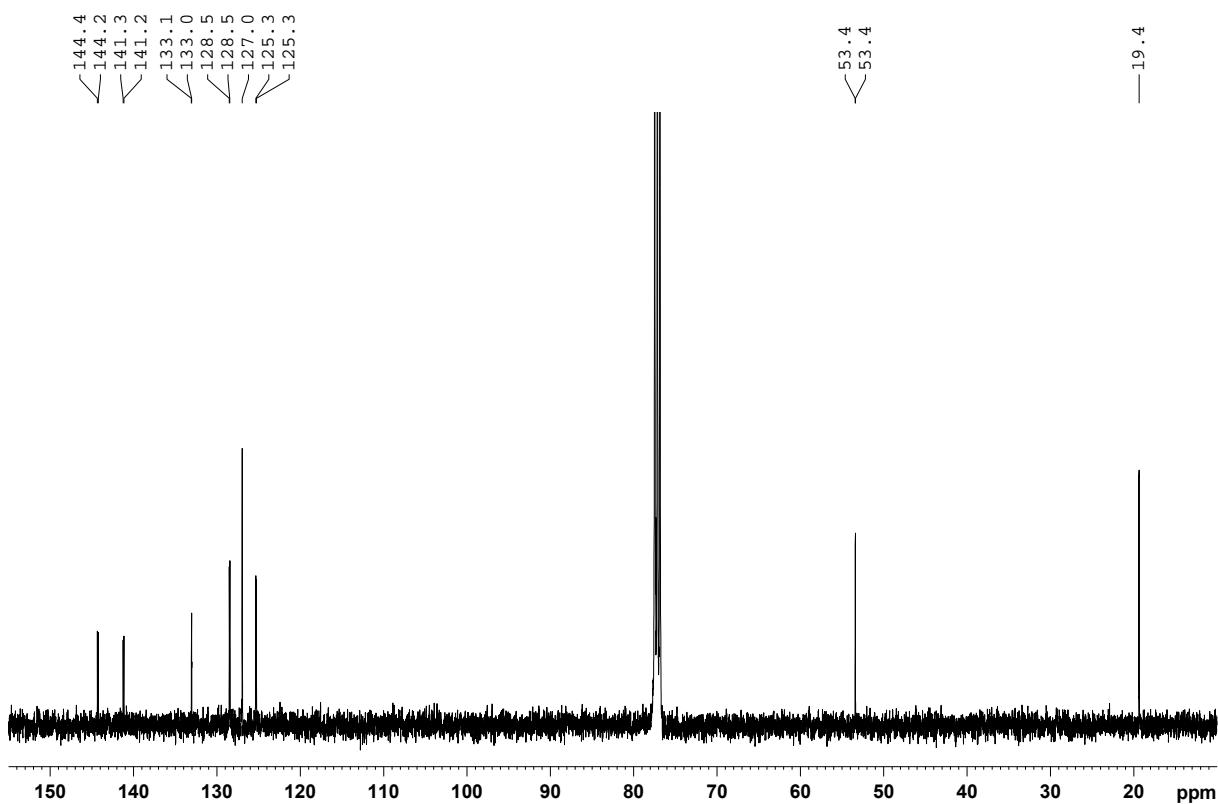


Figure S70. $^{13}\text{C}\{^1\text{H}\}$ -NMR spectrum of the *anti/syn* mixture of **39a/b** in CDCl_3

Supporting Information (SI)

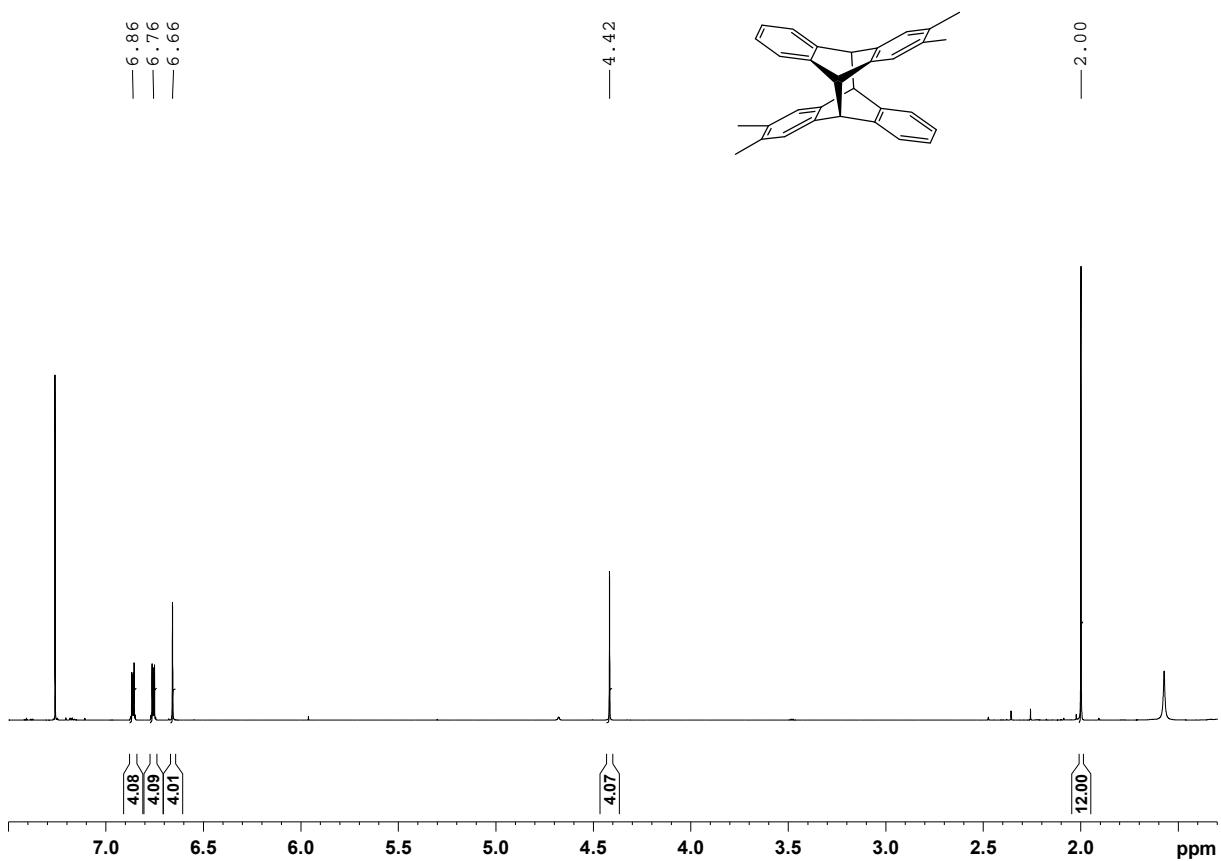


Figure S71. ¹H-NMR spectrum of **39a** in CDCl₃

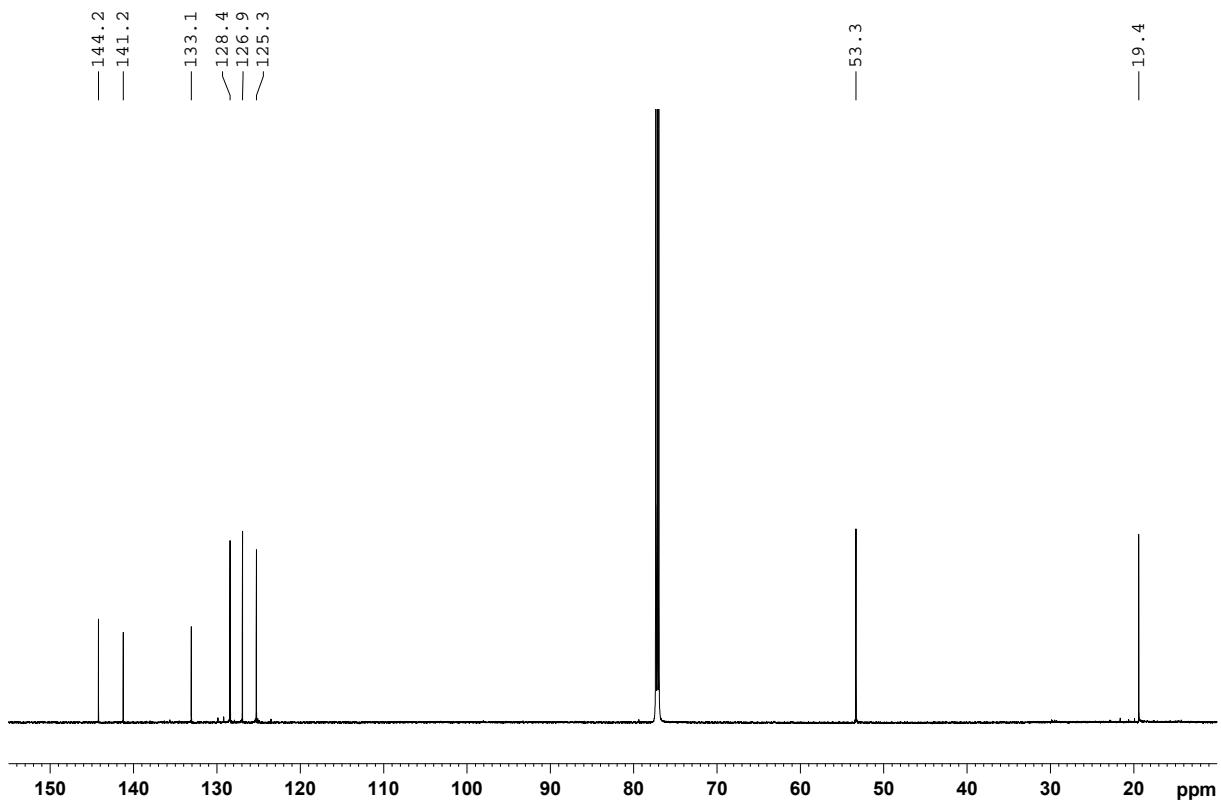


Figure S72. ¹³C{¹H}-NMR spectrum of **39a** in CDCl₃

Supporting Information (SI)

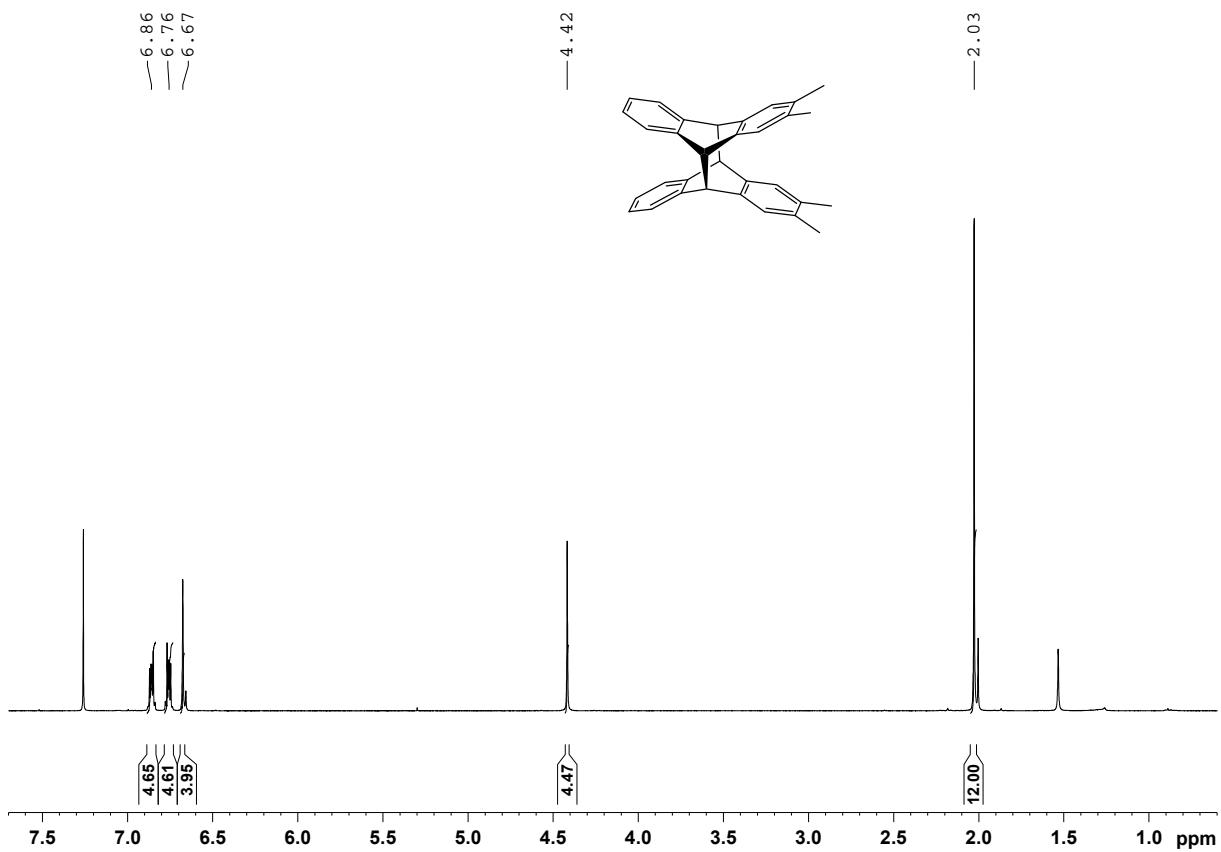


Figure S73. ^1H -NMR spectrum of **39b** in CDCl_3

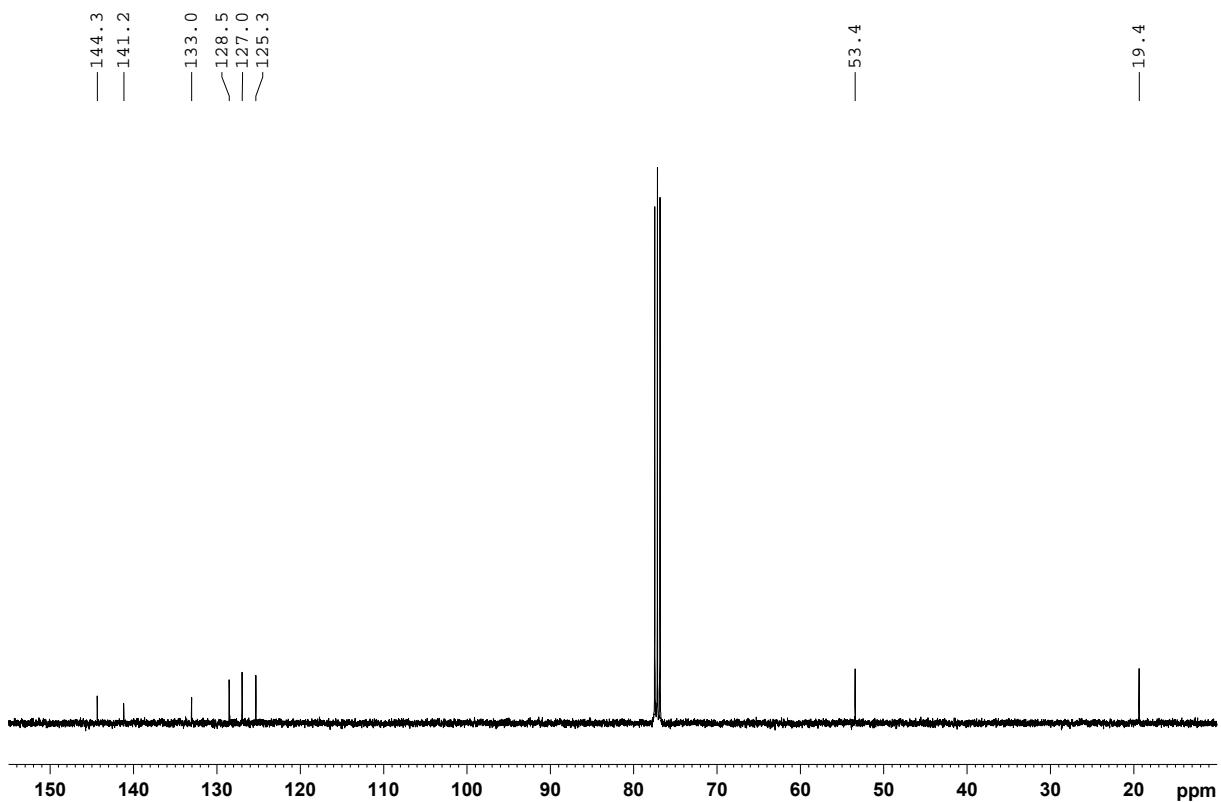


Figure S74. $^{13}\text{C}\{\text{H}\}$ -NMR spectrum of **39b** in CDCl_3

Supporting Information (SI)

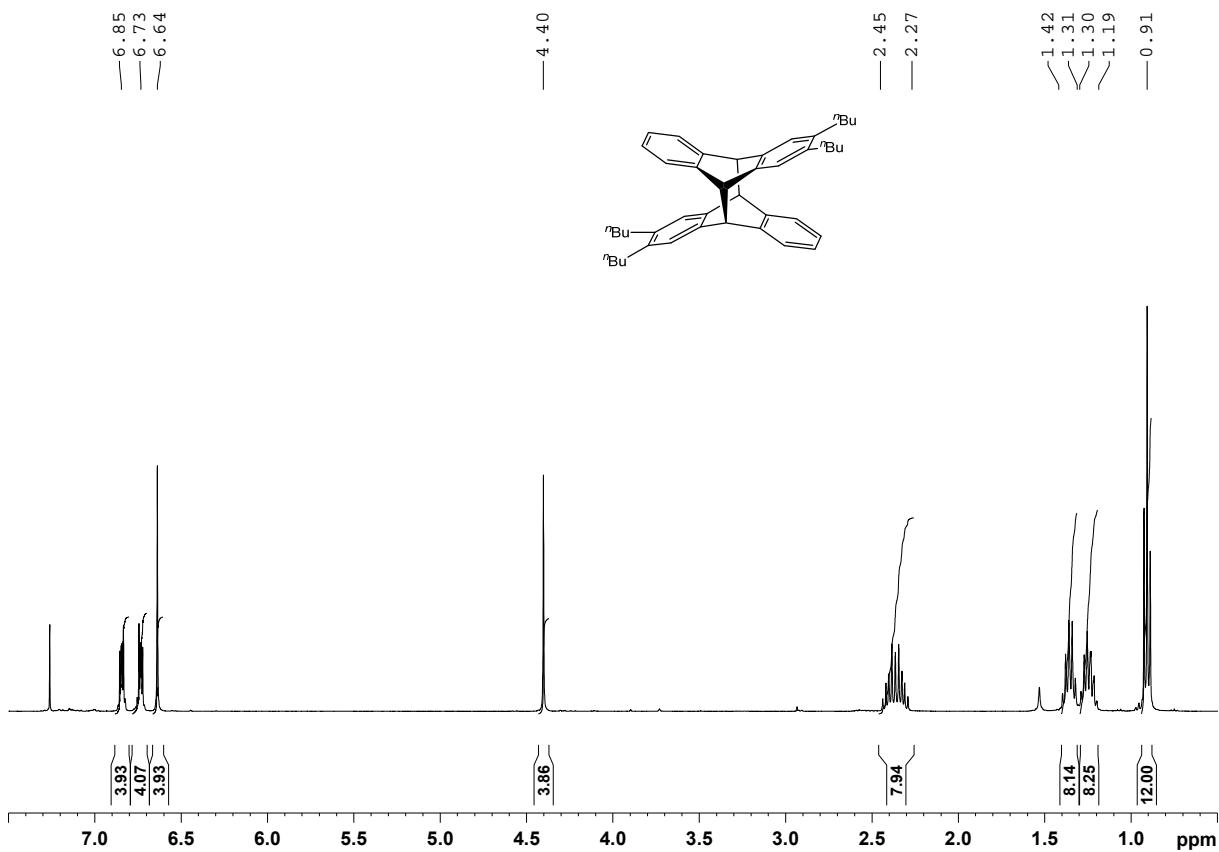


Figure S75. ^1H -NMR spectrum of **40a** in CDCl_3

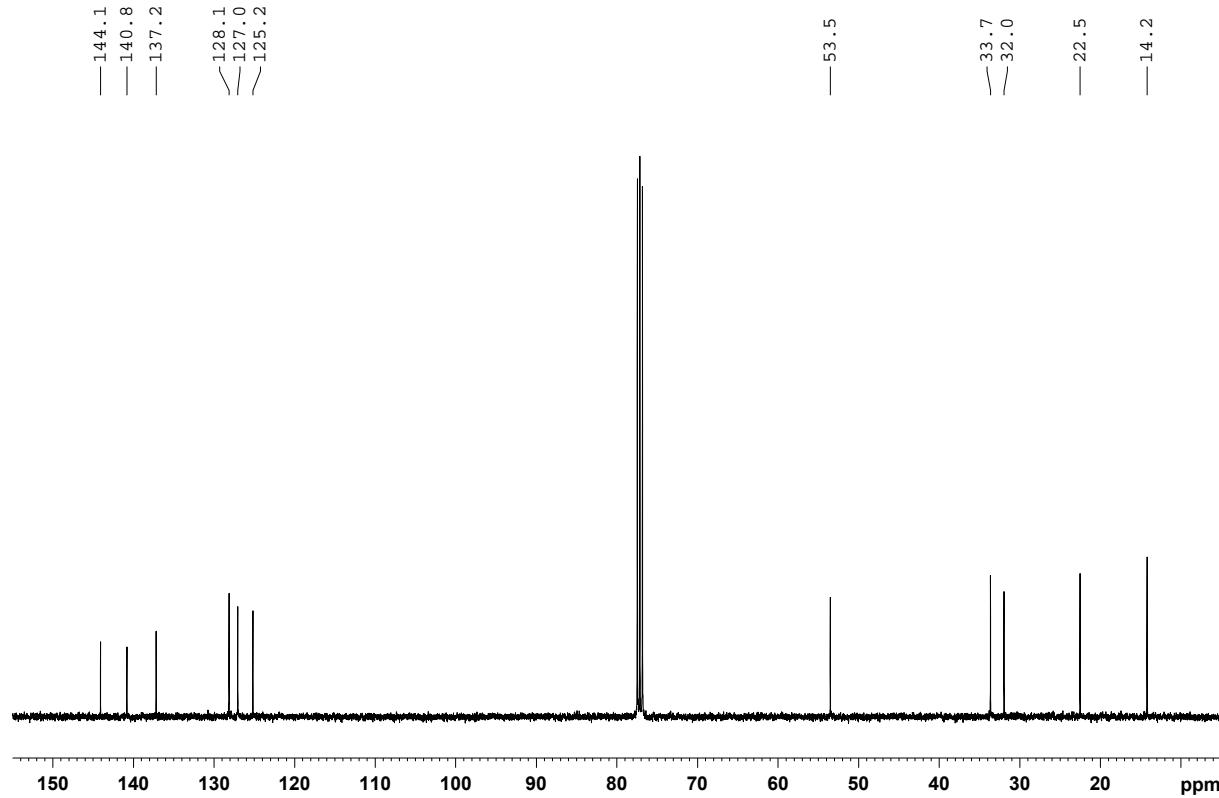


Figure S76. $^{13}\text{C}\{^1\text{H}\}$ -NMR spectrum of **40a** in CDCl_3

Supporting Information (SI)

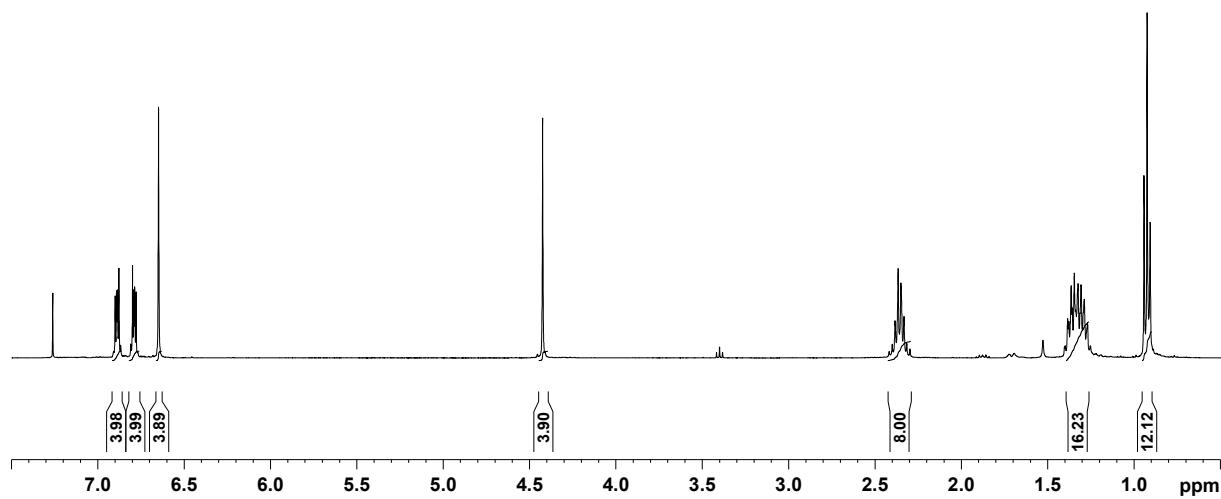
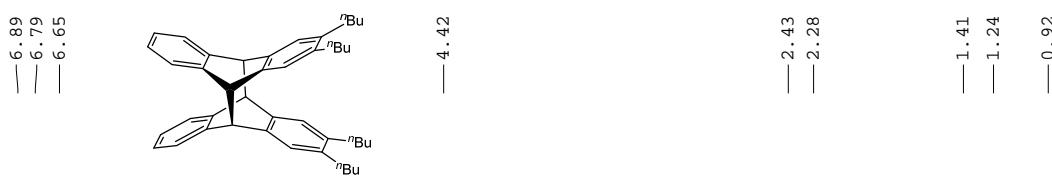


Figure S77. ¹H-NMR spectrum of **40b** in CDCl_3

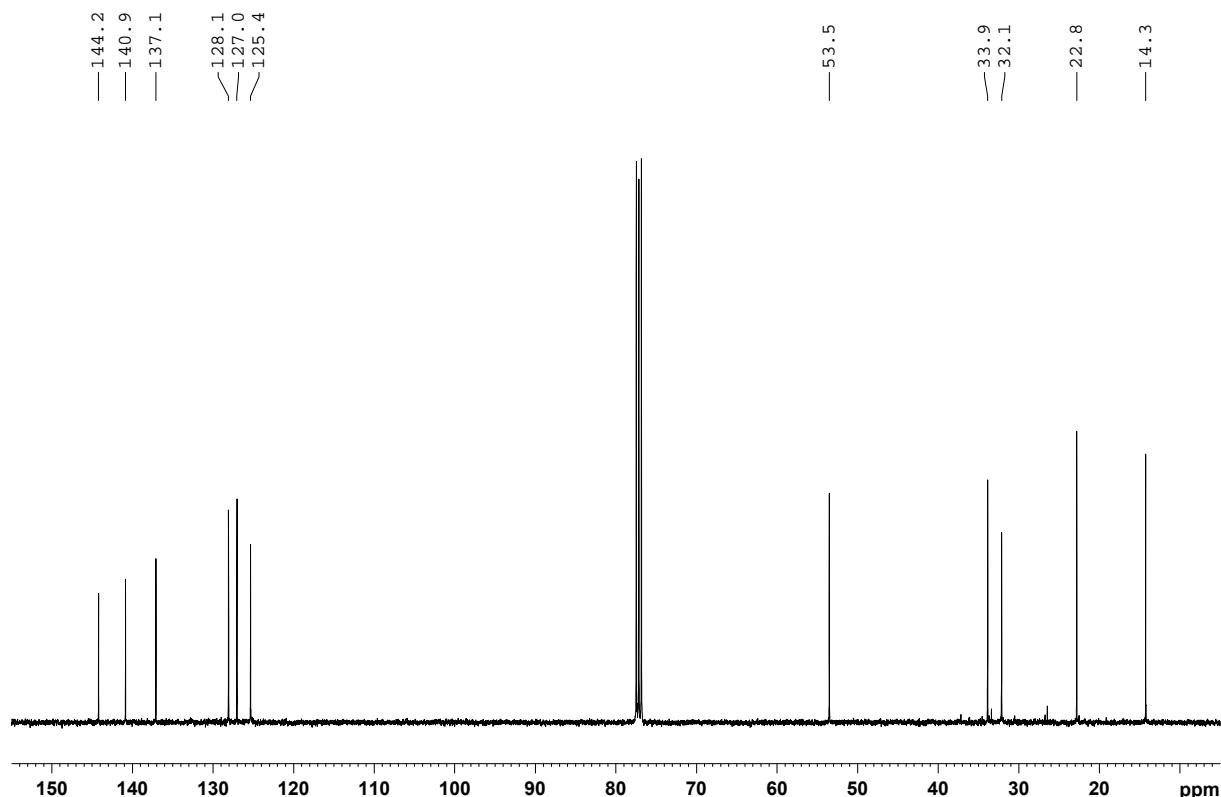


Figure S78. ¹³C{¹H}-NMR of **40b** in CDCl_3

Supporting Information (SI)

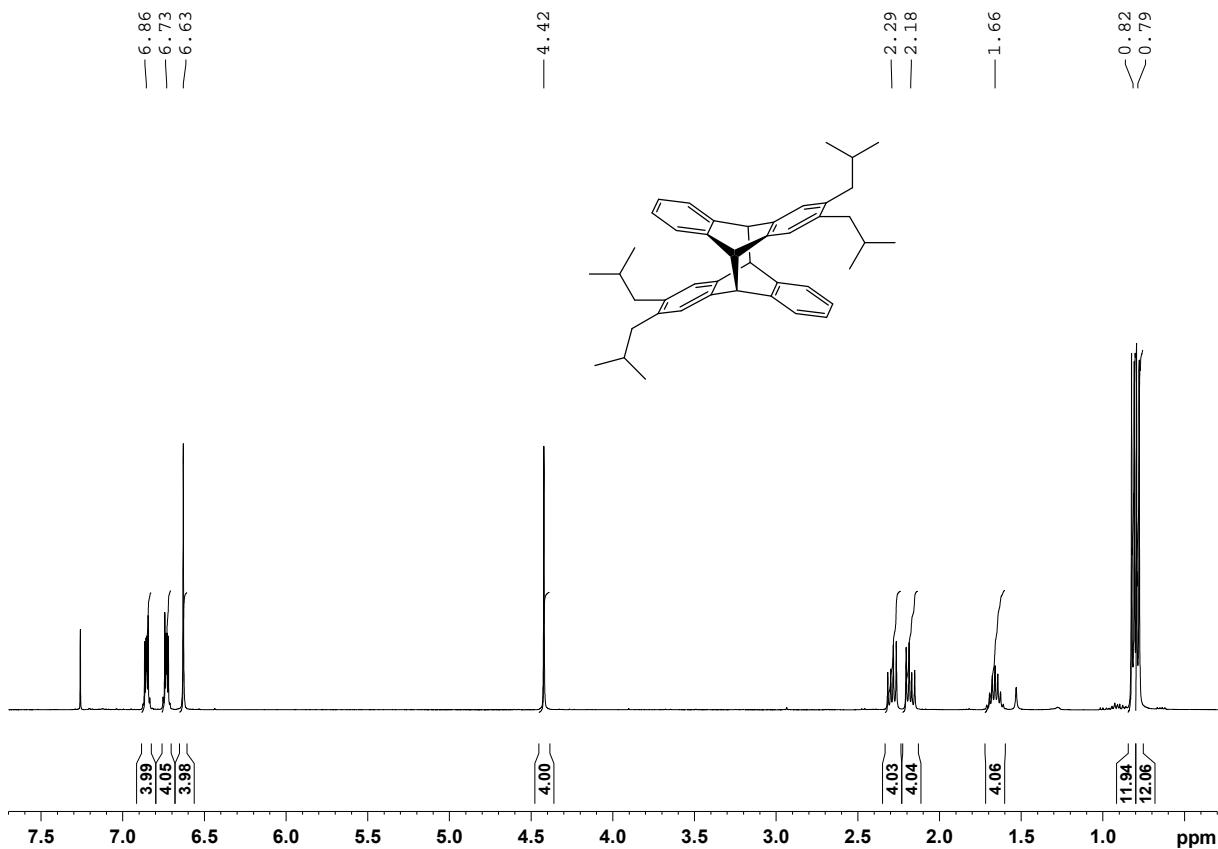


Figure S79. ^1H -NMR spectrum of **41a** in CDCl_3

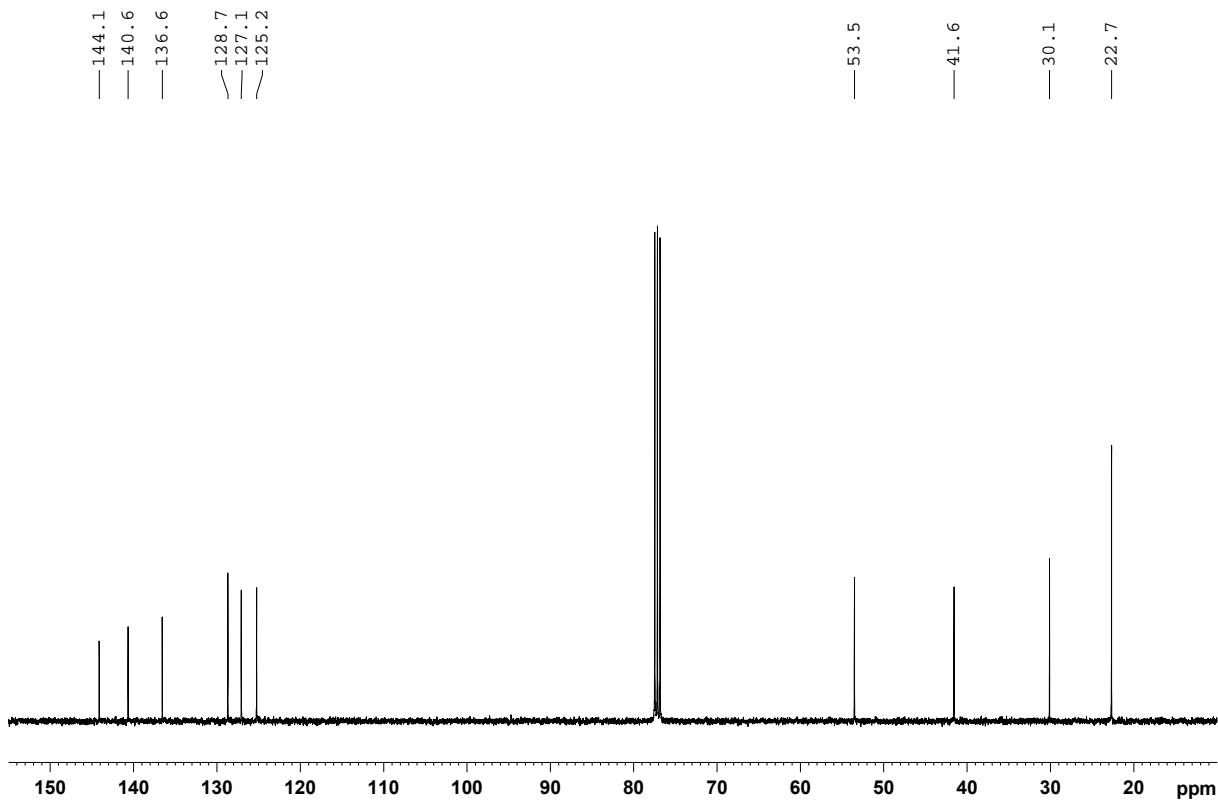


Figure S80. $^{13}\text{C}\{\text{H}\}$ -NMR of **41a** in CDCl_3

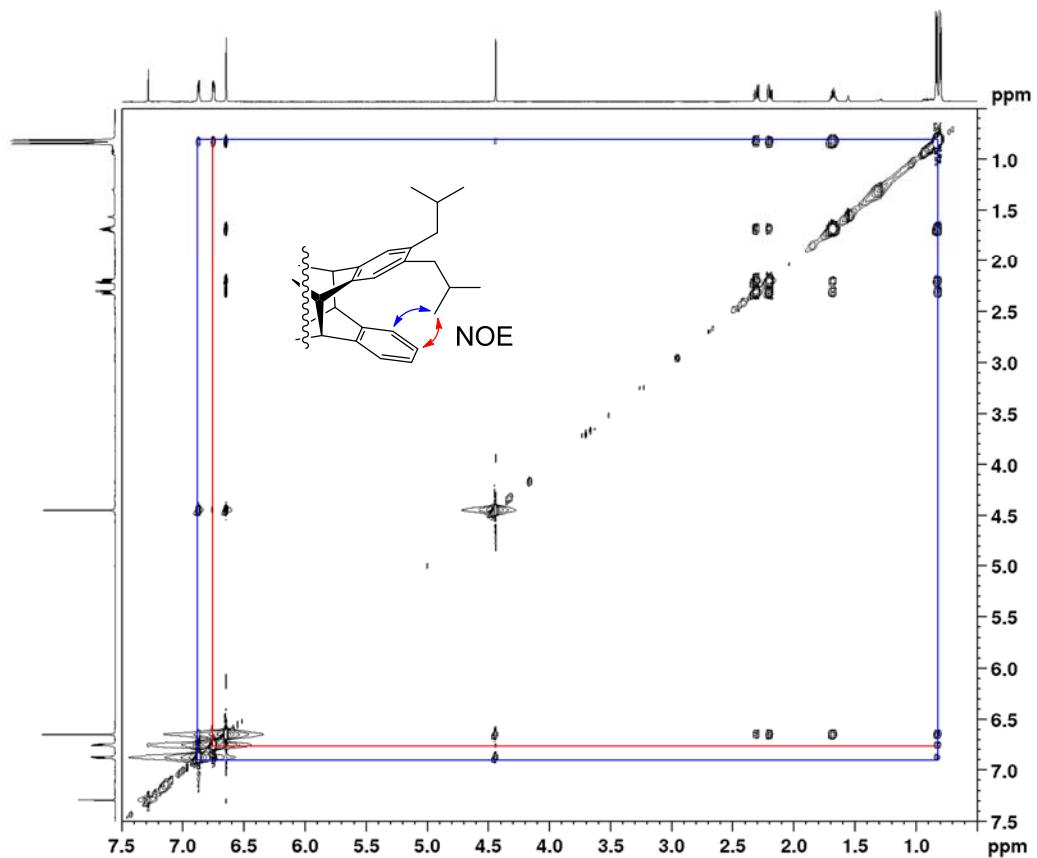


Figure S81. NOE spectrum of **41a** in CDCl_3

Supporting Information (SI)

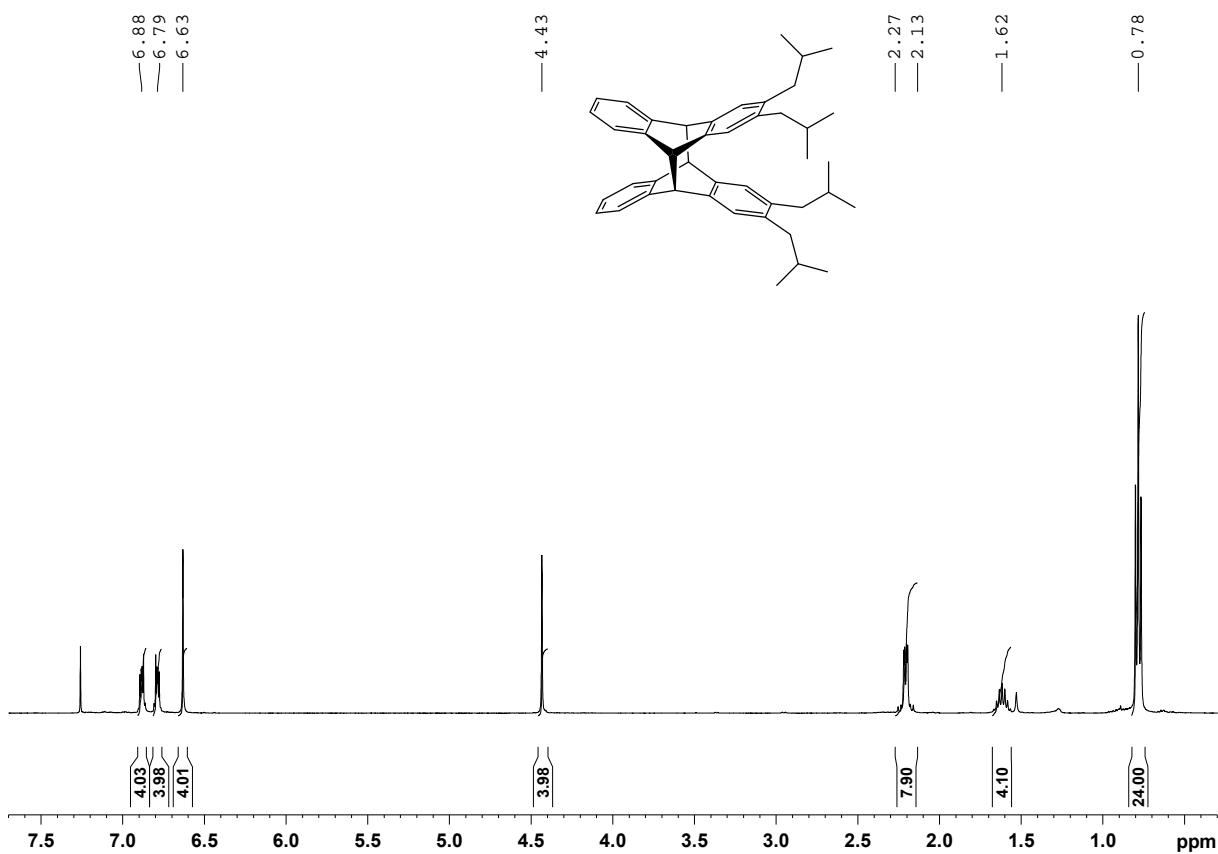


Figure S82. ^1H -NMR spectrum of **41b** in CDCl_3

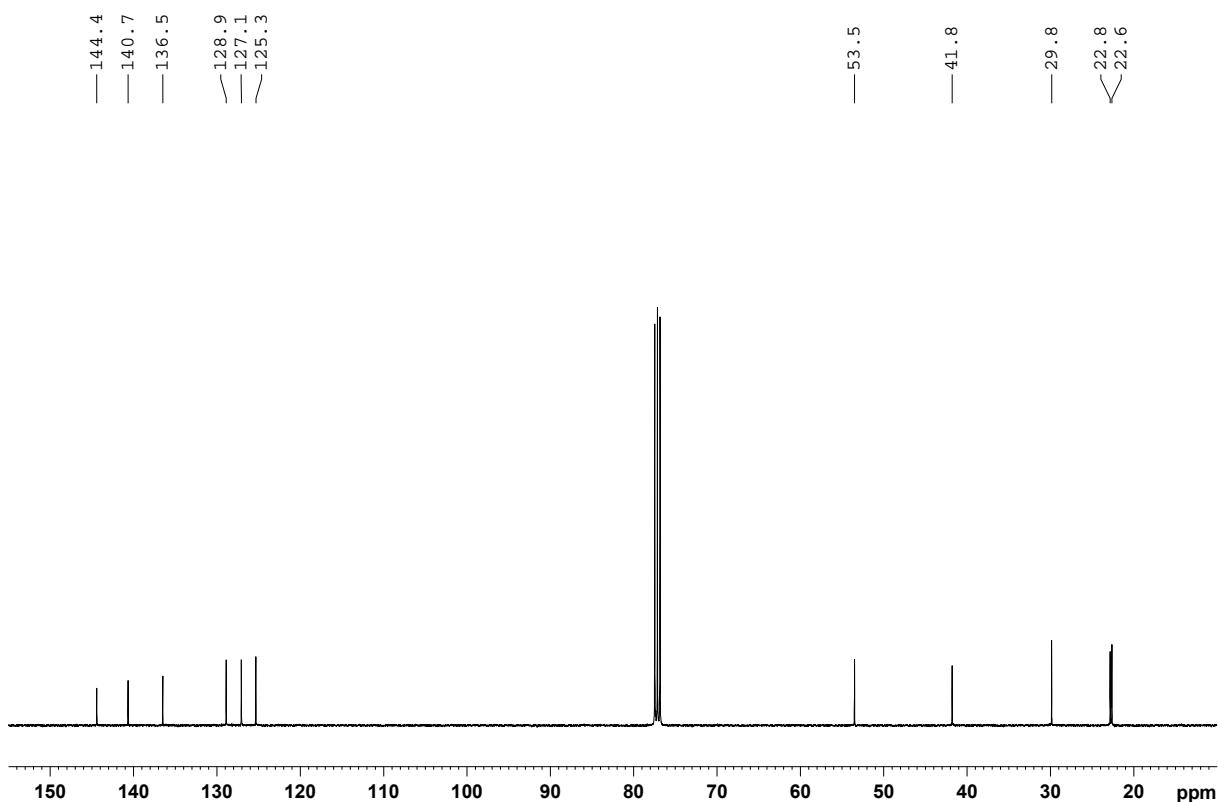


Figure S83. $^{13}\text{C}\{^1\text{H}\}$ -NMR spectrum of **41b** in CDCl_3

Supporting Information (SI)

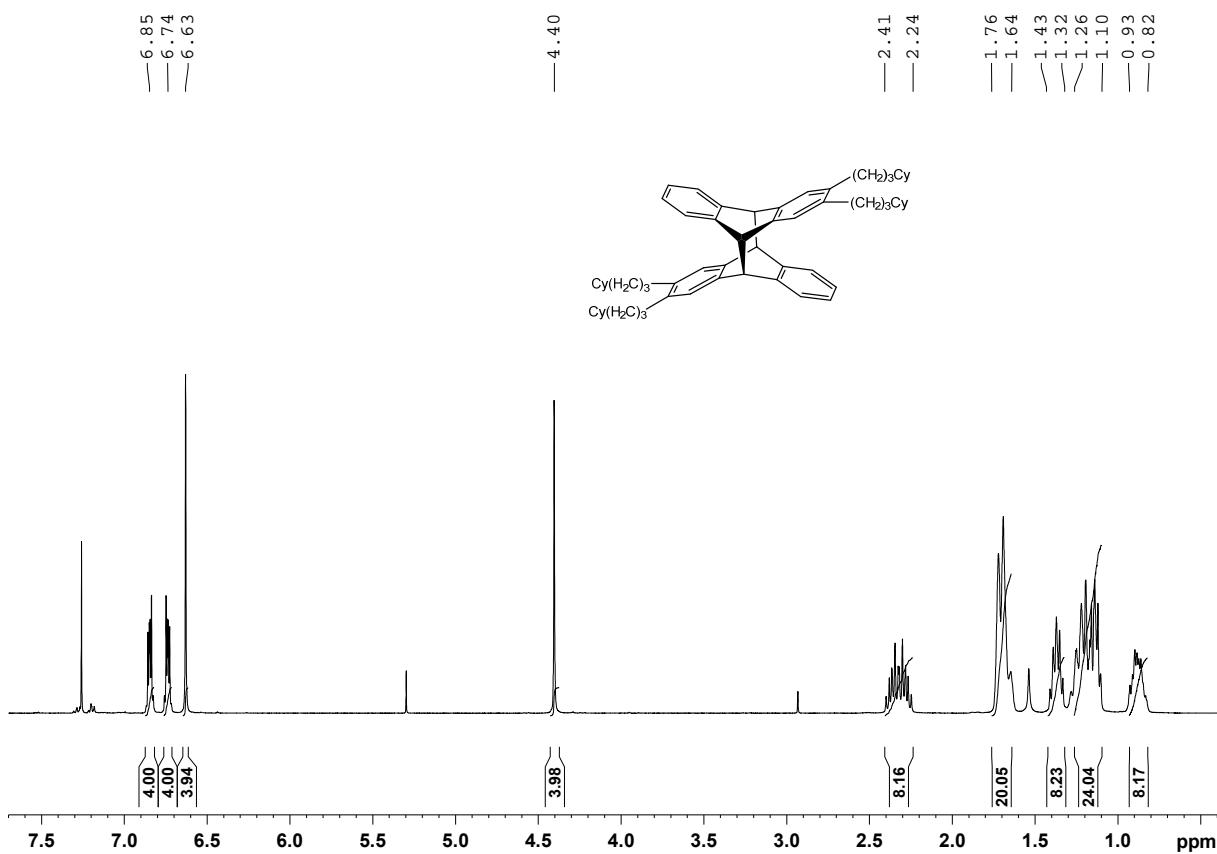


Figure S84. ^1H -NMR spectrum of **42a** in CDCl_3

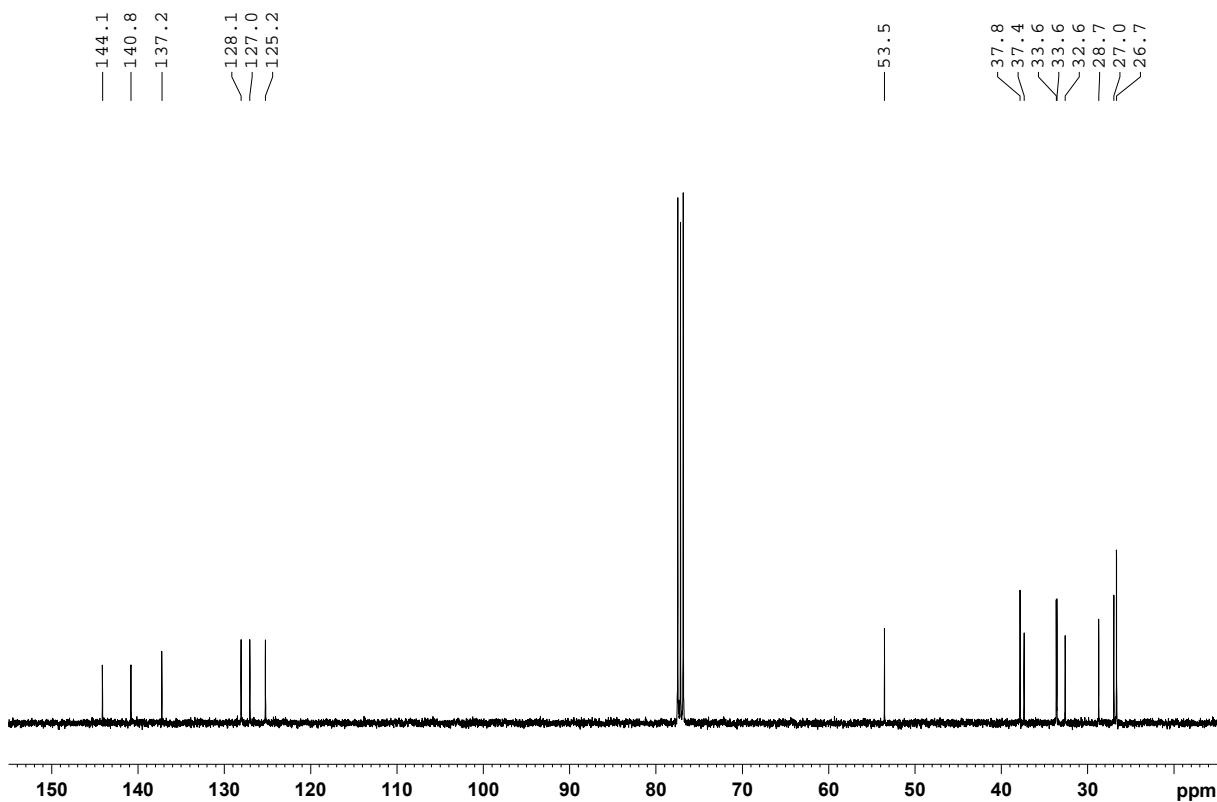


Figure S85. $^{13}\text{C}\{^1\text{H}\}$ -NMR spectrum of **42a** in CDCl_3

Supporting Information (SI)

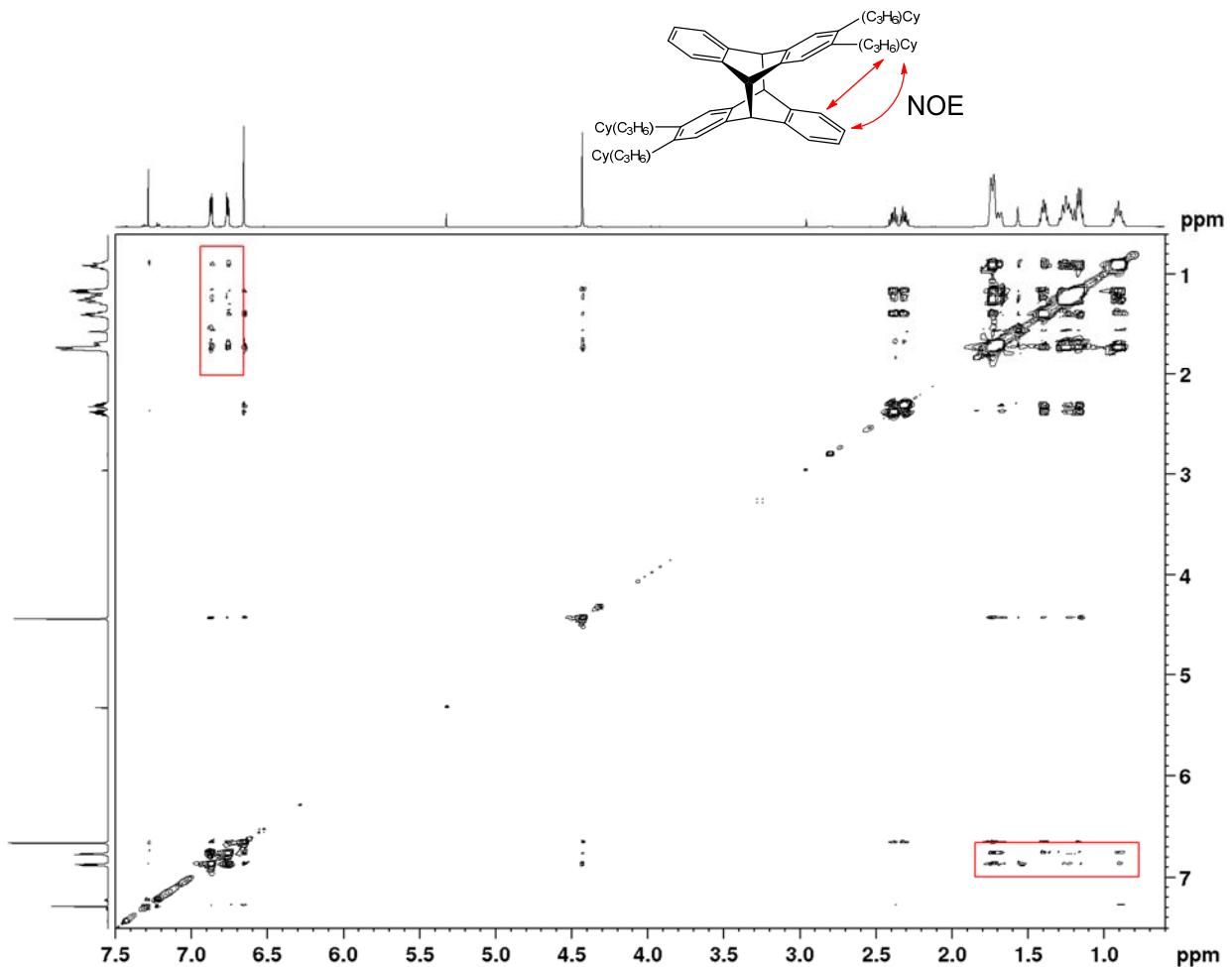


Figure S86. NOE spectrum of **42a** in CDCl_3

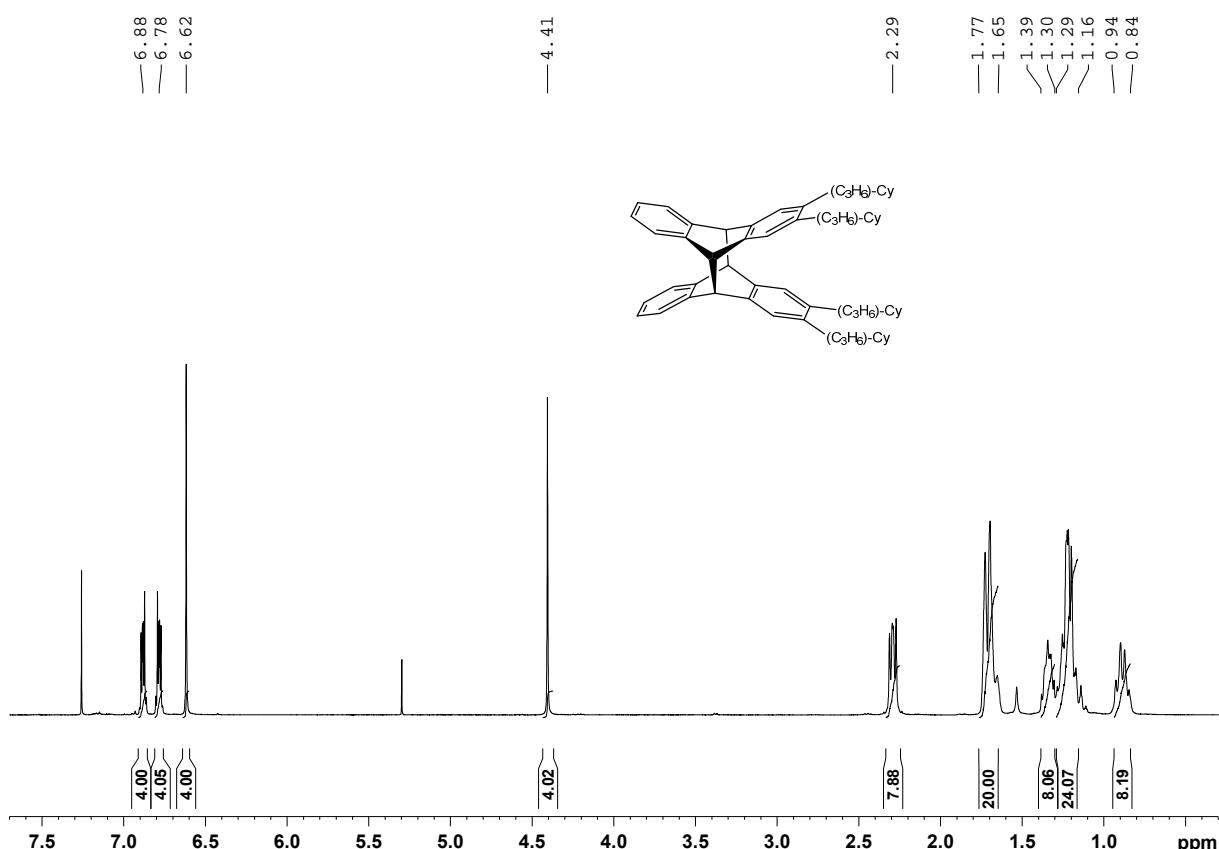


Figure S87. ^1H -NMR spectrum of **42b** in CDCl_3

Supporting Information (SI)

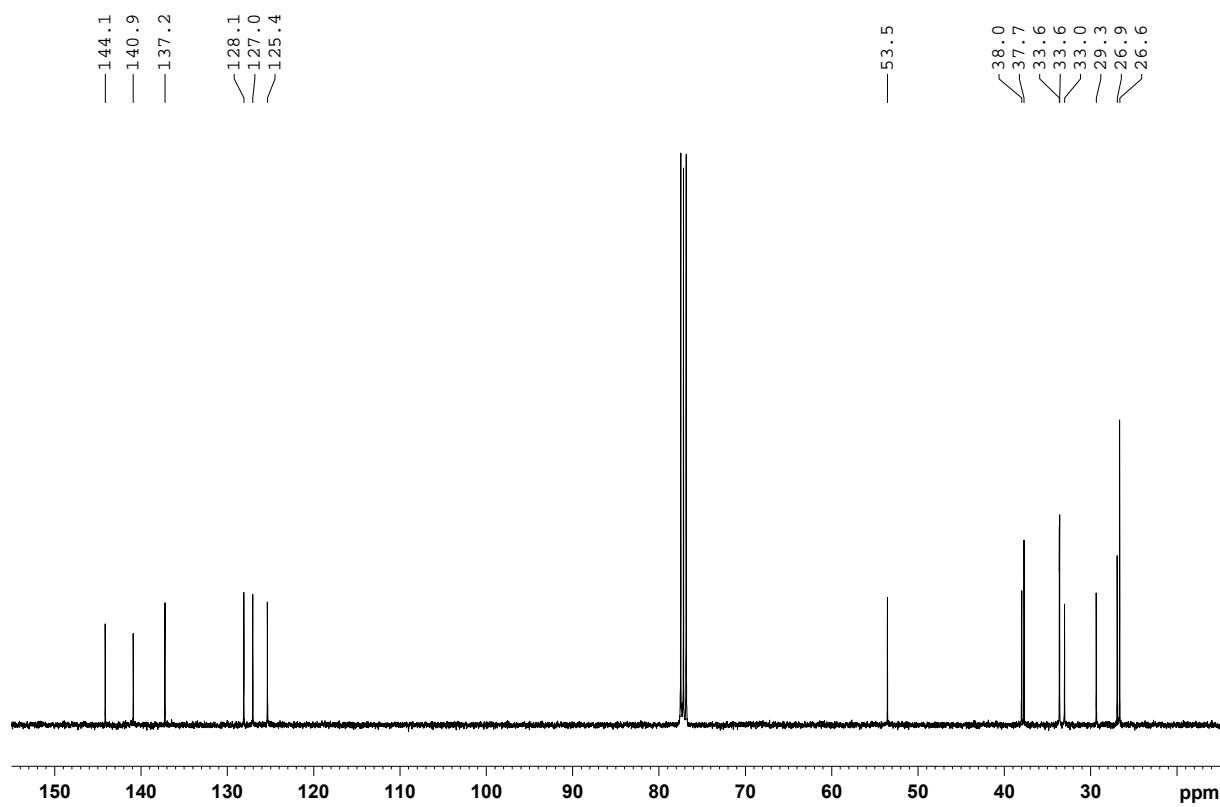


Figure S88. $^{13}\text{C}\{^1\text{H}\}$ -NMR spectrum of **42b** in CDCl_3

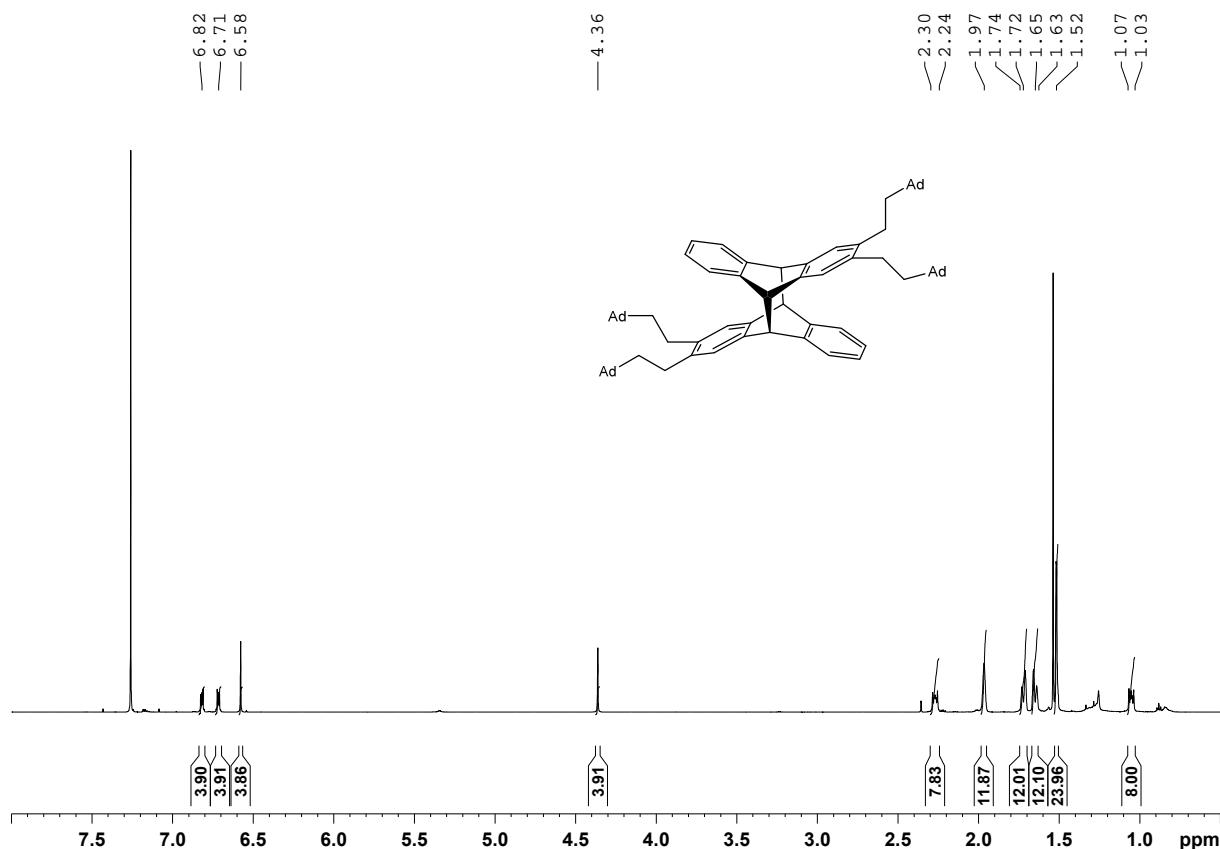


Figure S89. ^1H -NMR spectrum of **43a** in CDCl_3

Supporting Information (SI)

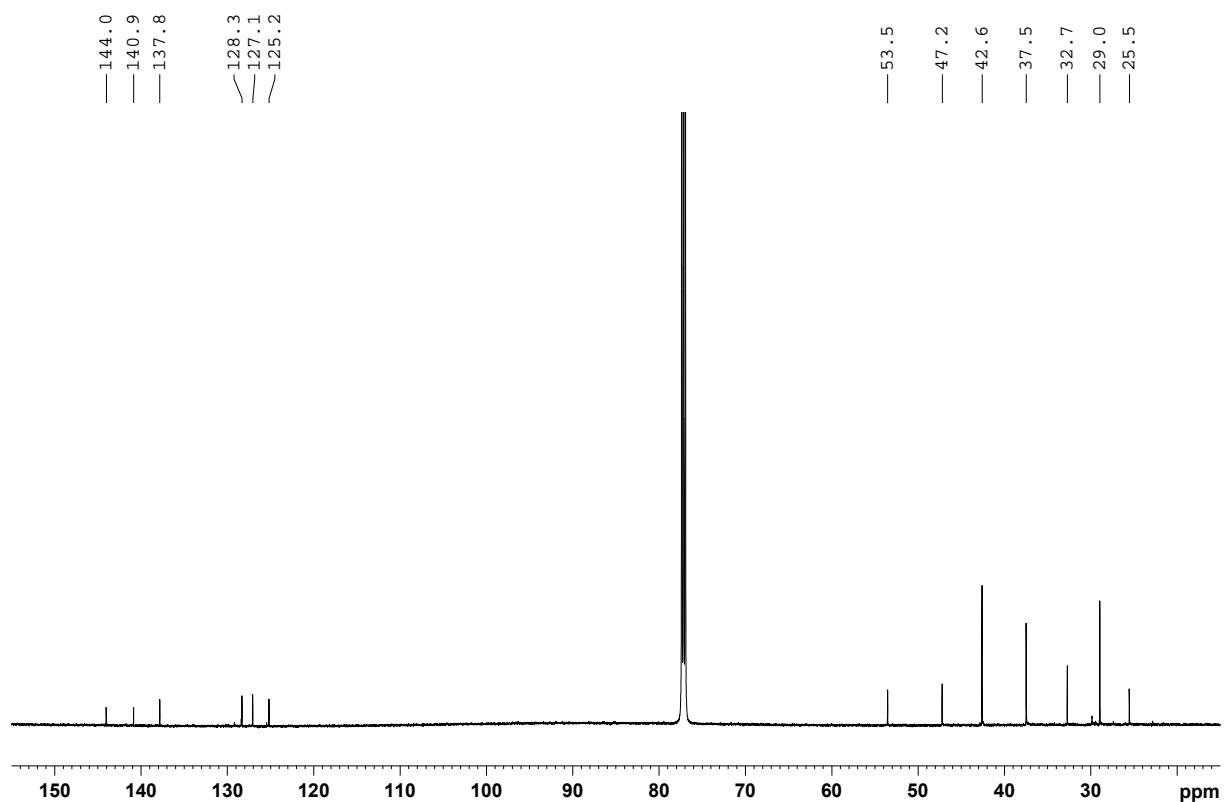


Figure S90. $^{13}\text{C}\{^1\text{H}\}$ -NMR spectrum of **43a** in CDCl_3

Supporting Information (SI)

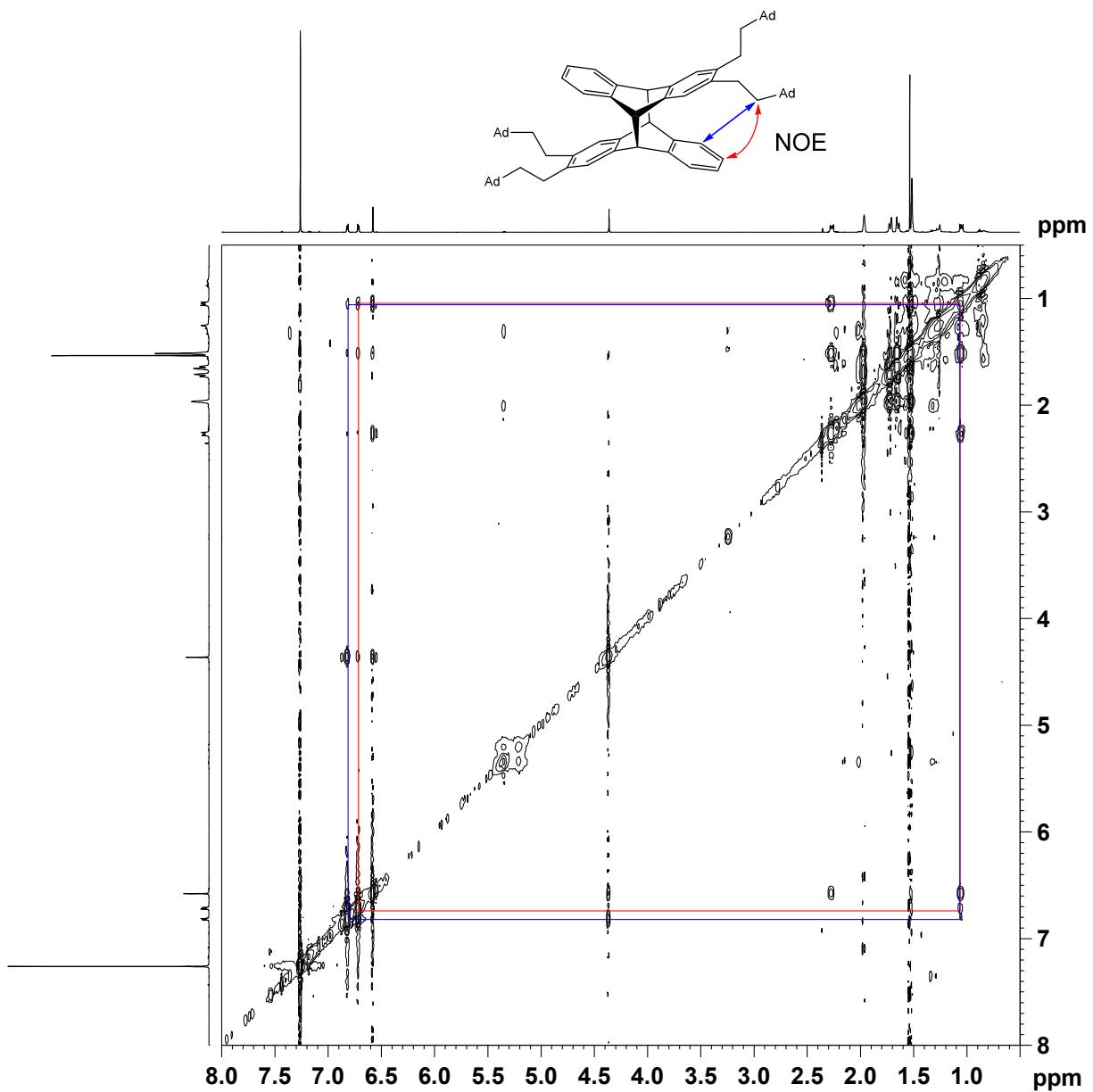


Figure S91. NOE spectrum of **43a** in CDCl_3

Supporting Information (SI)

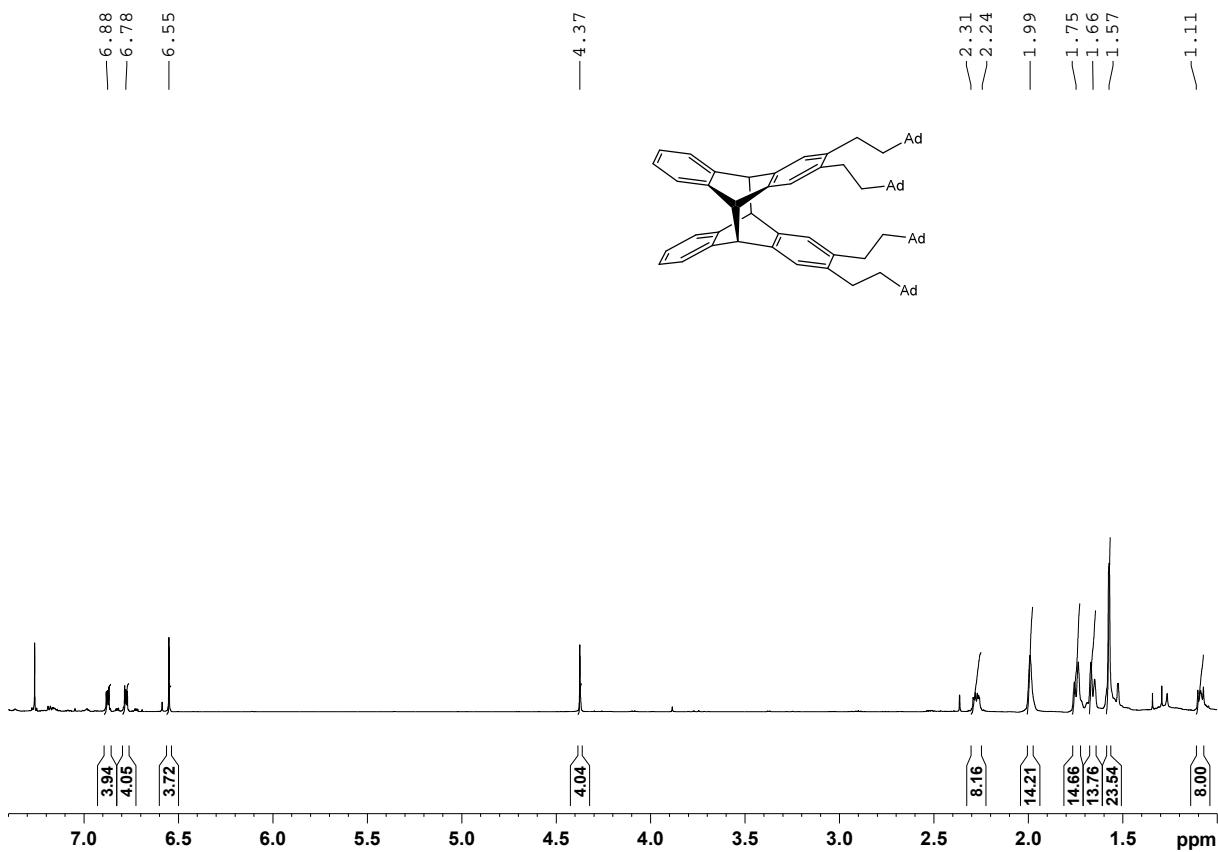


Figure S92. ^1H -NMR spectrum of **43b** in CDCl_3

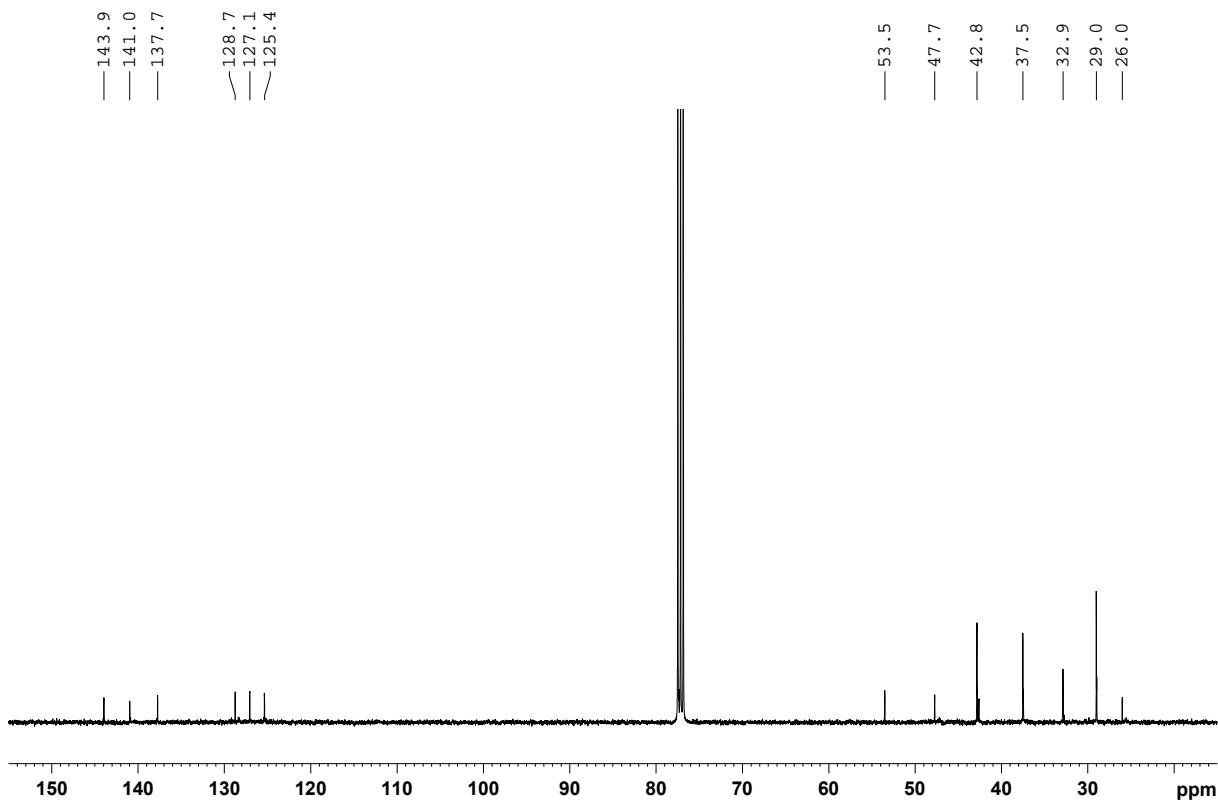


Figure S93. $^{13}\text{C}\{^1\text{H}\}$ -spectrum of **43b** in CDCl_3

Supporting Information (SI)

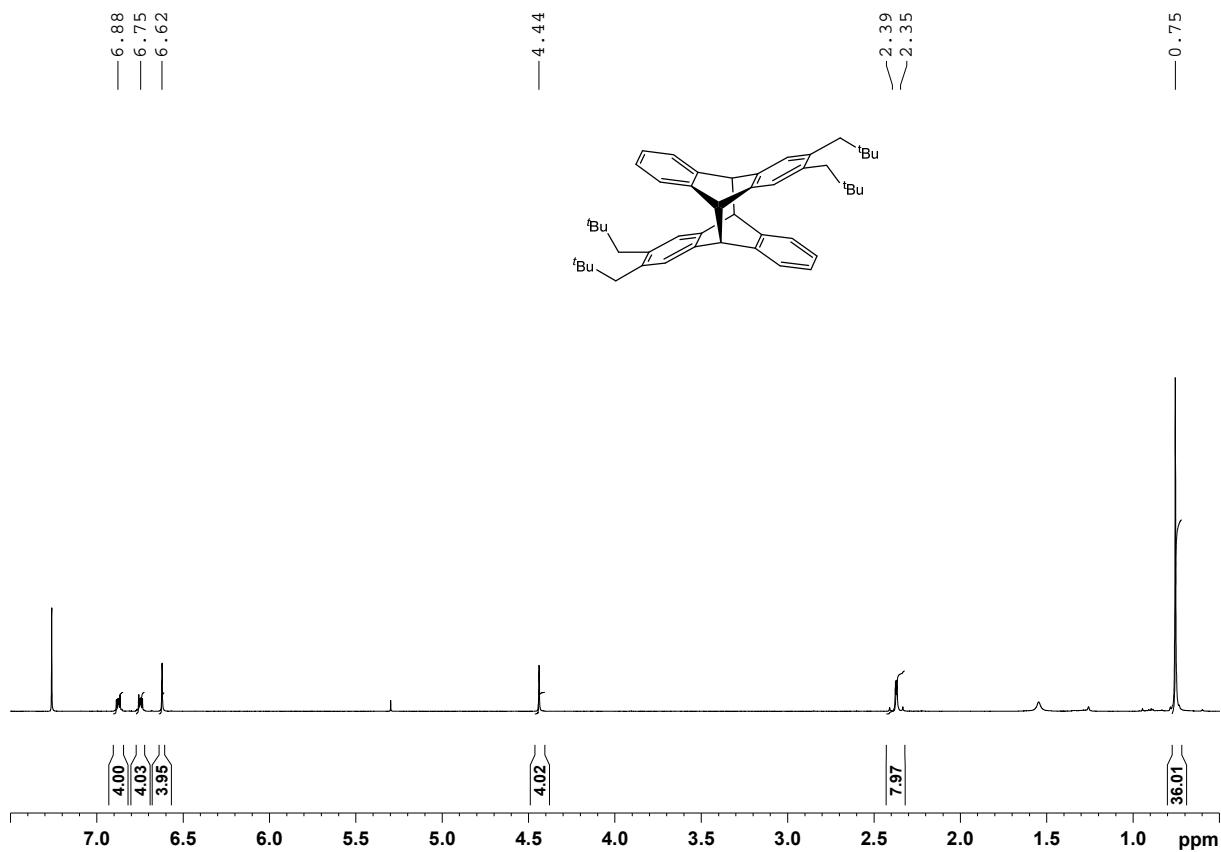


Figure S94. ^1H -NMR spectrum of **44a** in CDCl_3

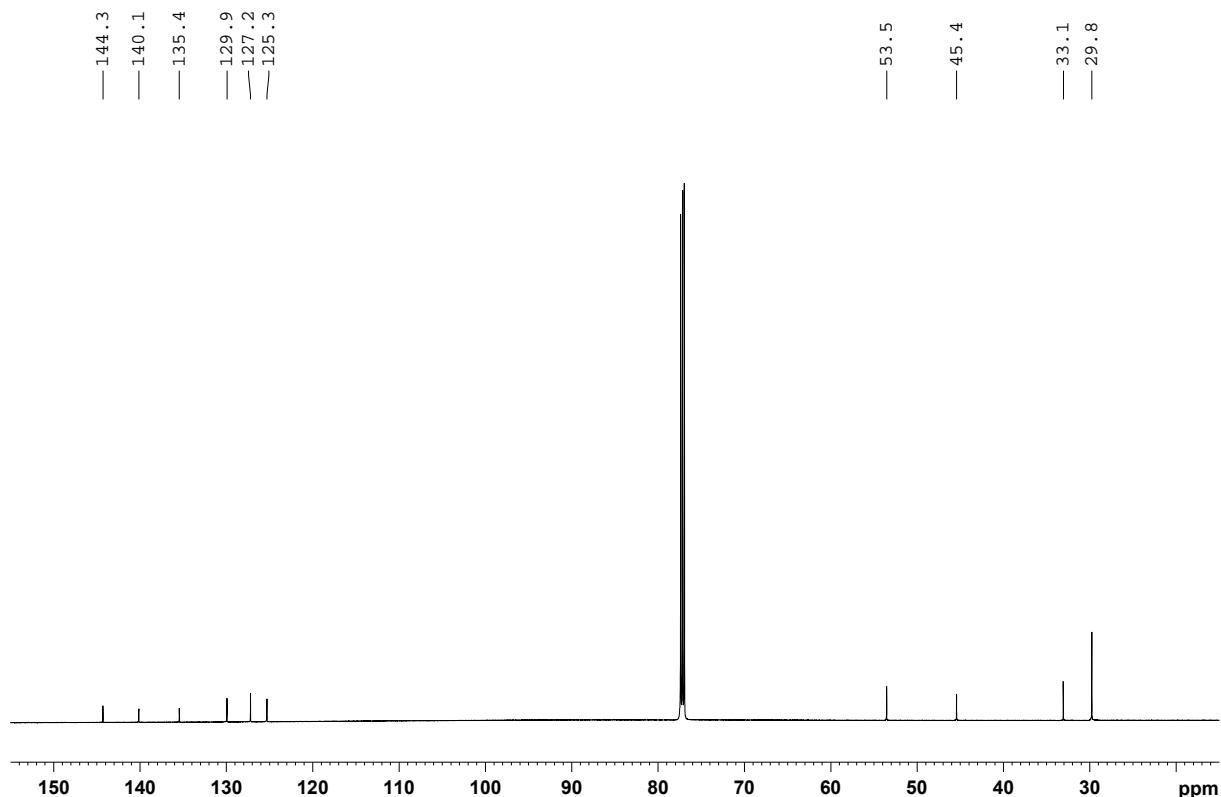


Figure S95. $^{13}\text{C}\{\text{H}\}$ -NMR spectrum of **44a** in CDCl_3

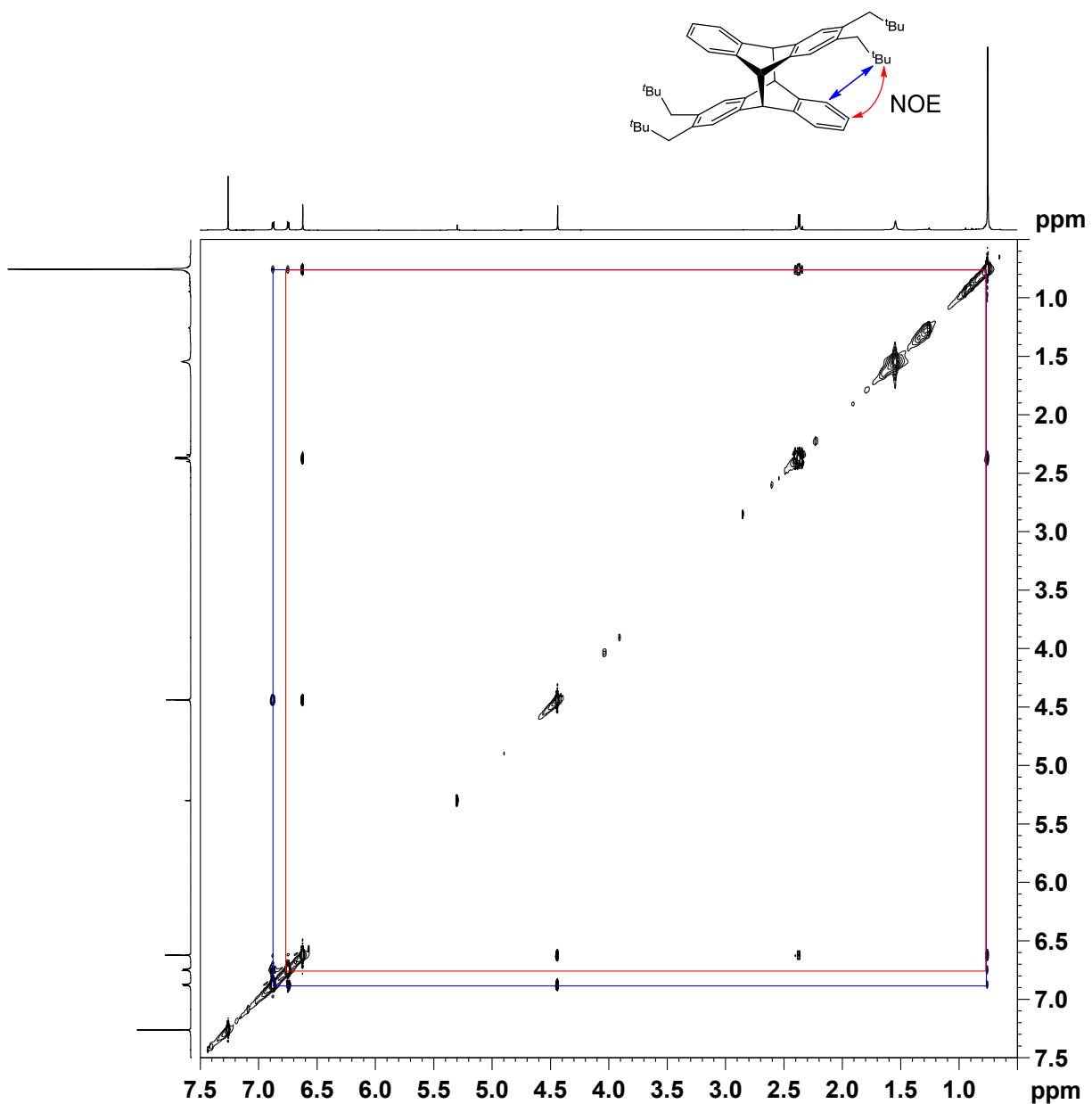


Figure S96. NOE spectrum of **44a** in CDCl_3

Supporting Information (SI)

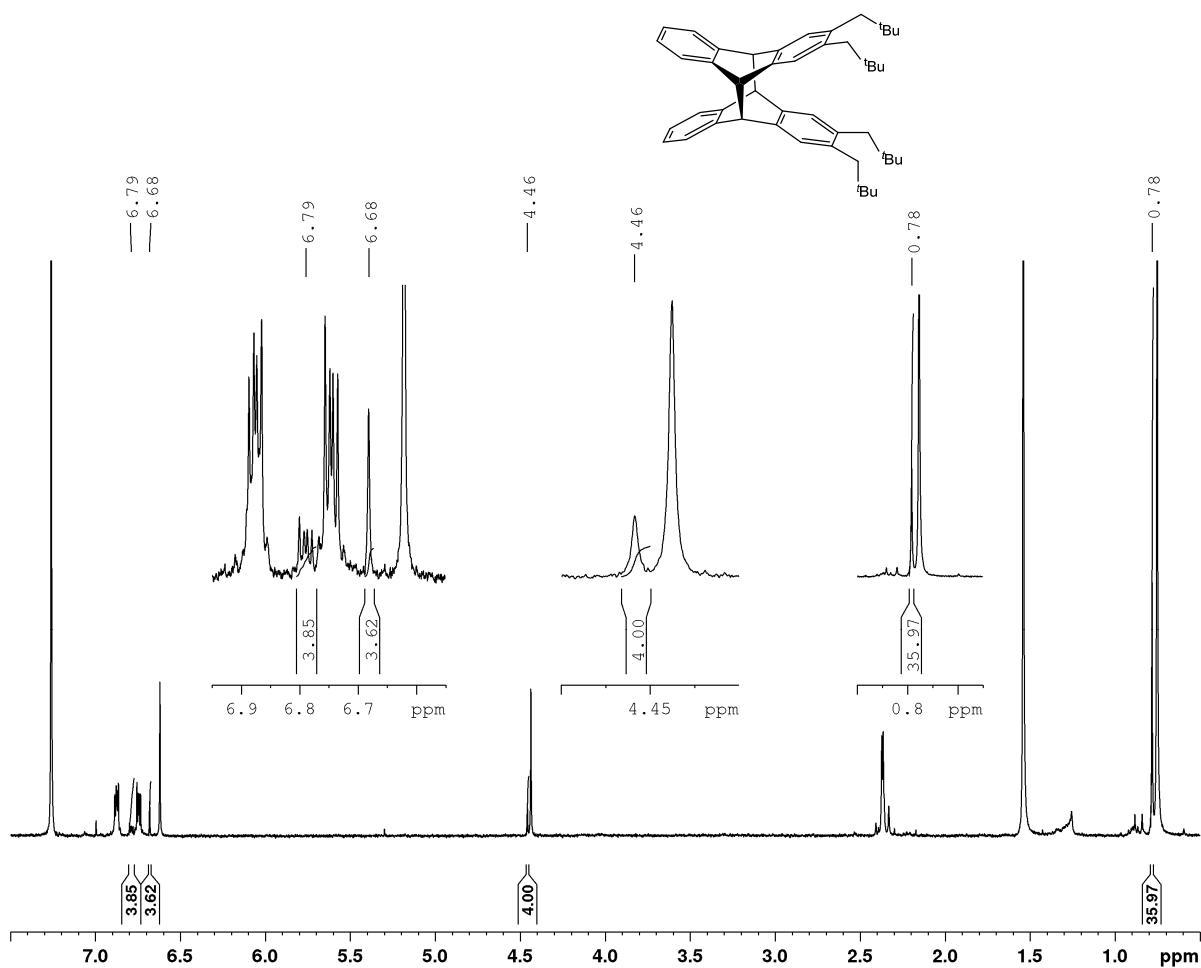


Figure S97. ¹H-NMR spectrum of **44b** in CDCl_3 . The CH_2 signals of the neopentyl groups could not be resolved due to overlap with signals for dimer **44a**.

2. UV/Vis and fluorescence data for newly prepared anthracene derivatives

Absorption spectra were obtained using a PerkinElmer Lambda1050 UV/Vis/NIR spectrometer, fluorescence spectra were recorded on a Varian Cary Eclipse fluorescence spectrometer. In both cases solutions of the monomers in *n*-hexane were used, individual concentrations as well as excitation wavelengths are reported for the individual spectra. The fluorescence spectra were scaled down to match the highest absorption band in intensity.

2,3-Di-*n*-butyl-anthracene (20)

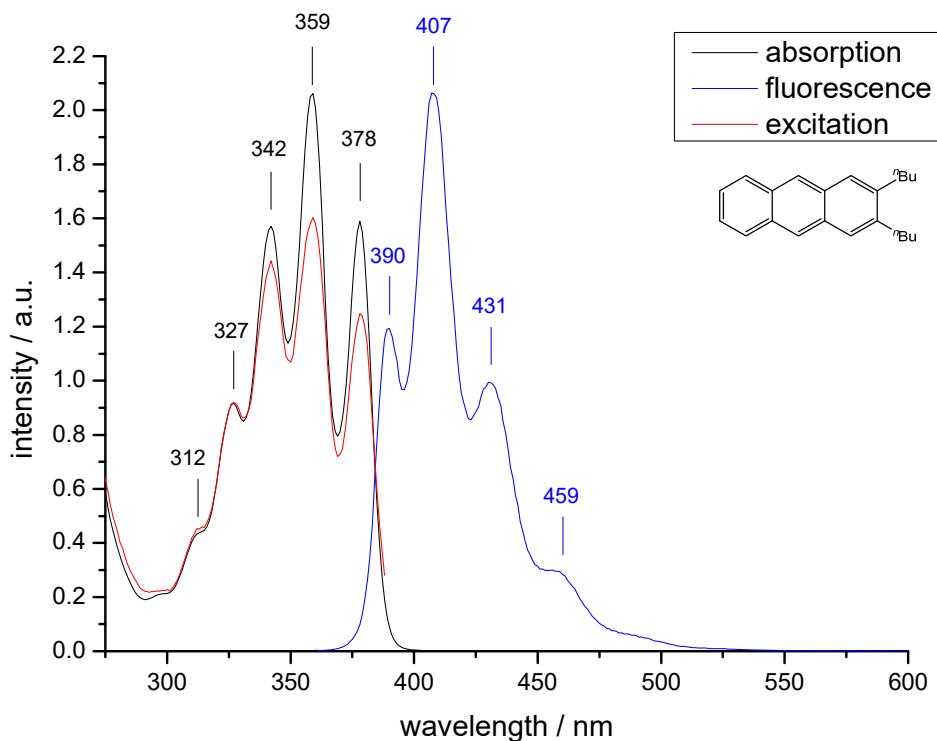


Figure S98. Absorption spectrum $c = 3.7 \cdot 10^{-4} \text{ mol} \cdot \text{L}^{-1}$, fluorescence spectrum: $c = 3.1 \cdot 10^{-4} \text{ mol} \cdot \text{L}^{-1}$, excitation wavelength: 359 nm

$\lambda_{\max} / \text{nm}$	312	327	342	359	378
$\epsilon / \text{L} \cdot \text{mol}^{-1} \cdot \text{cm}^{-1}$	1195.36 ± 2.40	2509.84 ± 11.61	4286.11 ± 13.79	5632.55 ± 6.28	4345.67 ± 5.27

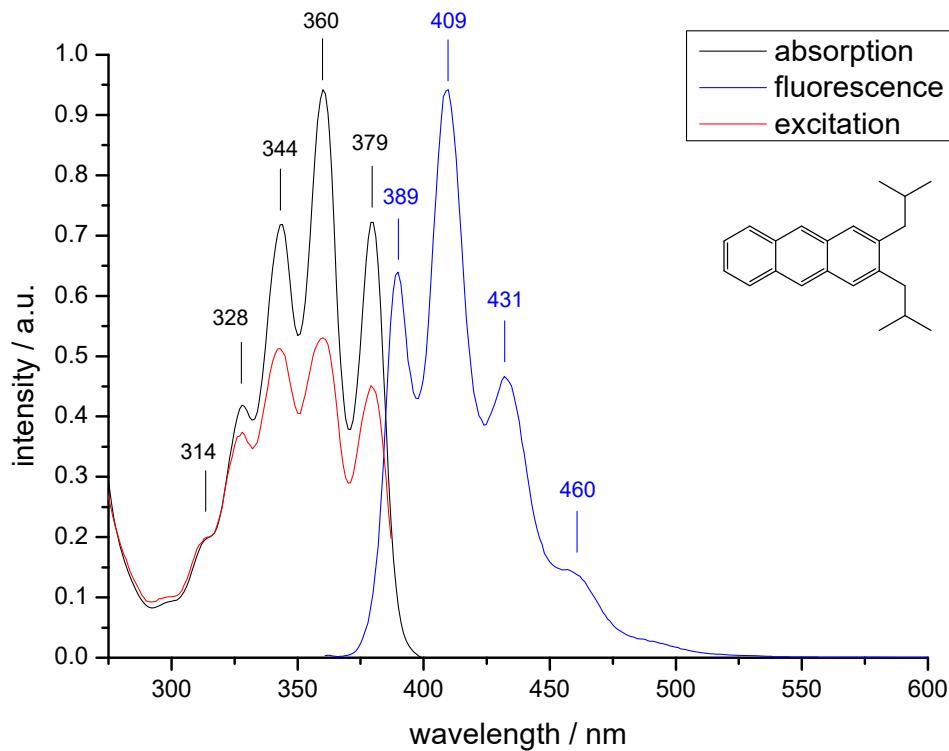
2,3-Di-*iso*-butyl-anthracene (21)

Figure S99. Absorption spectrum $c = 8.3 \cdot 10^{-4} \text{ mol} \cdot \text{L}^{-1}$, fluorescence spectrum: $c = 9.2 \cdot 10^{-5} \text{ mol} \cdot \text{L}^{-1}$, excitation wavelength: 360 nm

$\lambda_{\max} / \text{nm}$	314	328	344	360	379
$\varepsilon / \text{L} \cdot \text{mol}^{-1} \cdot \text{cm}^{-1}$	2410.06 ± 11.75	5030.07 ± 23.6	8506.54 ± 30.97	10966.07 ± 27.69	8526.11 ± 33.64

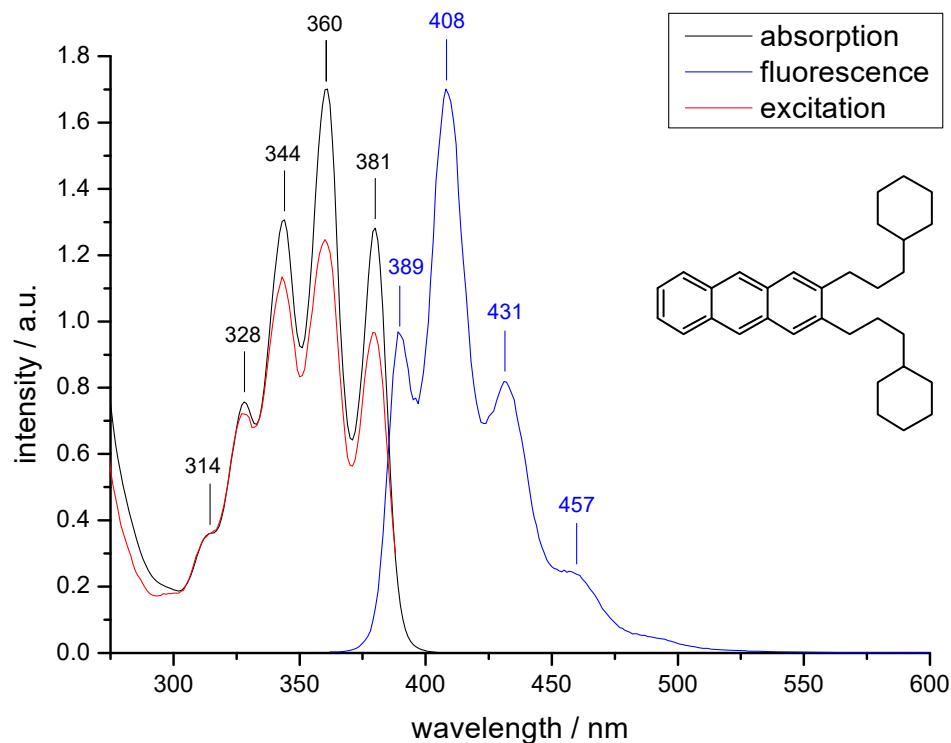
2,3-Di-(3-cyclohexylpropyl)-anthracene (32)

Figure S100. A solution ($c = 2.8 \cdot 10^{-4} \text{ mol} \cdot \text{L}^{-1}$) of **32** was used for both the absorption and fluorescence spectra, excitation wavelength: 361 nm

$\lambda_{\max} / \text{nm}$	314	328	344	361	380
$\varepsilon / \text{L} \cdot \text{mol}^{-1} \cdot \text{cm}^{-1}$	1296.35 ± 6.13	2725.76 ± 9.47	4703.86 ± 14.75	6132.11 ± 19.15	4619.46 ± 12.82

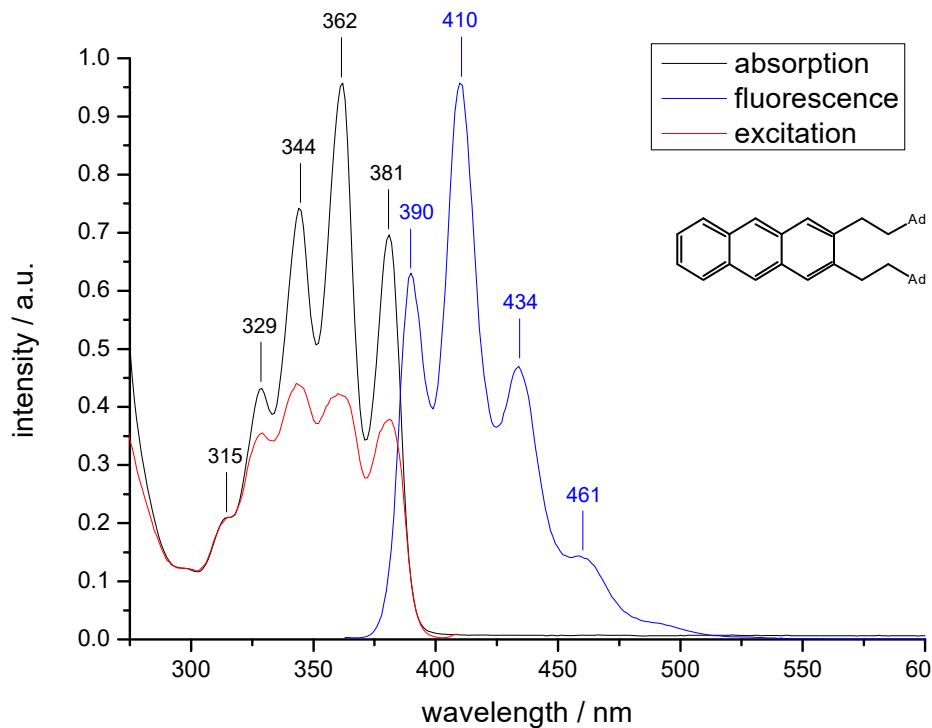
2,3-Di-(ethyl-2-(1-adamantyl))-anthracene (35)

Figure S 101. A solution ($c = 1.3 \cdot 10^{-4} \text{ mol} \cdot \text{L}^{-1}$) of **35** was used for both the absorption and fluorescence spectra, excitation wavelength: 362 nm

$\lambda_{\max} / \text{nm}$	315	329	344	362	381
$\varepsilon / \text{L} \cdot \text{mol}^{-1} \cdot \text{cm}^{-1}$	1570.01 ± 22.98	3232.32 ± 38.41	5558.19 ± 60.55	7178.88 ± 78.78	5185.50 ± 60.42

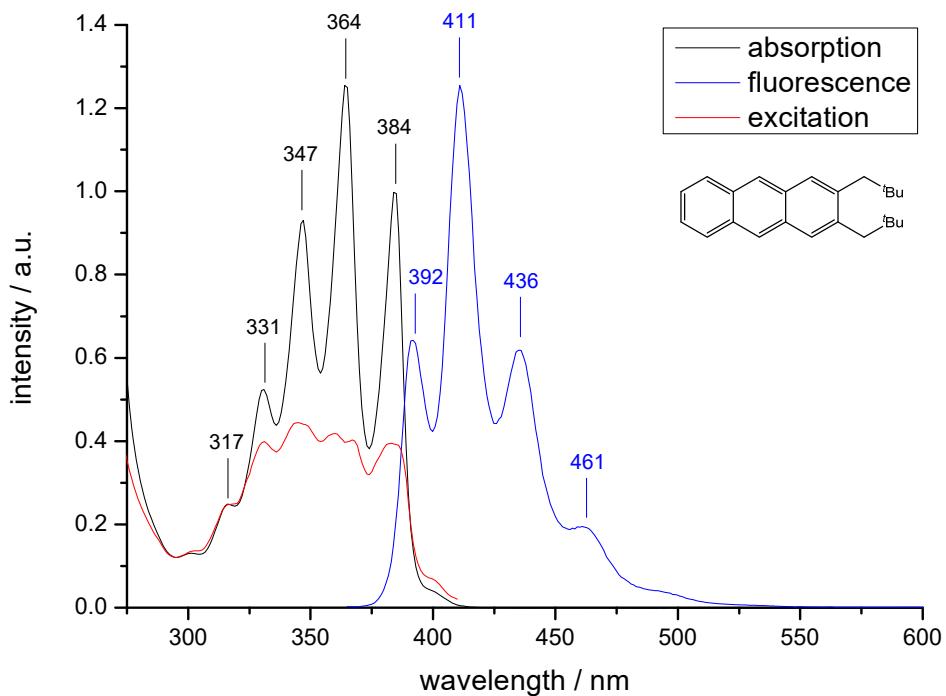
2,3-Di-neopentyl-anthracene (36)

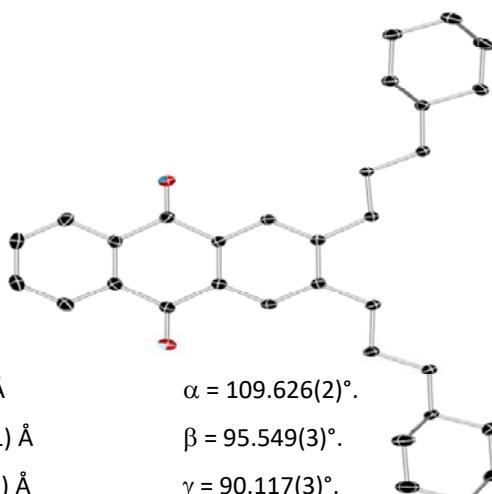
Figure S 102. A solution ($c = 1.9 \cdot 10^{-4} \text{ mol} \cdot \text{L}^{-1}$) of **36** was used for both the absorption and fluorescence spectra, excitation wavelength: 364 nm

$\lambda_{\max} / \text{nm}$	316	331	347	364	384
$\varepsilon / \text{L} \cdot \text{mol}^{-1} \cdot \text{cm}^{-1}$	1050.16 ± 22.98	2409.64 ± 26.56	4395.77 ± 45.53	5972.85 ± 62.93	4722.92 ± 48.88

3. Crystal structure data

Single crystals of the respective compounds were investigated on either a Bruker APEX II DUO instrument equipped with an $1\mu\text{S}$ microfocus sealed tube, a Bruker Smart APEX II diffractometer with graphite monochromator or a Bruker Smart APEX diffractometer with synchrotron radiation source ($\lambda = 0.8 \text{ \AA}$). The data collection strategy was determined using COSMO¹ employing ω - and φ -scans. Raw data were processed using APEX^{2,3} and SAINT,^{4,5} corrections for absorption effects were applied using SADABS.⁶ The structure was solved by direct methods and refined against all data by full-matrix least-squares methods on F^2 using SHELXTL⁷ and Shelxle.⁸

2,3-Di-(3-cyclohexylpropyl)-9,10-anthraquinone (31c)

Empirical formula	C32 H40 O2	
Formula weight	456.64	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P -1	
Unit cell dimensions	$a = 8.3688(7) \text{ \AA}$ $b = 12.6818(11) \text{ \AA}$ $c = 12.7859(11) \text{ \AA}$	$\alpha = 109.626(2)^\circ$. $\beta = 95.549(3)^\circ$. $\gamma = 90.117(3)^\circ$.
Volume	1271.30(19) Å ³	
Z	2	
Density (calculated)	1.193 Mg/m ³	
Absorption coefficient	0.072 mm ⁻¹	
F(000)	496	
Crystal size	0.278 x 0.136 x 0.064 mm ³	
Theta range for data collection	1.706 to 27.103°.	
Index ranges	-10≤h≤10, -16≤k≤16, -16≤l≤16	
Reflections collected	45809	
Independent reflections	5619 [R(int) = 0.0488]	
Completeness to theta = 25.242°	100.0 %	
Absorption correction	Numerical	
Max. and min. transmission	0.7458 and 0.6866	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	5619 / 0 / 307	
Goodness-of-fit on F^2	1.032	
Final R indices [$ I >2\sigma(I)$]	R1 = 0.0413, wR2 = 0.1081	
R indices (all data)	R1 = 0.0567, wR2 = 0.1187	

Supporting Information (SI)

Extinction coefficient	n/a
Largest diff. peak and hole	0.325 and -0.210 e. \AA^{-3}
CCDC	1915075
The ellipsoid probability was set to 50 %.	

2,3-Di-(ethyl-2-(1-adamantyl))-9,10-anthraquinone (31d)

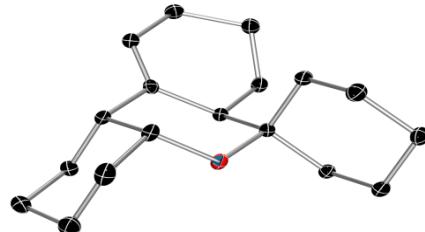
Empirical formula	C38 H44 O2	
Formula weight	532.73	
Temperature	100(2) K	
Wavelength	0.71073 \AA	
Crystal system	Monoclinic	
Space group	P2 ₁ /n	
Unit cell dimensions	a = 12.2567(12) \AA	$\alpha = 90^\circ$.
	b = 17.8763(18) \AA	$\beta = 103.004(2)^\circ$.
	c = 13.3141(13) \AA	$\gamma = 90^\circ$.
Volume	2842.4(5) \AA^3	
Z	4	
Density (calculated)	1.245 Mg/m ³	
Absorption coefficient	0.075 mm ⁻¹	
F(000)	1152	
Crystal size	0.362 x 0.129 x 0.078 mm ³	
Theta range for data collection	2.051 to 25.682°	
Index ranges	-14≤h≤14, -21≤k≤21, -16≤l≤16	
Reflections collected	45736	
Independent reflections	5393 [R(int) = 0.0672]	
Completeness to theta = 25.242°	99.9 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7458 and 0.6653	
Refinement method	Full-matrix least-squares on F ²	
Data / restraints / parameters	5393 / 0 / 361	
Goodness-of-fit on F ²	1.025	
Final R indices [I>2sigma(I)]	R1 = 0.0430, wR2 = 0.1045	
R indices (all data)	R1 = 0.0602, wR2 = 0.1183	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.221 and -0.223 e. \AA^{-3}	
CCDC	1915079	
The ellipsoid probability was set to 50 %.		

Supporting Information (SI)

9-Oxa-1,2,3,4*b*,5,6,7,8,8*a*,9,10,10*a*-dodecahydropheanthrene-10-spiro-1-cyclohexane (33)

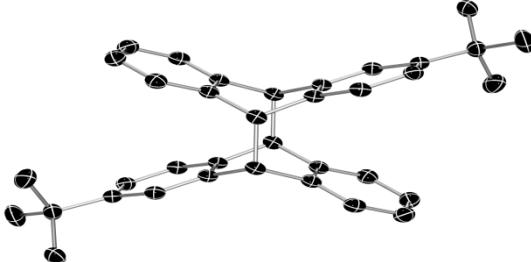
Empirical formula	C ₁₈ H ₂₈ O	
Formula weight	260.40	
Temperature	103(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P -1	
Unit cell dimensions	a = 8.4055(9) Å	α = 67.685(3)°.
	b = 9.6574(10) Å	β = 70.571(3)°.
	c = 10.6928(11) Å	γ = 66.514(3)°.
Volume	719.45(13) Å ³	
Z	2	
Density (calculated)	1.202 Mg/m ³	
Absorption coefficient	0.071 mm ⁻¹	
F(000)	288	
Crystal size	0.273 x 0.131 x 0.047 mm ³	
Theta range for data collection	2.107 to 28.803°.	
Index ranges	-11<=h<=11, -13<=k<=13, -14<=l<=14	
Reflections collected	16335	
Independent reflections	3756 [R(int) = 0.0414]	
Completeness to theta = 25.242°	99.9 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7458 and 0.6996	
Refinement method	Full-matrix least-squares on F ²	
Data / restraints / parameters	3756 / 0 / 172	
Goodness-of-fit on F ²	1.045	
Final R indices [I>2sigma(I)]	R1 = 0.0427, wR2 = 0.0998	
R indices (all data)	R1 = 0.0581, wR2 = 0.1095	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.347 and -0.243 e.Å ⁻³	
CCDC	1915074	

The ellipsoid probability was set to 50 %.



Supporting Information (SI)

2,6'-Di-*tert*-butyl-dianthracene (37a)

Empirical formula	C ₃₆ H ₃₆	
Formula weight	468.65	
Temperature/K	150	
Crystal system	Monoclinic	
Space group	P2 ₁ /c	
Unit cell dimensions	a = 13.8935(15) Å	α = 90°
	b = 7.9659(9) Å	β = 93.3580(10) °
	c = 11.9709(13) Å	γ = 90°
Volume/Å ³	1322.6(3)	
Z	2	
ρ _{calc} g/cm ³	1.177	
μ/mm ⁻¹	0.085	
F(000)	504.0	
Crystal size/mm ³	0.1 × 0.1 × 0.03	
Radiation	synchrotron (λ = 0.79942)	
2θ range for data collection/°	6.608 to 59.79	
Index ranges	-17 ≤ h ≤ 17, -7 ≤ k ≤ 9, -14 ≤ l ≤ 14	
Reflections collected	6924	
Independent reflections	2569 [R _{int} = 0.0274, R _{sigma} = 0.0286]	
Data/restraints/parameters	2569/0/166	
Goodness-of-fit on F ²	1.068	
Final R indexes [I>=2σ (I)]	R ₁ = 0.0407, wR ₂ = 0.1015	
Final R indexes [all data]	R ₁ = 0.0427, wR ₂ = 0.1032	
Largest diff. peak/hole / e Å ⁻³	0.25/-0.16	
CCDC	1915073	

The ellipsoid probability was set to 50 %.

Supporting Information (SI)

2,7'-Di-*tert*-butyl-dianthracene (37b)

Empirical formula	C36 H36
Formula weight	468.65
Temperature	100(2) K
Wavelength	0.71073 Å
Crystal system	Monoclinic
Space group	C 2
Unit cell dimensions	a = 30.492(3) Å α = 90°. b = 6.8073(8) Å β = 90.618(2)°. c = 12.6172(14) Å γ = 90°.
Volume	2618.8(5) Å ³
Z	4
Density (calculated)	1.189 Mg/m ³
Absorption coefficient	0.067 mm ⁻¹
F(000)	1008
Crystal size	0.425 x 0.106 x 0.074 mm ³
Theta range for data collection	1.336 to 28.278°.
Index ranges	-40<=h<=40, -9<=k<=9, -16<=l<=16
Reflections collected	26214
Independent reflections	6493 [R(int) = 0.0373]
Completeness to theta = 25.242°	100.0 %
Absorption correction	Numerical
Max. and min. transmission	0.7445 and 0.6789
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	6493 / 1 / 331
Goodness-of-fit on F ²	1.035
Final R indices [I>2sigma(I)]	R1 = 0.0377, wR2 = 0.0933
R indices (all data)	R1 = 0.0422, wR2 = 0.0968
Absolute structure parameter	-1.2(10)
Extinction coefficient	n/a
Largest diff. peak and hole	0.308 and -0.237 e.Å ⁻³
CCDC	1915078

The ellipsoid probability was set to 50 %.

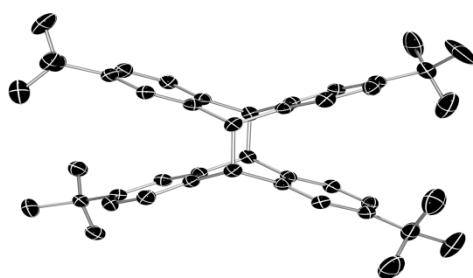


Supporting Information (SI)

2,3',6,7'-Tetra-*tert*-butyl-dianthracene (38a)

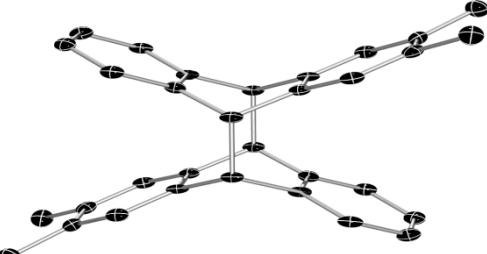
Empirical formula	C44 H52
Formula weight	580.85
Temperature	152(2) K
Wavelength	1.54178 Å
Crystal system	Orthorhombic
Space group	P 21 21 2
Unit cell dimensions	a = 18.9017(16) Å α = 90°. b = 26.689(3) Å β = 90°. c = 6.9776(6) Å γ = 90°.
Volume	3520.0(5) Å ³
Z	4
Density (calculated)	1.096 Mg/m ³
Absorption coefficient	0.453 mm ⁻¹
F(000)	1264
Crystal size	0.336 x 0.126 x 0.074 mm ³
Theta range for data collection	2.865 to 66.890°.
Index ranges	-22<=h<=22, -31<=k<=31, -8<=l<=8
Reflections collected	38920
Independent reflections	6218 [R(int) = 0.0923]
Completeness to theta = 66.890°	99.6 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.7528 and 0.6987
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	6218 / 0 / 424
Goodness-of-fit on F ²	1.016
Final R indices [I>2sigma(I)]	R1 = 0.0347, wR2 = 0.0789
R indices (all data)	R1 = 0.0598, wR2 = 0.0829
Absolute structure parameter	0.5(12)
Extinction coefficient	n/a
Largest diff. peak and hole	0.133 and -0.177 e.Å ⁻³
CCDC	1915076

The ellipsoid probability was set to 50 %.



Supporting Information (SI)

2,3,6',7'-Tetramethyl-dianthracene (39a)

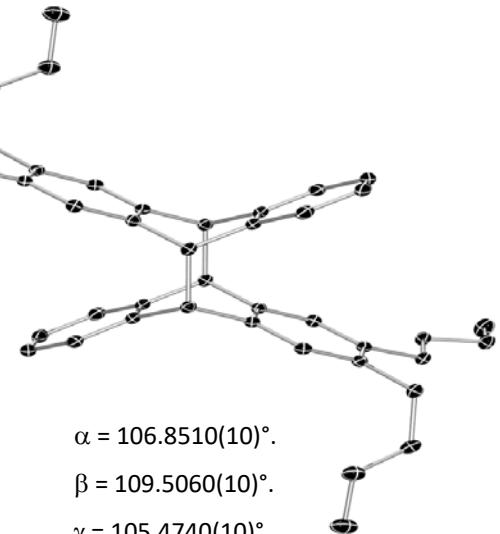
Empirical formula	C32 H28	
Formula weight	412.58	
Temperature	152(2) K	
Crystal system	Monoclinic	
Space group	P -1	
Unit cell dimensions	$a = 8.3036(12)$ Å $b = 8.4034(12)$ Å $c = 11.0420(17)$ Å	$\alpha = 83.627(7)^\circ$ $\beta = 87.534(7)^\circ$ $\gamma = 87.470(6)^\circ$
Volume/Å ³	764.422	

Due to a poor R-value no further structural information is given. The ellipsoid probability was set to 50 %.

Supporting Information (SI)

2,3,6',7'-Tetra-*n*-butyl-dianthracene (40a)

Empirical formula	C44 H52
Formula weight	580.86
Temperature	100(2) K
Wavelength	0.71073 Å
Crystal system	Triclinic
Space group	P -1
Unit cell dimensions	 a = 9.7346(2) Å b = 10.0564(2) Å c = 10.2632(2) Å
	$\alpha = 106.8510(10)^\circ$. $\beta = 109.5060(10)^\circ$. $\gamma = 105.4740(10)^\circ$.
Volume	829.51(3) Å ³
Z	1
Density (calculated)	1.163 Mg/m ³
Absorption coefficient	0.065 mm ⁻¹
F(000)	316
Crystal size	0.1 x 0.1 x 0.1 mm ³
Theta range for data collection	2.312 to 27.054°.
Index ranges	-12<=h<=12, -12<=k<=12, -13<=l<=12
Reflections collected	22418
Independent reflections	3631 [R(int) = 0.0138]
Completeness to theta = 25.242°	99.9 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.7455 and 0.7177
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	3631 / 0 / 201
Goodness-of-fit on F ²	1.008
Final R indices [I>2sigma(I)]	R1 = 0.0380, wR2 = 0.1053
R indices (all data)	R1 = 0.0412, wR2 = 0.1088
Extinction coefficient	n/a
Largest diff. peak and hole	0.363 and -0.192 e.Å ⁻³
CCDC	1915080

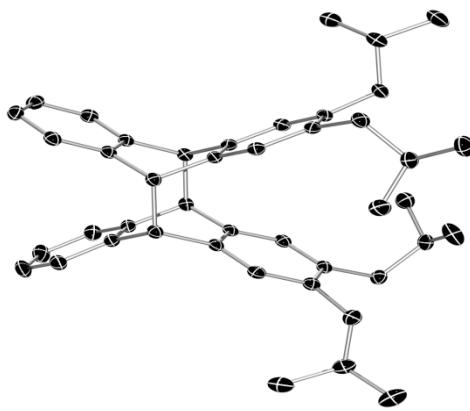


The ellipsoid probability was set to 50 %.

Supporting Information (SI)

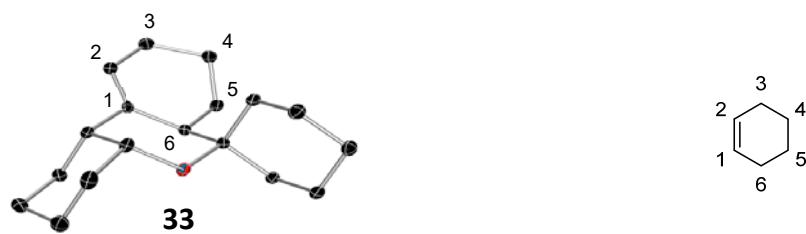
2,2',3,3'-Tetra-*iso*-butyl-dianthracene (41b)

Empirical formula	C44 H52
Formula weight	580.85
Temperature	100(2) K
Wavelength	0.71073 Å
Crystal system	Triclinic
Space group	P -1
Unit cell dimensions	a = 13.0562(4) Å α = 82.2500(10)°. b = 14.1031(4) Å β = 74.0370(10)°. c = 22.1469(6) Å γ = 62.8200(10)°.
Volume	3487.58(18) Å ³
Z	4
Density (calculated)	1.106 Mg/m ³
Absorption coefficient	0.062 mm ⁻¹
F(000)	1264
Crystal size	0.358 x 0.181 x 0.094 mm ³
Theta range for data collection	1.821 to 27.103°.
Index ranges	-16<=h<=16, -18<=k<=18, -28<=l<=28
Reflections collected	87232
Independent reflections	15369 [R(int) = 0.0394]
Completeness to theta = 25.242°	99.9 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.7458 and 0.7039
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	15369 / 0 / 809
Goodness-of-fit on F ²	1.023
Final R indices [I>2sigma(I)]	R1 = 0.0415, wR2 = 0.0993
R indices (all data)	R1 = 0.0565, wR2 = 0.1100
Extinction coefficient	n/a
Largest diff. peak and hole	0.294 and -0.223 e.Å ⁻³
CCDC	1915077
The ellipsoid probability was set to 50 %.	



4. Selected bond lengths and angles for compound 33

Table S1. Comparison of experimental and calculated (B3LYP/def2TZVP) bond lengths and angles for compound **33** (left) and cyclohexene (right). Numbering on the ring containing the double bond is adjusted to match the numbering in cyclohexene. Hydrogen atoms are omitted for clarity, the ellipsoid probability was set to 50 %.



r (C-C) / Å			\angle (C-C-C) / °				
33	calcd.	cyclohexene	33	calcd.	cyclohexene		
C1-C2	1.335(2)	1.387	1.335	C6-C1-C2	123.6(1)	120.9	123.5
C2-C3	1.501(2)	1.496	1.504	C1-C2-C3	124.4(1)	123.4	123.5
C3-C4	1.526(2)	1.527	1.515	C2-C3-C4	110.8(1)	111.2	112
C4-C5	1.529(2)	1.529	1.550	C3-C4-C5	110.9(1)	110.3	111
C5-C6	1.546(2)	1.510	1.515	C4-C5-C6	114.6(1)	112.6	111
C6-C1	1.515(2)	1.400	1.504	C5-C6-C1	112.0(1)	118.8	112

5. Cartesian coordinates

B3LYP/def2TZVP			
33			
E(SCF) = -777.64872911			
C	15.013653000	-8.659661000	-0.582093000
C	14.708960000	-9.977516000	0.135152000
C	13.877028000	-8.338952000	-1.571433000
C	14.443704000	-11.129899000	-0.840949000
C	13.579582000	-9.482192000	-2.545163000
C	13.293135000	-10.782947000	-1.791200000
C	16.427459000	-8.702522000	-1.155827000
C	17.385685000	-9.496756000	-0.514724000
O	15.699673000	-10.254524000	1.116286000
C	17.086169000	-10.302934000	0.733699000
C	16.768843000	-7.911819000	-2.242685000
C	18.137362000	-7.889498000	-2.846572000
C	18.815082000	-9.443708000	-0.998809000
C	18.916387000	-9.155232000	-2.497022000
H	13.800018000	-9.837878000	0.729620000
H	12.976091000	-8.140016000	-0.980174000
H	14.082023000	-7.414262000	-2.113135000
H	15.340227000	-11.335390000	-1.430250000
H	14.217684000	-12.033102000	-0.269083000
H	12.729272000	-9.215530000	-3.178676000
H	14.433654000	-9.630269000	-3.213291000
H	13.127105000	-11.604152000	-2.493092000
H	12.365438000	-10.672834000	-1.217320000
H	16.025961000	-7.260273000	-2.682049000
H	18.067718000	-7.765392000	-3.931793000
H	18.689216000	-7.007805000	-2.486948000
H	19.351295000	-8.654723000	-0.451567000
H	19.342194000	-10.369642000	-0.766456000
H	18.500489000	-10.000404000	-3.053637000
H	19.963641000	-9.059625000	-2.793333000
C	17.848324000	-9.699015000	1.942220000
C	17.634671000	-10.491129000	3.235061000
C	18.013589000	-11.963340000	3.062215000
C	17.496020000	-11.796172000	0.589966000
C	17.268831000	-12.588545000	1.880584000
H	17.523776000	-8.663705000	2.068569000
H	18.915812000	-9.677313000	1.704657000
H	18.224900000	-10.038948000	4.037238000
H	16.585904000	-10.415725000	3.531923000
H	19.094380000	-12.043185000	2.892137000
H	17.801745000	-12.518664000	3.979907000
H	16.942549000	-12.245820000	-0.235084000
H	18.554858000	-11.853723000	0.326670000

Supporting Information (SI)

H	17.593743000	-13.622158000	1.731671000
H	16.199065000	-12.620419000	2.100956000
H	15.007587000	-7.879684000	0.187836000

B3LYP-D3/def2TZVP			
2			
E(SCF) = -1079.46918356			
C	1.766546000	-0.531580000	0.701451000
C	1.766494000	-0.531804000	-0.699035000
C	2.690363000	-1.304327000	1.389608000
C	2.690217000	-1.304824000	-1.387014000
C	3.614669000	-2.081343000	0.695635000
C	3.614589000	-2.081612000	-0.692863000
C	0.735060000	0.338366000	1.386504000
C	0.745258000	1.687943000	0.701098000
C	0.735089000	0.338038000	-1.384567000
C	0.745446000	1.687841000	-0.699586000
C	0.757370000	2.892376000	1.389238000
C	0.766009000	4.099595000	0.694779000
C	0.757849000	2.892116000	-1.387947000
C	0.766257000	4.099476000	-0.693690000
C	-0.745258000	-1.687943000	0.701098000
C	-0.745446000	-1.687841000	-0.699586000
C	-0.757370000	-2.892376000	1.389238000
C	-0.757849000	-2.892116000	-1.387947000
C	-0.766009000	-4.099595000	0.694779000
C	-0.766257000	-4.099476000	-0.693690000
C	-0.735060000	-0.338366000	1.386504000
C	-1.766546000	0.531580000	0.701451000
C	-0.735089000	-0.338038000	-1.384567000
C	-1.766494000	0.531804000	-0.699035000
C	-2.690363000	1.304327000	1.389608000
C	-3.614669000	2.081343000	0.695635000
C	-2.690217000	1.304824000	-1.387014000
C	-3.614589000	2.081612000	-0.692863000
H	2.690187000	-1.301930000	2.473537000
H	2.689926000	-1.302870000	-2.470945000
H	4.333896000	-2.680387000	1.239764000
H	4.333661000	-2.680970000	-1.236847000
H	1.010550000	0.465438000	2.433207000
H	1.011079000	0.464634000	-2.431203000
H	0.758911000	2.890900000	2.473143000
H	0.759735000	2.890415000	-2.471852000
H	-0.758911000	-2.890900000	2.473143000
H	-0.759735000	-2.890415000	-2.471852000
H	-1.010550000	-0.465438000	2.433207000
H	-1.011079000	-0.464634000	-2.431203000
H	-2.690187000	1.301930000	2.473537000
H	-4.333896000	2.680387000	1.239764000

Supporting Information (SI)

H	-2.689926000	1.302870000	-2.470945000
H	-4.333661000	2.680970000	-1.236847000
H	0.775126000	5.035916000	1.238418000
H	0.775759000	5.035622000	-1.237628000
H	-0.775759000	-5.035622000	-1.237628000
H	-0.775126000	-5.035916000	1.238418000

37a

E(SCF) = -1394.12286731

C	1.643686000	-0.597861000	0.910966000
C	1.906570000	-0.270919000	-0.425651000
C	2.476547000	-1.482637000	1.580004000
C	3.001180000	-0.831788000	-1.067338000
C	3.571350000	-2.048083000	0.930722000
C	3.834335000	-1.721423000	-0.393032000
C	0.430205000	0.043230000	1.548185000
C	0.437154000	1.510381000	1.185503000
C	0.948323000	0.686424000	-1.100537000
C	0.693849000	1.836768000	-0.151351000
C	0.185321000	2.529702000	2.085514000
C	0.166790000	3.860200000	1.668260000
C	0.680395000	3.159686000	-0.554021000
C	0.405770000	4.203730000	0.339895000
C	-0.693849000	-1.836768000	0.151351000
C	-0.437154000	-1.510381000	-1.185503000
C	-0.680395000	-3.159686000	0.554021000
C	-0.185321000	-2.529702000	-2.085514000
C	-0.405770000	-4.203730000	-0.339895000
C	-0.166790000	-3.860200000	-1.668260000
C	-0.948323000	-0.686424000	1.100537000
C	-1.906570000	0.270919000	0.425651000
C	-0.430205000	-0.043230000	-1.548185000
C	-1.643686000	0.597861000	-0.910966000
C	-3.001180000	0.831788000	1.067338000
C	-3.834335000	1.721423000	0.393032000
C	-2.476547000	1.482637000	-1.580004000
C	-3.571350000	2.048083000	-0.930722000
C	-0.362776000	-5.647901000	0.173925000
C	0.362776000	5.647901000	-0.173925000
H	2.268336000	-1.737644000	2.612741000
H	3.204007000	-0.578943000	-2.101734000
H	4.216370000	-2.738146000	1.459948000
H	4.685985000	-2.155178000	-0.901822000
H	0.492482000	-0.061992000	2.631073000
H	1.402581000	1.066207000	-2.015442000
H	-0.012487000	2.293418000	3.124960000
H	0.874315000	3.380946000	-1.596677000
H	-0.874315000	-3.380946000	1.596677000
H	0.012487000	-2.293418000	-3.124960000

Supporting Information (SI)

H	-1.402581000	-1.066207000	2.015442000
H	-0.492482000	0.061992000	-2.631073000
H	-3.204007000	0.578943000	2.101734000
H	-4.685985000	2.155178000	0.901822000
H	-2.268336000	1.737644000	-2.612741000
H	-4.216370000	2.738146000	-1.459948000
H	-0.042226000	4.623721000	2.403100000
H	0.042226000	-4.623721000	-2.403100000
C	0.034039000	6.654974000	0.937049000
H	0.783292000	6.639373000	1.730772000
H	0.012569000	7.664613000	0.522387000
H	-0.943146000	6.459491000	1.382614000
C	1.731700000	6.024943000	-0.774803000
H	2.004471000	5.370478000	-1.603570000
H	1.711542000	7.050519000	-1.151680000
H	2.517718000	5.953740000	-0.020425000
C	-0.725055000	5.763287000	-1.262223000
H	-0.515196000	5.114589000	-2.113261000
H	-1.701369000	5.481885000	-0.863030000
H	-0.785902000	6.790062000	-1.631469000
C	0.725055000	-5.763287000	1.262223000
H	1.701369000	-5.481885000	0.863030000
H	0.515196000	-5.114589000	2.113261000
H	0.785902000	-6.790062000	1.631469000
C	-1.731700000	-6.024943000	0.774803000
H	-2.517718000	-5.953740000	0.020425000
H	-1.711542000	-7.050519000	1.151680000
H	-2.004471000	-5.370478000	1.603570000
C	-0.034039000	-6.654974000	-0.937049000
H	-0.012569000	-7.664613000	-0.522387000
H	-0.783292000	-6.639373000	-1.730772000
H	0.943146000	-6.459491000	-1.382614000

37b

E(SCF) = -1394.12235631

C	-0.497375000	1.775112000	-0.258356000
C	-0.497451000	1.775618000	1.142446000
C	-1.266390000	2.701836000	-0.946843000
C	-1.266005000	2.703525000	1.829835000
C	-2.040819000	3.628947000	-0.253243000
C	-2.040296000	3.629947000	1.135243000
C	0.354640000	0.729380000	-0.944141000
C	1.702140000	0.702542000	-0.257314000
C	0.355378000	0.729871000	1.827993000
C	1.700504000	0.705967000	1.138145000
C	2.901613000	0.650377000	-0.954399000
C	4.131151000	0.593650000	-0.294523000
C	2.913842000	0.667449000	1.809063000
C	4.108826000	0.610062000	1.102954000

Supporting Information (SI)

C	-1.702140000	-0.702528000	-0.257311000
C	-1.700504000	-0.705954000	1.138148000
C	-2.901613000	-0.650369000	-0.954396000
C	-2.913843000	-0.667454000	1.809066000
C	-4.131151000	-0.593646000	-0.294521000
C	-4.108828000	-0.610075000	1.102956000
C	-0.354640000	-0.729367000	-0.944138000
C	0.497376000	-1.775097000	-0.258350000
C	-0.355378000	-0.729852000	1.827995000
C	0.497451000	-1.775600000	1.142452000
C	1.266390000	-2.701825000	-0.946833000
C	2.040820000	-3.628933000	-0.253229000
C	1.266007000	-2.703502000	1.829844000
C	2.040298000	-3.629927000	1.135257000
H	-1.266431000	2.699154000	-2.030824000
H	-1.266513000	2.701772000	2.913774000
H	-2.638605000	4.349065000	-0.797734000
H	-2.638105000	4.350481000	1.679072000
H	0.487270000	1.002955000	-1.990665000
H	0.489629000	1.002919000	2.874445000
H	2.860566000	0.642210000	-2.034754000
H	2.930215000	0.671077000	2.893090000
H	-2.860565000	-0.642204000	-2.034751000
H	-2.930218000	-0.671094000	2.893093000
H	-0.487271000	-1.002946000	-1.990661000
H	-0.489627000	-1.002897000	2.874449000
H	1.266431000	-2.699147000	-2.030814000
H	2.638606000	-4.349052000	-0.797717000
H	1.266516000	-2.701744000	2.913784000
H	2.638108000	-4.350458000	1.679089000
C	5.468947000	0.498614000	-1.039525000
C	6.358711000	1.700087000	-0.662923000
C	6.178129000	-0.811129000	-0.637693000
C	5.290873000	0.496082000	-2.564344000
H	5.879607000	2.639578000	-0.945554000
H	6.556935000	1.735324000	0.408687000
H	7.320035000	1.637672000	-1.178997000
H	5.558409000	-1.676064000	-0.882028000
H	7.128533000	-0.906963000	-1.168582000
H	6.388176000	-0.843533000	0.431888000
H	6.267386000	0.429341000	-3.047717000
H	4.696846000	-0.356058000	-2.900309000
H	4.809914000	1.410724000	-2.916478000
H	5.037272000	0.572821000	1.658137000
C	-5.468948000	-0.498636000	-1.039523000
C	-5.290886000	-0.496318000	-2.564345000
C	-6.358768000	-1.700011000	-0.662750000
C	-6.178059000	0.811199000	-0.637861000
H	-4.696755000	0.355704000	-2.900422000
H	-4.810044000	-1.411066000	-2.916368000
H	-6.267393000	-0.429518000	-3.047719000
H	-6.556953000	-1.735112000	0.408872000

Supporting Information (SI)

H	-7.320108000	-1.637600000	-1.178794000
H	-5.879731000	-2.639564000	-0.945289000
H	-7.128443000	0.907029000	-1.168787000
H	-6.388134000	0.843741000	0.431710000
H	-5.558278000	1.676066000	-0.882281000
H	-5.037276000	-0.572860000	1.658138000

38a

E(SCF) = -1708.77787212

C	-1.378773000	-1.209637000	-0.693152000
C	-1.355430000	-1.241398000	0.701920000
C	-1.835080000	-2.322432000	-1.383983000
C	-1.758545000	-2.386347000	1.377394000
C	-2.227704000	-3.464470000	-0.699348000
C	-2.182208000	-3.529172000	0.696169000
C	-0.814565000	0.018717000	-1.363553000
C	-1.355534000	1.243329000	-0.656342000
C	-0.814685000	-0.017646000	1.411127000
C	-1.378773000	1.212023000	0.743328000
C	-1.766183000	2.382747000	-1.325147000
C	-2.200050000	3.527954000	-0.643214000
C	-1.839495000	2.319755000	1.431152000
C	-2.242551000	3.465838000	0.747412000
C	1.355534000	-1.243329000	-0.656342000
C	1.378773000	-1.212023000	0.743328000
C	1.766183000	-2.382747000	-1.325147000
C	1.839495000	-2.319755000	1.431152000
C	2.200050000	-3.527954000	-0.643214000
C	2.242551000	-3.465838000	0.747412000
C	0.814565000	-0.018717000	-1.363553000
C	1.378773000	1.209637000	-0.693152000
C	0.814685000	0.017646000	1.411127000
C	1.355430000	1.241398000	0.701920000
C	1.835080000	2.322432000	-1.383983000
C	2.227704000	3.464470000	-0.699348000
C	1.758545000	2.386347000	1.377394000
C	2.182208000	3.529172000	0.696169000
C	2.566107000	-4.788366000	-1.436020000
H	-1.858637000	-2.310831000	-2.467852000
H	-1.707090000	-2.382858000	2.457378000
H	-2.557564000	-4.322857000	-1.270090000
H	-1.118516000	0.040961000	-2.409994000
H	-1.118311000	-0.041193000	2.457600000
H	-1.718944000	2.387781000	-2.407604000
H	-1.863486000	2.308303000	2.515076000
H	1.718944000	-2.387781000	-2.407604000
H	1.863486000	-2.308303000	2.515076000
H	1.118516000	-0.040961000	-2.409994000
H	1.118311000	0.041193000	2.457600000

Supporting Information (SI)

H	1.858637000	2.310831000	-2.467852000
H	2.557564000	4.322857000	-1.270090000
H	1.707090000	2.382858000	2.457378000
H	2.579401000	-4.314384000	1.324690000
C	1.323505000	-5.264167000	-2.217773000
H	0.501468000	-5.487072000	-1.535486000
H	0.973987000	-4.506046000	-2.919543000
H	1.555210000	-6.167984000	-2.786799000
C	3.705573000	-4.471203000	-2.424529000
H	4.596818000	-4.133803000	-1.891753000
H	3.968137000	-5.361677000	-3.001126000
H	3.422574000	-3.689487000	-3.129962000
C	3.025216000	-5.938266000	-0.528194000
H	3.273920000	-6.809410000	-1.137340000
H	3.914360000	-5.670736000	0.046023000
H	2.241534000	-6.237216000	0.170450000
C	2.544274000	4.836956000	1.411279000
C	1.559510000	5.935997000	0.958954000
C	2.452224000	4.715457000	2.938998000
C	3.982661000	5.254459000	1.048695000
H	1.625652000	6.117551000	-0.114450000
H	0.531221000	5.647027000	1.185084000
H	1.774579000	6.876736000	1.472008000
H	3.132429000	3.953912000	3.325478000
H	2.724631000	5.667230000	3.399152000
H	1.439653000	4.469309000	3.264421000
H	4.241703000	6.193673000	1.543618000
H	4.697958000	4.492758000	1.365166000
H	4.102956000	5.399872000	-0.025166000
H	-2.579401000	4.314384000	1.324690000
C	-2.544274000	-4.836956000	1.411279000
C	-1.559510000	-5.935997000	0.958954000
C	-2.452224000	-4.715457000	2.938998000
C	-3.982661000	-5.254459000	1.048695000
H	-1.625652000	-6.117551000	-0.114450000
H	-0.531221000	-5.647027000	1.185084000
H	-1.774579000	-6.876736000	1.472008000
H	-3.132429000	-3.953912000	3.325478000
H	-2.724631000	-5.667230000	3.399152000
H	-1.439653000	-4.469309000	3.264421000
H	-4.241703000	-6.193673000	1.543618000
H	-4.697958000	-4.492758000	1.365166000
H	-4.102956000	-5.399872000	-0.025166000
C	-2.566107000	4.788366000	-1.436020000
C	-3.025216000	5.938266000	-0.528194000
C	-1.323505000	5.264167000	-2.217773000
C	-3.705573000	4.471203000	-2.424529000
H	-3.914360000	5.670736000	0.046023000
H	-2.241534000	6.237216000	0.170450000
H	-3.273920000	6.809410000	-1.137340000
H	-0.973987000	4.506046000	-2.919543000
H	-1.555210000	6.167984000	-2.786799000

Supporting Information (SI)

H	-0.501468000	5.487072000	-1.535486000			
H	-3.968137000	5.361677000	-3.001126000			
H	-3.422574000	3.689487000	-3.129962000			
H	-4.596818000	4.133803000	-1.891753000			
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E(SCF) = -1708.77545166						
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C	-0.012285000	0.301786000	1.926795000			
C	0.011982000	-1.060300000	1.598784000			
C	-0.515951000	0.704383000	3.154995000			
C	-0.467755000	-1.994267000	2.505216000			
C	-1.000400000	-0.236198000	4.061052000			
C	-0.976247000	-1.585791000	3.736013000			
C	0.526815000	1.266721000	0.893215000			
C	1.834328000	0.705555000	0.379991000			
C	0.575209000	-1.431260000	0.243671000			
C	1.857755000	-0.652803000	0.051500000			
C	2.977686000	1.462966000	0.200534000			
C	4.164004000	0.913972000	-0.299789000			
C	3.025383000	-1.206392000	-0.440248000			
C	4.189246000	-0.451344000	-0.620359000			
C	-1.816610000	0.755045000	-0.111577000			
C	-1.793480000	-0.603280000	-0.439789000			
C	-2.984687000	1.309995000	0.378209000			
C	-2.937679000	-1.360365000	-0.262003000			
C	-4.148990000	0.555717000	0.555868000			
C	-4.124085000	-0.810133000	0.235803000			
C	-0.533840000	1.533134000	-0.303377000			
C	0.029402000	1.161952000	-1.658477000			
C	-0.485870000	-1.164845000	-0.952655000			
C	0.053269000	-0.200147000	-1.986457000			
C	0.509230000	2.095753000	-2.565031000			
C	1.017418000	1.687095000	-3.795897000			
C	0.556599000	-0.602934000	-3.214727000			
C	1.041149000	0.337485000	-4.120903000			
H	-0.534254000	1.758515000	3.407030000			
H	-0.448607000	-3.047702000	2.250326000			
H	-1.390927000	0.086330000	5.018086000			
H	-1.348239000	-2.321440000	4.438062000			
H	0.707047000	2.233733000	1.362416000			
H	0.793958000	-2.498753000	0.224974000			
H	2.952582000	2.520254000	0.444084000			
H	3.040645000	-2.259785000	-0.701999000			
H	-2.999509000	2.363493000	0.639457000			
H	-2.912946000	-2.417701000	-0.505346000			
H	-0.752370000	2.600675000	-0.284909000			
H	-0.666296000	-2.131912000	-1.421663000			
H	0.490393000	3.149206000	-2.310184000			
H	1.389510000	2.422614000	-4.498030000			

Supporting Information (SI)

H	0.574542000	-1.657081000	-3.466726000
H	1.431450000	0.014822000	-5.077983000
C	-5.388715000	1.263358000	1.052141000
H	-6.131492000	0.540355000	1.384876000
H	-5.134134000	1.864285000	1.931595000
C	-6.009304000	2.192460000	-0.005438000
H	-6.155684000	1.634842000	-0.935571000
H	-5.288311000	2.979998000	-0.240908000
C	-7.336724000	2.824051000	0.424413000
H	-7.598337000	3.611971000	-0.288080000
H	-7.205390000	3.320018000	1.392418000
C	-8.496503000	1.829950000	0.509196000
H	-8.315201000	1.052209000	1.253570000
H	-9.427527000	2.331070000	0.781097000
H	-8.653665000	1.334253000	-0.452300000
C	-5.332512000	-1.704799000	0.389110000
H	-5.818450000	-1.524264000	1.352374000
H	-5.000952000	-2.746473000	0.413073000
C	-6.369697000	-1.543089000	-0.729956000
H	-6.690498000	-0.500262000	-0.781489000
H	-5.892650000	-1.760221000	-1.691402000
C	-7.597449000	-2.433261000	-0.547747000
H	-8.055029000	-2.217519000	0.423989000
H	-7.284495000	-3.482236000	-0.510050000
C	-8.634828000	-2.244165000	-1.652417000
H	-9.503911000	-2.887780000	-1.502054000
H	-8.987306000	-1.210033000	-1.683469000
H	-8.211756000	-2.477728000	-2.632694000
C	5.369208000	1.813083000	-0.451915000
H	5.862030000	1.632335000	-1.411458000
H	5.030814000	2.852487000	-0.481098000
C	6.399881000	1.664341000	0.675020000
H	6.760348000	0.632724000	0.705761000
H	5.903881000	1.839376000	1.635467000
C	7.591954000	2.608674000	0.530223000
H	8.072078000	2.435829000	-0.439219000
H	7.233975000	3.643659000	0.511011000
C	8.620181000	2.441883000	1.647082000
H	9.462777000	3.125021000	1.522461000
H	8.172744000	2.638410000	2.624655000
H	9.016385000	1.423366000	1.665422000
C	5.425043000	-1.161813000	-1.122738000
H	6.175828000	-0.445557000	-1.458675000
H	5.161996000	-1.759901000	-2.001538000
C	6.056068000	-2.088308000	-0.072321000
H	5.329542000	-2.855836000	0.212738000
H	6.258358000	-1.517439000	0.839093000
C	7.342501000	-2.754513000	-0.555384000
H	7.136006000	-3.316975000	-1.472413000
H	8.066016000	-1.979699000	-0.831787000
C	7.961013000	-3.682654000	0.487988000
H	8.880474000	-4.142916000	0.120618000

Supporting Information (SI)

H	8.203711000	-3.136933000	1.403314000
H	7.270553000	-4.485902000	0.757406000

ω B97XD/6-31G*			
8 (S₀-state)			
E(SCF) = -617.95466834			
C	0.000000000	-0.713041000	-4.404913000
C	0.000000000	-1.403117000	-3.229486000
C	0.000000000	-0.717402000	-1.974382000
C	0.000000000	0.717402000	-1.974382000
C	0.000000000	1.403117000	-3.229486000
C	0.000000000	0.713041000	-4.404913000
C	0.000000000	-1.398567000	-0.754737000
C	0.000000000	1.398567000	-0.754737000
C	0.000000000	0.715794000	0.461824000
C	0.000000000	-0.715794000	0.461824000
C	0.000000000	-1.392704000	1.720402000
H	0.000000000	-2.480959000	1.715261000
C	0.000000000	-0.721938000	2.908794000
C	0.000000000	0.721938000	2.908794000
C	0.000000000	1.392704000	1.720402000
H	0.000000000	-2.486817000	-0.754159000
H	0.000000000	-1.245464000	-5.351383000
H	0.000000000	-2.490302000	-3.225945000
H	0.000000000	2.490302000	-3.225945000
H	0.000000000	1.245464000	-5.351383000
H	0.000000000	2.486817000	-0.754159000
H	0.000000000	2.480959000	1.715261000
C	0.000000000	1.470318000	4.216081000
H	-0.881045000	1.222846000	4.820583000
H	0.881045000	1.222846000	4.820583000
H	0.000000000	2.550958000	4.049885000
C	0.000000000	-1.470318000	4.216081000
H	0.881045000	-1.222846000	4.820583000
H	-0.881045000	-1.222846000	4.820583000
H	0.000000000	-2.550958000	4.049885000
8 (S₁-state)			
E(SCF) = -617.82855617			
C	0.000000000	-0.692466000	-4.447964000
C	0.000000000	-1.394933000	-3.229340000
C	0.000000000	-0.720379000	-2.001600000
C	0.000000000	0.720379000	-2.001600000
C	0.000000000	1.394933000	-3.229340000
C	0.000000000	0.692466000	-4.447964000
C	0.000000000	-1.396438000	-0.758474000

Supporting Information (SI)

C	0.000000000	1.396438000	-0.758474000
C	0.000000000	0.718264000	0.480195000
C	0.000000000	-0.718264000	0.480195000
C	0.000000000	-1.382393000	1.712151000
H	0.000000000	-2.470622000	1.716655000
C	0.000000000	-0.698936000	2.944853000
C	0.000000000	0.698936000	2.944853000
C	0.000000000	1.382393000	1.712151000
H	0.000000000	-2.484764000	-0.757861000
H	0.000000000	-1.241595000	-5.384380000
H	0.000000000	-2.481986000	-3.233048000
H	0.000000000	2.481986000	-3.233048000
H	0.000000000	1.241595000	-5.384380000
H	0.000000000	2.484764000	-0.757861000
H	0.000000000	2.470622000	1.716655000
C	0.000000000	1.473510000	4.234831000
H	-0.880694000	1.237420000	4.845622000
H	0.880694000	1.237420000	4.845622000
H	0.000000000	2.551410000	4.051146000
C	0.000000000	-1.473510000	4.234831000
H	0.880694000	-1.237420000	4.845622000
H	-0.880694000	-1.237420000	4.845622000
H	0.000000000	-2.551410000	4.051146000

20 (S_0 -state)

E(SCF) = -853.77154446

C	-3.541632000	-1.264993000	0.545819000
C	-2.182924000	-1.133687000	0.513125000
C	-1.538291000	0.117087000	0.261436000
C	-2.352522000	1.272608000	0.043197000
C	-3.770782000	1.111094000	0.088430000
C	-4.364131000	-0.095651000	0.322321000
C	-0.149556000	0.243623000	0.223108000
C	-1.742660000	2.501914000	-0.207445000
C	-0.352061000	2.630737000	-0.251141000
C	0.465084000	1.472718000	-0.028386000
C	1.887239000	1.617327000	-0.073812000
H	2.502536000	0.737731000	0.097974000
C	2.460715000	2.827980000	-0.325546000
C	1.648708000	3.978427000	-0.549476000
C	0.289387000	3.881936000	-0.512556000
H	0.469144000	-0.635465000	0.392311000
H	-1.543783000	-1.995415000	0.681862000
H	-4.391158000	1.990044000	-0.078993000
H	-2.362603000	3.380114000	-0.376464000
H	3.541891000	2.924878000	-0.357943000
H	2.122818000	4.934485000	-0.750342000
H	-0.331467000	4.757759000	-0.683672000

Supporting Information (SI)

C	-5.871744000	-0.200880000	0.284435000
C	-6.398973000	-0.540528000	-1.118226000
H	-6.308464000	0.753318000	0.603041000
H	-6.229262000	-0.953184000	0.996936000
C	-7.909114000	-0.772145000	-1.146877000
H	-6.133012000	0.277268000	-1.801107000
H	-5.885804000	-1.432286000	-1.503202000
C	-8.436643000	-1.055952000	-2.552012000
H	-8.156466000	-1.612048000	-0.483586000
H	-8.419568000	0.107312000	-0.731590000
H	-9.517220000	-1.231791000	-2.546231000
H	-8.236759000	-0.212757000	-3.223073000
H	-7.955018000	-1.942300000	-2.980943000
C	-4.210447000	-2.595477000	0.827508000
C	-3.291767000	-3.809069000	0.952182000
H	-4.947377000	-2.798019000	0.038205000
H	-4.797601000	-2.506762000	1.753197000
C	-4.069993000	-5.105447000	1.181017000
H	-2.683532000	-3.908685000	0.042950000
H	-2.589158000	-3.662891000	1.783560000
C	-3.157904000	-6.323307000	1.314771000
H	-4.685449000	-5.005453000	2.085092000
H	-4.770180000	-5.259353000	0.349106000
H	-3.734390000	-7.239513000	1.478273000
H	-2.554552000	-6.462892000	0.410380000
H	-2.467727000	-6.206274000	2.158178000

20 (S_1 -state)

E(SCF) = -853.64842470

C	-3.218360000	-1.571335000	-0.190699000
C	-1.846328000	-1.289109000	-0.370720000
C	-1.317657000	0.002365000	-0.277880000
C	-2.217134000	1.085876000	0.011887000
C	-3.571329000	0.789541000	0.197254000
C	-4.088786000	-0.521628000	0.110087000
C	0.052510000	0.288282000	-0.457624000
C	-1.696369000	2.394569000	0.098709000
C	-0.323085000	2.685579000	-0.083573000
C	0.578949000	1.599306000	-0.368737000
C	1.939705000	1.881194000	-0.546580000
H	2.623594000	1.063478000	-0.759380000
C	2.430076000	3.195206000	-0.453954000
C	1.562009000	4.240427000	-0.182044000
C	0.192027000	3.985607000	0.002045000
H	0.733654000	-0.532568000	-0.673617000
H	-1.171082000	-2.113427000	-0.594197000
H	-4.256977000	1.605085000	0.421246000
H	-2.378044000	3.214964000	0.314757000
H	3.489637000	3.383823000	-0.595770000

Supporting Information (SI)

H	1.932903000	5.258113000	-0.110555000
H	-0.486290000	4.808021000	0.214572000
C	-5.572716000	-0.723432000	0.291481000
C	-6.350582000	-0.609491000	-1.028628000
H	-5.955133000	0.028121000	0.993857000
H	-5.779734000	-1.698165000	0.748428000
C	-7.852508000	-0.830127000	-0.852804000
H	-6.169079000	0.381564000	-1.466004000
H	-5.952575000	-1.336614000	-1.749349000
C	-8.626930000	-0.708565000	-2.163722000
H	-8.021562000	-1.823826000	-0.416017000
H	-8.241917000	-0.105434000	-0.125323000
H	-9.698353000	-0.874756000	-2.012259000
H	-8.500071000	0.287510000	-2.603135000
H	-8.273625000	-1.441744000	-2.897815000
C	-3.675440000	-3.006383000	-0.276697000
C	-3.617714000	-3.727466000	1.078826000
H	-3.039863000	-3.544534000	-0.991430000
H	-4.695610000	-3.066593000	-0.673415000
C	-4.096095000	-5.176731000	1.000339000
H	-2.586845000	-3.696161000	1.456661000
H	-4.225532000	-3.177195000	1.809795000
C	-4.030934000	-5.896135000	2.346156000
H	-5.127417000	-5.195308000	0.622413000
H	-3.489565000	-5.718463000	0.262303000
H	-4.382100000	-6.929833000	2.264568000
H	-3.004221000	-5.919143000	2.729137000
H	-4.651680000	-5.388327000	3.093199000

21 (S₀-state)

E(SCF) = -853.77594002

C	-5.921698000	-0.380349000	0.824656000
C	-4.759241000	-1.060778000	1.030766000
C	-3.501495000	-0.505741000	0.634170000
C	-3.486332000	0.787291000	0.010330000
C	-4.729396000	1.467884000	-0.186815000
C	-5.906520000	0.904918000	0.205894000
C	-2.295884000	-1.180560000	0.833062000
C	-2.266229000	1.340332000	-0.382009000
C	-1.061362000	0.663591000	-0.181452000
C	-1.076584000	-0.625515000	0.439195000
C	0.168175000	-1.294994000	0.625152000
H	0.152707000	-2.278596000	1.092032000
C	1.366280000	-0.756934000	0.240895000
C	1.382933000	0.549744000	-0.372865000
C	0.198702000	1.207357000	-0.567154000
H	-2.306636000	-2.161099000	1.304653000
H	-6.869665000	-0.813522000	1.129477000

Supporting Information (SI)

H	-4.767542000	-2.040400000	1.501873000
H	-4.714534000	2.447174000	-0.658449000
H	-6.842878000	1.432697000	0.051367000
H	-2.253765000	2.320779000	-0.853750000
H	0.207535000	2.191284000	-1.033521000
C	2.662370000	1.256345000	-0.768819000
H	3.474585000	0.544565000	-0.946997000
H	2.495855000	1.768181000	-1.724711000
C	3.129999000	2.303207000	0.263950000
H	2.304016000	3.015916000	0.397877000
C	4.342988000	3.068135000	-0.268795000
H	4.666722000	3.837009000	0.441194000
H	5.188813000	2.388166000	-0.431630000
H	4.120328000	3.560004000	-1.222403000
C	3.436986000	1.678493000	1.626123000
H	2.576481000	1.128641000	2.021072000
H	4.281716000	0.981660000	1.553304000
H	3.707551000	2.450028000	2.355218000
C	2.615449000	-1.590519000	0.435216000
H	3.512389000	-0.964575000	0.477240000
H	2.551926000	-2.090908000	1.409383000
C	2.807421000	-2.670383000	-0.650249000
H	1.903862000	-3.296247000	-0.646297000
C	4.007147000	-3.556455000	-0.309964000
H	3.890291000	-4.031208000	0.670768000
H	4.136313000	-4.348121000	-1.056042000
H	4.931525000	-2.965392000	-0.288419000
C	2.955825000	-2.068392000	-2.048687000
H	2.102778000	-1.432446000	-2.306897000
H	3.866579000	-1.459740000	-2.115837000
H	3.029508000	-2.857149000	-2.805313000

21 (S_1 -state)

E(SCF) = -853.65301888

C	-5.956551000	-0.371502000	0.796985000
C	-4.754900000	-1.074748000	0.981872000
C	-3.523144000	-0.518123000	0.613312000
C	-3.503284000	0.800461000	0.034670000
C	-4.716406000	1.479554000	-0.138730000
C	-5.937473000	0.897670000	0.239558000
C	-2.294679000	-1.200777000	0.784595000
C	-2.255768000	1.359086000	-0.334257000
C	-1.033955000	0.676669000	-0.160308000
C	-1.054138000	-0.641664000	0.414190000
C	0.163702000	-1.306967000	0.577440000
H	0.155870000	-2.303877000	1.015021000
C	1.410111000	-0.745542000	0.209860000
C	1.429590000	0.533839000	-0.349159000
C	0.202659000	1.219078000	-0.519428000

Supporting Information (SI)

H	-2.309635000	-2.197690000	1.220655000
H	-6.896628000	-0.827621000	1.091172000
H	-4.773411000	-2.069578000	1.419409000
H	-4.705035000	2.474737000	-0.575710000
H	-6.862260000	1.447204000	0.094245000
H	-2.240470000	2.355953000	-0.770409000
H	0.224673000	2.215249000	-0.958199000
C	2.685699000	1.266059000	-0.753056000
H	3.518012000	0.573317000	-0.914271000
H	2.507206000	1.756817000	-1.719220000
C	3.121228000	2.342723000	0.264758000
H	2.267489000	3.018964000	0.414340000
C	4.288047000	3.159154000	-0.293347000
H	4.593493000	3.940935000	0.410615000
H	5.158740000	2.516522000	-0.475298000
H	4.023903000	3.641409000	-1.241183000
C	3.481416000	1.730039000	1.618993000
H	2.653241000	1.141193000	2.026222000
H	4.353269000	1.069656000	1.525276000
H	3.732886000	2.509786000	2.346093000
C	2.635363000	-1.601967000	0.415884000
H	3.547246000	-0.996494000	0.438154000
H	2.563972000	-2.080386000	1.401874000
C	2.795557000	-2.708242000	-0.649625000
H	1.866130000	-3.295327000	-0.657033000
C	3.949243000	-3.640737000	-0.276836000
H	3.791870000	-4.102140000	0.704528000
H	4.060523000	-4.443189000	-1.014216000
H	4.897088000	-3.089001000	-0.239854000
C	2.995910000	-2.123360000	-2.048500000
H	2.176235000	-1.452079000	-2.324113000
H	3.932714000	-1.553391000	-2.099006000
H	3.050653000	-2.918289000	-2.800169000

32 (S_0 -state)

E(SCF) = -1244.40509121

C	-7.646798000	-0.764567000	1.077705000
C	-6.543776000	0.036161000	1.047354000
C	-5.311277000	-0.430807000	0.492110000
C	-5.255496000	-1.765081000	-0.032213000
C	-6.435240000	-2.572097000	0.017831000
C	-7.591993000	-2.089404000	0.553619000
C	-4.166569000	0.369373000	0.443050000
C	-4.056527000	-2.233864000	-0.574797000
C	-2.915584000	-1.432648000	-0.619741000
C	-2.971663000	-0.100083000	-0.103014000
C	-1.794819000	0.709142000	-0.176312000
H	-1.864889000	1.721884000	0.210062000
C	-0.624206000	0.253533000	-0.711871000

Supporting Information (SI)

C	-0.562342000	-1.103363000	-1.210698000
C	-1.676856000	-1.889730000	-1.163066000
H	-4.210141000	1.382157000	0.838882000
H	-8.576118000	-0.396894000	1.502518000
H	-6.583145000	1.046402000	1.447032000
H	-6.389448000	-3.581367000	-0.383569000
H	-8.481254000	-2.712055000	0.584668000
H	-4.011798000	-3.245922000	-0.972206000
H	-1.629843000	-2.907833000	-1.546045000
C	0.731936000	-1.688317000	-1.728178000
C	1.599122000	-2.275236000	-0.603473000
H	1.310961000	-0.938619000	-2.279879000
H	0.502946000	-2.486086000	-2.445296000
C	2.898025000	-2.889547000	-1.125232000
H	1.831155000	-1.495350000	0.134551000
H	1.005052000	-3.028148000	-0.072462000
H	2.657095000	-3.749764000	-1.767858000
H	3.403293000	-2.158368000	-1.772490000
C	0.602377000	1.135625000	-0.825875000
C	0.500131000	2.537529000	-0.228196000
H	0.861960000	1.233651000	-1.890125000
H	1.459147000	0.624571000	-0.366739000
C	1.798449000	3.322774000	-0.422580000
H	-0.332770000	3.075064000	-0.696837000
H	0.270950000	2.468958000	0.844024000
H	2.638070000	2.714801000	-0.056070000
H	1.975048000	3.467762000	-1.498909000
C	1.847530000	4.685716000	0.276618000
C	3.235291000	5.322104000	0.113316000
C	0.763375000	5.651688000	-0.223428000
H	1.678547000	4.521718000	1.353408000
C	3.334000000	6.690295000	0.792276000
H	3.444413000	5.437708000	-0.961054000
H	4.002039000	4.644722000	0.510196000
C	0.859100000	7.023462000	0.451931000
H	0.874896000	5.772953000	-1.311898000
H	-0.233197000	5.227652000	-0.054804000
C	2.249041000	7.639915000	0.278346000
H	4.328323000	7.122456000	0.629985000
H	3.217269000	6.563772000	1.877978000
H	0.091028000	7.694849000	0.050520000
H	0.648749000	6.909345000	1.524939000
H	2.306737000	8.603623000	0.797523000
H	2.423161000	7.842663000	-0.788057000
C	3.882999000	-3.336684000	-0.038783000
C	3.286811000	-4.383671000	0.913219000
C	5.176888000	-3.871683000	-0.669029000
H	4.145700000	-2.451340000	0.563697000
C	4.298317000	-4.850877000	1.964326000
H	2.950386000	-5.248544000	0.320640000
H	2.398865000	-3.981426000	1.413694000
C	6.190564000	-4.334534000	0.380287000

Supporting Information (SI)

H	4.923795000	-4.719069000	-1.324282000
H	5.621682000	-3.101923000	-1.312478000
C	5.580589000	-5.379490000	1.317864000
H	3.847692000	-5.619526000	2.602954000
H	4.549892000	-4.005241000	2.620446000
H	7.084296000	-4.737502000	-0.110218000
H	6.519002000	-3.467940000	0.971874000
H	6.304575000	-5.670016000	2.087947000
H	5.347479000	-6.287597000	0.743542000

32 (S_1 -state)

E(SCF) = -1244.28228608

C	-7.977735000	1.146122000	0.355865000
C	-6.749142000	1.547111000	0.908701000
C	-5.539246000	0.995297000	0.467682000
C	-5.569814000	0.000292000	-0.573134000
C	-6.807788000	-0.380919000	-1.106821000
C	-8.007039000	0.188530000	-0.645104000
C	-4.285554000	1.375919000	1.003906000
C	-4.344509000	-0.552932000	-1.016012000
C	-3.096609000	-0.170219000	-0.479835000
C	-3.065948000	0.821511000	0.560546000
C	-1.823614000	1.189953000	1.087385000
H	-1.794084000	1.939115000	1.876628000
C	-0.605621000	0.631521000	0.641088000
C	-0.634433000	-0.320288000	-0.380059000
C	-1.881945000	-0.708964000	-0.915971000
H	-4.262753000	2.127738000	1.790286000
H	-8.899262000	1.590849000	0.718329000
H	-6.730198000	2.299238000	1.693128000
H	-6.833781000	-1.132190000	-1.891872000
H	-8.951679000	-0.126351000	-1.077382000
H	-4.366632000	-1.304506000	-1.802647000
H	-1.897579000	-1.458397000	-1.705418000
C	0.610541000	-0.997875000	-0.896028000
C	0.934655000	-2.287209000	-0.125251000
H	1.472374000	-0.322007000	-0.852527000
H	0.471614000	-1.246026000	-1.956111000
C	2.186725000	-2.983941000	-0.657277000
H	1.065478000	-2.051497000	0.939734000
H	0.066188000	-2.953993000	-0.186518000
H	2.034406000	-3.242187000	-1.716080000
H	3.022048000	-2.269127000	-0.636230000
C	0.683084000	1.136400000	1.240510000
C	1.254621000	2.332578000	0.462839000
H	1.434541000	0.339092000	1.278346000
H	0.506064000	1.438185000	2.280595000
C	2.582306000	2.826821000	1.036256000
H	1.376974000	2.042996000	-0.587790000

Supporting Information (SI)

H	0.517413000	3.146814000	0.471101000
H	2.457472000	3.007561000	2.113546000
H	3.335506000	2.029420000	0.946374000
C	3.127378000	4.103760000	0.386196000
C	4.392306000	4.585996000	1.111386000
C	3.413398000	3.929808000	-1.112820000
H	2.361653000	4.889862000	0.490281000
C	4.971466000	5.858855000	0.488810000
H	5.148922000	3.787851000	1.069361000
H	4.171064000	4.751107000	2.173477000
C	3.996144000	5.199738000	-1.740093000
H	4.125476000	3.100021000	-1.241680000
H	2.499081000	3.646169000	-1.645994000
C	5.254073000	5.664678000	-1.002892000
H	5.886166000	6.153991000	1.016049000
H	4.253355000	6.681443000	0.615835000
H	4.215716000	5.027179000	-2.800169000
H	3.240776000	5.997388000	-1.701101000
H	5.634463000	6.593254000	-1.444312000
H	6.043516000	4.909085000	-1.124576000
C	2.602516000	-4.246699000	0.106801000
C	1.542842000	-5.356235000	0.033780000
C	3.949604000	-4.768640000	-0.414280000
H	2.734690000	-3.978241000	1.167530000
C	1.992578000	-6.635350000	0.746609000
H	1.342996000	-5.580689000	-1.025393000
H	0.597174000	-5.010349000	0.466091000
C	4.400582000	-6.044540000	0.301471000
H	3.852915000	-4.974434000	-1.491135000
H	4.713516000	-3.987276000	-0.313028000
C	3.333188000	-7.137273000	0.206111000
H	1.224373000	-7.410787000	0.644663000
H	2.093221000	-6.431438000	1.822154000
H	5.348477000	-6.398534000	-0.120568000
H	4.590555000	-5.818482000	1.360414000
H	3.653012000	-8.033415000	0.750526000
H	3.210705000	-7.431271000	-0.846088000
<hr/>			
35 (S₀-state)			
<hr/>			
E(SCF) = -1475.43395497			
<hr/>			
C	-1.595976000	1.048139000	-0.789532000
C	-2.793035000	1.661575000	-0.556504000
C	-3.996317000	0.930240000	-0.317685000
C	-3.928549000	-0.499119000	-0.324960000
C	-2.665500000	-1.117529000	-0.576294000
C	-1.527120000	-0.397880000	-0.802883000
C	-5.220027000	1.555721000	-0.077620000
C	-5.088143000	-1.238221000	-0.088352000
C	-6.314605000	-0.615117000	0.154110000

Supporting Information (SI)

C	-6.382718000	0.818200000	0.158895000
C	-7.644845000	1.443833000	0.406091000
H	-7.693892000	2.529915000	0.407629000
C	-8.763389000	0.699096000	0.635180000
C	-8.695271000	-0.725306000	0.632685000
C	-7.511174000	-1.359081000	0.400100000
H	-5.270663000	2.642799000	-0.072955000
H	-2.844985000	2.748823000	-0.542914000
H	-2.630068000	-2.204490000	-0.586276000
H	-5.035851000	-2.325213000	-0.092776000
H	-9.715803000	1.186695000	0.820659000
H	-9.596976000	-1.301387000	0.818072000
H	-7.455435000	-2.444816000	0.397160000
C	-0.214331000	-1.097732000	-1.096488000
H	-0.131174000	-1.252447000	-2.180941000
H	0.609529000	-0.429375000	-0.844779000
C	0.001514000	-2.436537000	-0.370032000
H	-0.501622000	-2.404099000	0.605678000
H	-0.475796000	-3.248472000	-0.935326000
C	-0.346867000	1.879885000	-0.976501000
H	0.240861000	1.480256000	-1.809448000
H	-0.630245000	2.898334000	-1.263362000
C	0.496802000	1.922226000	0.311298000
H	0.539613000	0.914744000	0.744897000
H	-0.043306000	2.530177000	1.050209000
C	1.477748000	-2.799850000	-0.129464000
C	2.102227000	-1.869468000	0.932568000
C	1.576588000	-4.244026000	0.405298000
C	2.309693000	-2.710838000	-1.425841000
H	1.527883000	-1.948718000	1.866336000
H	2.036975000	-0.823911000	0.613787000
C	3.571021000	-2.234329000	1.191072000
H	1.138991000	-4.938127000	-0.325975000
H	0.984397000	-4.334646000	1.326714000
C	3.039538000	-4.631404000	0.679210000
H	2.269379000	-1.693238000	-1.835605000
H	1.876216000	-3.377589000	-2.185029000
C	3.774275000	-3.092665000	-1.160789000
H	3.990264000	-1.543271000	1.933434000
C	3.643560000	-3.674871000	1.720237000
C	4.366465000	-2.129052000	-0.120131000
H	3.077813000	-5.659547000	1.058998000
C	3.843737000	-4.531727000	-0.626799000
H	4.342176000	-3.018470000	-2.096067000
H	3.096511000	-3.754373000	2.668794000
H	4.686529000	-3.951197000	1.923821000
H	4.333099000	-1.099773000	-0.502651000
H	5.422423000	-2.369274000	0.060477000
H	4.888942000	-4.816767000	-0.448578000
H	3.440899000	-5.229741000	-1.372630000
C	1.935449000	2.451904000	0.193237000
C	1.968680000	3.950339000	-0.169049000

Supporting Information (SI)

C	2.620096000	2.267107000	1.564923000
C	2.759590000	1.686373000	-0.864219000
H	1.384227000	4.519594000	0.567438000
H	1.495128000	4.110611000	-1.147255000
C	3.417446000	4.467304000	-0.203965000
H	2.607161000	1.202125000	1.837656000
H	2.043800000	2.799750000	2.334313000
C	4.065751000	2.779720000	1.538745000
H	2.315996000	1.816777000	-1.859420000
H	2.741984000	0.610898000	-0.647249000
C	4.211860000	2.188017000	-0.894132000
H	3.416117000	5.533138000	-0.462616000
C	4.066830000	4.273074000	1.175402000
C	4.217160000	3.681776000	-1.256152000
H	4.522086000	2.638965000	2.526043000
C	4.857996000	1.990637000	0.485432000
H	4.773377000	1.622627000	-1.648115000
H	3.515785000	4.843894000	1.934433000
H	5.094690000	4.659021000	1.163964000
H	3.775997000	3.828500000	-2.251000000
H	5.248136000	4.056631000	-1.301859000
H	5.902330000	2.328799000	0.463340000
H	4.869541000	0.923385000	0.746420000

35 (S_1 -state)

E(SCF) = -1475.30857902

C	-1.557520000	1.125083000	-0.569707000
C	-2.814302000	1.726798000	-0.357419000
C	-3.989797000	0.985776000	-0.191745000
C	-3.900331000	-0.446695000	-0.242245000
C	-2.643294000	-1.031712000	-0.437072000
C	-1.466055000	-0.272302000	-0.596293000
C	-5.254785000	1.580421000	0.006063000
C	-5.082381000	-1.204799000	-0.099162000
C	-6.353997000	-0.612831000	0.090165000
C	-6.442855000	0.823880000	0.146954000
C	-7.699168000	1.415069000	0.333495000
H	-7.770667000	2.498853000	0.378051000
C	-8.861549000	0.633524000	0.461143000
C	-8.776091000	-0.747765000	0.404701000
C	-7.527078000	-1.367180000	0.220712000
H	-5.321902000	2.665984000	0.045556000
H	-2.875483000	2.813379000	-0.332573000
H	-2.584154000	-2.116335000	-0.475197000
H	-5.014204000	-2.290195000	-0.141600000
H	-9.821853000	1.119357000	0.603137000
H	-9.668986000	-1.357617000	0.501018000
H	-7.462983000	-2.451408000	0.175572000
C	-0.132242000	-0.942370000	-0.837170000

Supporting Information (SI)

H	0.092846000	-0.899483000	-1.912987000
H	0.645841000	-0.340702000	-0.362655000
C	0.007072000	-2.390891000	-0.353112000
H	-0.533012000	-2.518159000	0.594984000
H	-0.469564000	-3.068352000	-1.074721000
C	-0.341633000	1.996977000	-0.770729000
H	0.269019000	1.579233000	-1.578698000
H	-0.662503000	2.985233000	-1.118041000
C	0.512183000	2.160254000	0.504975000
H	0.518642000	1.216329000	1.066572000
H	0.017621000	2.890007000	1.160339000
C	1.463097000	-2.842672000	-0.131453000
C	2.045222000	-2.208282000	1.150841000
C	1.502724000	-4.374730000	0.048233000
C	2.367569000	-2.474804000	-1.326761000
H	1.418736000	-2.489487000	2.008927000
H	2.015368000	-1.113511000	1.087852000
C	3.489972000	-2.675391000	1.385357000
H	1.091234000	-4.858725000	-0.848525000
H	0.857160000	-4.661585000	0.890407000
C	2.938797000	-4.864953000	0.291442000
H	2.376006000	-1.388068000	-1.477576000
H	1.961442000	-2.922968000	-2.245000000
C	3.805992000	-2.958973000	-1.090587000
H	3.884198000	-2.197740000	2.290560000
C	3.502540000	-4.202327000	1.558353000
C	4.359646000	-2.289997000	0.177785000
H	2.934709000	-5.954523000	0.416342000
C	3.813684000	-4.485082000	-0.913615000
H	4.426904000	-2.683860000	-1.951908000
H	2.901239000	-4.486100000	2.432259000
H	4.526222000	-4.553991000	1.742583000
H	4.370760000	-1.198429000	0.051937000
H	5.397933000	-2.603580000	0.347709000
H	4.840431000	-4.843210000	-0.761968000
H	3.433260000	-4.969758000	-1.822474000
C	1.969872000	2.594567000	0.277300000
C	2.057117000	3.903731000	-0.532221000
C	2.642805000	2.823486000	1.647654000
C	2.774474000	1.505981000	-0.464265000
H	1.490185000	4.692400000	-0.017257000
H	1.594239000	3.768505000	-1.518675000
C	3.522134000	4.335320000	-0.709910000
H	2.586736000	1.898921000	2.239736000
H	2.089140000	3.593074000	2.203321000
C	4.108333000	3.252012000	1.478702000
H	2.330962000	1.297950000	-1.446731000
H	2.733338000	0.570096000	0.107702000
C	4.238621000	1.930153000	-0.647100000
H	3.558496000	5.267198000	-1.286944000
C	4.164473000	4.557037000	0.668400000
C	4.290558000	3.233987000	-1.458574000

Supporting Information (SI)

H	4.557655000	3.411062000	2.466378000
C	4.878211000	2.151784000	0.731629000
H	4.778918000	1.138780000	-1.181982000
H	3.636306000	5.356156000	1.205322000
H	5.206428000	4.882178000	0.549478000
H	3.848942000	3.076083000	-2.451535000
H	5.333305000	3.540309000	-1.613385000
H	5.932178000	2.437091000	0.617557000
H	4.856806000	1.217113000	1.308550000
<hr/>			
36 (S₀-state)			
<hr/>			
E(SCF) = -932.37477634			
<hr/>			
C	-0.333267000	6.144485000	0.713473000
C	-0.171981000	4.980906000	1.403514000
C	0.001286000	3.736523000	0.718336000
C	0.001286000	3.736523000	-0.718336000
C	-0.171981000	4.980906000	-1.403514000
C	-0.333267000	6.144485000	-0.713473000
C	0.171061000	2.530676000	1.399781000
C	0.171061000	2.530676000	-1.399781000
C	0.335164000	1.325172000	-0.713651000
C	0.335164000	1.325172000	0.713651000
C	0.533993000	0.082396000	1.378574000
H	0.623416000	0.111658000	2.459967000
C	0.661379000	-1.117518000	0.726892000
C	0.661379000	-1.117518000	-0.726892000
C	0.533993000	0.082396000	-1.378574000
H	0.173445000	2.529276000	2.488045000
H	-0.463485000	7.082368000	1.245101000
H	-0.171675000	4.977554000	2.490674000
H	-0.171675000	4.977554000	-2.490674000
H	-0.463485000	7.082368000	-1.245101000
H	0.173445000	2.529276000	-2.488045000
H	0.623416000	0.111658000	-2.459967000
C	0.937647000	-2.353994000	-1.570623000
C	-0.167231000	-2.883823000	-2.530855000
H	1.220149000	-3.192768000	-0.929505000
H	1.825406000	-2.144297000	-2.183030000
C	0.937647000	-2.353994000	1.570623000
C	-0.167231000	-2.883823000	2.530855000
H	1.825406000	-2.144297000	2.183030000
H	1.220149000	-3.192768000	0.929505000
C	-1.448983000	-3.216387000	1.763768000
H	-1.830061000	-2.339692000	1.229414000
H	-1.273730000	-4.012392000	1.033918000
H	-2.229935000	-3.561240000	2.451597000
C	0.383837000	-4.168184000	3.171260000
H	1.297177000	-3.965045000	3.743311000
H	-0.350824000	-4.606996000	3.856252000

Supporting Information (SI)

H	0.623817000	-4.920056000	2.410087000
C	-0.508674000	-1.894711000	3.654594000
H	-1.165056000	-2.377708000	4.387864000
H	0.391892000	-1.559159000	4.183775000
H	-1.035922000	-1.014749000	3.275124000
C	-0.508674000	-1.894711000	-3.654594000
H	0.391892000	-1.559159000	-4.183775000
H	-1.165056000	-2.377708000	-4.387864000
H	-1.035922000	-1.014749000	-3.275124000
C	0.383837000	-4.168184000	-3.171260000
H	-0.350824000	-4.606996000	-3.856252000
H	1.297177000	-3.965045000	-3.743311000
H	0.623817000	-4.920056000	-2.410087000
C	-1.448983000	-3.216387000	-1.763768000
H	-1.273730000	-4.012392000	-1.033918000
H	-1.830061000	-2.339692000	-1.229414000
H	-2.229935000	-3.561240000	-2.451597000

36 (S_1 -state)

E(SCF) = -932.25293572

C	-0.326015000	6.190503000	0.693442000
C	-0.163575000	4.985359000	1.394785000
C	-0.001633000	3.768061000	0.720237000
C	-0.001633000	3.768061000	-0.720237000
C	-0.163575000	4.985359000	-1.394785000
C	-0.326015000	6.190503000	-0.693442000
C	0.168874000	2.536108000	1.397669000
C	0.168874000	2.536108000	-1.397669000
C	0.322544000	1.311434000	-0.717571000
C	0.322544000	1.311434000	0.717571000
C	0.518978000	0.092600000	1.369347000
H	0.608343000	0.110147000	2.450715000
C	0.653759000	-1.153132000	0.702108000
C	0.653759000	-1.153132000	-0.702108000
C	0.518978000	0.092600000	-1.369347000
H	0.182969000	2.537098000	2.485959000
H	-0.450472000	7.119340000	1.241280000
H	-0.161458000	4.989075000	2.481875000
H	-0.161458000	4.989075000	-2.481875000
H	-0.450472000	7.119340000	-1.241280000
H	0.182969000	2.537098000	-2.485959000
H	0.608343000	0.110147000	-2.450715000
C	0.937473000	-2.363345000	-1.569426000
C	-0.165015000	-2.893202000	-2.534913000
H	1.238398000	-3.209087000	-0.945425000
H	1.815869000	-2.122472000	-2.186818000
C	0.937473000	-2.363345000	1.569426000
C	-0.165015000	-2.893202000	2.534913000
H	1.815869000	-2.122472000	2.186818000

Supporting Information (SI)

H	1.238398000	-3.209087000	0.945425000
C	-1.428712000	-3.275189000	1.761418000
H	-1.829353000	-2.418139000	1.210141000
H	-1.222495000	-4.075931000	1.044802000
H	-2.205848000	-3.632610000	2.447137000
C	0.409418000	-4.146969000	3.213749000
H	1.310464000	-3.907144000	3.791115000
H	-0.322814000	-4.586276000	3.901033000
H	0.676482000	-4.911245000	2.474357000
C	-0.542975000	-1.883841000	3.628615000
H	-1.198864000	-2.362393000	4.365262000
H	0.342812000	-1.516466000	4.161592000
H	-1.082767000	-1.024226000	3.220297000
C	-0.542975000	-1.883841000	-3.628615000
H	0.342812000	-1.516466000	-4.161592000
H	-1.198864000	-2.362393000	-4.365262000
H	-1.082767000	-1.024226000	-3.220297000
C	0.409418000	-4.146969000	-3.213749000
H	-0.322814000	-4.586276000	-3.901033000
H	1.310464000	-3.907144000	-3.791115000
H	0.676482000	-4.911245000	-2.474357000
C	-1.428712000	-3.275189000	-1.761418000
H	-1.222495000	-4.075931000	-1.044802000
H	-1.829353000	-2.418139000	-1.210141000
H	-2.205848000	-3.632610000	-2.447137000

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