Supporting Information (SI)

2-Amino-aldononitriles: From Potential Prebiotic Synthons to Useful Chiral Scaffolds. A Synthetic and Structural Reinvestigation

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Summary

Table S1. Selected IR and Raman data for some acyl aminonitriles in the solid state.[a,b]

Comp	$\overline{\nu}_{NH}$[b]	$\overline{\nu}_{C\equiv N}$[b]	$\overline{\nu}_{C\equiv N}$[c]	$\overline{\nu}_{C=O}$[b,d]	$\overline{\nu}_{C=O}$[c,d]	$\overline{\nu}_{C=O}$[b,e]	$\overline{\nu}_{C=O}$[c,e]	δ_{NH}[b,f]
11		2239	2239	1755	1736	1649	1645	
13		2255	2254	1749	1743	1662	1661	
17	3349	2229		1771, 1747				1509
18		[g]	2250	1730	1732	1655	1658	
20		[g]	2246	1742, 1720	1716	1639	1639	
37		2247		1754		1672		
38		2240[h]		1750		1670		
42	3347	2239	2236	1763, 1743	1737			
43		2237	2243	1765, 1744	1751	1673	1671	
47	3237	2243	2243	1753, 1730	1753, 1728	1675, 1645	1643	1541
51	3278	2251	2245	1743	1734	1690, 1674	1679	1503

[a]In cm^{-1}; [b]IR (KBr disc); [c]Raman; [d]Ester; [e]Amide band I; [f]Amide band II; [g]Not observed; [h]Imperceptible.

Table S2. ^{1}H NMR data (δ, ppm) for some acyl aminonitriles.[a]

Compo	H-2	H-3	H-4	H-5	H-6	H-6´	H-7	H-7´	NCH_2	NH
11	5.48 d	5.57 t	5.57 t	5.11 m[c]	4.27 dd	4.07dd	--	--	3.41 m	--
12[b]	5.34 d	5.60 t	5.60 t	5.14 m[c]	4.27 dd	4.07dd	--	--	3.25 m	--
13	5.38 d	5.57 d	5.44 dd	5.40 d	5.23 dd	--	4.28 dd	3.85 dd	3.39 m	--
17	4.52 dd	5.62 dd	5.46 dd	5.40 dd	5.30 m[c]	--	4.37 dd	4.10 dd	--	4.11 d
18	5.76 bs	6.12 m	6.12 m	6.04 m	5.91 bs	--	4.60 dd	4.48 dd	3.36 m[d]	--
20	5.98 dd	6.54 bs	6.07 t	6.54 bs	5.85 m[c]	--	4.79 dd	4.48 dd	3.55 m[e]	--
37	5.38 d	5.53 d	5.58 d	5.32 dd	5.23 m	--	4.29 dd	3.86 dd	4.58 m[f]	--
38*Z*[i]	5.62 d	5.68 m	5.50 m	5.50 m	5.02 m		4.17 m	4.17 m	4.70 m[g]	
38*E*[i]	3.99 d	5.23 dd	5.73 dd	5.19 dd	5.02 m		4.32 dd	4.16 dd	3.94 m[h]	
42	4.72 dd	5.25 dd	5.60 dd	5.28 m[c]	4.26 m	4.26 m				4.60 d
43	5.73 d	5.68 dd	5.53 dd	5.09 m[c]	4.27 dd	4.04dd				
47[b]	5.47 dd	5.14 dd	5.39 dd	5.19 dt	4.25 m	4.25 m				6.77 d
51	5.47 dd	4.91 dd	5.44 dd	5.26 dd	5.39 m[c]		4.26 dd	3.85 dd		6.67 d

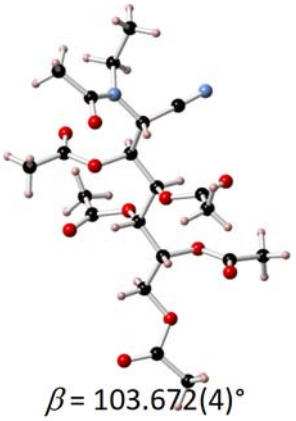
[a]In $CDCl_3$ at 500 MHz; [b]In $CDCl_3$ at 400 MHz; [c]m = ddd; [d]m = 3.47 m + 3.25 m; [e]m = 3.60 m + 3.49 m; [f]m= 4.67 d + 4.44 d; [g]dd = 4.82 d + 4.58 d; [h]dd = 4.08 d + 3.80 d; [i]In $CDCl_3$ at 200 MHz.

Table S3. ^{13}C NMR data (δ, ppm) for some acyl aminonitriles.[a]

Compound	C≡N	C-2	C-6	C-7	NCH_2	NC=O	Me[d]
11	114.57	45.37	61.35		42.83		
12[b]	114.70	45.94	61.57		50.21		
13	114.70	45.18		61.74	42.91		
17	116.67	47.01		61.60			
18	114.62	47.16		62.56	42.73		
20	114.60	47.38		62.32	43.26		
37	114.32	46.81		61.89	51.78	171.62	21.81
38*Z*[c]	116.94	49.35		61.26		172.06	21.76
38*E*[c]	114.42	46.92		61.10			
42	116.54	45.78	61.27				
43	114.25	49.05	61.38			170.91	22.42
47[b]	115.73	39.23	61.38				
51	115.75	38.97		61.90		173.01	22.95

[a]In $CDCl_3$ at 125 MHz; [b]In $CDCl_3$ at 100 MHz; [c]In $CDCl_3$ at 50 MHz; [d]Acetamido group.

Table S4. Crystal data and structure refinement details of **13**



Identification code	**2011acc0771**
Empirical formula	$C_{21}H_{30}N_2O_{11}$
Formula weight	486.47
Temperature	100(2) K
Wavelength	0.71075 Å
Crystal system	Monoclinic
Space group	$P2_1$
Unit cell dimensions	a = 8.689(2) Å
	b = 12.613(3) Å
	c = 11.114(3) Å
Volume	1183.4(5) Å^3
Z	2
Density (calculated)	1.365 Mg / m^3
Absorption coefficient	0.111 mm^{-1}
F(000)	516
Crystal	Fragment; Colourless
Crystal size	0.20 × 0.10 × 0.03 mm^3
θ range for data collection	3.14 – 27.48°
Index ranges	$-11 \le h \le 6$, $-10 \le k \le 16$, $-14 \le l \le 14$
Reflections collected	6306
Independent reflections	2828 [R_{int} = 0.0245]
Completeness to θ = 27.48°	99.5 %
Absorption correction	Semi–empirical from equivalents
Max. and min. transmission	0.9967 and 0.9781
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	2828 / 1 / 314
Goodness-of-fit on F^2	1.038
Final R indices [$F^2 > 2\sigma(F^2)$]	$R1$ = 0.0379, $wR2$ = 0.0855
R indices (all data)	$R1$ = 0.0424, $wR2$ = 0.0877
Largest diff. peak and hole	0.278 and –0.179 e Å^{-3}

Table S5. Crystal data and structure refinement details of **37**

Compound	**2012acc0031**
Formula	$C_{26}H_{32}O_{11}N_2$
$D_{calc.}$/ g cm^{-3}	1.315
m/mm^{-1}	0.103
Formula Weight	548.53
Colour	clear colourless
Shape	needle-shaped
Size/mm^3	0.20×0.20×0.20
T/K	100(2)
Crystal System	monoclinic
Flack Parameter	-0.7(10)
Hooft Parameter	-1.8(10)
Space Group	$C2$
a/Å	19.892(11)
b/Å	6.009(3)
c/Å	23.888(12)
a/°	90
b/°	103.91(3)
g/°	90
V/Å^3	2772(3)
Z	4
Z'	1
Wavelength/Å	0.71073
Radiation type	Mo K_a
Q_{min}/°	2.954
Q_{max}/°	25.026
Measured Refl's.	10256
Indep't Refl's	4095
Refl's I≥2 s(I)	2395
R_{int}	0.0995
Parameters	377
Restraints	648
Largest Peak	0.307
Deepest Hole	-0.209
GooF	1.070
wR_2 (all data)	0.2155
wR_2	0.1730
R_1 (all data)	0.1520
R_1	0.0903

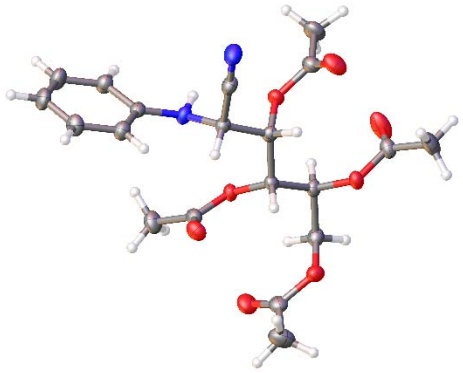


Table S6. Crystal data and structure refinement details of **42.**

Compound	2014acc0004
Formula	$C_{20}H_{24}N_2O_8$
$D_{calc.}$/ g cm^{-3}	1.292
μ/mm^{-1}	0.101
Formula Weight	420.41
Colour	clear colourless
Shape	prism
Max Size/mm	0.32
Mid Size/mm	0.28
Min Size/mm	0.20
T/K	120
Crystal System	monoclinic
Space Group	$P2_1$
a/Å	10.0041(8)
b/Å	10.3736(5)
c/Å	10.8552(7)
α/°	90
β/°	106.375(4)
γ/°	90
V/Å^3	1080.84(12)
Z	2
Z'	1.000
Θ_{min}/°	3.138
Θ_{max}/°	27.101
Measured Refl.	10823
Independent Refl.	4674
Reflections Used	4216
R_{int}	0.0315
Parameters	279
Restraints	1
Largest Peak	0.194
Deepest Hole	-0.245
GooF	1.167
wR_2 (all data)	0.1017
wR_2	0.0892
R_1 (all data)	0.0466
R_1	0.0391

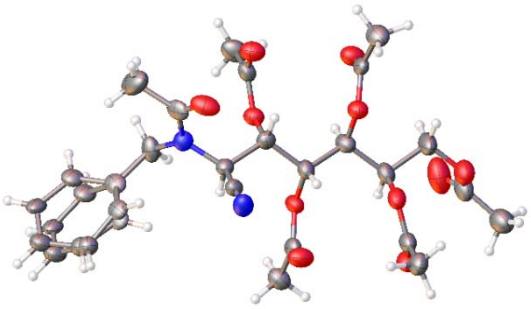
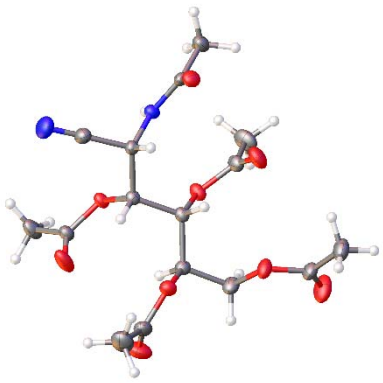


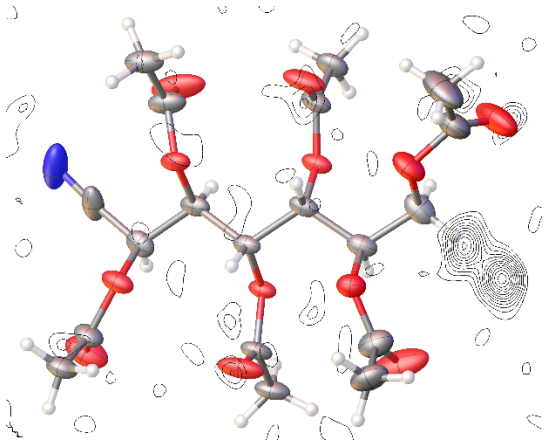
Table S7. Crystal data and structure refinement details of **47**

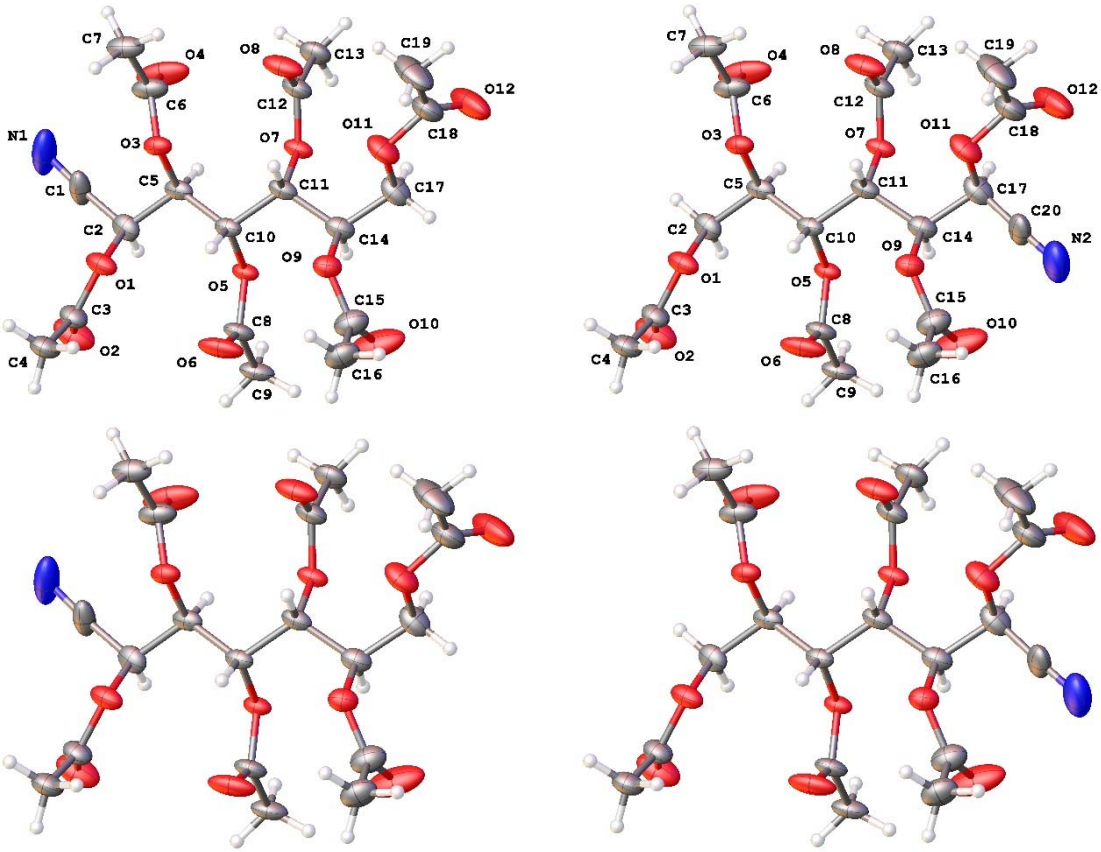


Identification code	adona_0m
Empirical formula	$C_{16}H_{22}N_2O_9$
Formula weight	386.36
Temperature/K	170(2)
Crystal system	Orthorhombic
Space group	$P2_12_12_1$
a/Å	8.3036(3)
b/Å	14.5478(5)
c/Å	15.9656(5)
α/°	90
β/°	90
γ/°	90
Volume/Å^3	1928.63(11)
Z	4
ρ_{calc}g/cm^3	1.331
μ/mm^{-1}	0.11
F(000)	816.0
Crystal size/mm^3	0.2 × 0.18 × 0.12
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	3.78 to 60.38
Index ranges	-11 ≤ h ≤ 11, -11 ≤ k ≤ 20, -22 ≤ l ≤ 18
Reflections collected	12536
Independent reflections	5693 [R_{int} = 0.0281, R_{sigma} = 0.0484]
Data/restraints/parameters	5693/0/250
Goodness-of-fit on F^2	0.804
Final R indexes [I>=2σ (I)]	R_1 = 0.0444, wR_2 = 0.1170
Final R indexes [all data]	R_1 = 0.0617, wR_2 = 0.1334
Largest diff. peak/hole / e Å^{-3}	0.25/-0.21

Table S8. Crystal data and structure refinement details of **63.**

Compound	**2015acc0013_K_100K**
Formula	$C_{19}H_{24}NO_{12}$
$D_{calc.}$/ g cm^{-3}	1.383
m/mm^{-1}	0.117
Formula Weight	458.39
Colour	clear colourless
Shape	block-shaped
Size/mm^3	0.13×0.05×0.02
T/K	100(2)
Crystal System	orthorhombic
Flack Parameter	-0.4(14)
Hooft Parameter	-0.4(14)
Space Group	$P2_12_12_1$
a/Å	8.6244(3)
b/Å	12.0277(4)
c/Å	21.2251(10)
a/°	90.00
b/°	90.00
g/°	90.00
V/Å^3	2201.73(15)
Z	4
Z'	1
Wavelength/Å	0.71073
Radiation type	Mo K_a
Q_{min}/°	3.04
Q_{max}/°	28.70
Measured Refl's.	12046
Indep't Refl's	5634
Refl's I≥2 s(I)	4355
R_{int}	0.0363
Parameters	313
Restraints	0
Largest Peak	0.445
Deepest Hole	-0.305
GooF	1.040
wR_2 (all data)	0.1707
wR_2	0.1575
R_1 (all data)	0.0883
R_1	0.0671





(a) (b)

Solid-state Orientations in the Crystal Structure for Compound 63: Major component (a) and minor component (b), thermal ellipsoids drawn at the 50% probability level.

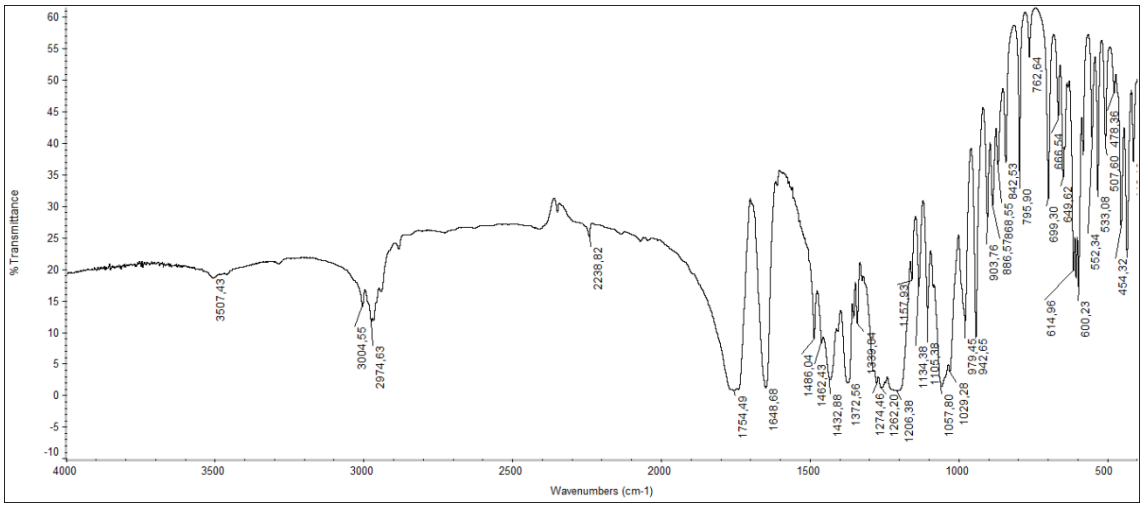


Figure S1. IR spectrum of **11**.

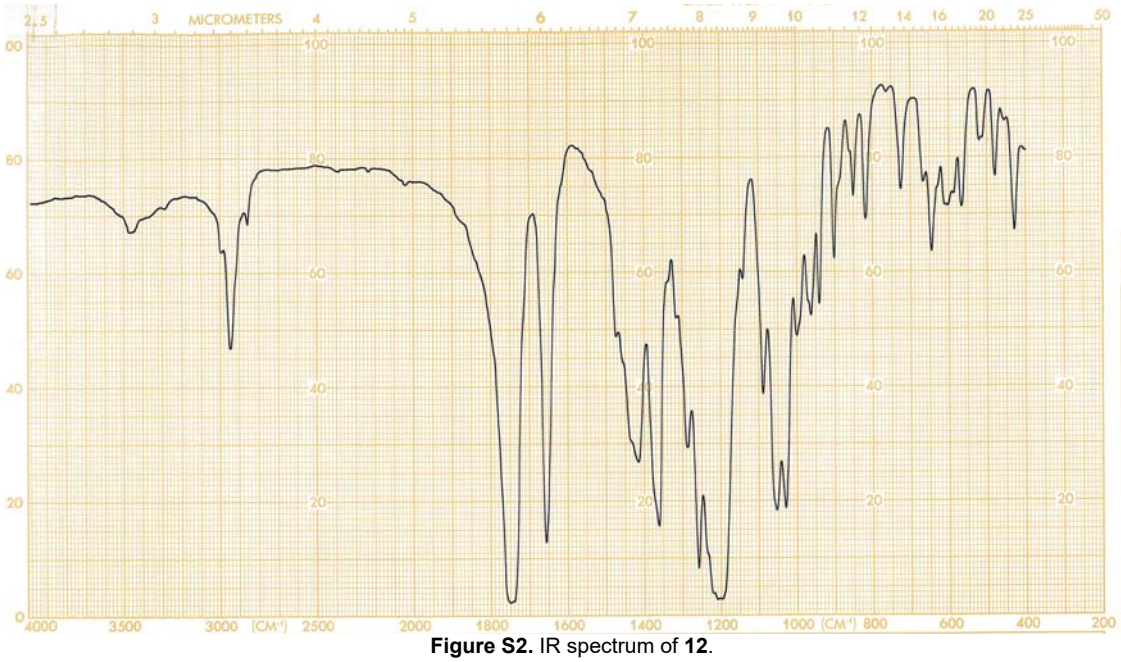


Figure S2. IR spectrum of **12**.

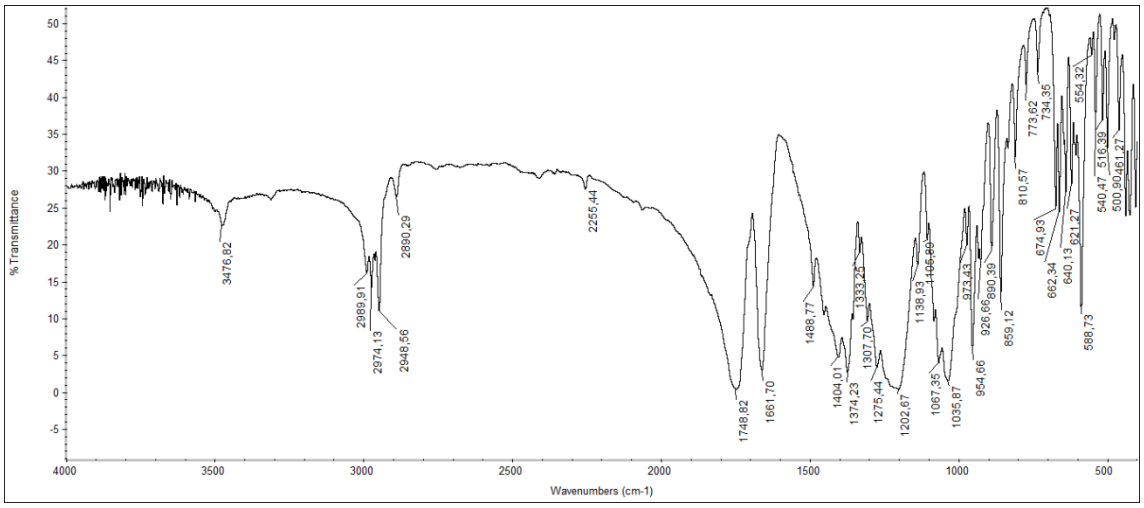


Figure S3. IR spectrum of **13**.

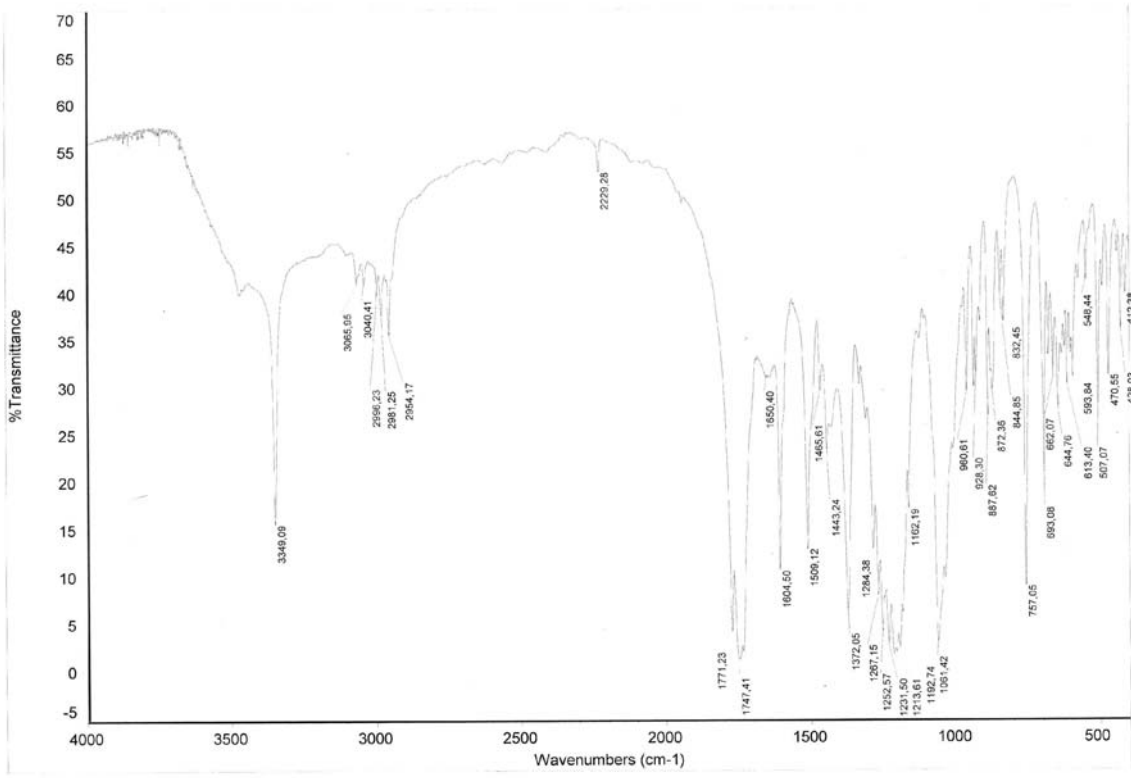


Figure S4. IR spectrum of **17**.

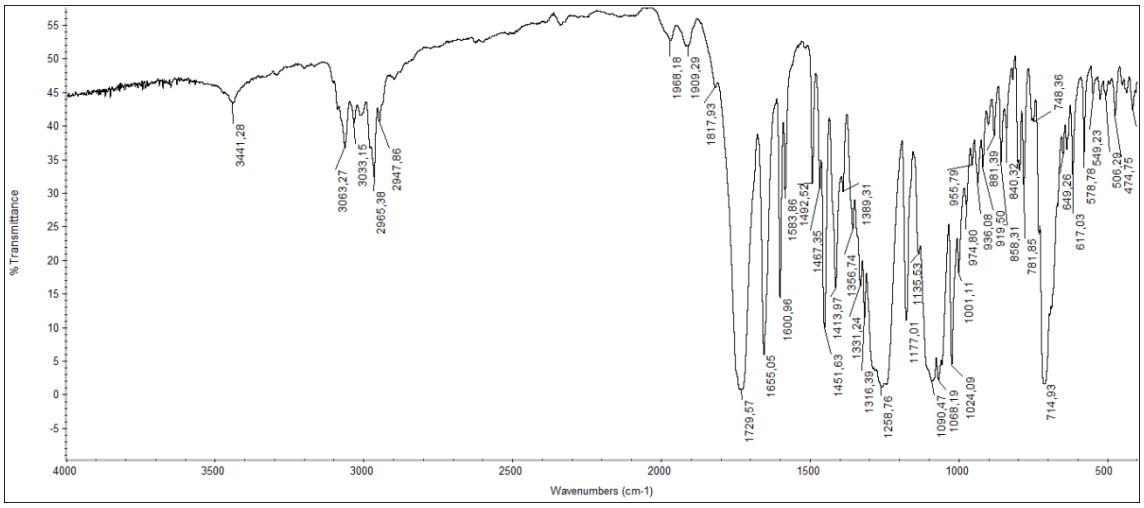


Figure S5. IR spectrum of **18**.

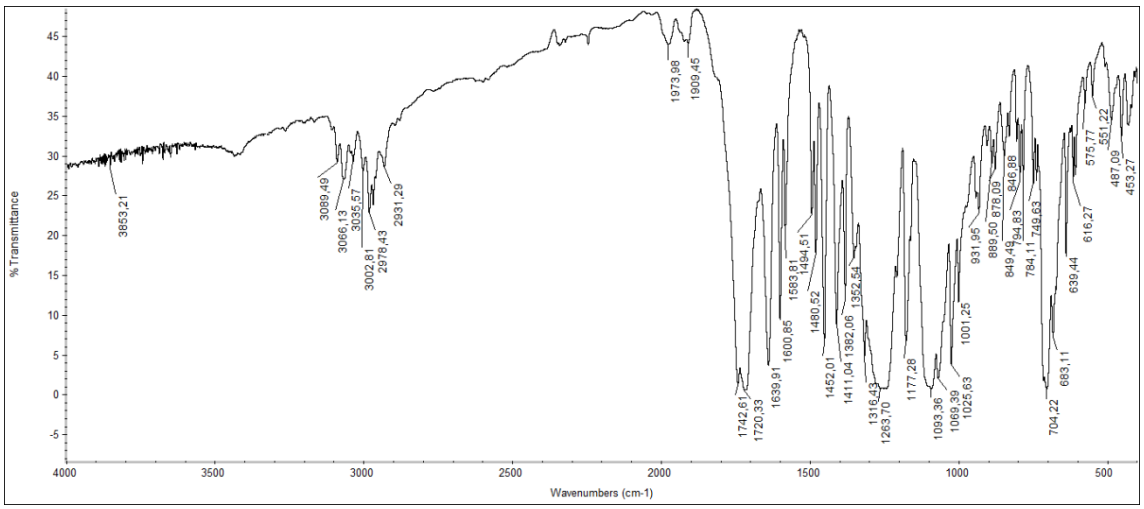


Figure S6. IR spectrum of **20**.

Figure S7. IR spectrum of **26.**

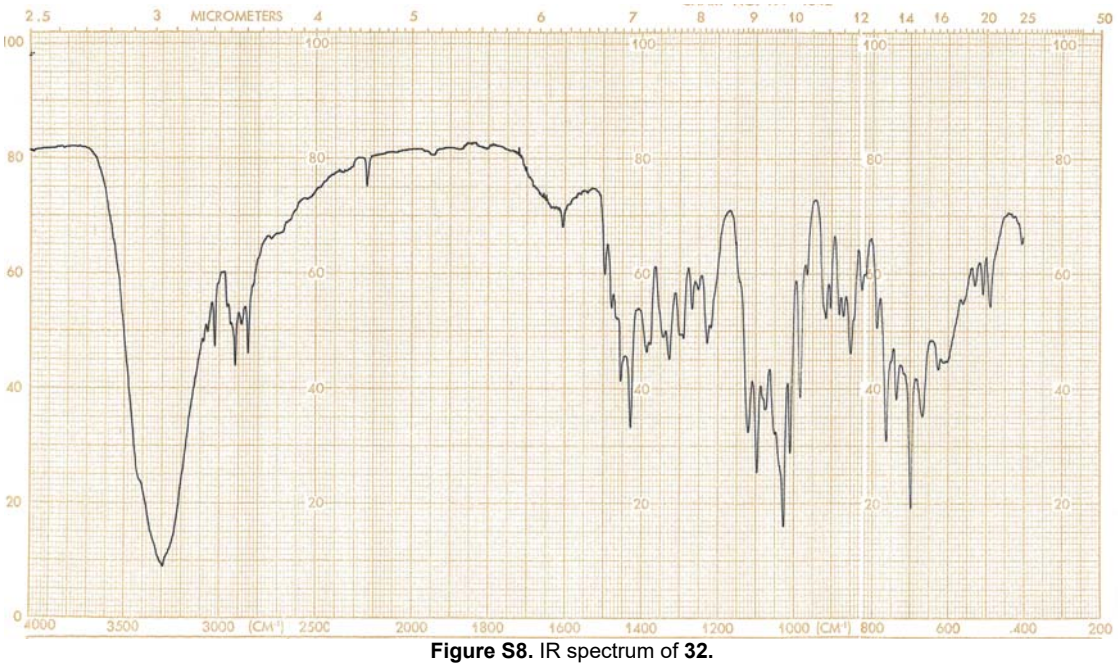


Figure S8. IR spectrum of **32.**

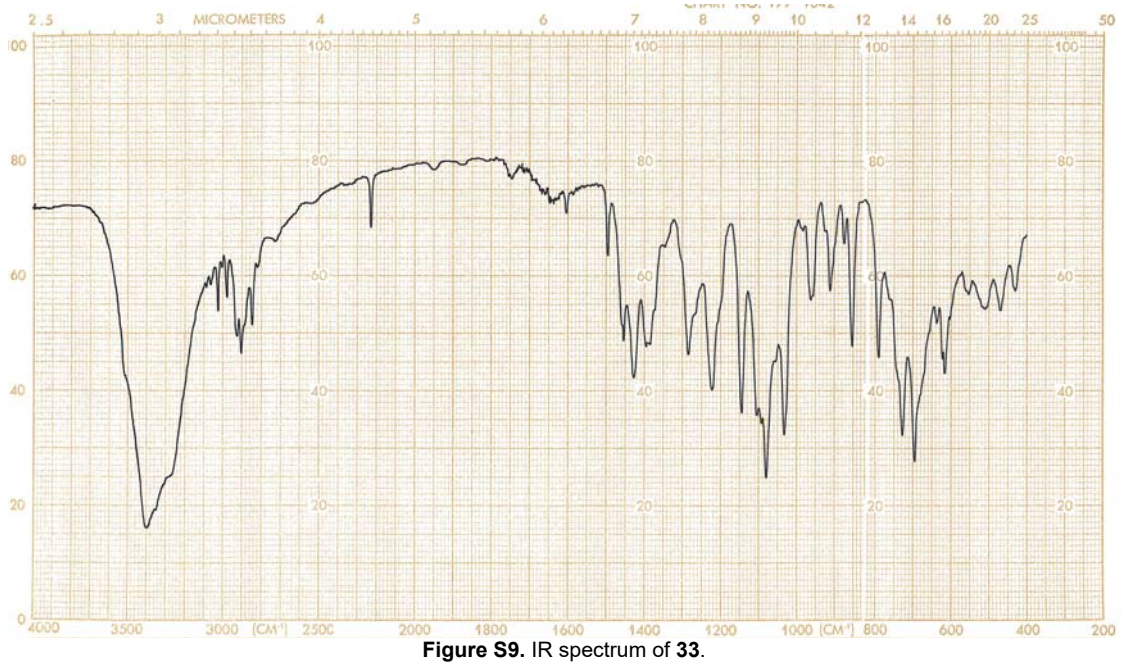


Figure S9. IR spectrum of **33**.

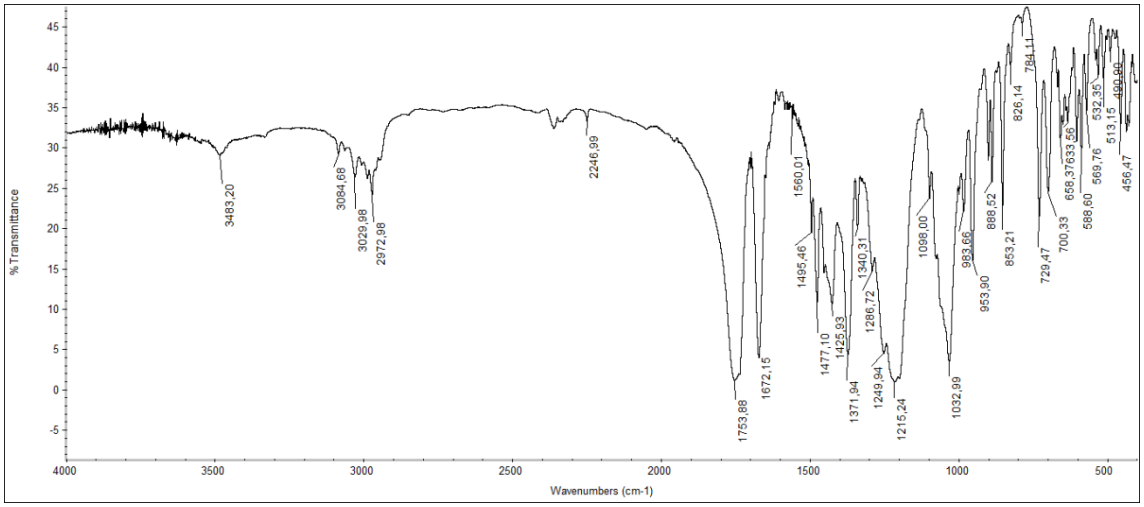


Figure S10. IR spectrum of **37**.

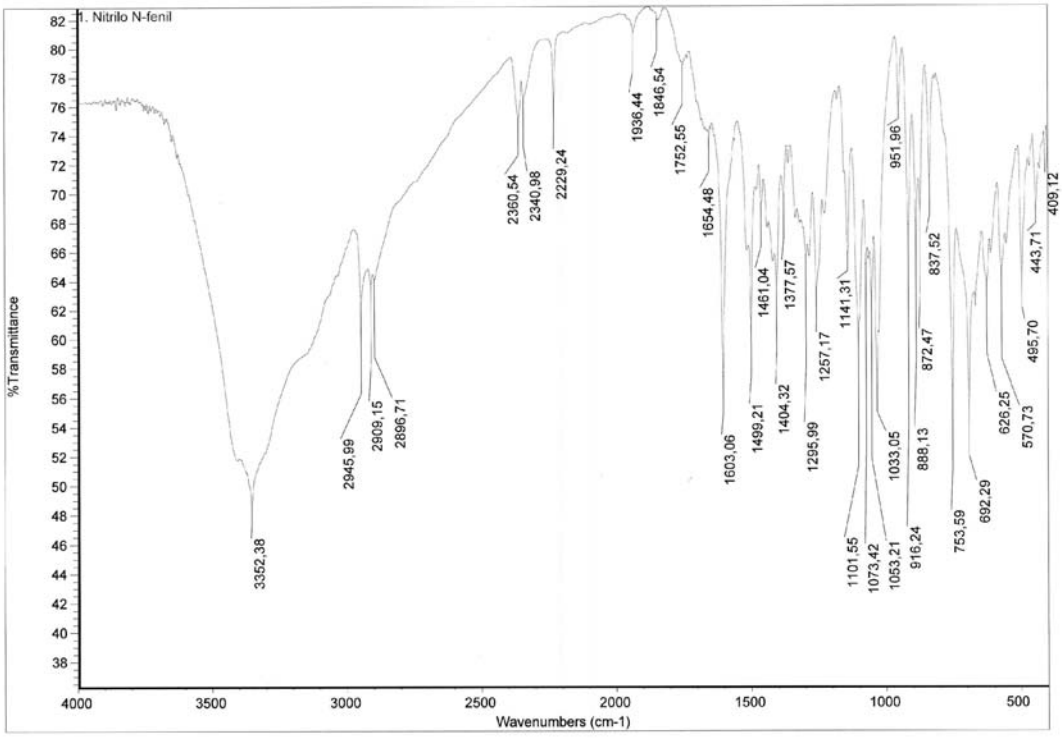


Figure S11. IR spectrum of **41**.

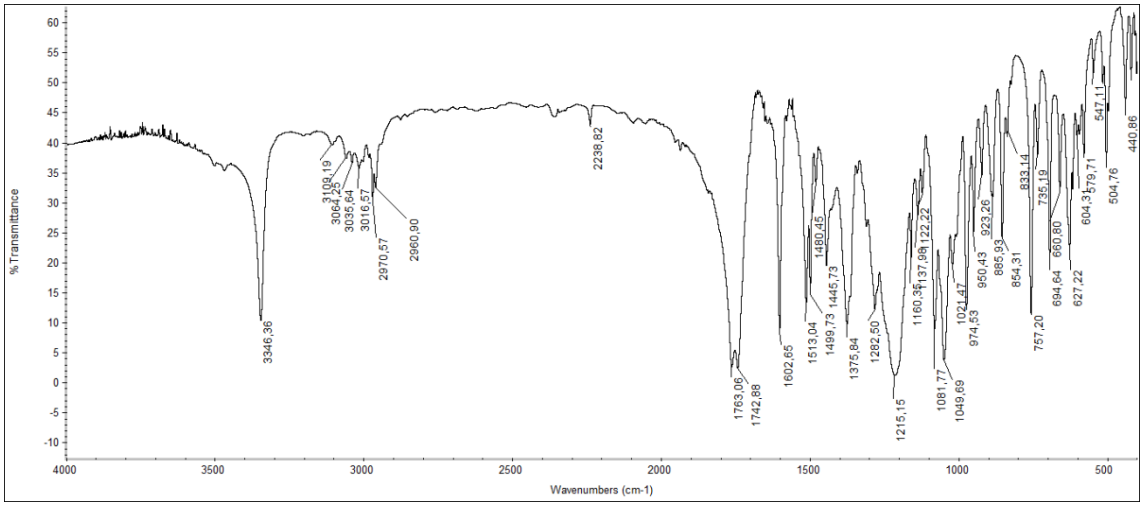


Figure S12. IR spectrum of **42**.

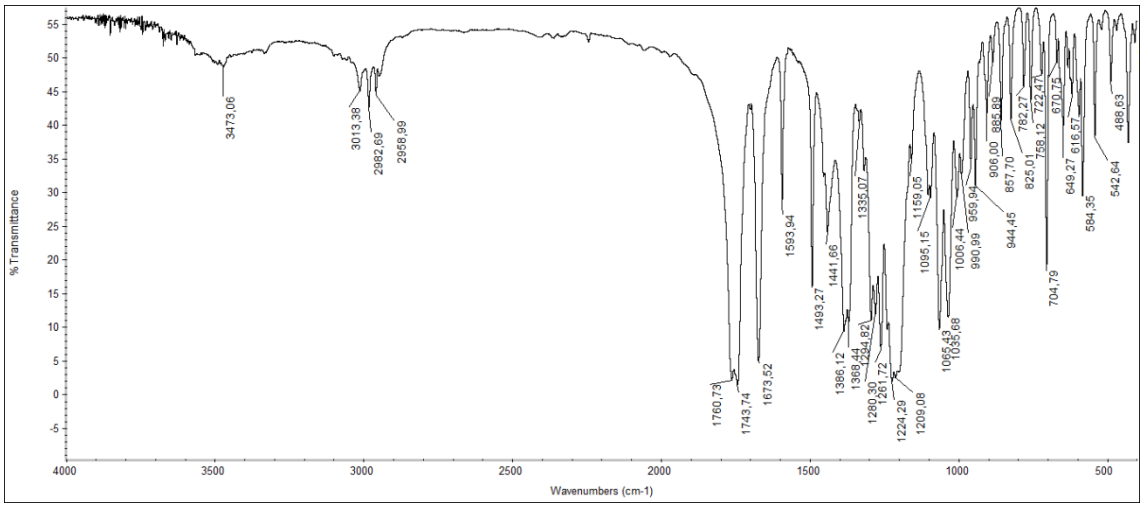


Figure S13. IR spectrum of **43.**

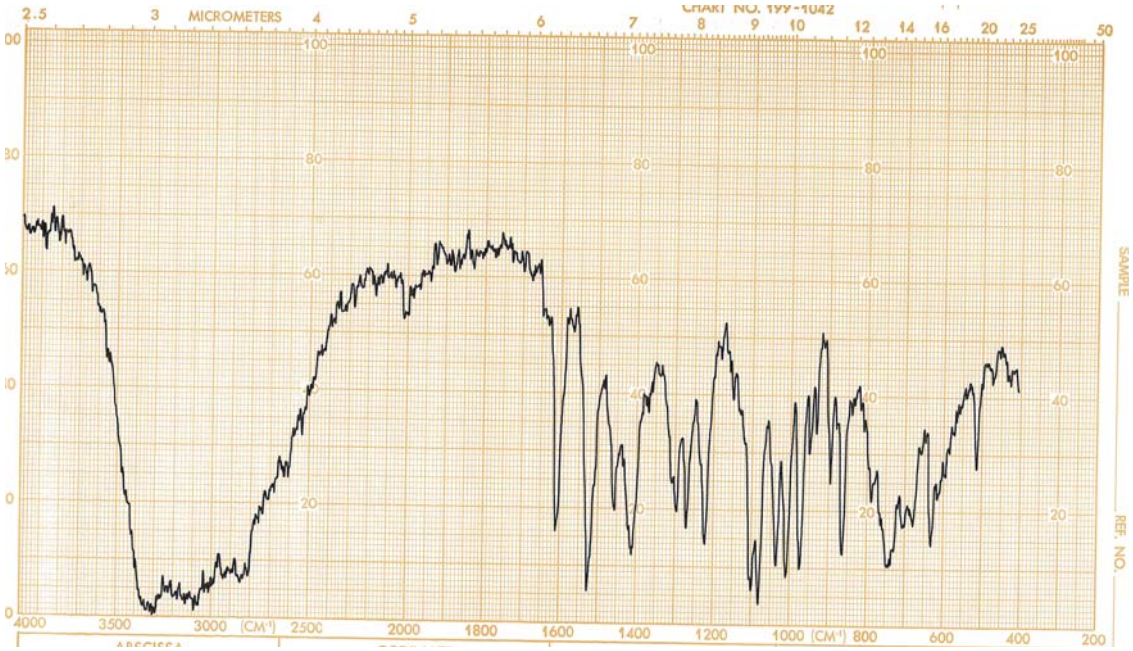


Figure S14. IR spectrum of **45.**

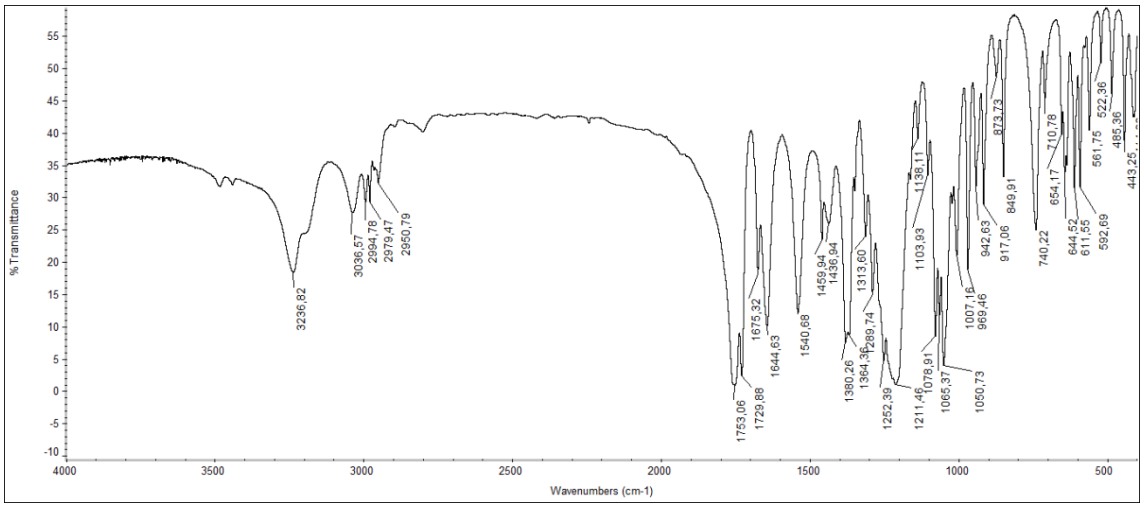


Figure S15. IR spectrum of **47**.

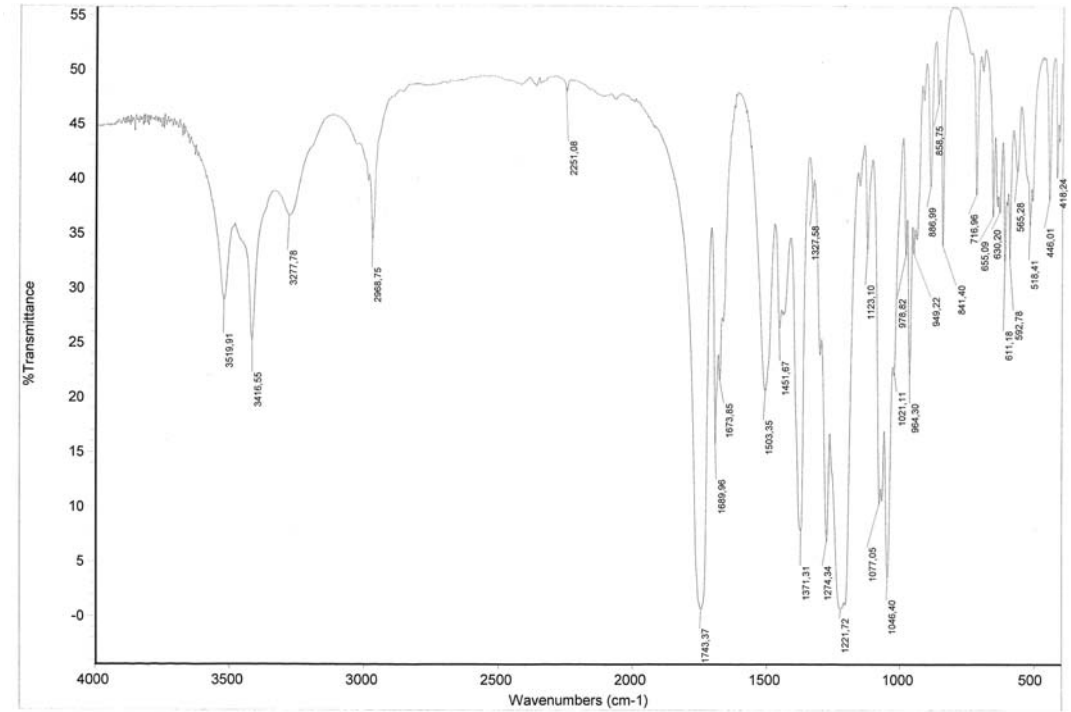


Figure S16. IR spectrum of **51**.

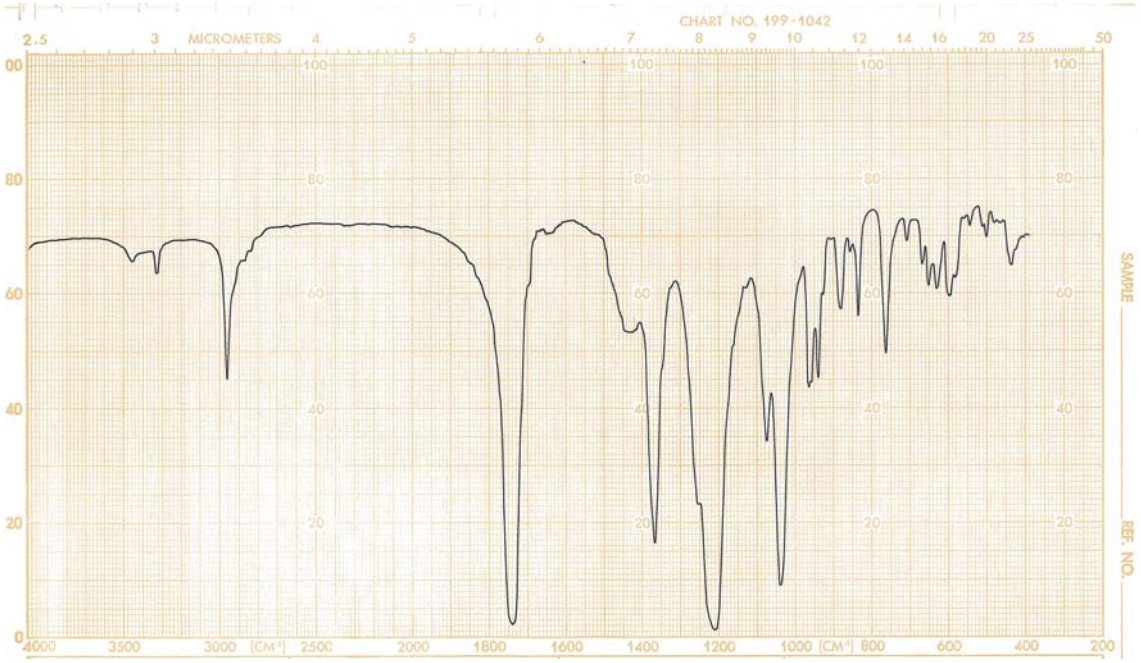


Figure S17. IR spectrum of **58.**

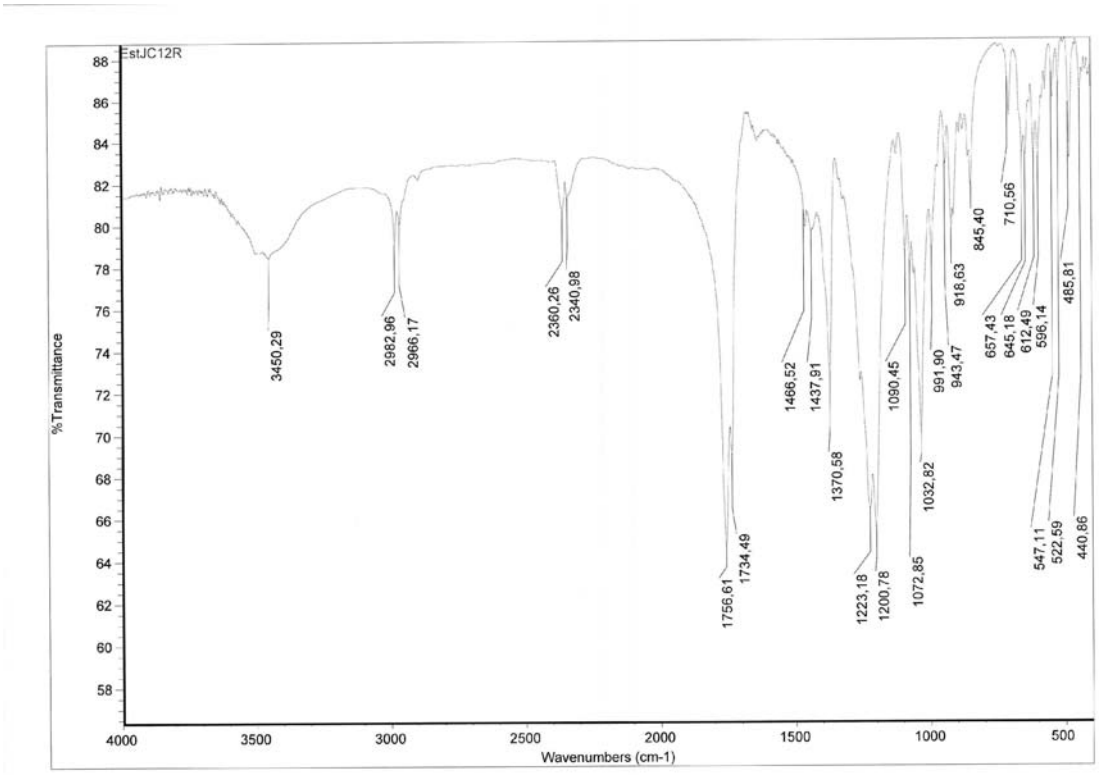


Figure S18. IR spectrum of **63.**

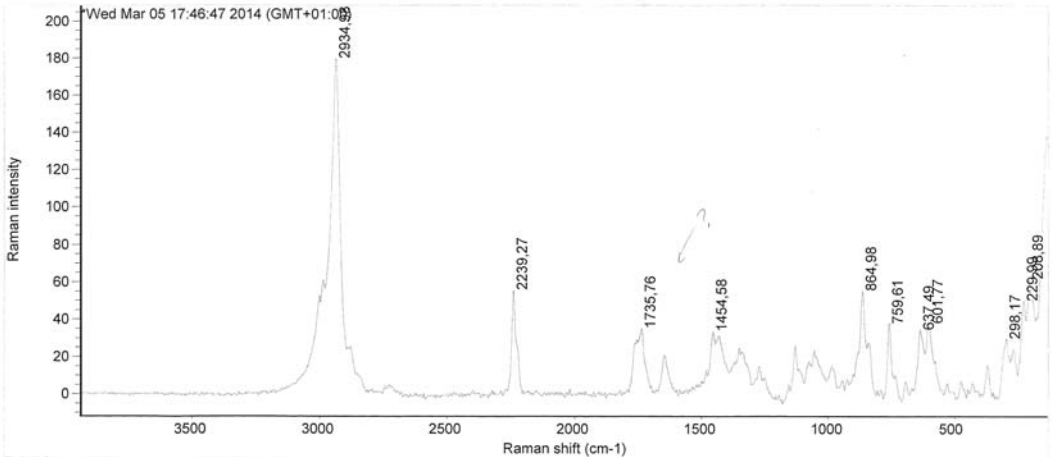


Figure S19. Raman spectrum of **11**.

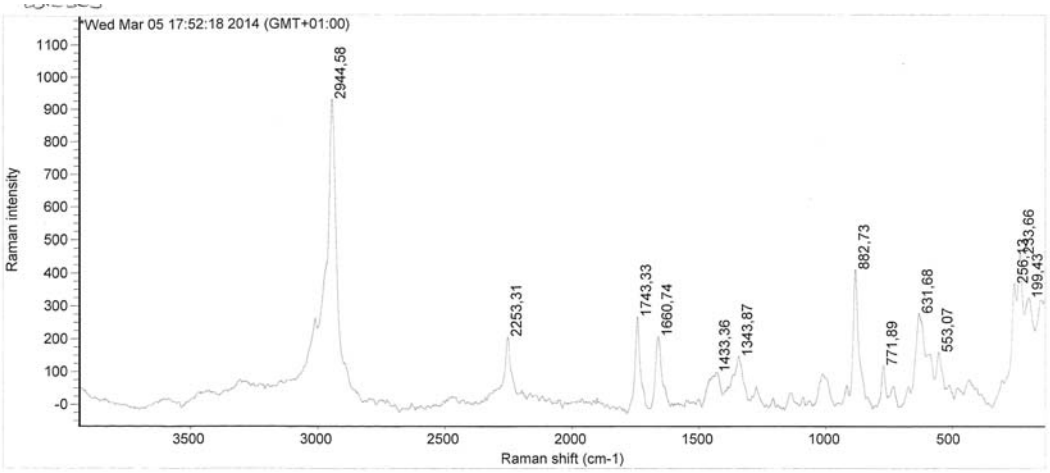


Figure S20. Raman spectrum of **13**.

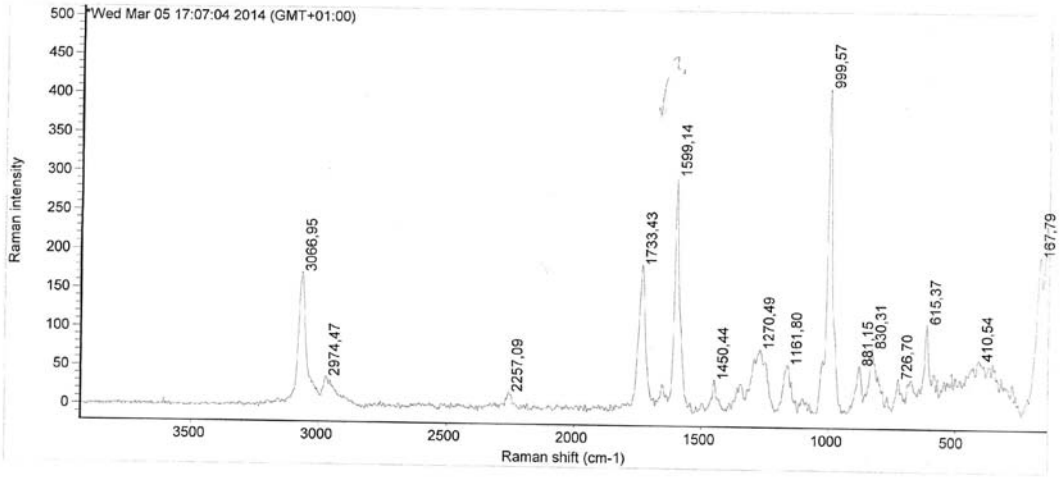


Figure S21. Raman spectrum of **18**.

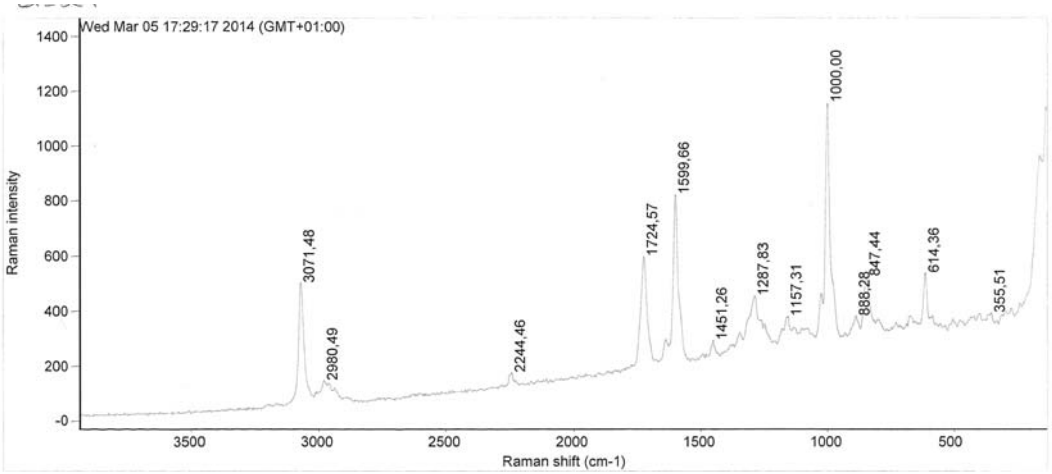


Figure S22. Raman spectrum of **20**.

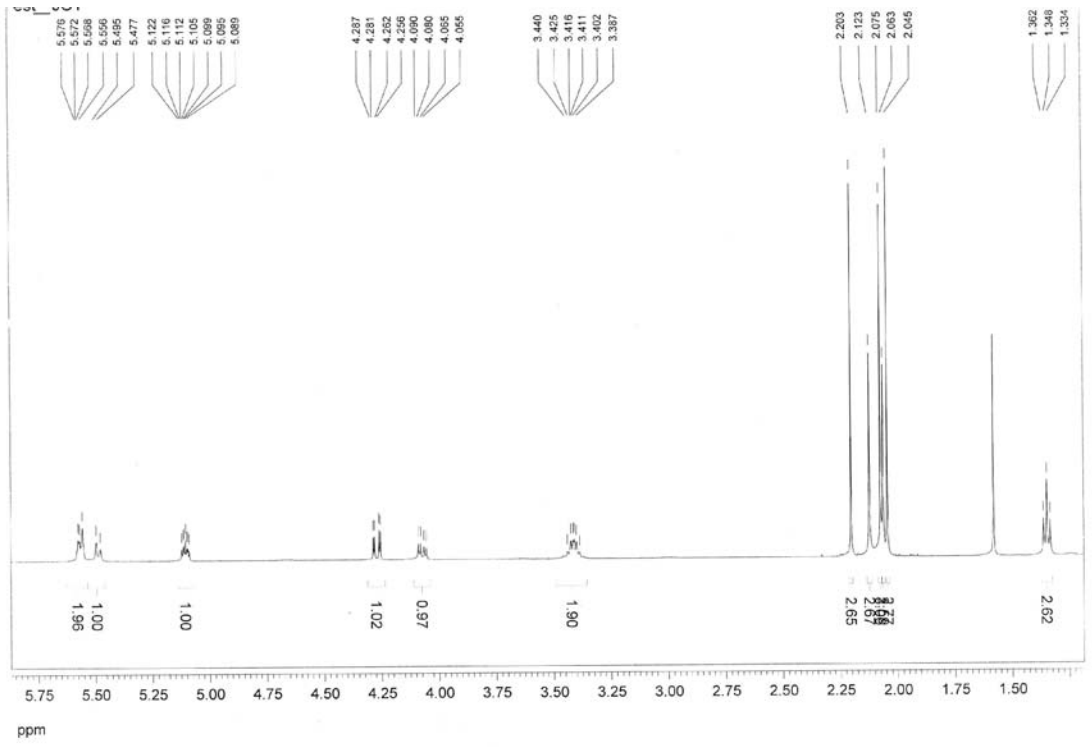


Figure S23. ^{1}H NMR spectrum of **11** in $CDCl_3$.

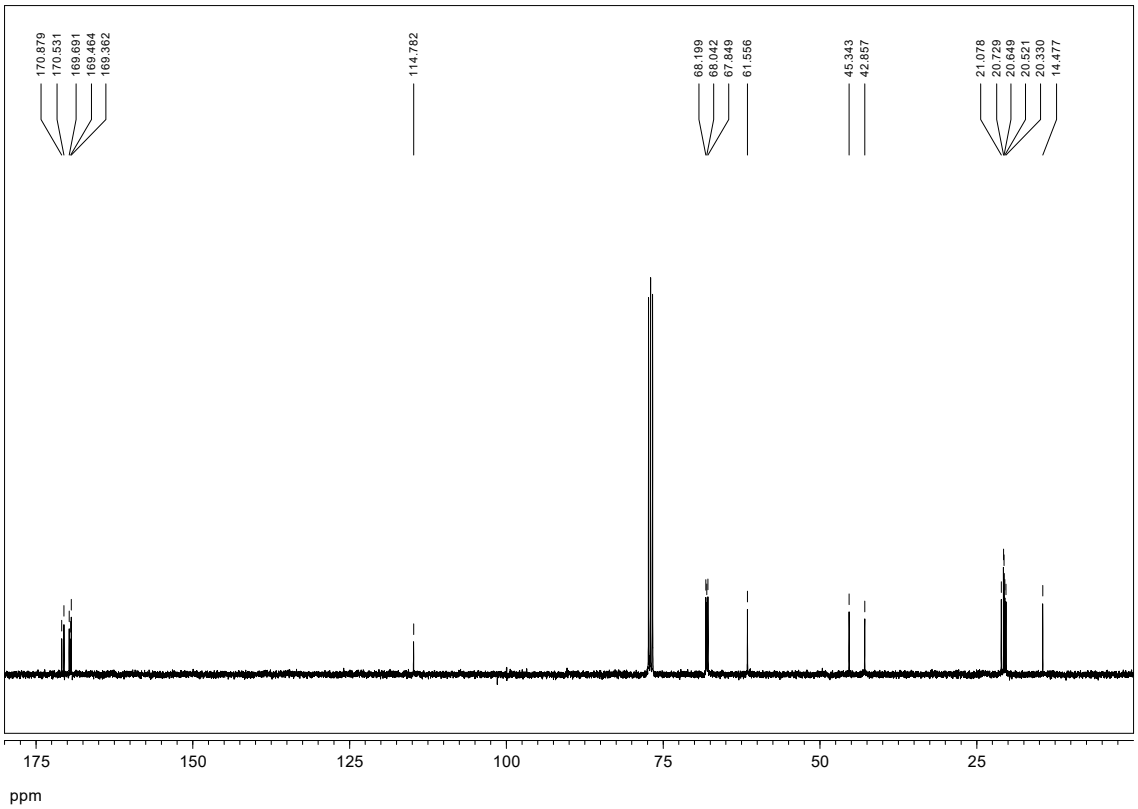


Figure S24. $^{13}C\{^{1}H\}$ NMR spectrum of **11** in $CDCl_3$.

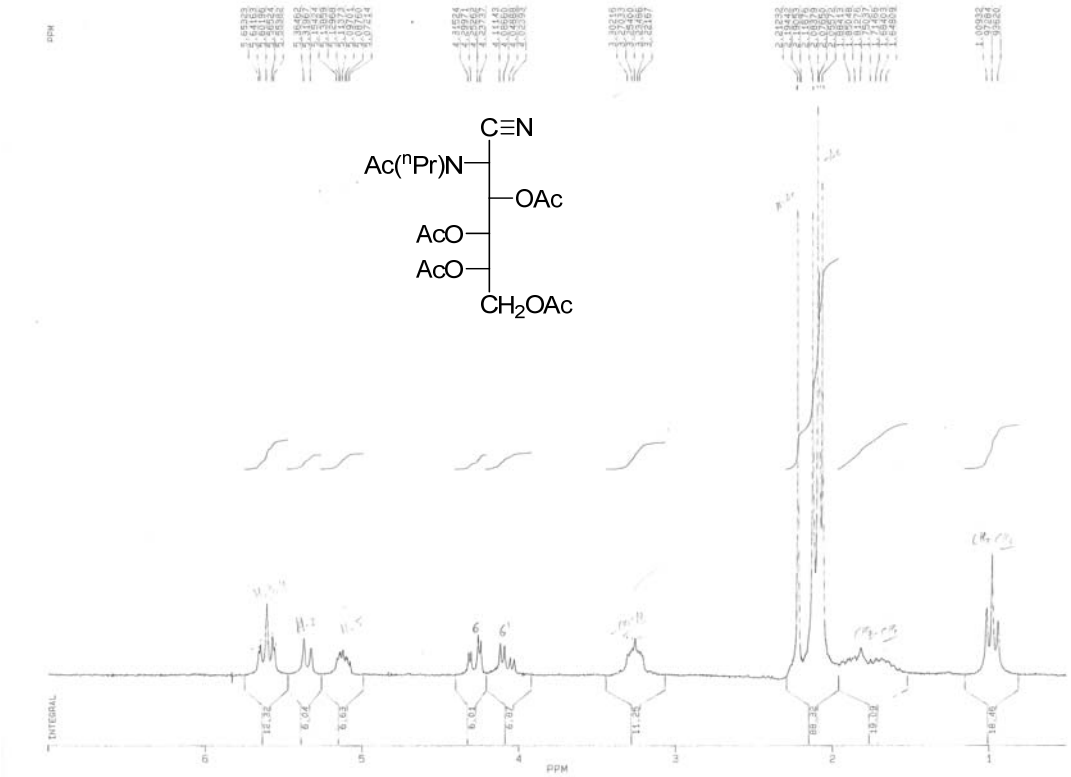


Figure S25. ^{1}H NMR spectrum of **12** in $CDCl_3$

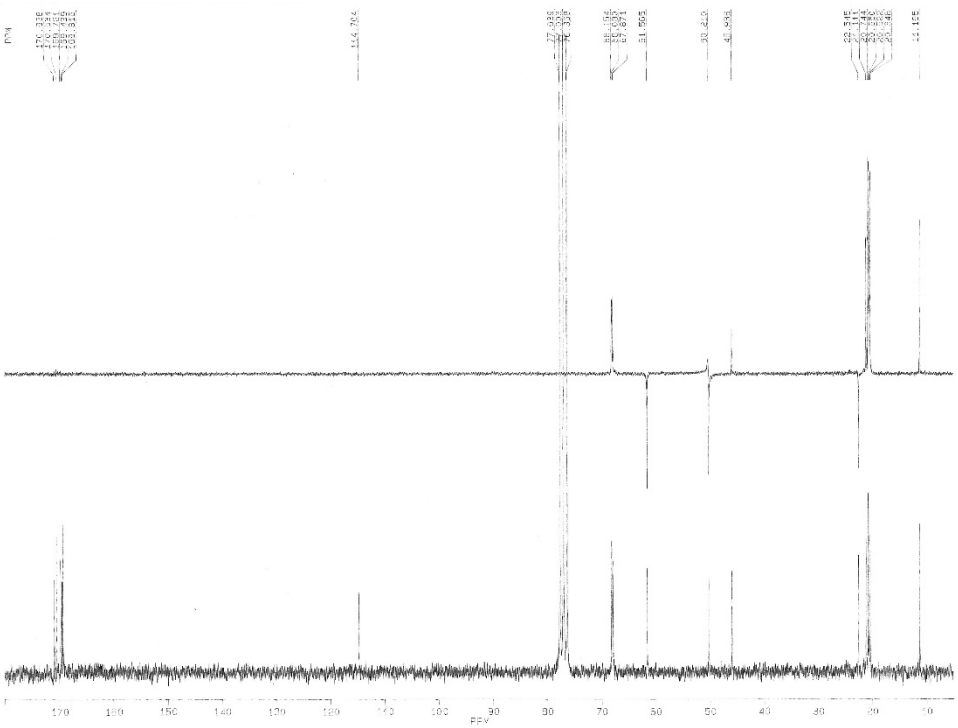


Figure S26. $^{13}C\{^{1}H\}$ NMR and DEPT spectra of **12** in $CDCl_3$

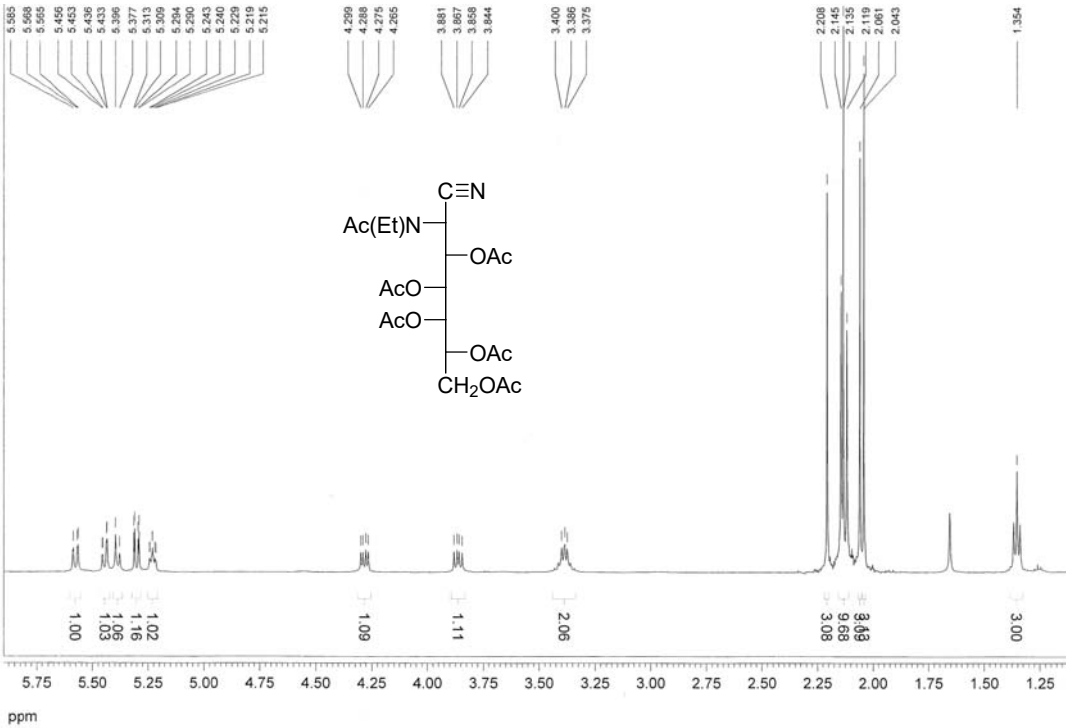


Figure S27. ^{1}H NMR spectrum of **13** in $CDCl_3$.

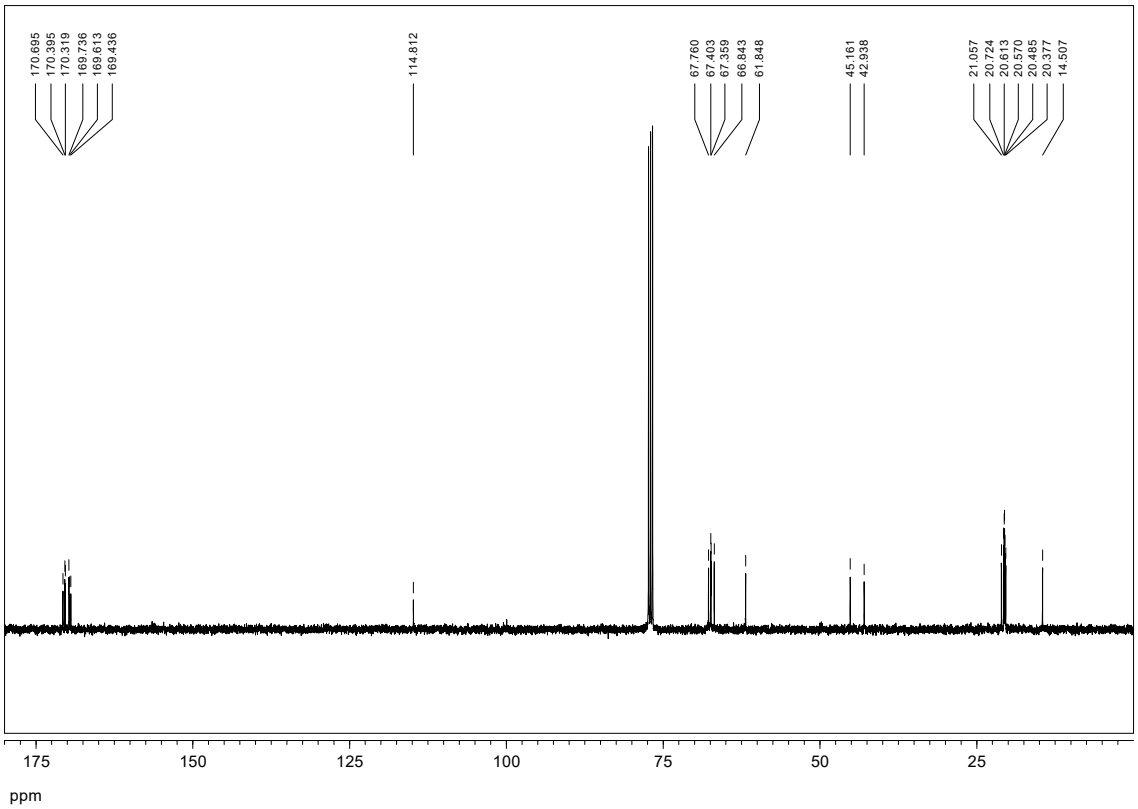


Figure S28. $^{13}C\{^{1}H\}$ NMR spectrum of **13** in $CDCl_3$.

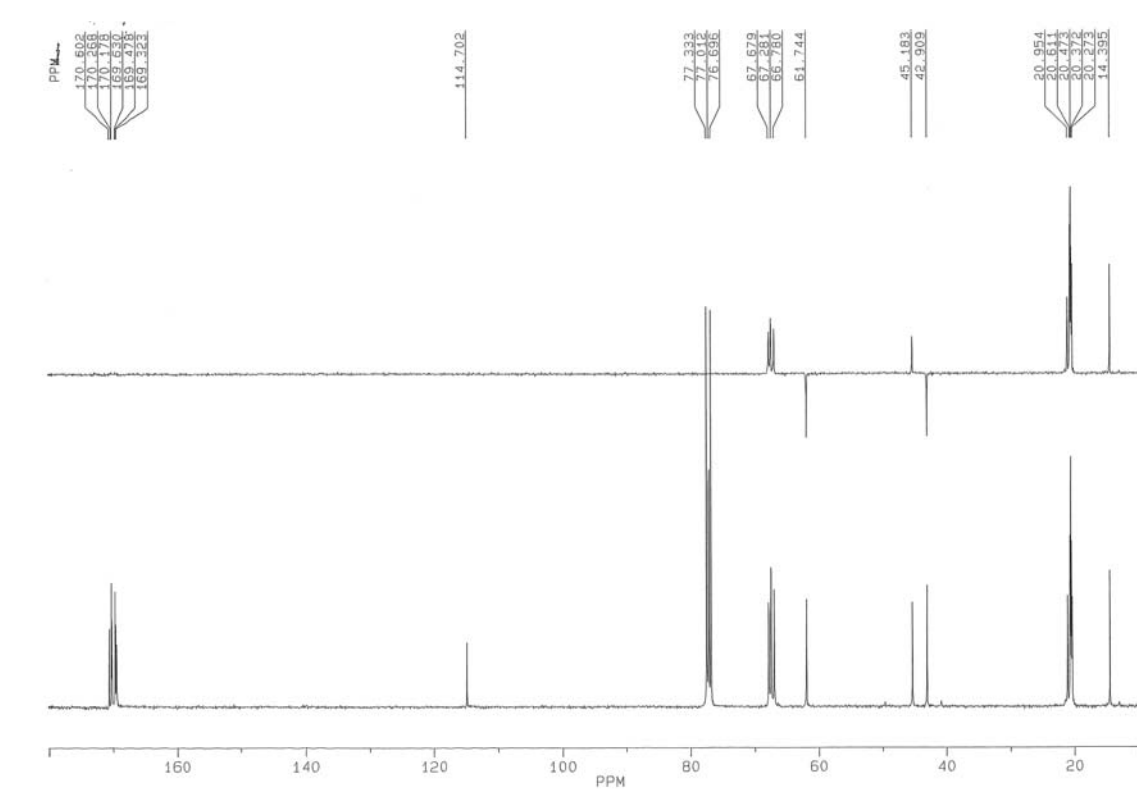


Figure S29. $^{13}C\{^{1}H\}$ NMR and DEPT spectra of **13** in $CDCl_3$.

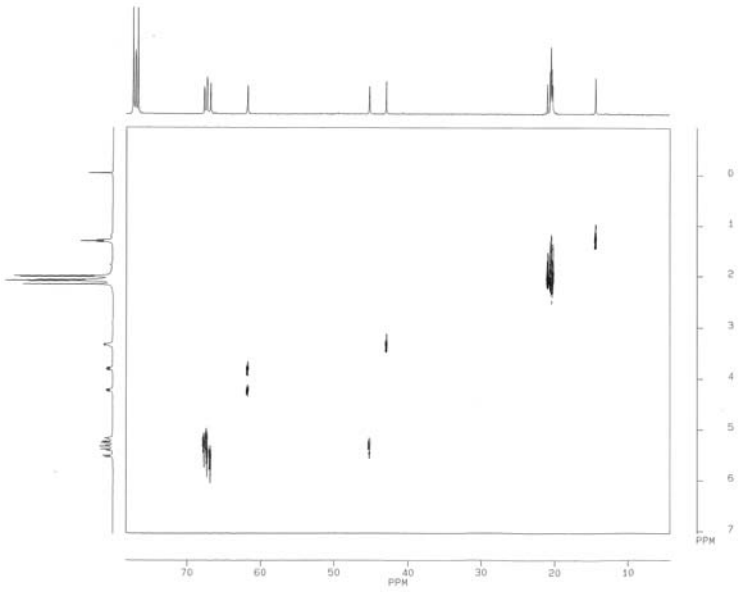


Figure S30. HMQC spectrum of **13** in $CDCl_3$.

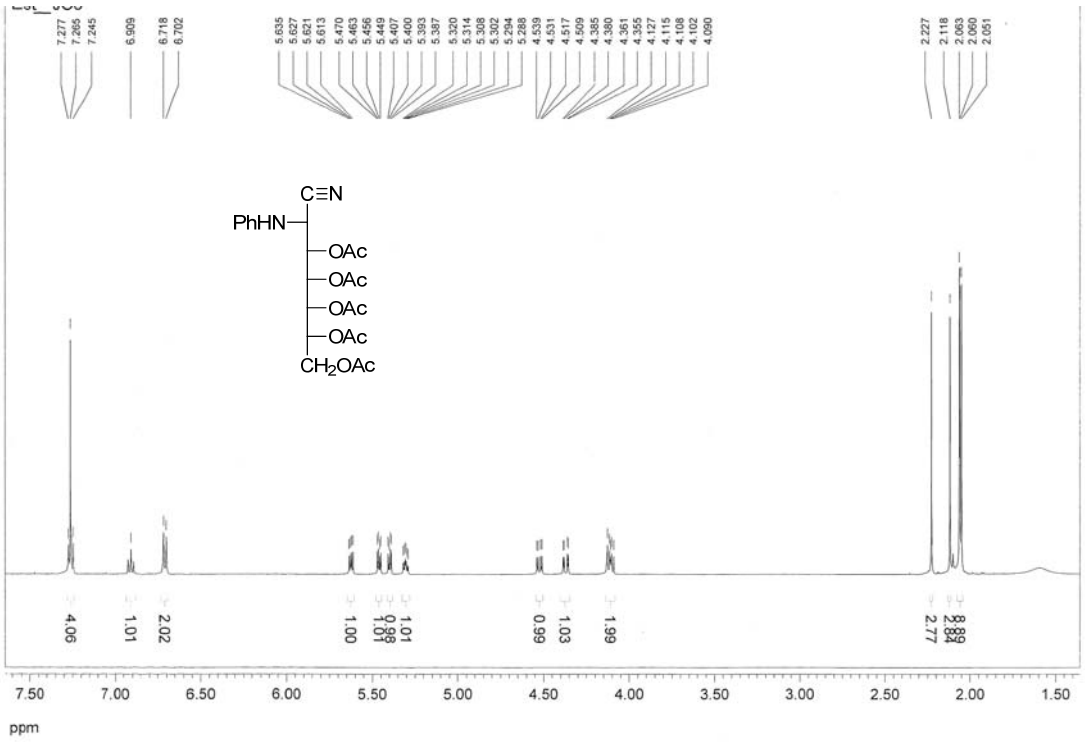


Figure S31. ^1H NMR spectrum of **17** in $CDCl_3$.

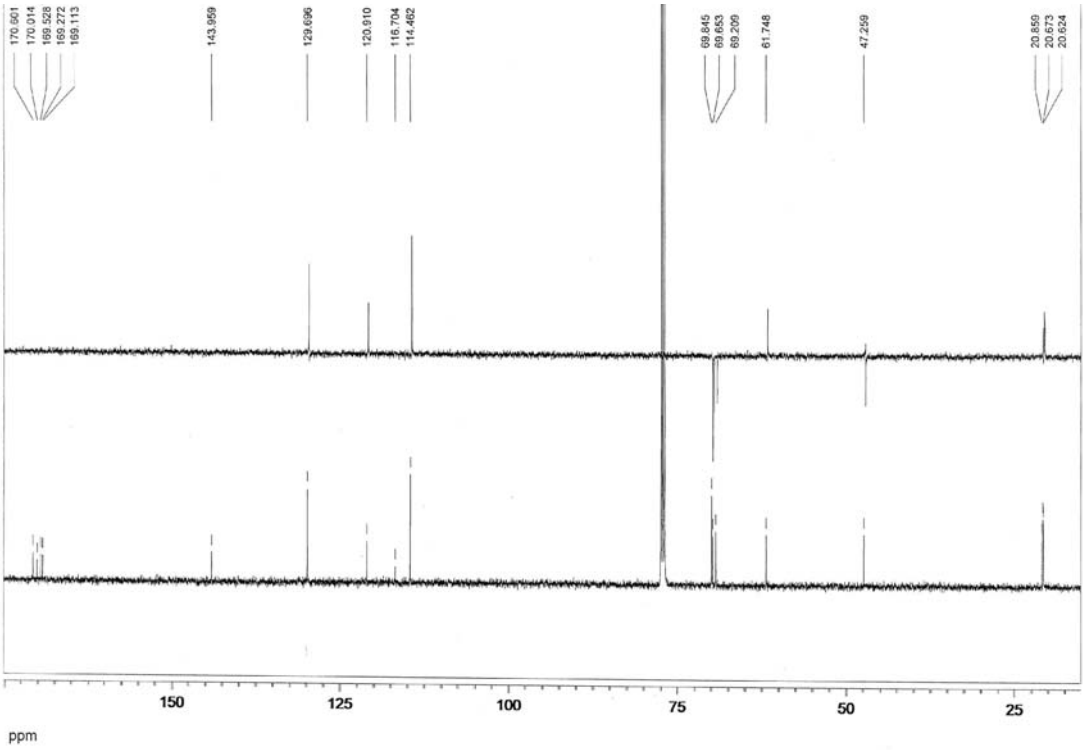


Figure S32. $^{13}C\{^{1}H\}$ NMR and DEPT spectra of **17** in $CDCl_3$.

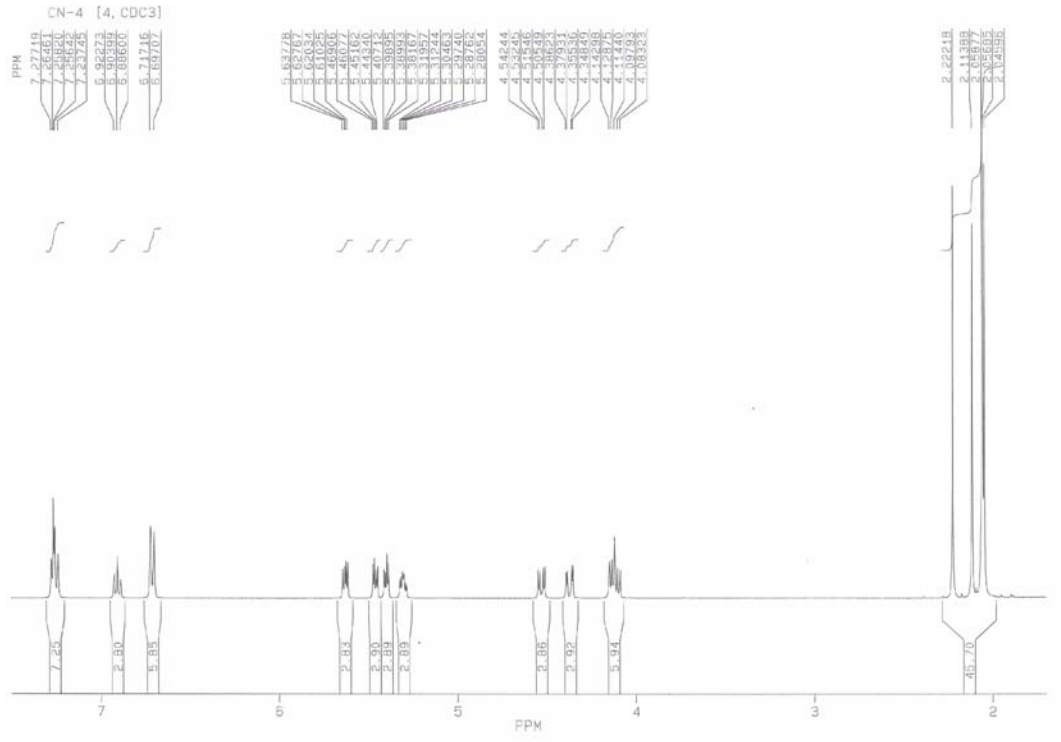


Figure S33. ^{1}H NMR spectrum of **17** in $CDCl_3$

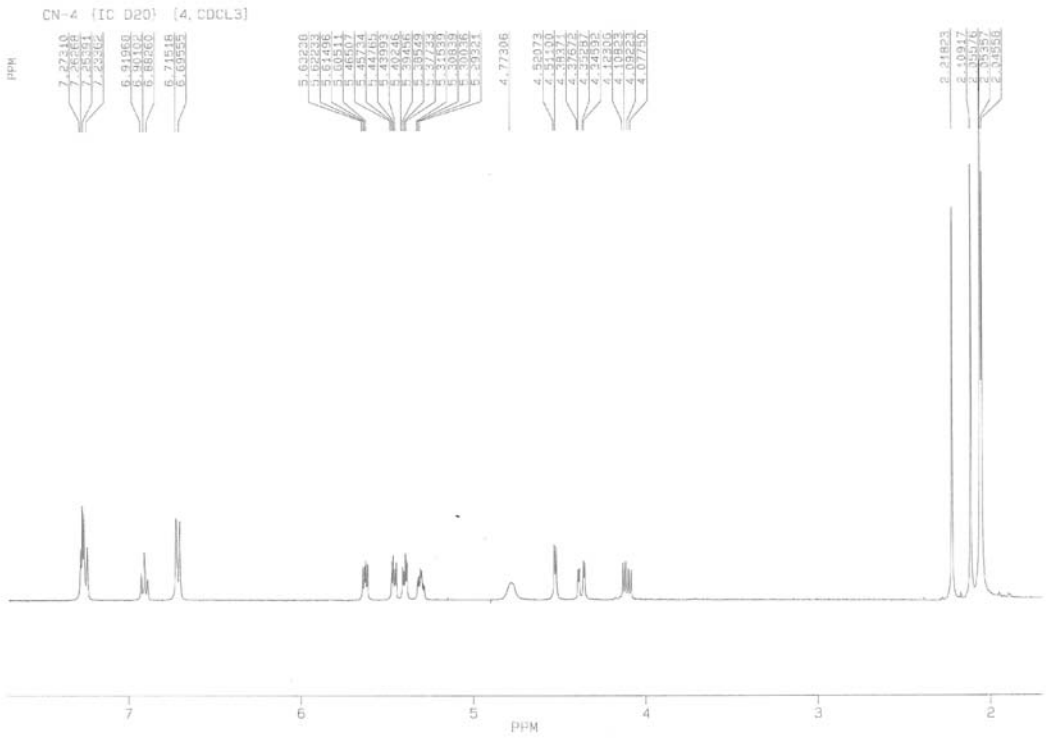


Figure S34. ^{1}H NMR spectrum of **17** in $CDCl_3$

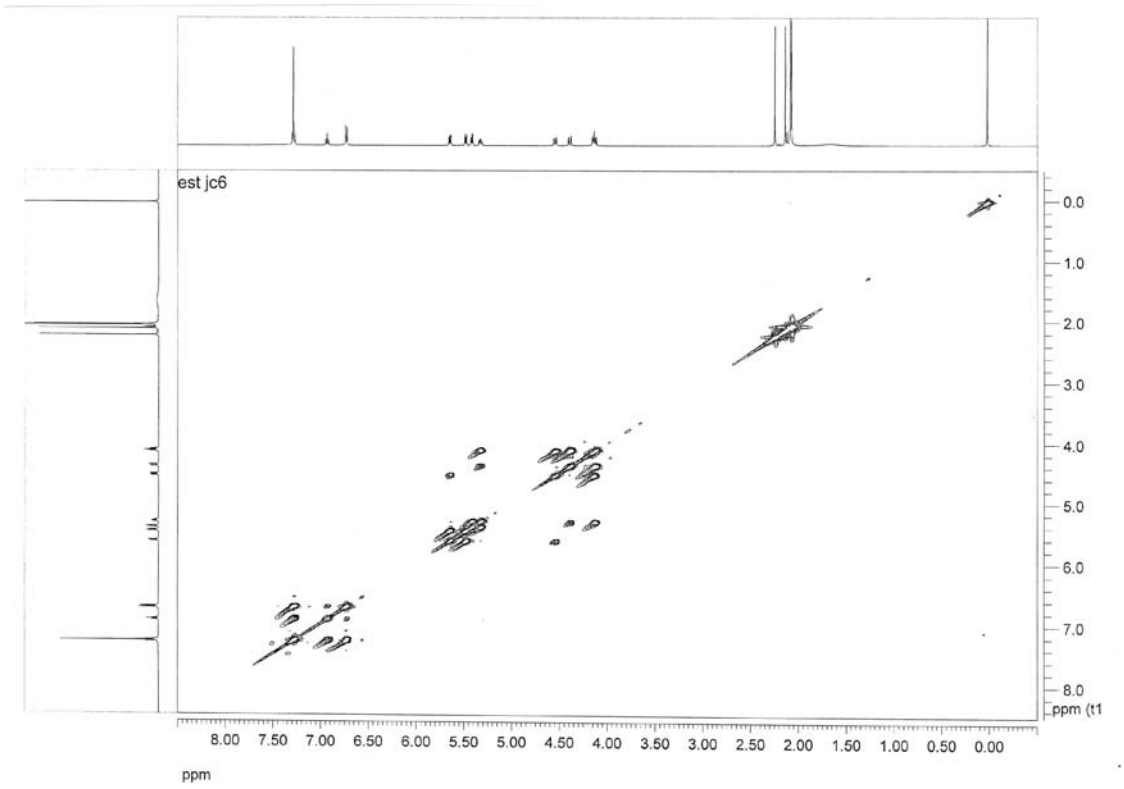


Figure S35. COSY spectrum of **17** in $CDCl_3$

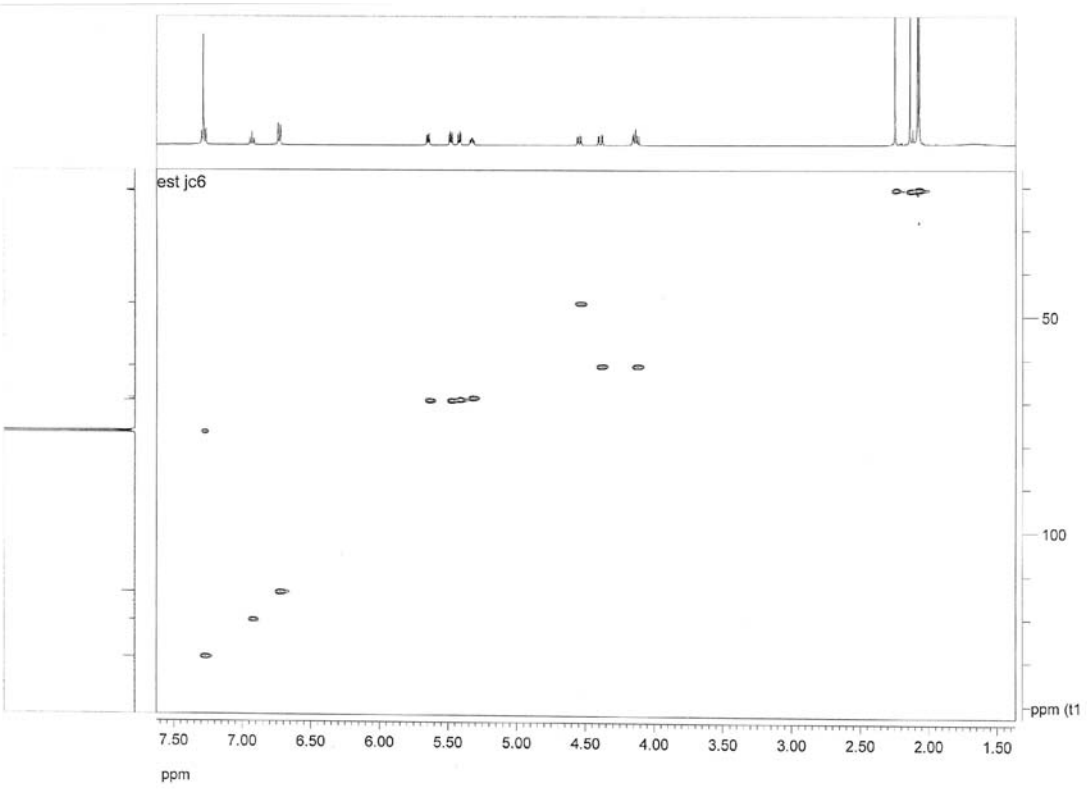


Figure S36. HMQC spectrum of **17** in $CDCl_3$

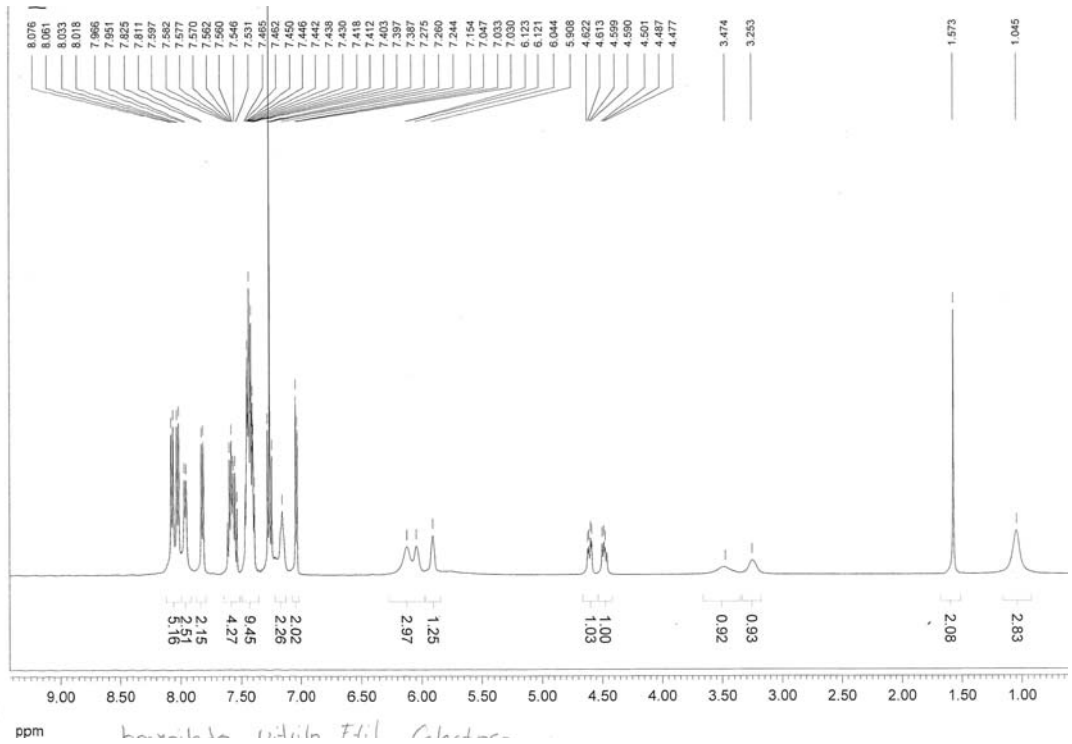


Figure S37. ^1H NMR spectrum of **18** in $CDCl_3$.

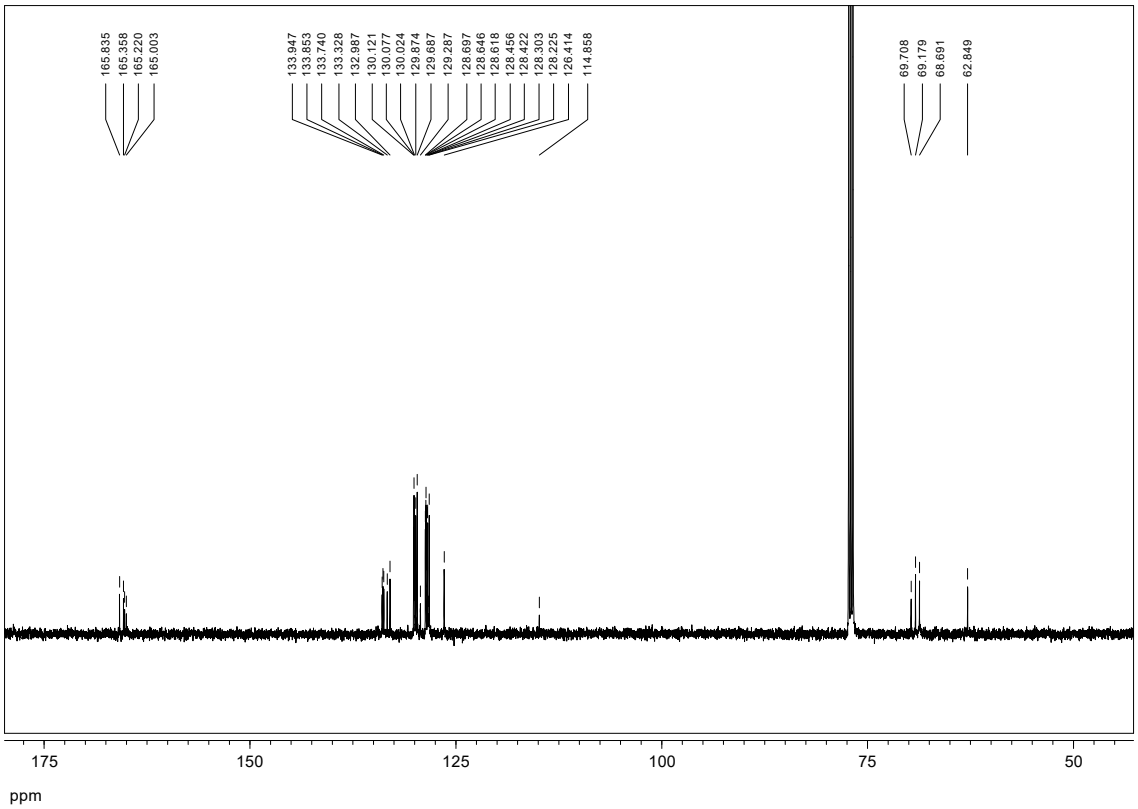


Figure S38. $^{13}C\{^{1}H\}$ NMR spectrum of **18** in $CDCl_3$.

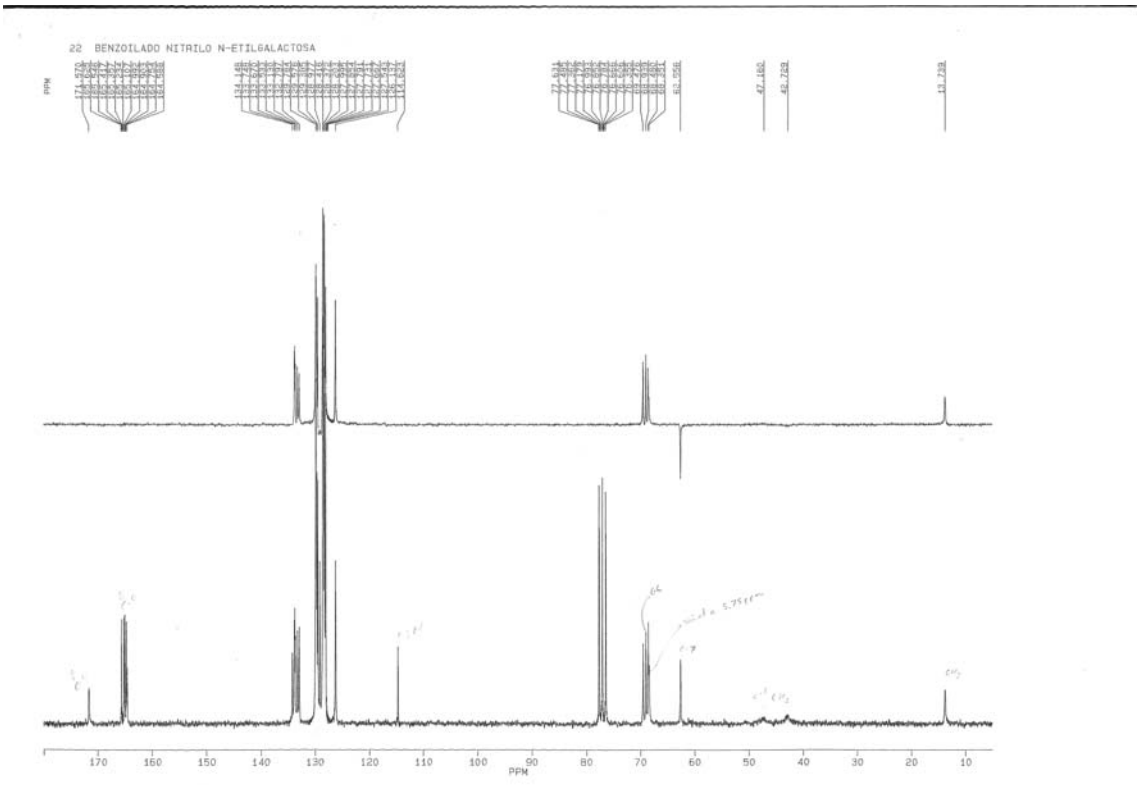


Figure S39. $^{13}C\{^{1}H\}$ NMR and DEPT spectra of **18** in $CDCl_3$.

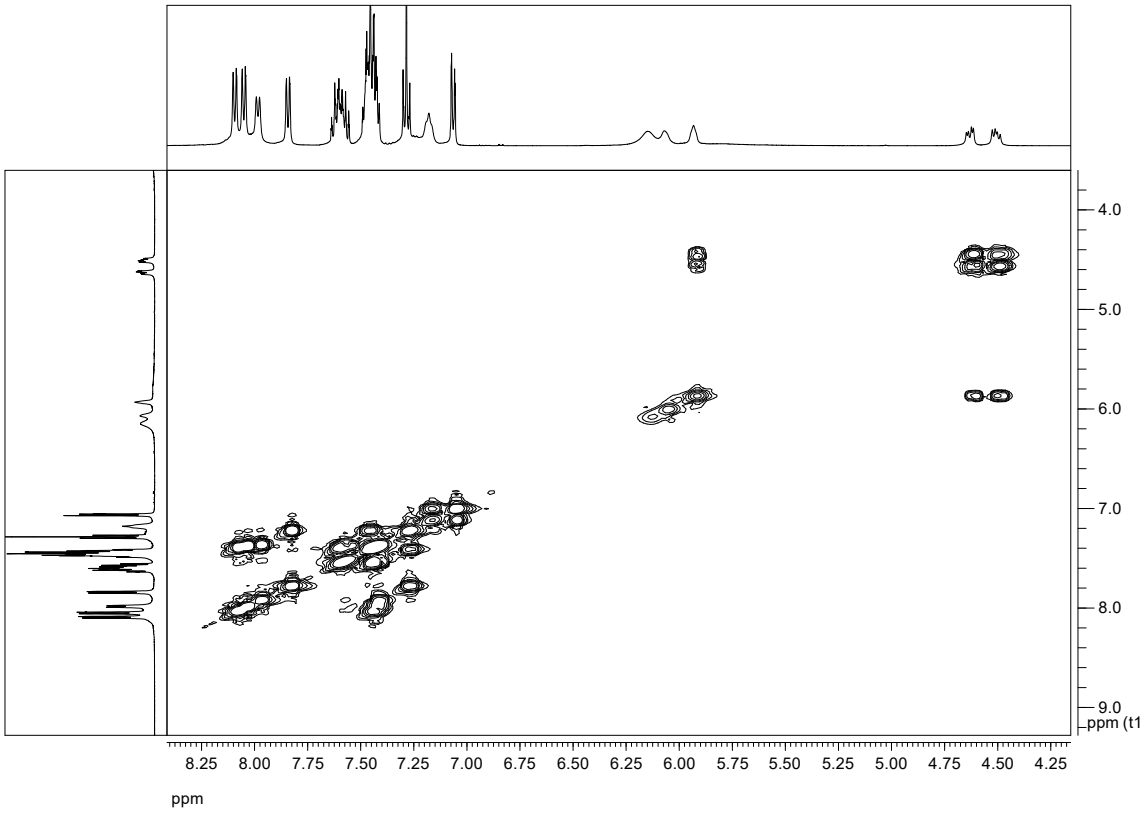


Figure S40. COSY spectrum of **18** in $CDCl_3$.

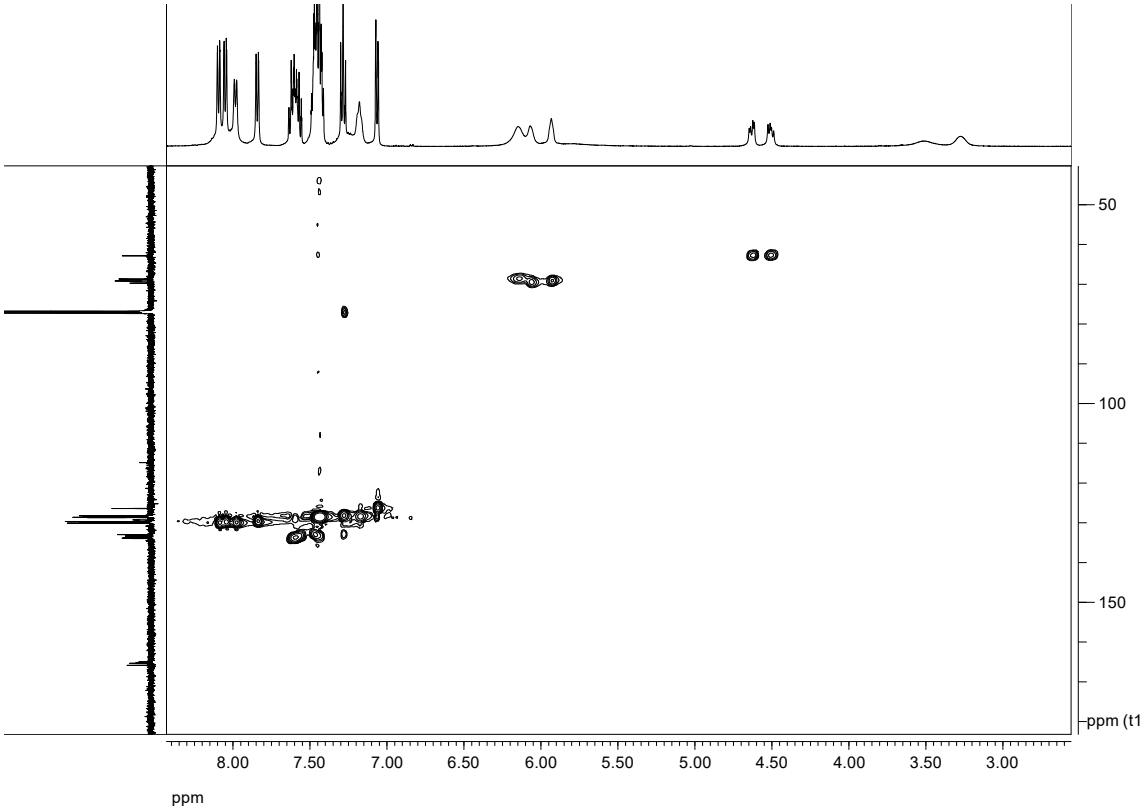


Figure S41. HMQC spectrum of **18** in $CDCl_3$.

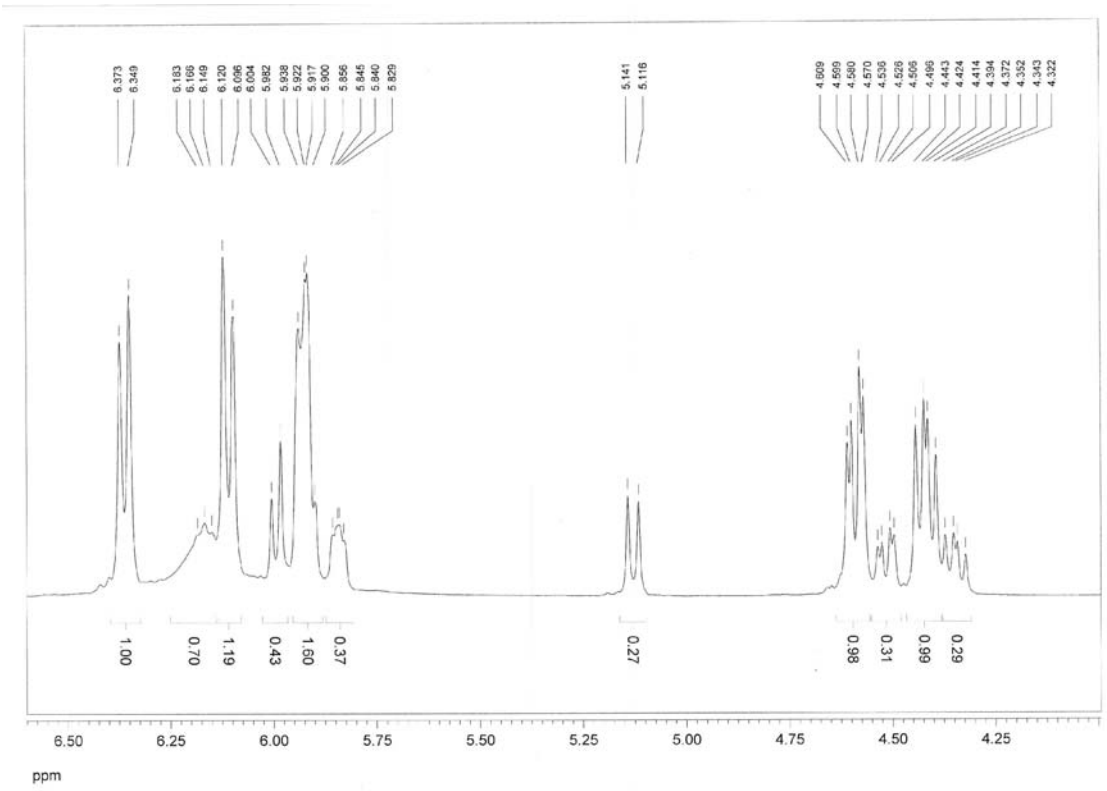


Figure S42. Magnified ^{1}H NMR espectral zone of **18** in $CDCl_3$ (240K).

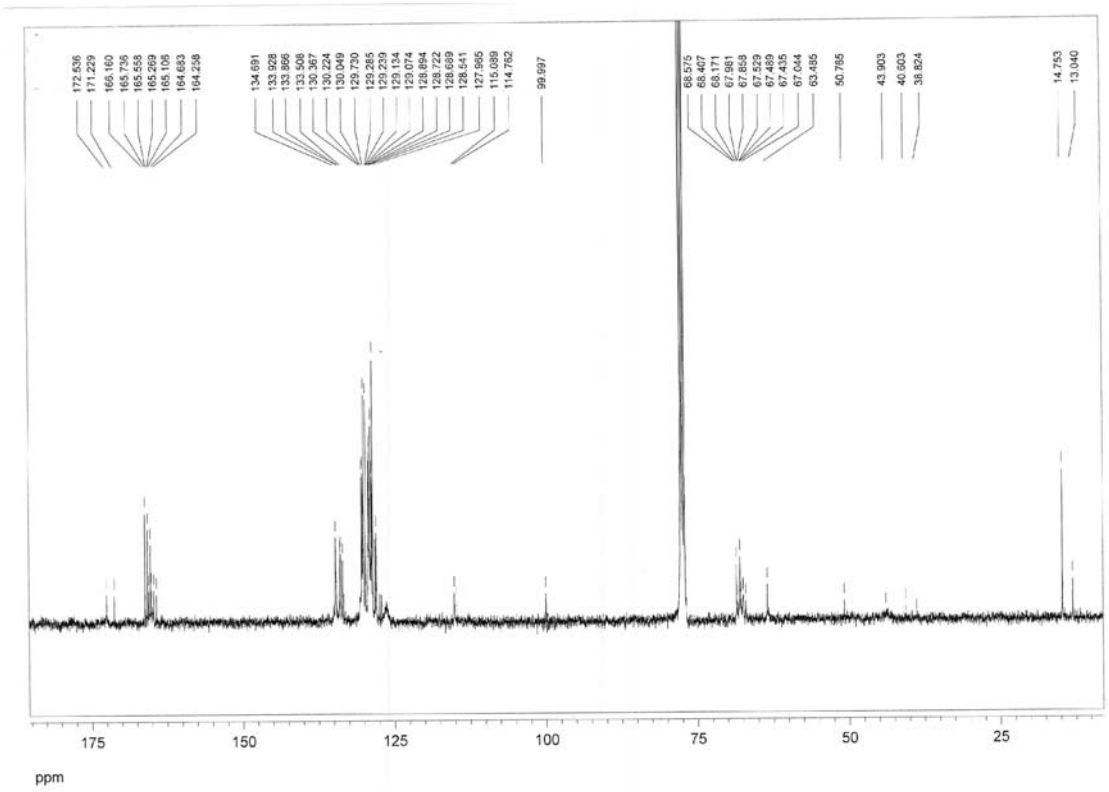


Figure S43. $^{13}C\{^{1}H\}$ NMR spectrum of **18** in $CDCl_3$ (240K).

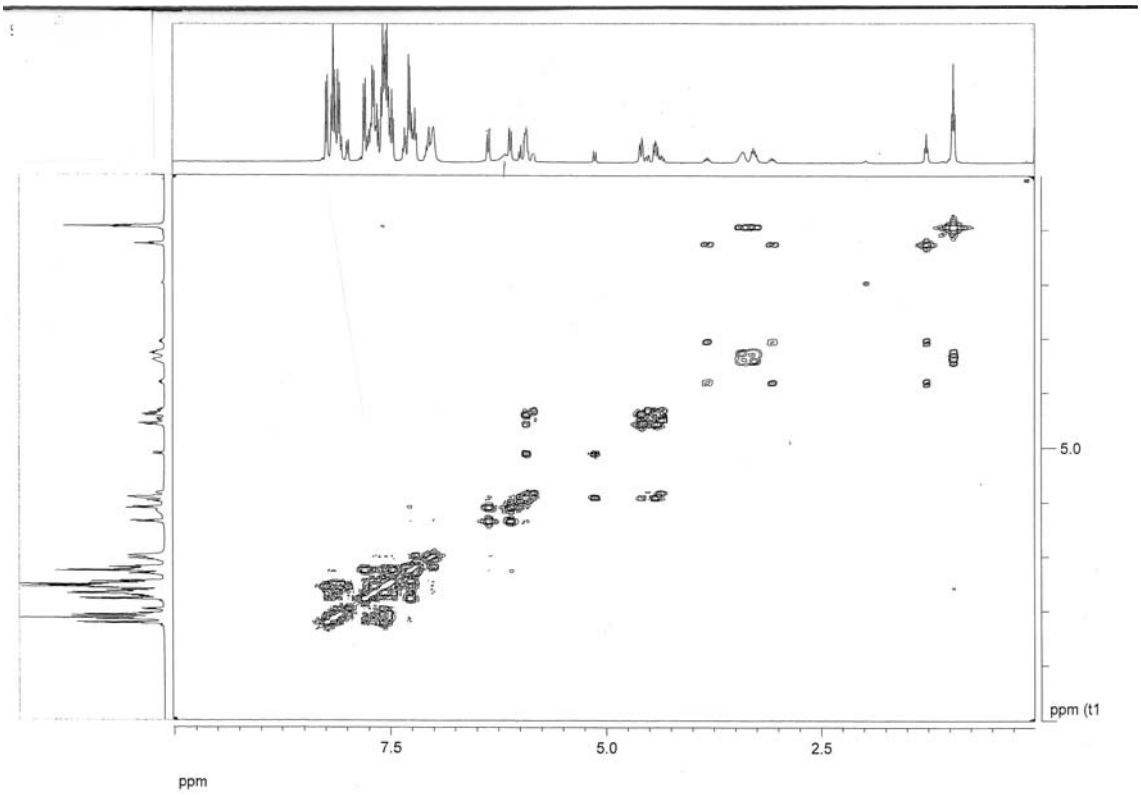


Figure S44. COSY spectrum of **18** in $CDCl_3$ (240K).

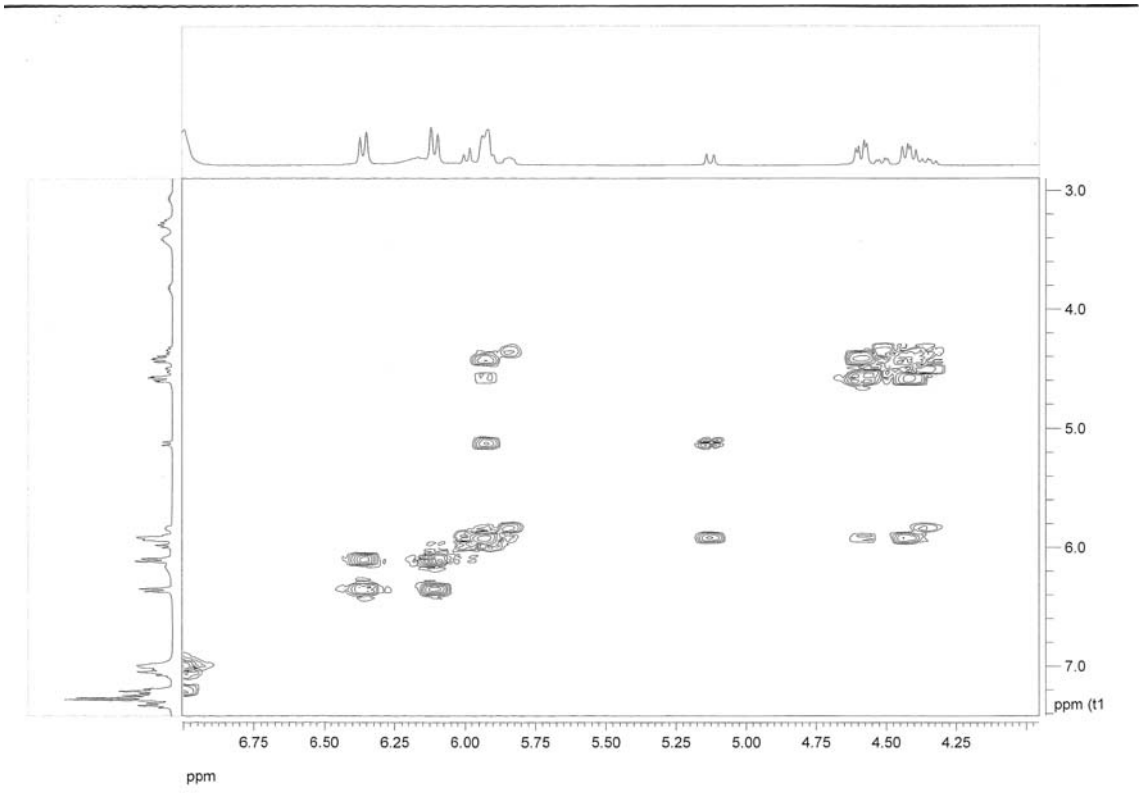


Figure S45. Magnified COSY espectral zone of **18** in $CDCl_3$ (240K).

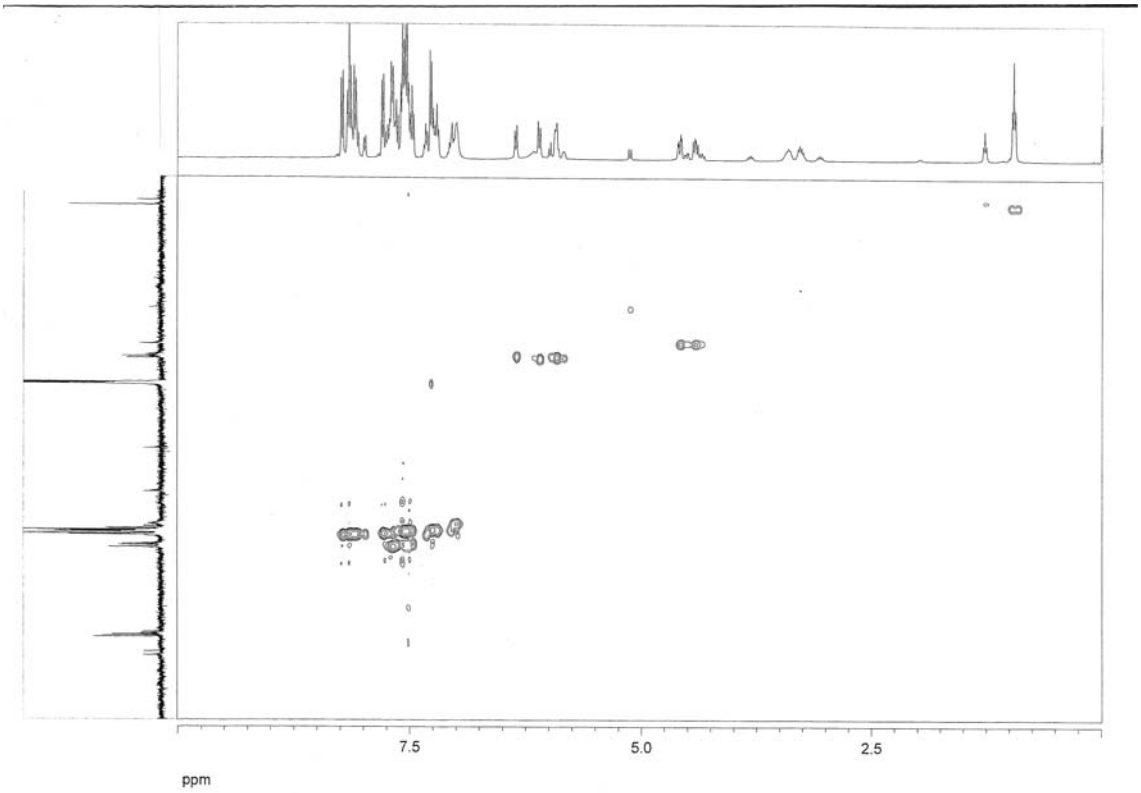


Figure S46. HMQC spectrum of **18** in $CDCl_3$ (240K).

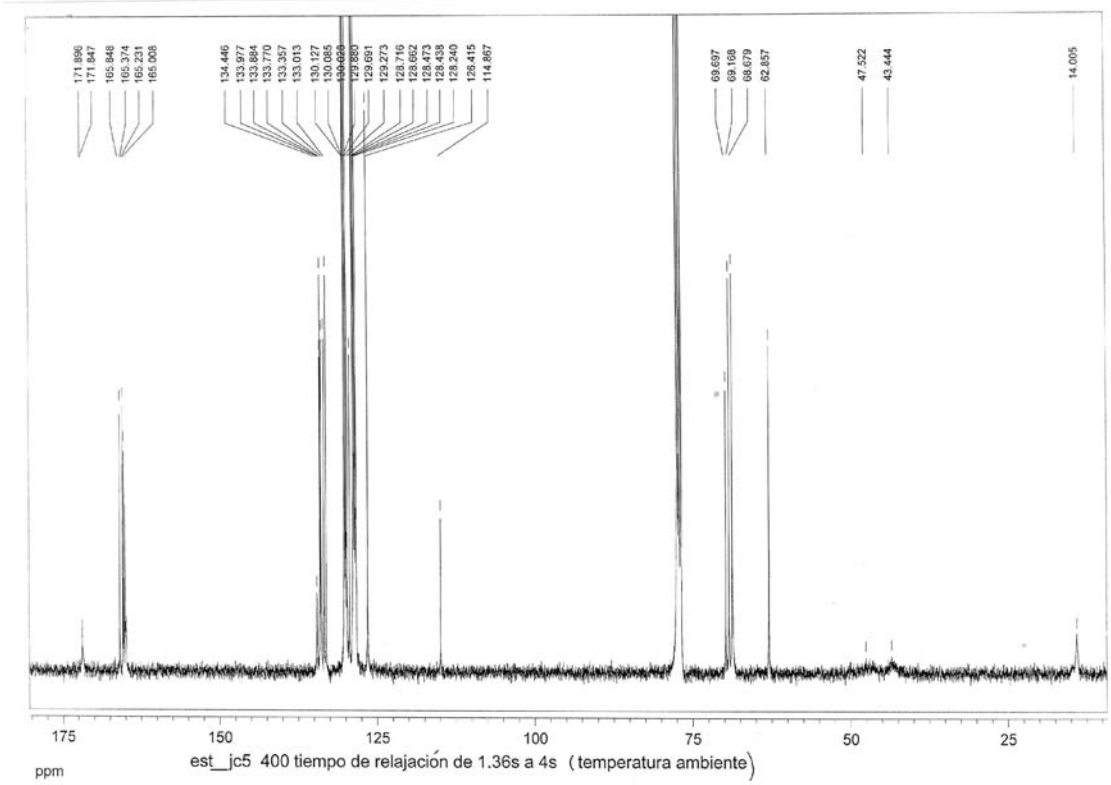


Figure S47. $^{13}C\{^1H\}$ NMR spectrum of **18** in $CDCl_3$.

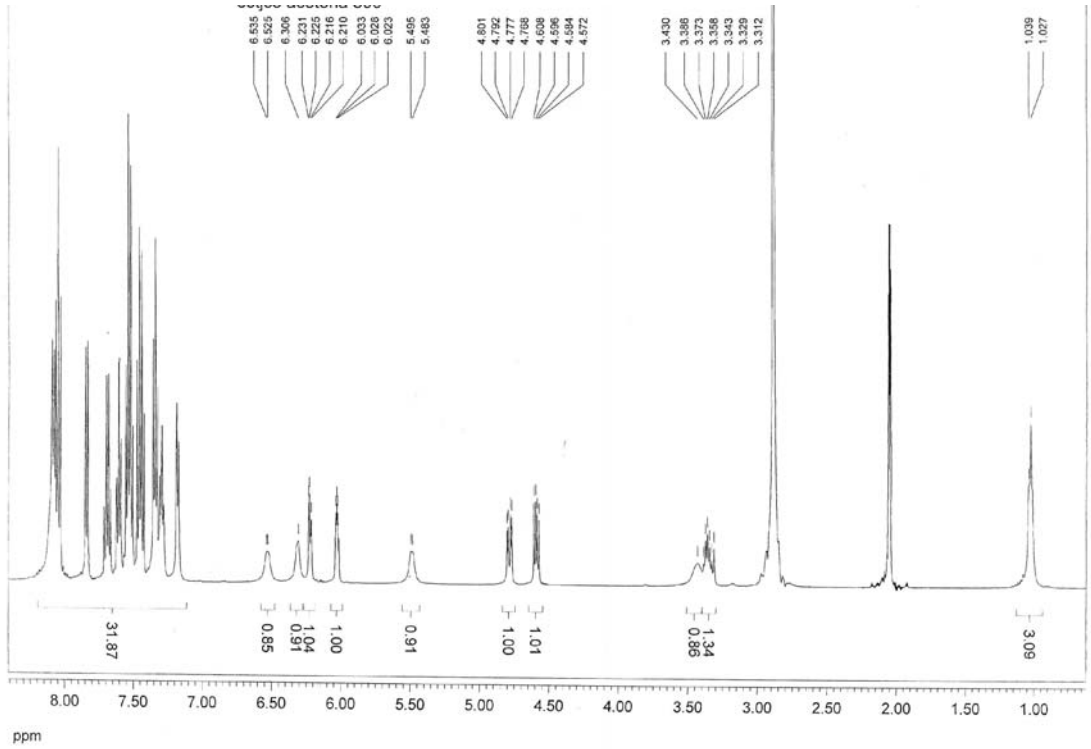


Figure S48. ^{1}H NMR spectrum of **18** in Acetone-d_6.

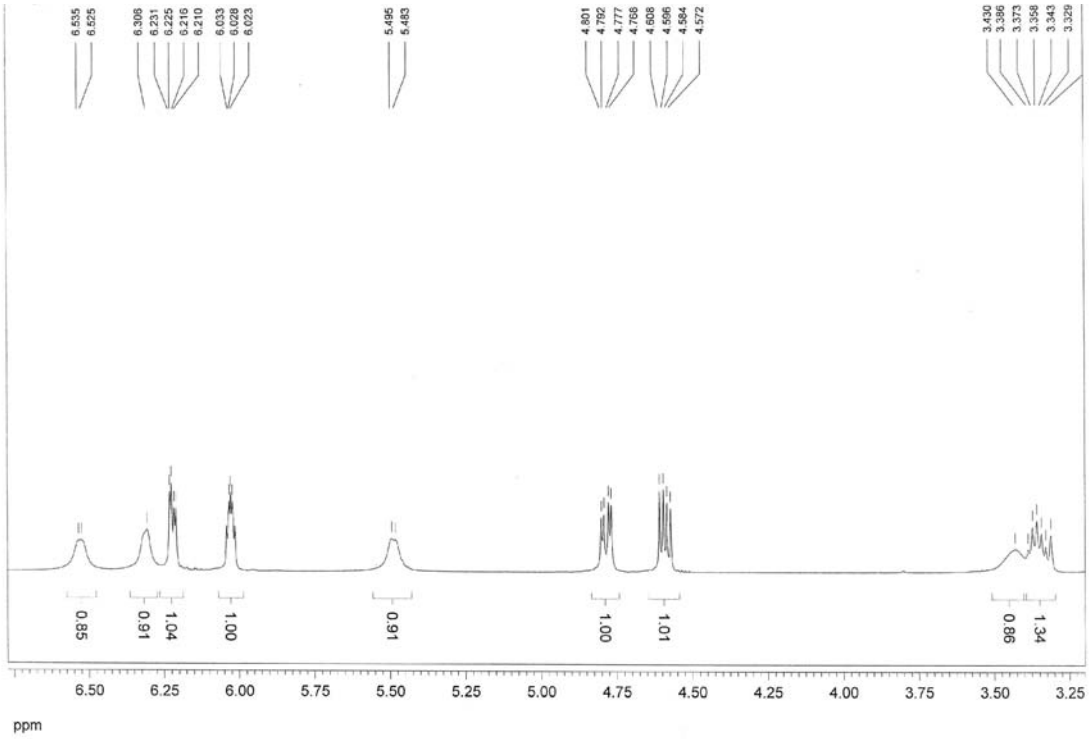


Figure S49. Magnified ^{1}H NMR espectral zone of **18** in Acetone-d_6.

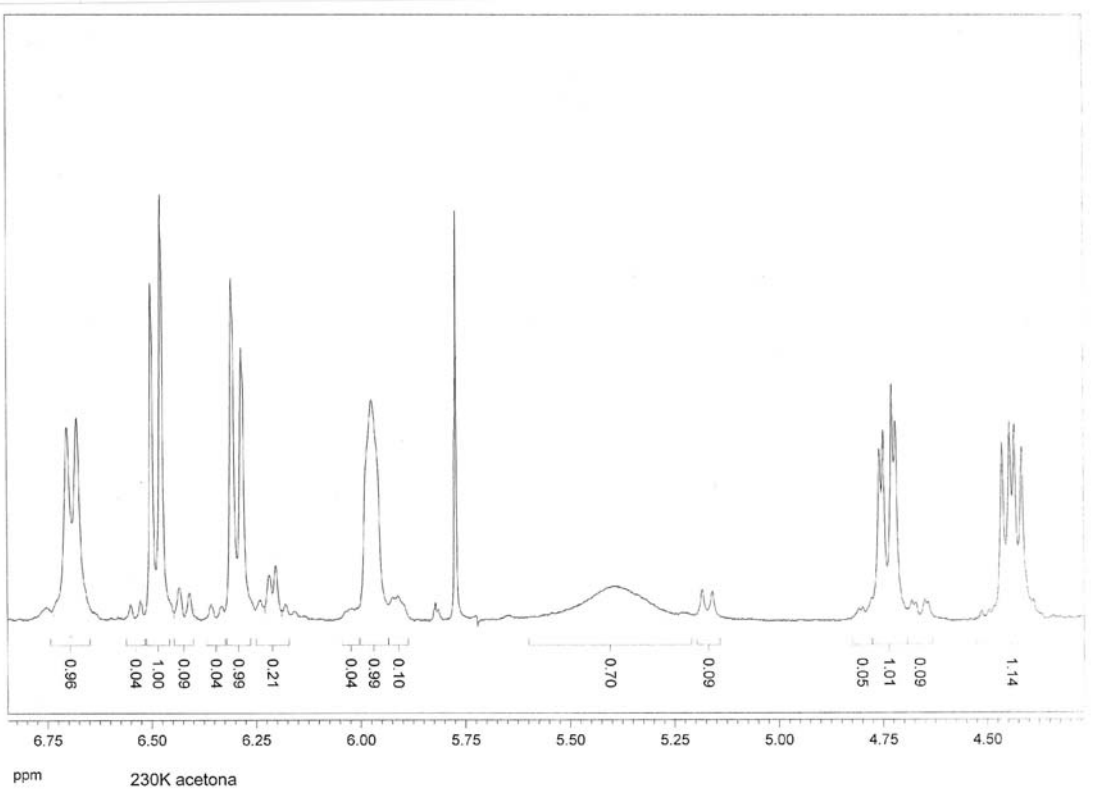


Figure S50. Magnified ^{1}H NMR espectral zone of **18** in Acetone-d_6 (230K).

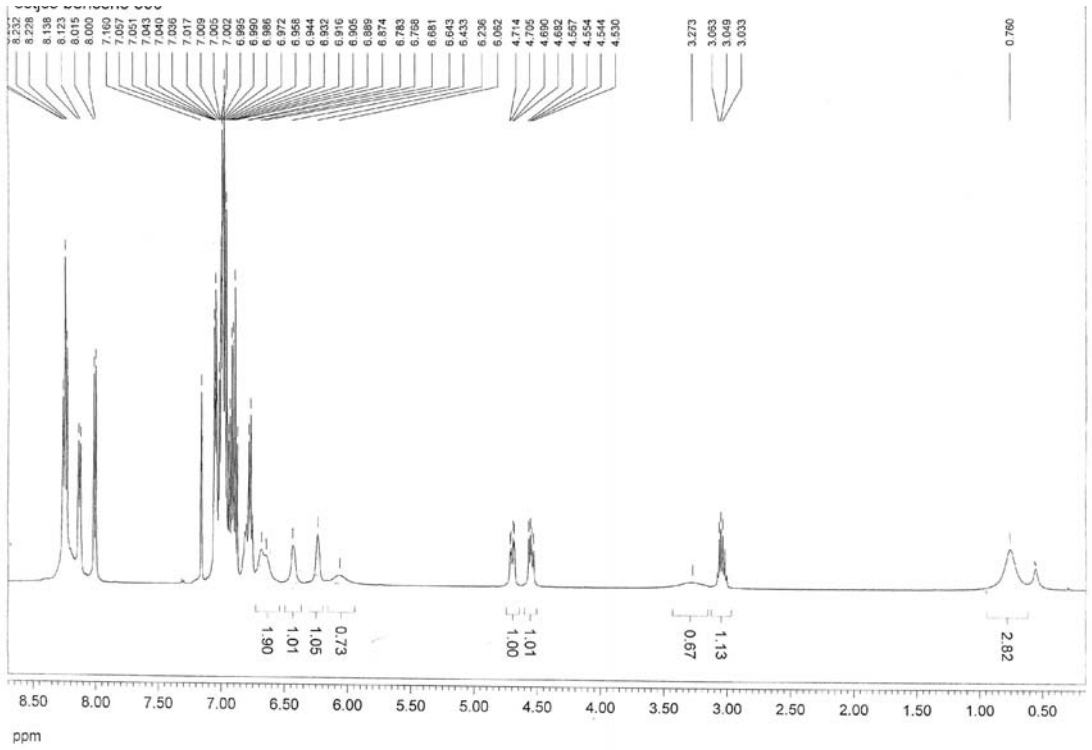


Figure S51. ^{1}H NMR spectrum of **18** in Benzene-d_6.

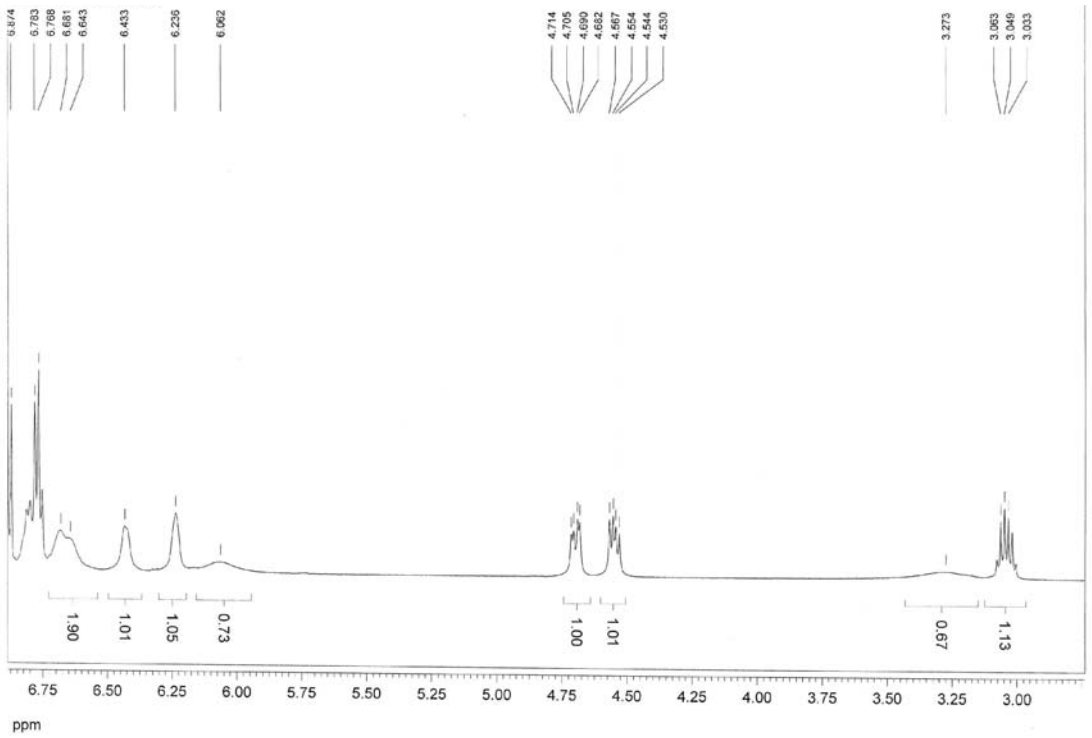


Figure S52. Magnified ^{1}H NMR espectral zone of **18** in Benzene-d_6.

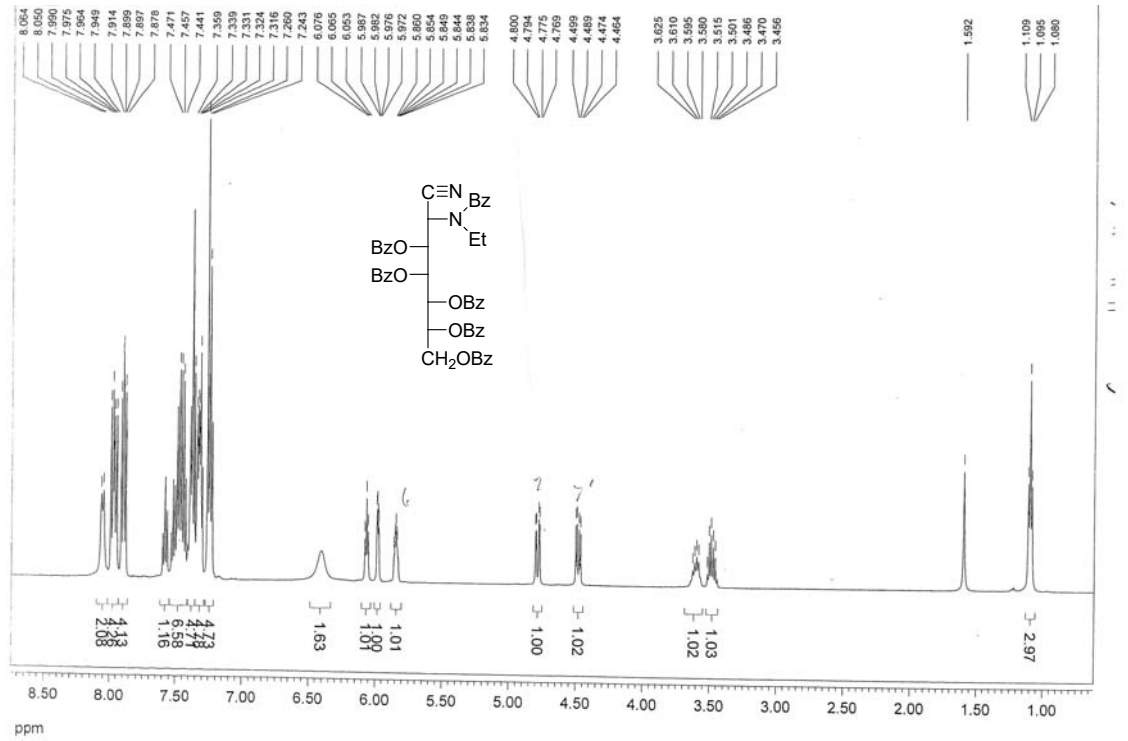


Figure S53. ^{1}H NMR spectrum of **20** in $CDCl_3$.

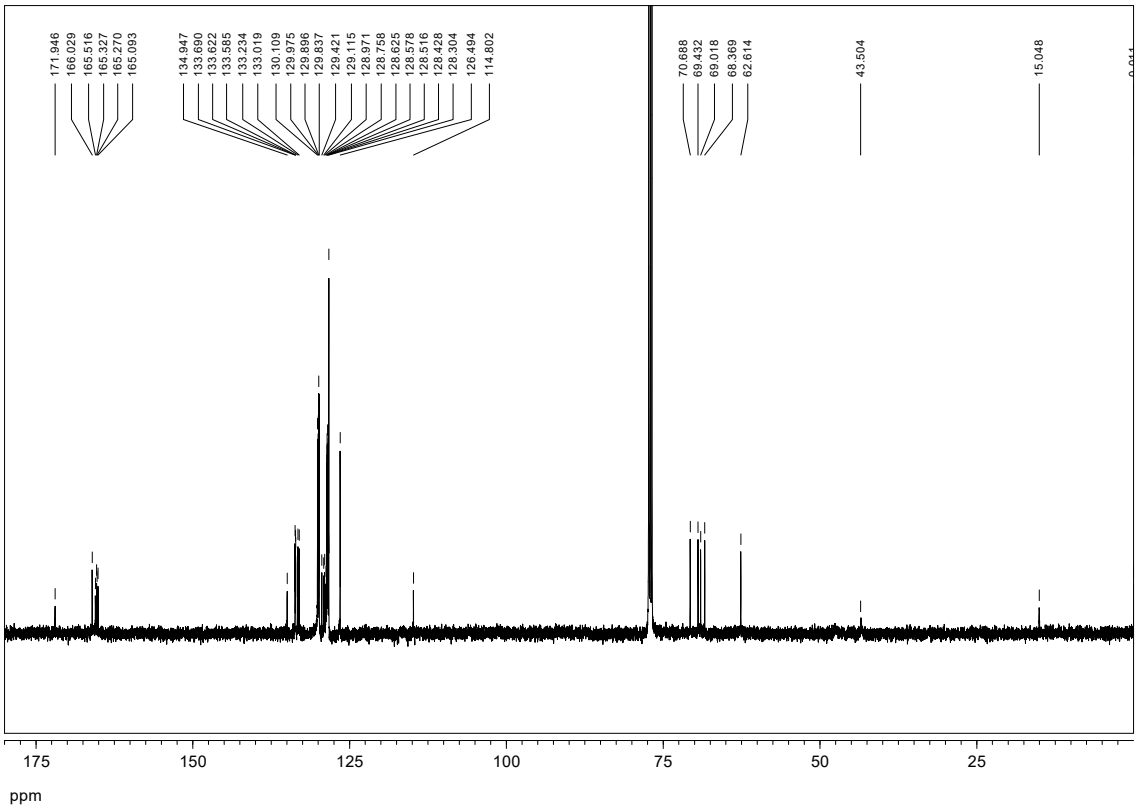


Figure S54. $^{13}C\{^{1}H\}$ NMR spectrum of **20** in $CDCl_3$.

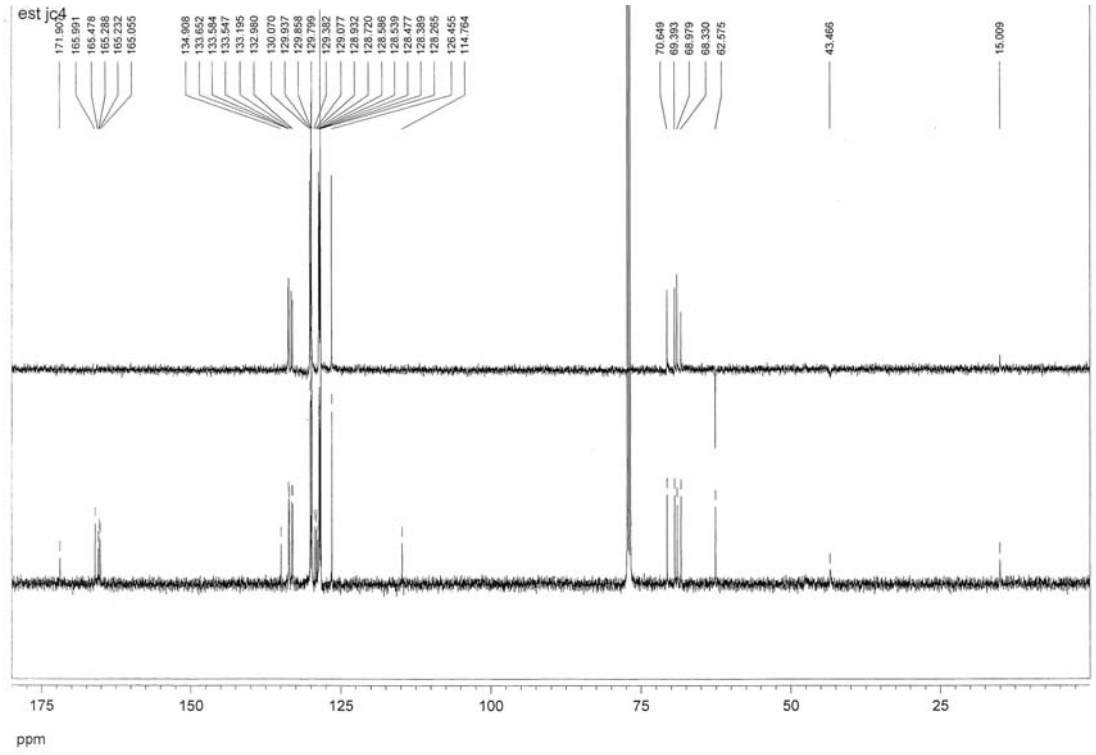


Figure S55. $^{13}C\{^{1}H\}$ NMR and DEPT spectra of **20** in $CDCl_3$.

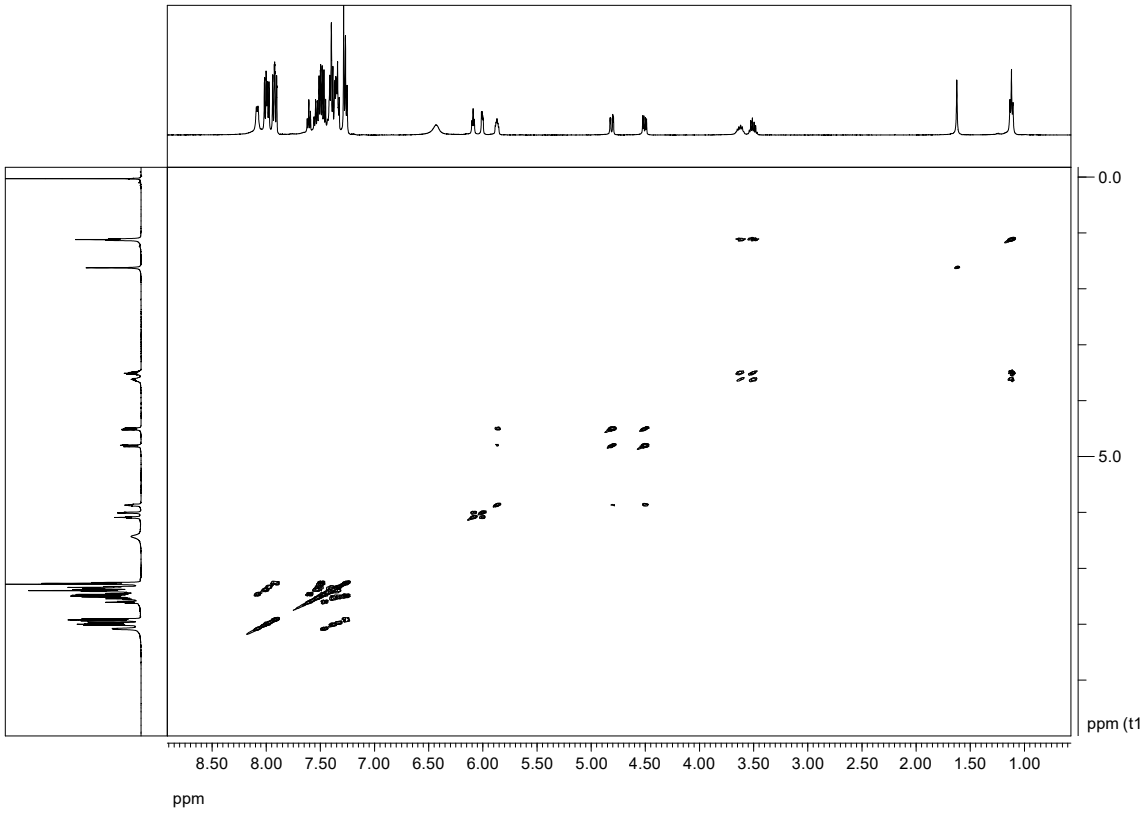


Figure S56. COSY spectrum of **20** in $CDCl_3$.

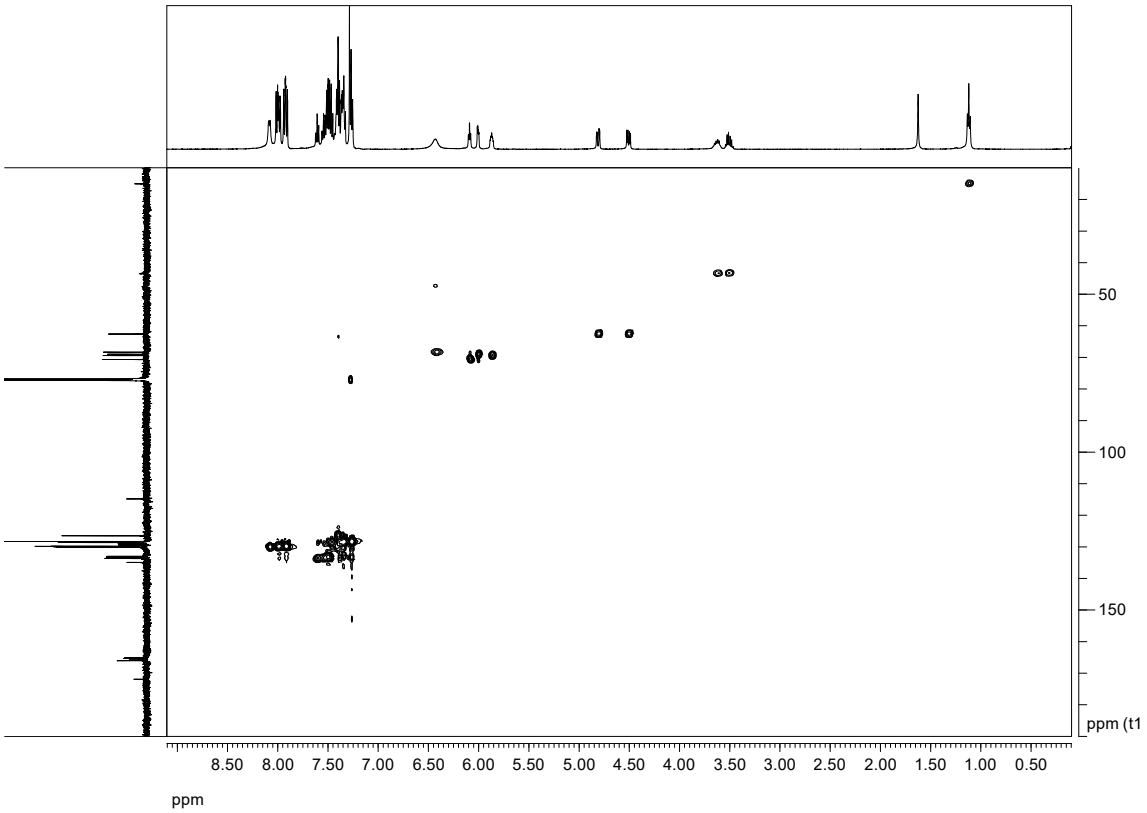


Figure S57. HMQC spectrum of **20** in $CDCl_3$.

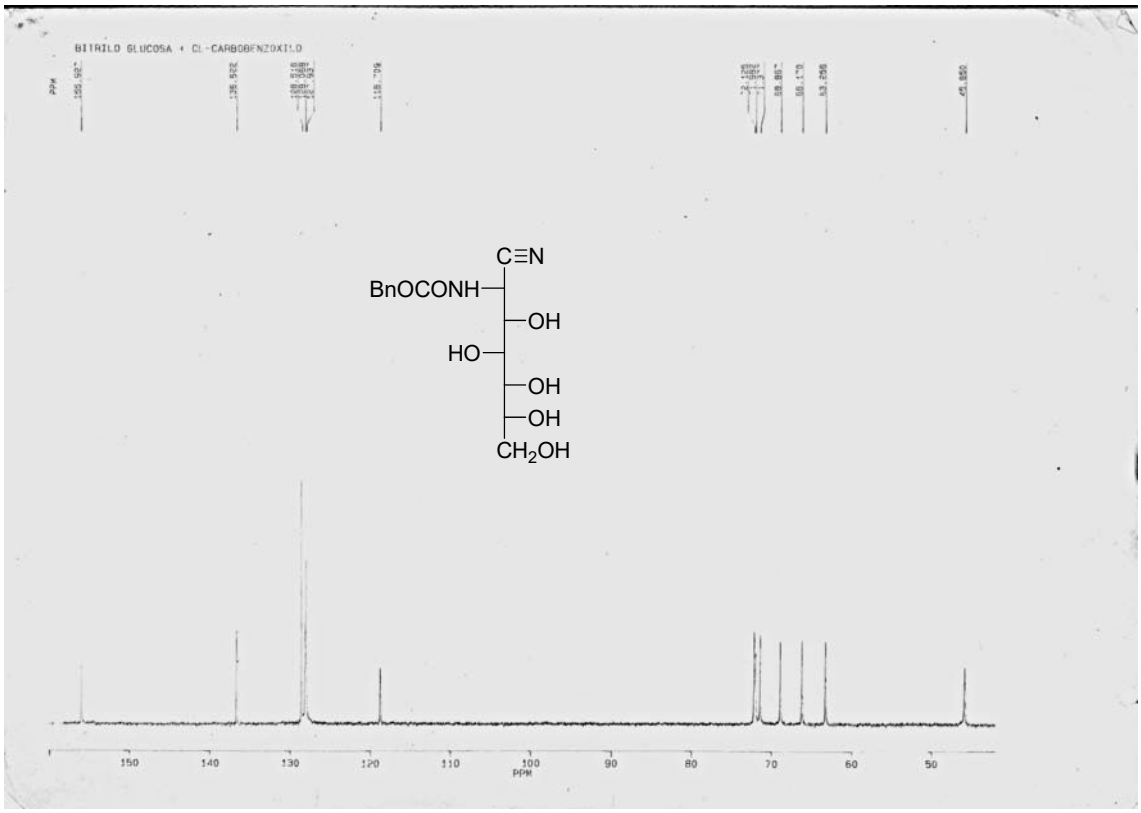


Figure S58. $^{13}C\{^{1}H\}$ NMR spectrum of **26** in DMSO-d_6.

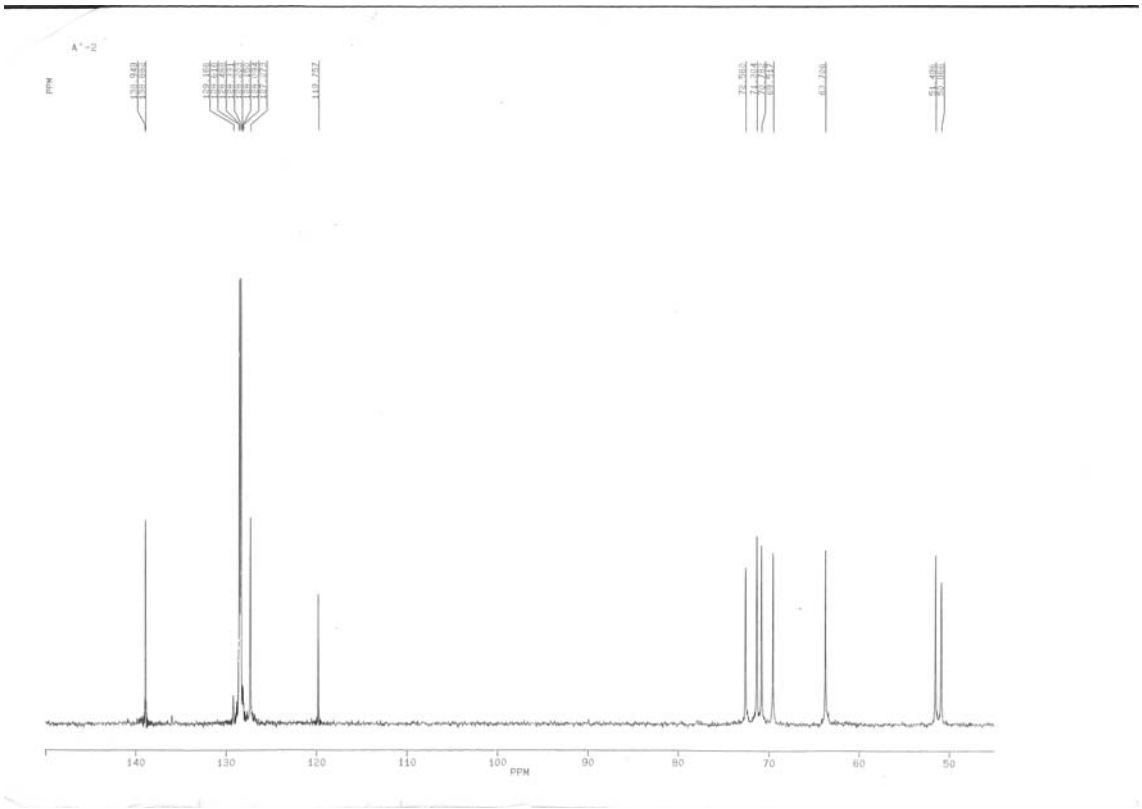


Figure S59. $^{13}C\{^{1}H\}$ NMR spectrum of **33** in $CDCl_3$.

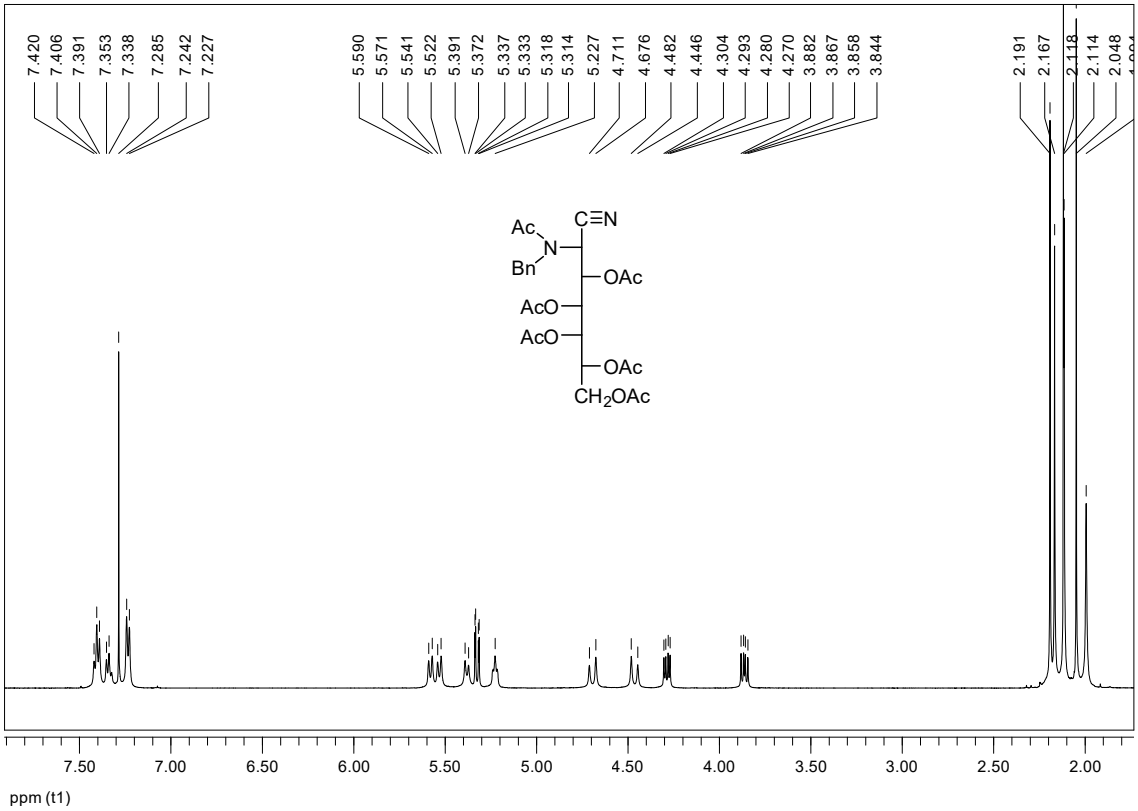


Figure S60. ^{1}H NMR spectrum of **37** in $CDCl_3$.

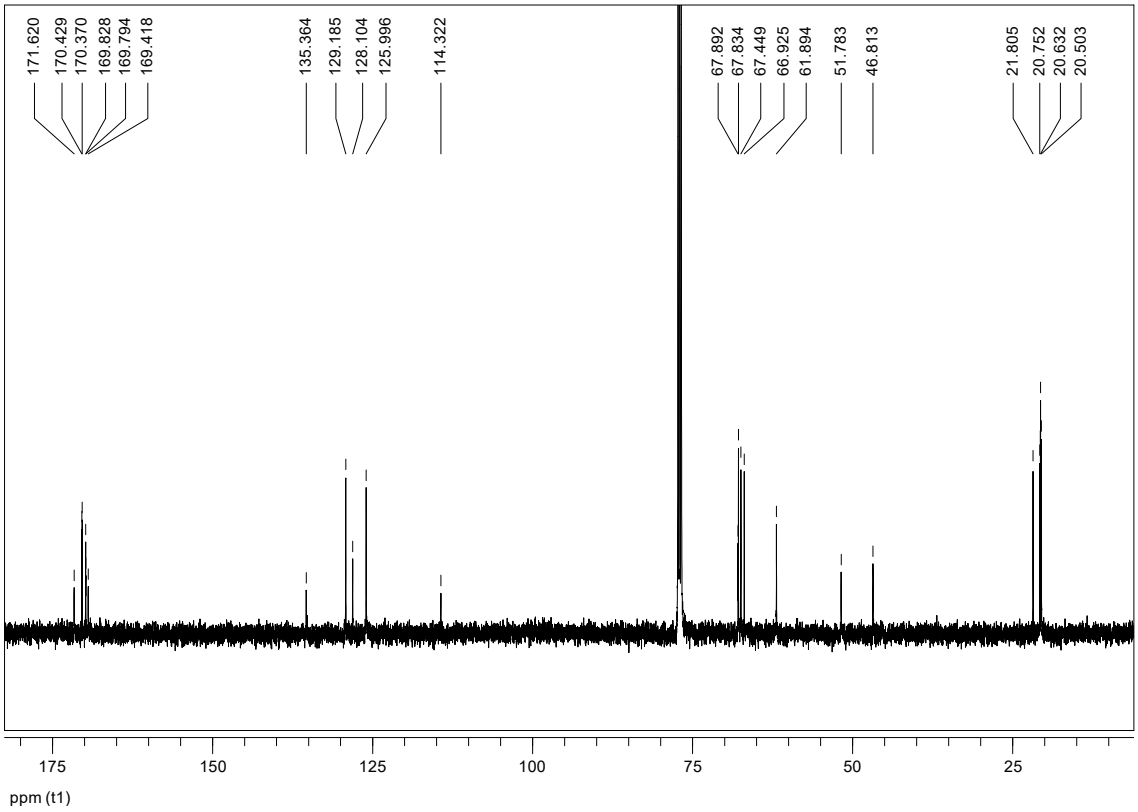


Figure S61. $^{13}C\{^{1}H\}$ NMR spectrum of **37** in $CDCl_3$.

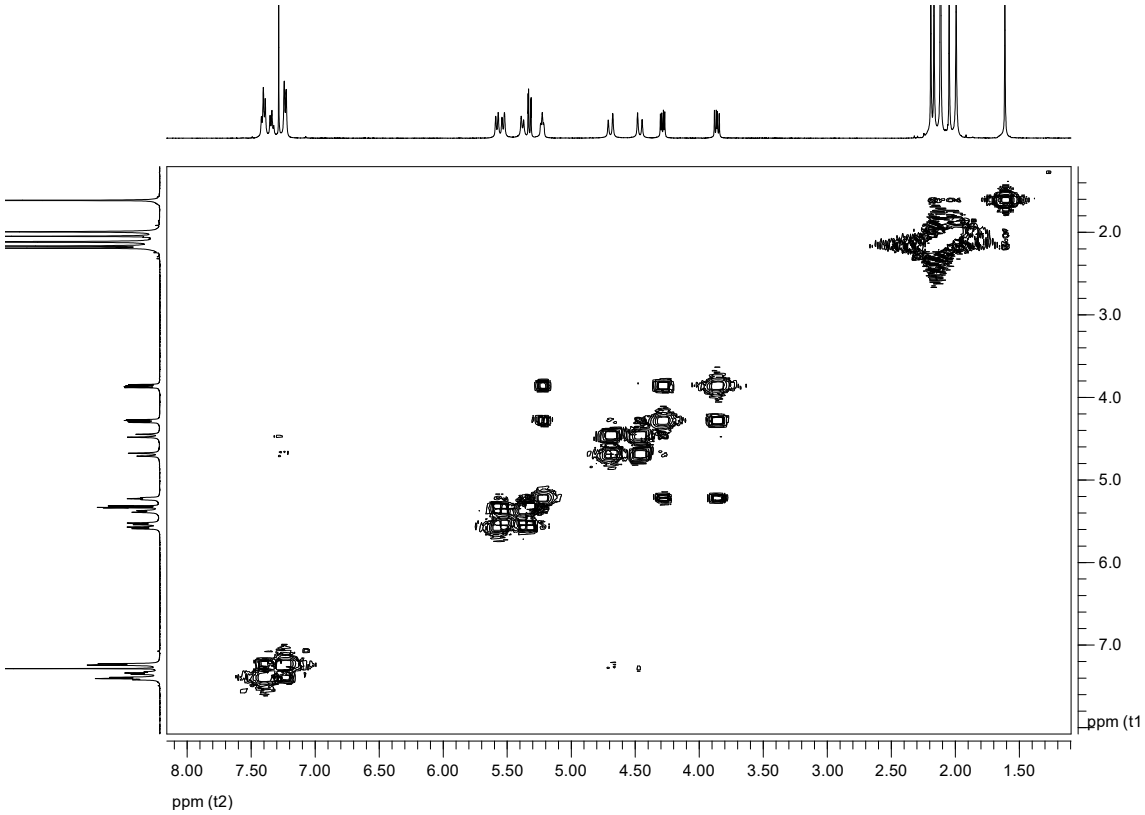


Figure S62. COSY spectrum of **37** in $CDCl_3$.

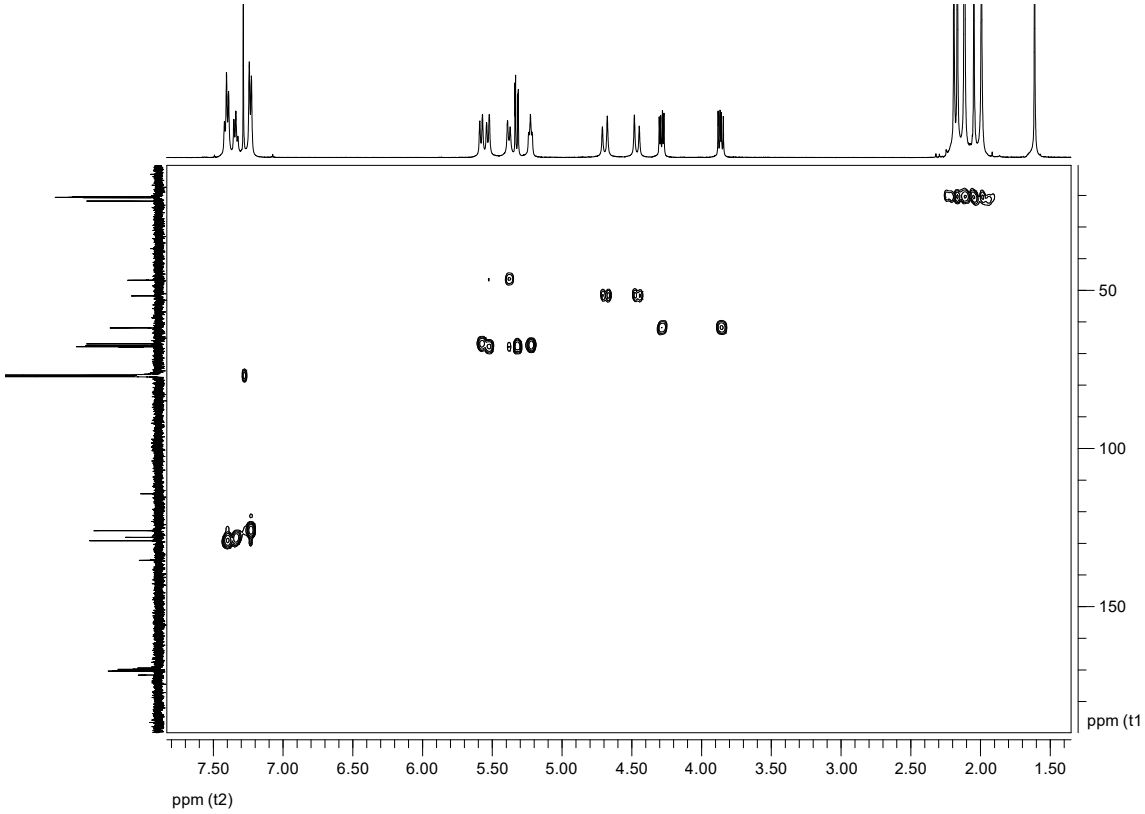


Figure S63. HMQC spectrum of **37** in $CDCl_3$.

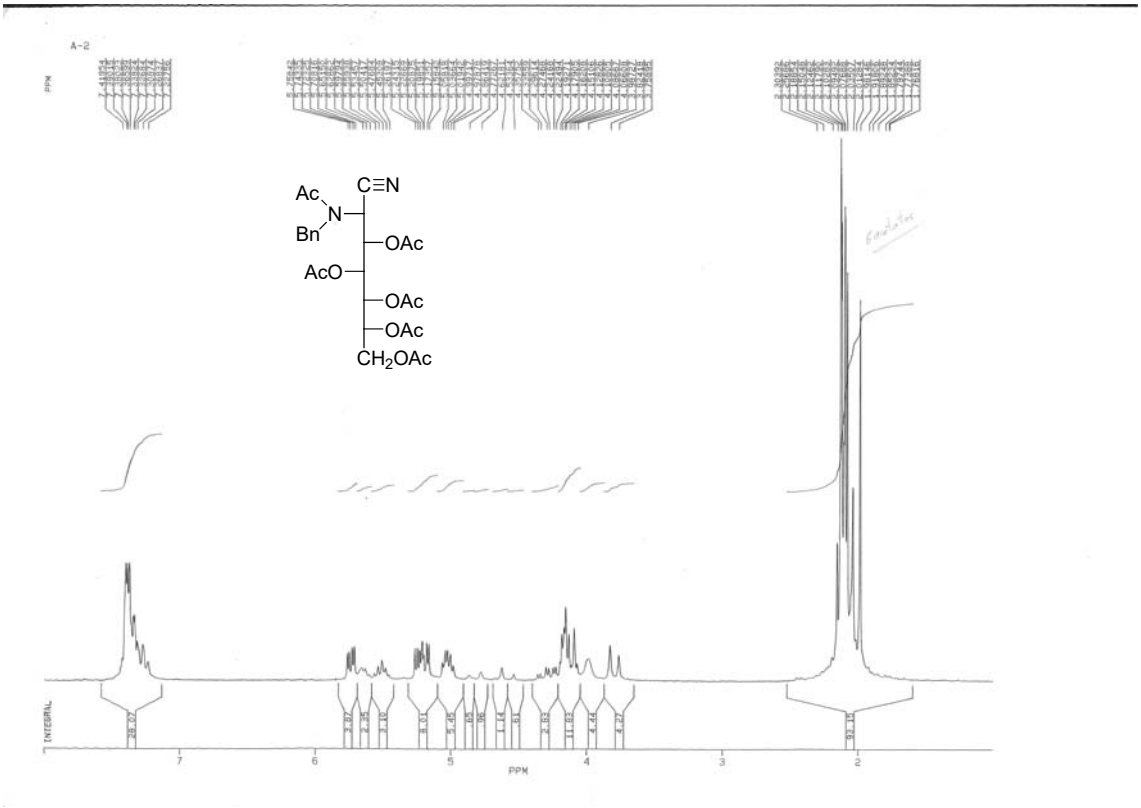


Figure S64. ^{1}H NMR spectrum of **38** in $CDCl_3$.

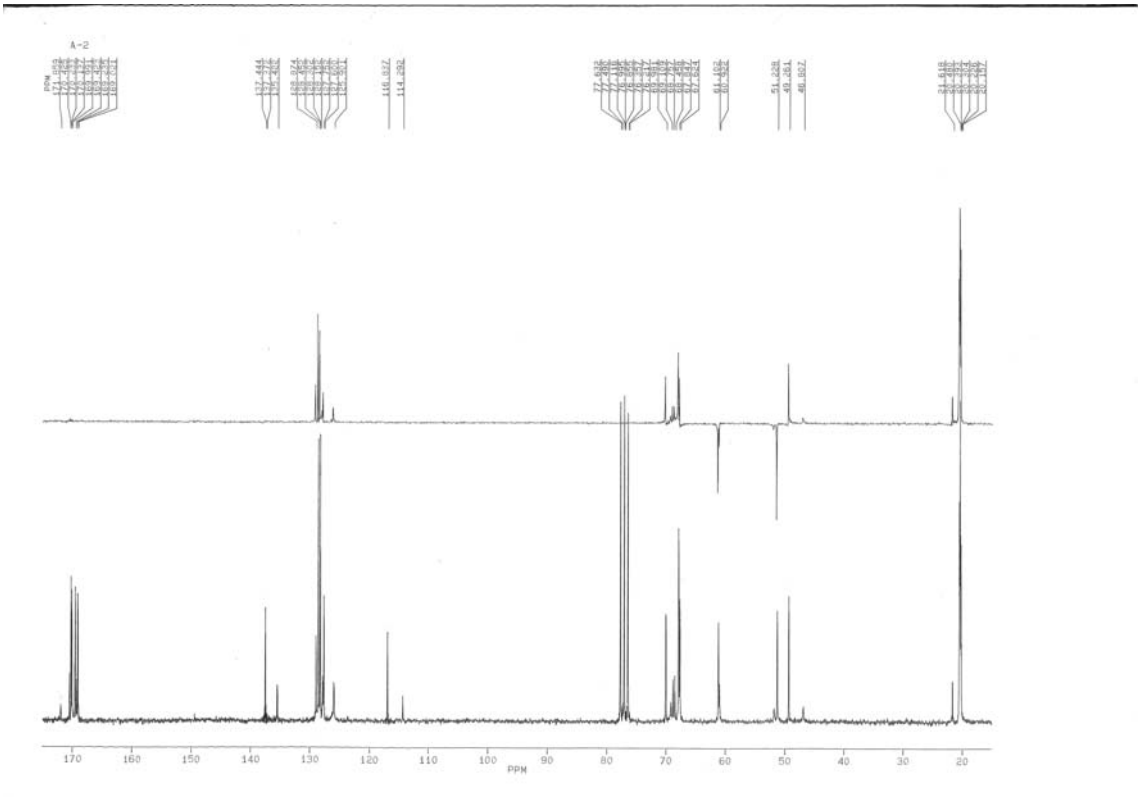


Figure S65. $^{13}C\{^{1}H\}$ NMR and DEPT spectra of **38** in $CDCl_3$

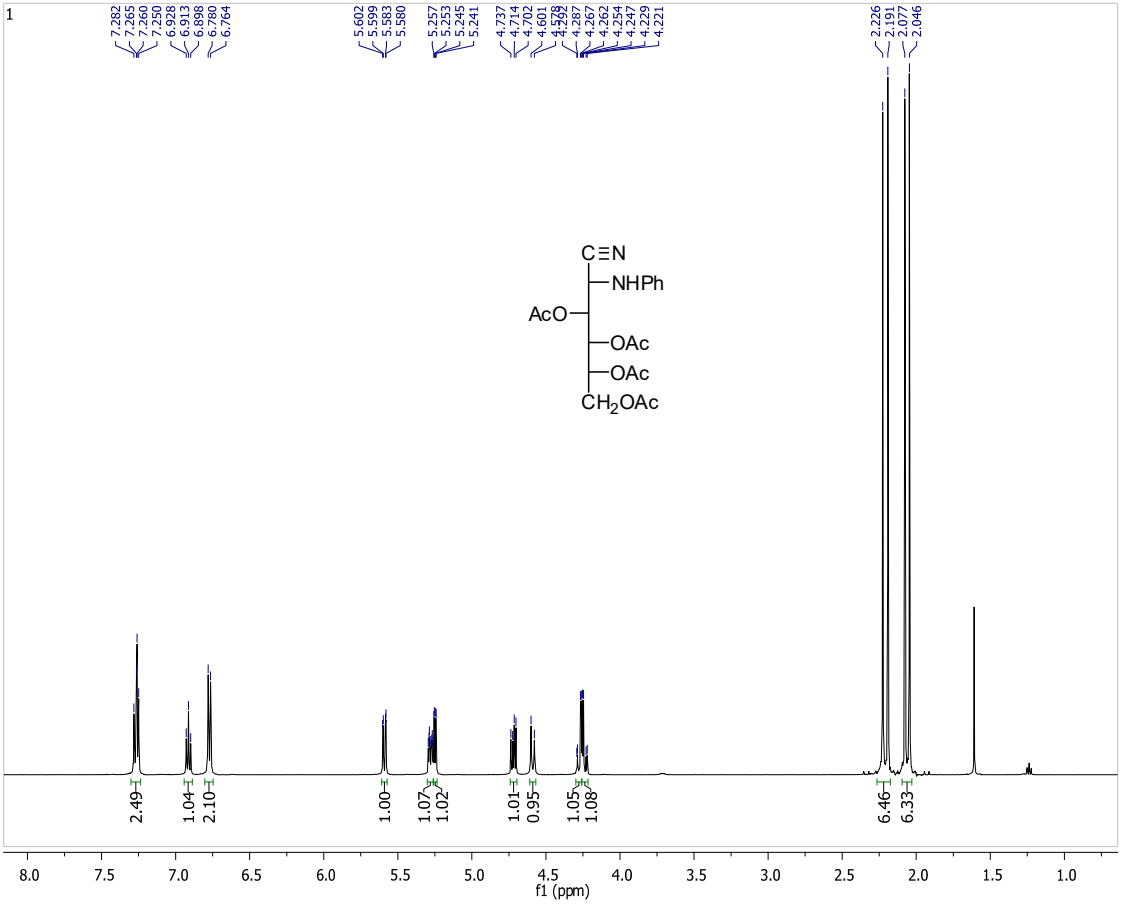


Figure S66. ^{1}H NMR spectrum of **42** in $CDCl_3$.

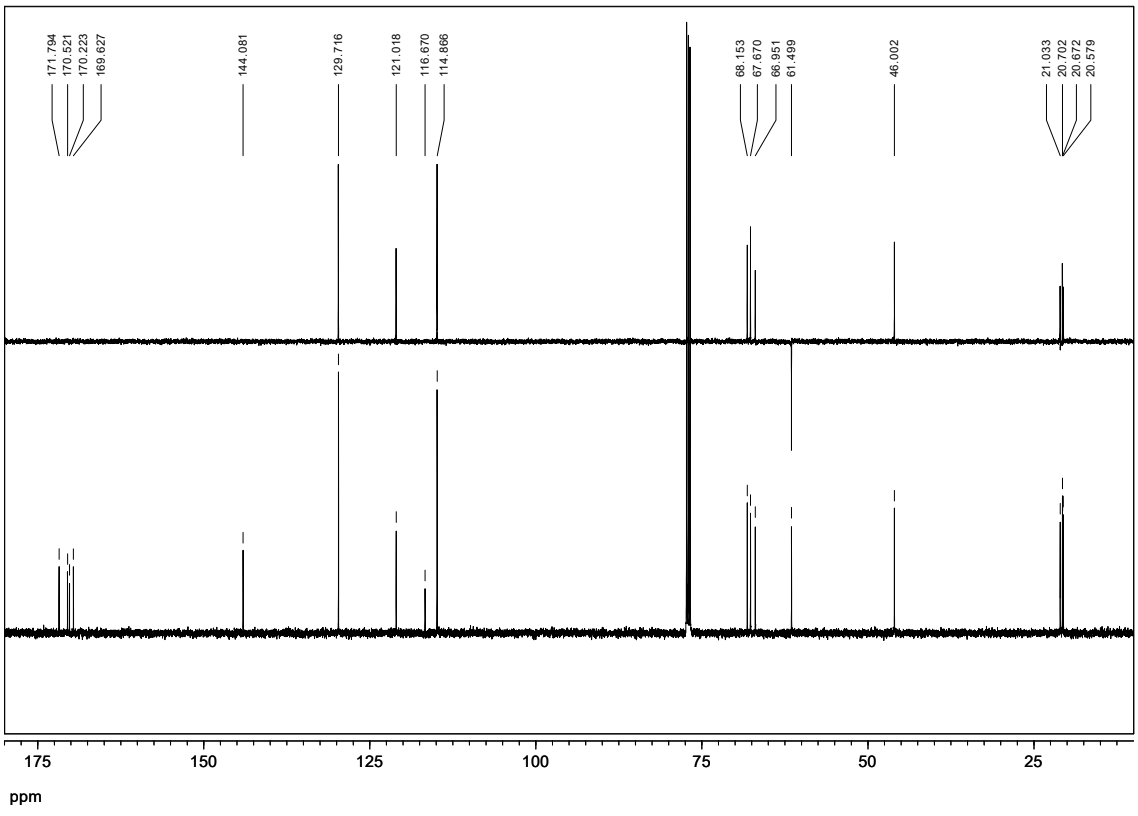


Figure S67. $^{13}C\{^{1}H\}$ NMR and DEPT spectra of **42** in $CDCl_3$.

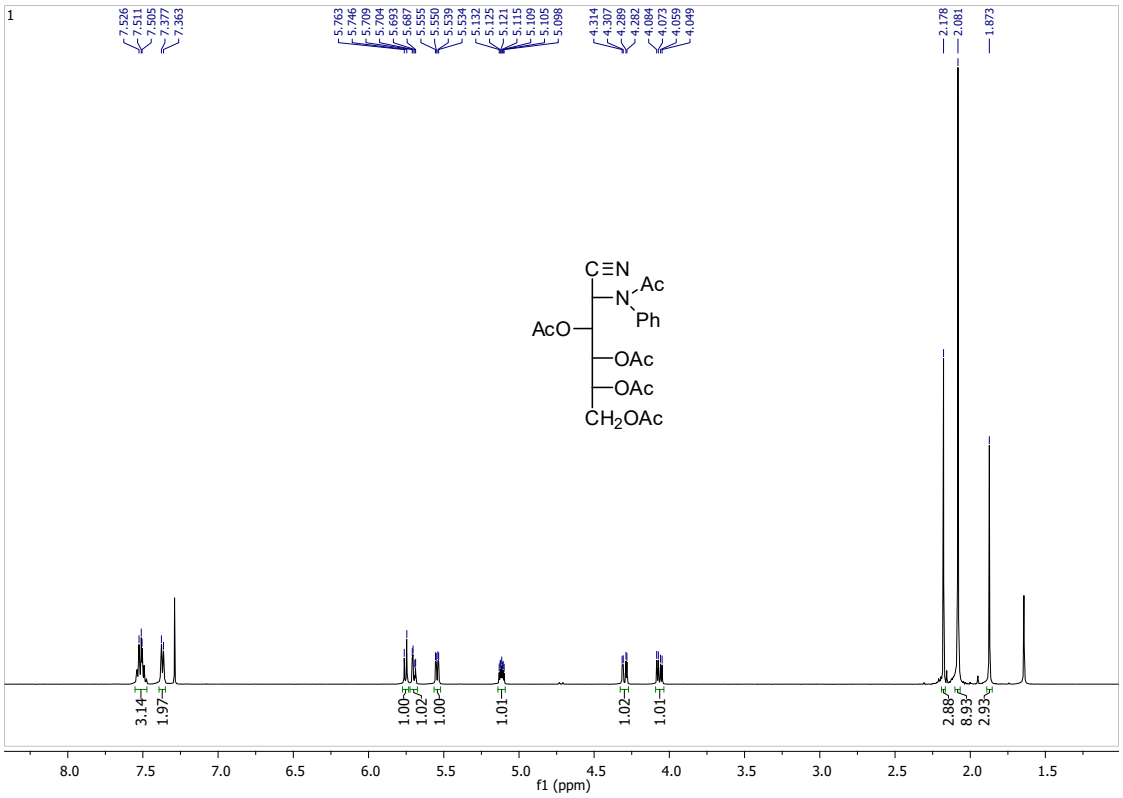


Figure S68. ^{1}H NMR spectrum of **43** in $CDCl_3$.

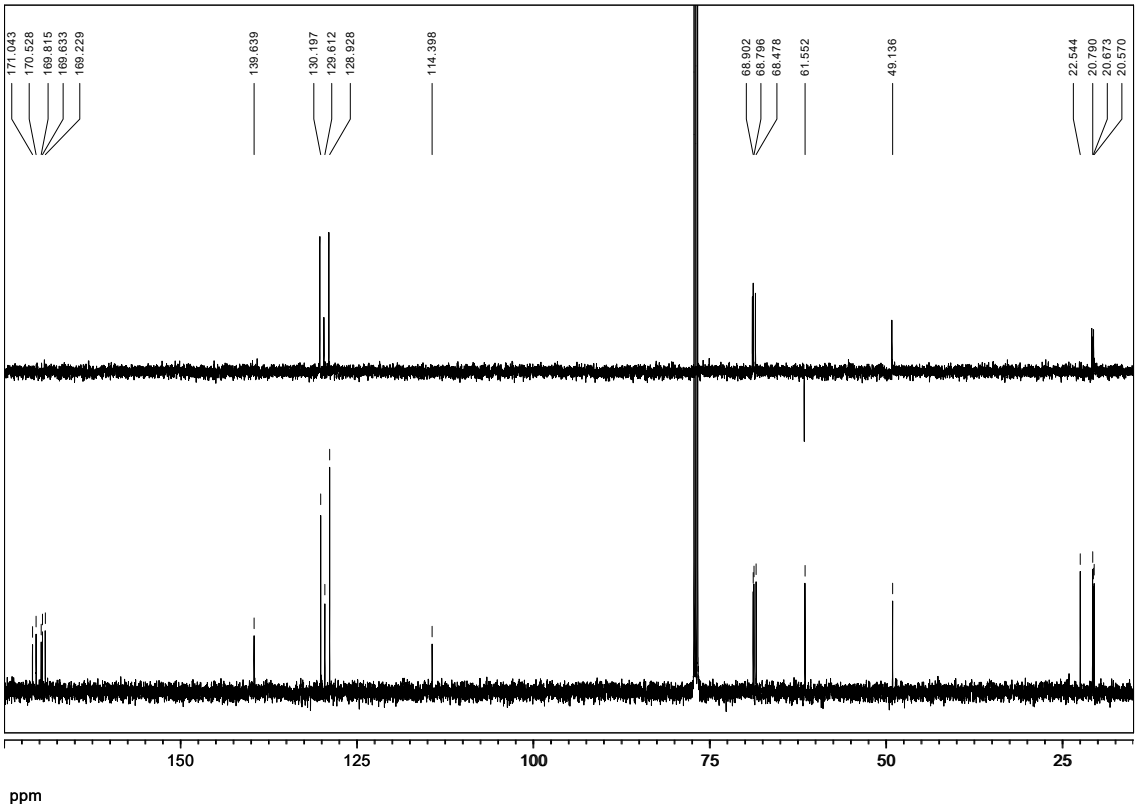


Figure S69. $^{13}C\{^{1}H\}$ NMR and DEPT spectra of **43** in $CDCl_3$.

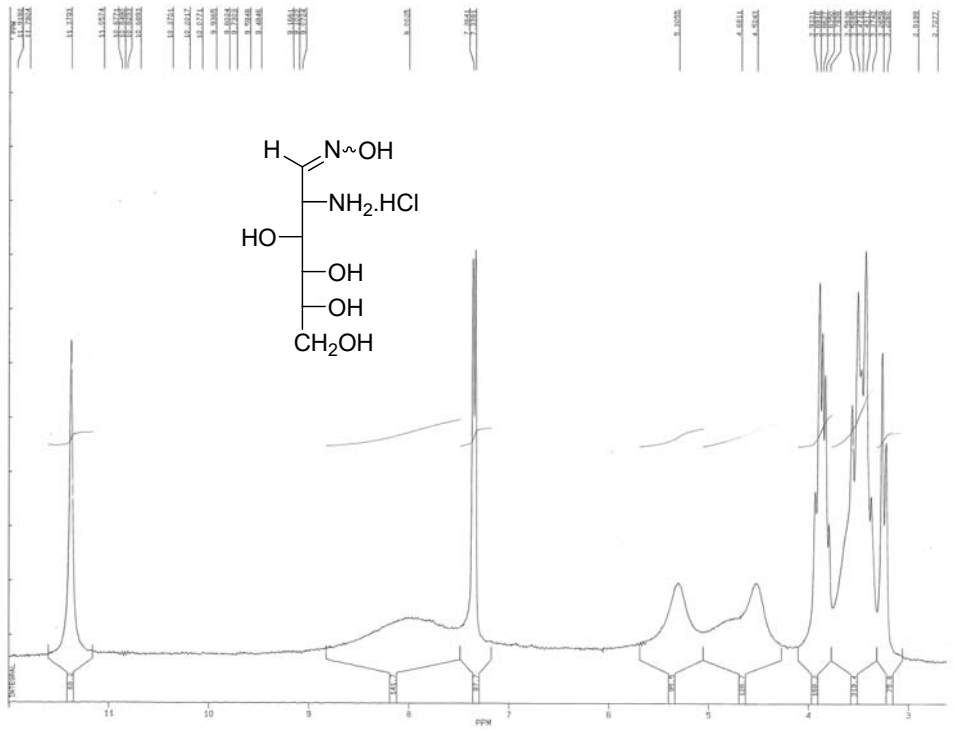


Figure S70. ^{1}H NMR spectrum of **45** in DMSO-d_6.

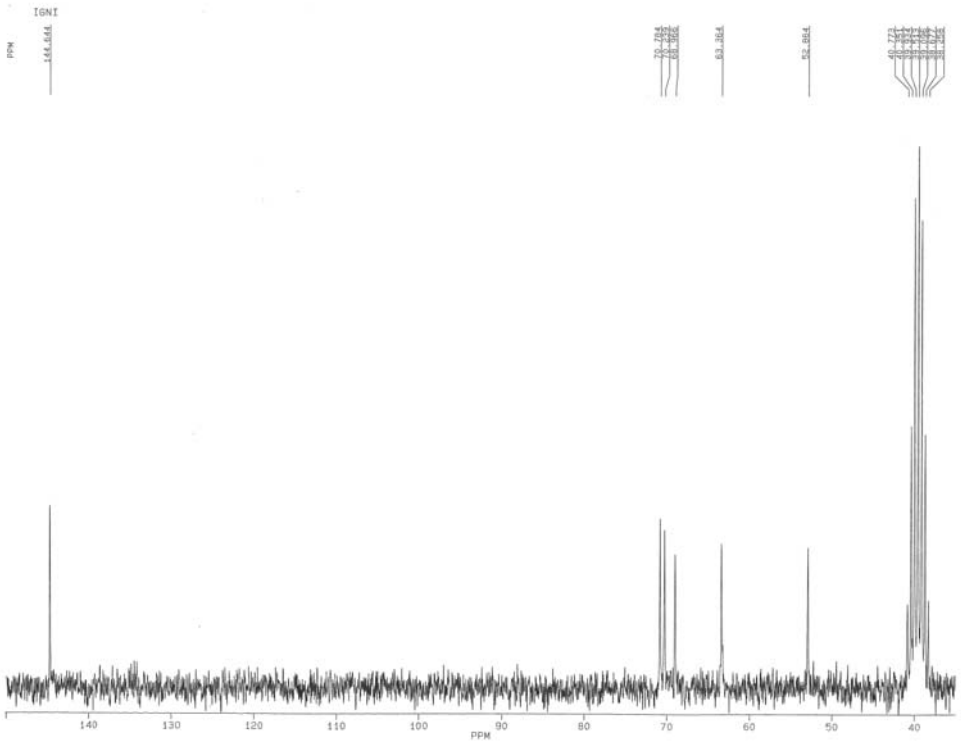


Figure S71. ^{13}C{^{1}H} NMR spectrum of **45** in DMSO-d_6..

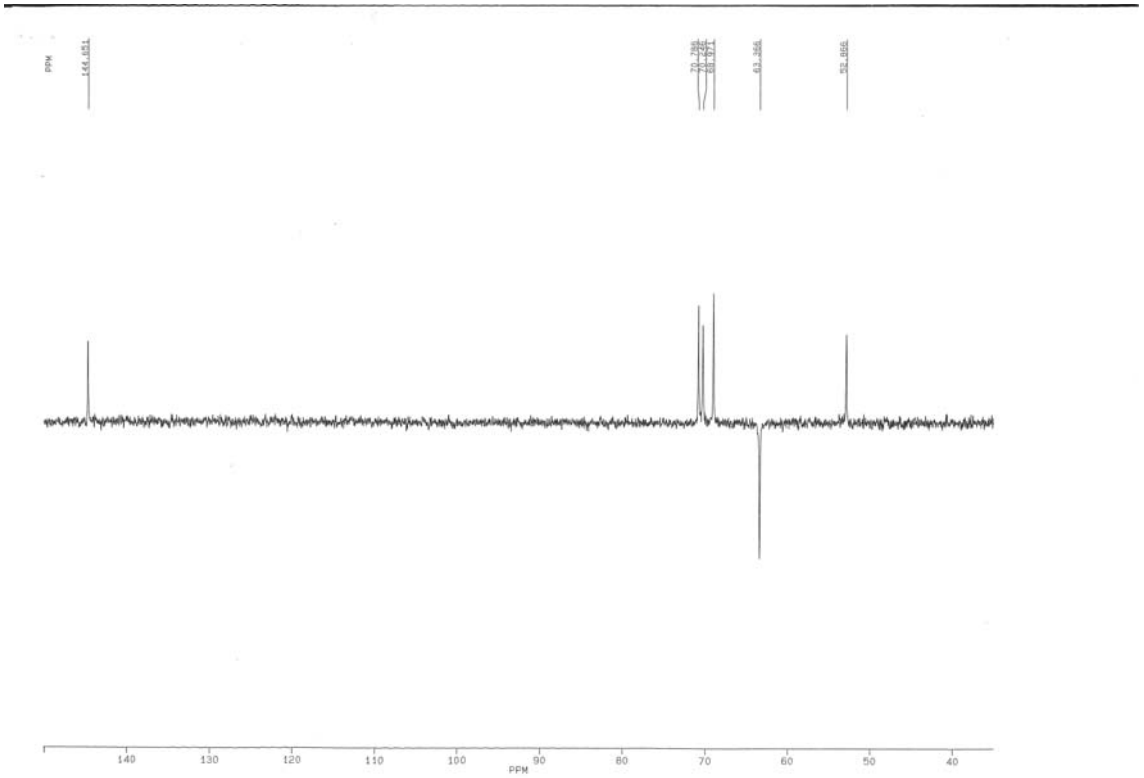


Figure S72. DEPT spectrum of **45** in DMSO-d_6.

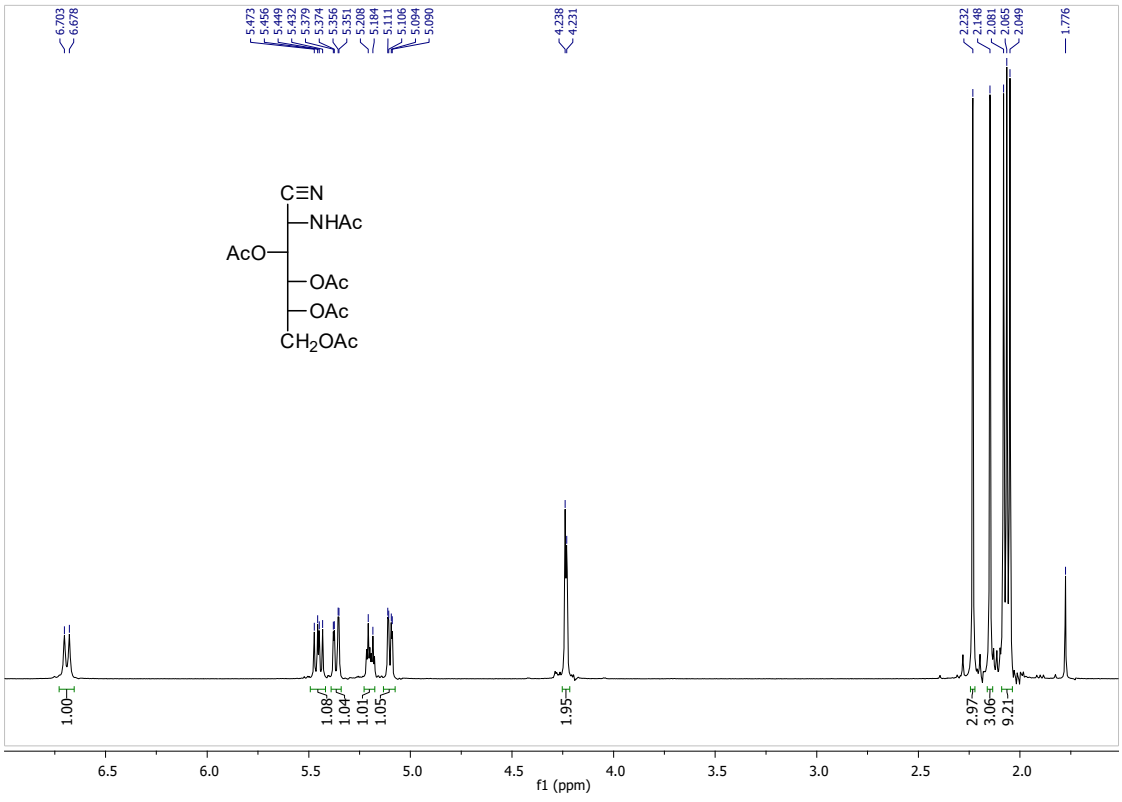


Figure S73. ^{1}H NMR spectrum of **47** in $CDCl_3$.

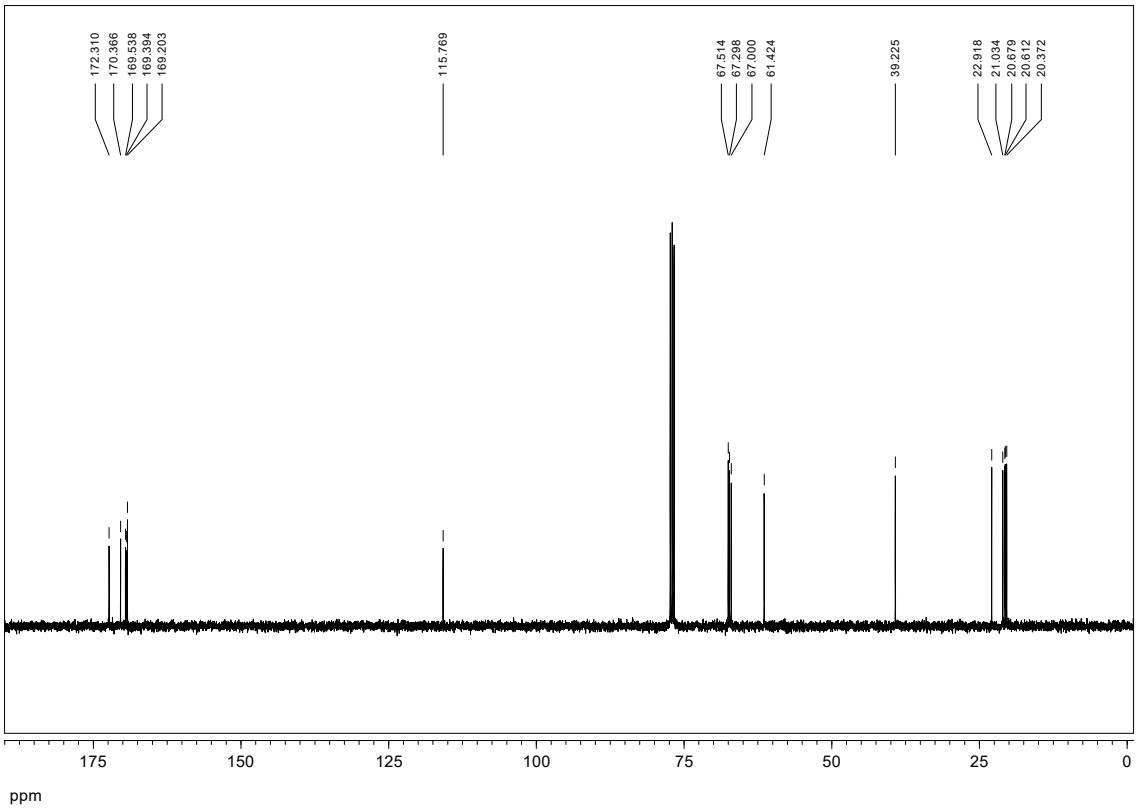


Figure S74. $^{13}C\{^{1}H\}$ NMR spectrum of **47** in $CDCl_3$.

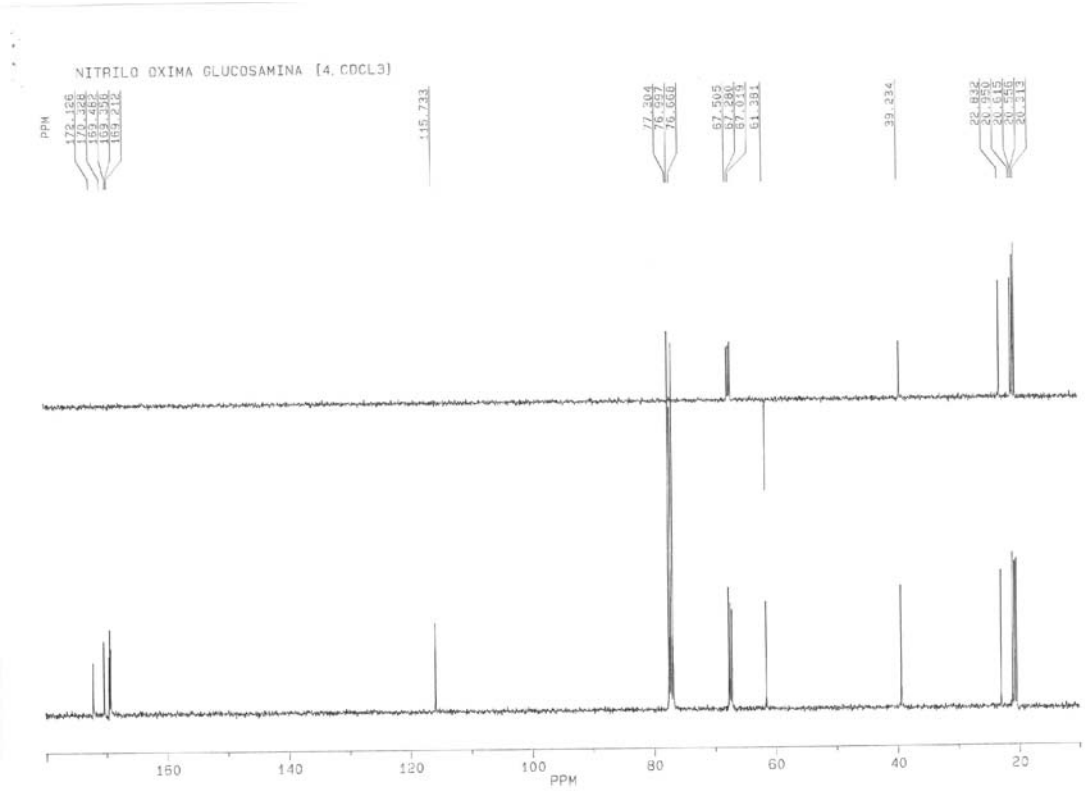


Figure S75. $^{13}C\{^{1}H\}$ NMR and DEPT spectra of **47** in $CDCl_3$.

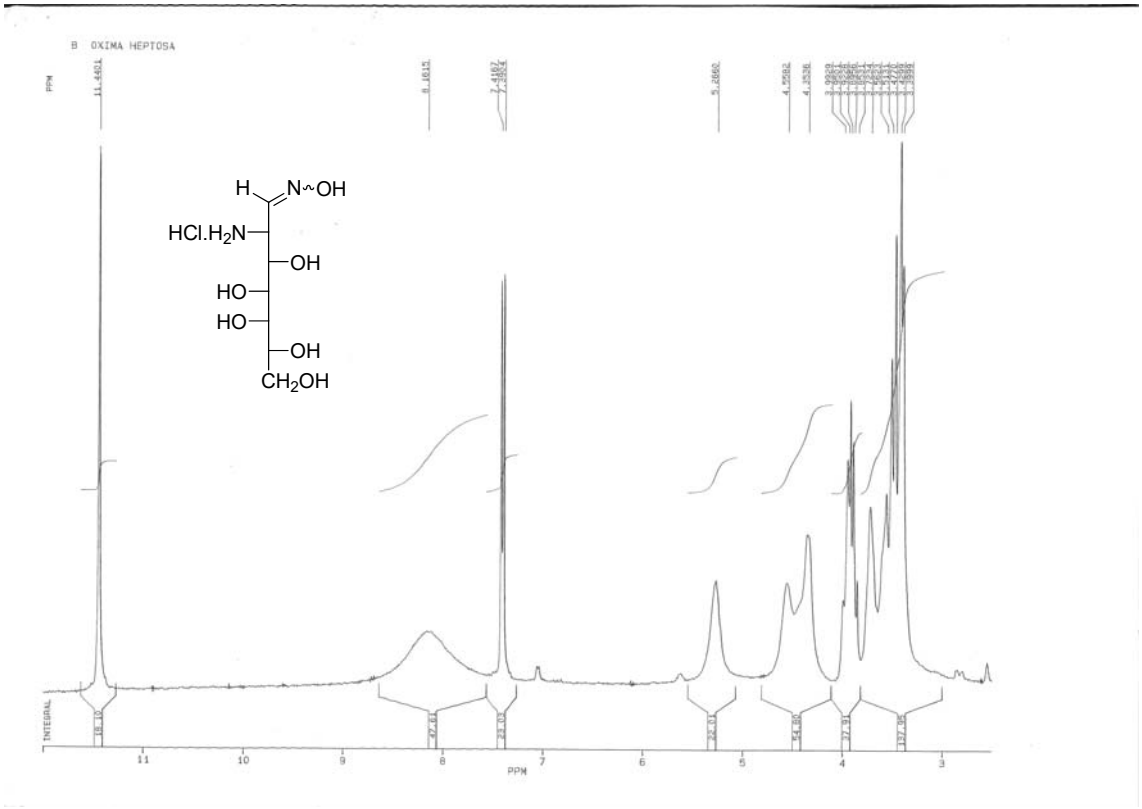


Figure S76. ^{1}H NMR spectrum of **49** in DMSO-d_6.

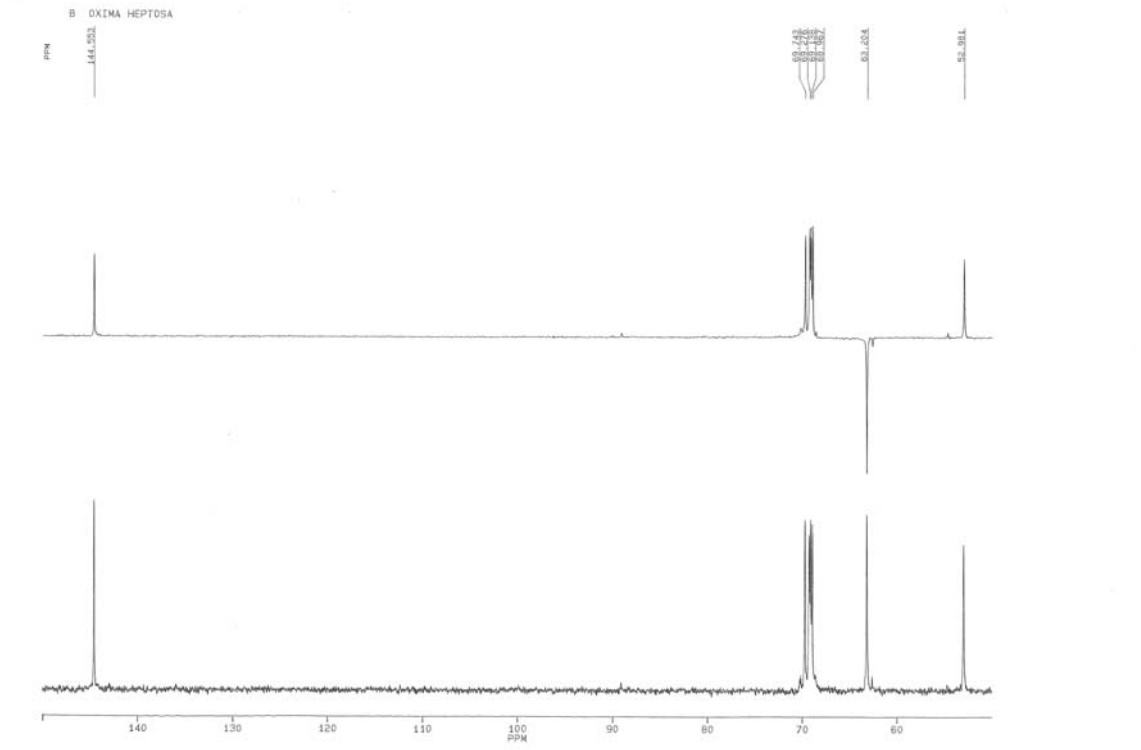


Figure S77. ^{13}C{^{1}H} NMR and DEPT spectra of **49** in DMSO-d_6..

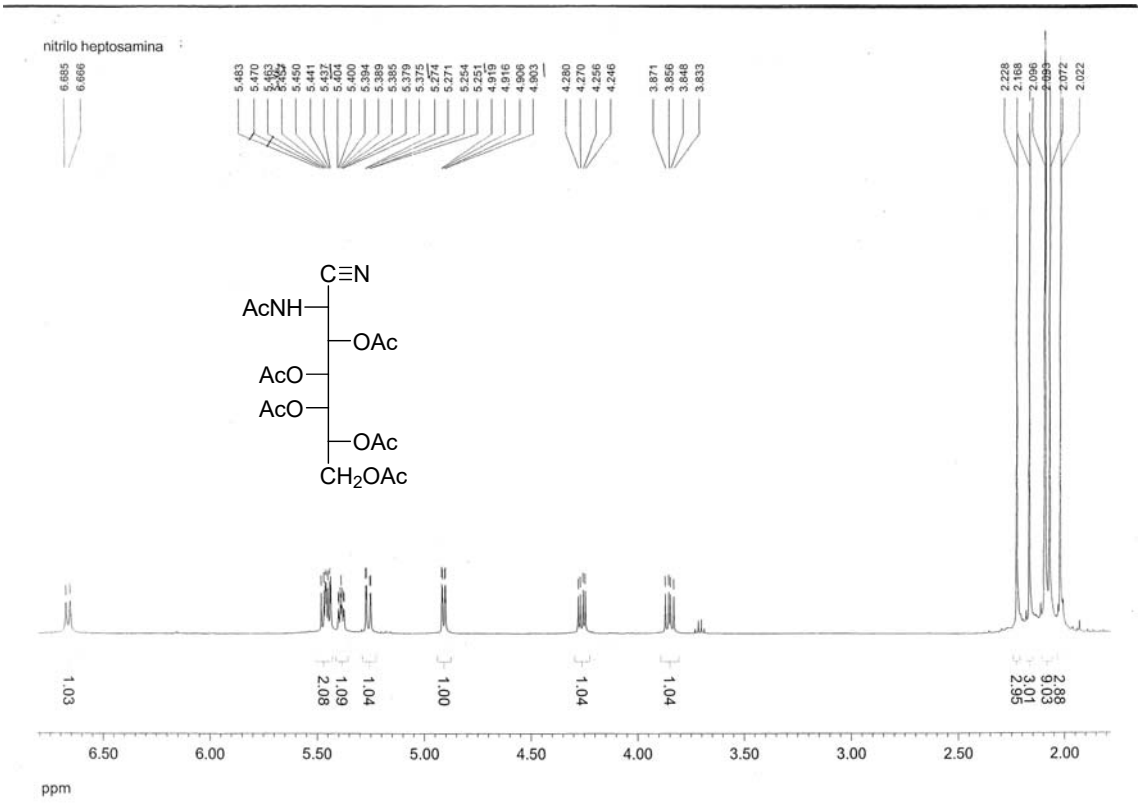


Figure S78. ^{1}H NMR spectrum of **51** in $CDCl_3$.

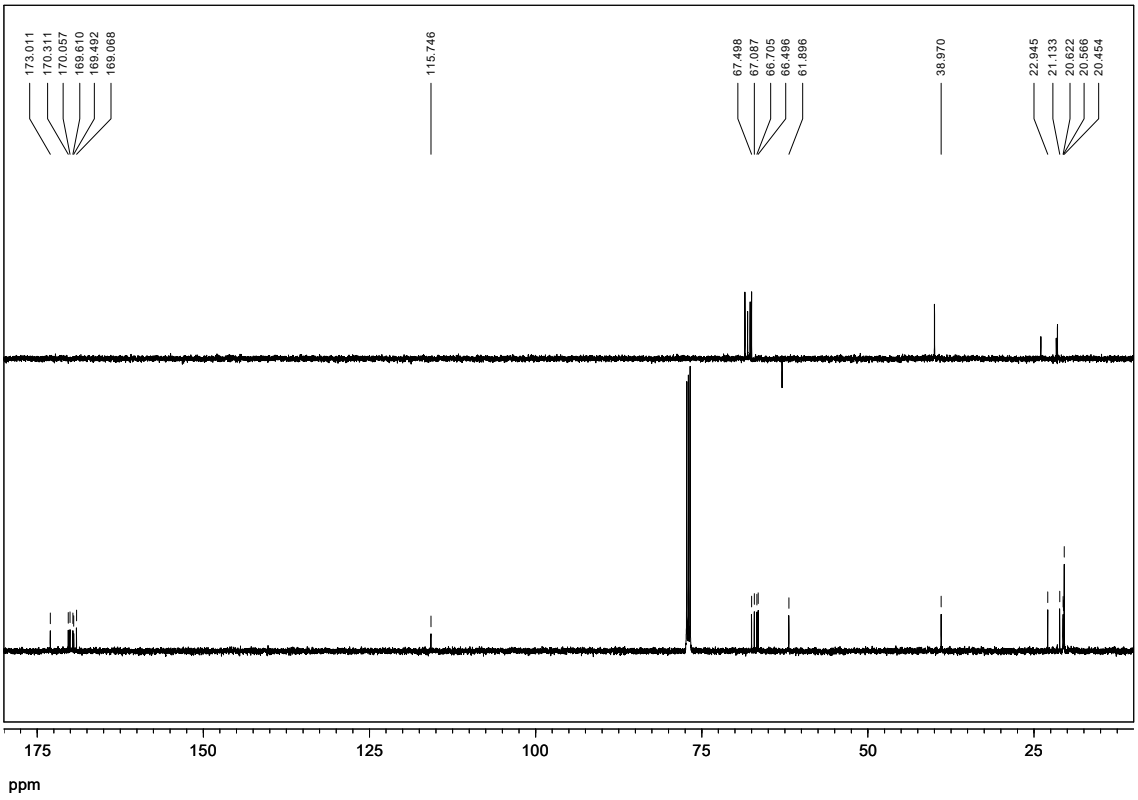


Figure S79. $^{13}C\{^{1}H\}$ NMR and DEPT spectra of **51** in $CDCl_3$.

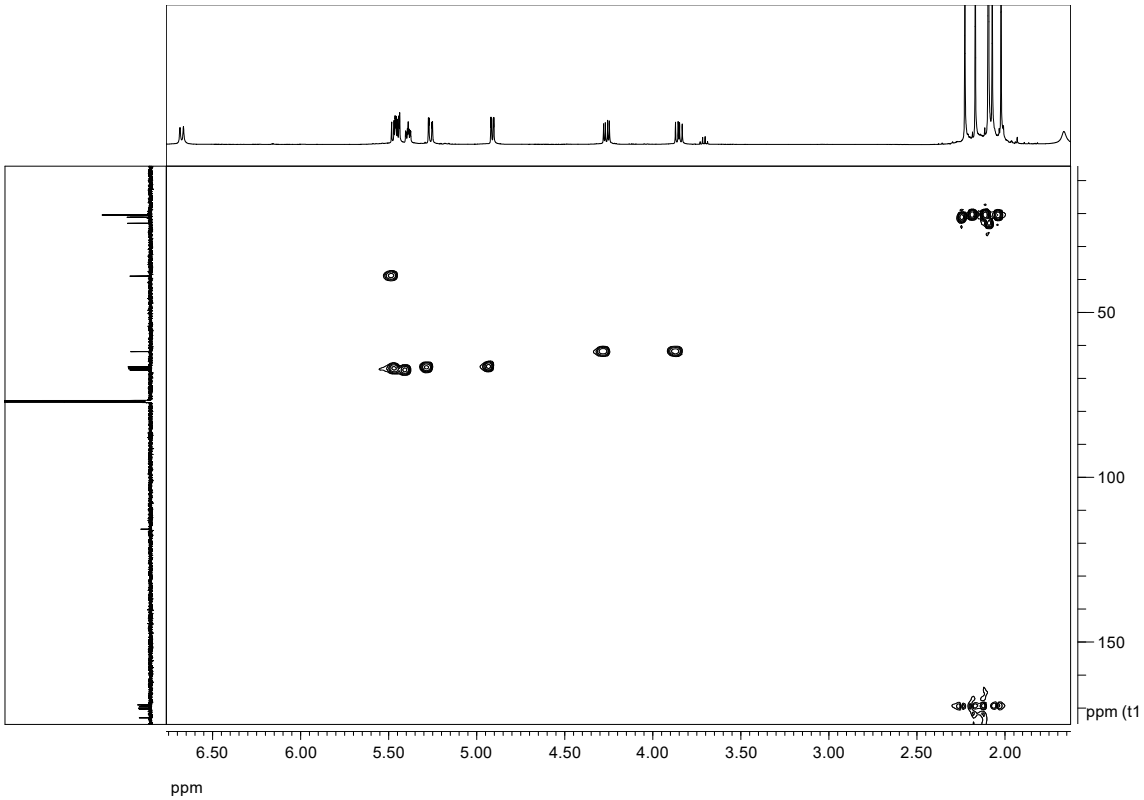


Figure S80. HMQC spectrum of **51** in $CDCl_3$.

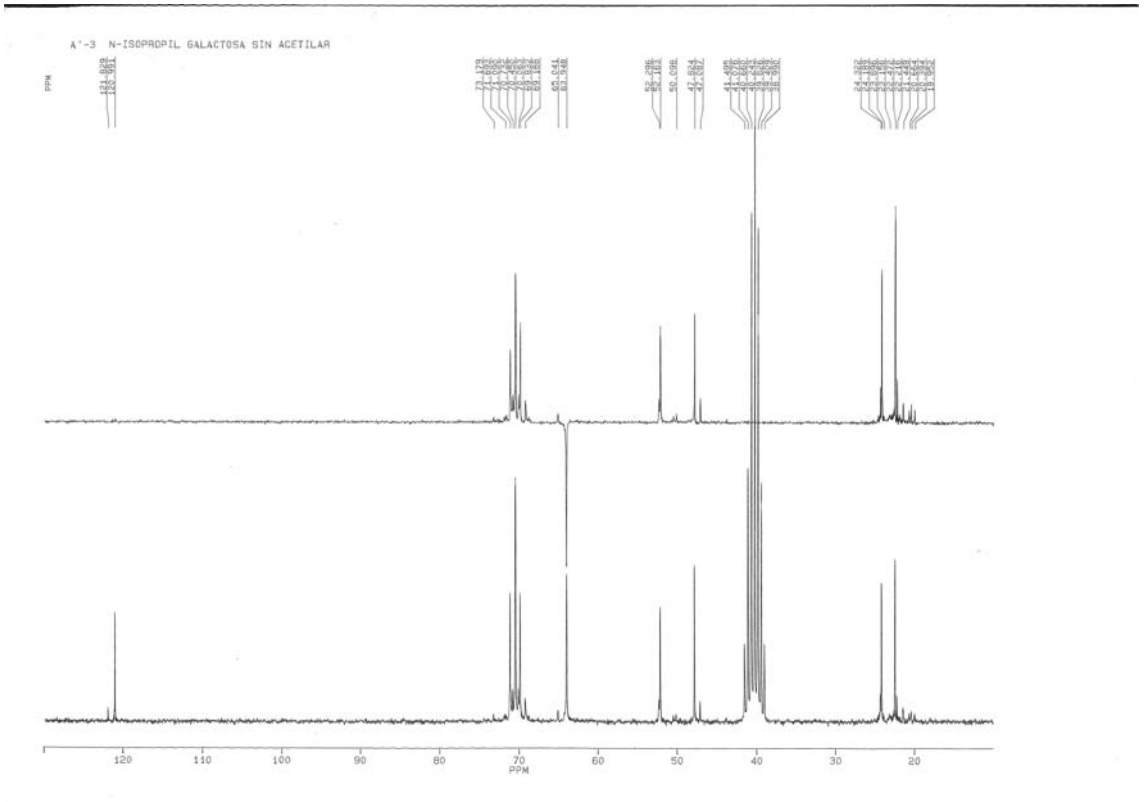


Figure S81. $^{13}C\{^1H\}$ NMR and DEPT spectra of **54** in DMSO-d_6.

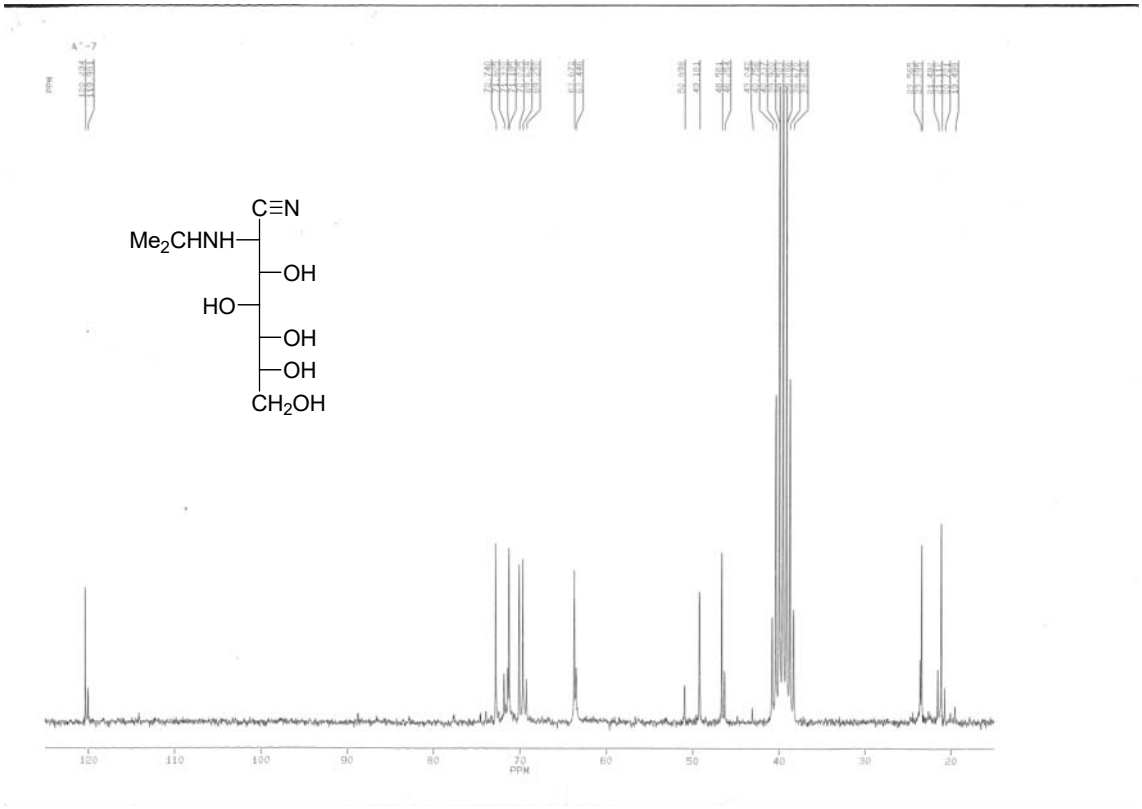


Figure S82. $^{13}C\{^{1}H\}$ NMR spectrum of **55** in DMSO-d_6.

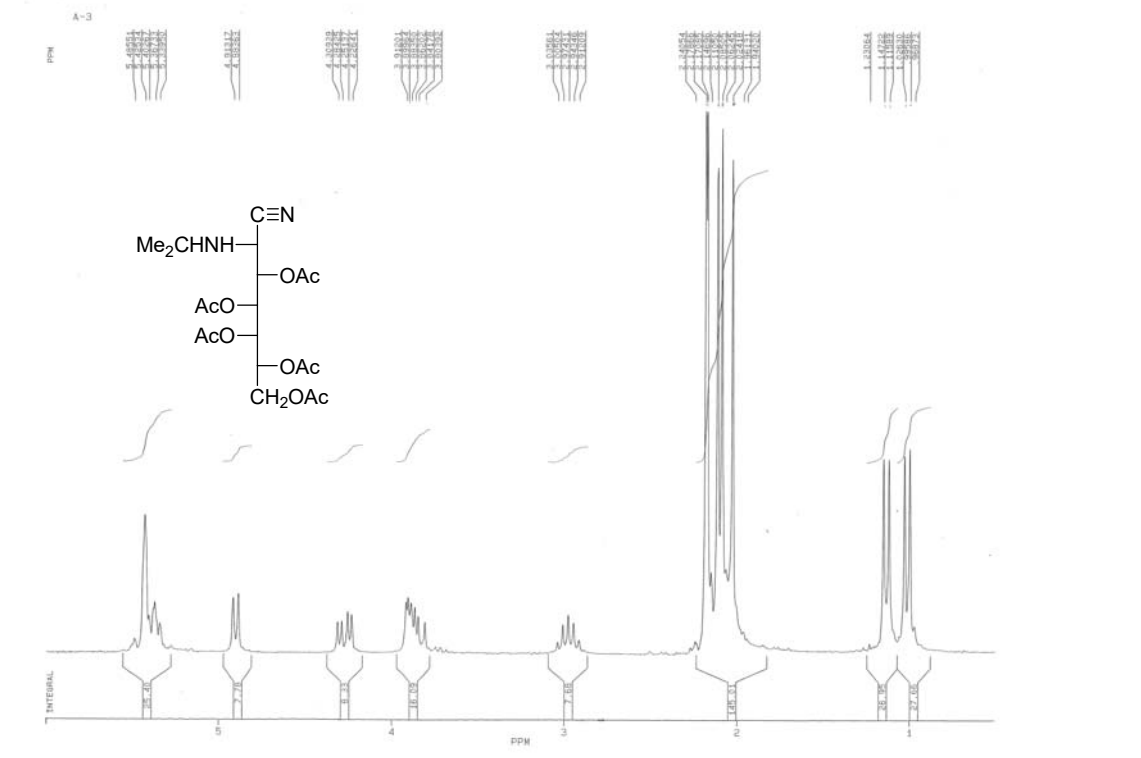


Figure S83. ^{1}H NMR spectrum of **58** in $CDCl_3$.

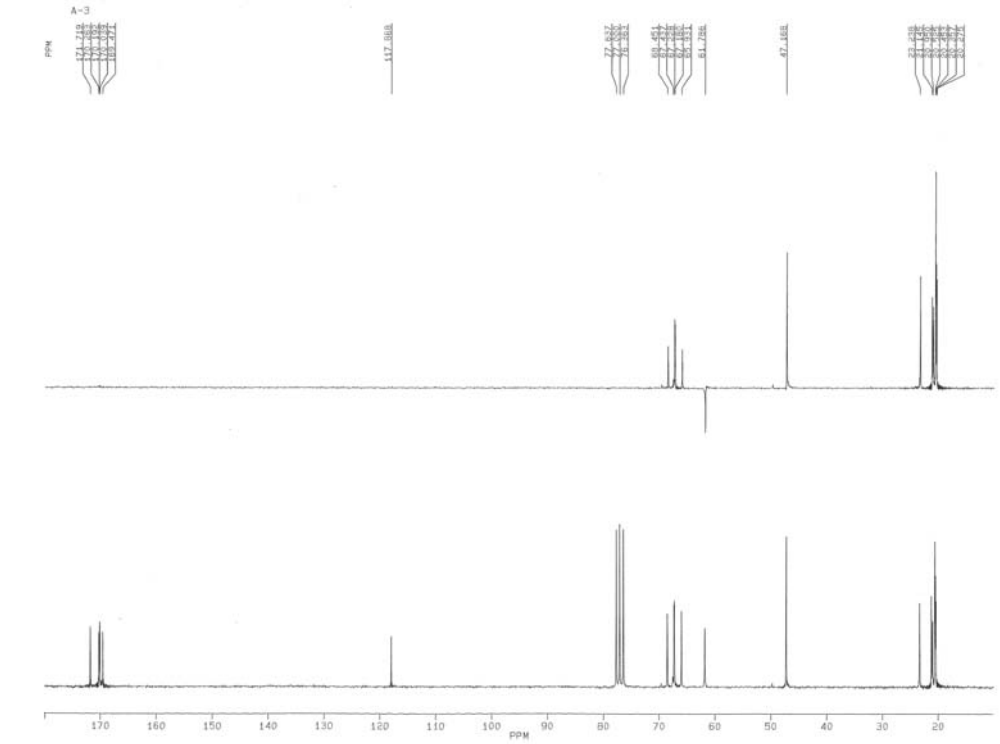


Figure S84. $^{13}C\{^{1}H\}$ NMR and DEPT spectra of **58** in $CDCl_3$.

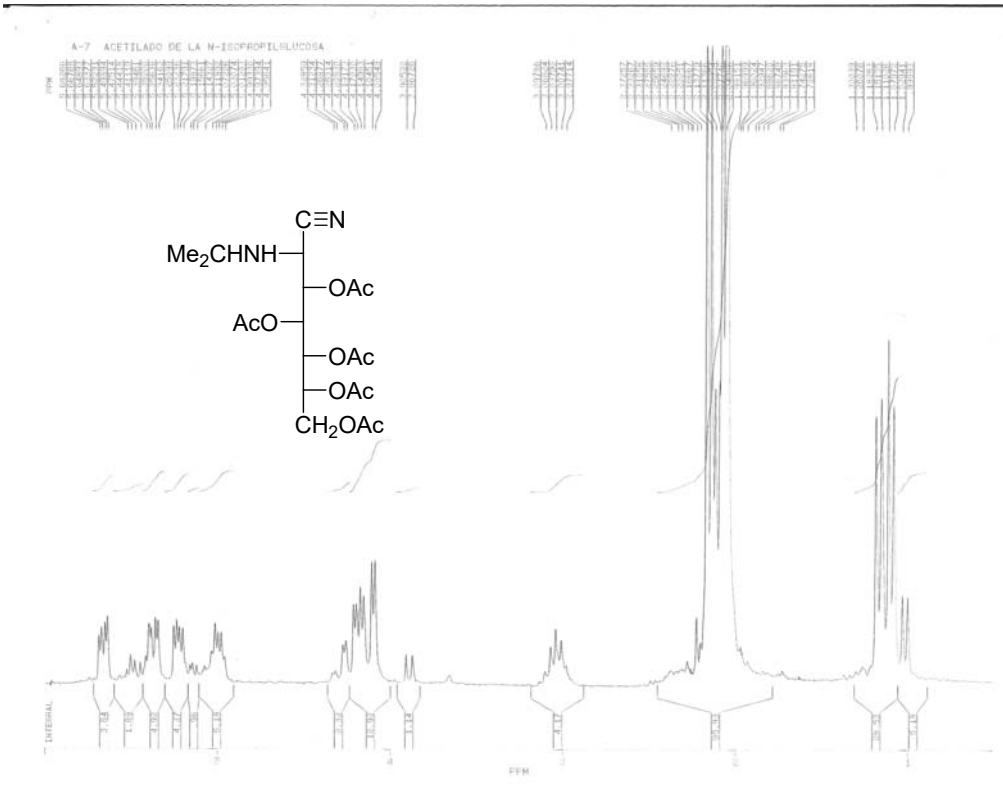


Figure S85. ^{1}H NMR spectrum of **59** and **61** in $CDCl_3$

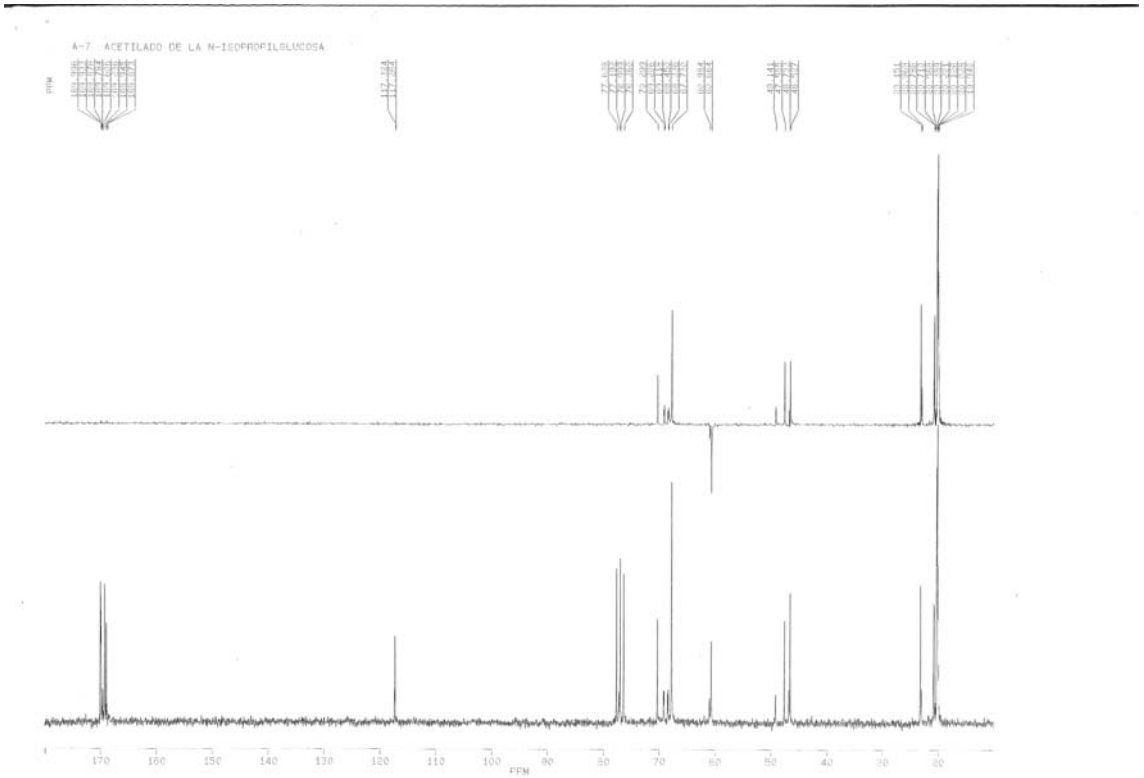


Figure S86. $^{13}C\{^{1}H\}$ NMR and DEPT spectra of **59** and **61** in $CDCl_3$

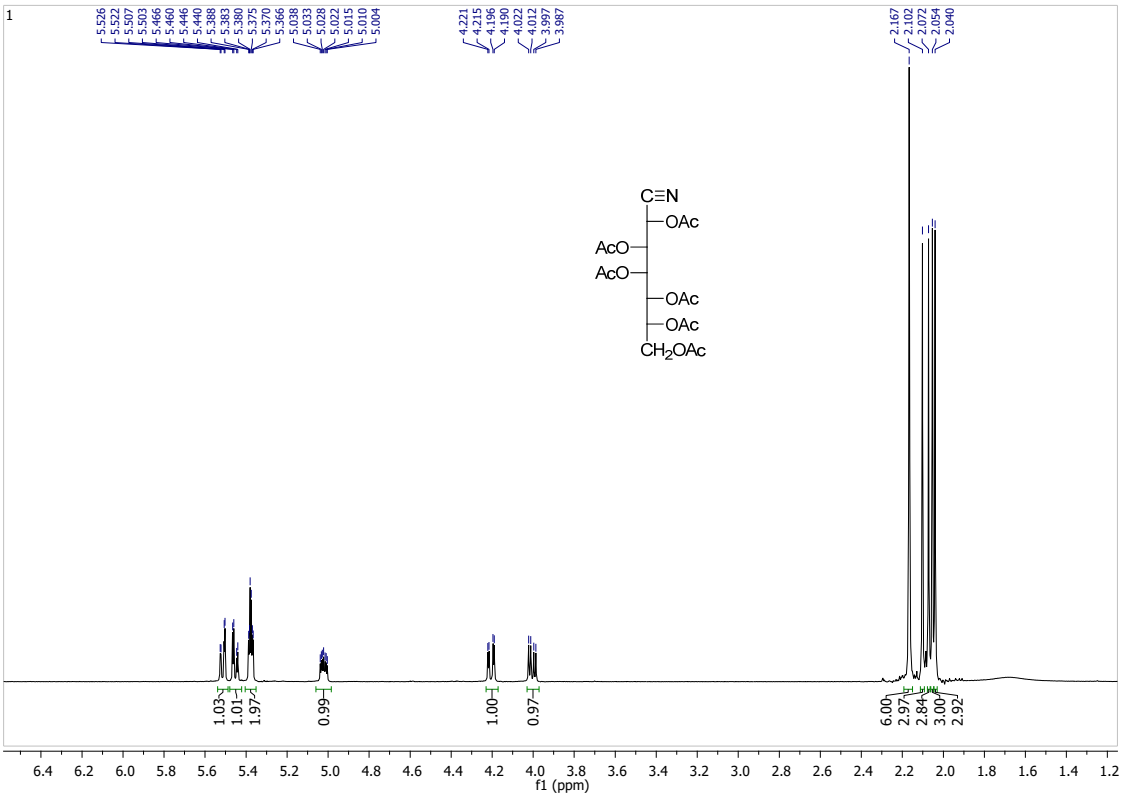


Figure S87. ^{1}H NMR spectrum of **63** in $CDCl_3$

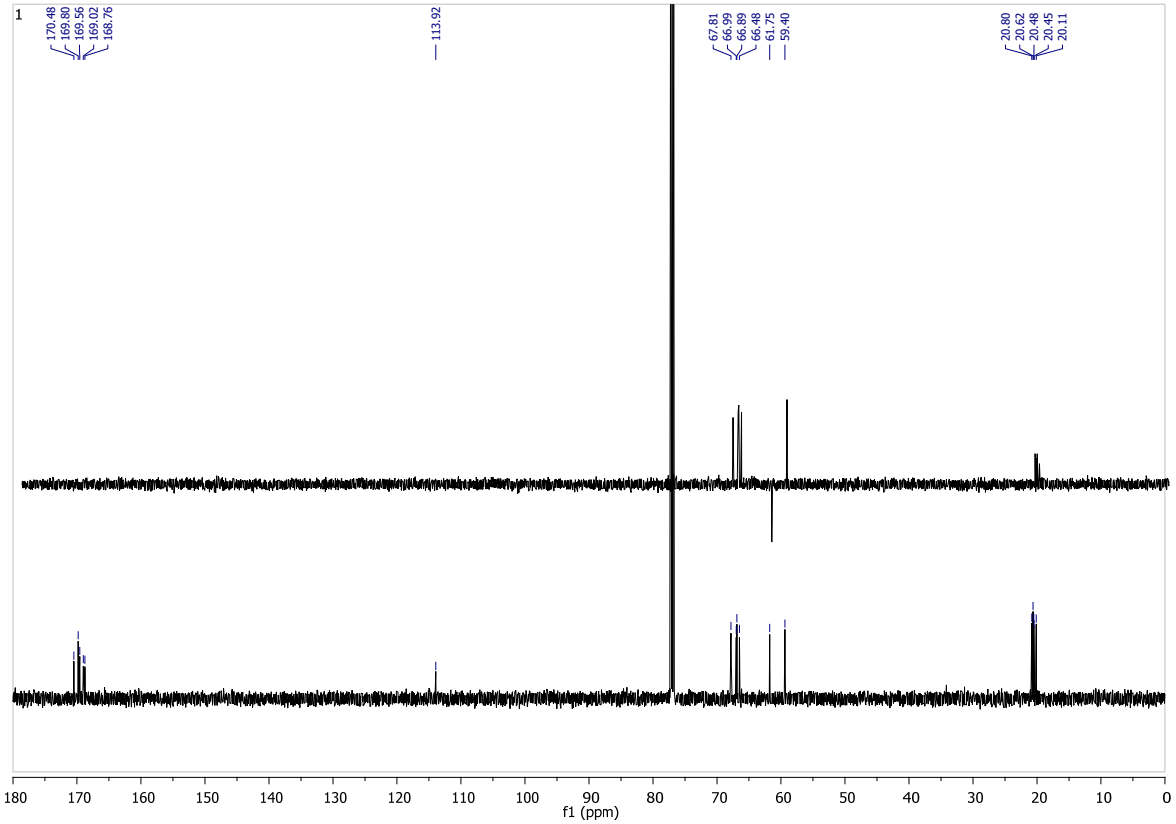


Figure S88. $^{13}C\{^{1}H\}$ NMR and DEPT spectra of **63** in $CDCl_3$

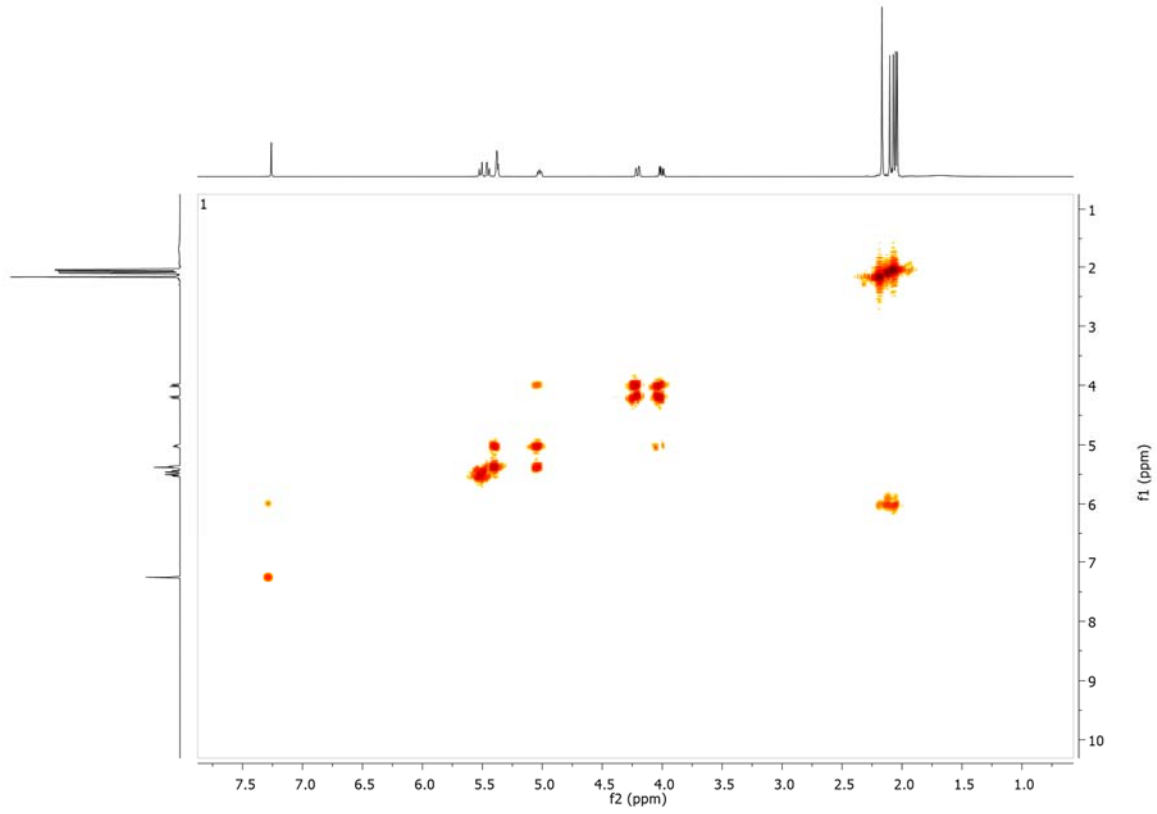


Figure S89. COSY spectrum of **63** in $CDCl_3$

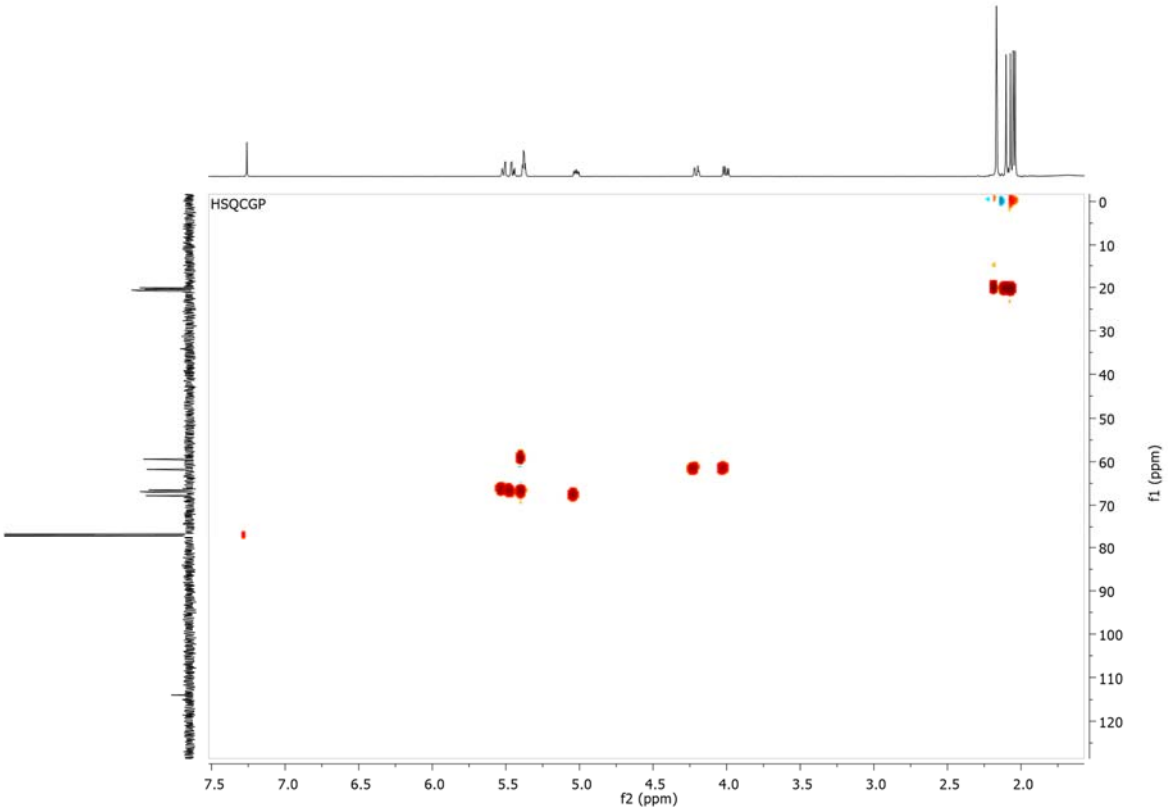


Figure S90. HMQC spectrum of **63** in $CDCl_3$

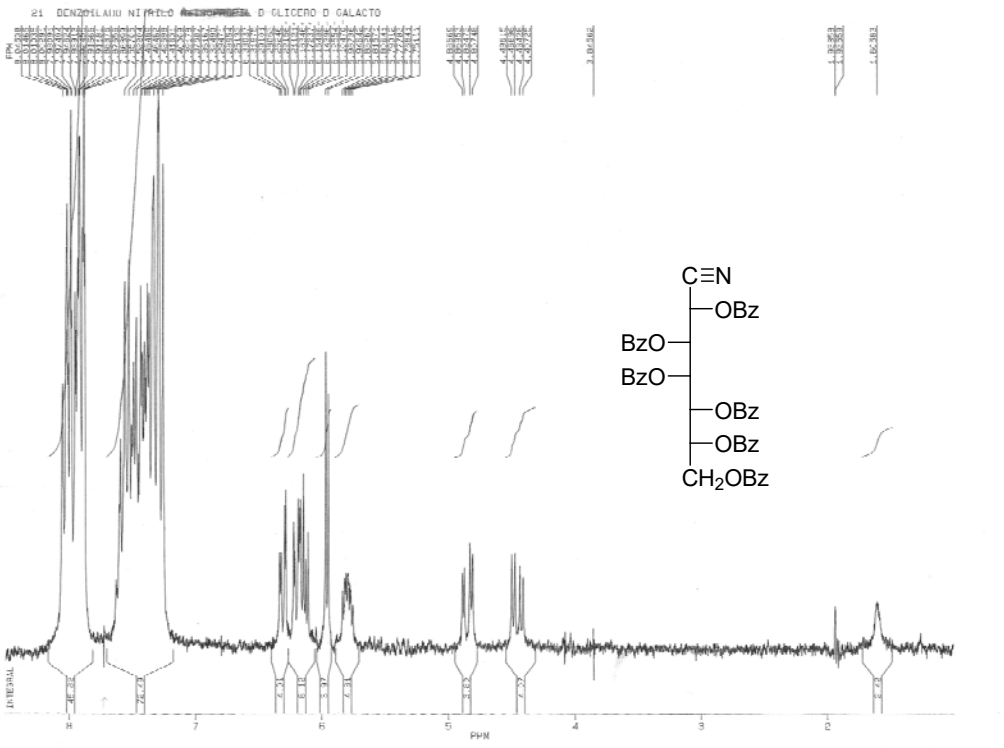


Figure S91. ^1H NMR spectrum of **64** in $CDCl_3$

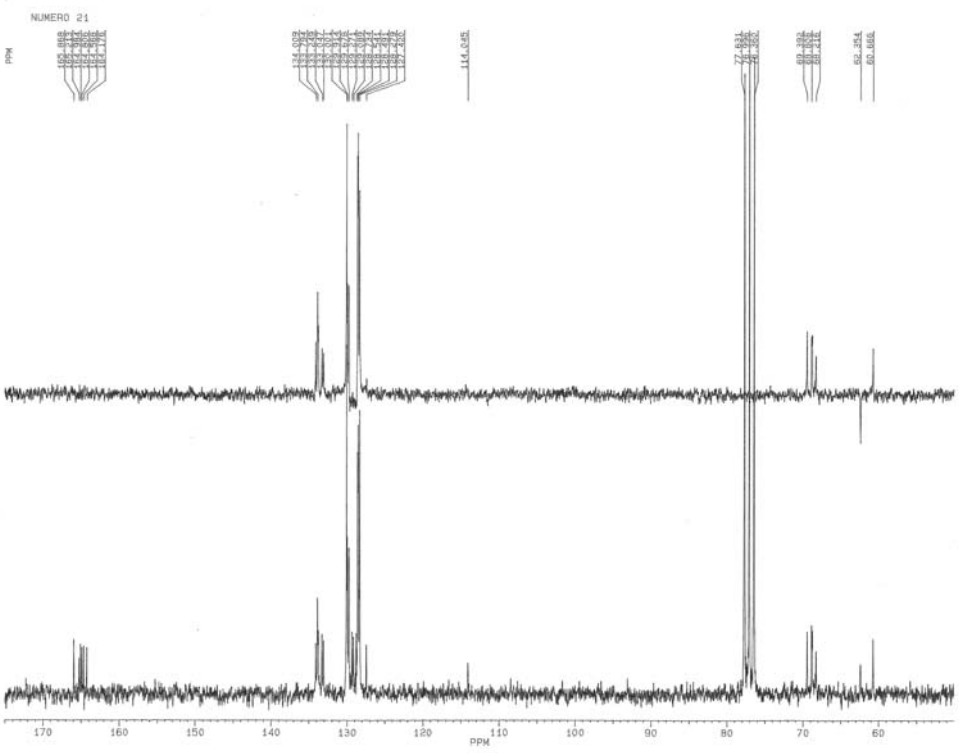


Figure S92. $^{13}C\{^{1}H\}$ NMR and DEPT spectra of **64** in $CDCl_3$

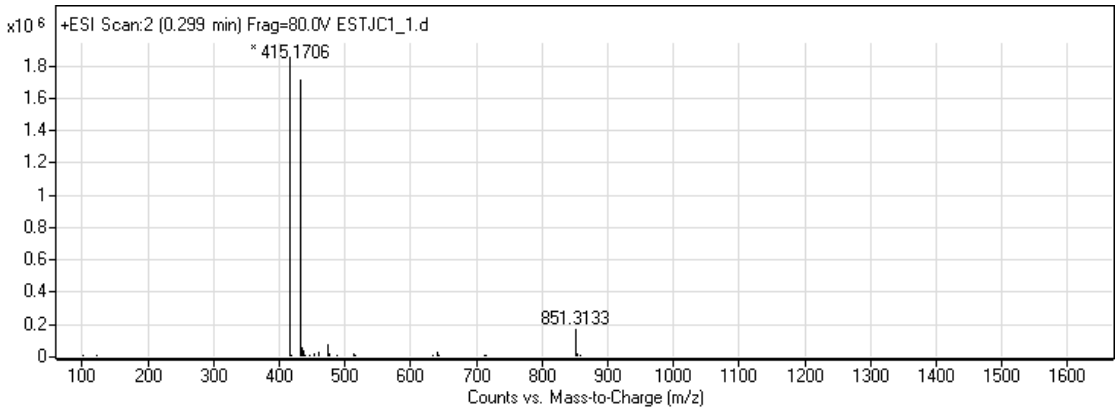


Figure S93. Mass spectrum of **11**.

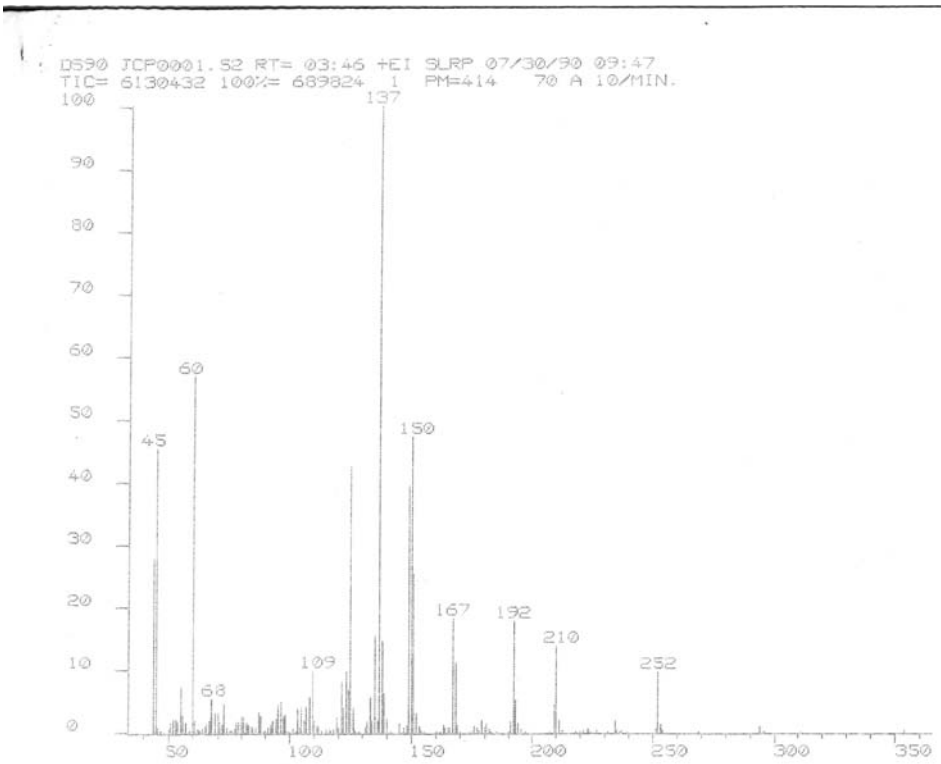


Figure S94. Mass spectrum (EI) of **11**.

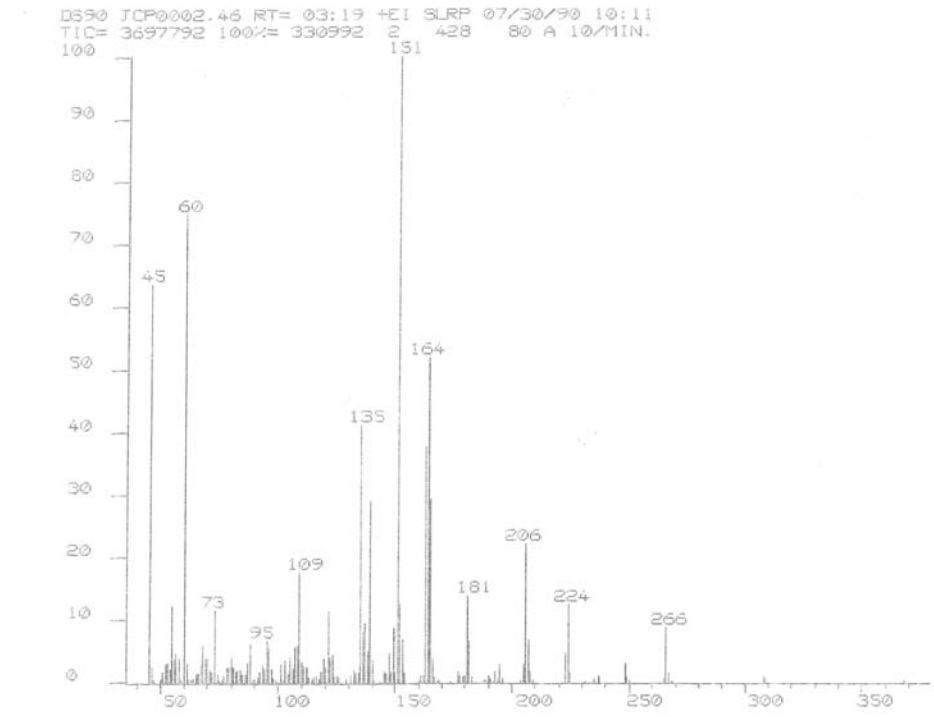


Figure S95. Mass spectrum (EI) of **12**.

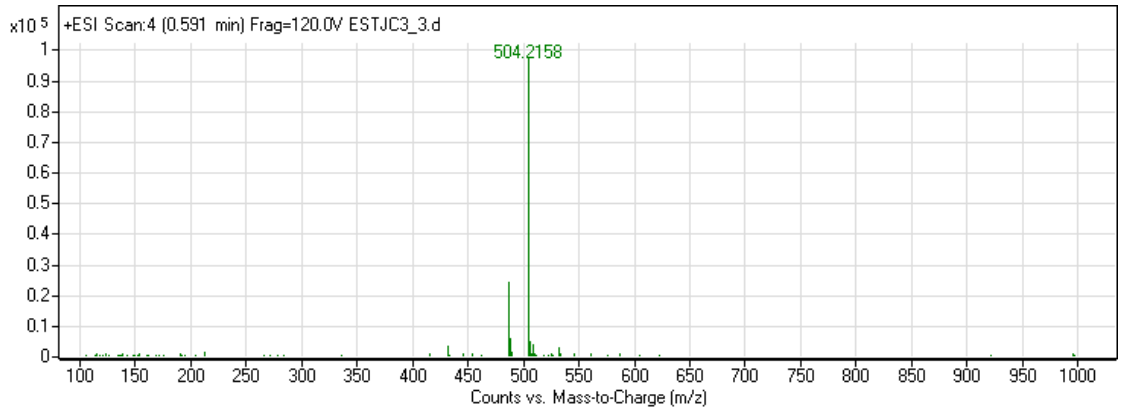


Figure S96. Mass spectrum of **13**.

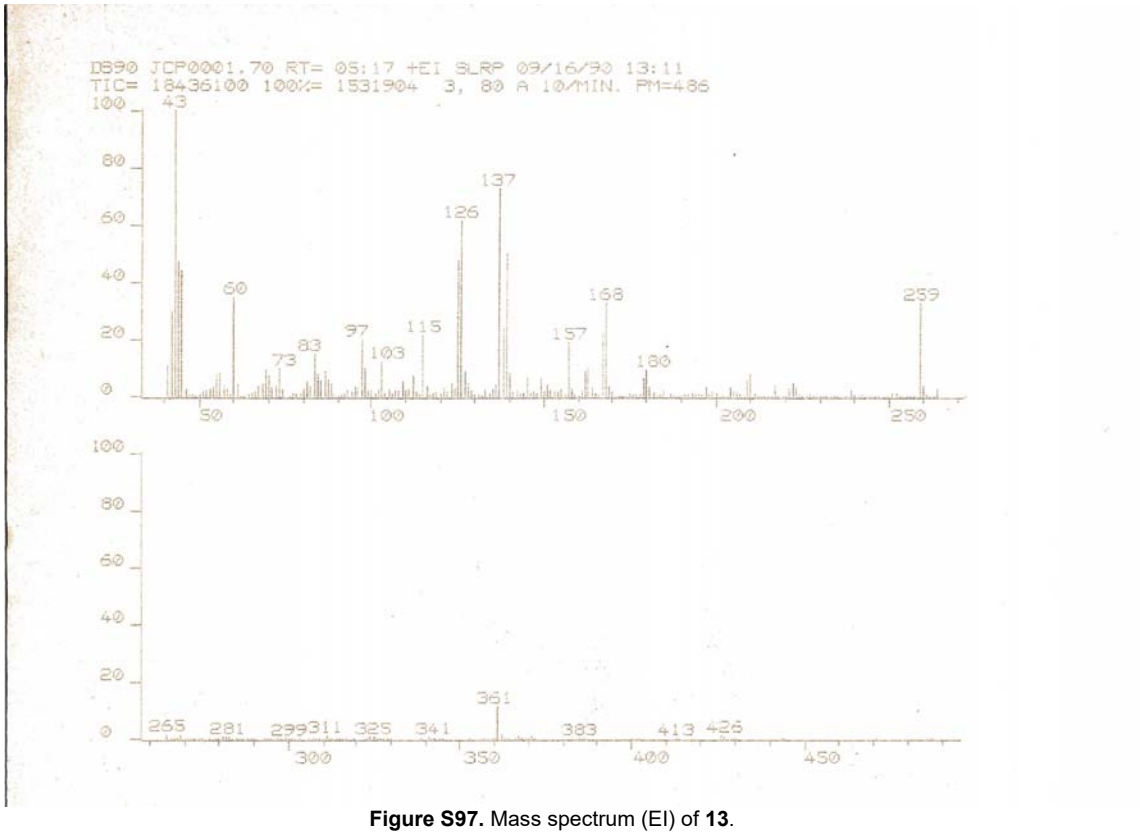


Figure S97. Mass spectrum (EI) of **13**.

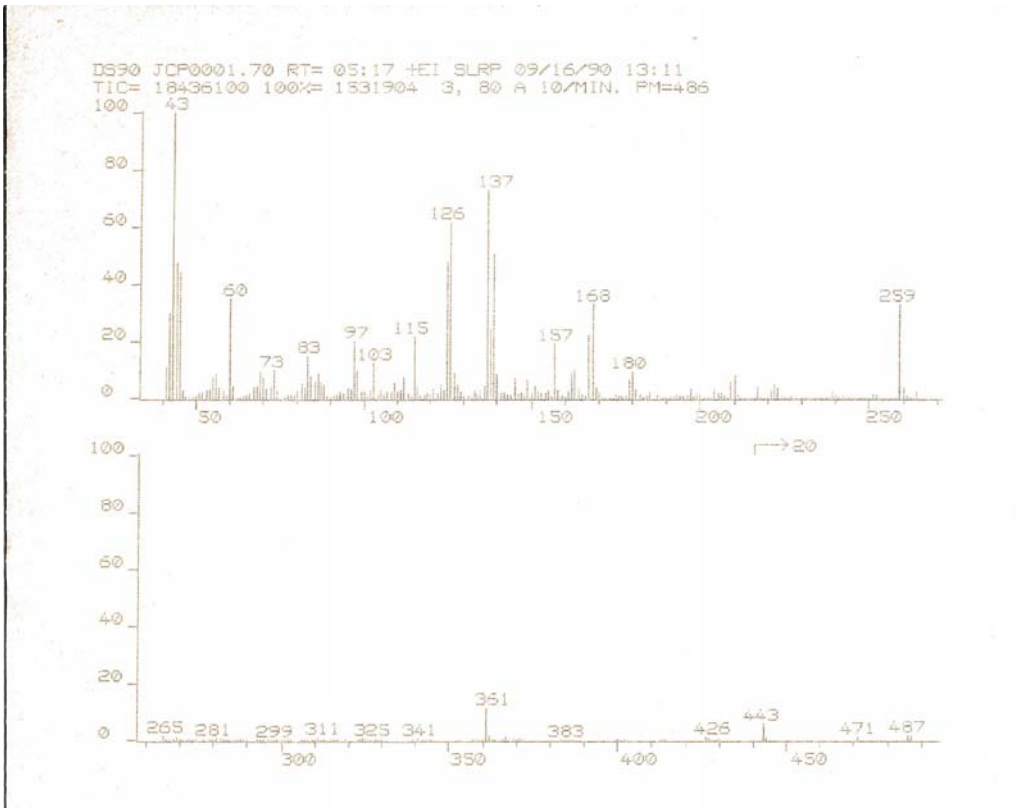


Figure S98. Mass spectrum (EI) of **13**.

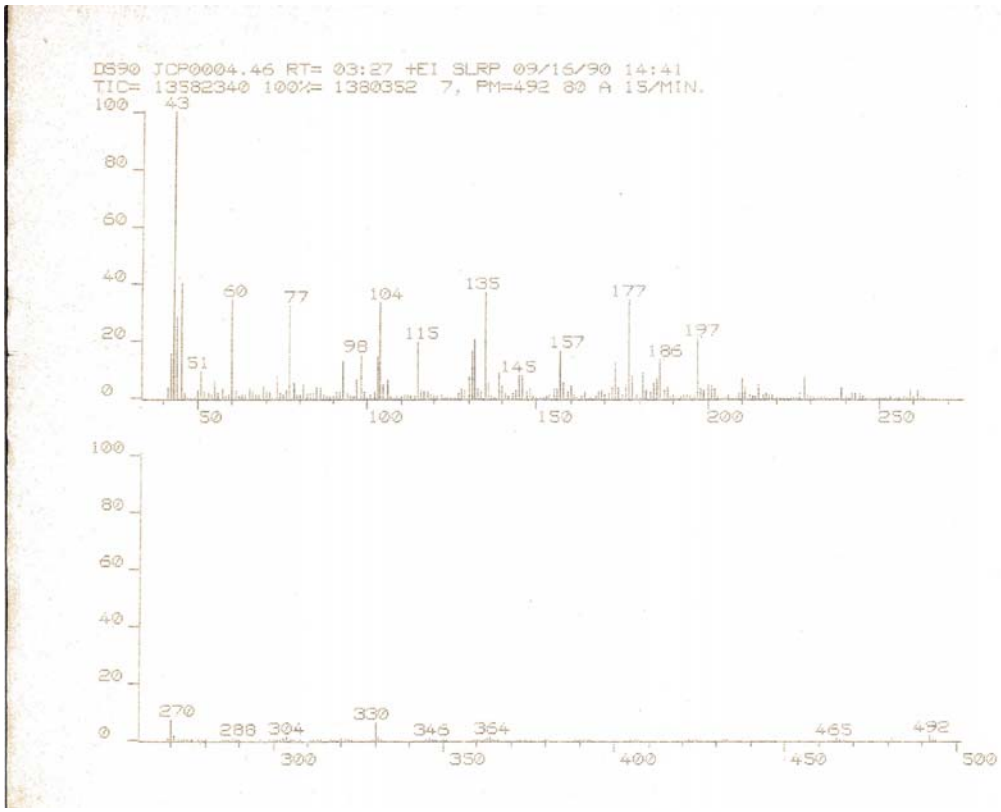


Figure S99. Mass spectrum (EI) of **17.**

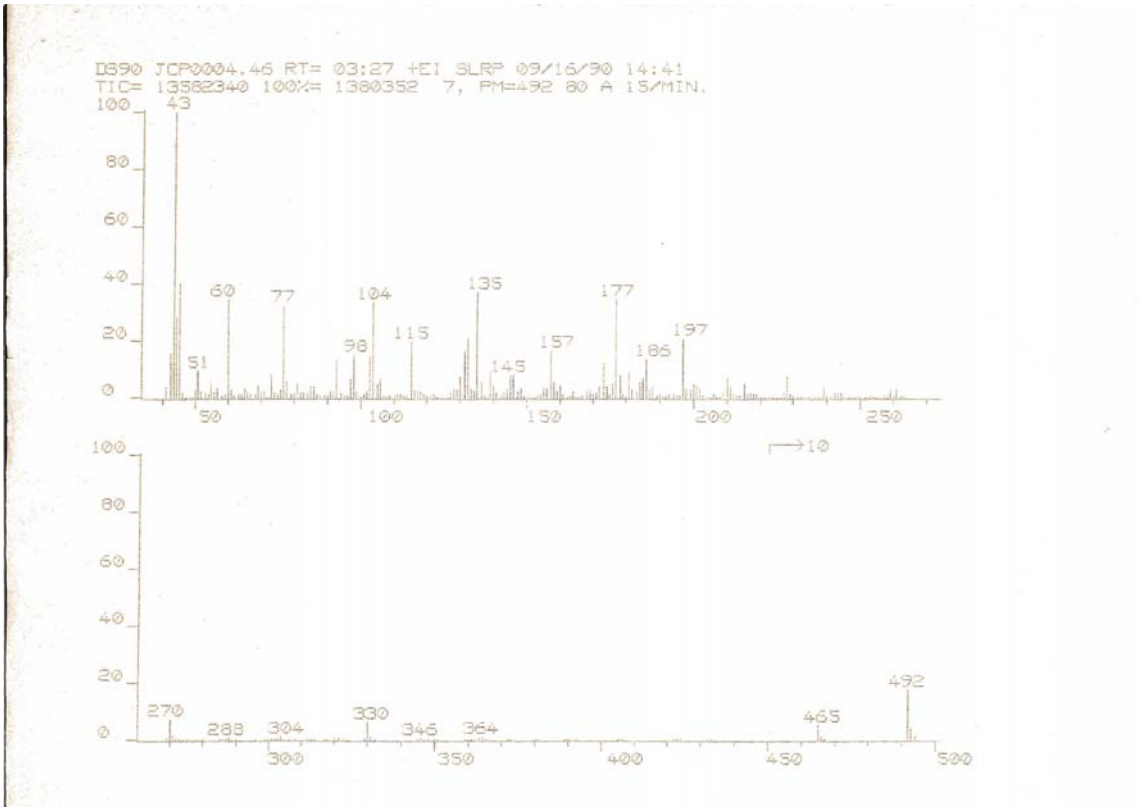


Figure S100. Mass spectrum (EI) of **17.**

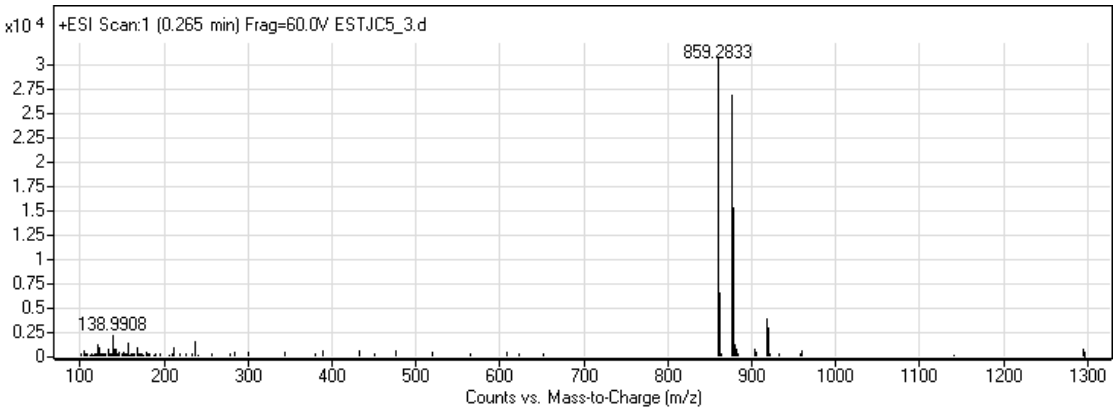


Figure S101. Mass spectrum of **18**.

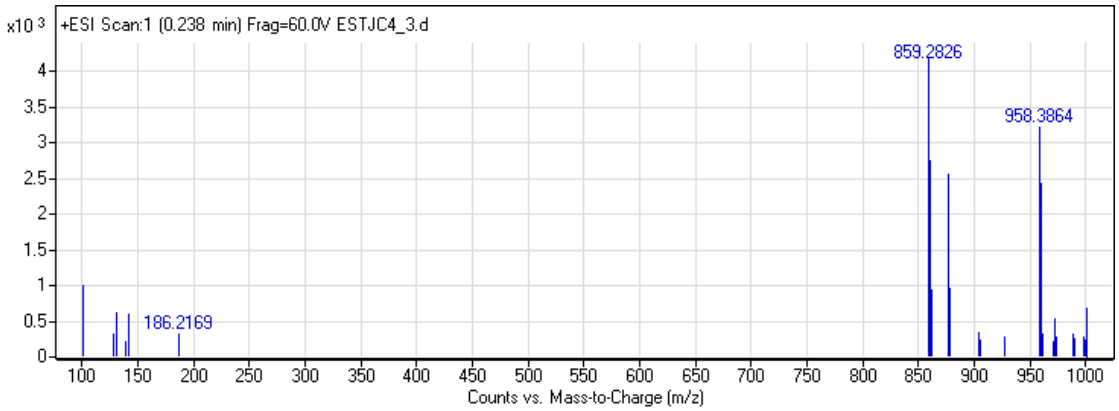


Figure S102. Mass spectrum of **20**.

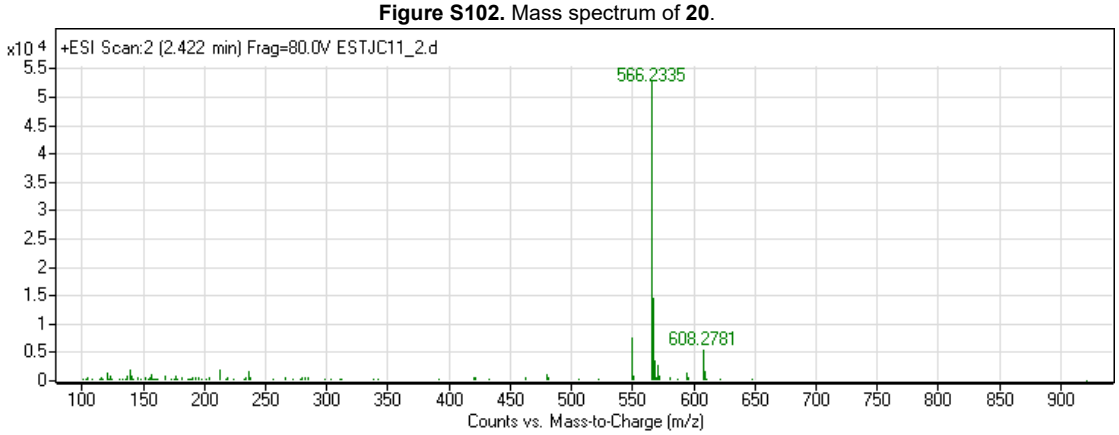


Figure S103. Mass spectrum of **37**

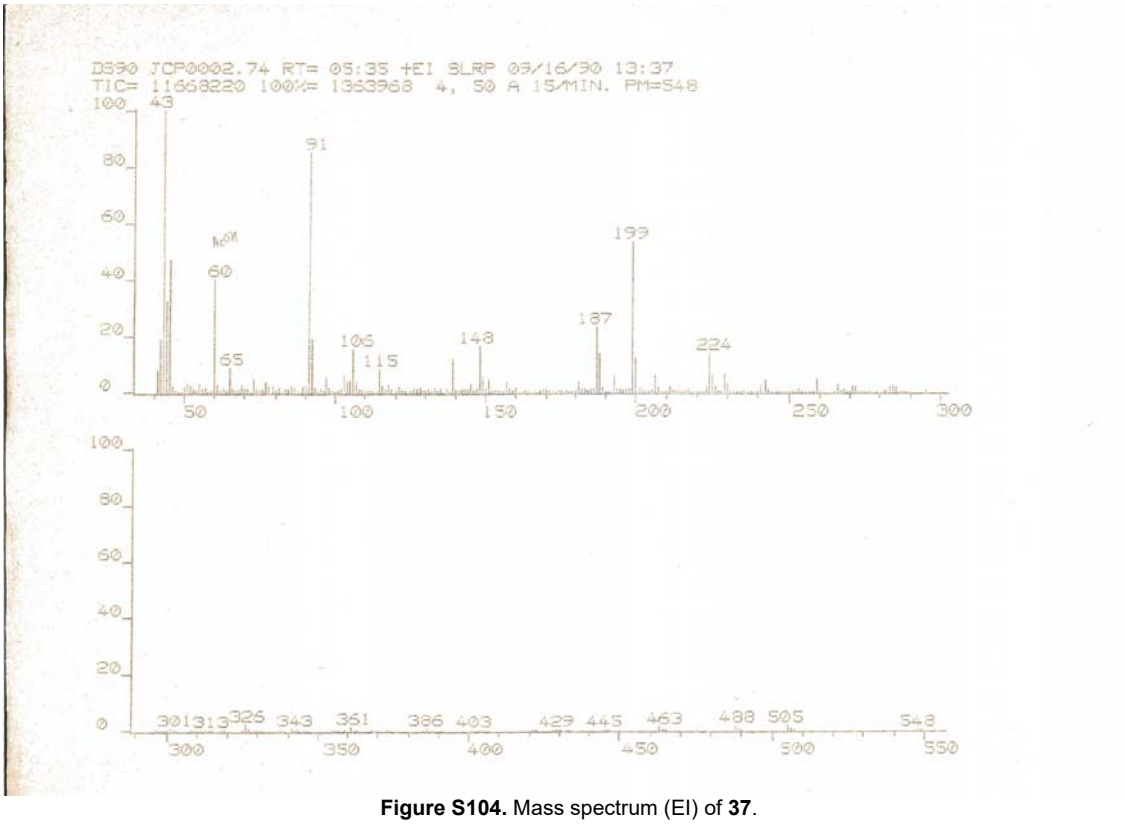


Figure S104. Mass spectrum (EI) of **37**.

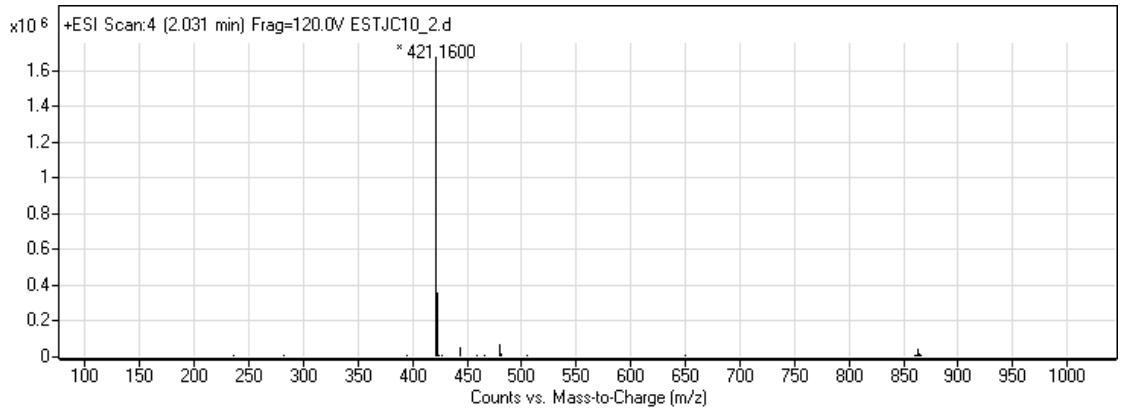


Figure S105. Mass spectrum of **42**.

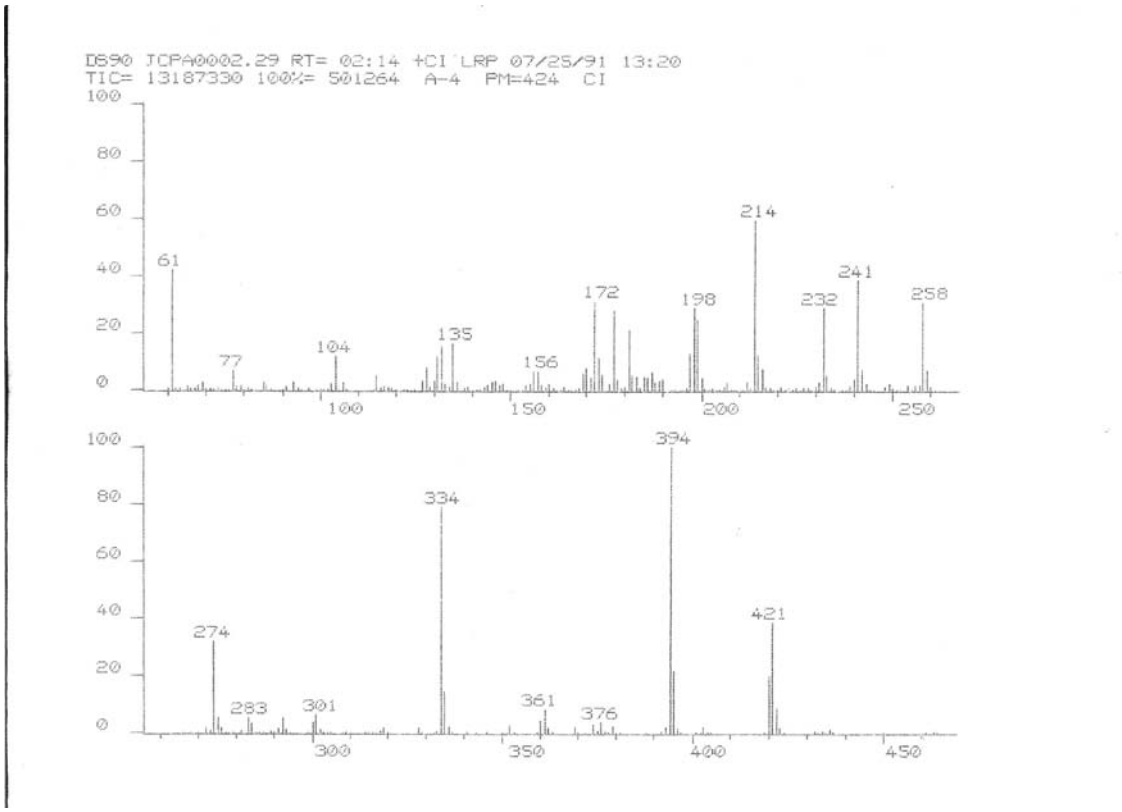


Figure S106. Mass spectrum (EI) of **42**.

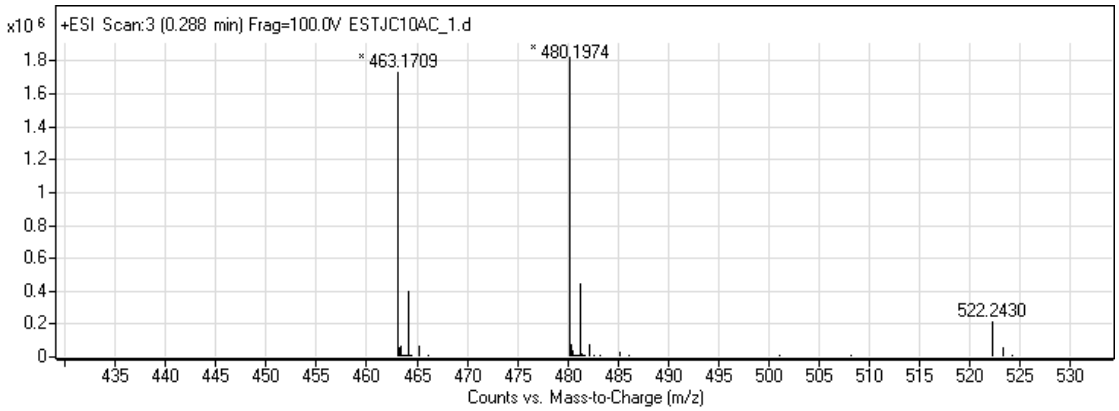


Figure S107. Mass spectrum of **43**.

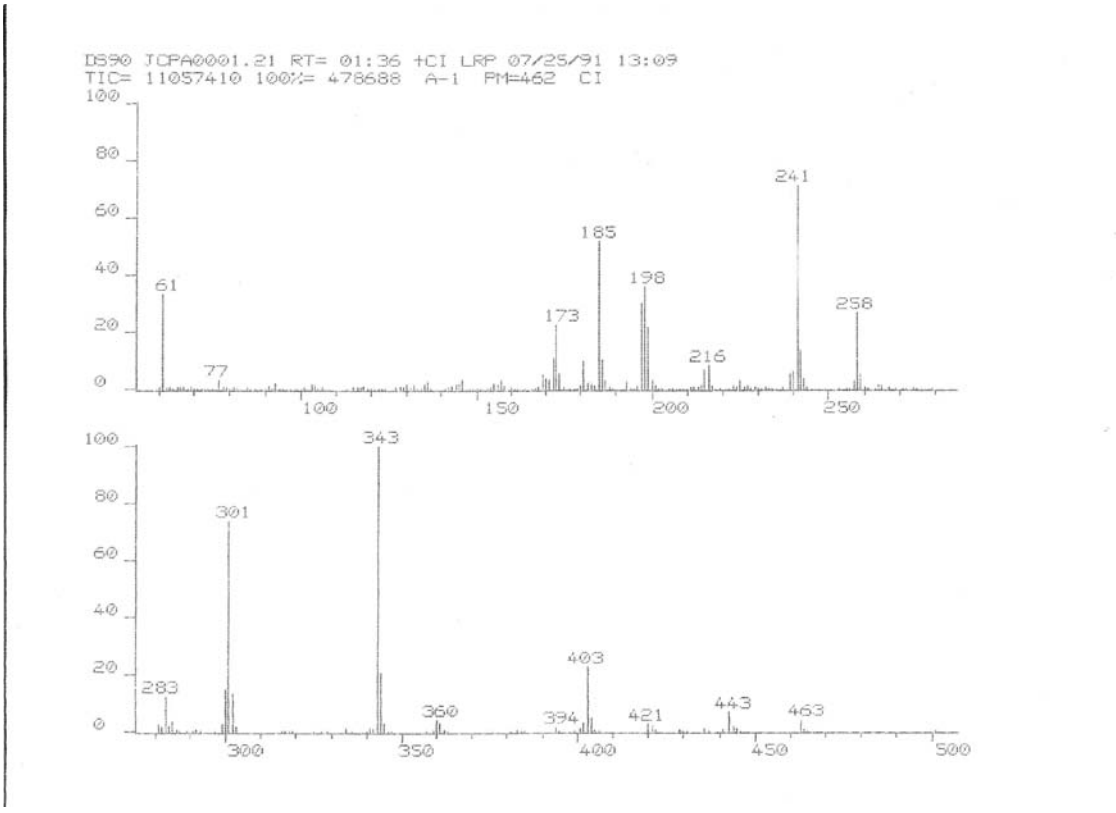


Figure S108. Mass spectrum (EI) of **43**.

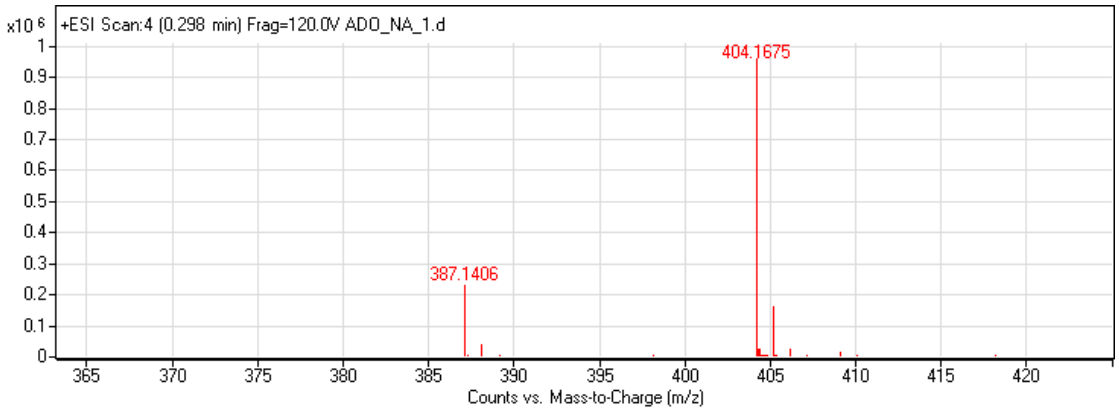


Figure S109. Mass spectrum of **47**.

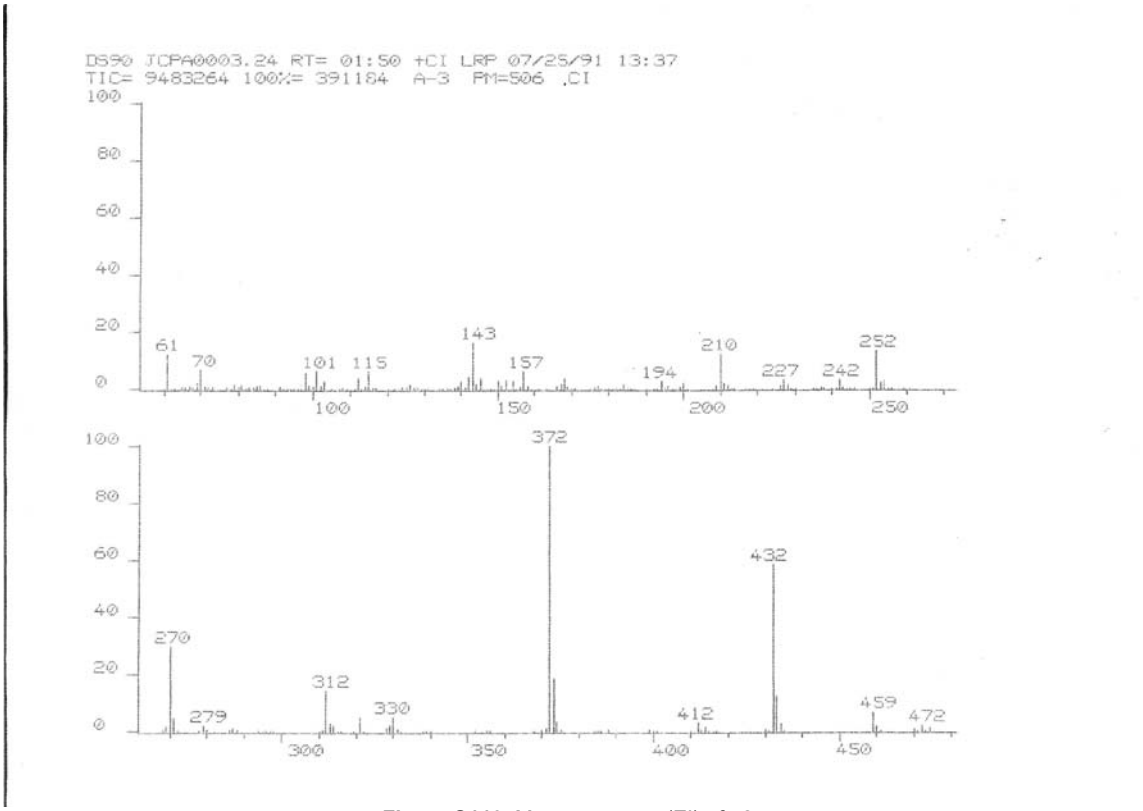


Figure S110. Mass spectrum (EI) of **58**.

Structure 13 A_1G^+Z (M06-2X, Gas Phase)

Energy (Hartrees): = -1755.1525901
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.189721	1.650763	-0.244558
2	1	0	2.737969	2.440834	-0.846097
3	1	0	3.315478	1.983199	0.786914
4	6	0	2.315620	0.406248	-0.283086
5	1	0	2.474921	-0.104293	-1.235837
6	6	0	0.844192	0.753099	-0.165541
7	1	0	0.538950	1.271784	-1.074457
8	6	0	-0.038903	-0.478999	0.029917
9	1	0	0.253576	-1.018881	0.932404
10	6	0	-1.498428	-0.058720	0.145118
11	1	0	-1.647951	0.386680	1.130323
12	6	0	-2.505680	-1.204885	-0.081752
13	1	0	-2.419276	-1.521295	-1.123517
14	6	0	-2.203275	-2.345970	0.794032
15	7	0	-1.966782	-3.215881	1.504909
16	8	0	4.458853	1.380894	-0.840242
17	8	0	2.661597	-0.475690	0.784392
18	8	0	0.605219	1.602829	0.964288
19	8	0	0.154506	-1.317471	-1.109264
20	8	0	-1.778717	0.913859	-0.855446
21	6	0	5.430754	0.889262	-0.042260
22	6	0	3.521246	-1.482600	0.507229
23	6	0	0.800577	-2.506506	-0.916940
24	6	0	0.188016	2.871521	0.726777
25	6	0	-2.553450	1.971842	-0.524337
26	6	0	6.618557	0.468789	-0.855011
27	6	0	3.821939	-2.273435	1.738969
28	6	0	1.149975	-3.143333	-2.226721
29	6	0	-2.851346	2.794100	-1.737755
30	1	0	7.482534	0.360271	-0.204565
31	1	0	6.371612	-0.496217	-1.304558
32	1	0	6.811744	1.182114	-1.654408
33	1	0	1.176391	-4.223181	-2.101389
34	1	0	0.457286	-2.848897	-3.011829
35	1	0	2.155344	-2.798373	-2.485228
36	1	0	2.885610	-2.636332	2.163377
37	1	0	4.472681	-3.104845	1.482855
38	1	0	4.307273	-1.611126	2.457931
39	1	0	-3.506401	3.617763	-1.467042
40	1	0	-1.908741	3.175811	-2.133669
41	1	0	-3.311537	2.150758	-2.490513
42	6	0	-0.190991	3.557749	2.003605
43	1	0	0.459046	3.247246	2.819407
44	1	0	-0.157170	4.634170	1.855938
45	1	0	-1.217044	3.260841	2.236732
46	7	0	-3.865759	-0.734713	0.122235
47	6	0	-4.572537	-0.351239	-0.997613
48	6	0	-5.889829	0.354642	-0.756918
49	1	0	-6.392871	0.438805	-1.716570
50	1	0	-6.528823	-0.168482	-0.046551
51	1	0	-5.693645	1.356158	-0.362793
52	8	0	5.322370	0.780724	1.147712
53	8	0	3.970336	-1.673639	-0.592255
54	8	0	0.111728	3.346041	-0.372945
55	8	0	1.078132	-2.935616	0.163530
56	8	0	-2.929900	2.186172	0.597984
57	8	0	-4.141803	-0.521578	-2.119919
58	6	0	-4.334815	-0.518307	1.494605
59	1	0	-3.451723	-0.416702	2.129277
60	1	0	-4.846861	0.442723	1.548234
61	6	0	-5.208807	-1.656298	2.014285
62	1	0	-5.534897	-1.439635	3.033549
63	1	0	-6.096051	-1.790629	1.393111
64	1	0	-4.653411	-2.594641	2.024009

Structure 13 A_1G^+Z (M06-2X, $CHCl_3$)

Energy (Hartrees): = -1755.1837422
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.225785	1.577620	-0.378356

2	1	0	2.808616	2.312859	-1.067614
3	1	0	3.312479	2.006757	0.620544
4	6	0	2.337038	0.343959	-0.348317
5	1	0	2.487021	-0.224859	-1.269230
6	6	0	0.871920	0.728941	-0.244497
7	1	0	0.579260	1.238517	-1.162877
8	6	0	-0.040045	-0.478401	-0.023210
9	1	0	0.271389	-1.030290	0.865172
10	6	0	-1.483585	-0.029028	0.147934
11	1	0	-1.581814	0.451513	1.122106
12	6	0	-2.510581	-1.174624	0.010477
13	1	0	-2.441437	-1.567506	-1.006223
14	6	0	-2.198108	-2.265076	0.945421
15	7	0	-1.932579	-3.102276	1.684441
16	8	0	4.519618	1.254683	-0.895029
17	8	0	2.656179	-0.479859	0.776206
18	8	0	0.669449	1.601727	0.874043
19	8	0	0.071966	-1.315085	-1.175629
20	8	0	-1.803386	0.902254	-0.879997
21	6	0	5.463746	0.851441	-0.022880
22	6	0	3.508058	-1.509450	0.582981
23	6	0	0.672322	-2.528917	-1.033701
24	6	0	0.270040	2.875696	0.633755
25	6	0	-2.526656	1.998049	-0.547852
26	6	0	6.701003	0.412361	-0.742453
27	6	0	3.709214	-2.277048	1.849363
28	6	0	0.771990	-3.226082	-2.353137
29	6	0	-2.901743	2.766333	-1.773257
30	1	0	7.512328	0.283566	-0.030076
31	1	0	6.483803	-0.540447	-1.231444
32	1	0	6.971346	1.134926	-1.512373
33	1	0	1.027114	-4.270422	-2.191054
34	1	0	-0.162729	-3.133172	-2.905908
35	1	0	1.562352	-2.744328	-2.934738
36	1	0	2.741519	-2.613364	2.223736
37	1	0	4.359282	-3.127705	1.659709
38	1	0	4.158205	-1.615804	2.593316
39	1	0	-3.461010	3.655614	-1.493152
40	1	0	-1.994443	3.042770	-2.312923
41	1	0	-3.498672	2.122740	-2.424231
42	6	0	0.002302	3.598525	1.915042
43	1	0	0.818533	3.436729	2.619310
44	1	0	-0.132158	4.658233	1.712765
45	1	0	-0.912661	3.190750	2.351449
46	7	0	-3.859609	-0.675107	0.200485
47	6	0	-4.592520	-0.401259	-0.931277
48	6	0	-5.886393	0.351363	-0.733301
49	1	0	-6.406963	0.374231	-1.687763
50	1	0	-6.527086	-0.099960	0.024101
51	1	0	-5.662874	1.376096	-0.420950
52	8	0	5.303297	0.837871	1.168895
53	8	0	4.028337	-1.739674	-0.477193
54	8	0	0.142050	3.326322	-0.472643
55	8	0	1.074325	-2.942532	0.017359
56	8	0	-2.808357	2.277996	0.587571
57	8	0	-4.193738	-0.701923	-2.042674
58	6	0	-4.312795	-0.361496	1.561808
59	1	0	-3.422060	-0.211449	2.175344
60	1	0	-4.833677	0.595811	1.550379
61	6	0	-5.179647	-1.458720	2.169257
62	1	0	-5.492744	-1.166394	3.174068
63	1	0	-6.075117	-1.635267	1.570056
64	1	0	-4.628476	-2.397816	2.243950

Structure 13 A_1G^+E (M06-2X, Gas Phase)

Energy (Hartrees): = -1755.1511944
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.220967	1.622364	0.299021
2	1	0	-2.774262	2.418517	0.896416
3	1	0	-3.402557	1.966832	-0.720017
4	6	0	-2.304481	0.409214	0.282786
5	1	0	-2.426701	-0.132759	1.222931
6	6	0	-0.843719	0.796812	0.143564
7	1	0	-0.523134	1.269867	1.072358
8	6	0	0.042156	-0.416340	-0.135934
9	1	0	-0.267944	-0.914634	-1.056149
10	6	0	1.498457	0.000638	-0.261199
11	1	0	1.623672	0.540566	-1.200661
12	6	0	2.482150	-1.195332	-0.205584

13	1	0	2.225744	-1.796026	0.666556
14	6	0	2.295955	-2.046747	-1.392405
15	7	0	2.151977	-2.678756	-2.339467
16	8	0	-4.453323	1.294470	0.942880
17	8	0	-2.648946	-0.455139	-0.801506
18	8	0	-0.650148	1.710239	-0.939938
19	8	0	-0.138930	-1.304599	0.971011
20	8	0	1.840446	0.856733	0.821527
21	6	0	-5.433037	0.762007	0.181058
22	6	0	-3.446891	-1.512337	-0.532240
23	6	0	-0.705251	-2.522411	0.715379
24	6	0	-0.245179	2.972214	-0.635005
25	6	0	2.538132	1.990874	0.522287
26	6	0	-6.564650	0.279534	1.038222
27	6	0	-3.776559	-2.259175	-1.783486
28	6	0	-1.096010	-3.208304	1.987973
29	6	0	3.016560	2.664687	1.767938
30	1	0	-7.447236	0.126941	0.422652
31	1	0	-6.250261	-0.672510	1.473239
32	1	0	-6.762594	0.979867	1.847835
33	1	0	-1.103514	-4.283637	1.827620
34	1	0	-0.437604	-2.931159	2.808707
35	1	0	-2.113527	-2.880383	2.220198
36	1	0	-2.852306	-2.519951	-2.299172
37	1	0	-4.340968	-3.152687	-1.531414
38	1	0	-4.367246	-1.599590	-2.422110
39	1	0	3.256972	3.700281	1.542842
40	1	0	2.260103	2.599456	2.548110
41	1	0	3.921144	2.144932	2.099420
42	6	0	0.059008	3.750244	-1.877308
43	1	0	-0.623731	3.482235	-2.681385
44	1	0	0.014428	4.813280	-1.654570
45	1	0	1.077556	3.489948	-2.176478
46	7	0	3.852568	-0.748924	-0.097714
47	6	0	4.467167	-0.576467	1.124756
48	6	0	3.799149	-1.167266	2.352151
49	1	0	4.451827	-0.959871	3.196135
50	1	0	2.818999	-0.719716	2.527472
51	1	0	3.678694	-2.248654	2.252020
52	8	0	-5.367452	0.664868	-1.012977
53	8	0	-3.826783	-1.777069	0.578743
54	8	0	-0.127689	3.368560	0.490882
55	8	0	-0.885837	-2.938809	-0.390726
56	8	0	2.737963	2.348820	-0.603592
57	8	0	5.519917	0.021855	1.206771
58	6	0	4.516089	-0.186898	-1.285230
59	1	0	3.750024	-0.007321	-2.042379
60	1	0	4.938995	0.778474	-1.007725
61	6	0	5.596452	-1.120367	-1.813561
62	1	0	6.079199	-0.678390	-2.687138
63	1	0	6.353452	-1.278926	-1.044516
64	1	0	5.170021	-2.082334	-2.104229

Structure 13 A_1G^+E (M06-2X, $CHCl_3$)

Energy (Hartrees): = -1755.1825417
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.238597	1.527747	0.435855
2	1	0	-2.822450	2.253888	1.135183
3	1	0	-3.360635	1.982330	-0.548016
4	6	0	-2.323500	0.316590	0.348377
5	1	0	-2.448778	-0.288519	1.249620
6	6	0	-0.866648	0.732179	0.240335
7	1	0	-0.570323	1.209710	1.174902
8	6	0	0.056315	-0.455633	-0.034257
9	1	0	-0.260205	-0.984962	-0.934445
10	6	0	1.494982	0.007611	-0.211749
11	1	0	1.584529	0.495065	-1.182697
12	6	0	2.525405	-1.140548	-0.095679
13	1	0	2.373371	-1.627563	0.867567
14	6	0	2.266564	-2.158881	-1.128423
15	7	0	2.054126	-2.935444	-1.946288
16	8	0	-4.511191	1.158463	0.974285
17	8	0	-2.643099	-0.472448	-0.801180
18	8	0	-0.691727	1.651077	-0.843421
19	8	0	-0.041918	-1.328706	1.094468
20	8	0	1.829219	0.930537	0.818531
21	6	0	-5.468588	0.762077	0.113055
22	6	0	-3.469550	-1.527238	-0.632800
23	6	0	-0.617732	-2.550413	0.910305

24	6	0	-0.335797	2.928525	-0.553284
25	6	0	2.485900	2.066962	0.455611
26	6	0	-6.677625	0.272962	0.847977
27	6	0	-3.682086	-2.246585	-1.925172
28	6	0	-0.741351	-3.278889	2.210523
29	6	0	2.946845	2.823100	1.658341
30	1	0	-7.510164	0.171425	0.155945
31	1	0	-6.434273	-0.702700	1.276132
32	1	0	-6.930124	0.949246	1.664364
33	1	0	-0.987805	-4.320247	2.018731
34	1	0	0.181195	-3.196154	2.785287
35	1	0	-1.545510	-2.814293	2.787055
36	1	0	-2.718575	-2.592091	-2.303214
37	1	0	-4.350181	-3.089491	-1.766873
38	1	0	-4.109638	-1.552623	-2.651290
39	1	0	3.120459	3.862230	1.388449
40	1	0	2.219824	2.744657	2.465159
41	1	0	3.890575	2.378261	1.990424
42	6	0	-0.146258	3.721275	-1.806225
43	1	0	-1.059403	3.686768	-2.403011
44	1	0	0.105231	4.747893	-1.552022
45	1	0	0.658992	3.270744	-2.389273
46	7	0	3.881709	-0.646080	-0.183816
47	6	0	4.657576	-0.411547	0.928067
48	6	0	4.136628	-0.854748	2.277628
49	1	0	4.884627	-0.579506	3.017412
50	1	0	3.188337	-0.372927	2.522505
51	1	0	3.992847	-1.937707	2.304474
52	8	0	-5.337127	0.787492	-1.081979
53	8	0	-3.957063	-1.814137	0.429093
54	8	0	-0.196771	3.330858	0.570141
55	8	0	-0.981612	-2.946210	-0.160589
56	8	0	2.667674	2.371801	-0.690816
57	8	0	5.740327	0.134190	0.814424
58	6	0	4.400227	-0.220383	-1.493018
59	1	0	3.551121	-0.121181	-2.171747
60	1	0	4.842075	0.768786	-1.372904
61	6	0	5.418284	-1.206124	-2.049503
62	1	0	5.786315	-0.854914	-3.016044
63	1	0	6.266879	-1.294139	-1.369583
64	1	0	4.971195	-2.192900	-2.190788

Structure 13 B_1G^+Z (M06-2X, Gas Phase)

Energy (Hartrees): = -1755.1479943
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.190226	1.579712	-0.382641
2	1	0	2.762887	2.321612	-1.058401
3	1	0	3.310422	2.001103	0.616418
4	6	0	2.291057	0.353221	-0.321482
5	1	0	2.457214	-0.246515	-1.219817
6	6	0	0.825815	0.738337	-0.262597
7	1	0	0.556688	1.202463	-1.211943
8	6	0	-0.096598	-0.452368	-0.000533
9	1	0	0.144966	-0.915270	0.958570
10	6	0	-1.546234	0.004093	0.019506
11	1	0	-1.728448	0.570478	0.931086
12	6	0	-2.565761	-1.140486	-0.084380
13	1	0	-2.456543	-1.562832	-1.086781
14	6	0	-2.291357	-2.240596	0.856635
15	7	0	-2.059747	-3.145205	1.523825
16	8	0	4.460909	1.231175	-0.932738
17	8	0	2.599779	-0.429712	0.830405
18	8	0	0.583327	1.665436	0.802338
19	8	0	0.113189	-1.396918	-1.054457
20	8	0	-1.796411	0.832886	-1.124503
21	6	0	5.412053	0.798501	-0.076918
22	6	0	3.443244	-1.473865	0.668169
23	6	0	0.749721	-2.564478	-0.737284
24	6	0	0.223826	2.929660	0.477431
25	6	0	-2.448165	2.005452	-0.927579
26	6	0	6.593297	0.262105	-0.828418
27	6	0	3.691288	-2.158811	1.972749
28	6	0	1.113321	-3.332424	-1.971918
29	6	0	-2.552638	2.776958	-2.208348
30	1	0	7.447318	0.192088	-0.159773
31	1	0	6.316795	-0.735016	-1.180258
32	1	0	6.818081	0.883467	-1.693798
33	1	0	1.066363	-4.397196	-1.754486
34	1	0	0.476836	-3.068944	-2.813383

35	1	0	2.149822	-3.073908	-2.207152
36	1	0	2.739287	-2.525465	2.358493
37	1	0	4.383450	-2.982329	1.820693
38	1	0	4.103390	-1.431123	2.673201
39	1	0	-3.324714	3.535737	-2.108597
40	1	0	-1.586348	3.261432	-2.367803
41	1	0	-2.754016	2.113375	-3.047963
42	6	0	-0.198416	3.694891	1.692746
43	1	0	0.415846	3.427086	2.550561
44	1	0	-0.149245	4.760346	1.483476
45	1	0	-1.234092	3.414827	1.904211
46	7	0	-3.916436	-0.615874	0.028441
47	6	0	-4.295810	-0.111814	1.255424
48	6	0	-5.670721	0.506372	1.354663
49	1	0	-5.843210	0.737732	2.402177
50	1	0	-5.695975	1.431986	0.774678
51	1	0	-6.453658	-0.160718	0.990859
52	8	0	5.289774	0.815062	1.116194
53	8	0	3.914277	-1.773250	-0.397824
54	8	0	0.222385	3.342858	-0.651152
55	8	0	1.013194	-2.887478	0.381951
56	8	0	-2.846007	2.368938	0.144194
57	8	0	-3.535014	-0.148219	2.197686
58	6	0	-4.776391	-0.704267	-1.147430
59	1	0	-5.546353	0.062689	-1.072211
60	1	0	-4.171002	-0.449171	-2.022297
61	6	0	-5.401333	-2.086205	-1.310390
62	1	0	-6.021327	-2.126922	-2.208043
63	1	0	-4.628203	-2.853842	-1.393876
64	1	0	-6.020705	-2.329772	-0.444890

Structure 13 B_1G^+Z (M06-2X, $CHCl_3$)

Energy (Hartrees): =-1755.1821906
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.228364	1.478007	-0.477055
2	1	0	2.833733	2.173455	-1.218423
3	1	0	3.318394	1.974540	0.490277
4	6	0	2.309555	0.270663	-0.362833
5	1	0	2.469803	-0.382487	-1.224537
6	6	0	0.852670	0.697762	-0.334261
7	1	0	0.605520	1.150491	-1.295181
8	6	0	-0.104027	-0.462226	-0.056977
9	1	0	0.156016	-0.949699	0.884443
10	6	0	-1.538896	0.035423	0.019472
11	1	0	-1.674454	0.595631	0.942633
12	6	0	-2.587382	-1.087487	-0.062354
13	1	0	-2.512020	-1.524606	-1.061507
14	6	0	-2.302734	-2.184140	0.881338
15	7	0	-2.048700	-3.078845	1.554002
16	8	0	4.518707	1.091895	-0.958106
17	8	0	2.577504	-0.453314	0.839897
18	8	0	0.641755	1.649978	0.715261
19	8	0	0.019579	-1.394954	-1.135560
20	8	0	-1.805354	0.878754	-1.106030
21	6	0	5.450164	0.740589	-0.050197
22	6	0	3.419907	-1.505387	0.767977
23	6	0	0.623393	-2.590006	-0.887862
24	6	0	0.337826	2.926363	0.378964
25	6	0	-2.417918	2.067426	-0.876948
26	6	0	6.685438	0.230801	-0.724811
27	6	0	3.564498	-2.159506	2.103596
28	6	0	0.754097	-3.394218	-2.142625
29	6	0	-2.606084	2.822809	-2.154287
30	1	0	7.496884	0.167341	-0.003709
31	1	0	6.462611	-0.765179	-1.115825
32	1	0	6.958296	0.872412	-1.562455
33	1	0	0.823166	-4.449258	-1.886987
34	1	0	-0.076400	-3.207495	-2.821077
35	1	0	1.681558	-3.090926	-2.636783
36	1	0	2.581185	-2.472193	2.457770
37	1	0	4.228529	-3.016281	2.020534
38	1	0	3.970343	-1.432145	2.809680
39	1	0	-3.208092	3.708248	-1.965108
40	1	0	-1.621324	3.117717	-2.522851
41	1	0	-3.076960	2.188133	-2.905777
42	6	0	0.052081	3.743660	1.597222
43	1	0	0.849823	3.615673	2.329776
44	1	0	-0.052972	4.788905	1.317592
45	1	0	-0.878447	3.382431	2.041353

46	7	0	-3.926887	-0.546026	0.081682
47	6	0	-4.294264	-0.079312	1.319099
48	6	0	-5.675713	0.508309	1.455584
49	1	0	-5.838547	0.728628	2.507820
50	1	0	-5.745433	1.434637	0.880409
51	1	0	-6.445343	-0.179248	1.100655
52	8	0	5.280022	0.816110	1.137690
53	8	0	3.974245	-1.833370	-0.248464
54	8	0	0.298788	3.312349	-0.759381
55	8	0	1.016743	-2.915929	0.195825
56	8	0	-2.731593	2.442362	0.219792
57	8	0	-3.515871	-0.133776	2.255029
58	6	0	-4.814545	-0.627613	-1.080452
59	1	0	-5.577657	0.143786	-0.987229
60	1	0	-4.222404	-0.377603	-1.964306
61	6	0	-5.446217	-2.005248	-1.229744
62	1	0	-6.090380	-2.035343	-2.111159
63	1	0	-4.678191	-2.774932	-1.344139
64	1	0	-6.045617	-2.251385	-0.350344

Structure 13 B_1G^+E (M06-2X, Gas Phase)

Energy (Hartrees): =-1755.1465438
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.249372	1.498185	-0.405234
2	1	0	2.853388	2.256609	-1.081493
3	1	0	3.408478	1.919965	0.588494
4	6	0	2.286998	0.322471	-0.322596
5	1	0	2.408239	-0.289391	-1.219591
6	6	0	0.840205	0.773027	-0.244739
7	1	0	0.576051	1.233360	-1.197364
8	6	0	-0.115288	-0.385663	0.042551
9	1	0	0.124412	-0.846904	1.003009
10	6	0	-1.558997	0.104031	0.067353
11	1	0	-1.704296	0.690743	0.972952
12	6	0	-2.587090	-1.038516	-0.021023
13	1	0	-2.374742	-1.547487	-0.965119
14	6	0	-2.373584	-2.048898	1.031940
15	7	0	-2.213025	-2.838218	1.850211
16	8	0	4.490151	1.075750	-0.971905
17	8	0	2.573986	-0.471049	0.829161
18	8	0	0.650813	1.725153	0.808094
19	8	0	0.070896	-1.343993	-1.001415
20	8	0	-1.804207	0.926116	-1.071786
21	6	0	5.426671	0.587268	-0.130459
22	6	0	3.351802	-1.563814	0.656705
23	6	0	0.641822	-2.542425	-0.664655
24	6	0	0.411074	3.013454	0.457245
25	6	0	-2.329262	2.158943	-0.854087
26	6	0	6.568548	-0.006735	-0.899047
27	6	0	3.620770	-2.234130	1.964246
28	6	0	1.028744	-3.314077	-1.888273
29	6	0	-2.489134	2.912307	-2.136856
30	1	0	7.422090	-0.135489	-0.238723
31	1	0	6.232885	-0.981101	-1.262979
32	1	0	6.822312	0.612807	-1.757726
33	1	0	0.982730	-4.378202	-1.668678
34	1	0	0.405118	-3.054306	-2.740792
35	1	0	2.067459	-3.048671	-2.106942
36	1	0	2.675042	-2.417745	2.473619
37	1	0	4.150007	-3.166494	1.788487
38	1	0	4.226998	-1.557303	2.569631
39	1	0	-3.236250	3.690491	-2.002465
40	1	0	-1.523050	3.375139	-2.354843
41	1	0	-2.754834	2.243937	-2.953475
42	6	0	0.102322	3.850014	1.659478
43	1	0	0.701287	3.537684	2.513044
44	1	0	0.267920	4.897258	1.419970
45	1	0	-0.954061	3.697550	1.894136
46	7	0	-3.954893	-0.563019	-0.110569
47	6	0	-4.705244	-0.067655	0.948437
48	6	0	-3.996598	0.322941	2.226382
49	1	0	-4.758126	0.394346	2.999035
50	1	0	-3.225087	-0.376419	2.545028
51	1	0	-3.550637	1.309285	2.079081
52	8	0	5.318652	0.602564	1.064341
53	8	0	3.763723	-1.907672	-0.420501
54	8	0	0.425013	3.395157	-0.681324
55	8	0	0.833186	-2.880267	0.464997
56	8	0	-2.575845	2.580462	0.242044

57	8	0	-5.897289	0.099057	0.818313
58	6	0	-4.683435	-0.923445	-1.332046
59	1	0	-5.497039	-0.208906	-1.439609
60	1	0	-3.998068	-0.790043	-2.173017
61	6	0	-5.231124	-2.344557	-1.275846
62	1	0	-5.754521	-2.592530	-2.201060
63	1	0	-4.429630	-3.074548	-1.131897
64	1	0	-5.932711	-2.431534	-0.445226

Structure 13 A_1G^-Z (M06-2X, Gas Phase)

Energy (Hartrees): = - 1755.1499916
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.242478	1.263626	0.109783
2	1	0	3.091142	2.204596	-0.419945
3	1	0	3.296960	1.436513	1.185536
4	6	0	2.108274	0.302630	-0.207375
5	1	0	2.281775	-0.130991	-1.193903
6	6	0	0.753998	0.990577	-0.222822
7	1	0	0.710035	1.620243	-1.112942
8	6	0	-0.390602	-0.022148	-0.263600
9	1	0	-0.362701	-0.665864	0.616509
10	6	0	-1.731551	0.688289	-0.325017
11	1	0	-1.859836	1.268161	0.588849
12	6	0	-2.973832	-0.222487	-0.421155
13	1	0	-3.827288	0.462858	-0.475779
14	6	0	-2.978777	-1.022702	-1.654131
15	7	0	-3.001021	-1.650580	-2.615031
16	8	0	4.478416	0.733195	-0.373676
17	8	0	2.068945	-0.750358	0.759480
18	8	0	0.556811	1.801694	0.937566
19	8	0	-0.164610	-0.796385	-1.442253
20	8	0	-1.737707	1.565948	-1.449196
21	6	0	5.166631	-0.092875	0.441192
22	6	0	2.674211	-1.915028	0.438931
23	6	0	0.011890	-2.133511	-1.319432
24	6	0	0.570286	3.150194	0.766301
25	6	0	-1.962884	2.886778	-1.205094
26	6	0	6.305792	-0.732701	-0.294637
27	6	0	2.620915	-2.871240	1.587024
28	6	0	0.346545	-2.742849	-2.643451
29	6	0	-1.738419	3.704220	-2.439180
30	1	0	7.023613	-1.128615	0.419242
31	1	0	5.880963	-1.551277	-0.881566
32	1	0	6.773375	-0.025475	-0.977381
33	1	0	0.330260	-3.825467	-2.553925
34	1	0	-0.368260	-2.399022	-3.391329
35	1	0	1.347553	-2.410952	-2.927796
36	1	0	1.591160	-2.962414	1.931503
37	1	0	3.007576	-3.836039	1.270508
38	1	0	3.232054	-2.458324	2.392220
39	1	0	-2.325519	4.617352	-2.377895
40	1	0	-0.677021	3.968363	-2.448522
41	1	0	-1.973538	3.136735	-3.337005
42	6	0	0.126999	3.851211	2.011172
43	1	0	0.517560	3.351605	2.896069
44	1	0	0.440965	4.890950	1.970257
45	1	0	-0.964892	3.801780	2.031409
46	7	0	-3.120791	-1.056193	0.773563
47	6	0	-3.592163	-0.381856	1.882216
48	6	0	-3.782873	-1.181099	3.153742
49	1	0	-4.177945	-0.498656	3.901432
50	1	0	-4.471645	-2.015263	3.018361
51	1	0	-2.827028	-1.581636	3.497990
52	8	0	4.865973	-0.304057	1.583890
53	8	0	3.190751	-2.113924	-0.628953
54	8	0	0.874295	3.672915	-0.270378
55	8	0	-0.085953	-2.716587	-0.272985
56	8	0	-2.252112	3.312741	-0.124580
57	8	0	-3.802487	0.813235	1.844969
58	6	0	-3.129033	-2.522259	0.687386
59	1	0	-2.382973	-2.824343	-0.043855
60	1	0	-2.776585	-2.912421	1.641731
61	6	0	-4.496928	-3.095532	0.327878
62	1	0	-4.450441	-4.186113	0.308658
63	1	0	-5.257884	-2.797300	1.052171
64	1	0	-4.813064	-2.756336	-0.659792

Structure 13 A_1G-Z (M06-2X, $CHCl_3$)

Energy (Hartrees): = -1755.1802673
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.235010	1.248901	-0.018582
2	1	0	3.070072	2.157783	-0.597898
3	1	0	3.300603	1.488211	1.043498
4	6	0	2.101994	0.267224	-0.270721
5	1	0	2.247155	-0.196443	-1.248537
6	6	0	0.750094	0.961316	-0.259418
7	1	0	0.697423	1.612550	-1.133165
8	6	0	-0.414171	-0.032360	-0.298228
9	1	0	-0.358980	-0.717330	0.548881
10	6	0	-1.740931	0.706710	-0.265073
11	1	0	-1.807688	1.257771	0.671939
12	6	0	-3.008982	-0.173927	-0.322458
13	1	0	-3.851313	0.524524	-0.264371
14	6	0	-3.130320	-0.868564	-1.611911
15	7	0	-3.245344	-1.400328	-2.622584
16	8	0	4.477512	0.715412	-0.487477
17	8	0	2.085950	-0.748892	0.736971
18	8	0	0.591088	1.741499	0.929293
19	8	0	-0.279317	-0.752970	-1.524975
20	8	0	-1.785252	1.614678	-1.364177
21	6	0	5.199387	-0.043108	0.358486
22	6	0	2.707450	-1.915039	0.464384
23	6	0	-0.007452	-2.079401	-1.479774
24	6	0	0.557714	3.093463	0.803488
25	6	0	-2.071609	2.917084	-1.095662
26	6	0	6.396472	-0.618960	-0.332561
27	6	0	2.615630	-2.852139	1.625029
28	6	0	0.138180	-2.633723	-2.859880
29	6	0	-1.977177	3.747006	-2.334819
30	1	0	7.074661	-1.045117	0.402801
31	1	0	6.047984	-1.402135	-1.010312
32	1	0	6.898296	0.145215	-0.925833
33	1	0	0.365167	-3.695177	-2.803288
34	1	0	-0.790964	-2.467923	-3.409509
35	1	0	0.937934	-2.103313	-3.379939
36	1	0	1.589175	-2.894104	1.988376
37	1	0	2.957836	-3.839130	1.323632
38	1	0	3.251660	-2.464881	2.424711
39	1	0	-2.453527	4.709530	-2.165201
40	1	0	-0.917219	3.901778	-2.552965
41	1	0	-2.429768	3.228452	-3.179285
42	6	0	0.200630	3.738765	2.102817
43	1	0	0.787666	3.307616	2.913886
44	1	0	0.361721	4.811595	2.033240
45	1	0	-0.855469	3.537567	2.299512
46	7	0	-3.082774	-1.095323	0.809907
47	6	0	-3.443121	-0.517064	2.003988
48	6	0	-3.533456	-1.416163	3.213225
49	1	0	-3.881879	-0.810059	4.046011
50	1	0	-4.217686	-2.250497	3.056716
51	1	0	-2.548491	-1.823864	3.452613
52	8	0	4.892484	-0.232451	1.506108
53	8	0	3.271825	-2.131203	-0.576302
54	8	0	0.775122	3.657365	-0.234828
55	8	0	0.089636	-2.696838	-0.452411
56	8	0	-2.330207	3.313141	0.006433
57	8	0	-3.641449	0.683894	2.081150
58	6	0	-3.036412	-2.551845	0.616209
59	1	0	-2.342767	-2.764049	-0.195465
60	1	0	-2.594762	-2.995111	1.507895
61	6	0	-4.402615	-3.160002	0.320255
62	1	0	-4.307575	-4.241736	0.202862
63	1	0	-5.107819	-2.963517	1.130566
64	1	0	-4.821660	-2.756782	-0.603686

Structure 13 A_1G-E (M06-2X, Gas Phase)

Energy (Hartrees): = -1755.1482904
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	6	0	-3.186157	1.450259	-0.121254
2	1	0	-2.965466	2.361432	0.436770
3	1	0	-3.191736	1.652361	-1.193240
4	6	0	-2.148720	0.383685	0.198655
5	1	0	-2.385416	-0.053950	1.171444
6	6	0	-0.748318	0.967339	0.259507
7	1	0	-0.678960	1.596501	1.147800
8	6	0	0.330012	-0.117177	0.335995
9	1	0	0.245985	-0.796930	-0.514583
10	6	0	1.708940	0.522984	0.351250
11	1	0	1.824915	1.075479	-0.581851
12	6	0	2.932332	-0.419855	0.424914
13	1	0	3.783257	0.233247	0.633376
14	6	0	2.869101	-1.351454	1.566931
15	7	0	2.842192	-2.089431	2.445503
16	8	0	-4.478438	1.028270	0.312892
17	8	0	-2.165039	-0.642701	-0.792167
18	8	0	-0.476123	1.762440	-0.900507
19	8	0	0.093540	-0.812856	1.557563
20	8	0	1.758688	1.431520	1.451144
21	6	0	-5.215242	0.295361	-0.550394
22	6	0	-2.899477	-1.750571	-0.528787
23	6	0	-0.285043	-2.118319	1.509242
24	6	0	-0.293026	3.094861	-0.719157
25	6	0	2.250929	2.671019	1.202662
26	6	0	-6.431325	-0.257030	0.129469
27	6	0	-2.844429	-2.702389	-1.679825
28	6	0	-0.524797	-2.644773	2.887989
29	6	0	2.093833	3.567042	2.389602
30	1	0	-7.155130	-0.570355	-0.618441
31	1	0	-6.101153	-1.123779	0.708054
32	1	0	-6.858830	0.473096	0.814559
33	1	0	-0.916801	-3.655437	2.819355
34	1	0	0.424387	-2.636251	3.427744
35	1	0	-1.226366	-1.994535	3.410947
36	1	0	-1.802309	-2.922047	-1.912258
37	1	0	-3.379019	-3.611930	-1.420584
38	1	0	-3.306620	-2.218394	-2.542169
39	1	0	2.810824	4.381355	2.323039
40	1	0	1.080857	3.975285	2.342920
41	1	0	2.207253	3.009058	3.316907
42	6	0	0.185311	3.750979	-1.976806
43	1	0	-0.221964	3.257870	-2.856954
44	1	0	-0.075244	4.806288	-1.953674
45	1	0	1.274926	3.656812	-1.987511
46	7	0	3.170231	-1.128330	-0.816130
47	6	0	4.003412	-0.625638	-1.799677
48	6	0	4.707328	0.691103	-1.537084
49	1	0	5.196540	0.973956	-2.465249
50	1	0	4.033269	1.488937	-1.219545
51	1	0	5.473000	0.563457	-0.766589
52	8	0	-4.897326	0.095527	-1.689801
53	8	0	-3.510214	-1.900469	0.494359
54	8	0	-0.462480	3.643241	0.335489
55	8	0	-0.390740	-2.731745	0.484351
56	8	0	2.713670	2.984475	0.138920
57	8	0	4.166051	-1.235005	-2.833051
58	6	0	2.561693	-2.446603	-1.058220
59	1	0	1.710761	-2.559856	-0.388233
60	1	0	2.184751	-2.445767	-2.081585
61	6	0	3.555136	-3.586280	-0.863665
62	1	0	3.062232	-4.541451	-1.054299
63	1	0	4.385289	-3.479605	-1.561771
64	1	0	3.938142	-3.599341	0.158408

Structure 13 A_1G-E (M06-2X, $CHCl_3$)

Energy (Hartrees): = -1755.1789547
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.201792	1.341580	0.057207
2	1	0	-3.006998	2.199649	0.702139
3	1	0	-3.201629	1.652116	-0.988395
4	6	0	-2.136828	0.279761	0.288818
5	1	0	-2.331747	-0.223151	1.239466
6	6	0	-0.755660	0.912792	0.334660
7	1	0	-0.695428	1.545495	1.221227
8	6	0	0.373234	-0.122923	0.387261
9	1	0	0.273613	-0.836006	-0.433270
10	6	0	1.721349	0.573887	0.304320

11	1	0	1.757023	1.108782	-0.645023
12	6	0	2.984109	-0.318371	0.324836
13	1	0	3.829227	0.370561	0.401837
14	6	0	3.070238	-1.157678	1.533856
15	7	0	3.165222	-1.824230	2.463220
16	8	0	-4.494962	0.862263	0.431660
17	8	0	-2.140562	-0.682245	-0.767881
18	8	0	-0.549765	1.710255	-0.836750
19	8	0	0.258136	-0.784888	1.646861
20	8	0	1.799644	1.500492	1.385437
21	6	0	-5.229980	0.235229	-0.507010
22	6	0	-2.858902	-1.812175	-0.589119
23	6	0	-0.167632	-2.073159	1.677682
24	6	0	-0.415626	3.052288	-0.682013
25	6	0	2.244470	2.752362	1.103816
26	6	0	-6.489588	-0.317051	0.083503
27	6	0	-2.721482	-2.718568	-1.769555
28	6	0	-0.223789	-2.573244	3.084621
29	6	0	2.160892	3.633448	2.305921
30	1	0	-7.184463	-0.575245	-0.712035
31	1	0	-6.224178	-1.217396	0.643780
32	1	0	-6.935754	0.396353	0.775778
33	1	0	-0.599420	-3.593040	3.092596
34	1	0	0.780262	-2.531631	3.512608
35	1	0	-0.870141	-1.924005	3.677722
36	1	0	-1.665372	-2.888568	-1.981778
37	1	0	-3.226020	-3.659928	-1.566813
38	1	0	-3.173593	-2.229731	-2.635503
39	1	0	2.690057	4.563372	2.113764
40	1	0	1.104989	3.842634	2.493953
41	1	0	2.570149	3.123738	3.178185
42	6	0	-0.073623	3.705302	-1.981980
43	1	0	-0.723745	3.334527	-2.774656
44	1	0	-0.158713	4.784377	-1.880250
45	1	0	0.957453	3.442603	-2.233367
46	7	0	3.125860	-1.120586	-0.876427
47	6	0	3.797360	-0.651072	-1.984605
48	6	0	4.439438	0.715618	-1.911378
49	1	0	4.781785	0.964066	-2.913121
50	1	0	3.762764	1.495455	-1.556871
51	1	0	5.305122	0.687724	-1.243335
52	8	0	-4.887863	0.127590	-1.654884
53	8	0	-3.526632	-2.018195	0.389211
54	8	0	-0.541496	3.603872	0.378113
55	8	0	-0.442388	-2.695940	0.687775
56	8	0	2.623029	3.072911	0.008887
57	8	0	3.876574	-1.336678	-2.986560
58	6	0	2.586458	-2.488658	-0.936824
59	1	0	1.826692	-2.592566	-0.162967
60	1	0	2.091464	-2.606262	-1.901462
61	6	0	3.669720	-3.545020	-0.761584
62	1	0	3.227271	-4.541610	-0.824797
63	1	0	4.420373	-3.451695	-1.547501
64	1	0	4.157453	-3.448484	0.211013

Structure 13 B_1G^-Z (M06-2X, Gas Phase)

Energy (Hartrees): = -1755.146382
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.253446	1.266257	0.181607
2	1	0	-3.035575	2.110425	0.837846
3	1	0	-3.296530	1.598409	-0.856758
4	6	0	-2.163850	0.209281	0.332682
5	1	0	-2.318277	-0.343787	1.263400
6	6	0	-0.798890	0.879687	0.353849
7	1	0	-0.726398	1.521584	1.232408
8	6	0	0.385706	-0.097280	0.363359
9	1	0	0.251967	-0.862298	-0.404291
10	6	0	1.670297	0.676821	0.108716
11	1	0	1.617183	1.098725	-0.895380
12	6	0	3.004159	-0.089188	0.169330
13	1	0	3.763724	0.690884	0.053095
14	6	0	3.300231	-0.702730	1.476204
15	7	0	3.630645	-1.111126	2.496383
16	8	0	-4.522802	0.769565	0.591067
17	8	0	-2.167645	-0.705688	-0.760762
18	8	0	-0.667214	1.686946	-0.830140
19	8	0	0.480595	-0.703957	1.642194
20	8	0	1.733318	1.738766	1.063179
21	6	0	-5.283655	0.178022	-0.356083

22	6	0	-2.877068	-1.847975	-0.608609
23	6	0	0.016259	-1.979443	1.769050
24	6	0	-0.600586	3.029421	-0.689852
25	6	0	2.250207	2.913459	0.635232
26	6	0	-6.484838	-0.472018	0.261243
27	6	0	-2.536897	-2.824023	-1.691954
28	6	0	0.580552	-2.623566	2.993753
29	6	0	2.191661	3.952917	1.709673
30	1	0	-7.229990	-0.661687	-0.507247
31	1	0	-6.143763	-1.417637	0.688796
32	1	0	-6.889960	0.144940	1.061572
33	1	0	-0.006966	-3.502369	3.246149
34	1	0	1.607678	-2.909453	2.753007
35	1	0	0.618056	-1.915454	3.820382
36	1	0	-1.550478	-3.231678	-1.458523
37	1	0	-3.273036	-3.623164	-1.704608
38	1	0	-2.494686	-2.316069	-2.654704
39	1	0	2.810100	4.800374	1.426094
40	1	0	1.149816	4.266154	1.805763
41	1	0	2.514493	3.528565	2.659632
42	6	0	-0.329529	3.692655	-2.007484
43	1	0	-0.844454	3.173447	-2.813888
44	1	0	-0.630932	4.735732	-1.952725
45	1	0	0.748034	3.639966	-2.184987
46	7	0	3.180165	-0.993359	-0.958240
47	6	0	2.692216	-2.274904	-0.876706
48	6	0	2.983145	-3.204787	-2.034156
49	1	0	2.654074	-4.196596	-1.736389
50	1	0	2.423046	-2.895487	-2.919632
51	1	0	4.043365	-3.227817	-2.289225
52	8	0	-5.001309	0.167561	-1.521658
53	8	0	-3.653971	-2.027954	0.285548
54	8	0	-0.713866	3.593276	0.364582
55	8	0	-0.731342	-2.477862	0.978876
56	8	0	2.673824	3.064326	-0.480994
57	8	0	2.039036	-2.634879	0.080910
58	6	0	4.019174	-0.493204	-2.049229
59	1	0	3.744486	-1.012156	-2.966377
60	1	0	3.765278	0.560122	-2.200523
61	6	0	5.509157	-0.645398	-1.760071
62	1	0	6.101451	-0.225186	-2.574723
63	1	0	5.783104	-0.124890	-0.839584
64	1	0	5.776494	-1.697048	-1.641314

Structure 13 B_1G^-Z (M06-2X, $CHCl_3$)

Energy (Hartrees): = -1755.1803446
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.241745	1.194086	0.272713
2	1	0	-3.055773	1.995611	0.988542
3	1	0	-3.287942	1.600612	-0.738765
4	6	0	-2.127056	0.159733	0.371481
5	1	0	-2.238069	-0.411711	1.296512
6	6	0	-0.775800	0.859509	0.361674
7	1	0	-0.705257	1.501748	1.240346
8	6	0	0.428849	-0.092375	0.353120
9	1	0	0.310757	-0.856116	-0.417773
10	6	0	1.699351	0.706835	0.098885
11	1	0	1.638982	1.131248	-0.903213
12	6	0	3.043153	-0.044680	0.153439
13	1	0	3.801029	0.736002	0.030076
14	6	0	3.348484	-0.634844	1.470217
15	7	0	3.673846	-1.011170	2.504472
16	8	0	-4.507010	0.641487	0.636500
17	8	0	-2.146918	-0.732683	-0.744150
18	8	0	-0.684194	1.661680	-0.826887
19	8	0	0.538918	-0.703589	1.632417
20	8	0	1.752707	1.760240	1.063870
21	6	0	-5.251206	0.086561	-0.338575
22	6	0	-2.826117	-1.890327	-0.610904
23	6	0	0.093119	-1.979176	1.766827
24	6	0	-0.714280	3.009188	-0.704655
25	6	0	2.099395	2.995402	0.625874
26	6	0	-6.471000	-0.568204	0.230950
27	6	0	-2.543991	-2.803580	-1.762006
28	6	0	0.641209	-2.607049	3.006584
29	6	0	2.076133	3.985069	1.744280
30	1	0	-7.153217	-0.835361	-0.572508
31	1	0	-6.148396	-1.468699	0.758694
32	1	0	-6.957213	0.091918	0.949389
33	1	0	0.003248	-3.433516	3.312417

34	1	0	1.635249	-2.986126	2.754251
35	1	0	0.749476	-1.873463	3.804368
36	1	0	-1.514532	-3.158124	-1.670340
37	1	0	-3.227814	-3.648432	-1.735803
38	1	0	-2.641223	-2.260075	-2.702382
39	1	0	2.427356	4.949114	1.385073
40	1	0	1.050118	4.070429	2.107324
41	1	0	2.699681	3.628478	2.565248
42	6	0	-0.564097	3.667287	-2.039368
43	1	0	-1.299214	3.263142	-2.736821
44	1	0	-0.687986	4.741774	-1.929675
45	1	0	0.432518	3.446044	-2.427071
46	7	0	3.218798	-0.961594	-0.961382
47	6	0	2.767865	-2.250139	-0.858899
48	6	0	3.047856	-3.179298	-2.014063
49	1	0	2.741210	-4.178003	-1.712570
50	1	0	2.469530	-2.878456	-2.891029
51	1	0	4.104239	-3.185139	-2.287006
52	8	0	-4.948825	0.115348	-1.502493
53	8	0	-3.555008	-2.127993	0.313861
54	8	0	-0.837956	3.570995	0.351079
55	8	0	-0.638040	-2.501420	0.972527
56	8	0	2.369581	3.223395	-0.523796
57	8	0	2.151516	-2.618209	0.127159
58	6	0	4.013105	-0.451136	-2.085213
59	1	0	3.729710	-0.995469	-2.984089
60	1	0	3.720481	0.590226	-2.246122
61	6	0	5.510814	-0.554244	-1.831294
62	1	0	6.065526	-0.153356	-2.682109
63	1	0	5.798906	0.013783	-0.943116
64	1	0	5.807703	-1.594471	-1.680589

Structure 13 B_1G^-E (M06-2X, Gas Phase)

Energy (Hartrees): = -1755.1411518
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.189307	1.463807	-0.097061
2	1	0	-2.954999	2.362193	0.476209
3	1	0	-3.173312	1.681612	-1.165818
4	6	0	-2.174088	0.372927	0.218118
5	1	0	-2.419885	-0.071351	1.186587
6	6	0	-0.768743	0.944800	0.279291
7	1	0	-0.697244	1.596191	1.151342
8	6	0	0.310649	-0.138104	0.392399
9	1	0	0.199882	-0.867943	-0.412358
10	6	0	1.686451	0.503312	0.334487
11	1	0	1.765266	1.027324	-0.617973
12	6	0	2.929187	-0.419317	0.385393
13	1	0	3.743670	0.242280	0.706879
14	6	0	2.872471	-1.435297	1.447588
15	7	0	2.866925	-2.191356	2.310950
16	8	0	-4.497156	1.068660	0.310010
17	8	0	-2.196018	-0.642866	-0.782028
18	8	0	-0.494593	1.709280	-0.901231
19	8	0	0.121508	-0.755927	1.663536
20	8	0	1.760201	1.448517	1.401831
21	6	0	-5.242801	0.382132	-0.583981
22	6	0	-2.973364	-1.728145	-0.547969
23	6	0	-0.344150	-2.032000	1.709099
24	6	0	-0.270545	3.039096	-0.752294
25	6	0	2.320087	2.649205	1.109540
26	6	0	-6.488235	-0.145392	0.061238
27	6	0	-2.879145	-2.694943	-1.684484
28	6	0	-0.448438	-2.504247	3.124638
29	6	0	2.201675	3.599366	2.258433
30	1	0	-7.208604	-0.415451	-0.706604
31	1	0	-6.196994	-1.036085	0.623851
32	1	0	-6.903388	0.582401	0.756430
33	1	0	-1.008910	-3.434577	3.149013
34	1	0	0.565121	-2.662689	3.500374
35	1	0	-0.926453	-1.742935	3.740013
36	1	0	-1.831282	-2.921074	-1.881289
37	1	0	-3.427022	-3.598931	-1.433731
38	1	0	-3.310307	-2.220794	-2.568405
39	1	0	2.946643	4.384134	2.154281
40	1	0	1.202390	4.038570	2.203088
41	1	0	2.303626	3.075634	3.206998
42	6	0	0.210483	3.652296	-2.030826
43	1	0	-0.221975	3.150698	-2.894031

44	1	0	-0.020034	4.714772	-2.029375
45	1	0	1.297044	3.527352	-2.052592
46	7	0	3.303755	-0.905932	-0.932508
47	6	0	3.152292	-2.174123	-1.476235
48	6	0	2.304940	-3.199472	-0.763634
49	1	0	2.034318	-3.942958	-1.509945
50	1	0	2.886542	-3.687858	0.020033
51	1	0	1.401376	-2.794566	-0.313279
52	8	0	-4.912325	0.202067	-1.722961
53	8	0	-3.649618	-1.847905	0.436037
54	8	0	-0.409157	3.615991	0.291477
55	8	0	-0.606557	-2.668550	0.727366
56	8	0	2.809742	2.890884	0.039026
57	8	0	3.693782	-2.434022	-2.528641
58	6	0	4.153770	0.031350	-1.685194
59	1	0	3.942787	-0.117862	-2.742246
60	1	0	3.853685	1.046281	-1.412155
61	6	0	5.634708	-0.195326	-1.405623
62	1	0	6.239608	0.531045	-1.951219
63	1	0	5.859118	-0.086965	-0.340720
64	1	0	5.918713	-1.198019	-1.725352

Structure 13 B_1G^-E (M06-2X, $CHCl_3$)

Energy (Hartrees): = -1755.1721466
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.185818	1.486848	-0.037175
2	1	0	-2.948981	2.366685	0.562859
3	1	0	-3.172085	1.743173	-1.096793
4	6	0	-2.173264	0.387476	0.249258
5	1	0	-2.400002	-0.065460	1.217717
6	6	0	-0.765868	0.959193	0.280328
7	1	0	-0.688092	1.648961	1.122153
8	6	0	0.317700	-0.118134	0.424055
9	1	0	0.205546	-0.874845	-0.355199
10	6	0	1.696842	0.513717	0.340374
11	1	0	1.761299	1.055027	-0.604286
12	6	0	2.925327	-0.430994	0.339401
13	1	0	3.772000	0.211927	0.609573
14	6	0	2.901927	-1.430295	1.417793
15	7	0	2.921337	-2.177108	2.288856
16	8	0	-4.499673	1.090790	0.361512
17	8	0	-2.210707	-0.617053	-0.766590
18	8	0	-0.529723	1.666047	-0.942263
19	8	0	0.152091	-0.693204	1.720857
20	8	0	1.804553	1.429027	1.427226
21	6	0	-5.269307	0.463634	-0.549134
22	6	0	-2.986926	-1.701078	-0.551176
23	6	0	-0.365946	-1.941597	1.829280
24	6	0	-0.170574	2.972253	-0.867598
25	6	0	2.491984	2.574766	1.190748
26	6	0	-6.547807	-0.010456	0.067962
27	6	0	-2.856233	-2.678486	-1.674713
28	6	0	-0.434715	-2.360403	3.262053
29	6	0	2.408092	3.504431	2.356071
30	1	0	-7.262369	-0.257239	-0.713715
31	1	0	-6.318700	-0.907046	0.649882
32	1	0	-6.953266	0.741396	0.744321
33	1	0	-0.955678	-3.311418	3.337479
34	1	0	0.584082	-2.456347	3.644912
35	1	0	-0.945191	-1.593871	3.846559
36	1	0	-1.802649	-2.896320	-1.853392
37	1	0	-3.398867	-3.588275	-1.430426
38	1	0	-3.271874	-2.226988	-2.578483
39	1	0	3.135802	4.303541	2.237689
40	1	0	1.399083	3.923379	2.374017
41	1	0	2.571279	2.963187	3.287913
42	6	0	0.132245	3.521504	-2.224835
43	1	0	-0.589873	3.158004	-2.955287
44	1	0	0.136855	4.608015	-2.184114
45	1	0	1.124247	3.169026	-2.521350
46	7	0	3.223387	-0.945253	-0.989648
47	6	0	2.992735	-2.201787	-1.510629
48	6	0	2.178565	-3.207655	-0.737165
49	1	0	1.809372	-3.932564	-1.460772
50	1	0	2.818356	-3.729368	-0.022354
51	1	0	1.333890	-2.784419	-0.199150
52	8	0	-4.940548	0.299303	-1.694110
53	8	0	-3.695052	-1.820811	0.412712
54	8	0	-0.091853	3.572821	0.169946

55	8	0	-0.703611	-2.595341	0.879514
56	8	0	3.063648	2.779483	0.153410
57	8	0	3.452732	-2.488844	-2.601207
58	6	0	4.054399	-0.033178	-1.796136
59	1	0	3.777217	-0.173274	-2.839164
60	1	0	3.799204	0.988803	-1.507360
61	6	0	5.540948	-0.292972	-1.596559
62	1	0	6.129351	0.407768	-2.192669
63	1	0	5.825414	-0.165092	-0.548297
64	1	0	5.790861	-1.308283	-1.907991

Structure 13 R-X (M06-2X, Gas Phase)

Energy (Hartrees): = - 1755.1495784
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	4.083786	0.431345	-2.127391
2	8	0	1.641957	-0.932021	-0.890158
3	8	0	2.588269	-2.431894	0.493053
4	8	0	-0.033079	1.431818	-1.096139
5	8	0	-0.414460	3.243722	0.186560
6	8	0	-0.813171	-1.413430	0.975632
7	8	0	-0.499185	-3.160297	-0.410316
8	8	0	-2.631561	0.964293	0.808512
9	8	0	-3.310110	2.481018	-0.711448
10	8	0	-4.673949	-0.577399	-0.376411
11	8	0	-5.608110	-2.501105	0.285202
12	7	0	2.376730	2.827795	1.937587
13	7	0	3.890909	0.369053	0.133123
14	6	0	5.405801	0.883636	2.049944
15	1	0	6.282411	0.977114	1.406421
16	1	0	5.734817	0.509285	3.021426
17	1	0	4.978134	1.876487	2.191521
18	6	0	4.375611	-0.067288	1.447312
19	1	0	4.764884	-1.081946	1.363292
20	1	0	3.508529	-0.139255	2.107188
21	6	0	4.512404	0.053400	-1.056829
22	6	0	5.727867	-0.844966	-0.964330
23	1	0	5.416739	-1.848196	-0.658932
24	1	0	6.463289	-0.486954	-0.244493
25	1	0	6.171971	-0.892315	-1.954992
26	6	0	2.598366	1.029146	0.048949
27	1	0	2.529779	1.492071	-0.937940
28	6	0	2.469883	2.060327	1.089010
29	6	0	1.457553	-0.004379	0.171445
30	1	0	1.529472	-0.526765	1.127256
31	6	0	2.263904	-2.101503	-0.616991
32	6	0	2.465312	-2.886421	-1.874347
33	1	0	3.055637	-3.772948	-1.657985
34	1	0	2.952493	-2.252290	-2.617228
35	1	0	1.482885	-3.175327	-2.252710
36	6	0	0.061185	0.592004	0.053422
37	1	0	-0.160631	1.170742	0.952139
38	6	0	-0.327435	2.749760	-0.899961
39	6	0	-0.557426	3.441891	-2.206668
40	1	0	-1.595857	3.247467	-2.487160
41	1	0	0.100331	3.047903	-2.979170
42	1	0	-0.418474	4.511627	-2.072579
43	6	0	-0.969204	-0.521104	-0.134878
44	1	0	-0.749571	-1.061325	-1.056262
45	6	0	-0.529851	-2.714106	0.702524
46	6	0	-0.228607	-3.472096	1.958681
47	1	0	-0.377287	-4.533910	1.779896
48	1	0	-0.843377	-3.118694	2.784296
49	1	0	0.823263	-3.292888	2.196643
50	6	0	-2.395227	-0.000375	-0.219605
51	1	0	-2.531728	0.480254	-1.189557
52	6	0	-3.108237	2.177902	0.431023
53	6	0	-3.284424	3.071043	1.620013
54	1	0	-3.894778	3.925352	1.339076
55	1	0	-2.290860	3.415699	1.915808
56	1	0	-3.727956	2.523480	2.450200
57	6	0	-3.395702	-1.122985	-0.057994
58	1	0	-3.159129	-1.955396	-0.727844
59	1	0	-3.394649	-1.489581	0.969755
60	6	0	-5.725944	-1.388907	-0.143794
61	6	0	-7.016547	-0.705659	-0.496926
62	1	0	-7.846611	-1.374366	-0.286731
63	1	0	-7.004886	-0.432654	-1.552880
64	1	0	-7.111088	0.215054	0.079802

Structure 37 A_1G^+Z (M06-2X, Gas Phase)

Energy (Hartrees): = -1946.8556253
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.287250	0.837451	-0.281266
2	1	0	-4.228215	1.718137	0.365130
3	1	0	-4.194319	1.159577	-1.320216
4	6	0	-3.202206	-0.158491	0.062088
5	1	0	-3.402350	-0.601420	1.039259
6	6	0	-1.839841	0.512392	0.108187
7	1	0	-1.805081	1.146111	0.994526
8	6	0	-0.681386	-0.482783	0.156499
9	1	0	-0.705440	-1.142074	-0.713384
10	6	0	0.645214	0.267021	0.179244
11	1	0	0.817022	0.693958	-0.810844
12	6	0	1.851877	-0.594806	0.601751
13	1	0	1.691282	-0.905464	1.636807
14	6	0	1.976685	-1.783942	-0.253328
15	7	0	2.088686	-2.686968	-0.953264
16	8	0	-5.530197	0.165074	-0.092840
17	8	0	-3.208458	-1.193803	-0.921986
18	8	0	-1.623431	1.322641	-1.053828
19	8	0	-0.845361	-1.254590	1.345297
20	8	0	0.560264	1.315254	1.137598
21	6	0	-6.626915	0.866322	-0.445522
22	6	0	-3.638263	-2.422039	-0.534025
23	6	0	-1.026833	-2.601592	1.208006
24	6	0	-1.547226	2.667991	-0.880898
25	6	0	1.093933	2.517916	0.824078
26	6	0	-7.873966	0.061116	-0.214788
27	6	0	-3.572420	-3.389489	-1.675199
28	6	0	-1.363009	-3.230174	2.523647
29	6	0	1.016773	3.440234	1.998743
30	1	0	-8.741689	0.657313	-0.483320
31	1	0	-7.836282	-0.848025	-0.816319
32	1	0	-7.924417	-0.239287	0.832331
33	1	0	-1.090464	-4.282382	2.495669
34	1	0	-0.873424	-2.712368	3.346032
35	1	0	-2.447070	-3.147641	2.640543
36	1	0	-2.522259	-3.656803	-1.812567
37	1	0	-4.143755	-4.279260	-1.423968
38	1	0	-3.939607	-2.929060	-2.591185
39	1	0	1.520150	4.373620	1.761835
40	1	0	-0.036860	3.625775	2.215442
41	1	0	1.470715	2.951272	2.862665
42	6	0	-1.156167	3.351129	-2.155244
43	1	0	-1.584545	2.843058	-3.017028
44	1	0	-1.467893	4.391734	-2.113160
45	1	0	-0.065884	3.306384	-2.222135
46	7	0	3.076159	0.189215	0.569905
47	6	0	3.516184	0.732485	1.763372
48	6	0	4.672795	1.700377	1.664185
49	1	0	4.955505	1.976820	2.676389
50	1	0	5.525134	1.264110	1.141598
51	1	0	4.359805	2.593834	1.116029
52	8	0	-6.574501	1.981600	-0.879449
53	8	0	-3.979632	-2.678388	0.586328
54	8	0	-1.739730	3.207386	0.172945
55	8	0	-0.958881	-3.165293	0.155328
56	8	0	1.551210	2.772248	-0.259307
57	8	0	2.979290	0.472234	2.819279
58	6	0	5.026854	-0.161554	-0.955446
59	6	0	5.913909	0.406054	-1.869159
60	6	0	5.385302	-1.338632	-0.303913
61	6	0	7.136770	-0.198232	-2.135682
62	1	0	5.645458	1.328890	-2.374024
63	6	0	6.610291	-1.941796	-0.567086
64	1	0	4.707699	-1.787674	0.412846
65	6	0	7.488206	-1.375337	-1.483711
66	1	0	7.817784	0.253068	-2.847504
67	1	0	6.876415	-2.858238	-0.054341
68	1	0	8.442428	-1.846401	-1.686289
69	6	0	3.684925	0.505086	-0.719359
70	1	0	2.988623	0.173320	-1.495177
71	1	0	3.767636	1.588245	-0.838097

Structure 37 A_1G^+Z (M06-2X, $CHCl_3$)

Energy (Hartrees): = -1946.8943881
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.335244	-0.755981	-0.300746
2	1	0	4.330991	-1.641697	0.340333
3	1	0	4.265535	-1.069384	-1.344237
4	6	0	3.195918	0.168858	0.060844
5	1	0	3.362124	0.587365	1.053849
6	6	0	1.861665	-0.559347	0.070909
7	1	0	1.843020	-1.220977	0.937179
8	6	0	0.677325	0.403776	0.138511
9	1	0	0.691871	1.084056	-0.714933
10	6	0	-0.636893	-0.365263	0.136936
11	1	0	-0.781037	-0.806013	-0.850956
12	6	0	-1.860497	0.501577	0.511405
13	1	0	-1.679402	0.946559	1.492953
14	6	0	-2.050586	1.579958	-0.470162
15	7	0	-2.206079	2.395360	-1.262583
16	8	0	5.534972	-0.006085	-0.100586
17	8	0	3.161077	1.236235	-0.892912
18	8	0	1.687059	-1.333614	-1.120828
19	8	0	0.829271	1.141348	1.351207
20	8	0	-0.561647	-1.391797	1.117908
21	6	0	6.681720	-0.640330	-0.404572
22	6	0	3.474454	2.481161	-0.460838
23	6	0	0.841995	2.501158	1.278565
24	6	0	1.611431	-2.684237	-0.999688
25	6	0	-1.048454	-2.615280	0.799015
26	6	0	7.869221	0.237811	-0.152687
27	6	0	3.389434	3.467424	-1.581749
28	6	0	1.104058	3.097031	2.623197
29	6	0	-0.960466	-3.535196	1.973247
30	1	0	8.776667	-0.279728	-0.453292
31	1	0	7.761337	1.171453	-0.706570
32	1	0	7.912500	0.485460	0.909766
33	1	0	1.035271	4.179975	2.558610
34	1	0	0.389012	2.706833	3.349133
35	1	0	2.107272	2.805511	2.940415
36	1	0	2.349875	3.528352	-1.910690
37	1	0	3.725266	4.441472	-1.235009
38	1	0	3.994325	3.128466	-2.423693
39	1	0	-1.449880	-4.477107	1.738338
40	1	0	0.094510	-3.709469	2.196288
41	1	0	-1.417816	-3.062648	2.844283
42	6	0	1.281681	-3.318880	-2.312237
43	1	0	1.850815	-2.854430	-3.117019
44	1	0	1.479401	-4.386679	-2.259595
45	1	0	0.217844	-3.156117	-2.504600
46	7	0	-3.055768	-0.316800	0.621273
47	6	0	-3.462847	-0.679912	1.887876
48	6	0	-4.621451	-1.643328	1.966004
49	1	0	-4.903819	-1.740409	3.011554
50	1	0	-5.478594	-1.304352	1.381844
51	1	0	-4.312489	-2.620932	1.584163
52	8	0	6.708648	-1.769582	-0.815080
53	8	0	3.756062	2.733041	0.679831
54	8	0	1.767392	-3.258547	0.043547
55	8	0	0.671305	3.099041	0.253169
56	8	0	-1.471411	-2.887616	-0.293190
57	8	0	-2.893323	-0.270939	2.882299
58	6	0	-4.984797	0.098433	-0.918356
59	6	0	-5.757536	-0.266109	-2.022950
60	6	0	-5.369927	1.199200	-0.157743
61	6	0	-6.891587	0.460571	-2.363317
62	1	0	-5.465809	-1.125498	-2.619588
63	6	0	-6.507174	1.928189	-0.497925
64	1	0	-4.784448	1.497930	0.705562
65	6	0	-7.270265	1.562613	-1.599881
66	1	0	-7.481102	0.168006	-3.224807
67	1	0	-6.792299	2.785315	0.101272
68	1	0	-8.154232	2.131264	-1.864151
69	6	0	-3.752559	-0.728315	-0.592121
70	1	0	-3.044104	-0.663745	-1.422189
71	1	0	-4.019561	-1.784114	-0.517182

Structure 37 A_1G^+E (M06-2X, Gas Phase)

Energy (Hartrees): = -1946.8535335

No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.348100	-0.846599	-0.272672
2	1	0	4.284985	-1.739821	0.356335
3	1	0	4.269818	-1.150010	-1.318078
4	6	0	3.253534	0.133384	0.078233
5	1	0	3.447591	0.580387	1.053914
6	6	0	1.891410	-0.548911	0.117526
7	1	0	1.834586	-1.154984	1.022835
8	6	0	0.748396	0.461724	0.113456
9	1	0	0.831945	1.134428	-0.742414
10	6	0	-0.602155	-0.231368	0.056107
11	1	0	-0.688509	-0.758418	-0.895249
12	6	0	-1.789469	0.762215	0.202533
13	1	0	-1.572046	1.451455	1.018030
14	6	0	-1.878917	1.569047	-1.024062
15	7	0	-1.918370	2.152228	-2.011551
16	8	0	5.585453	-0.172594	-0.053594
17	8	0	3.248632	1.171063	-0.907699
18	8	0	1.712152	-1.392271	-1.021970
19	8	0	0.889239	1.200137	1.330658
20	8	0	-0.679596	-1.164535	1.123346
21	6	0	6.688831	-0.867234	-0.401976
22	6	0	3.446998	2.443212	-0.487359
23	6	0	0.821912	2.558266	1.255998
24	6	0	1.613441	-2.733435	-0.798316
25	6	0	-1.131867	-2.418819	0.826748
26	6	0	7.931914	-0.063093	-0.148063
27	6	0	3.298167	3.411313	-1.620519
28	6	0	1.167939	3.184438	2.570253
29	6	0	-1.312435	-3.225799	2.071098
30	1	0	8.803030	-0.655463	-0.414025
31	1	0	7.899924	0.852140	-0.740578
32	1	0	7.971499	0.225093	0.902969
33	1	0	0.838423	4.220134	2.571023
34	1	0	0.723158	2.626538	3.393491
35	1	0	2.255332	3.146543	2.665557
36	1	0	2.228701	3.609481	-1.734740
37	1	0	3.805037	4.339376	-1.368729
38	1	0	3.678489	2.988656	-2.548400
39	1	0	-1.387367	-4.276699	1.805590
40	1	0	-0.483117	-3.054449	2.755421
41	1	0	-2.242154	-2.898008	2.546353
42	6	0	1.301556	-3.465352	-2.065789
43	1	0	1.784485	-2.992484	-2.918728
44	1	0	1.605649	-4.503841	-1.962746
45	1	0	0.217795	-3.421994	-2.201288
46	7	0	-3.033430	0.077773	0.486612
47	6	0	-3.360650	-0.250499	1.787873
48	6	0	-2.696564	0.527167	2.907470
49	1	0	-3.155510	0.198541	3.836261
50	1	0	-1.623560	0.328856	2.942361
51	1	0	-2.856273	1.601238	2.787110
52	8	0	6.642997	-1.976832	-0.850160
53	8	0	3.660369	2.736163	0.657055
54	8	0	1.733419	-3.223676	0.288603
55	8	0	0.529320	3.135282	0.247543
56	8	0	-1.364400	-2.772242	-0.294370
57	8	0	-4.170784	-1.123795	2.021491
58	6	0	-5.092210	-0.124678	-0.888397
59	6	0	-6.212197	-0.668874	-0.260106
60	6	0	-5.260801	0.921587	-1.795764
61	6	0	-7.480924	-0.169188	-0.531360
62	1	0	-6.076786	-1.472646	0.453399
63	6	0	-6.529698	1.421063	-2.065473
64	1	0	-4.397895	1.344905	-2.297999
65	6	0	-7.642252	0.877289	-1.432725
66	1	0	-8.344819	-0.599643	-0.038821
67	1	0	-6.648980	2.230669	-2.775635
68	1	0	-8.631733	1.265095	-1.644574
69	6	0	-3.712927	-0.670116	-0.591446
70	1	0	-3.084745	-0.610538	-1.482234
71	1	0	-3.773570	-1.718594	-0.298676

Structure 37 A_1G^+E (M06-2X, $CHCl_3$)

Energy (Hartrees): = - 1946.8914331
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.320843	0.873277	-0.256503
2	1	0	-4.257082	1.751989	0.390902
3	1	0	-4.249140	1.191430	-1.298242
4	6	0	-3.227279	-0.114040	0.079966
5	1	0	-3.407515	-0.544358	1.064988
6	6	0	-1.857729	0.551391	0.089386
7	1	0	-1.787090	1.170373	0.984091
8	6	0	-0.722710	-0.470191	0.083595
9	1	0	-0.805737	-1.126282	-0.784454
10	6	0	0.633786	0.220572	0.052233
11	1	0	0.757520	0.713100	-0.913051
12	6	0	1.814858	-0.759668	0.289667
13	1	0	1.586952	-1.377690	1.158800
14	6	0	1.925228	-1.671779	-0.859432
15	7	0	1.993490	-2.354875	-1.778818
16	8	0	-5.557942	0.191108	-0.042741
17	8	0	-3.252809	-1.162073	-0.896622
18	8	0	-1.679891	1.371098	-1.069194
19	8	0	-0.874494	-1.227105	1.286487
20	8	0	0.676246	1.186906	1.093222
21	6	0	-6.669448	0.890405	-0.338172
22	6	0	-3.542881	-2.415636	-0.476403
23	6	0	-0.885937	-2.585439	1.192652
24	6	0	-1.580823	2.715189	-0.886806
25	6	0	1.109628	2.441172	0.781473
26	6	0	-7.903608	0.076174	-0.096236
27	6	0	-3.505722	-3.381905	-1.617029
28	6	0	-1.168215	-3.204899	2.522457
29	6	0	1.198298	3.289542	2.006404
30	1	0	-8.783749	0.672892	-0.322038
31	1	0	-7.880638	-0.815310	-0.725312
32	1	0	-7.925028	-0.251800	0.944258
33	1	0	-1.120055	-4.287239	2.435316
34	1	0	-0.447430	-2.846323	3.259382
35	1	0	-2.165781	-2.899032	2.842096
36	1	0	-2.466402	-3.492382	-1.935762
37	1	0	-3.891205	-4.344405	-1.290257
38	1	0	-4.082134	-2.996533	-2.458070
39	1	0	1.270620	4.334875	1.716755
40	1	0	0.332590	3.122135	2.646225
41	1	0	2.099501	2.998752	2.554891
42	6	0	-1.309010	3.406950	-2.182706
43	1	0	-2.029035	3.086661	-2.936473
44	1	0	-1.355574	4.482898	-2.035812
45	1	0	-0.310061	3.122772	-2.520925
46	7	0	3.060199	-0.056954	0.529489
47	6	0	3.408108	0.321719	1.810472
48	6	0	2.736948	-0.375039	2.973321
49	1	0	3.209112	-0.010820	3.882612
50	1	0	1.668386	-0.153408	3.010070
51	1	0	2.870119	-1.457452	2.909368
52	8	0	-6.633984	2.021961	-0.741420
53	8	0	-3.765078	-2.691677	0.672282
54	8	0	-1.687141	3.236787	0.189530
55	8	0	-0.688118	-3.163464	0.160286
56	8	0	1.389837	2.768526	-0.338508
57	8	0	4.252631	1.179800	1.987636
58	6	0	5.110552	0.088459	-0.878633
59	6	0	6.239206	0.675005	-0.303071
60	6	0	5.277162	-0.997824	-1.739764
61	6	0	7.509309	0.175964	-0.574236
62	1	0	6.111958	1.517836	0.365342
63	6	0	6.546730	-1.498012	-2.010492
64	1	0	4.410587	-1.450343	-2.209169
65	6	0	7.666014	-0.913031	-1.426181
66	1	0	8.377752	0.640705	-0.121520
67	1	0	6.661171	-2.339640	-2.683888
68	1	0	8.655929	-1.300157	-1.638851
69	6	0	3.728304	0.636470	-0.590471
70	1	0	3.095698	0.526702	-1.473082
71	1	0	3.786332	1.698974	-0.353484

Structure 37 B_1G^+Z (M06-2X, Gas Phase)

Energy (Hartrees): = -1946.8517449
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	6	0	4.255481	0.556201	-0.409607
2	1	0	4.118400	1.281437	-1.216826
3	1	0	4.430269	1.098684	0.521706
4	6	0	3.046145	-0.343388	-0.275336
5	1	0	2.982209	-1.005206	-1.140938
6	6	0	1.767874	0.472810	-0.192450
7	1	0	1.586509	0.911971	-1.174210
8	6	0	0.547090	-0.343365	0.231019
9	1	0	0.707830	-0.783894	1.216987
10	6	0	-0.683891	0.548891	0.279192
11	1	0	-0.596991	1.236747	1.118699
12	6	0	-2.013263	-0.214072	0.386317
13	1	0	-2.135820	-0.786317	-0.537627
14	6	0	-2.026357	-1.195180	1.485859
15	7	0	-2.057500	-2.008796	2.294522
16	8	0	5.364506	-0.295757	-0.687288
17	8	0	3.200736	-1.138071	0.900466
18	8	0	1.891418	1.523204	0.774404
19	8	0	0.370742	-1.381365	-0.736059
20	8	0	-0.766500	1.287665	-0.947823
21	6	0	6.561010	0.318923	-0.779435
22	6	0	3.466624	-2.458410	0.730870
23	6	0	0.519464	-2.673153	-0.314322
24	6	0	1.881657	2.802931	0.325411
25	6	0	-1.021963	2.617580	-0.875270
26	6	0	7.652855	-0.677105	-1.050218
27	6	0	3.606158	-3.142091	2.055773
28	6	0	0.497197	-3.620121	-1.473821
29	6	0	-0.989714	3.241027	-2.237886
30	1	0	8.594894	-0.152496	-1.183073
31	1	0	7.721982	-1.371929	-0.212040
32	1	0	7.405893	-1.257937	-1.939211
33	1	0	0.160021	-4.594798	-1.129615
34	1	0	-0.127397	-3.245595	-2.282052
35	1	0	1.528775	-3.706862	-1.825766
36	1	0	2.603008	-3.246502	2.474708
37	1	0	4.044628	-4.125522	1.907637
38	1	0	4.207819	-2.539317	2.734590
39	1	0	-1.547251	4.174283	-2.220062
40	1	0	0.058300	3.451797	-2.464546
41	1	0	-1.380431	2.558453	-2.990777
42	6	0	1.794691	3.769964	1.464279
43	1	0	2.380409	3.422928	2.313578
44	1	0	2.122175	4.750560	1.129172
45	1	0	0.743381	3.820194	1.761276
46	7	0	-3.121476	0.725661	0.467224
47	6	0	-3.245363	1.468420	1.625995
48	6	0	-4.375483	2.468042	1.686188
49	1	0	-4.429097	2.830539	2.709128
50	1	0	-4.153954	3.307907	1.022955
51	1	0	-5.330876	2.026664	1.396820
52	8	0	6.696913	1.502448	-0.654208
53	8	0	3.537400	-2.984578	-0.344426
54	8	0	1.903012	3.087854	-0.841157
55	8	0	0.684192	-2.972026	0.830902
56	8	0	-1.212478	3.198961	0.156528
57	8	0	-2.464892	1.314039	2.538720
58	6	0	-5.038818	-0.272036	-0.778250
59	6	0	-5.722555	-0.453866	-1.981075
60	6	0	-5.343585	-1.087795	0.307642
61	6	0	-6.703440	-1.428742	-2.095032
62	1	0	-5.481671	0.173407	-2.834223
63	6	0	-6.324688	-2.069955	0.191469
64	1	0	-4.810877	-0.969658	1.245066
65	6	0	-7.007149	-2.241089	-1.005430
66	1	0	-7.226816	-1.560524	-3.034505
67	1	0	-6.549203	-2.703223	1.041273
68	1	0	-7.768351	-3.006695	-1.094770
69	6	0	-3.996783	0.827952	-0.686621
70	1	0	-4.487382	1.802161	-0.668045
71	1	0	-3.377132	0.817460	-1.589603

Structure 37 B_1G^+Z (M06-2X, $CHCl_3$)

Energy (Hartrees): = - 1946.892829
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.292691	0.576772	-0.406993
2	1	0	4.164268	1.283935	-1.230792
3	1	0	4.457165	1.131833	0.518954
4	6	0	3.083079	-0.322652	-0.281119
5	1	0	3.017903	-0.974937	-1.153085

6	6	0	1.802134	0.488652	-0.190117
7	1	0	1.627031	0.946110	-1.164508
8	6	0	0.587587	-0.349682	0.210576
9	1	0	0.748810	-0.803228	1.190220
10	6	0	-0.657268	0.523139	0.266843
11	1	0	-0.577423	1.203235	1.113195
12	6	0	-1.978447	-0.260833	0.366572
13	1	0	-2.079032	-0.858080	-0.543841
14	6	0	-1.984969	-1.220692	1.485498
15	7	0	-1.993890	-2.021576	2.307289
16	8	0	5.407494	-0.280121	-0.659730
17	8	0	3.233361	-1.125869	0.892371
18	8	0	1.916192	1.514534	0.802724
19	8	0	0.433650	-1.370784	-0.778132
20	8	0	-0.752169	1.268472	-0.951554
21	6	0	6.601043	0.328990	-0.779814
22	6	0	3.509079	-2.441586	0.726162
23	6	0	0.553353	-2.670758	-0.385191
24	6	0	1.888731	2.807475	0.393509
25	6	0	-1.030424	2.594217	-0.869827
26	6	0	7.692737	-0.665147	-1.034857
27	6	0	3.672898	-3.115560	2.050924
28	6	0	0.508670	-3.589358	-1.563476
29	6	0	-1.048664	3.219464	-2.228420
30	1	0	8.640272	-0.145730	-1.153710
31	1	0	7.748379	-1.364385	-0.198517
32	1	0	7.459221	-1.239948	-1.932626
33	1	0	0.234755	-4.588411	-1.232172
34	1	0	-0.182228	-3.223458	-2.321501
35	1	0	1.515209	-3.618890	-1.990256
36	1	0	2.747714	-3.003139	2.618521
37	1	0	3.893810	-4.168936	1.898349
38	1	0	4.477162	-2.632620	2.608545
39	1	0	-1.588751	4.162696	-2.187830
40	1	0	-0.010109	3.413368	-2.509849
41	1	0	-1.486362	2.546533	-2.964743
42	6	0	1.850238	3.736579	1.563175
43	1	0	2.627379	3.470675	2.280278
44	1	0	1.974971	4.759509	1.217404
45	1	0	0.880510	3.627116	2.055105
46	7	0	-3.104312	0.658395	0.417477
47	6	0	-3.277124	1.400634	1.563700
48	6	0	-4.424737	2.376688	1.586031
49	1	0	-4.520896	2.749919	2.602827
50	1	0	-4.208344	3.215781	0.919466
51	1	0	-5.361621	1.913237	1.271174
52	8	0	6.732967	1.520270	-0.690079
53	8	0	3.592169	-2.967748	-0.350717
54	8	0	1.879421	3.125470	-0.765741
55	8	0	0.703401	-2.996955	0.757966
56	8	0	-1.200801	3.166036	0.172213
57	8	0	-2.519300	1.261241	2.505626
58	6	0	-5.095111	-0.277715	-0.770381
59	6	0	-5.806671	-0.462618	-1.957639
60	6	0	-5.449502	-1.016824	0.355748
61	6	0	-6.861085	-1.364173	-2.016809
62	1	0	-5.529651	0.106364	-2.840355
63	6	0	-6.505766	-1.924477	0.295451
64	1	0	-4.903554	-0.894055	1.285322
65	6	0	-7.213383	-2.100150	-0.886999
66	1	0	-7.404192	-1.498679	-2.945169
67	1	0	-6.769844	-2.496697	1.177410
68	1	0	-8.032850	-2.807882	-0.932365
69	6	0	-3.968705	0.739247	-0.751007
70	1	0	-4.377604	1.748951	-0.816098
71	1	0	-3.348068	0.607915	-1.641517

Structure 37 B_1G^+E (M06-2X, Gas Phase)

Energy (Hartrees): = -1946.85037
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.200539	0.304945	-0.378031
2	1	0	4.152740	0.982726	-1.234984
3	1	0	4.425049	0.888456	0.517232
4	6	0	2.898395	-0.445731	-0.208624
5	1	0	2.766985	-1.147655	-1.033421
6	6	0	1.711777	0.505686	-0.186513
7	1	0	1.571522	0.894400	-1.195600
8	6	0	0.422930	-0.165450	0.282048
9	1	0	0.547234	-0.567828	1.289335

10	6	0	-0.732503	0.832916	0.276249
11	1	0	-0.572758	1.554145	1.076941
12	6	0	-2.109068	0.155331	0.411000
13	1	0	-2.162564	-0.589420	-0.389062
14	6	0	-2.217803	-0.606194	1.667933
15	7	0	-2.294159	-1.188731	2.654072
16	8	0	5.213102	-0.678619	-0.578527
17	8	0	2.955747	-1.180317	1.015646
18	8	0	1.943978	1.599319	0.708473
19	8	0	0.161725	-1.231952	-0.631420
20	8	0	-0.751039	1.510863	-0.978633
21	6	0	6.472318	-0.201227	-0.662482
22	6	0	3.027903	-2.532921	0.931049
23	6	0	0.077054	-2.499218	-0.125049
24	6	0	2.176544	2.820852	0.161175
25	6	0	-0.766082	2.868420	-0.962804
26	6	0	7.458140	-1.318297	-0.854439
27	6	0	3.078766	-3.148568	2.295187
28	6	0	-0.056426	-3.505424	-1.224968
29	6	0	-0.732970	3.423973	-2.351697
30	1	0	8.453370	-0.900342	-0.978452
31	1	0	7.430714	-1.977403	0.014473
32	1	0	7.177523	-1.909731	-1.726317
33	1	0	-0.559196	-4.388805	-0.839025
34	1	0	-0.584213	-3.089097	-2.080640
35	1	0	0.959227	-3.775945	-1.525844
36	1	0	2.057469	-3.156939	2.683286
37	1	0	3.441811	-4.169843	2.213877
38	1	0	3.703625	-2.557334	2.962309
39	1	0	-1.088131	4.451001	-2.333529
40	1	0	0.310626	3.408271	-2.676686
41	1	0	-1.324376	2.812602	-3.030983
42	6	0	2.295383	3.872314	1.219786
43	1	0	2.771369	3.472795	2.113153
44	1	0	2.846928	4.720063	0.821356
45	1	0	1.280465	4.190677	1.470875
46	7	0	-3.219507	1.063799	0.182940
47	6	0	-3.716187	1.988244	1.092295
48	6	0	-2.872850	2.340402	2.296564
49	1	0	-3.521409	2.867700	2.991563
50	1	0	-2.429795	1.481873	2.797790
51	1	0	-2.078933	3.015154	1.969634
52	8	0	6.731218	0.965716	-0.586967
53	8	0	3.006831	-3.130833	-0.108340
54	8	0	2.241749	3.004085	-1.022953
55	8	0	0.139332	-2.737792	1.044690
56	8	0	-0.758855	3.511242	0.050584
57	8	0	-4.776008	2.538836	0.888069
58	6	0	-4.717103	-0.530854	-0.960783
59	6	0	-4.435846	-1.557019	-1.858117
60	6	0	-5.662972	-0.742056	0.044939
61	6	0	-5.092369	-2.781849	-1.759639
62	1	0	-3.702953	-1.396359	-2.643486
63	6	0	-6.315367	-1.962360	0.145433
64	1	0	-5.881541	0.062628	0.740035
65	6	0	-6.030850	-2.985270	-0.756777
66	1	0	-4.868324	-3.574241	-2.463923
67	1	0	-7.048565	-2.118445	0.927615
68	1	0	-6.540217	-3.937900	-0.674817
69	6	0	-3.993725	0.793726	-1.033831
70	1	0	-4.700328	1.614682	-1.141689
71	1	0	-3.305707	0.804014	-1.884508

Structure 37 B_1G^+E (M06-2X, $CHCl_3$)

Energy (Hartrees): = -1946.8886364
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.181040	0.339068	-0.480721
2	1	0	4.086071	0.954749	-1.379068
3	1	0	4.426223	0.979957	0.369067
4	6	0	2.902869	-0.427943	-0.221568
5	1	0	2.745899	-1.156602	-1.017805
6	6	0	1.700922	0.500760	-0.173952
7	1	0	1.538008	0.884397	-1.181274
8	6	0	0.430830	-0.189349	0.322892
9	1	0	0.574466	-0.562916	1.338600
10	6	0	-0.743126	0.788310	0.311339
11	1	0	-0.604186	1.501919	1.121902
12	6	0	-2.112850	0.090516	0.414623
13	1	0	-2.158180	-0.618671	-0.418002

14	6	0	-2.228900	-0.736500	1.628111
15	7	0	-2.318641	-1.387655	2.569021
16	8	0	5.208015	-0.637978	-0.658364
17	8	0	3.029579	-1.117663	1.024559
18	8	0	1.929362	1.594760	0.721359
19	8	0	0.172275	-1.282395	-0.558772
20	8	0	-0.765969	1.480431	-0.935772
21	6	0	6.453183	-0.156014	-0.826860
22	6	0	3.188739	-2.463271	0.986053
23	6	0	0.185199	-2.545331	-0.038448
24	6	0	2.142092	2.824446	0.185740
25	6	0	-0.807245	2.838776	-0.908048
26	6	0	7.444064	-1.265995	-1.001417
27	6	0	3.348818	-3.013588	2.367122
28	6	0	-0.036113	-3.558035	-1.114488
29	6	0	-0.825427	3.400806	-2.291773
30	1	0	8.440295	-0.848511	-1.125226
31	1	0	7.414352	-1.923091	-0.130541
32	1	0	7.172435	-1.860242	-1.875779
33	1	0	0.037302	-4.555653	-0.689280
34	1	0	-1.023883	-3.408488	-1.556588
35	1	0	0.711974	-3.424014	-1.897270
36	1	0	2.431933	-2.819405	2.927045
37	1	0	3.532821	-4.083674	2.313824
38	1	0	4.171757	-2.507048	2.873517
39	1	0	-0.799265	4.486146	-2.239613
40	1	0	0.039600	3.027573	-2.842006
41	1	0	-1.729457	3.070436	-2.807378
42	6	0	2.285212	3.854246	1.258944
43	1	0	2.989887	3.510361	2.016617
44	1	0	2.615473	4.792569	0.820519
45	1	0	1.310158	3.990758	1.732681
46	7	0	-3.229606	1.002366	0.230154
47	6	0	-3.667464	1.943544	1.141162
48	6	0	-2.846995	2.207767	2.380848
49	1	0	-3.523898	2.607870	3.133265
50	1	0	-2.330975	1.342146	2.790634
51	1	0	-2.109590	2.975340	2.134002
52	8	0	6.697089	1.020711	-0.834706
53	8	0	3.179551	-3.099726	-0.032216
54	8	0	2.185214	3.020578	-0.998680
55	8	0	0.350606	-2.766911	1.126973
56	8	0	-0.813724	3.468157	0.114968
57	8	0	-4.680367	2.582733	0.926519
58	6	0	-4.781345	-0.497938	-0.971872
59	6	0	-4.582265	-1.480985	-1.938620
60	6	0	-5.710579	-0.720968	0.047434
61	6	0	-5.306956	-2.670887	-1.896507
62	1	0	-3.858926	-1.313343	-2.730980
63	6	0	-6.430847	-1.907197	0.092444
64	1	0	-5.867007	0.043945	0.802082
65	6	0	-6.231613	-2.884792	-0.881461
66	1	0	-5.146584	-3.428757	-2.654828
67	1	0	-7.151590	-2.070463	0.885288
68	1	0	-6.794806	-3.810005	-0.845106
69	6	0	-3.996723	0.793914	-1.003671
70	1	0	-4.663987	1.647484	-1.108412
71	1	0	-3.298759	0.790525	-1.844876

Structure 37 A_1G^-Z (M06-2X, Gas Phase)

Energy (Hartrees): = - 1946.8560818
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.261016	0.302857	0.138238
2	1	0	4.442504	1.246715	-0.376711
3	1	0	4.350950	0.434013	1.217638
4	6	0	2.877858	-0.220958	-0.211072
5	1	0	2.916484	-0.673843	-1.203155
6	6	0	1.826680	0.876958	-0.226605
7	1	0	1.991807	1.487556	-1.115962
8	6	0	0.414276	0.294815	-0.266673
9	1	0	0.228775	-0.316408	0.617362
10	6	0	-0.623822	1.401136	-0.335398
11	1	0	-0.554471	1.999882	0.572893
12	6	0	-2.092723	0.936858	-0.419081
13	1	0	-2.683053	1.858712	-0.481477
14	6	0	-2.366940	0.161313	-1.637017
15	7	0	-2.587163	-0.440394	-2.589344
16	8	0	5.257840	-0.603645	-0.339333
17	8	0	2.476680	-1.215071	0.735831
18	8	0	1.907369	1.707114	0.934027

19	8	0	0.381802	-0.518345	-1.440406
20	8	0	-0.352250	2.223910	-1.467809
21	6	0	5.615938	-1.624222	0.466789
22	6	0	2.658178	-2.511030	0.399205
23	6	0	0.081842	-1.832367	-1.314352
24	6	0	2.372896	2.973151	0.763532
25	6	0	-0.114731	3.544078	-1.232172
26	6	0	6.496055	-2.592721	-0.265548
27	6	0	2.285504	-3.408138	1.535917
28	6	0	0.189424	-2.525644	-2.634548
29	6	0	0.356426	4.233430	-2.474940
30	1	0	7.020408	-3.220005	0.450650
31	1	0	5.841906	-3.210691	-0.885985
32	1	0	7.192505	-2.067508	-0.916751
33	1	0	-0.031674	-3.581054	-2.503151
34	1	0	-0.517218	-2.065141	-3.327719
35	1	0	1.200642	-2.396596	-3.022572
36	1	0	1.284306	-3.152735	1.881914
37	1	0	2.326746	-4.442889	1.206978
38	1	0	2.998870	-3.233914	2.343978
39	1	0	0.118769	5.292410	-2.410406
40	1	0	1.443705	4.118396	-2.503286
41	1	0	-0.073138	3.779981	-3.365524
42	6	0	2.179723	3.783920	2.005732
43	1	0	2.391426	3.187888	2.892066
44	1	0	2.810796	4.667658	1.961802
45	1	0	1.129641	4.087188	2.027491
46	7	0	-2.486827	0.211417	0.791621
47	6	0	-2.750162	1.021138	1.883582
48	6	0	-3.257945	0.343515	3.135849
49	1	0	-3.423980	1.120684	3.876921
50	1	0	-4.190097	-0.192084	2.945624
51	1	0	-2.522157	-0.368642	3.515144
52	8	0	5.239045	-1.741788	1.600274
53	8	0	3.078870	-2.857982	-0.672707
54	8	0	2.843012	3.361150	-0.270200
55	8	0	-0.231981	-2.337009	-0.269004
56	8	0	-0.229593	4.047575	-0.152100
57	8	0	-2.560320	2.218266	1.829385
58	6	0	-4.479348	-1.253371	0.390971
59	6	0	-5.039830	-2.522696	0.240672
60	6	0	-5.293189	-0.134349	0.243029
61	6	0	-6.389021	-2.670226	-0.046911
62	1	0	-4.408534	-3.399728	0.345153
63	6	0	-6.647342	-0.281272	-0.048521
64	1	0	-4.881187	0.863626	0.354158
65	6	0	-7.198569	-1.546830	-0.192390
66	1	0	-6.810534	-3.661781	-0.162413
67	1	0	-7.268551	0.598862	-0.163500
68	1	0	-8.251510	-1.660374	-0.419623
69	6	0	-2.999918	-1.152800	0.716213
70	1	0	-2.421037	-1.702088	-0.024520
71	1	0	-2.792630	-1.647910	1.666379

Structure 37 A_1G-Z (M06-2X, $CHCl_3$)

Energy (Hartrees): = -1946.8927614
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.191914	0.171781	-0.084182
2	1	0	4.369164	1.033289	-0.728657
3	1	0	4.347921	0.446438	0.960107
4	6	0	2.774330	-0.337662	-0.291505
5	1	0	2.722895	-0.869074	-1.244537
6	6	0	1.775204	0.808050	-0.316118
7	1	0	1.959050	1.398934	-1.214948
8	6	0	0.325525	0.317164	-0.336021
9	1	0	0.129791	-0.342872	0.511335
10	6	0	-0.637486	1.492277	-0.296829
11	1	0	-0.477666	2.045446	0.628936
12	6	0	-2.138201	1.134833	-0.306708
13	1	0	-2.668037	2.092737	-0.333615
14	6	0	-2.540756	0.395977	-1.512528
15	7	0	-2.866727	-0.171150	-2.455561
16	8	0	5.145922	-0.814474	-0.486601
17	8	0	2.398585	-1.227270	0.764727
18	8	0	1.930312	1.635004	0.840098
19	8	0	0.172953	-0.393127	-1.567730
20	8	0	-0.367942	2.335356	-1.414691
21	6	0	5.560490	-1.706259	0.433118
22	6	0	2.556528	-2.551746	0.559489
23	6	0	-0.026120	-1.732374	-1.539014

24	6	0	2.434747	2.883905	0.663316
25	6	0	-0.107348	3.647609	-1.165554
26	6	0	6.434875	-2.747759	-0.192771
27	6	0	2.109121	-3.333576	1.752464
28	6	0	-0.113331	-2.281772	-2.925688
29	6	0	0.278247	4.360137	-2.421033
30	1	0	6.933027	-3.323643	0.583450
31	1	0	5.795231	-3.404556	-0.787698
32	1	0	7.161914	-2.286335	-0.860719
33	1	0	-0.332570	-3.345476	-2.881652
34	1	0	-0.891726	-1.749623	-3.475522
35	1	0	0.838573	-2.115740	-3.435004
36	1	0	1.142044	-2.970499	2.099578
37	1	0	2.054879	-4.388787	1.495496
38	1	0	2.840826	-3.184310	2.550434
39	1	0	0.222512	5.434065	-2.260387
40	1	0	1.309956	4.083758	-2.655347
41	1	0	-0.357328	4.053019	-3.250931
42	6	0	2.399171	3.656007	1.941767
43	1	0	2.902340	3.093583	2.729789
44	1	0	2.875318	4.622304	1.795680
45	1	0	1.356129	3.795263	2.233844
46	7	0	-2.527550	0.435924	0.915415
47	6	0	-2.766523	1.245475	2.005182
48	6	0	-3.250635	0.579389	3.268544
49	1	0	-3.461887	1.363167	3.991977
50	1	0	-4.152752	-0.009308	3.090708
51	1	0	-2.482552	-0.083837	3.672589
52	8	0	5.239806	-1.663078	1.591747
53	8	0	3.023233	-3.009937	-0.450082
54	8	0	2.838997	3.279066	-0.396735
55	8	0	-0.113151	-2.362305	-0.517783
56	8	0	-0.156855	4.124336	-0.066279
57	8	0	-2.576058	2.446473	1.937286
58	6	0	-4.265713	-1.316817	0.474582
59	6	0	-4.584004	-2.649107	0.206083
60	6	0	-5.254741	-0.344681	0.350457
61	6	0	-5.870681	-3.003867	-0.177376
62	1	0	-3.812916	-3.409111	0.291713
63	6	0	-6.545023	-0.699449	-0.037930
64	1	0	-5.024678	0.698127	0.545680
65	6	0	-6.856799	-2.027415	-0.301412
66	1	0	-6.103821	-4.041608	-0.387140
67	1	0	-7.304753	0.067344	-0.138001
68	1	0	-7.859771	-2.302370	-0.606173
69	6	0	-2.843970	-0.987559	0.895314
70	1	0	-2.143907	-1.492270	0.227630
71	1	0	-2.646601	-1.397184	1.886901

Structure 37 A_1G-E (M06-2X, Gas Phase)

Energy (Hartrees): = -1946.8533995
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.166917	0.226172	-0.111708
2	1	0	-4.369093	1.126923	0.469848
3	1	0	-4.256473	0.434456	-1.178850
4	6	0	-2.769252	-0.288551	0.198755
5	1	0	-2.790751	-0.809110	1.158687
6	6	0	-1.759487	0.843330	0.284428
7	1	0	-1.955300	1.407318	1.196969
8	6	0	-0.321316	0.320265	0.320310
9	1	0	-0.127802	-0.294257	-0.560174
10	6	0	0.659067	1.482914	0.366062
11	1	0	0.518604	2.063478	-0.546485
12	6	0	2.172216	1.154782	0.421583
13	1	0	2.654410	2.099174	0.683360
14	6	0	2.508121	0.239843	1.528513
15	7	0	2.762796	-0.444226	2.413794
16	8	0	-5.145853	-0.729975	0.293053
17	8	0	-2.338348	-1.199447	-0.812901
18	8	0	-1.870602	1.720123	-0.841608
19	8	0	-0.235908	-0.462181	1.508968
20	8	0	0.327006	2.287673	1.498192
21	6	0	-5.490904	-1.683776	-0.599538
22	6	0	-2.518758	-2.521590	-0.579205
23	6	0	0.046012	-1.785996	1.410337
24	6	0	-2.310002	2.984071	-0.610627
25	6	0	0.182392	3.620453	1.290059
26	6	0	-6.352929	-2.725344	0.047361
27	6	0	-2.069307	-3.329047	-1.753923

28	6	0	0.060512	-2.426977	2.760444
29	6	0	-0.325269	4.308775	2.516603
30	1	0	-6.852835	-3.310408	-0.720138
31	1	0	-5.688348	-3.369254	0.629024
32	1	0	-7.070455	-2.268313	0.726728
33	1	0	0.089438	-3.506461	2.640778
34	1	0	0.952117	-2.078430	3.287397
35	1	0	-0.819254	-2.123348	3.327021
36	1	0	-1.028475	-3.089838	-1.973807
37	1	0	-2.178135	-4.385892	-1.527089
38	1	0	-2.685543	-3.054098	-2.611724
39	1	0	-0.086356	5.367686	2.460543
40	1	0	-1.411410	4.185543	2.519622
41	1	0	0.084387	3.853276	3.416020
42	6	0	-2.194689	3.828524	-1.841036
43	1	0	-2.378354	3.240055	-2.737865
44	1	0	-2.882500	4.666964	-1.766818
45	1	0	-1.170541	4.210393	-1.870172
46	7	0	2.701513	0.697464	-0.849004
47	6	0	3.224789	1.582709	-1.776500
48	6	0	3.246311	3.057118	-1.423950
49	1	0	3.552055	3.587178	-2.321914
50	1	0	2.283603	3.440961	-1.081878
51	1	0	3.988468	3.243848	-0.642452
52	8	0	-5.113356	-1.694441	-1.738275
53	8	0	-2.990331	-2.945078	0.441202
54	8	0	-2.701595	3.355820	0.461555
55	8	0	0.263915	-2.333300	0.363483
56	8	0	0.405735	4.141189	0.230358
57	8	0	3.667202	1.185085	-2.831755
58	6	0	3.941957	-1.468401	-0.660017
59	6	0	3.786171	-2.619255	0.108325
60	6	0	5.226882	-1.018515	-0.965601
61	6	0	4.898915	-3.310352	0.574981
62	1	0	2.786140	-2.966846	0.348216
63	6	0	6.338132	-1.706703	-0.494710
64	1	0	5.349713	-0.140676	-1.589969
65	6	0	6.176896	-2.853085	0.277413
66	1	0	4.766568	-4.200961	1.177701
67	1	0	7.332906	-1.352222	-0.737791
68	1	0	7.045240	-3.387590	0.644026
69	6	0	2.719690	-0.737922	-1.174618
70	1	0	1.822733	-1.206556	-0.770811
71	1	0	2.676767	-0.800059	-2.262145

Structure 37 A_1G-E (M06-2X, $CHCl_3$)

Energy (Hartrees): = - 1946.8904742
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.150182	0.252801	0.131560
2	1	0	-4.284751	1.090475	0.817315
3	1	0	-4.334648	0.574929	-0.894212
4	6	0	-2.737864	-0.295872	0.266802
5	1	0	-2.671473	-0.888308	1.182539
6	6	0	-1.720219	0.830122	0.336927
7	1	0	-1.869069	1.367828	1.273878
8	6	0	-0.277889	0.316413	0.278008
9	1	0	-0.134249	-0.283812	-0.621639
10	6	0	0.695379	1.485096	0.279421
11	1	0	0.512073	2.069051	-0.623286
12	6	0	2.211510	1.169903	0.275774
13	1	0	2.698145	2.128838	0.469312
14	6	0	2.612436	0.323228	1.416099
15	7	0	2.941452	-0.301911	2.320377
16	8	0	-5.114029	-0.726197	0.526724
17	8	0	-2.408679	-1.121677	-0.853745
18	8	0	-1.900307	1.726273	-0.764396
19	8	0	-0.093317	-0.474110	1.452256
20	8	0	0.415822	2.276745	1.433421
21	6	0	-5.574260	-1.574635	-0.412966
22	6	0	-2.592275	-2.453973	-0.727374
23	6	0	0.093626	-1.811451	1.328609
24	6	0	-2.292827	2.998084	-0.496181
25	6	0	0.346186	3.622555	1.264914
26	6	0	-6.460278	-2.614338	0.198690
27	6	0	-2.216057	-3.166393	-1.985944
28	6	0	0.241121	-2.452222	2.669436
29	6	0	-0.047689	4.302848	2.533941
30	1	0	-6.976300	-3.163722	-0.584996

31	1	0	-5.828077	-3.295388	0.773674
32	1	0	-7.172749	-2.153950	0.883125
33	1	0	0.296787	-3.531271	2.550120
34	1	0	1.152027	-2.073941	3.139561
35	1	0	-0.605873	-2.179937	3.301072
36	1	0	-1.260845	-2.797953	-2.359440
37	1	0	-2.170660	-4.236364	-1.798287
38	1	0	-2.984569	-2.954254	-2.733853
39	1	0	0.102444	5.374950	2.433530
40	1	0	-1.106150	4.094223	2.708061
41	1	0	0.523824	3.904119	3.372143
42	6	0	-2.324208	3.820478	-1.743616
43	1	0	-2.825975	3.276815	-2.544312
44	1	0	-2.822586	4.765701	-1.543626
45	1	0	-1.293214	4.009915	-2.053356
46	7	0	2.700415	0.647390	-0.988200
47	6	0	3.236348	1.479131	-1.953742
48	6	0	3.257062	2.966486	-1.685571
49	1	0	3.553706	3.455317	-2.610402
50	1	0	2.293213	3.359310	-1.356864
51	1	0	4.000419	3.197390	-0.916832
52	8	0	-5.281092	-1.497141	-1.576794
53	8	0	-3.031664	-2.963049	0.269803
54	8	0	-2.554164	3.381398	0.612084
55	8	0	0.135878	-2.370788	0.264799
56	8	0	0.556748	4.152232	0.206544
57	8	0	3.688564	1.017928	-2.983630
58	6	0	3.861918	-1.538321	-0.633266
59	6	0	3.647446	-2.767598	-0.011411
60	6	0	5.153684	-1.015825	-0.683176
61	6	0	4.708468	-3.464900	0.556961
62	1	0	2.640043	-3.169653	0.042067
63	6	0	6.213923	-1.709659	-0.110013
64	1	0	5.331132	-0.065551	-1.175419
65	6	0	5.993736	-2.934702	0.513551
66	1	0	4.528984	-4.415720	1.045829
67	1	0	7.214304	-1.294030	-0.151060
68	1	0	6.820027	-3.471095	0.965661
69	6	0	2.690042	-0.797575	-1.243378
70	1	0	1.760139	-1.225812	-0.869615
71	1	0	2.695935	-0.917447	-2.326790

Structure 37 B_1G^-Z (M06-2X, Gas Phase)

Energy (Hartrees): = -1946.8534931
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.136704	1.138598	-0.008869
2	1	0	-4.013109	1.974604	0.681250
3	1	0	-4.109176	1.494320	-1.039960
4	6	0	-3.014491	0.127707	0.211374
5	1	0	-3.223428	-0.456136	1.112001
6	6	0	-1.690984	0.858696	0.369529
7	1	0	-1.729651	1.479953	1.264624
8	6	0	-0.464942	-0.060332	0.468189
9	1	0	-0.480636	-0.800621	-0.335164
10	6	0	0.796877	0.785456	0.374270
11	1	0	0.834921	1.230798	-0.620013
12	6	0	2.150501	0.080492	0.565025
13	1	0	2.890754	0.888992	0.556298
14	6	0	2.329811	-0.564121	1.878322
15	7	0	2.572597	-0.999653	2.911981
16	8	0	-5.412077	0.577125	0.282366
17	8	0	-2.882481	-0.756511	-0.899119
18	8	0	-1.490765	1.700866	-0.779875
19	8	0	-0.468858	-0.710674	1.729018
20	8	0	0.704315	1.823508	1.351090
21	6	0	-6.059104	-0.033258	-0.734881
22	6	0	-3.552227	-1.930309	-0.832540
23	6	0	-0.873285	-2.012441	1.765238
24	6	0	-1.510497	3.041198	-0.606579
25	6	0	1.182742	3.039595	0.996574
26	6	0	-7.274817	-0.750458	-0.231413
27	6	0	-3.102456	-2.854317	-1.921234
28	6	0	-0.415330	-2.670363	3.026571
29	6	0	0.973543	4.040423	2.088740
30	1	0	-7.925263	-0.993608	-1.067639
31	1	0	-6.922542	-1.668457	0.244318
32	1	0	-7.795694	-0.151669	0.514145
33	1	0	-1.006974	-3.564205	3.206107

34	1	0	0.633661	-2.937286	2.874888
35	1	0	-0.465554	-1.979031	3.866186
36	1	0	-2.106734	-3.212833	-1.651497
37	1	0	-3.791192	-3.691844	-1.991425
38	1	0	-3.044667	-2.316303	-2.866818
39	1	0	1.546584	4.937351	1.869547
40	1	0	-0.092509	4.275275	2.119240
41	1	0	1.261787	3.612345	3.048175
42	6	0	-1.156883	3.751426	-1.879161
43	1	0	-1.567522	3.227488	-2.740385
44	1	0	-1.518197	4.775487	-1.829985
45	1	0	-0.066445	3.759502	-1.956957
46	7	0	2.488091	-0.781710	-0.560487
47	6	0	2.103275	-2.103433	-0.549943
48	6	0	2.638694	-2.984209	-1.655942
49	1	0	2.375690	-4.008420	-1.405414
50	1	0	2.176229	-2.723412	-2.610612
51	1	0	3.721690	-2.890452	-1.757670
52	8	0	-5.677332	-0.010061	-1.871594
53	8	0	-4.380947	-2.169335	-0.000570
54	8	0	-1.751539	3.571013	0.443909
55	8	0	-1.496713	-2.522132	0.880540
56	8	0	1.685896	3.247912	-0.075993
57	8	0	1.366318	-2.529760	0.313760
58	6	0	4.853162	-0.228914	-1.148525
59	6	0	5.768562	0.489657	-1.918837
60	6	0	5.309700	-0.955835	-0.052849
61	6	0	7.119991	0.474062	-1.605488
62	1	0	5.417471	1.067202	-2.768613
63	6	0	6.666257	-0.966765	0.264747
64	1	0	4.613666	-1.510574	0.567799
65	6	0	7.572991	-0.256763	-0.509990
66	1	0	7.820196	1.036455	-2.211438
67	1	0	7.007553	-1.531546	1.123892
68	1	0	8.627216	-0.266156	-0.261018
69	6	0	3.387948	-0.202296	-1.547122
70	1	0	3.249265	-0.718717	-2.497710
71	1	0	3.077256	0.834440	-1.716084

Structure 37 B_1G^-Z (M06-2X, $CHCl_3$)

Energy (Hartrees): = - 1946.8932059
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.126124	1.107596	0.040471
2	1	0	-4.033453	1.908098	0.775082
3	1	0	-4.093066	1.521490	-0.968308
4	6	0	-2.990941	0.109188	0.234992
5	1	0	-3.175417	-0.484020	1.133882
6	6	0	-1.671351	0.853050	0.375205
7	1	0	-1.714396	1.480723	1.265669
8	6	0	-0.438461	-0.056546	0.478584
9	1	0	-0.443181	-0.803724	-0.317368
10	6	0	0.821505	0.793794	0.384795
11	1	0	0.853285	1.244460	-0.606863
12	6	0	2.178379	0.087435	0.570604
13	1	0	2.921752	0.892332	0.551995
14	6	0	2.355204	-0.529057	1.898647
15	7	0	2.579858	-0.925396	2.952180
16	8	0	-5.399782	0.508997	0.283157
17	8	0	-2.869959	-0.761569	-0.891250
18	8	0	-1.487123	1.680485	-0.785129
19	8	0	-0.446511	-0.695259	1.748900
20	8	0	0.728741	1.818740	1.375556
21	6	0	-6.027587	-0.067001	-0.759290
22	6	0	-3.522288	-1.941314	-0.842805
23	6	0	-0.850814	-1.990723	1.806533
24	6	0	-1.546513	3.024966	-0.638492
25	6	0	1.107188	3.071268	1.019085
26	6	0	-7.271329	-0.768257	-0.310063
27	6	0	-3.114523	-2.817323	-1.985010
28	6	0	-0.431999	-2.619805	3.094922
29	6	0	0.922103	4.027002	2.151822
30	1	0	-7.869090	-1.045427	-1.175035
31	1	0	-6.966647	-1.666113	0.232565
32	1	0	-7.842675	-0.135617	0.369123
33	1	0	-1.031708	-3.507735	3.281258
34	1	0	0.619387	-2.898771	2.986443
35	1	0	-0.510361	-1.911085	3.918490
36	1	0	-2.071907	-3.108422	-1.838931

37	1	0	-3.745522	-3.702318	-2.011854
38	1	0	-3.191475	-2.263281	-2.921417
39	1	0	1.281525	5.010507	1.860268
40	1	0	-0.140839	4.071452	2.395553
41	1	0	1.459256	3.664398	3.029414
42	6	0	-1.264140	3.715119	-1.935178
43	1	0	-1.860400	3.272849	-2.733655
44	1	0	-1.476639	4.776549	-1.834926
45	1	0	-0.207982	3.573508	-2.176209
46	7	0	2.508308	-0.796214	-0.538373
47	6	0	2.112493	-2.110361	-0.506630
48	6	0	2.585584	-3.003832	-1.625673
49	1	0	2.309437	-4.023643	-1.368977
50	1	0	2.096465	-2.727659	-2.562969
51	1	0	3.665775	-2.938110	-1.768698
52	8	0	-5.616060	-0.022228	-1.888696
53	8	0	-4.321751	-2.220628	0.009353
54	8	0	-1.780885	3.562526	0.410966
55	8	0	-1.456812	-2.524394	0.920347
56	8	0	1.521613	3.334308	-0.078881
57	8	0	1.403320	-2.521817	0.394154
58	6	0	4.859115	-0.236523	-1.178842
59	6	0	5.737929	0.575231	-1.899188
60	6	0	5.360216	-1.038209	-0.155484
61	6	0	7.095716	0.579606	-1.606837
62	1	0	5.352308	1.208836	-2.692082
63	6	0	6.721805	-1.030203	0.141120
64	1	0	4.693529	-1.669664	0.422635
65	6	0	7.591922	-0.224723	-0.583157
66	1	0	7.766904	1.215388	-2.172580
67	1	0	7.097955	-1.655114	0.942703
68	1	0	8.650111	-0.218125	-0.349979
69	6	0	3.387846	-0.231530	-1.555697
70	1	0	3.238283	-0.774023	-2.489266
71	1	0	3.067695	0.797147	-1.747031

Structure 37 B_1G^-E (M06-2X, Gas Phase)

Energy (Hartrees): = -1946.8497931
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.951981	1.539559	-0.150143
2	1	0	-3.686660	2.446793	0.395133
3	1	0	-3.931629	1.723440	-1.225077
4	6	0	-2.974485	0.425162	0.198257
5	1	0	-3.239476	0.016302	1.176916
6	6	0	-1.551138	0.949839	0.254773
7	1	0	-1.461552	1.610081	1.118411
8	6	0	-0.510527	-0.168923	0.383469
9	1	0	-0.634643	-0.893635	-0.423867
10	6	0	0.887147	0.425657	0.340174
11	1	0	0.989924	0.939960	-0.614918
12	6	0	2.103662	-0.529518	0.418054
13	1	0	2.927185	0.102188	0.778965
14	6	0	1.985563	-1.562425	1.456755
15	7	0	1.924404	-2.334133	2.304063
16	8	0	-5.271195	1.201572	0.272676
17	8	0	-3.029457	-0.615723	-0.774826
18	8	0	-1.246423	1.690754	-0.933547
19	8	0	-0.744656	-0.780875	1.649140
20	8	0	0.975437	1.378399	1.400671
21	6	0	-6.042624	0.510196	-0.595043
22	6	0	-3.832815	-1.673950	-0.507025
23	6	0	-1.219273	-2.054781	1.682132
24	6	0	-0.953603	3.008195	-0.794175
25	6	0	1.608834	2.541646	1.118833
26	6	0	-7.305565	0.052759	0.069670
27	6	0	-3.783573	-2.665425	-1.624710
28	6	0	-1.384615	-2.518663	3.094228
29	6	0	1.516874	3.502081	2.261188
30	1	0	-8.035796	-0.220665	-0.687577
31	1	0	-7.047291	-0.825515	0.666560
32	1	0	-7.693861	0.821001	0.736115
33	1	0	-1.952338	-3.444891	3.099997
34	1	0	-0.388189	-2.682794	3.511006
35	1	0	-1.883019	-1.750787	3.684790
36	1	0	-2.745310	-2.926492	-1.829134
37	1	0	-4.354461	-3.547596	-1.348542
38	1	0	-4.211961	-2.195972	-2.512419
39	1	0	2.284051	4.264636	2.154285
40	1	0	0.529959	3.968099	2.204111

41	1	0	1.603933	2.979815	3.212227
42	6	0	-0.442021	3.588033	-2.076706
43	1	0	-0.883969	3.090991	-2.937608
44	1	0	-0.635893	4.657727	-2.090096
45	1	0	0.640069	3.427706	-2.087869
46	7	0	2.522061	-1.002833	-0.893378
47	6	0	2.376650	-2.267746	-1.448125
48	6	0	1.439791	-3.258166	-0.801680
49	1	0	1.156996	-3.963104	-1.580299
50	1	0	1.964224	-3.802890	-0.014512
51	1	0	0.545482	-2.816600	-0.368795
52	8	0	-5.721290	0.276497	-1.726942
53	8	0	-4.494702	-1.755311	0.490961
54	8	0	-1.061346	3.599362	0.245113
55	8	0	-1.447018	-2.694046	0.693613
56	8	0	2.137288	2.750336	0.058199
57	8	0	2.987435	-2.559847	-2.453932
58	6	0	4.778623	0.019363	-0.936240
59	6	0	5.220414	1.201238	-0.345175
60	6	0	5.600742	-1.110275	-0.911580
61	6	0	6.472941	1.258082	0.262005
62	1	0	4.579699	2.077950	-0.363157
63	6	0	6.847149	-1.052225	-0.303971
64	1	0	5.255250	-2.024424	-1.383250
65	6	0	7.285897	0.132446	0.283946
66	1	0	6.810629	2.181536	0.717502
67	1	0	7.481950	-1.930371	-0.292673
68	1	0	8.260106	0.175524	0.756200
69	6	0	3.414462	-0.054069	-1.582113
70	1	0	3.490281	-0.391944	-2.613338
71	1	0	2.949283	0.935213	-1.563677

Structure 37 B_1G^-E (M06-2X, $CHCl_3$)

Energy (Hartrees): = -1946.8856788

No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.984230	1.504757	-0.069280
2	1	0	-3.744715	2.381596	0.533939
3	1	0	-3.959500	1.762252	-1.128452
4	6	0	-2.985495	0.394996	0.224305
5	1	0	-3.225869	-0.056917	1.190009
6	6	0	-1.571903	0.949547	0.271002
7	1	0	-1.496781	1.638676	1.113441
8	6	0	-0.506128	-0.143225	0.428408
9	1	0	-0.612604	-0.889555	-0.361145
10	6	0	0.882418	0.471138	0.377281
11	1	0	0.977909	0.993094	-0.575479
12	6	0	2.107432	-0.477183	0.445196
13	1	0	2.932272	0.162820	0.785772
14	6	0	2.018588	-1.496906	1.499751
15	7	0	1.985413	-2.265909	2.350847
16	8	0	-5.304704	1.119782	0.318714
17	8	0	-3.026281	-0.607502	-0.793645
18	8	0	-1.307657	1.651603	-0.948452
19	8	0	-0.713371	-0.729063	1.713715
20	8	0	0.963958	1.409167	1.448238
21	6	0	-6.073551	0.500062	-0.597663
22	6	0	-3.814972	-1.684127	-0.585415
23	6	0	-1.233673	-1.979812	1.790788
24	6	0	-0.953346	2.959162	-0.871890
25	6	0	1.672725	2.540792	1.212193
26	6	0	-7.359111	0.034911	0.011396
27	6	0	-3.701901	-2.651422	-1.719337
28	6	0	-1.369201	-2.408040	3.215702
29	6	0	1.585512	3.483711	2.366117
30	1	0	-8.071171	-0.205512	-0.774509
31	1	0	-7.139793	-0.864115	0.593377
32	1	0	-7.762575	0.788839	0.686630
33	1	0	-1.911490	-3.349028	3.261176
34	1	0	-0.368470	-2.530016	3.637299
35	1	0	-1.886448	-1.636086	3.786785
36	1	0	-2.651741	-2.870423	-1.915284
37	1	0	-4.244264	-3.561782	-1.476577
38	1	0	-4.129621	-2.188999	-2.612007
39	1	0	2.316640	4.278938	2.243120
40	1	0	0.577711	3.905709	2.375164
41	1	0	1.742868	2.951419	3.304171
42	6	0	-0.629146	3.504576	-2.225733
43	1	0	-1.347596	3.147597	-2.963146

44	1	0	-0.615408	4.590992	-2.185443
45	1	0	0.362019	3.142388	-2.512599
46	7	0	2.512977	-0.972229	-0.863319
47	6	0	2.294709	-2.214487	-1.427281
48	6	0	1.389732	-3.205009	-0.740576
49	1	0	1.054994	-3.903333	-1.505516
50	1	0	1.958910	-3.761603	0.007434
51	1	0	0.521676	-2.767471	-0.254280
52	8	0	-5.738797	0.334182	-1.740722
53	8	0	-4.520913	-1.804230	0.380119
54	8	0	-0.896320	3.564215	0.164429
55	8	0	-1.525238	-2.627778	0.821994
56	8	0	2.264236	2.725255	0.181077
57	8	0	2.839679	-2.508170	-2.475940
58	6	0	4.795255	-0.011408	-0.977628
59	6	0	5.312290	1.167762	-0.443612
60	6	0	5.571184	-1.173919	-0.948080
61	6	0	6.592172	1.190678	0.106992
62	1	0	4.705945	2.068354	-0.454891
63	6	0	6.845564	-1.151357	-0.396486
64	1	0	5.170711	-2.091015	-1.368442
65	6	0	7.359700	0.032280	0.131174
66	1	0	6.985757	2.113064	0.518772
67	1	0	7.442309	-2.056221	-0.381320
68	1	0	8.355133	0.048104	0.559659
69	6	0	3.404807	-0.037987	-1.571474
70	1	0	3.432918	-0.353775	-2.611940
71	1	0	2.968229	0.962338	-1.519732

Structure 13 R-X (M06-2X, Gas Phase)

Energy (Hartrees): = -1946.8575287
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.897709	-0.550001	-1.915356
2	1	0	-5.775511	0.209141	-2.682491
3	6	0	-6.910733	-1.490477	-2.030121
4	1	0	-7.577531	-1.464894	-2.883713
5	6	0	-7.068260	-2.466467	-1.048717
6	1	0	-7.857197	-3.203472	-1.137196
7	6	0	-6.209412	-2.489882	0.041414
8	1	0	-6.324958	-3.246240	0.808501
9	6	0	-5.193481	-1.542973	0.158894
10	1	0	-4.530845	-1.570160	1.017460
11	6	0	-5.031475	-0.568466	-0.820936
12	6	0	-3.938291	0.481911	-0.746266
13	1	0	-3.287622	0.392408	-1.621813
14	1	0	-4.381196	1.478694	-0.806058
15	6	0	-4.591766	1.954651	1.643729
16	1	0	-4.756293	2.244899	2.677929
17	1	0	-5.468671	1.432370	1.257166
18	1	0	-4.419255	2.854100	1.046861
19	6	0	-3.352164	1.093873	1.610319
20	6	0	-1.880061	-0.380832	0.371622
21	1	0	-1.894779	-0.938065	-0.568436
22	6	0	-1.789151	-1.391154	1.439830
23	6	0	-0.657843	0.548684	0.328360
24	1	0	-0.702964	1.241871	1.166590
25	6	0	-1.198232	2.558415	-0.851922
26	6	0	-1.204865	3.170435	-2.219798
27	1	0	-1.807626	4.075027	-2.206877
28	1	0	-1.571179	2.460336	-2.960125
29	1	0	-0.170427	3.424699	-2.462615
30	6	0	0.674691	-0.181096	0.352592
31	1	0	0.854831	-0.557703	1.361737
32	6	0	1.111801	-2.479122	-0.125751
33	6	0	1.269100	-3.444547	-1.259577
34	1	0	2.273950	-3.297464	-1.666309
35	1	0	0.540242	-3.258971	-2.045667
36	1	0	1.192600	-4.458854	-0.875908
37	6	0	1.802700	0.760314	-0.072523
38	1	0	1.600322	1.135930	-1.076491
39	6	0	1.648594	3.103351	0.365203
40	6	0	1.432564	4.093838	1.467486
41	1	0	1.692917	5.088399	1.114415
42	1	0	2.005301	3.821450	2.352035
43	1	0	0.368539	4.067435	1.718003
44	6	0	3.159602	0.088761	-0.088799

45	1	0	3.142427	-0.693620	-0.849654
46	6	0	4.004383	-1.708972	1.210650
47	6	0	4.103276	-2.228436	2.611150
48	1	0	4.759651	-3.094335	2.629167
49	1	0	3.097783	-2.519114	2.921466
50	1	0	4.462504	-1.448302	3.281068
51	6	0	4.270183	1.072325	-0.418566
52	1	0	4.050960	1.582121	-1.359078
53	1	0	4.380469	1.795274	0.388752
54	6	0	5.703000	-0.372017	-1.596626
55	6	0	6.948107	-1.197403	-1.479778
56	1	0	7.260568	-1.523047	-2.468673
57	1	0	6.694218	-2.068394	-0.870946
58	1	0	7.737981	-0.639876	-0.979253
59	8	0	-2.593787	1.002477	2.549881
60	8	0	-1.490162	3.115778	0.169787
61	8	0	-0.780058	1.269647	-0.905596
62	8	0	0.649298	-1.272524	-0.569996
63	8	0	1.390769	-2.692450	1.016726
64	8	0	1.672756	3.353614	-0.809414
65	8	0	1.778877	1.849117	0.858257
66	8	0	3.410089	-0.493918	1.191252
67	8	0	4.367383	-2.282196	0.218887
68	8	0	5.519205	0.390129	-0.493409
69	8	0	4.935133	-0.380376	-2.517852
70	7	0	-3.100373	0.406951	0.437618
71	7	0	-1.712852	-2.236137	2.212798

Structure 42 $_1G^+{}_5G^-$ (M06-2X, Gas Phase)

Energy (Hartrees): = -1487.7521796
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.078094	-0.503828	-2.264113
2	1	0	-2.007488	-0.611160	-3.346868
3	6	0	-0.745564	-0.856956	-1.635196
4	1	0	-0.564894	-1.928737	-1.737530
5	6	0	-0.686661	-0.442052	-0.163971
6	1	0	-0.743963	0.647032	-0.117640
7	6	0	0.607817	-0.887880	0.491912
8	1	0	1.432055	-0.444389	-0.070247
9	6	0	0.802373	-0.401091	1.947092
10	1	0	1.801172	-0.728802	2.250706
11	6	0	-0.132725	-1.056724	2.874874
12	7	0	-0.858263	-1.574799	3.597473
13	8	0	-2.396647	0.861557	-1.985699
14	8	0	0.284414	-0.124302	-2.309139
15	8	0	-1.825235	-1.017168	0.475677
16	8	0	0.696981	-2.302484	0.408845
17	6	0	-3.533271	1.120132	-1.300546
18	6	0	-2.556554	-0.226290	1.294366
19	6	0	1.444483	-0.762280	-2.586671
20	6	0	1.956204	-2.804809	0.341646
21	6	0	-3.653497	2.582266	-0.991158
22	6	0	-3.712905	-0.969111	1.874839
23	6	0	1.938303	-4.250754	-0.039594
24	1	0	-4.370822	-0.265300	2.376935
25	1	0	-4.241144	-1.495856	1.081751
26	1	0	-3.317596	-1.692401	2.592099
27	1	0	-3.208000	3.187527	-1.777827
28	1	0	-4.701380	2.831230	-0.842224
29	1	0	-3.112479	2.756655	-0.057416
30	1	0	2.901434	-4.699513	0.187831
31	1	0	1.128462	-4.770774	0.470044
32	1	0	1.756879	-4.291032	-1.116111
33	6	0	2.458360	0.203198	-3.123968
34	1	0	2.747771	0.878938	-2.313927
35	1	0	3.326441	-0.344749	-3.479797
36	1	0	2.019139	0.805892	-3.918333
37	7	0	0.704747	1.036094	2.081322
38	8	0	-4.310542	0.271817	-0.958654
39	8	0	1.621357	-1.932421	-2.386855
40	8	0	-2.263272	0.921802	1.518224
41	8	0	2.928890	-2.133338	0.547133
42	1	0	-2.858842	-1.152504	-1.870569
43	1	0	-0.254753	1.365661	2.070332
44	6	0	1.595774	1.849466	1.370730
45	6	0	1.218362	3.168209	1.084573
46	6	0	2.860349	1.406089	0.962138
47	6	0	2.082893	4.019732	0.415682
48	1	0	0.240117	3.516176	1.399589

49	6	0	3.718047	2.274185	0.293784
50	1	0	3.184444	0.387857	1.147864
51	6	0	3.341625	3.581534	0.012862
52	1	0	1.768760	5.035480	0.205888
53	1	0	4.693923	1.912762	-0.009840
54	1	0	4.015888	4.249024	-0.508232

Structure 42 $_1G^+{}_5G^-$ (M06-2X, $CHCl_3$)

Energy (Hartrees): = -1487.7794703
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.335857	-0.883629	1.962560
2	1	0	2.374575	-1.282909	2.976298
3	6	0	0.988855	-1.200442	1.345623
4	1	0	0.921046	-2.274112	1.162583
5	6	0	0.758745	-0.419125	0.049690
6	1	0	0.746247	0.646623	0.285342
7	6	0	-0.562004	-0.781988	-0.604346
8	1	0	-1.358495	-0.560655	0.109587
9	6	0	-0.906443	0.023889	-1.879524
10	1	0	-1.899329	-0.309401	-2.198884
11	6	0	-0.011926	-0.312984	-3.000528
12	7	0	0.673198	-0.572608	-3.883761
13	8	0	2.503200	0.536401	2.050745
14	8	0	-0.035078	-0.798458	2.264419
15	8	0	1.863876	-0.721131	-0.804653
16	8	0	-0.556416	-2.173737	-0.894843
17	6	0	3.533780	1.102201	1.388363
18	6	0	2.490667	0.302576	-1.426977
19	6	0	-1.064347	-1.646846	2.489272
20	6	0	-1.759860	-2.797318	-0.846971
21	6	0	3.496812	2.593056	1.515392
22	6	0	3.652810	-0.179240	-2.227804
23	6	0	-1.605303	-4.277863	-0.962154
24	1	0	4.249887	0.672534	-2.544091
25	1	0	4.249587	-0.872183	-1.636224
26	1	0	3.265423	-0.706333	-3.103673
27	1	0	3.334326	2.881142	2.553983
28	1	0	4.425186	3.013314	1.136186
29	1	0	2.658100	2.965595	0.922099
30	1	0	-2.578440	-4.735681	-1.122037
31	1	0	-0.920936	-4.524507	-1.774068
32	1	0	-1.174458	-4.641940	-0.026398
33	6	0	-2.067898	-1.031005	3.412553
34	1	0	-2.591375	-0.236528	2.873667
35	1	0	-2.780667	-1.786509	3.733423
36	1	0	-1.566061	-0.579623	4.268365
37	7	0	-0.920455	1.453646	-1.684476
38	8	0	4.348073	0.471953	0.766642
39	8	0	-1.146339	-2.733041	1.980920
40	8	0	2.108804	1.443391	-1.342402
41	8	0	-2.790783	-2.193737	-0.717851
42	1	0	3.134929	-1.316913	1.363799
43	1	0	0.004039	1.864496	-1.605397
44	6	0	-1.892369	2.043698	-0.869792
45	6	0	-1.679698	3.357772	-0.428171
46	6	0	-3.080247	1.394367	-0.510093
47	6	0	-2.633119	4.005122	0.341805
48	1	0	-0.759892	3.863183	-0.704517
49	6	0	-4.029982	2.060062	0.260613
50	1	0	-3.275993	0.371345	-0.811470
51	6	0	-3.820018	3.363535	0.692039
52	1	0	-2.446915	5.021697	0.669487
53	1	0	-4.943833	1.539894	0.524813
54	1	0	-4.564719	3.872048	1.291660

Structure 42 $_1G^-{}_5G^-$ (M06-2X, Gas Phase)

Energy (Hartrees): = -1487.7463848
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.126738	1.104582	-1.198370
2	1	0	-3.519177	2.080130	-1.484179

3	6	0	-1.681884	1.250062	-0.752701
4	1	0	-1.051361	1.416796	-1.627373
5	6	0	-1.190535	0.012775	-0.000419
6	1	0	-1.873138	-0.229699	0.817207
7	6	0	0.194548	0.227404	0.583565
8	1	0	0.141188	1.039850	1.310873
9	6	0	0.765881	-1.021802	1.303749
10	1	0	0.619759	-1.907884	0.686008
11	6	0	-0.006097	-1.221252	2.542253
12	7	0	-0.613167	-1.298466	3.512868
13	8	0	-3.930072	0.619730	-0.120246
14	8	0	-1.557023	2.363384	0.137511
15	8	0	-1.189812	-1.040092	-0.967730
16	8	0	1.067014	0.593292	-0.473925
17	6	0	-4.415185	-0.638988	-0.221711
18	6	0	-1.681728	-2.246511	-0.584652
19	6	0	-0.670443	3.337027	-0.193614
20	6	0	1.993450	1.551458	-0.211563
21	6	0	-5.019269	-1.093117	1.071449
22	6	0	-1.811968	-3.171467	-1.753984
23	6	0	2.845361	1.800599	-1.412870
24	1	0	-1.836849	-4.198770	-1.399354
25	1	0	-2.761520	-2.931904	-2.238172
26	1	0	-1.003946	-3.014688	-2.466599
27	1	0	-5.447427	-0.257800	1.621256
28	1	0	-5.760784	-1.863127	0.872905
29	1	0	-4.209495	-1.531460	1.663142
30	1	0	3.650061	2.480324	-1.146483
31	1	0	3.244660	0.850616	-1.774643
32	1	0	2.215906	2.242408	-2.187750
33	6	0	-0.510710	4.318970	0.926575
34	1	0	0.246066	3.911737	1.602781
35	1	0	-0.150723	5.263988	0.527362
36	1	0	-1.442786	4.444825	1.473591
37	7	0	2.171041	-0.896033	1.629618
38	8	0	-4.317428	-1.306250	-1.215901
39	8	0	-0.075746	3.363486	-1.234541
40	8	0	-1.974500	-2.494545	0.551479
41	8	0	2.076731	2.097930	0.855469
42	1	0	-3.187598	0.414351	-2.038537
43	1	0	2.353967	-0.091835	2.217768
44	6	0	3.158969	-1.081728	0.651664
45	6	0	4.384443	-0.421933	0.811778
46	6	0	2.986926	-1.911898	-0.460654
47	6	0	5.408304	-0.595676	-0.108167
48	1	0	4.521664	0.237602	1.662242
49	6	0	4.018746	-2.075358	-1.376707
50	1	0	2.050428	-2.425829	-0.632676
51	6	0	5.234983	-1.421782	-1.213700
52	1	0	6.346400	-0.073862	0.040100
53	1	0	3.862035	-2.723062	-2.231347
54	1	0	6.031921	-1.554881	-1.933970

Structure 42 $_1$G$^-$$_5G^-$ (M06-2X, $CHCl_3$)

Energy (Hartrees): = -1487.7756752
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.121811	1.121298	-1.169599
2	1	0	-3.481892	2.105999	-1.467252
3	6	0	-1.680256	1.226054	-0.710548
4	1	0	-1.049934	1.417725	-1.579665
5	6	0	-1.199908	-0.041362	-0.002214
6	1	0	-1.879819	-0.306647	0.811160
7	6	0	0.193367	0.147356	0.577923
8	1	0	0.145852	0.917329	1.350197
9	6	0	0.803401	-1.133228	1.200071
10	1	0	0.712664	-1.964519	0.499280
11	6	0	0.037222	-1.488683	2.407625
12	7	0	-0.544484	-1.709292	3.371585
13	8	0	-3.955137	0.672275	-0.095304
14	8	0	-1.546391	2.304169	0.222749
15	8	0	-1.214443	-1.057104	-1.007222
16	8	0	1.052542	0.572007	-0.472638
17	6	0	-4.465570	-0.574652	-0.174200
18	6	0	-1.700304	-2.278570	-0.669604
19	6	0	-0.731384	3.334518	-0.109209
20	6	0	1.940948	1.562453	-0.202146
21	6	0	-5.165577	-0.957237	1.091672
22	6	0	-1.830729	-3.152161	-1.874557

23	6	0	2.791040	1.847758	-1.395768
24	1	0	-2.120081	-4.153958	-1.567371
25	1	0	-2.596264	-2.724054	-2.524227
26	1	0	-0.888651	-3.174610	-2.424327
27	1	0	-5.657419	-0.098185	1.544947
28	1	0	-5.875429	-1.755640	0.887629
29	1	0	-4.408190	-1.330646	1.787602
30	1	0	3.577552	2.547379	-1.123787
31	1	0	3.216699	0.915126	-1.772441
32	1	0	2.157844	2.278980	-2.174508
33	6	0	-0.614208	4.311027	1.017433
34	1	0	0.099351	3.902235	1.738065
35	1	0	-0.234427	5.257442	0.639158
36	1	0	-1.573116	4.443646	1.516751
37	7	0	2.192874	-0.967416	1.575453
38	8	0	-4.329920	-1.285894	-1.135361
39	8	0	-0.166545	3.412939	-1.166886
40	8	0	-1.969556	-2.576782	0.461679
41	8	0	1.996225	2.111333	0.865990
42	1	0	-3.194661	0.432748	-2.009892
43	1	0	2.324604	-0.204114	2.229965
44	6	0	3.226266	-1.057788	0.631348
45	6	0	4.400827	-0.329917	0.867136
46	6	0	3.151827	-1.861886	-0.511894
47	6	0	5.471114	-0.408747	-0.012629
48	1	0	4.460194	0.304677	1.745872
49	6	0	4.229452	-1.927923	-1.388174
50	1	0	2.260862	-2.436174	-0.732565
51	6	0	5.395002	-1.206052	-1.151292
52	1	0	6.367898	0.164517	0.193928
53	1	0	4.151280	-2.555587	-2.268876
54	1	0	6.227838	-1.263805	-1.841195

Structure 42 $_5G^-$ (M06-2X, Gas Phase)

Energy (Hartrees): = -1487.746178
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.795103	2.299104	-0.976062
2	1	0	2.765019	2.579575	-1.389646
3	6	0	1.810077	0.827361	-0.610889
4	1	0	1.855445	0.237210	-1.526975
5	6	0	0.596221	0.425308	0.218600
6	1	0	0.587794	1.001253	1.145326
7	6	0	0.636874	-1.052409	0.604326
8	1	0	1.380899	-1.169048	1.392696
9	6	0	-0.731103	-1.567777	1.101160
10	1	0	-1.177578	-0.764212	1.694481
11	6	0	-0.520407	-2.724893	2.002750
12	7	0	-0.344694	-3.627939	2.689285
13	8	0	1.576276	3.078960	0.201224
14	8	0	2.946946	0.536169	0.208693
15	8	0	-0.558432	0.765008	-0.549500
16	8	0	1.031620	-1.856491	-0.510674
17	6	0	0.504901	3.903805	0.221095
18	6	0	-1.525482	1.498010	0.072965
19	6	0	4.001828	-0.082063	-0.374347
20	6	0	2.180594	-2.587575	-0.396565
21	6	0	0.336374	4.536765	1.569214
22	6	0	-2.583119	1.935785	-0.886375
23	6	0	2.486033	-3.299907	-1.676946
24	1	0	-3.442913	2.289301	-0.323436
25	1	0	-2.165754	2.751281	-1.481052
26	1	0	-2.865958	1.113894	-1.542968
27	1	0	1.297968	4.681484	2.057110
28	1	0	-0.198507	5.476993	1.459125
29	1	0	-0.269635	3.852719	2.168996
30	1	0	3.223056	-4.075275	-1.485568
31	1	0	1.580903	-3.719271	-2.113286
32	1	0	2.905325	-2.563404	-2.366666
33	6	0	5.094575	-0.328357	0.619670
34	1	0	4.801389	-1.193338	1.218829
35	1	0	6.018311	-0.547538	0.090531
36	1	0	5.210759	0.529718	1.279686
37	7	0	-1.598165	-1.926592	0.010095
38	8	0	-0.224663	4.064782	-0.718327
39	8	0	4.014349	-0.401721	-1.531631
40	8	0	-1.477167	1.759553	1.245181
41	8	0	2.847525	-2.598372	0.596122
42	1	0	1.011229	2.499536	-1.705037
43	1	0	-1.107549	-2.202446	-0.826691

44	6	0	-2.879194	-1.425166	-0.168697
45	6	0	-3.470277	-1.534870	-1.437193
46	6	0	-3.615430	-0.833704	0.863711
47	6	0	-4.743753	-1.041906	-1.668473
48	1	0	-2.914038	-2.007153	-2.240209
49	6	0	-4.888861	-0.333665	0.613787
50	1	0	-3.213092	-0.767589	1.866632
51	6	0	-5.462635	-0.424048	-0.647609
52	1	0	-5.176221	-1.137450	-2.657752
53	1	0	-5.436765	0.127752	1.427115
54	1	0	-6.455620	-0.034161	-0.830303

Structure 42 $_5G^-$ (M06-2X, $CHCl_3$)

Energy (Hartrees): = -1487.7750899
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.859171	2.291857	-0.980605
2	1	0	2.834605	2.550213	-1.395746
3	6	0	1.832838	0.819379	-0.624729
4	1	0	1.860786	0.237653	-1.546483
5	6	0	0.607220	0.441750	0.201839
6	1	0	0.595061	1.022812	1.125055
7	6	0	0.626617	-1.032362	0.599222
8	1	0	1.366182	-1.145327	1.391780
9	6	0	-0.745904	-1.527538	1.102798
10	1	0	-1.174269	-0.730028	1.716784
11	6	0	-0.543787	-2.699647	1.989322
12	7	0	-0.384355	-3.620221	2.656417
13	8	0	1.665595	3.074178	0.202648
14	8	0	2.964846	0.491095	0.190684
15	8	0	-0.536028	0.786034	-0.583347
16	8	0	1.008568	-1.846680	-0.511651
17	6	0	0.623321	3.930062	0.237276
18	6	0	-1.497181	1.546763	0.006049
19	6	0	3.982315	-0.195579	-0.380362
20	6	0	2.106276	-2.646697	-0.380034
21	6	0	0.499818	4.581224	1.578965
22	6	0	-2.538322	1.967568	-0.977467
23	6	0	2.357941	-3.408482	-1.640232
24	1	0	-3.417606	2.317683	-0.441688
25	1	0	-2.118679	2.786455	-1.567418
26	1	0	-2.792396	1.145428	-1.645607
27	1	0	1.475960	4.720766	2.040241
28	1	0	-0.023462	5.529301	1.474436
29	1	0	-0.096607	3.917300	2.210878
30	1	0	3.279031	-3.976662	-1.538348
31	1	0	1.519122	-4.081472	-1.829330
32	1	0	2.434409	-2.709802	-2.474271
33	6	0	5.083199	-0.433835	0.602850
34	1	0	4.687542	-0.997928	1.448856
35	1	0	5.884800	-0.988884	0.122003
36	1	0	5.452986	0.523473	0.974406
37	7	0	-1.627938	-1.873345	0.021108
38	8	0	-0.117669	4.110391	-0.693049
39	8	0	3.966266	-0.556120	-1.527033
40	8	0	-1.460668	1.845958	1.170788
41	8	0	2.755099	-2.695593	0.626494
42	1	0	1.082590	2.515576	-1.710317
43	1	0	-1.157628	-2.176904	-0.819394
44	6	0	-2.912450	-1.375033	-0.140296
45	6	0	-3.523948	-1.503235	-1.398481
46	6	0	-3.630483	-0.767243	0.896574
47	6	0	-4.802187	-1.013894	-1.614354
48	1	0	-2.978407	-1.986033	-2.203248
49	6	0	-4.910249	-0.273377	0.661854
50	1	0	-3.208266	-0.684218	1.890349
51	6	0	-5.505870	-0.383474	-0.588845
52	1	0	-5.250929	-1.121814	-2.595609
53	1	0	-5.444100	0.200681	1.477928
54	1	0	-6.502752	0.003337	-0.760276

Structure 42 R-X (M06-2X, Gas Phase)

Energy (Hartrees): = -1487.747819
No imaginary frequencies

Standard orientation:

Center	Atomic	Atomic	Coordinates (Angstroms)

Number	Number	Type	X	Y	Z
1	8	0	-0.603280	-1.801717	0.677977
2	8	0	-1.950736	-3.147480	-0.524408
3	8	0	-0.079492	1.122153	0.825614
4	8	0	1.132487	2.049936	-0.822436
5	8	0	-3.139180	-0.162866	-0.514603
6	8	0	-4.087030	-1.414003	1.094911
7	8	0	-2.504322	2.728514	-0.384231
8	8	0	-1.081341	3.991720	0.822356
9	7	0	1.578677	-3.389195	-1.880599
10	7	0	1.922029	-0.746975	0.289113
11	6	0	1.360834	-2.347340	-1.449759
12	6	0	1.078719	-1.020029	-0.847957
13	1	0	1.243766	-0.252663	-1.609807
14	6	0	3.304604	-0.579612	0.146213
15	6	0	4.100448	-0.585763	1.299306
16	1	0	3.634739	-0.764535	2.263283
17	6	0	5.464756	-0.363219	1.212894
18	1	0	6.062759	-0.374684	2.116609
19	6	0	6.066572	-0.127029	-0.020535
20	1	0	7.133002	0.045707	-0.086862
21	6	0	5.279374	-0.123494	-1.163590
22	1	0	5.731763	0.050101	-2.132801
23	6	0	3.908711	-0.349638	-1.091657
24	1	0	3.326005	-0.350624	-2.003647
25	6	0	-0.405366	-0.951978	-0.454163
26	1	0	-1.005725	-1.326448	-1.284519
27	6	0	-1.435603	-2.873455	0.520023
28	6	0	-1.645337	-3.587834	1.817819
29	1	0	-2.450934	-3.065741	2.340870
30	1	0	-0.747196	-3.564560	2.431625
31	1	0	-1.957545	-4.609026	1.614368
32	6	0	-0.888981	0.462264	-0.138949
33	1	0	-0.882535	1.027504	-1.073264
34	6	0	0.950654	1.866946	0.351494
35	6	0	1.759660	2.439233	1.469060
36	1	0	1.915474	1.684623	2.239116
37	1	0	1.191431	3.270211	1.894180
38	1	0	2.709234	2.795188	1.077186
39	6	0	-2.293047	0.469521	0.449673
40	1	0	-2.313476	-0.101228	1.378873
41	6	0	-3.997479	-1.110728	-0.062754
42	6	0	-4.759192	-1.729683	-1.193547
43	1	0	-4.122592	-2.510678	-1.616001
44	1	0	-4.973286	-0.992952	-1.965480
45	1	0	-5.671484	-2.178595	-0.808760
46	6	0	-2.769388	1.884133	0.738526
47	1	0	-3.847651	1.878428	0.899402
48	1	0	-2.260280	2.276185	1.617483
49	6	0	-1.593545	3.717408	-0.227452
50	6	0	-1.285020	4.375075	-1.539448
51	1	0	-2.153048	4.369257	-2.195348
52	1	0	-0.481176	3.798669	-2.005696
53	1	0	-0.929945	5.386814	-1.358883
54	1	0	1.638661	-1.256492	1.115862

Structure 42 $_{1}G^{+}{}_{5}G^{-}$ (M06-2X, Gas Phase)

Energy (Hartrees): =-1409.3879334
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.456049	2.860554	-0.038276
2	1	0	-0.085360	3.757643	-0.339001
3	6	0	-0.515368	1.698066	0.063104
4	1	0	-1.121419	1.833585	0.959604
5	6	0	0.196828	0.350115	0.125995
6	1	0	0.824409	0.219836	-0.757003
7	6	0	-0.803807	-0.798057	0.180838
8	1	0	-1.338064	-0.823601	-0.769859
9	6	0	-0.188075	-2.196058	0.370666
10	1	0	-1.003735	-2.919123	0.271540
11	6	0	0.405712	-2.372792	1.709321
12	7	0	0.888433	-2.518267	2.740660
13	8	0	1.443876	2.597730	-1.038616
14	8	0	-1.367124	1.650052	-1.084485
15	8	0	1.012013	0.411682	1.297566
16	8	0	-1.723616	-0.560057	1.241740
17	6	0	2.725977	2.463411	-0.630524
18	6	0	2.279112	-0.048701	1.224596

19	6	0	-2.662233	2.020858	-0.914341
20	6	0	-3.046999	-0.518714	0.927207
21	6	0	3.614212	2.043406	-1.763238
22	6	0	3.004422	0.158314	2.511499
23	6	0	-3.866746	-0.116995	2.112821
24	1	0	4.023322	-0.203890	2.409128
25	1	0	2.997621	1.222486	2.747515
26	1	0	2.478658	-0.390087	3.295243
27	1	0	3.233569	2.399506	-2.717817
28	1	0	4.623864	2.402439	-1.578210
29	1	0	3.628661	0.950214	-1.766013
30	1	0	-4.884784	-0.475430	1.982893
31	1	0	-3.426884	-0.488297	3.036043
32	1	0	-3.873834	0.976109	2.134294
33	6	0	-3.451574	1.804912	-2.167908
34	1	0	-3.731209	0.748785	-2.190321
35	1	0	-4.351391	2.413778	-2.134740
36	1	0	-2.851594	2.030097	-3.047602
37	7	0	0.763703	-2.507298	-0.667778
38	6	0	0.459642	-3.435821	-1.632326
39	6	0	1.577598	-3.722608	-2.607530
40	1	0	2.084402	-4.635917	-2.289704
41	1	0	1.142023	-3.899301	-3.588911
42	1	0	2.307966	-2.915232	-2.659910
43	8	0	3.083216	2.620563	0.504720
44	8	0	-3.092627	2.432682	0.126997
45	8	0	2.725719	-0.566179	0.229470
46	8	0	-3.461867	-0.738011	-0.175521
47	8	0	-0.615379	-3.988847	-1.681053
48	1	0	0.943071	3.023451	0.921625
49	1	0	1.673552	-2.064370	-0.626934

Structure 42 $_1G^+{}_5G^-$ (M06-2X, $CHCl_3$)

Energy (Hartrees): = -1409.4123463
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.899162	2.804278	0.033026
2	1	0	0.499014	3.784077	-0.227755
3	6	0	-0.234875	1.800346	0.105918
4	1	0	-0.830702	2.019477	0.992473
5	6	0	0.262825	0.356511	0.166049
6	1	0	0.904539	0.146218	-0.691774
7	6	0	-0.900552	-0.625893	0.144429
8	1	0	-1.395725	-0.537003	-0.823014
9	6	0	-0.518858	-2.111012	0.294249
10	1	0	-1.434472	-2.692199	0.147537
11	6	0	-0.019495	-2.422677	1.647417
12	7	0	0.383892	-2.674924	2.692074
13	8	0	1.828497	2.438143	-0.993077
14	8	0	-1.057340	1.900579	-1.062011
15	8	0	1.017954	0.271728	1.376908
16	8	0	-1.805263	-0.282826	1.188946
17	6	0	3.069344	2.061193	-0.617356
18	6	0	2.201923	-0.377570	1.355565
19	6	0	-2.332978	2.332226	-0.903618
20	6	0	-3.124694	-0.181093	0.871509
21	6	0	3.882162	1.641777	-1.802446
22	6	0	2.903492	-0.266129	2.666217
23	6	0	-3.922811	0.251074	2.057350
24	1	0	3.861998	-0.775220	2.608168
25	1	0	3.043916	0.788598	2.905384
26	1	0	2.279397	-0.719386	3.439445
27	1	0	3.848789	2.415667	-2.570109
28	1	0	4.906376	1.451740	-1.491892
29	1	0	3.449835	0.731313	-2.223479
30	1	0	-4.982455	0.196521	1.821042
31	1	0	-3.683954	-0.374195	2.918102
32	1	0	-3.648568	1.281511	2.293786
33	6	0	-3.080205	2.277528	-2.197146
34	1	0	-3.291934	1.228345	-2.418322
35	1	0	-4.016210	2.821754	-2.099236
36	1	0	-2.474122	2.684457	-3.006275
37	7	0	0.415909	-2.537274	-0.716158
38	6	0	0.042802	-3.410375	-1.701022
39	6	0	1.129331	-3.760752	-2.684585
40	1	0	1.118807	-4.839188	-2.841991
41	1	0	0.896859	-3.280363	-3.637447
42	1	0	2.119235	-3.444992	-2.355621
43	8	0	3.444025	2.056844	0.525563
44	8	0	-2.780479	2.680606	0.155642

45	8	0	2.597801	-0.974764	0.384719
46	8	0	-3.543556	-0.400362	-0.231461
47	8	0	-1.087893	-3.848219	-1.786352
48	1	0	1.408668	2.858737	0.993387
49	1	0	1.372696	-2.210910	-0.648168

Structure 42 $_1G^-{}_5G^-$ (M06-2X, Gas Phase)

Energy (Hartrees): =-1409.3787268
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.579844	1.285724	0.411472
2	1	0	-2.849183	0.946455	1.413856
3	6	0	-1.095053	1.115904	0.145497
4	1	0	-0.868703	1.339481	-0.896815
5	6	0	-0.538055	-0.265953	0.504350
6	1	0	-0.867043	-0.559666	1.505159
7	6	0	0.984840	-0.255421	0.462640
8	1	0	1.361855	0.299487	1.323420
9	6	0	1.612892	-1.663282	0.432858
10	1	0	1.468599	-2.065488	-0.572831
11	6	0	0.960354	-2.559533	1.398699
12	7	0	0.435385	-3.234436	2.164592
13	8	0	-3.279657	0.513546	-0.562389
14	8	0	-0.418642	2.043150	1.004971
15	8	0	-0.986741	-1.236990	-0.439147
16	8	0	1.396883	0.391075	-0.737892
17	6	0	-4.604797	0.379387	-0.326417
18	6	0	-2.080020	-1.971831	-0.108408
19	6	0	0.260867	3.070786	0.434659
20	6	0	2.475381	1.206343	-0.694989
21	6	0	-5.221541	-0.626184	-1.255111
22	6	0	-2.395179	-2.944921	-1.205098
23	6	0	2.819679	1.691459	-2.065548
24	1	0	-3.215273	-3.587529	-0.895381
25	1	0	-2.666430	-2.383015	-2.101057
26	1	0	-1.511842	-3.540215	-1.438017
27	1	0	-5.010280	-1.619307	-0.850143
28	1	0	-6.297425	-0.475366	-1.287056
29	1	0	-4.786798	-0.554101	-2.251229
30	1	0	3.634202	2.407841	-2.001116
31	1	0	3.111129	0.824826	-2.662860
32	1	0	1.936652	2.150232	-2.510483
33	6	0	0.989626	3.867786	1.475132
34	1	0	1.939893	3.361980	1.664991
35	1	0	1.188261	4.863917	1.087557
36	1	0	0.421167	3.909442	2.402104
37	7	0	3.039580	-1.616223	0.674643
38	6	0	3.921234	-1.465218	-0.372499
39	6	0	5.327585	-1.114580	0.048040
40	1	0	6.004147	-1.335532	-0.773582
41	1	0	5.357421	-0.043084	0.264381
42	1	0	5.630537	-1.661039	0.941976
43	8	0	-5.172897	0.978647	0.539072
44	8	0	0.288847	3.269665	-0.746353
45	8	0	-2.688411	-1.829985	0.911223
46	8	0	3.055373	1.467580	0.326942
47	8	0	3.577050	-1.579626	-1.527458
48	1	0	-2.848703	2.340219	0.312426
49	1	0	3.340810	-1.304218	1.586648

Structure 42 $_1G^-{}_5G^-$ (M06-2X, $CHCl_3$)

Energy (Hartrees): = -1409.4072708
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.598209	1.262887	-0.348326
2	1	0	2.882553	0.933233	-1.349365
3	6	0	1.102346	1.127215	-0.123930
4	1	0	0.857302	1.330052	0.918517
5	6	0	0.526304	-0.229511	-0.536060
6	1	0	0.852176	-0.480913	-1.548667
7	6	0	-0.996778	-0.207117	-0.505646
8	1	0	-1.361334	0.354338	-1.366189

9	6	0	-1.630704	-1.611041	-0.489378
10	1	0	-1.427643	-2.062502	0.485029
11	6	0	-1.034110	-2.473418	-1.520477
12	7	0	-0.534062	-3.122341	-2.324364
13	8	0	3.248259	0.456902	0.636414
14	8	0	0.470271	2.090139	-0.976554
15	8	0	0.966321	-1.242443	0.368561
16	8	0	-1.438367	0.417156	0.696866
17	6	0	4.567367	0.262093	0.445847
18	6	0	2.025804	-2.003893	-0.002643
19	6	0	-0.181228	3.133493	-0.406163
20	6	0	-2.448980	1.316394	0.622903
21	6	0	5.129363	-0.707235	1.440690
22	6	0	2.286577	-3.064137	1.020414
23	6	0	-2.867069	1.748342	1.990234
24	1	0	3.163270	-3.642009	0.738044
25	1	0	2.425256	-2.603006	1.999798
26	1	0	1.414177	-3.719213	1.079468
27	1	0	4.938167	-1.718937	1.072497
28	1	0	6.204281	-0.560298	1.520828
29	1	0	4.649276	-0.593506	2.411803
30	1	0	-3.628814	2.520430	1.913540
31	1	0	-3.253604	0.879006	2.527670
32	1	0	-1.996187	2.122197	2.530099
33	6	0	-0.803530	4.001774	-1.453248
34	1	0	-1.522761	3.410128	-2.022283
35	1	0	-1.304437	4.840907	-0.976905
36	1	0	-0.033693	4.356809	-2.140347
37	7	0	-3.063622	-1.528569	-0.635479
38	6	0	-3.885067	-1.572858	0.463385
39	6	0	-5.312908	-1.178508	0.187331
40	1	0	-5.952853	-1.587356	0.966360
41	1	0	-5.379304	-0.086599	0.209286
42	1	0	-5.646466	-1.522840	-0.792257
43	8	0	5.181022	0.799352	-0.435797
44	8	0	-0.240134	3.301586	0.781002
45	8	0	2.632694	-1.831281	-1.022609
46	8	0	-2.920854	1.684764	-0.420398
47	8	0	-3.475851	-1.878095	1.565564
48	1	0	2.891494	2.307912	-0.219347
49	1	0	-3.427538	-1.132997	-1.492668

Structure 42 $_5G^-$ (M06-2X, Gas Phase)

Energy (Hartrees): = -1409.3826589
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.079380	-2.316540	-0.926493
2	1	0	0.748182	-3.270786	-1.340224
3	6	0	-0.131400	-1.491618	-0.543011
4	1	0	-0.668140	-1.223393	-1.453774
5	6	0	0.232124	-0.236529	0.244852
6	1	0	0.707599	-0.526299	1.183440
7	6	0	-1.009861	0.583297	0.594326
8	1	0	-1.517789	0.079497	1.417108
9	6	0	-0.680133	2.033746	0.998603
10	1	0	0.238983	2.054880	1.593579
11	6	0	-1.788070	2.570753	1.813091
12	7	0	-2.673697	2.976573	2.419913
13	8	0	1.866483	-2.579508	0.235116
14	8	0	-0.992535	-2.245352	0.317685
15	8	0	1.169520	0.502267	-0.536441
16	8	0	-1.912740	0.655010	-0.515573
17	6	0	3.186542	-2.288989	0.175246
18	6	0	2.395227	0.737414	0.027836
19	6	0	-2.092406	-2.809962	-0.233251
20	6	0	-3.150709	0.096916	-0.368397
21	6	0	3.851611	-2.536199	1.494599
22	6	0	3.345874	1.354614	-0.947849
23	6	0	-3.924941	0.169354	-1.648011
24	1	0	4.025667	0.563328	-1.272273
25	1	0	2.822169	1.763946	-1.808671
26	1	0	3.905536	2.132733	-0.433843
27	1	0	3.420858	-3.404143	1.990054
28	1	0	4.920692	-2.658209	1.339892
29	1	0	3.675040	-1.651537	2.110853
30	1	0	-4.982825	0.048118	-1.430118
31	1	0	-3.736290	1.105779	-2.169753
32	1	0	-3.588665	-0.661154	-2.273833
33	6	0	-2.893742	-3.541755	0.798726
34	1	0	-3.432076	-2.793687	1.384546
35	1	0	-3.603500	-4.198619	0.302829

36	1	0	-2.237501	-4.099810	1.464709
37	7	0	-0.465306	2.882350	-0.149569
38	6	0	0.742077	3.478053	-0.389644
39	6	0	0.834290	4.180669	-1.724267
40	1	0	1.747379	4.769800	-1.746068
41	1	0	0.863896	3.434372	-2.522222
42	1	0	-0.029350	4.826356	-1.890209
43	8	0	3.722634	-1.858719	-0.809144
44	8	0	-2.373605	-2.695581	-1.395388
45	8	0	2.654778	0.427680	1.155514
46	8	0	-3.519227	-0.411846	0.649385
47	8	0	1.659402	3.424449	0.400575
48	1	0	1.676312	-1.786543	-1.667344
49	1	0	-1.156023	2.836365	-0.883059

Structure 42 $_5G^-$ (M06-2X, $CHCl_3$)

Energy (Hartrees): =-1409.4095537
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.337384	-2.198527	-0.902042
2	1	0	1.115373	-3.188320	-1.306459
3	6	0	0.044452	-1.506772	-0.530025
4	1	0	-0.506704	-1.305338	-1.449077
5	6	0	0.259475	-0.209487	0.246409
6	1	0	0.767627	-0.424505	1.187952
7	6	0	-1.073288	0.457694	0.582517
8	1	0	-1.524185	-0.107540	1.398492
9	6	0	-0.926332	1.931719	1.003845
10	1	0	-0.049737	2.045073	1.649455
11	6	0	-2.120040	2.333473	1.775179
12	7	0	-3.064383	2.640779	2.350448
13	8	0	2.151374	-2.360327	0.262403
14	8	0	-0.740839	-2.342379	0.329322
15	8	0	1.092624	0.628696	-0.554366
16	8	0	-1.955918	0.426668	-0.543752
17	6	0	3.440973	-1.967854	0.189905
18	6	0	2.304384	0.988855	-0.043276
19	6	0	-1.786026	-3.006088	-0.216257
20	6	0	-3.145394	-0.225567	-0.409154
21	6	0	4.133055	-2.160248	1.502268
22	6	0	3.128057	1.722467	-1.051996
23	6	0	-3.911025	-0.196866	-1.691881
24	1	0	3.830520	1.000168	-1.477646
25	1	0	2.512867	2.138988	-1.847250
26	1	0	3.688389	2.506057	-0.545777
27	1	0	3.966565	-3.173073	1.870234
28	1	0	5.195853	-1.963601	1.384374
29	1	0	3.704874	-1.458238	2.220594
30	1	0	-4.877265	-0.673472	-1.546747
31	1	0	-4.040294	0.834792	-2.022793
32	1	0	-3.340934	-0.733493	-2.452534
33	6	0	-2.489642	-3.831990	0.812459
34	1	0	-2.878579	-3.169097	1.587250
35	1	0	-3.304386	-4.378299	0.343615
36	1	0	-1.782325	-4.522147	1.275000
37	7	0	-0.760806	2.819149	-0.120333
38	6	0	0.374145	3.555902	-0.299001
39	6	0	0.410700	4.336901	-1.587592
40	1	0	1.354915	4.872671	-1.652455
41	1	0	0.308474	3.660457	-2.439295
42	1	0	-0.417289	5.048674	-1.618202
43	8	0	3.937544	-1.515713	-0.807969
44	8	0	-2.086916	-2.911387	-1.376506
45	8	0	2.658737	0.692159	1.064221
46	8	0	-3.487761	-0.747955	0.614042
47	8	0	1.273884	3.565435	0.520112
48	1	0	1.868602	-1.616743	-1.654014
49	1	0	-1.443116	2.764237	-0.863717

Structure 42 R-X (M06-2X, Gas Phase)

Energy (Hartrees): = -1409.3803048
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	6	0	-1.576754	1.218634	-0.922864
2	1	0	-1.749201	0.514540	-1.741909
3	6	0	-0.131391	1.101562	-0.420917
4	1	0	0.544635	1.511843	-1.172771
5	6	0	0.312411	-0.328183	-0.138240
6	1	0	0.251743	-0.889974	-1.072363
7	6	0	1.741219	-0.391541	0.386056
8	1	0	1.851791	0.216956	1.287528
9	6	0	2.158172	-1.813453	0.724007
10	1	0	3.236732	-1.846257	0.874161
11	1	0	1.643403	-2.153161	1.621162
12	6	0	0.937600	-3.659583	-0.161820
13	6	0	0.613861	-4.375063	-1.439026
14	1	0	-0.196216	-3.821628	-1.921517
15	1	0	0.265036	-5.378939	-1.209209
16	1	0	1.474417	-4.395864	-2.104368
17	6	0	3.687713	0.772381	-0.268256
18	6	0	4.330061	1.485749	-1.417232
19	1	0	4.284895	0.877087	-2.319349
20	1	0	5.357403	1.731326	-1.161064
21	1	0	3.762270	2.403059	-1.587126
22	6	0	-1.490582	-1.766849	0.401514
23	6	0	-2.279195	-2.327496	1.542406
24	1	0	-1.665854	-3.097030	2.016206
25	1	0	-3.194929	-2.771529	1.159738
26	1	0	-2.492290	-1.548807	2.274785
27	6	0	0.938078	2.830046	0.841909
28	6	0	0.788578	3.665277	2.077216
29	1	0	0.532632	3.039424	2.931073
30	1	0	-0.026263	4.374199	1.915344
31	1	0	1.713230	4.207209	2.255134
32	6	0	-3.815197	0.569009	-0.219279
33	6	0	-4.763243	0.366813	0.940495
34	1	0	-4.340148	0.655258	1.902885
35	1	0	-5.043039	-0.687352	0.971283
36	1	0	-5.666380	0.944977	0.747608
37	6	0	-1.778287	2.594564	-1.430398
38	7	0	-2.528158	0.915289	0.123120
39	1	0	-2.311541	1.251771	1.049507
40	7	0	-1.899004	3.682596	-1.775566
41	8	0	1.840186	-2.676913	-0.371590
42	8	0	0.441483	-3.890304	0.907598
43	8	0	2.543901	0.154168	-0.658636
44	8	0	4.083981	0.740582	0.861725
45	8	0	-0.506734	-0.945596	0.849636
46	8	0	-1.659511	-2.007668	-0.761091
47	8	0	-0.053664	1.900116	0.765883
48	8	0	1.791251	2.946285	0.011560
49	8	0	-4.140951	0.407641	-1.370466