Supporting Information File 1

for

Fluorescent hexaaryl- and hexa-heteroaryl[3]radialenes: Synthesis, structures, and properties

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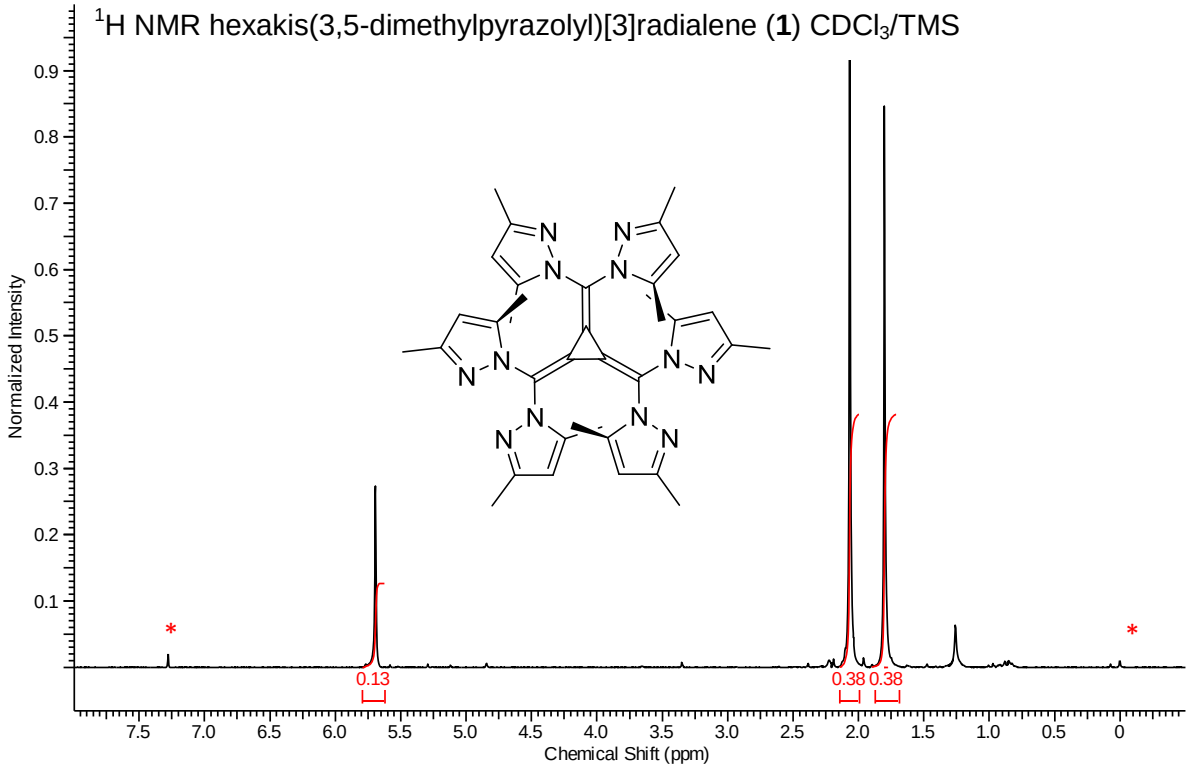
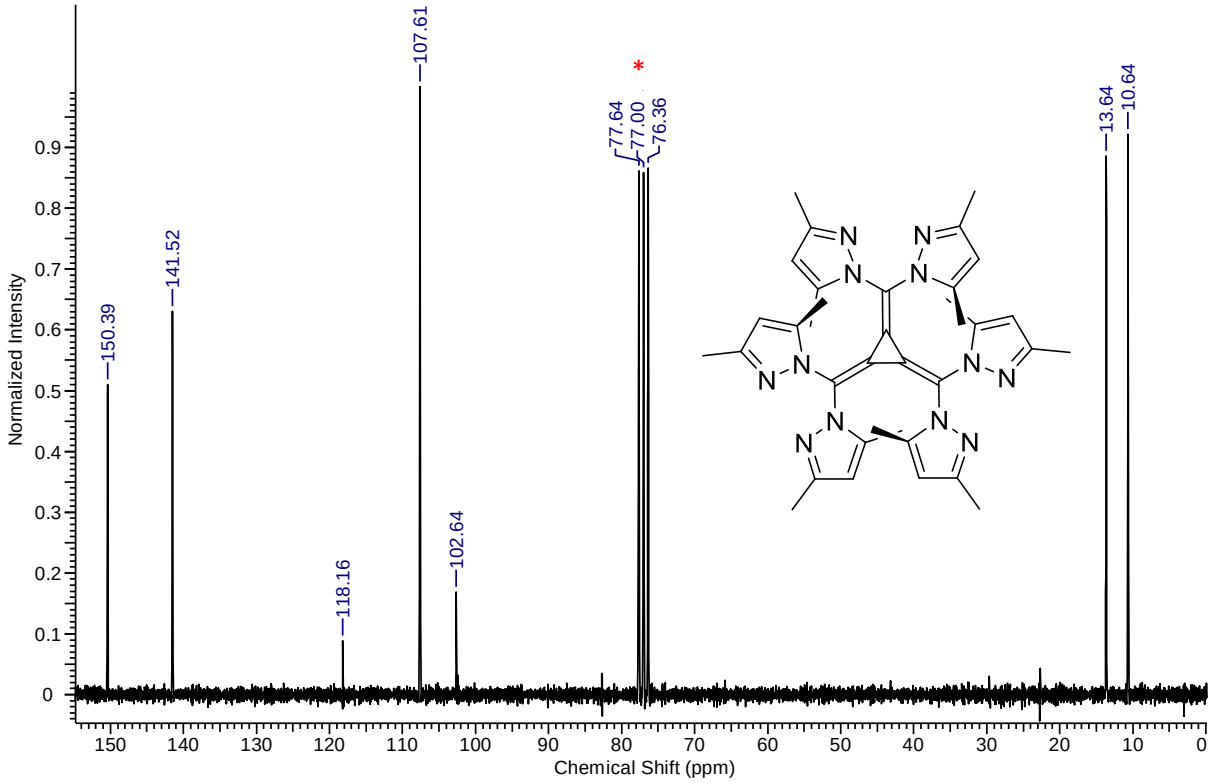
^{1}H and ^{13}C NMR spectra of all compounds

Solvent peaks are marked with an asterisk.

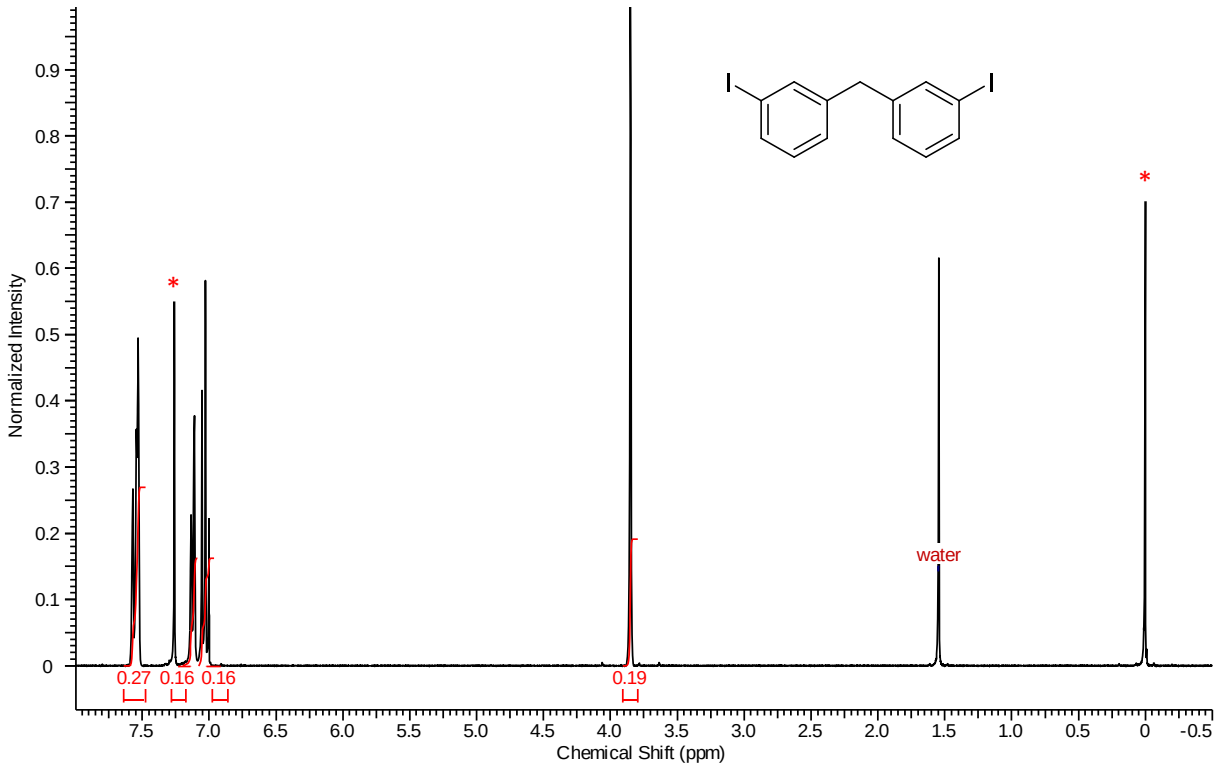
^{1}H NMR hexakis(3,5-dimethylpyrazolyl)[3]radialene (**1**) $CDCl_3$/TMS



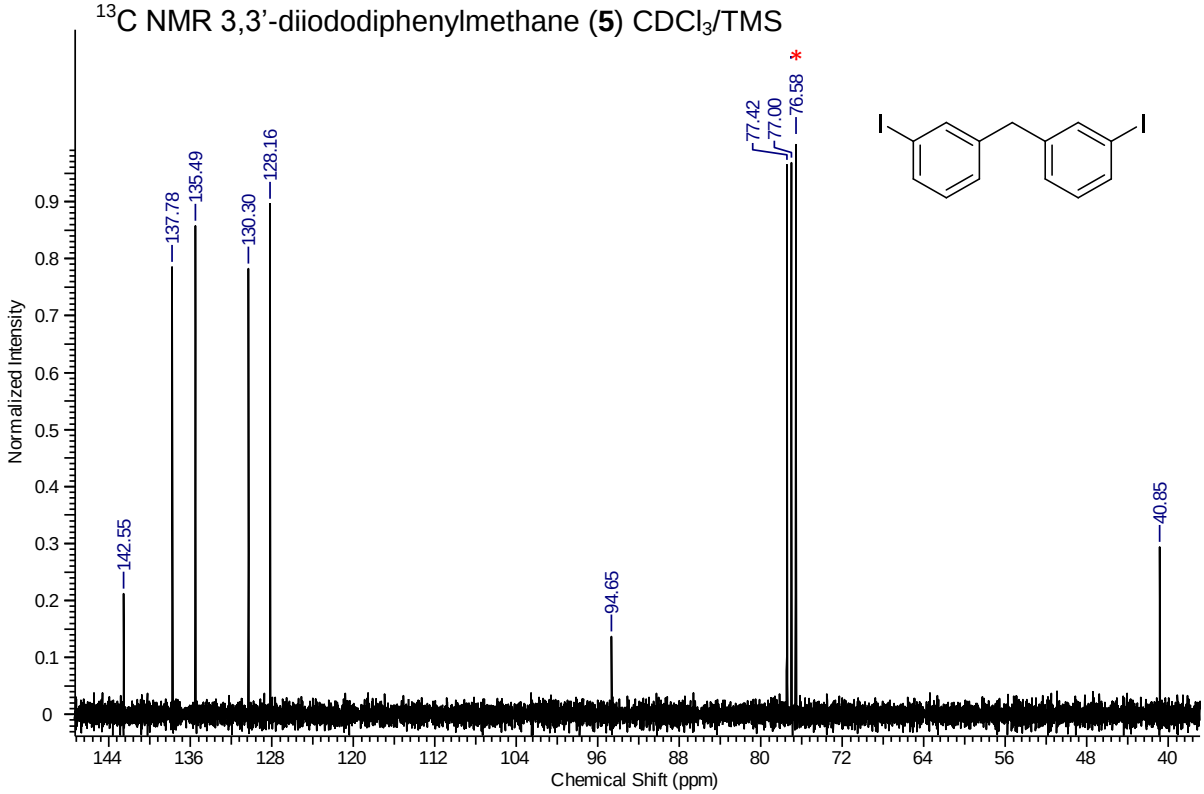
^{13}C NMR hexakis(3,5-dimethylpyrazolyl)[3]radialene (**1**) $CDCl_3$/TMS



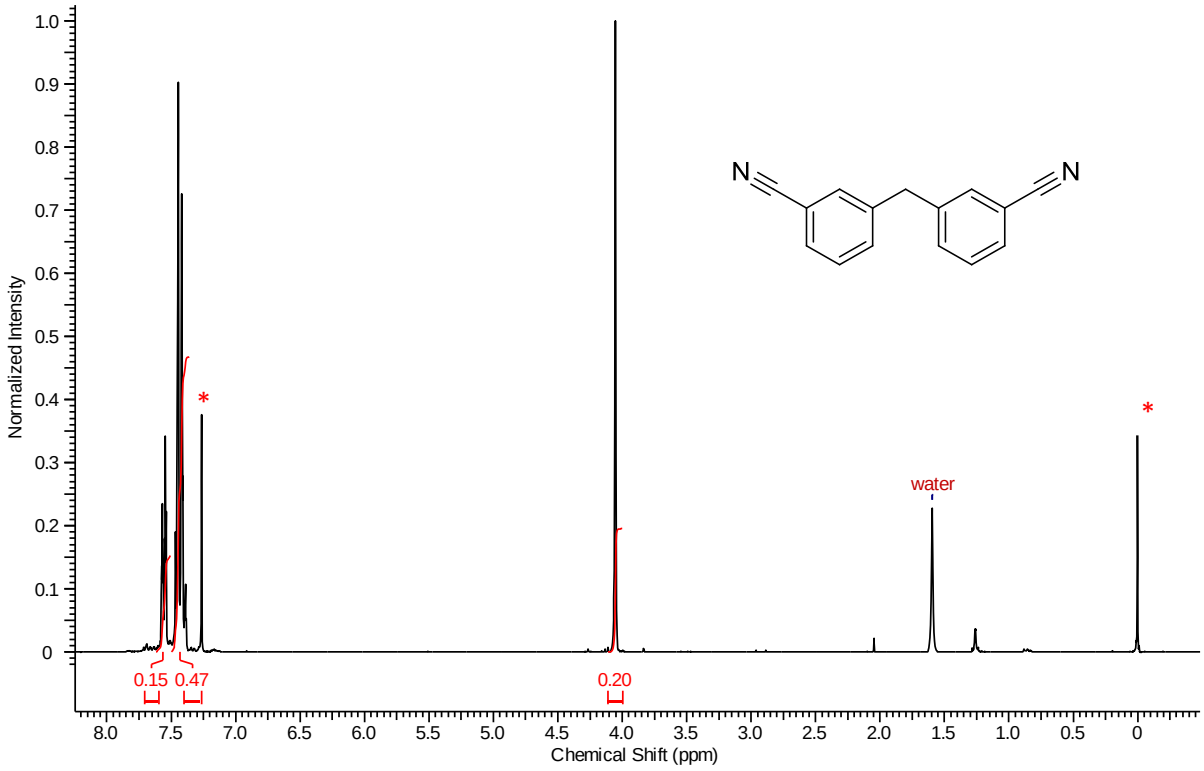
^{1}H NMR 3,3'-diiododiphenylmethane (**5**) $CDCl_3$/TMS



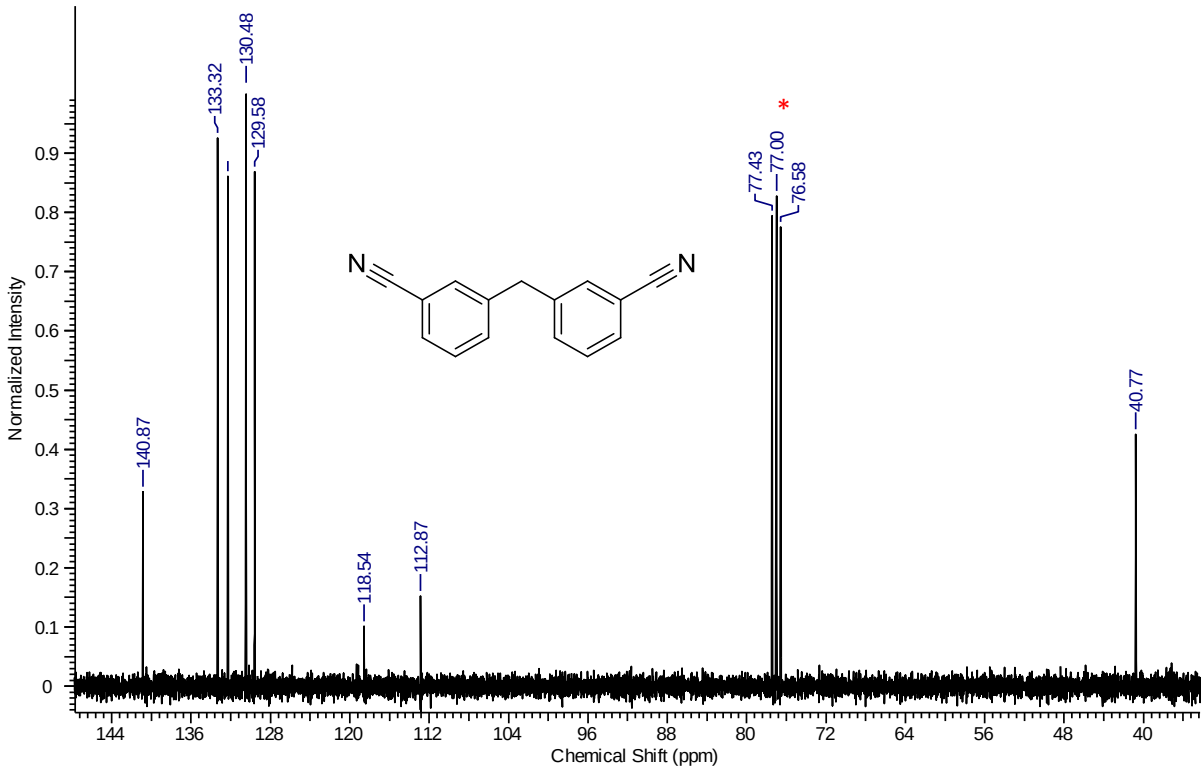
^{13}C NMR 3,3'-diiododiphenylmethane (**5**) $CDCl_3$/TMS

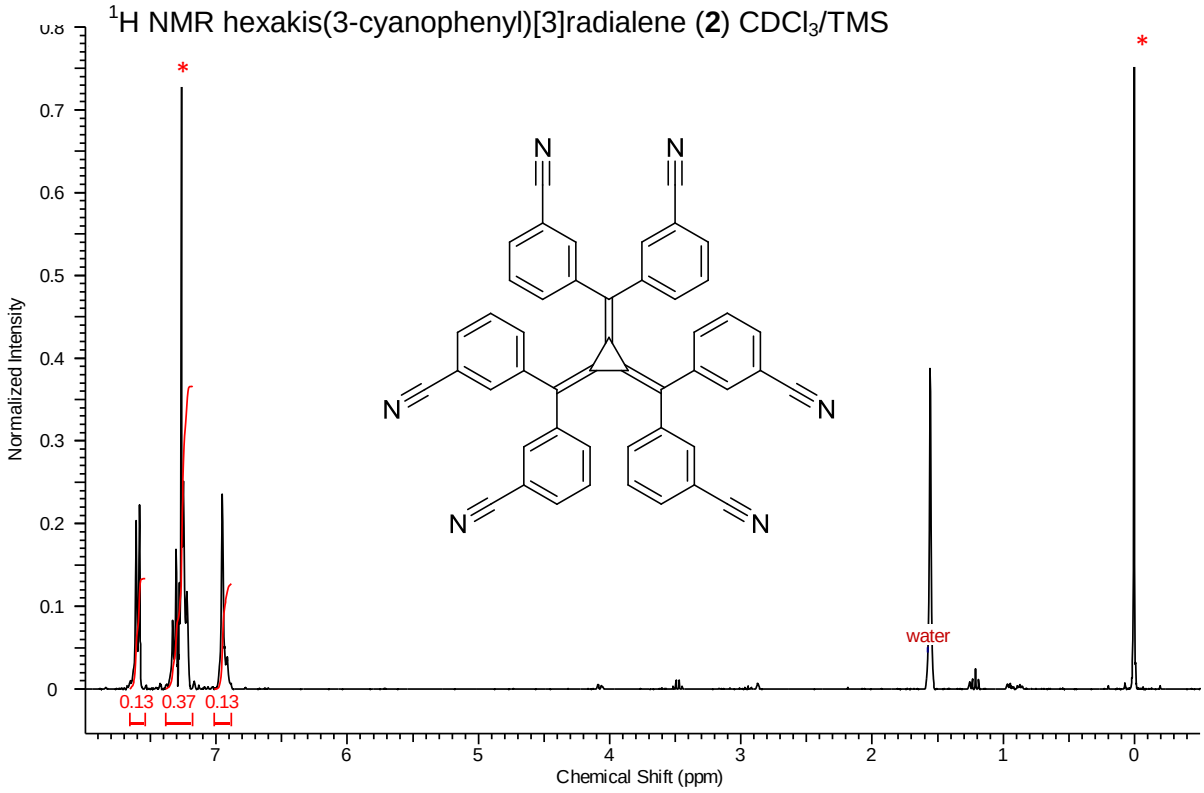


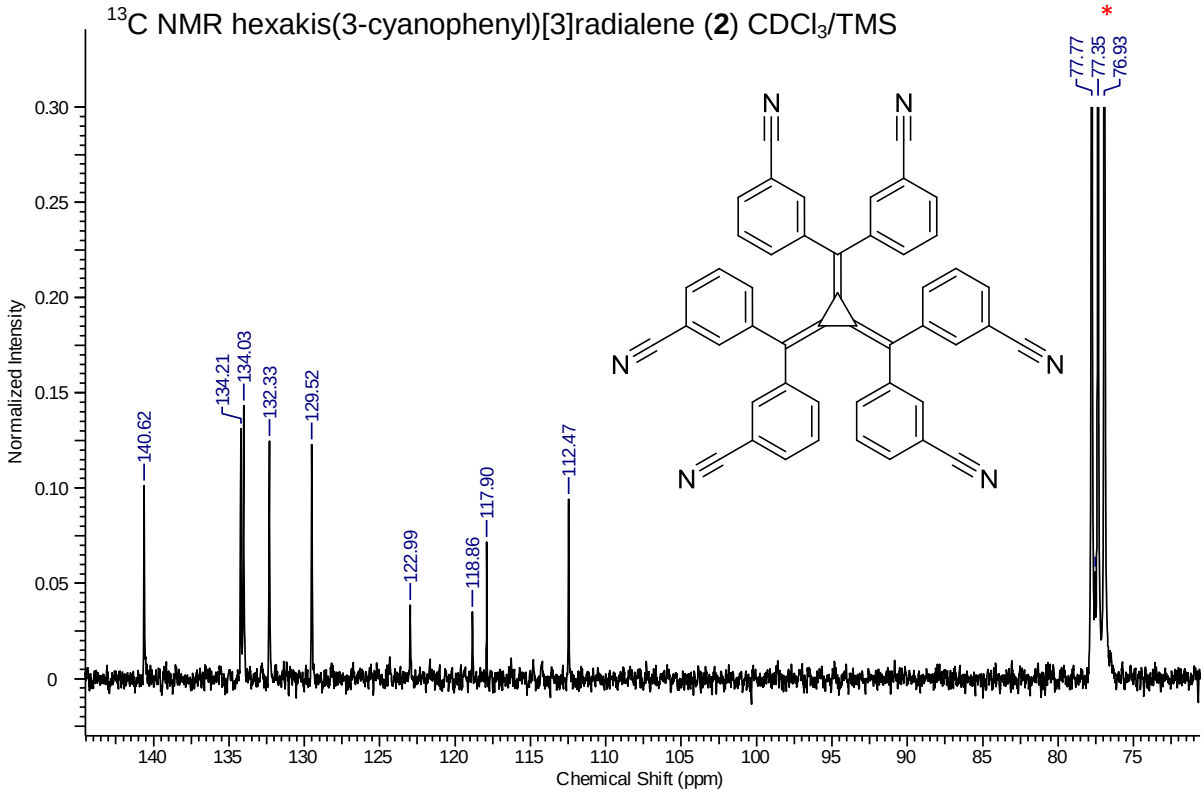
^{1}H NMR 3,3'-dicyanodiphenylmethane (**6**) $CDCl_3$/TMS

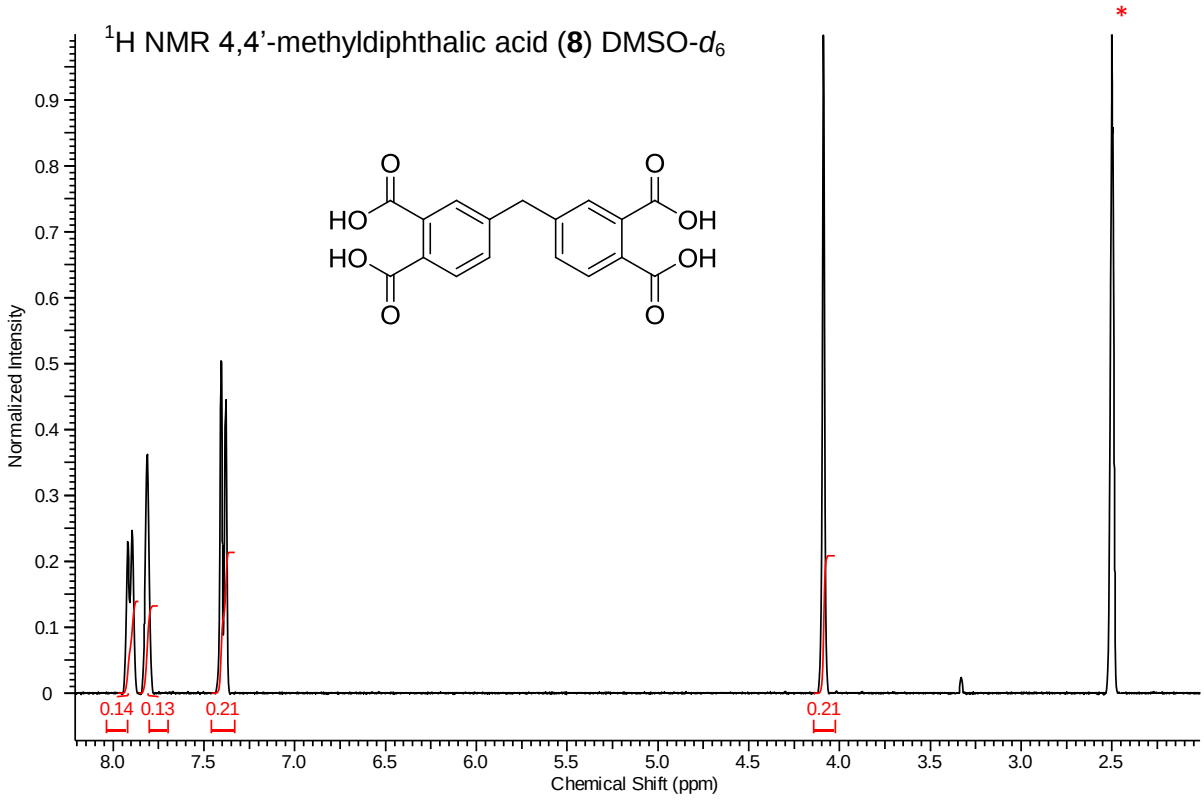


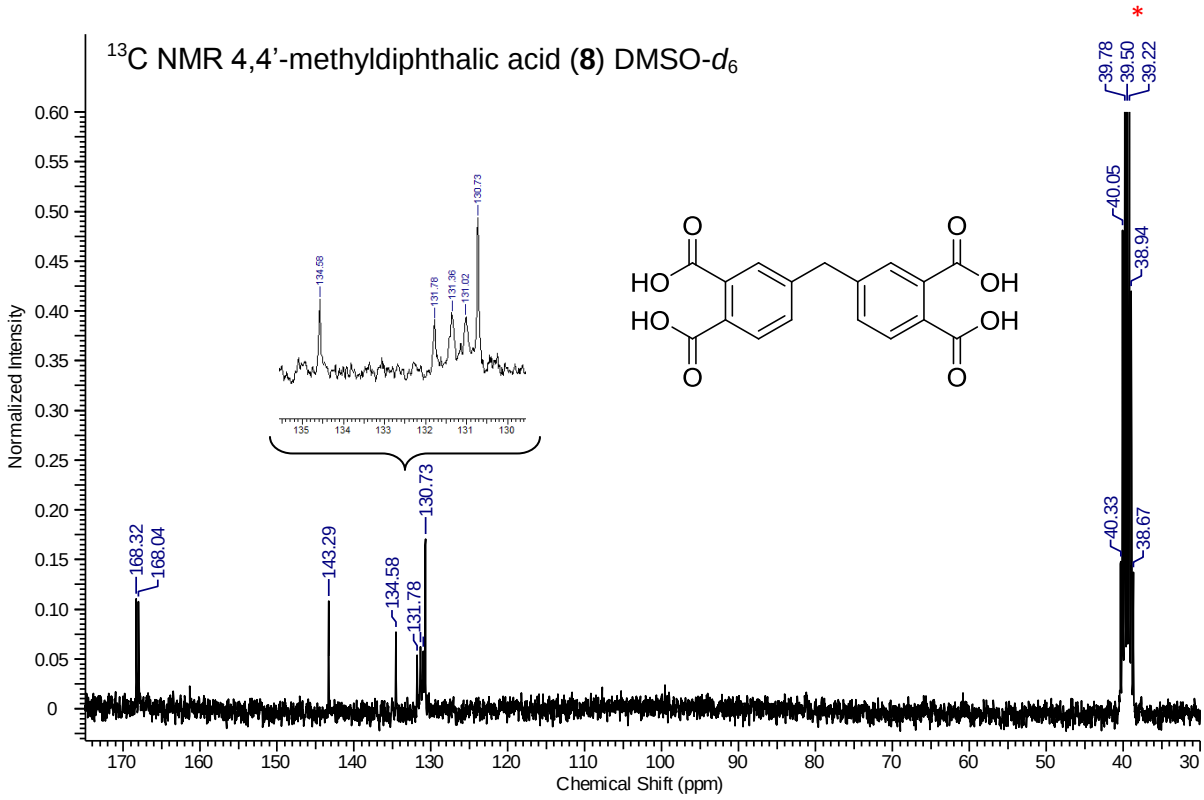
^{13}C NMR 3,3'-dicyanodiphenylmethane (**6**) $CDCl_3$/TMS



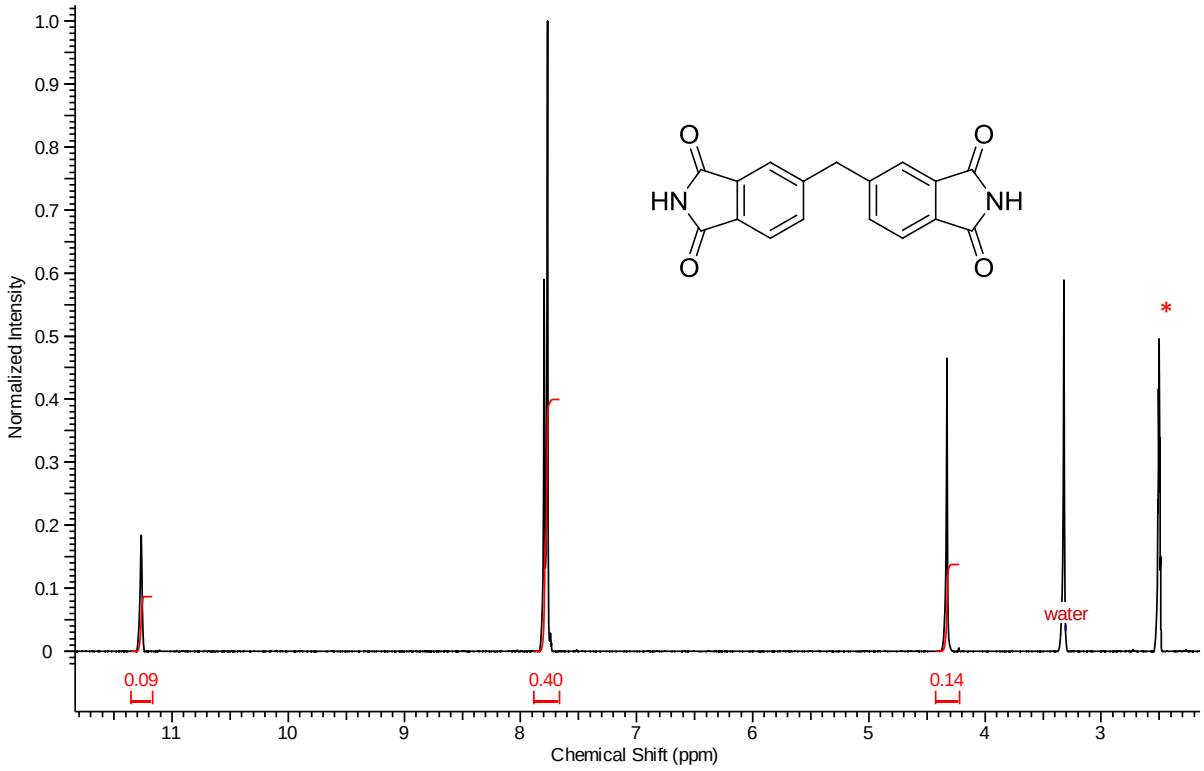

^{1}H NMR hexakis(3-cyanophenyl)[3]radialene (**2**) $CDCl_3$/TMS
Normalized Intensity
Chemical Shift (ppm)
water
0.13
0.37
0.13
*
*


^{13}C NMR hexakis(3-cyanophenyl)[3]radialene (**2**) $CDCl_3$/TMS
Normalized Intensity
Chemical Shift (ppm)
140.62
134.21
134.03
132.33
129.52
122.99
118.86
117.90
112.47
77.77
77.35
76.93
*

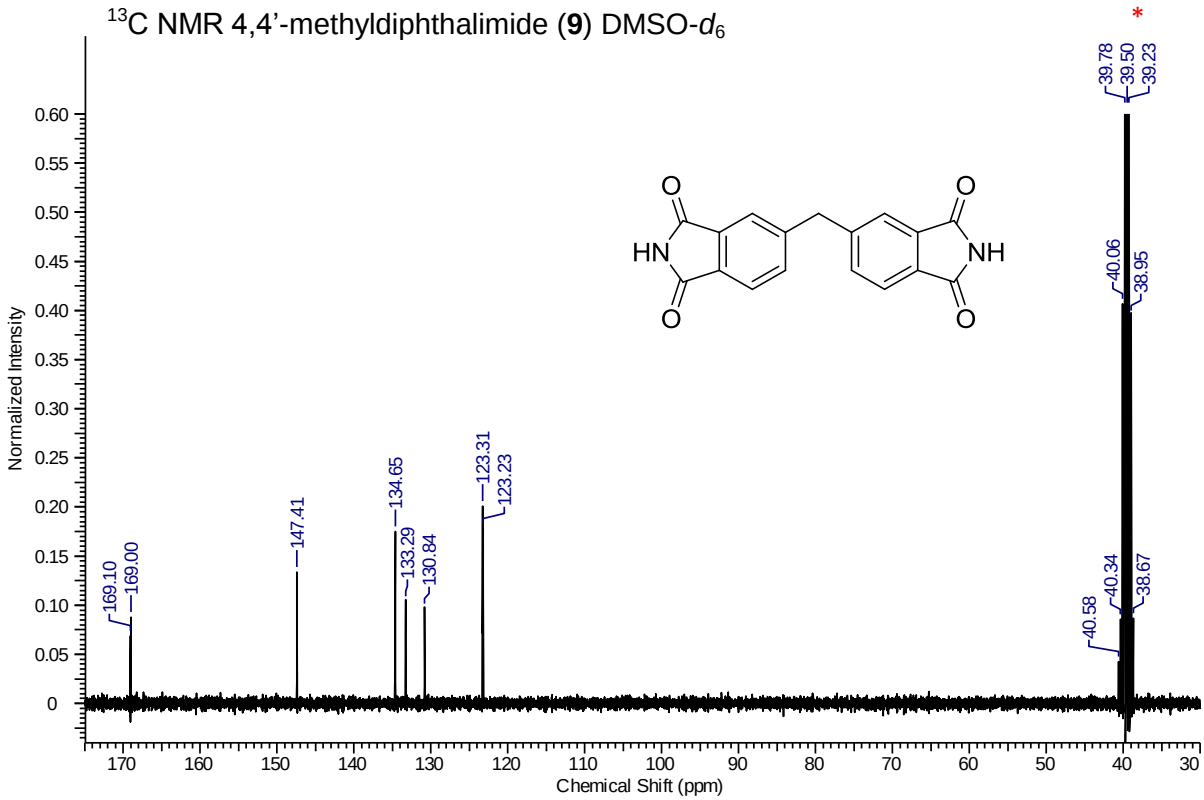

^{1}H NMR 4,4'-methyldiphthalic acid (**8**) DMSO-d_6
*
HO
HO
OH
OH
O
Normalized Intensity
0.14
0.13
0.21
0.21
Chemical Shift (ppm)

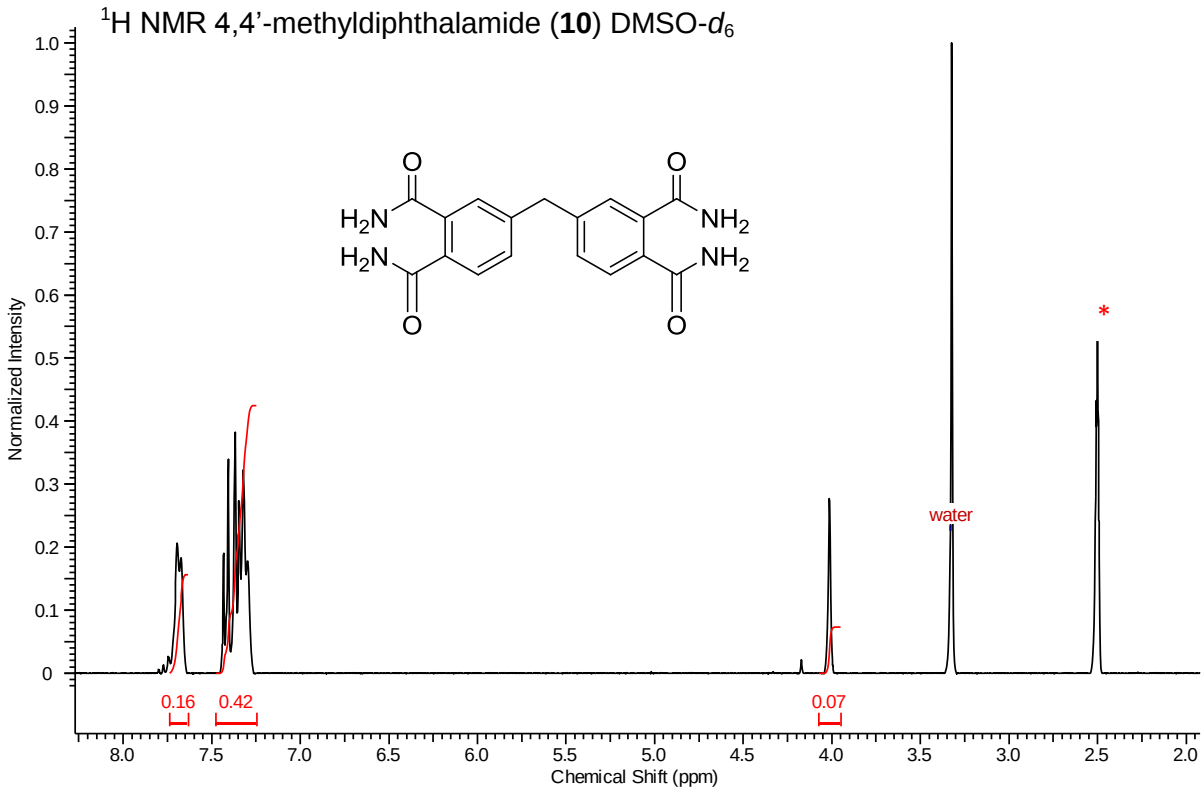

^{13}C NMR 4,4'-methyldiphthalic acid (**8**) DMSO-d_6
*
HO
HO
OH
OH
O
Normalized Intensity
168.32
168.04
143.29
134.58
131.78
130.73
40.33
38.67
40.05
38.94
39.78
39.50
39.22
Chemical Shift (ppm)

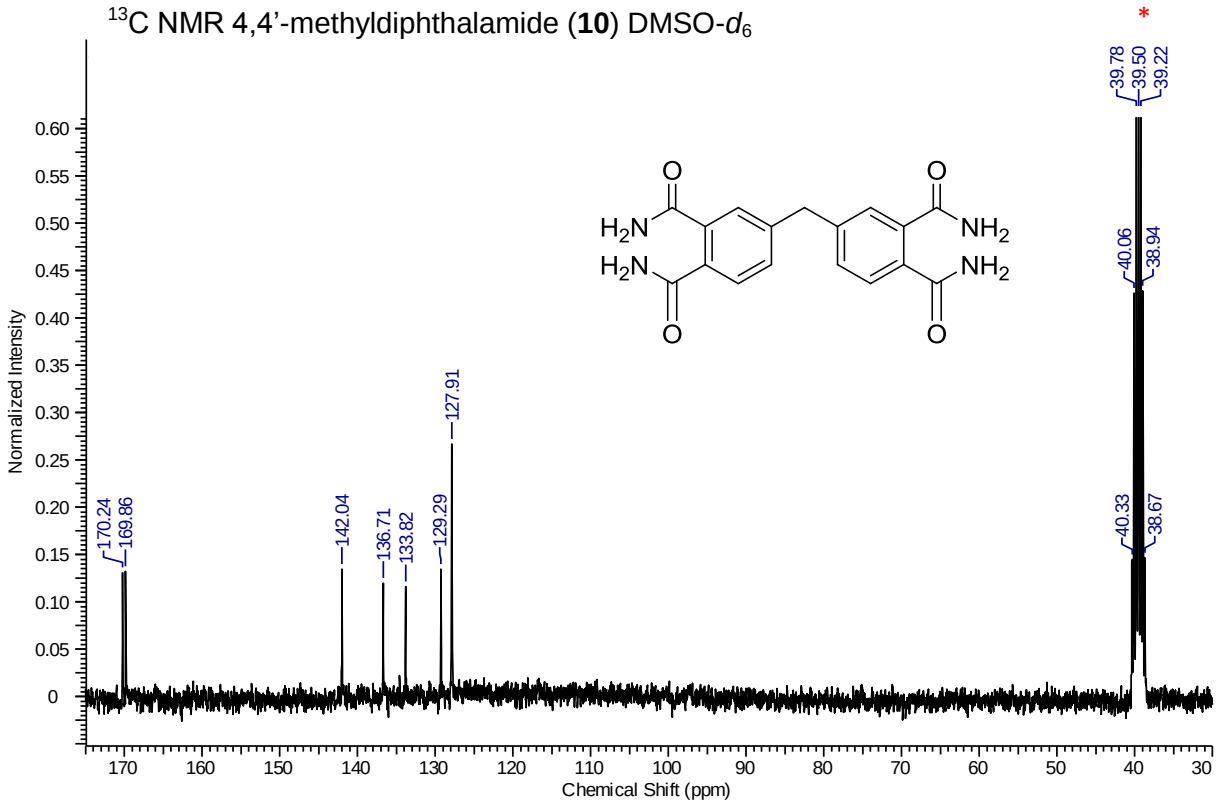
^{1}H NMR 4,4'-methyldiphthalimide (**9**) DMSO-d_6



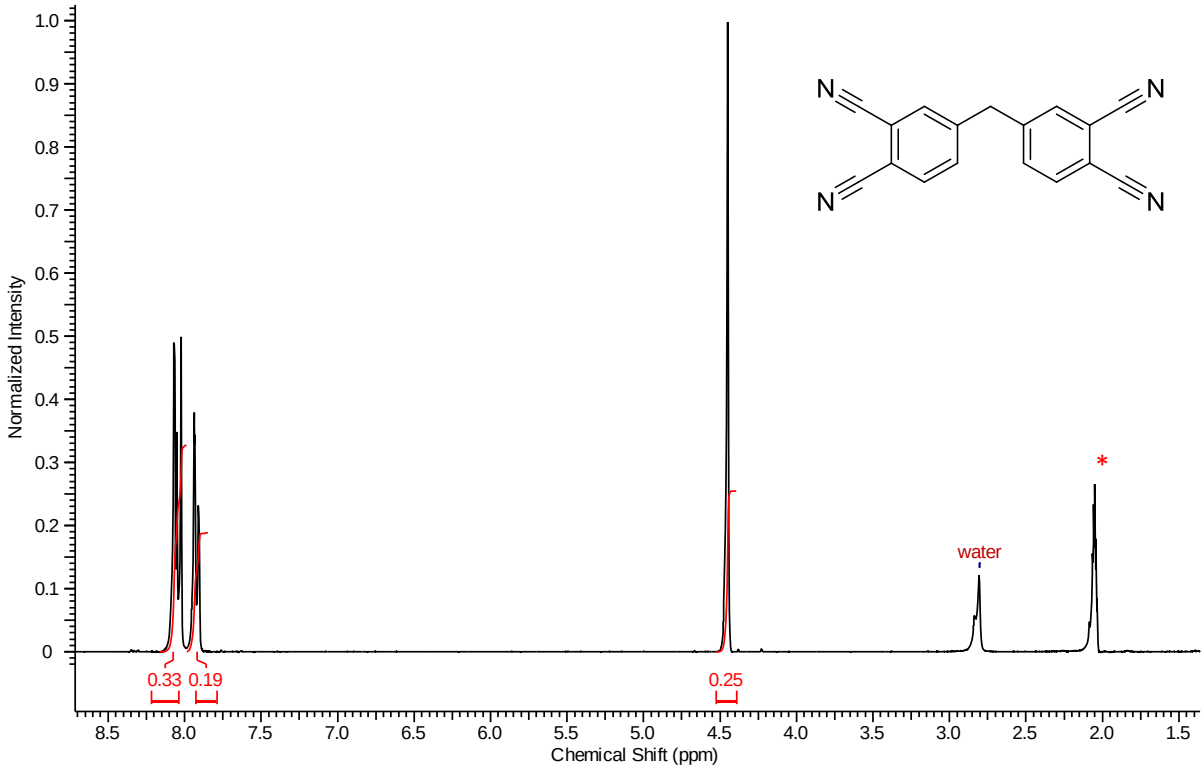
^{13}C NMR 4,4'-methyldiphthalimide (**9**) DMSO-d_6



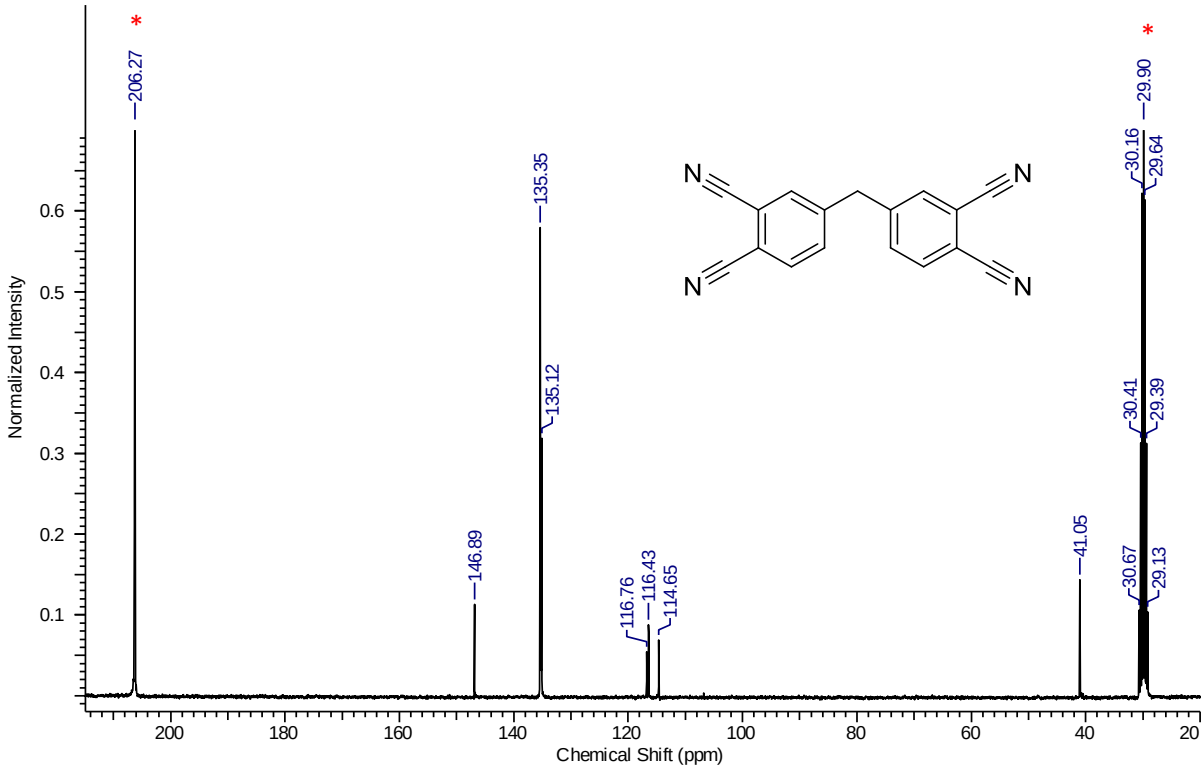

^{1}H NMR 4,4'-methyldiphthalamide (**10**) DMSO-d_6
Normalized Intensity
Chemical Shift (ppm)
water
*
0.16
0.42
0.07

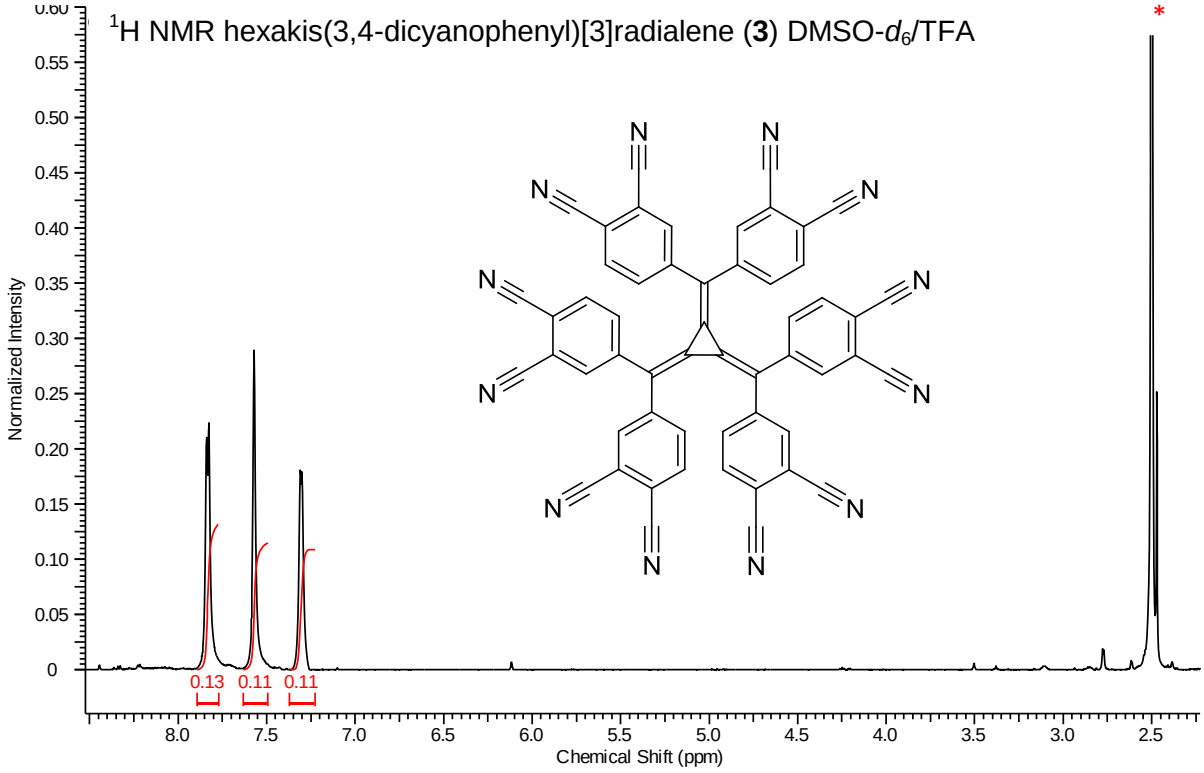

^{13}C NMR 4,4'-methyldiphthalamide (**10**) DMSO-d_6
Normalized Intensity
Chemical Shift (ppm)
*
170.24
169.86
142.04
136.71
133.82
129.29
127.91
39.78
39.50
39.22
40.06
38.94
40.33
38.67

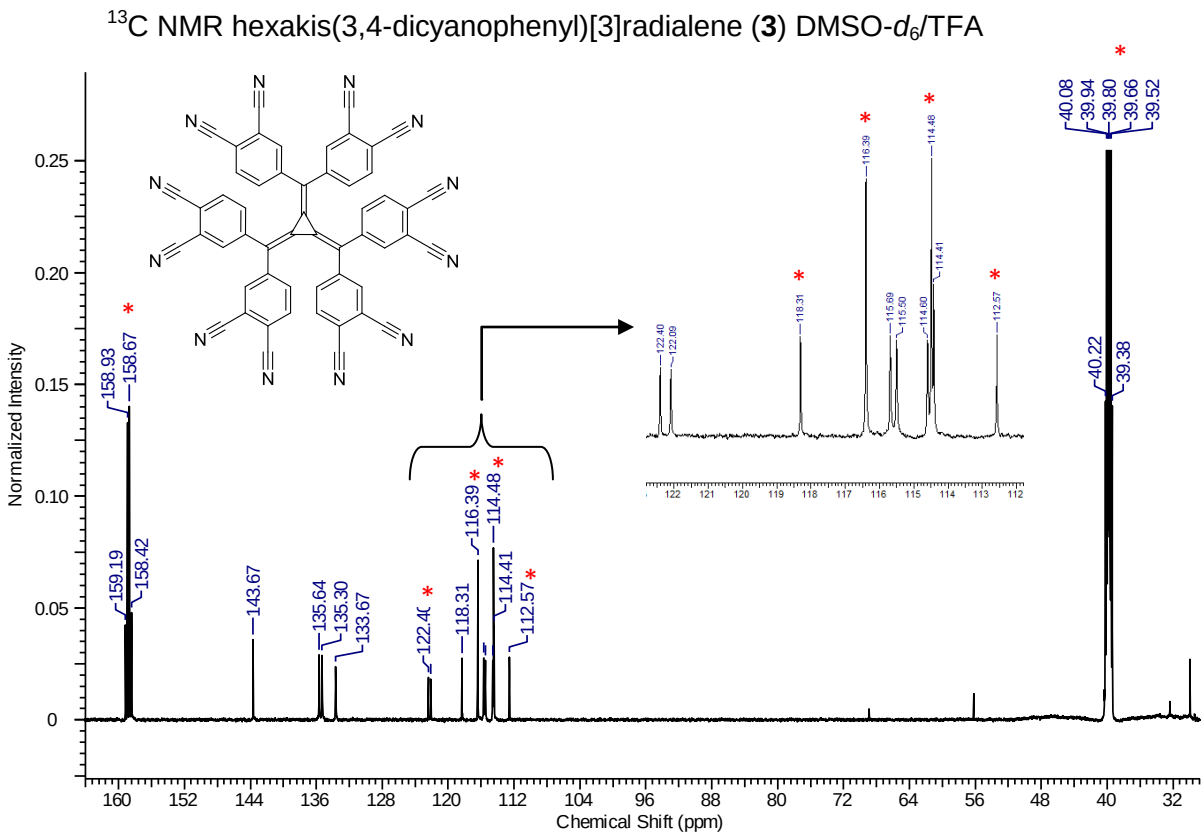
^{1}H NMR 4,4'-methyldiphthalonitrile (**11**) acetone-d_6



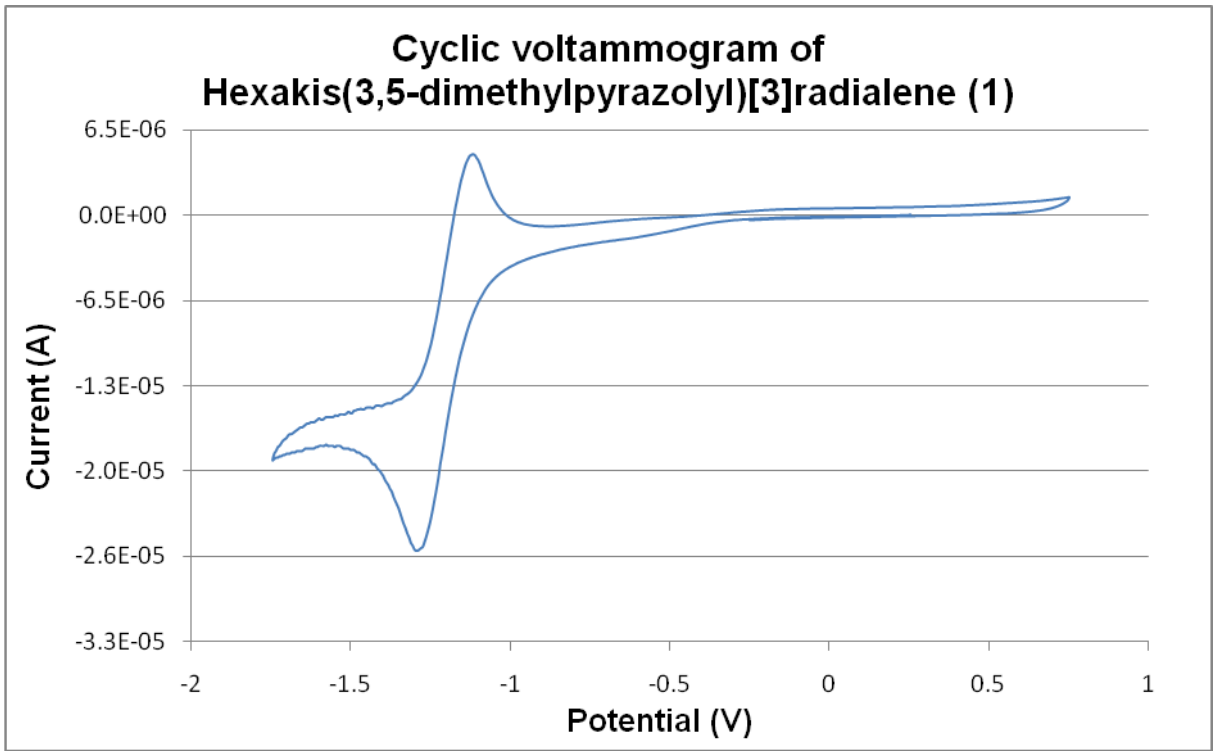
^{13}C NMR 4,4'-methyldiphthalonitrile (**11**) acetone-d_6

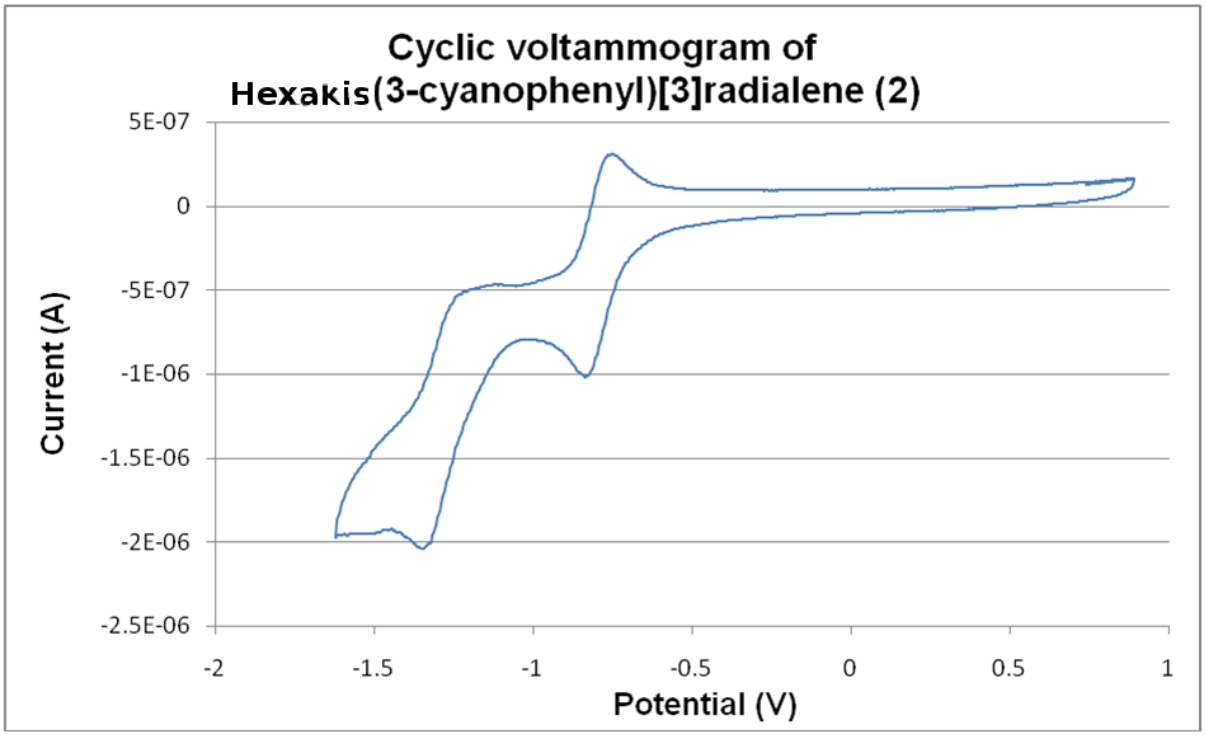


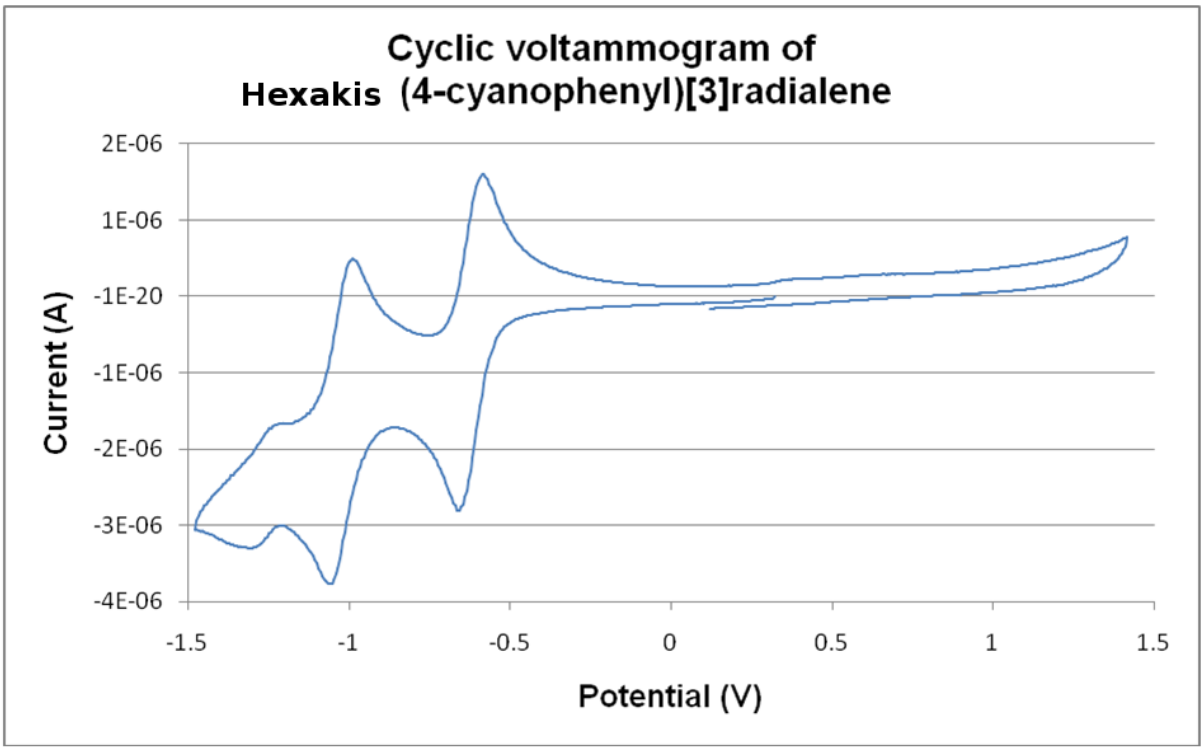

^{1}H NMR hexakis(3,4-dicyanophenyl)[3]radialene (**3**) DMSO-d_6/TFA
Normalized Intensity
Chemical Shift (ppm)
0.13
0.11
0.11
*


^{13}C NMR hexakis(3,4-dicyanophenyl)[3]radialene (**3**) DMSO-d_6/TFA
Normalized Intensity
Chemical Shift (ppm)
158.93
158.67
159.19
158.42
143.67
135.64
135.30
133.67
122.40
118.31
116.39
114.48
114.41
112.57
40.08
39.94
39.80
39.66
39.52
40.22
39.38
*

Cyclic voltammograms of hexaaryl[3]radialenes






Cyclic voltammogram of
Hexakis (4-cyanophenyl)[3]radialene
2E-06
1E-06
-1E-20
-1E-06
-2E-06
-3E-06
-4E-06
Current (A)
-1.5
-1
-0.5
0
0.5
1
1.5
Potential (V)

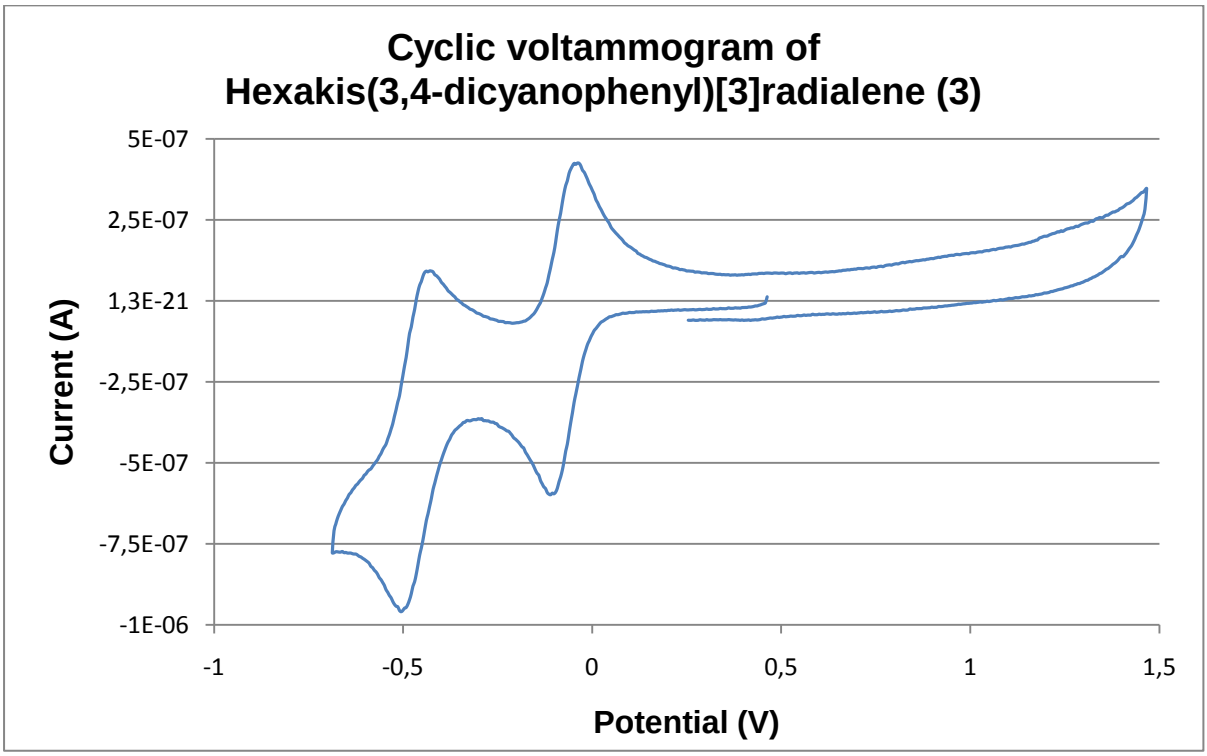

Cyclic voltammogram of
Hexakis(3,4-dicyanophenyl)[3]radialene (3)
5E-07
2,5E-07
1,3E-21
-2,5E-07
-5E-07
-7,5E-07
-1E-06
Current (A)
-1
-0,5
0
0,5
1
1,5
Potential (V)

Table 1: Crystal data and structure refinement for 3.

Empirical formula	$C_{56}H_{21}N_{13}$	
Formula weight	875.86	
Temperature	150(2) K	
Wavelength	0.7107 Å	
Crystal system	Monoclinic	
Space group	$P2_1/c$	
Unit cell dimensions	a = 13.7345(13) Å	α = 90°
	b = 12.6611(9) Å	β = 93.942(8)°
	c = 25.128(2) Å	γ = 90°
Volume	4359.3(6) Å3	
Z	4	
Density (calculated)	1.335 Mg/m^3	
Absorption coefficient	0.084 mm^{-1}	
F(000)	1792	
Crystal size	0.150 × 0.128 × 0.040 mm^3	
Theta range for data collection	2.67 to 23.26°	
Index ranges	−15<=h<=15, −14<=k<=14, −27<=l<=27	
Reflections collected	28680	
Independent reflections	6241 [R_{int} = 0.1149]	
Completeness to theta = 23.26°	99.9%	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	1.00000 and 0.84680	
Refinement method	Full-matrix least-squares on F2	
Data / restraints / parameters	6241/0/623	
Goodness-of-fit on F2	1.025	
Final R indices [I>2sigma(I)]	R_1 = 0.0682, wR_2 = 0.1296	
R indices (all data)	R_1 = 0.1324, wR_2 = 0.1608	
Largest diff. peak and hole	0.362 and −0.320 e.$Å^{-3}$	