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Table 1. FQ data of polymers 1-3.^a

	1		2		3	
	25 Å	200 Å	25 Å	200 Å	25 Å	200 Å
TNT	30,70,90	7,32,65	20,50,65	2,15,20	15,35,65	5,10,15
DNT	80,93,99	50,80,95	70	25	65,85,96	25,45,80
CDNB	85,90,98	55,68,95	75	30	60,80,97	20,40,75
DNT*	75,85,95	55,75,95	55	30	65,85,97	35,65,85
pDNB	65,75,90	40,60,85	50	25	55,70,85	25,40,70
mDNB	75,90,98	60,85,97	80	60	75,90,97	45,60,95
NT	40,50,65	37,47,65	20	30	30,55,70	35,60,70
CNB	10,30,60	25,70,80	5	25	5,35,60	25,55,80
NB	0,3,15	2,10,30	-	-	5,15,45	20,20,25
BQ	2,10,20	15,35,65	5	5	2,10,20	9,25,35
CA	5,10,20	5,11,20	0	2	2,6,15	3,10,15
DQ	20,45,80	50,85,90	7	16	6,15,50	40,60,80
AQ	0,0,0	-,3,-	0	1	0,0,0	0,1,3
BP	0,0,0	-,0,-	0	0	0,0,0	0,0,0
DCNB	0,0,0	-,3,-	0	6	0,0,0	-,6,-
DCIB	0,0,0	-,5,-	0	10	0,5,5	-,2,-
DMB	0,0,0	-,2,-	5	5	0,0,0	-,3,-

^a Data (Num1, Num2, Num3) for polymers 1 and 3 are the FQ with exposure times of 10s, 1 min, and 5 min, respectively. FQ data for 2 are at 1 min only except for TNT at (1 min, 5 min, 10 min).

A. Crystal Data

Identification code	97069
Empirical formula	$C_{46}H_{42}Cl_4Si_2$
Formula weight	792.78
Temperature	293(2) K
Wavelength	0.71073 Å
Crystal morphology	?
Crystal size	? x ? x ? mm
Crystal system	Orthorhombic
Space group	Cmca
Unit cell dimensions	$a = 25.259(2)$ Å $\alpha = 90^\circ$ $b = 15.6271(11)$ Å $\beta = 90^\circ$ $c = 10.8201(8)$ Å $\gamma = 90^\circ$
Volume, Z	$4270.9(5)$ Å ³ , 4
Density (calculated)	1.233 Mg/m ³
Absorption coefficient	0.364 mm ⁻¹
F(000)	1656

B. Data Collection and Reduction

Diffractometer	Siemens SMART/CCD
Scan Type	ω Scans
Scan angle	0.30°
θ range for data collection	1.61 to 20.00°
Limiting indices	$-27 \leq h \leq 26$, $-17 \leq k \leq 17$, $-11 \leq l \leq 7$
Reflections collected	3644
Independent reflections	1011 ($R_{int} = 0.0301$)
Absorption correction	None

C. Solution and Refinement

Refinement method	Full-matrix least-squares on F^2
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Data / restraints / parameters 1000 / 0 / 127

Goodness-of-fit on F^2 1.095

Final R indices [$I > 2\sigma(I)$] $R1 = 0.0670$, $wR2 = 0.1718$

R indices (all data) $R1 = 0.0696$, $wR2 = 0.1755$

Extinction coefficient 0.0021(5)

Largest diff. peak and hole 0.810 and $-0.653 \text{ e}\text{\AA}^{-3}$

Weighting Scheme $\text{calc } w = 1 / [\sigma^2(F_o^2) + (0.0847P)^2 + 23.5701P]$
where $P = (F_o^2 + F_c^2) / 2$

Notes Cell constants based upon three sets of fifteen (15) 0.30° ω scans. Refle were harvested using the Siemens XSCANS algorithm.

Table 2. Atomic coordinates [$\times 10^4$] and equivalent isotropic displacement parameters [$\text{\AA}^2 \times 10^3$] for 1. $U(\text{eq})$ is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
Si(1)	5000	3390(1)	-106(2)	36(1)
C(1)	5000	4037(4)	-1523(7)	34(2)
C(2)	5000	4400(4)	-2516(7)	29(2)
C(3)	5000	4747(4)	-3739(6)	24(2)
C(4)	5472(2)	4887(3)	-4383(4)	24(1)
C(5)	6027(2)	4806(3)	-3840(4)	29(1)
C(6)	6310(2)	5645(3)	-4105(4)	29(1)
C(7)	6307(2)	5861(3)	-5365(4)	28(1)
C(8)	6546(2)	6603(3)	-5771(5)	40(1)
C(9)	6802(2)	7126(3)	-4926(6)	47(2)
C(10)	6811(2)	6915(3)	-3699(6)	47(2)
C(11)	6567(2)	6171(3)	-3271(5)	38(1)
C(14)	4400(2)	3653(4)	785(5)	62(2)
C(13)	5000	2254(5)	-586(9)	76(3)
Cl(1)	6994(2)	9437(2)	-3982(4)	228(2)
C(1S)	7358(3)	10000	-5000	82(3)

Table 3. Bond lengths [Å] and angles [°] for 1.

Si(1)-C(1)	1.837(8)	Si(1)-C(14)	1.843(5)
Si(1)-C(14)#1	1.843(6)	Si(1)-C(13)	1.848(8)
C(1)-C(2)	1.215(9)	C(2)-C(3)	1.430(10)
C(3)-C(4)#1	1.399(5)	C(3)-C(4)	1.399(5)
C(4)-C(4)#2	1.380(9)	C(4)-C(5)	1.526(6)
C(5)-C(6)	1.520(6)	C(5)-C(7)#2	1.524(6)
C(6)-C(11)	1.382(6)	C(6)-C(7)	1.405(6)
C(7)-C(8)	1.380(7)	C(7)-C(5)#2	1.524(6)
C(8)-C(9)	1.385(7)	C(9)-C(10)	1.368(8)
C(10)-C(11)	1.395(7)	Cl(1)-C(1S)	1.684(5)
C(1S)-Cl(1)#3	1.684(5)		
C(1)-Si(1)-C(14)	108.3(2)	C(1)-Si(1)-C(14)#1	108.3(2)
C(14)-Si(1)-C(14)#1	110.6(4)	C(1)-Si(1)-C(13)	107.1(4)
C(14)-Si(1)-C(13)	111.2(2)	C(14)#1-Si(1)-C(13)	111.2(2)
C(2)-C(1)-Si(1)	174.3(6)	C(1)-C(2)-C(3)	174.5(6)
C(4)#1-C(3)-C(4)	117.0(5)	C(4)#1-C(3)-C(2)	121.4(3)
C(4)-C(3)-C(2)	121.4(3)	C(4)#2-C(4)-C(3)	121.5(3)
C(4)#2-C(4)-C(5)	113.2(2)	C(3)-C(4)-C(5)	125.3(4)
C(6)-C(5)-C(7)#2	105.4(3)	C(6)-C(5)-C(4)	106.7(3)
C(7)#2-C(5)-C(4)	105.4(4)	C(11)-C(6)-C(7)	119.5(4)
C(11)-C(6)-C(5)	127.7(4)	C(7)-C(6)-C(5)	112.8(4)
C(8)-C(7)-C(6)	120.6(4)	C(8)-C(7)-C(5)#2	126.7(5)
C(6)-C(7)-C(5)#2	112.7(4)	C(7)-C(8)-C(9)	119.3(5)
C(10)-C(9)-C(8)	120.4(5)	C(9)-C(10)-C(11)	121.0(5)
C(6)-C(11)-C(10)	119.1(5)	Cl(1)#3-C(1S)-Cl(1)	113.7(6)

Symmetry transformations used to generate equivalent atoms:

#1 -x+1,y,z #2 x,-y+1,-z-1 #3 x,-y+2,-z-1

Table 4. Anisotropic displacement parameters [$\text{\AA}^2 \times 10^3$] for 1.

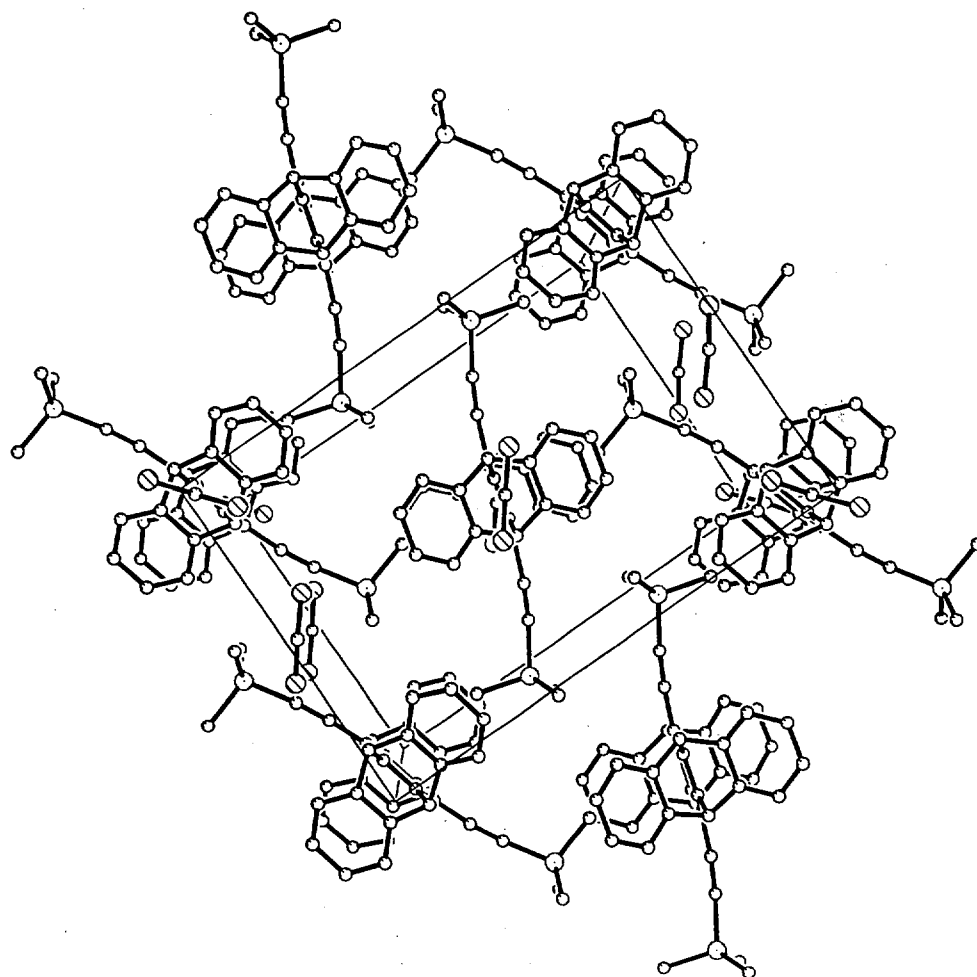
The anisotropic displacement factor exponent takes the form:

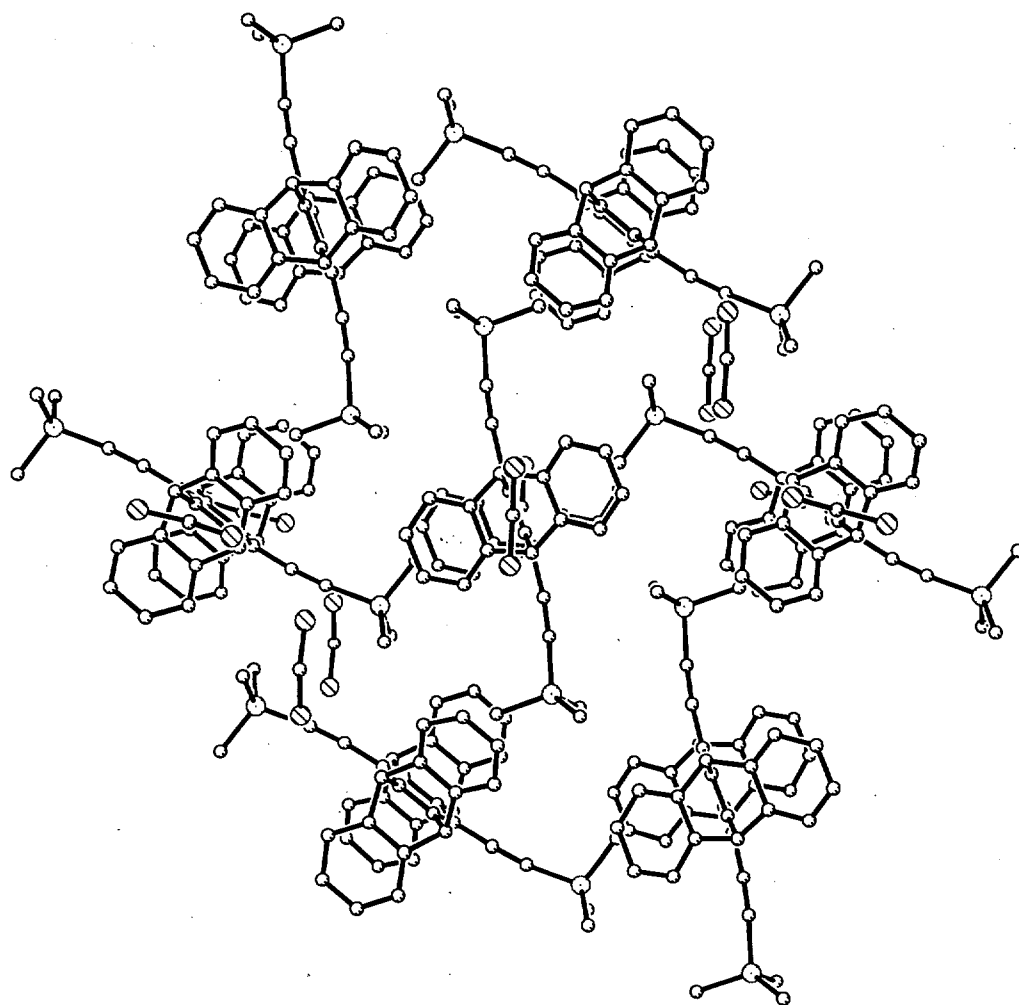
$$-2\pi^2 [(h a^*)^2 U_{11} + \dots + 2 h k a^* b^* U_{12}]$$

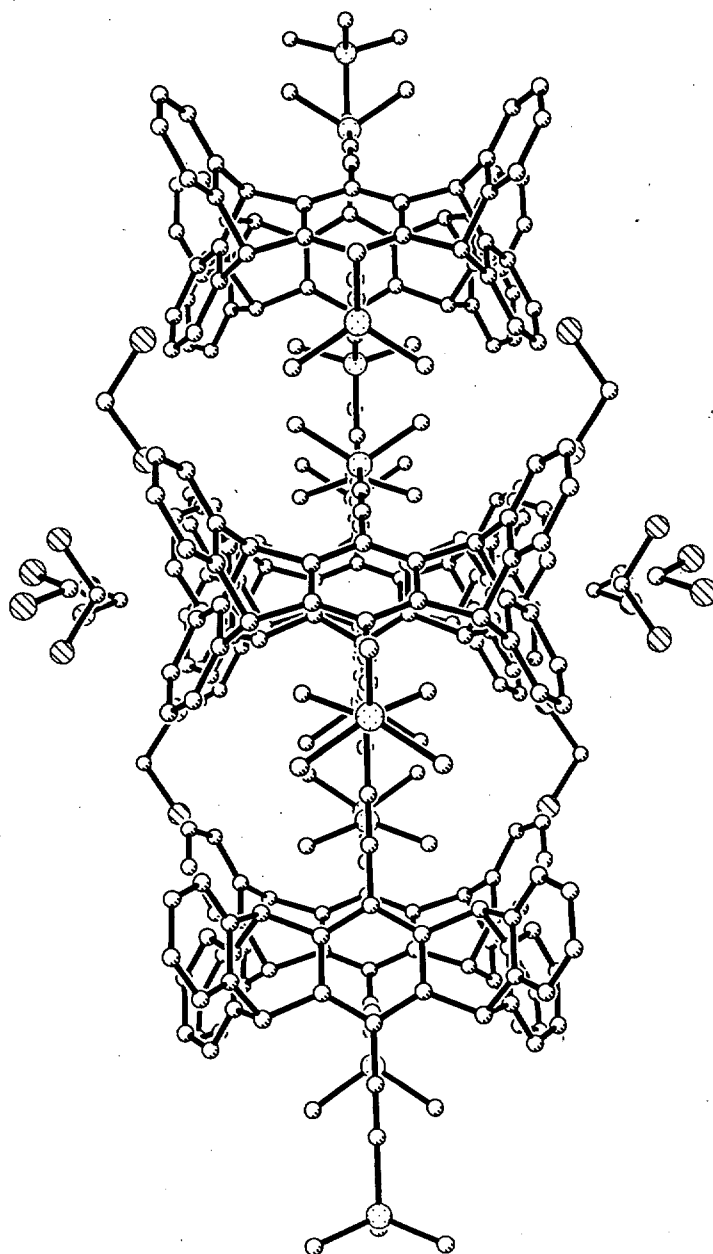
	U11	U22	U33	U23	U13	U12
Si(1)	45(1)	37(1)	27(1)	7(1)	0	0
C(1)	30(4)	35(4)	38(5)	-1(4)	0	0
C(2)	25(4)	29(4)	32(5)	-3(4)	0	0
C(3)	32(4)	21(4)	20(4)	1(3)	0	0
C(4)	25(3)	21(2)	25(3)	1(2)	-1(2)	0(2)
C(5)	23(3)	35(3)	29(3)	5(2)	-2(2)	-1(2)
C(6)	20(3)	32(3)	35(4)	-6(2)	0(2)	3(2)
C(7)	19(3)	27(3)	39(4)	0(2)	3(2)	0(2)
C(8)	30(3)	40(3)	52(4)	4(3)	6(3)	-1(2)
C(9)	38(3)	29(3)	73(5)	-2(3)	11(3)	-12(3)
C(10)	30(3)	44(4)	67(5)	-22(3)	1(3)	-8(3)
C(11)	24(3)	47(3)	41(3)	-9(3)	2(2)	2(2)
C(14)	59(4)	78(4)	47(4)	3(3)	10(3)	-9(3)
C(13)	115(8)	41(5)	71(7)	10(5)	0	0
Cl(1)	253(4)	102(2)	329(5)	-61(2)	217(4)	-48(2)
C(1S)	32(5)	93(7)	122(9)	-29(6)	0	0

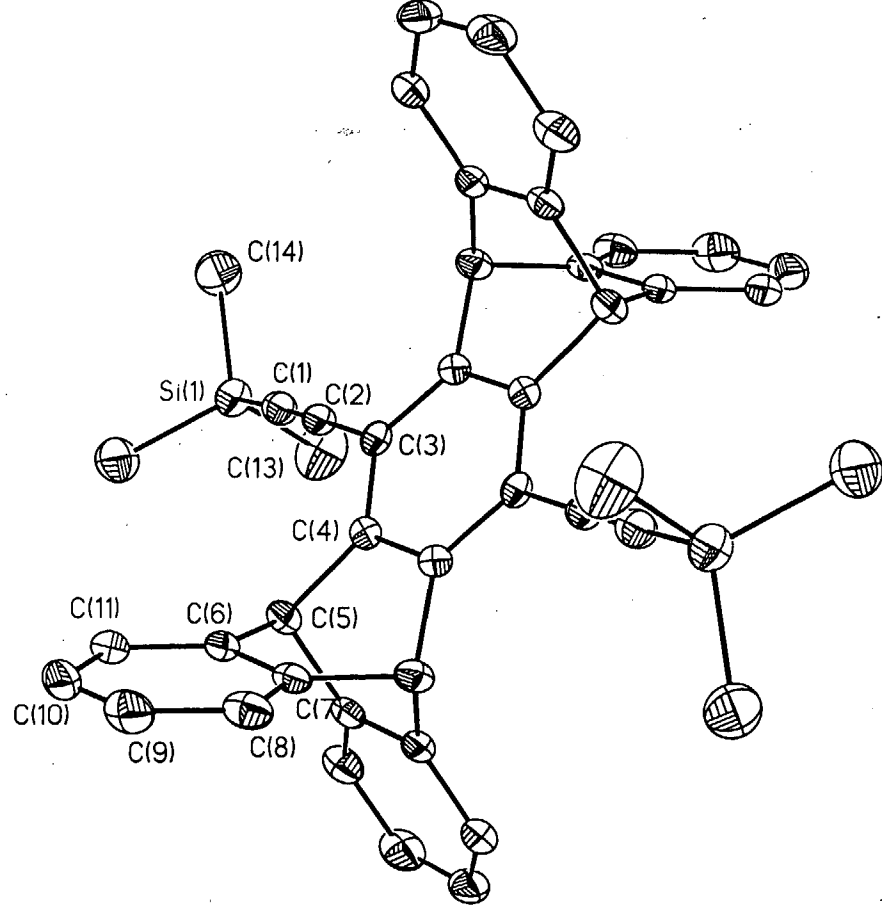
Table 5. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for 1.

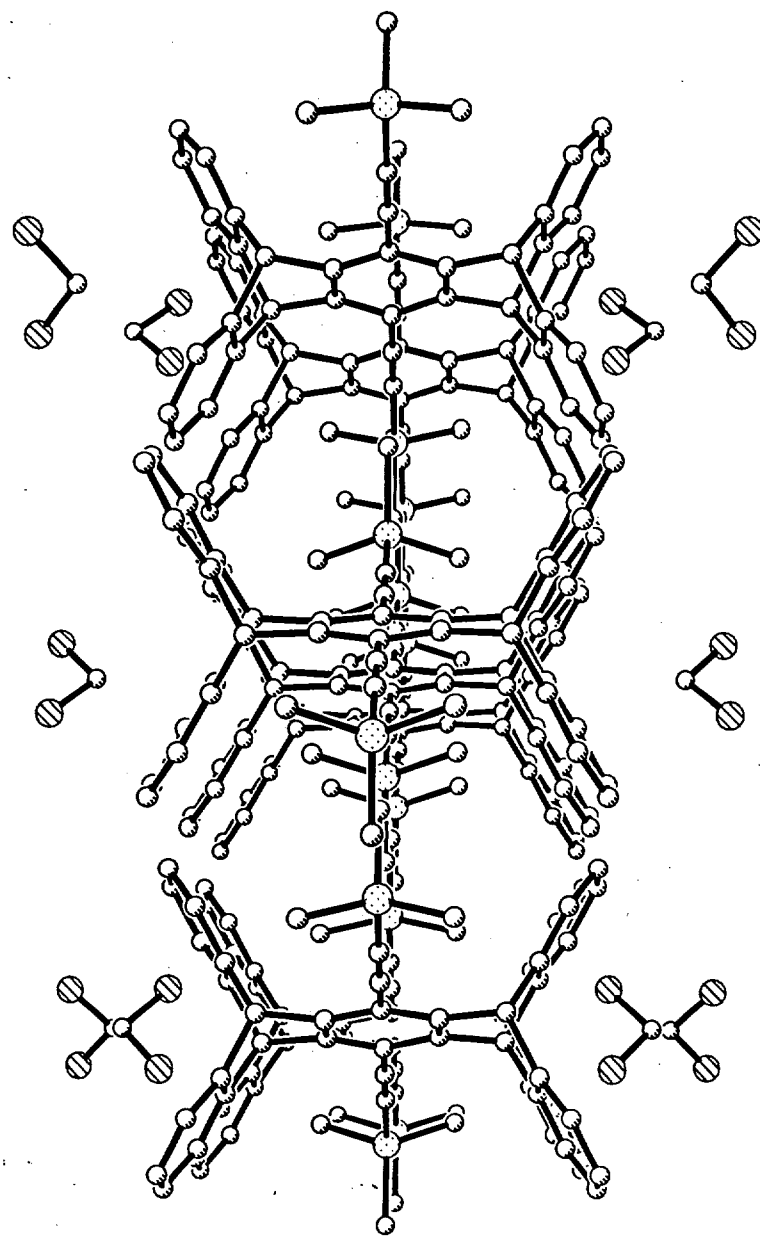
	x	y	z	U(eq)
H(5)	6025(2)	4658(3)	-2960(4)	35
H(8)	6537(2)	6751(3)	-6603(5)	48
H(9)	6968(2)	7624(3)	-5194(6)	56
H(10)	6983(2)	7273(3)	-3142(6)	56
H(11)	6576(2)	6032(3)	-2436(5)	45
H(14A)	4393(2)	3320(4)	1530(5)	92
H(14B)	4092(2)	3526(4)	298(5)	92
H(14C)	4403(2)	4250(4)	990(5)	92
H(13A)	5000	1895(5)	133(9)	114
H(13B)	5310	2139(5)	-1071(9)	114
H(13C)	4690	2139(5)	-1071(9)	114
H(1S1)	7585(3)	10392	-4548	99
H(1S2)	7585(3)	9608	-5452	99

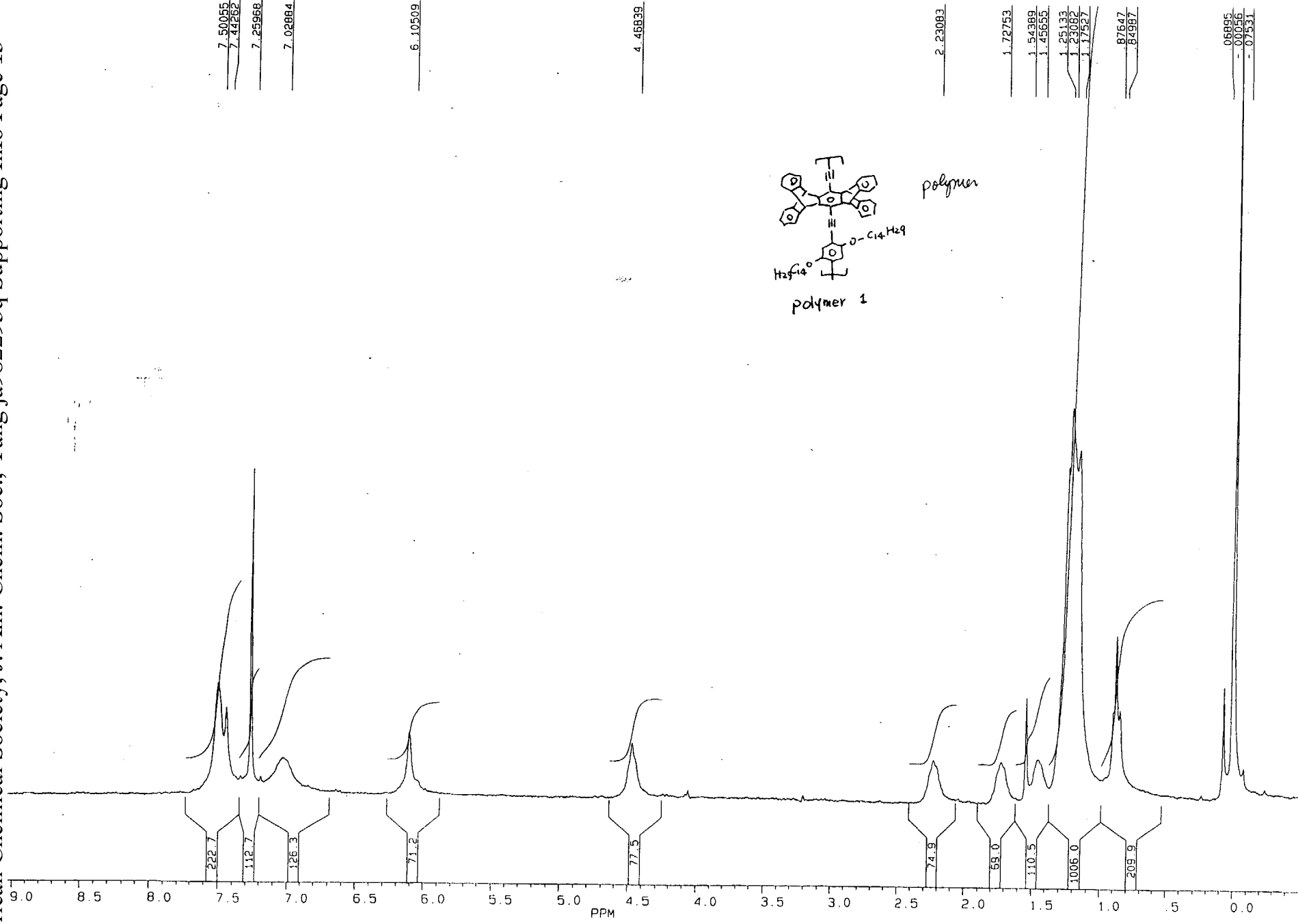


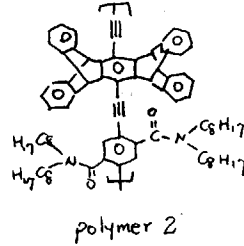


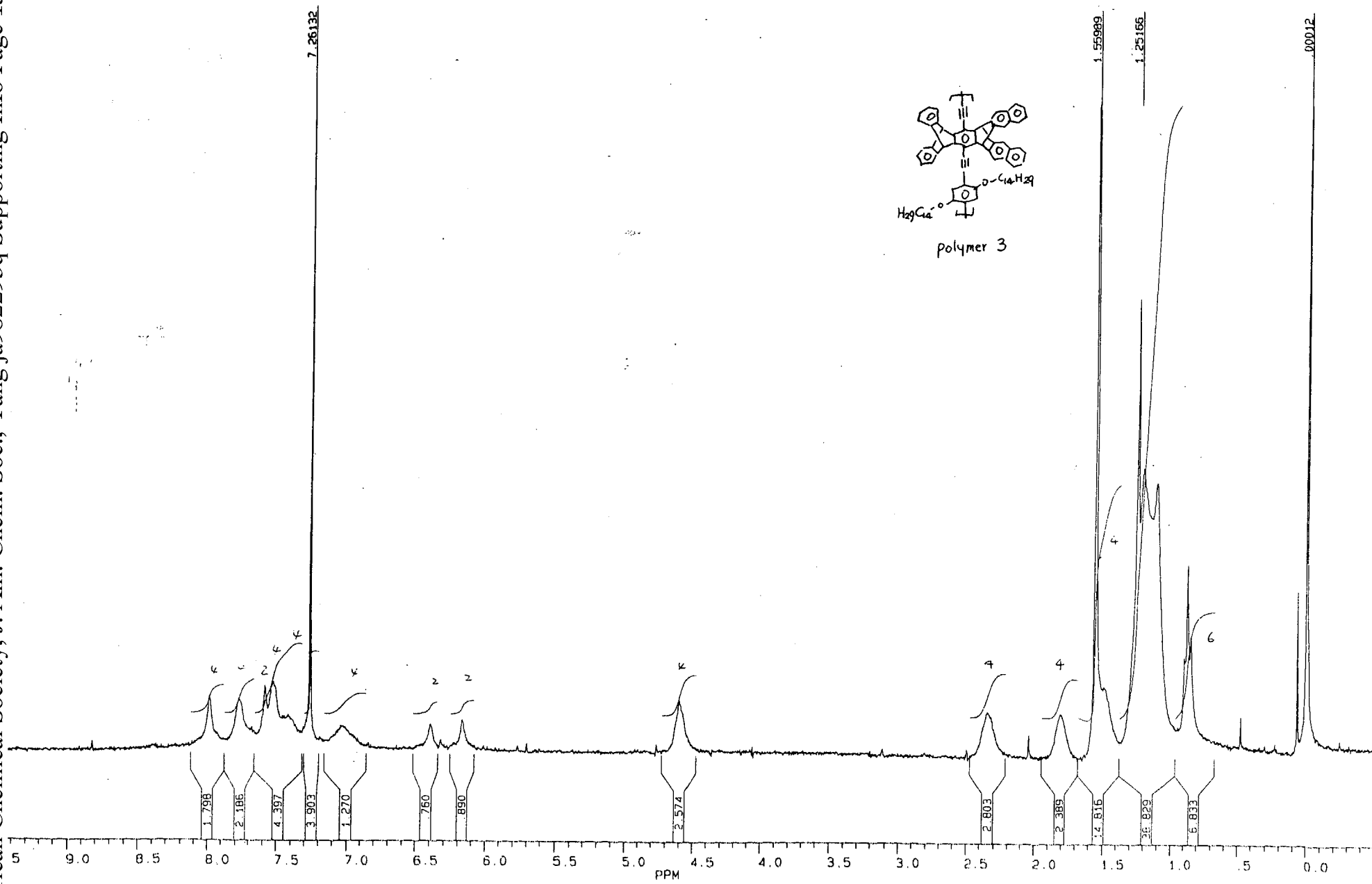


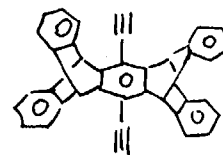
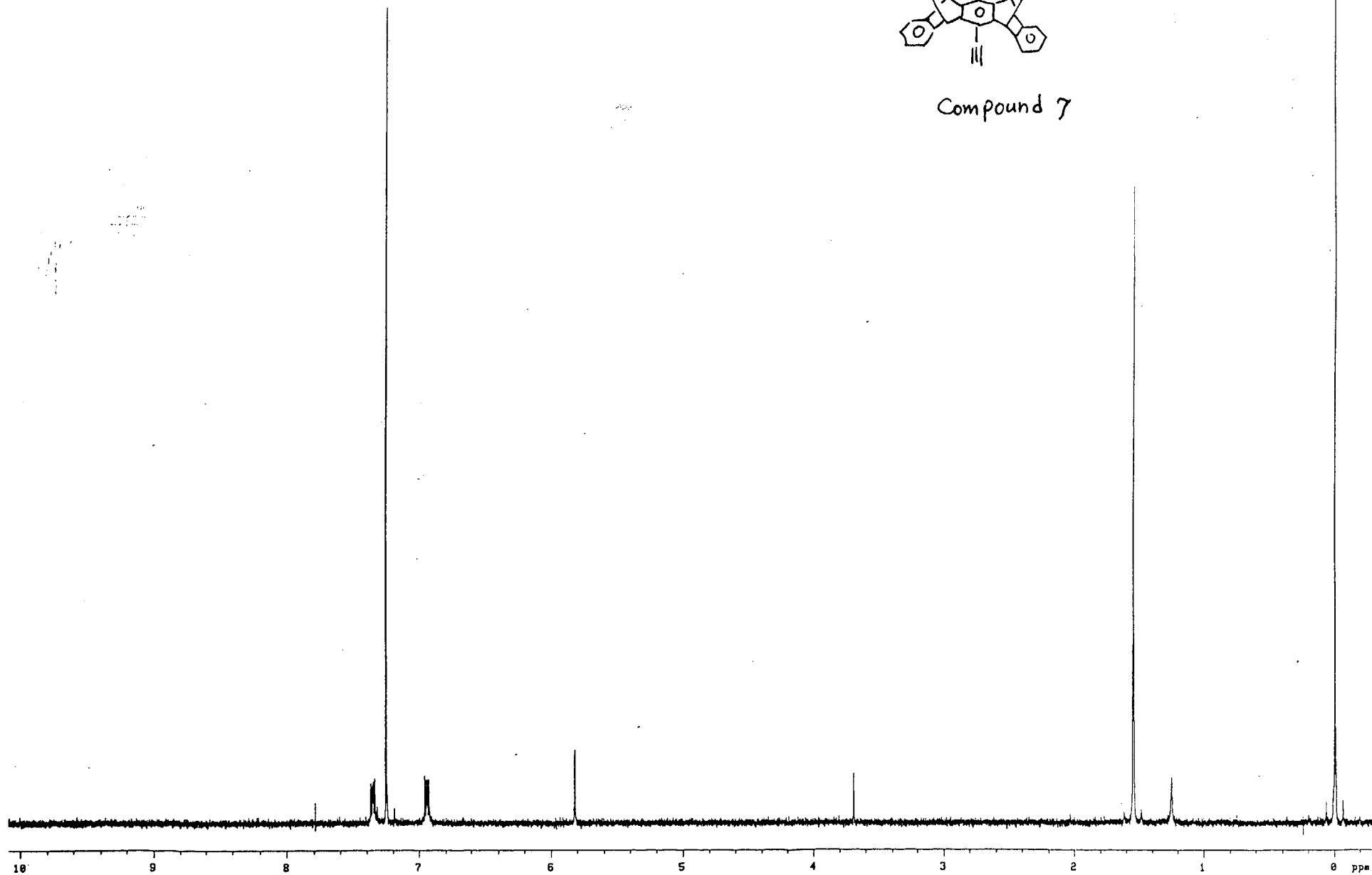






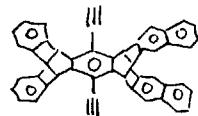
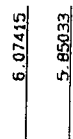




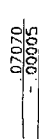
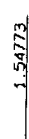


Compound 7

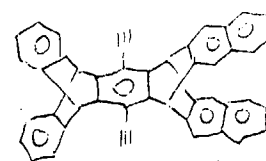
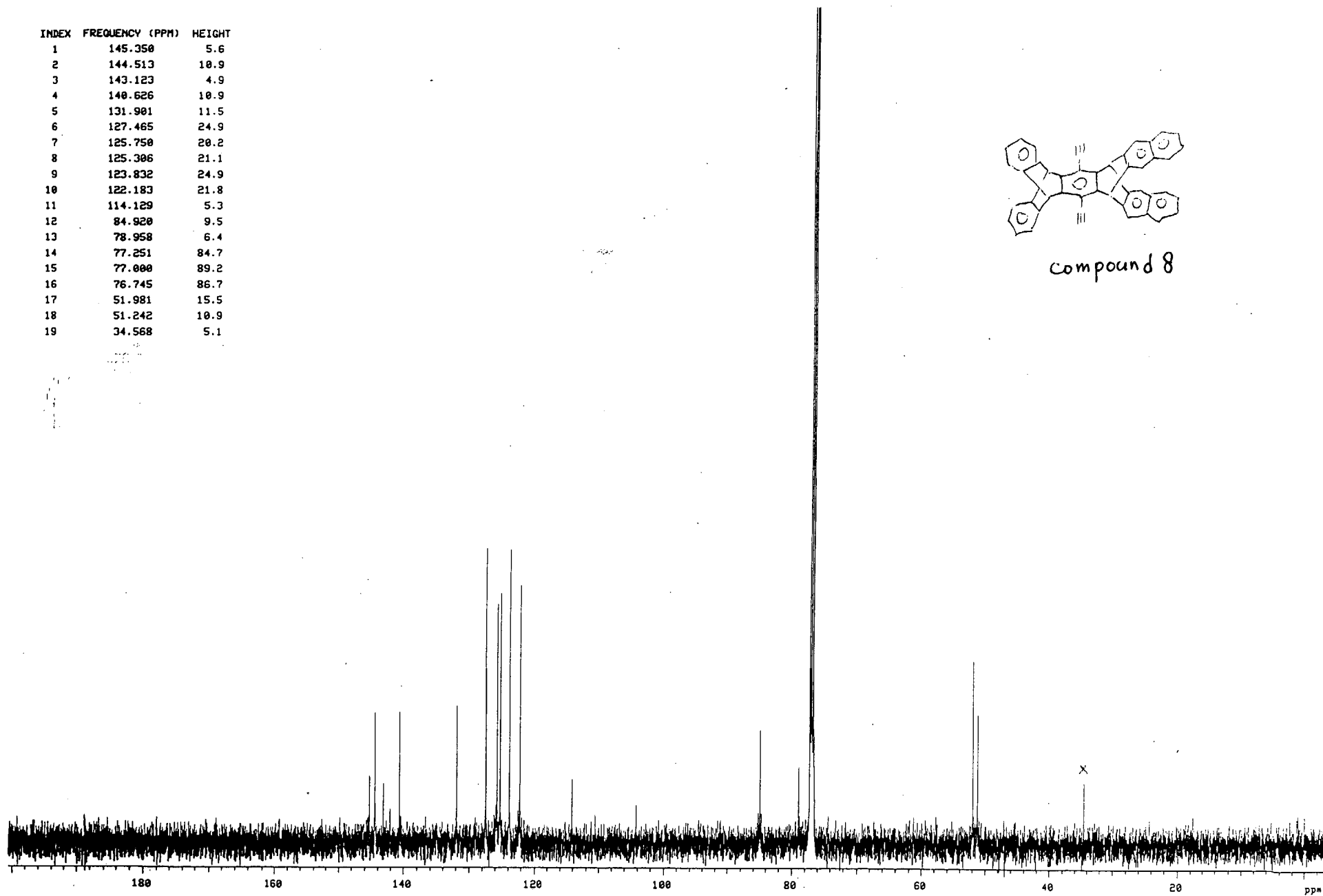
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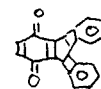
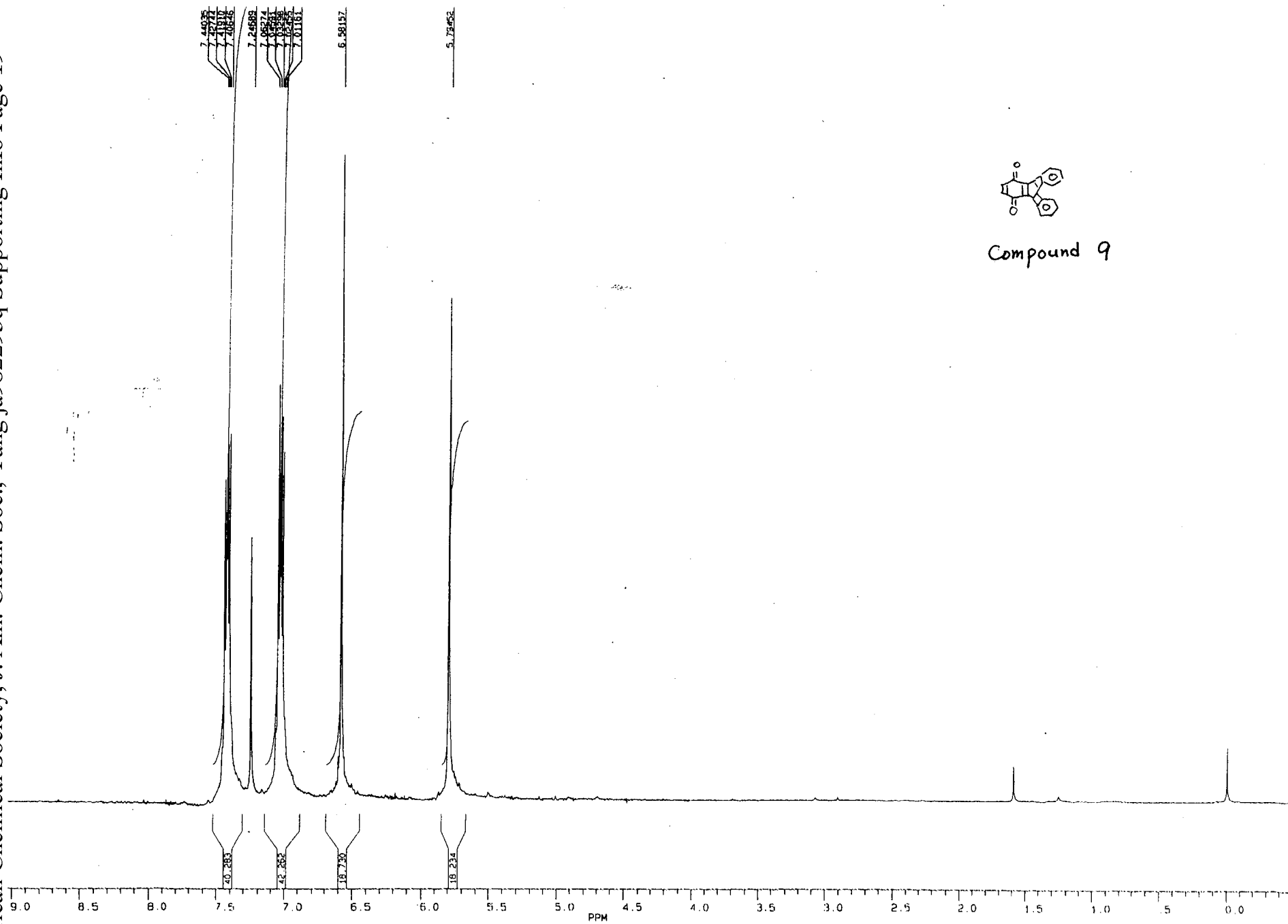
Compound 8



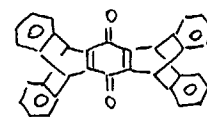
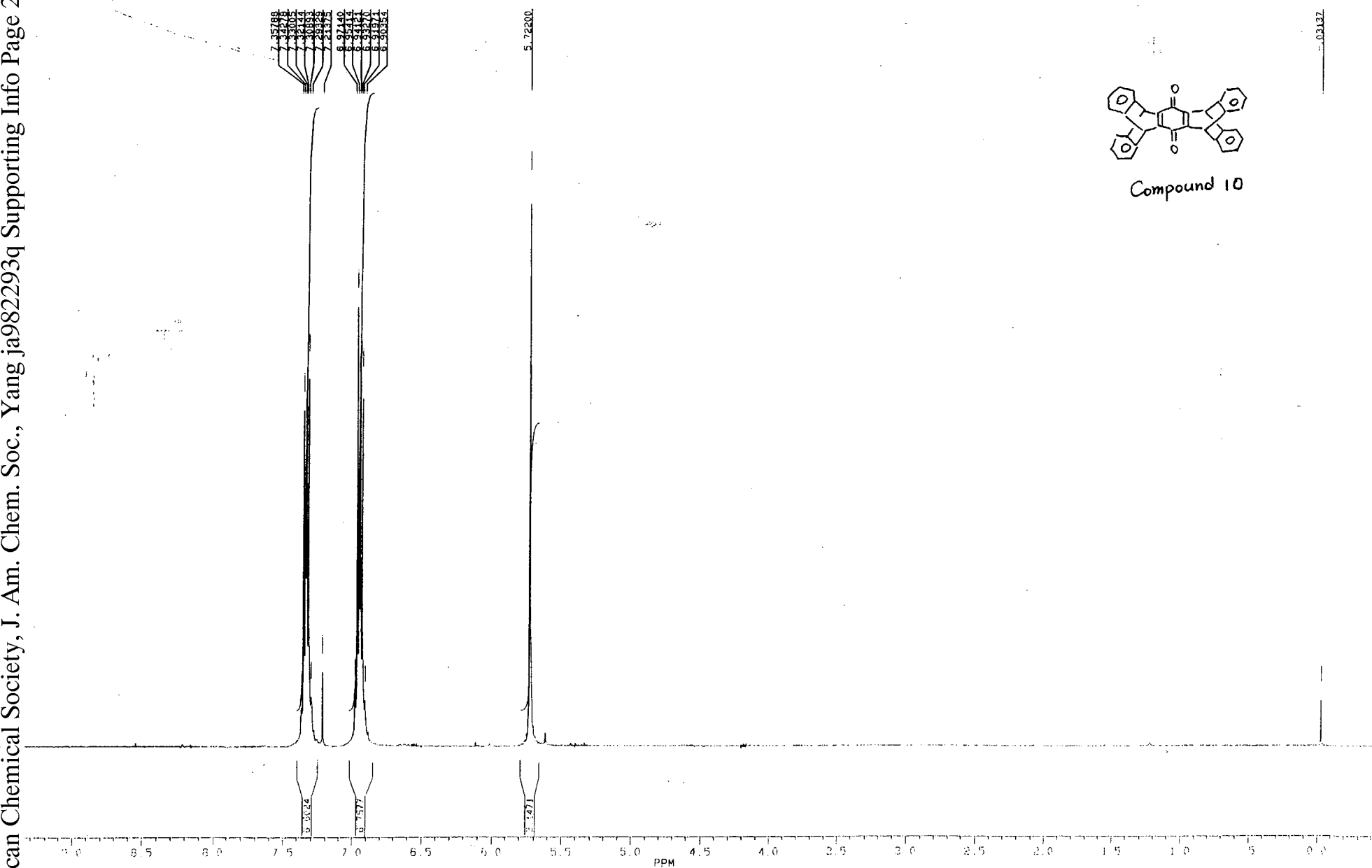
INDEX	FREQUENCY (PPM)	HEIGHT
1	145.350	5.6
2	144.513	10.9
3	143.123	4.9
4	140.626	10.9
5	131.901	11.5
6	127.465	24.9
7	125.750	20.2
8	125.306	21.1
9	123.832	24.9
10	122.183	21.8
11	114.129	5.3
12	84.920	9.5
13	78.958	6.4
14	77.251	84.7
15	77.000	89.2
16	76.745	86.7
17	51.981	15.5
18	51.242	10.9
19	34.568	5.1



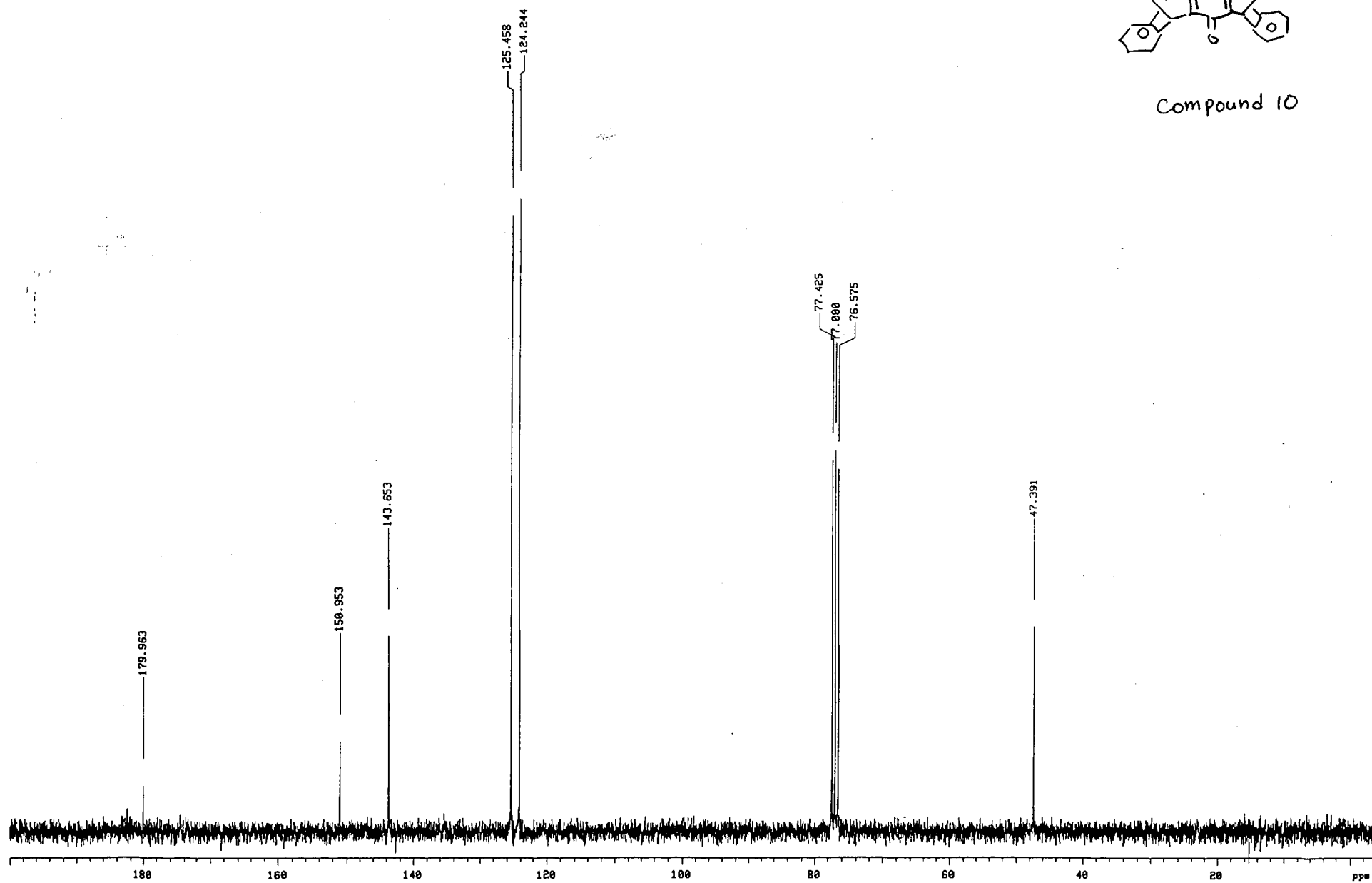
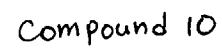
compound 8



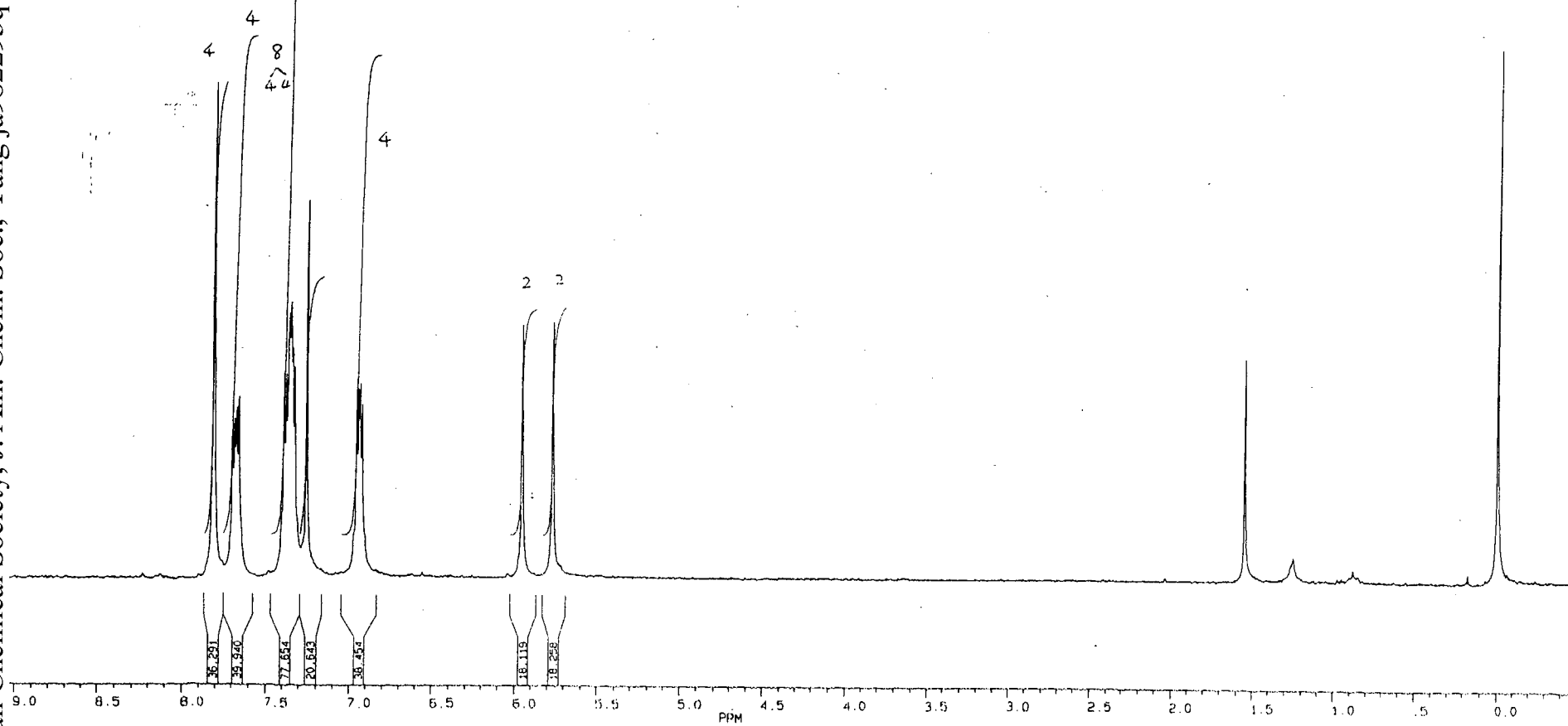
Compound 9



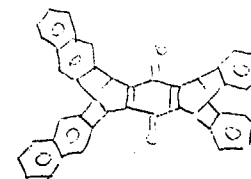
Compound 10



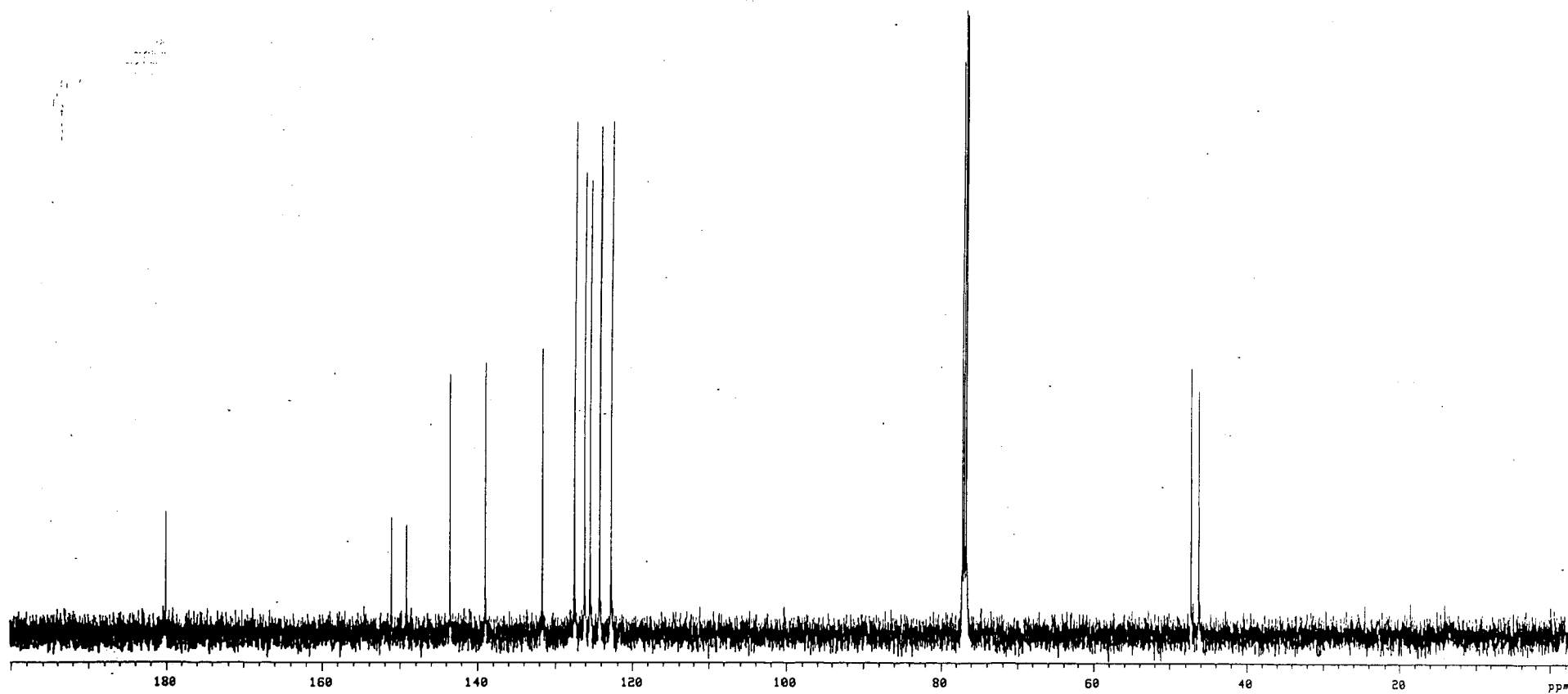
Compound II

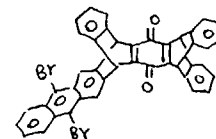
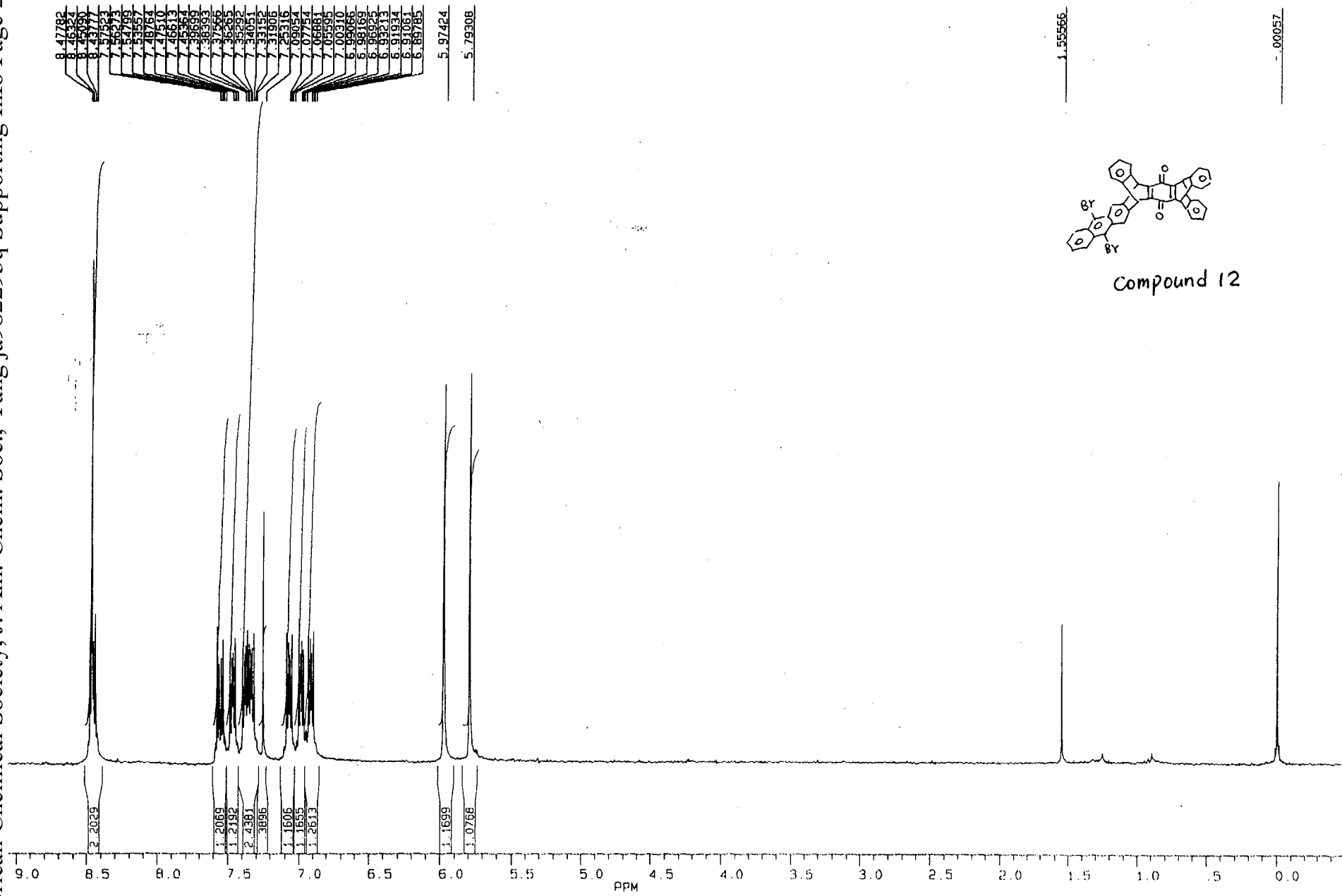


INDEX	FREQUENCY (PPM)	HEIGHT
1	180.186	6.9
2	151.163	6.6
3	149.205	6.2
4	143.545	14.9
5	139.079	15.5
6	131.679	16.4
7	127.530	29.6
8	126.180	26.6
9	125.426	26.1
10	124.232	29.3
11	122.886	29.6
12	77.255	33.1
13	77.000	36.1
14	76.745	35.8
15	47.376	15.3
16	46.343	14.0



Compound 11



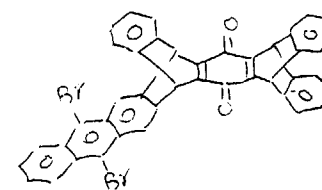


Compound 12

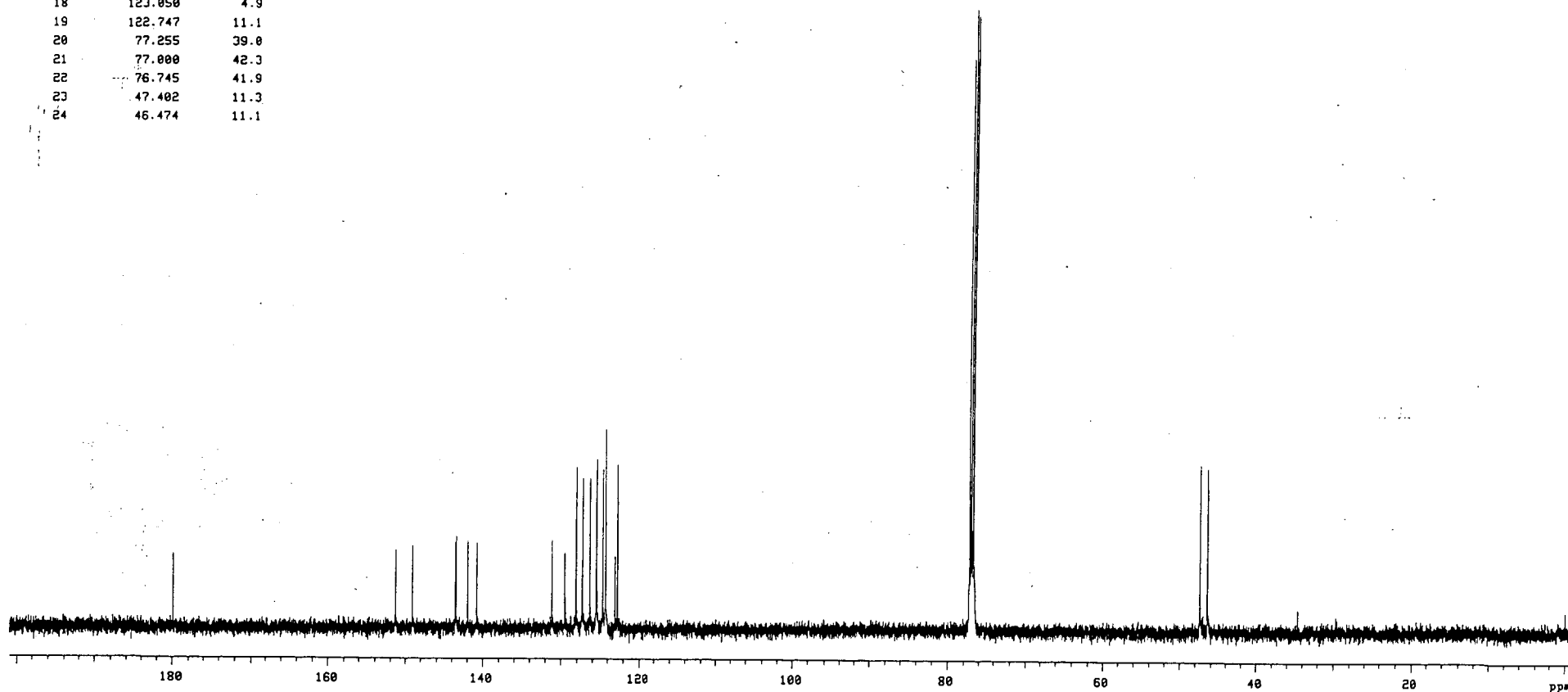
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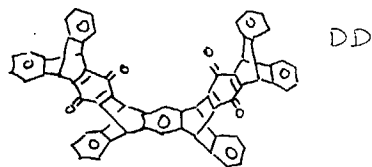
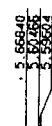
5.97424

INDEX	FREQUENCY (PPM)	HEIGHT
1	179.905	5.0
2	151.272	5.3
3	149.066	5.5
4	143.559	5.8
5	143.443	6.2
6	141.940	5.9
7	140.753	5.8
8	131.148	6.0
9	129.546	5.1
10	128.163	10.9
11	127.337	10.2
12	126.351	10.2
13	125.503	10.6
14	125.455	11.5
15	124.644	10.8
16	124.283	13.5
17	124.265	12.8
18	123.050	4.9
19	122.747	11.1
20	77.255	39.0
21	77.000	42.3
22	76.745	41.9
23	47.402	11.3
24	46.474	11.1

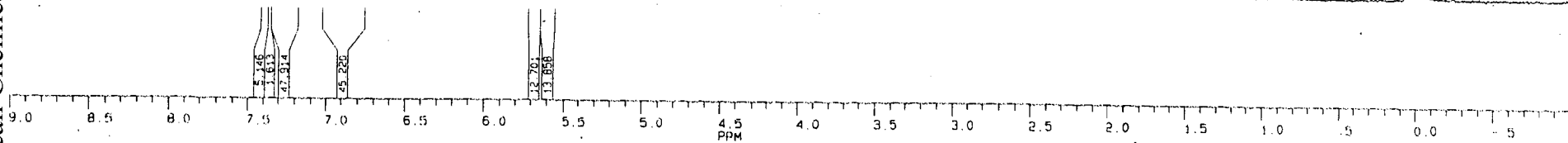
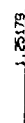
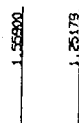


Compound 12

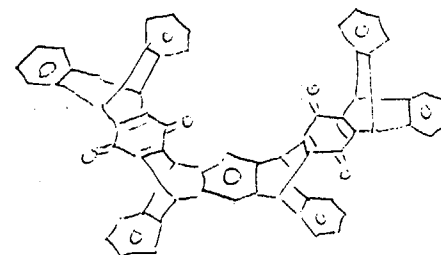




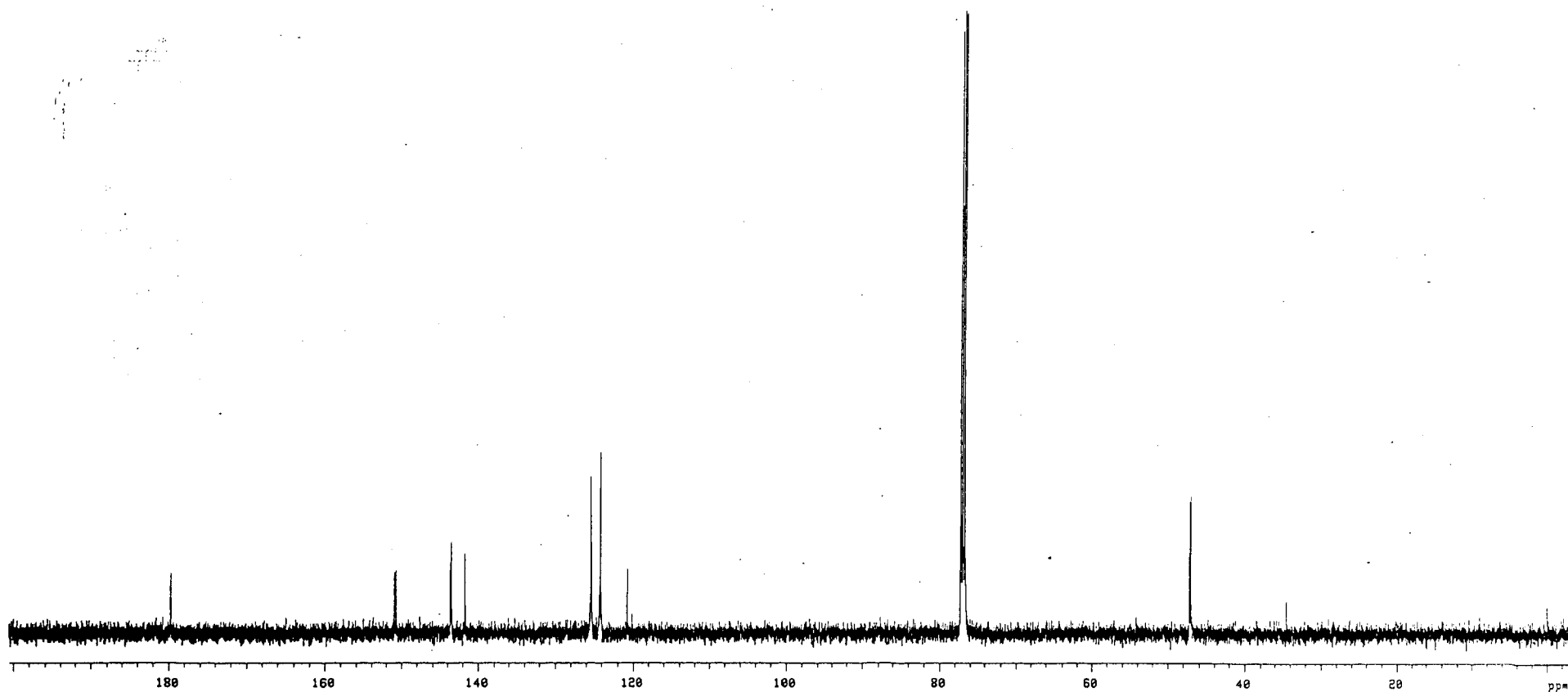
compound 13



INDEX	FREQUENCY (PPM)	HEIGHT
1	179.713	3.1
2	158.977	3.2
3	158.755	3.3
4	143.614	3.7
5	143.581	4.5
6	143.472	4.7
7	141.656	4.1
8	125.412	8.2
9	125.321	6.4
10	124.185	7.6
11	124.112	9.5
12	120.811	3.3
13	77.251	31.8
14	77.000	32.9
15	76.745	32.8
16	47.234	6.9
17	47.085	7.2



compound 13



HUMPH

7.37175
7.35905
7.35072
7.33767
7.32195

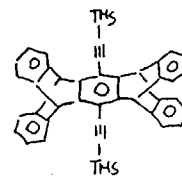
6.98158
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6.96035
6.94762

5.80019

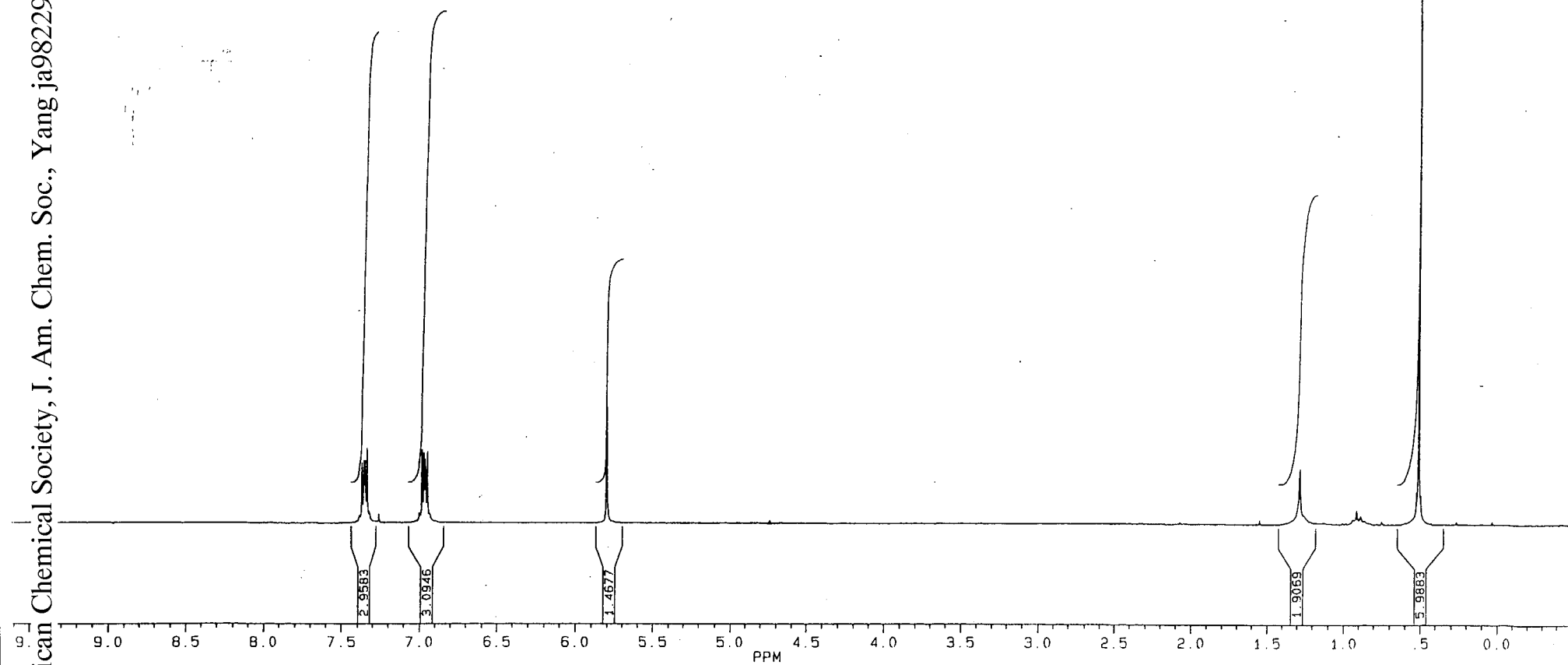
1.28370

91275

52382
51025
49862



Compound 14



III-BHM 39

144.923
144.108

125.204
123.759

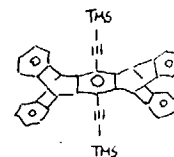
114.841

102.699
100.675

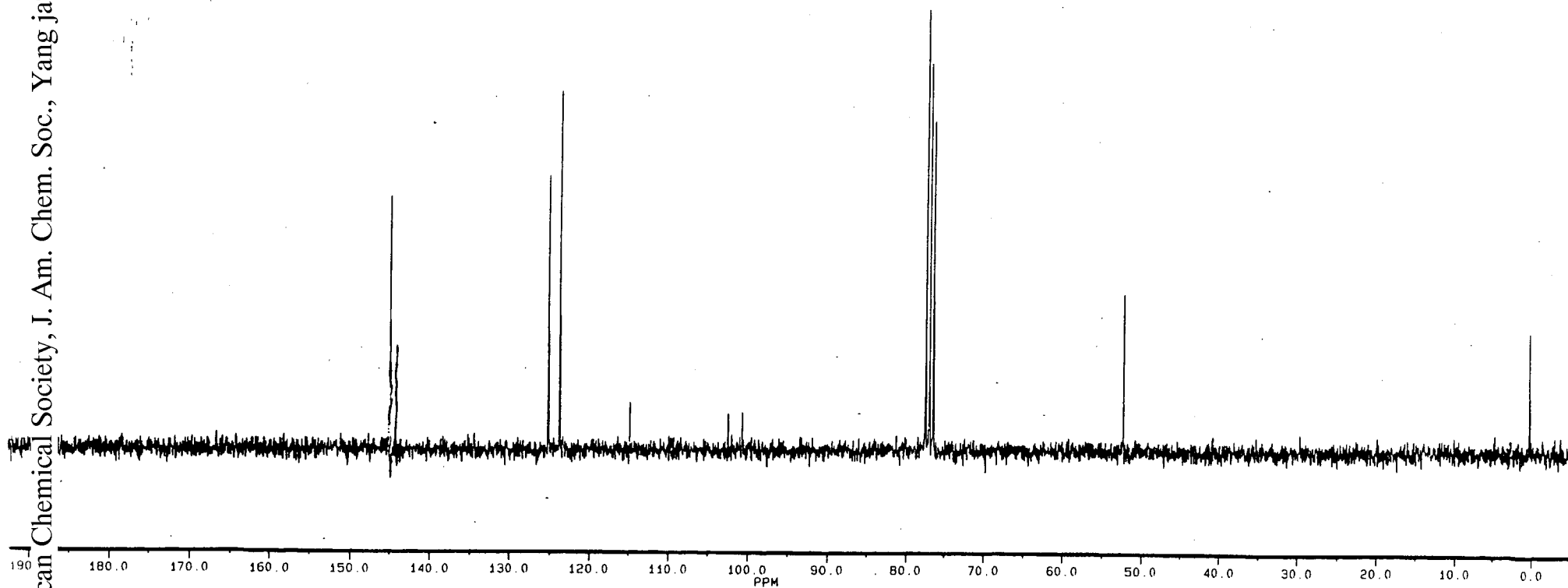
77.505
77.001
76.594

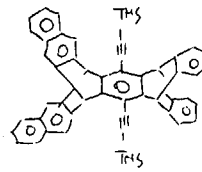
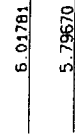
52.239

309



Compound 14

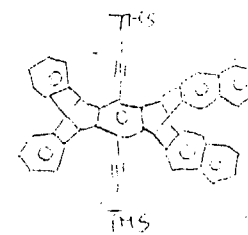
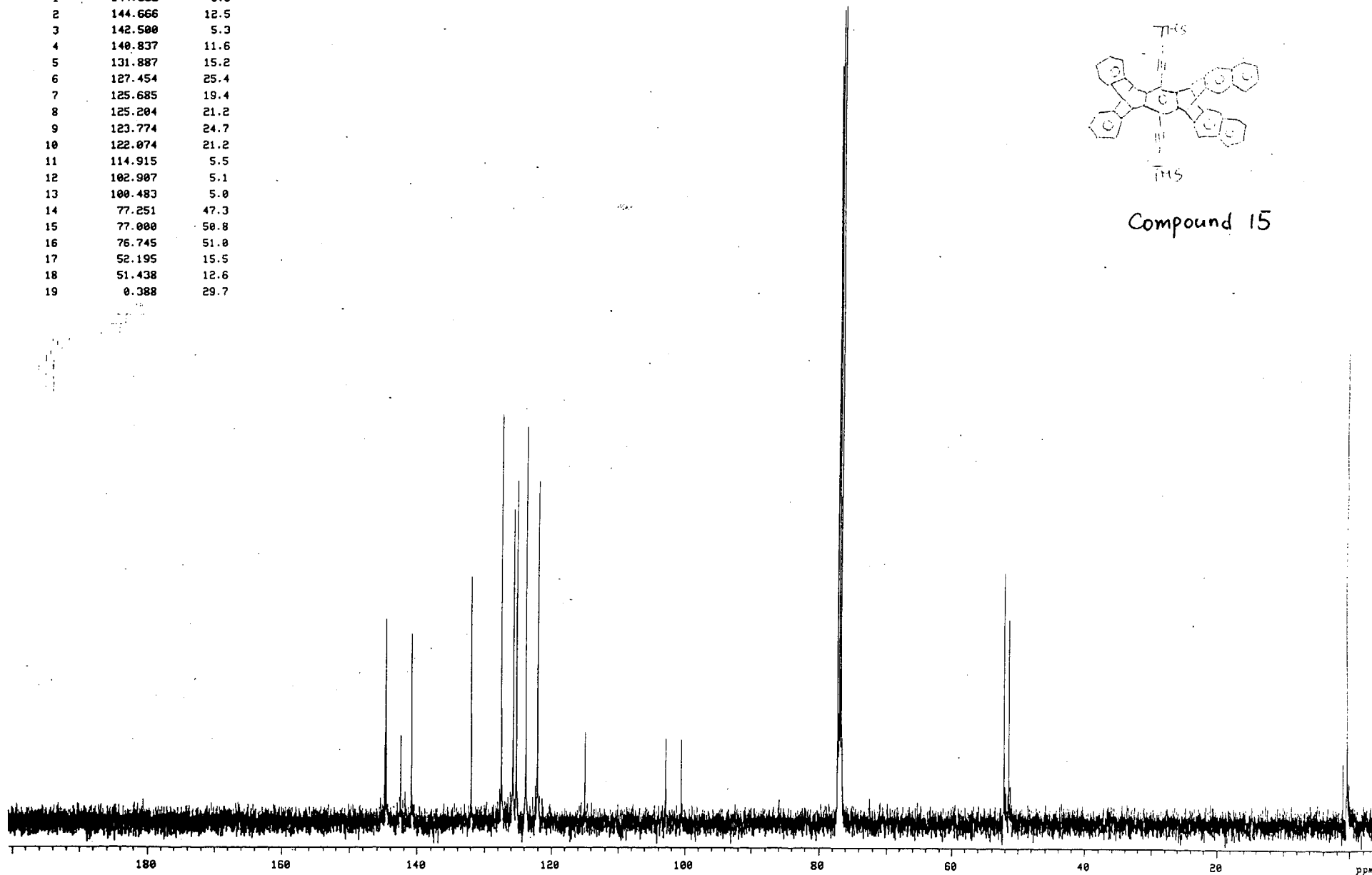




62436
56152
54834
47184

.07390
.00041

INDEX	FREQUENCY (PPM)	HEIGHT
1	144.862	5.5
2	144.666	12.5
3	142.500	5.3
4	140.837	11.6
5	131.887	15.2
6	127.454	25.4
7	125.685	19.4
8	125.204	21.2
9	123.774	24.7
10	122.074	21.2
11	114.915	5.5
12	102.907	5.1
13	100.483	5.0
14	77.251	47.3
15	77.000	50.8
16	76.745	51.0
17	52.195	15.5
18	51.438	12.6
19	0.388	29.7



Compound 15