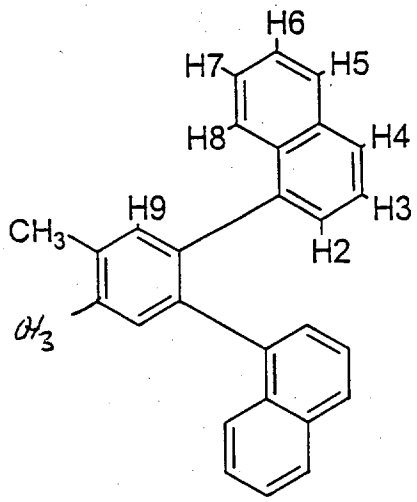
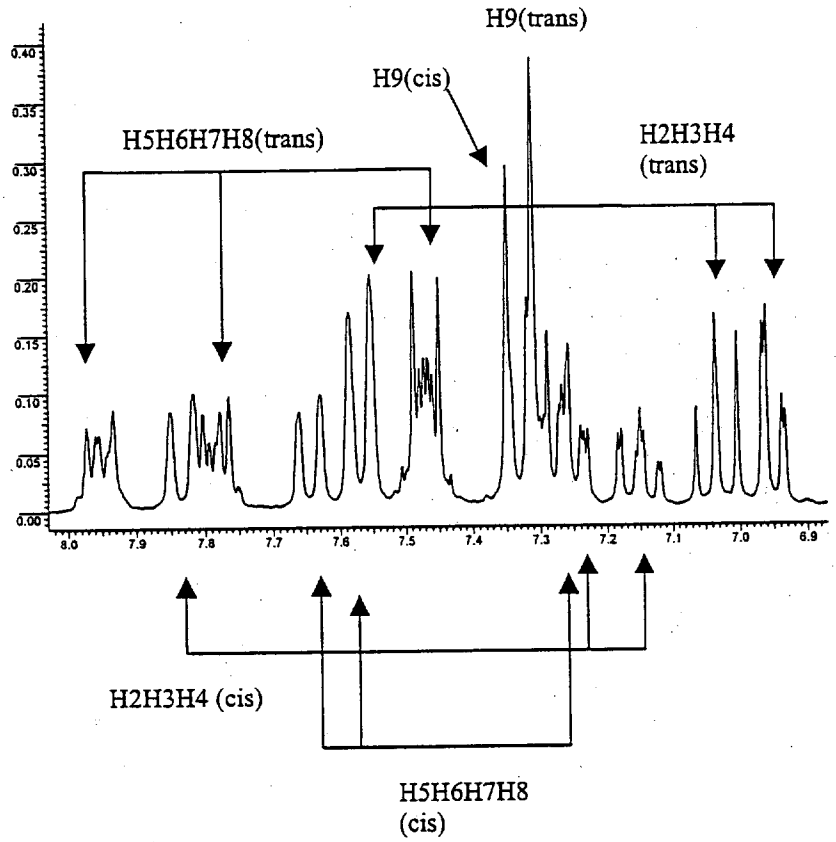
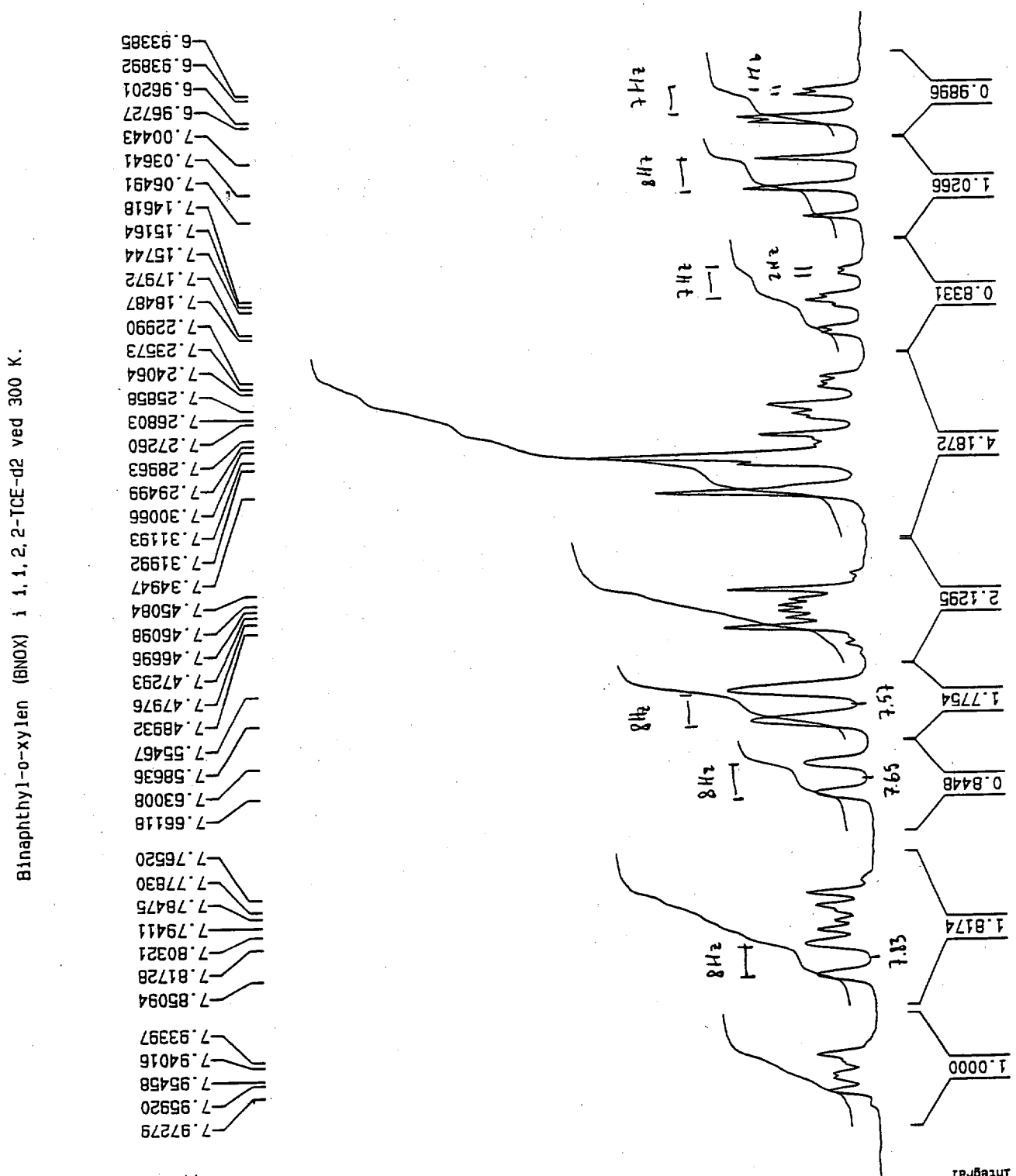
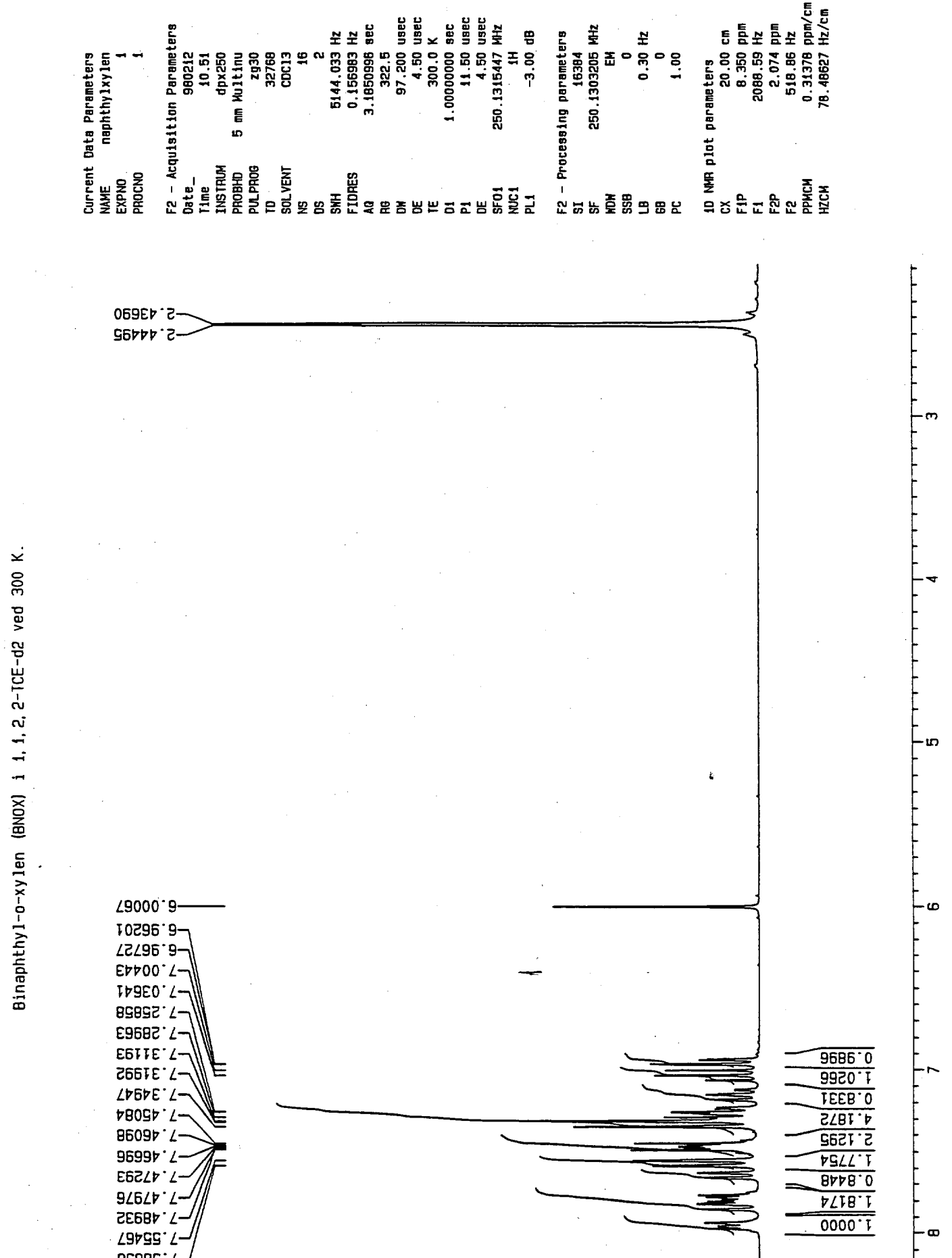
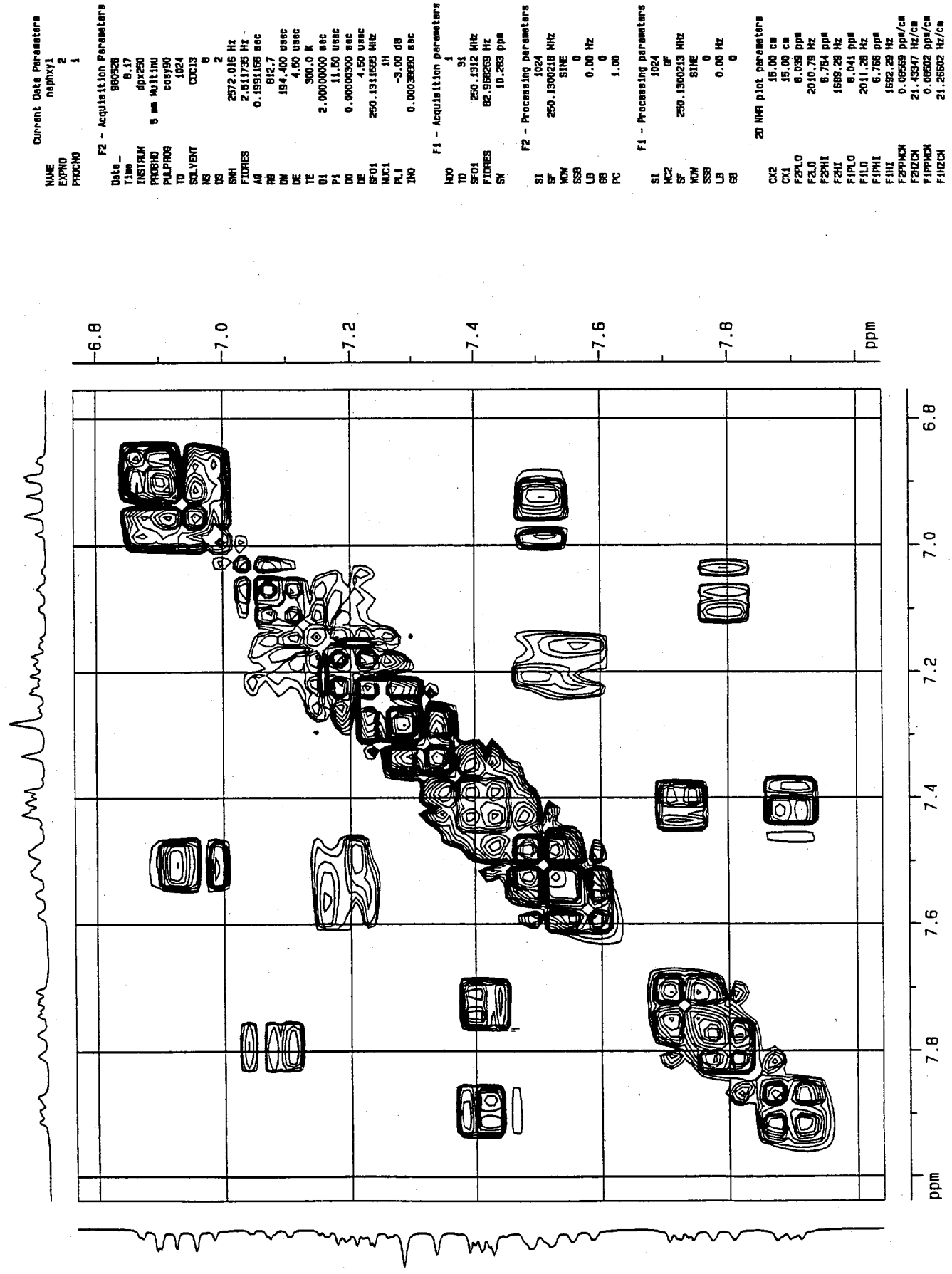
Assignment of the low field part of the 1H spectrum of 1,2-Bis(1-Naphthyl)-4,5-dimethyl-benzene (1).

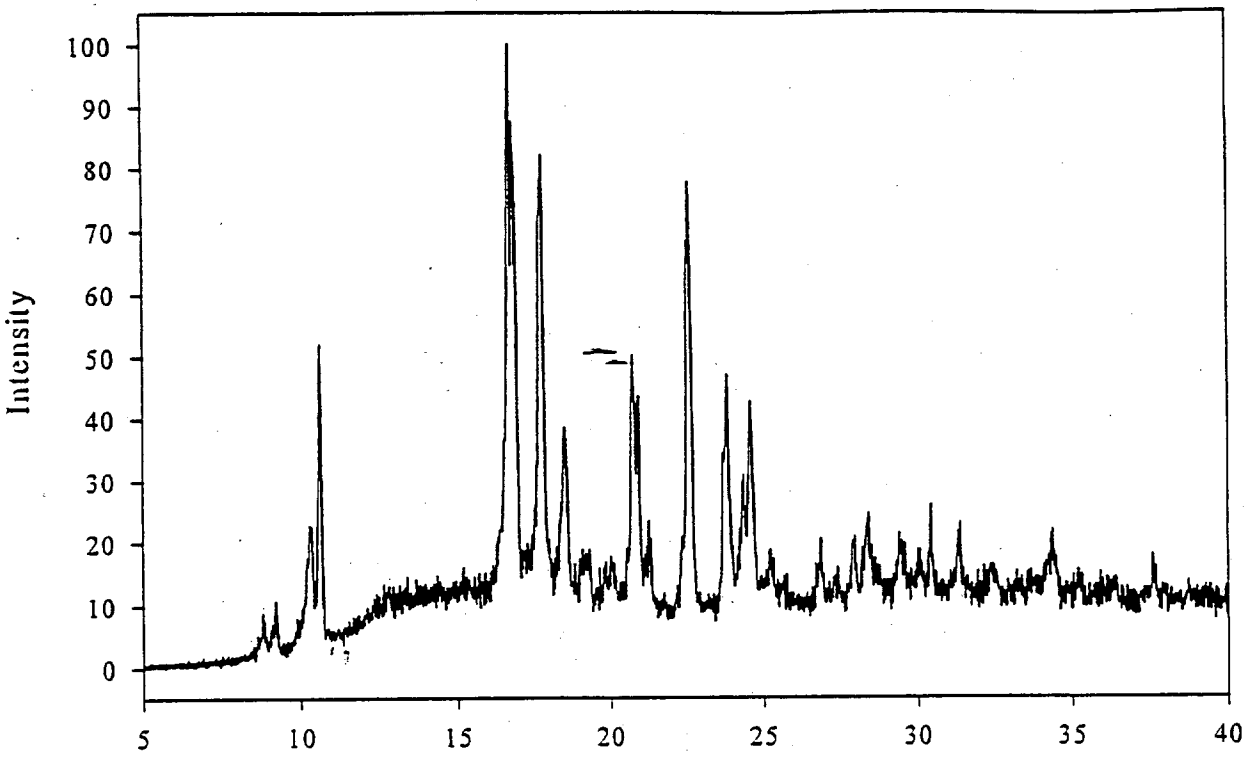


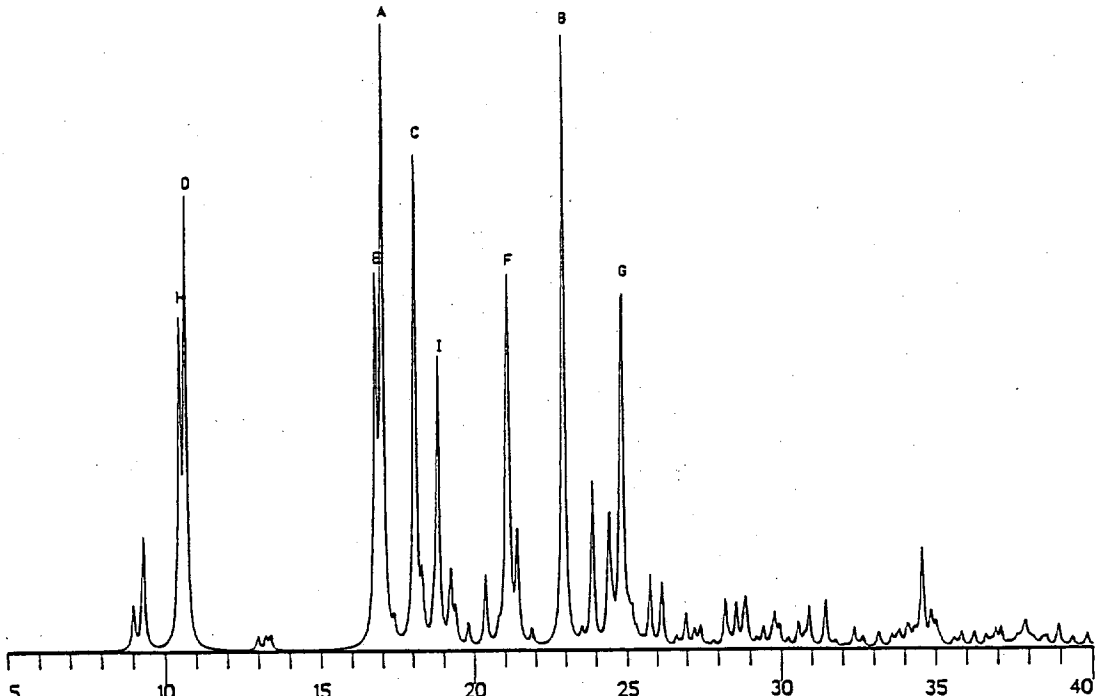








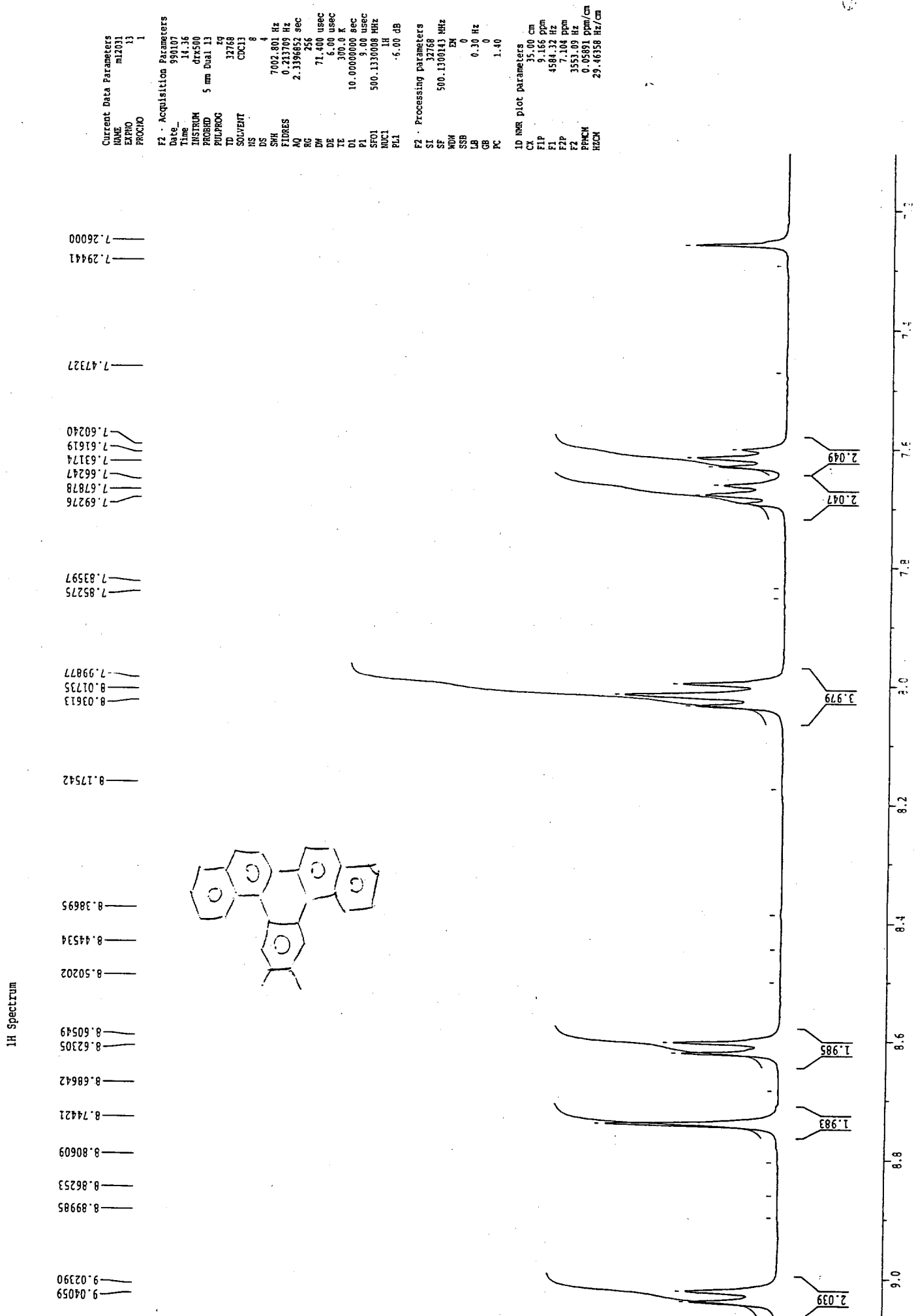




LIST OF THE 9 HIGHEST PEAKS

A.	-1	3	1	16.996	100.000	B.	2	3	0	22.927	97.516	C.	2	0	0	18.066	79.893
D.	-1	1	1	10.664	72.268	E.	-2	1	1	16.770	60.653	F.	1	3	1	21.087	60.186
G.	-3	1	1	24.829	58.349	H.	0	1	1	10.474	54.638	I.	0	0	2	18.818	46.827

Supplementary Calculated and observed powder diffractograms. Above, the powder diffractogram calculated from the single crystal data. Below, the observed powder diffractogram of the fully crystallised sample



Compound 1

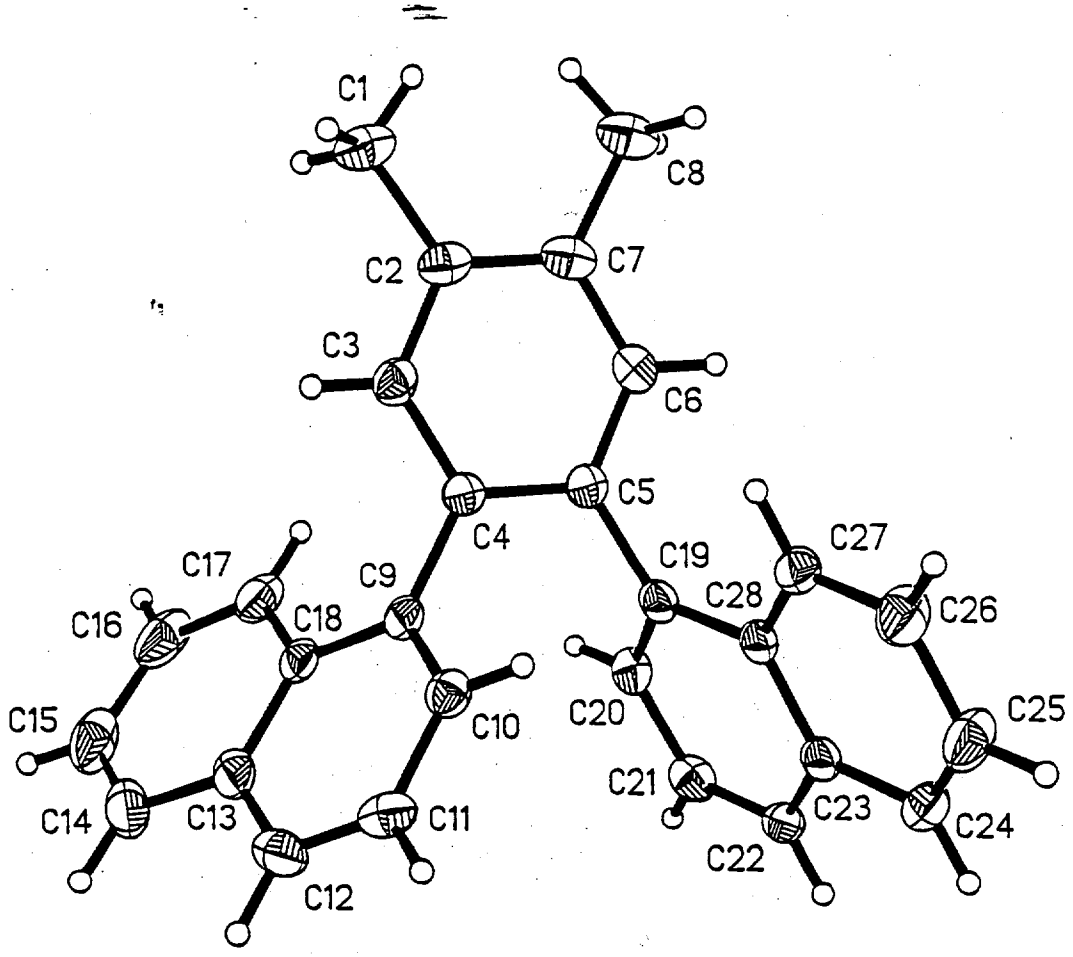

C1
C8
C2
C7
C3
C6
C5
C4
C17
C9
C19
C27
C16
C18
C28
C26
C15
C10
C20
C25
C21
C14
C13
C11
C23
C24
C22
C12

Table 1. Crystal data and structure refinement for 1.

Identification code	compound 1
Empirical formula	C28 H22
Formula weight	358.46
Temperature	120(2) K
Wavelength	0.71073 A
Crystal system	monoclinic
Space group	P2(1)/c
Unit cell dimensions	a = 11.037(2) A alpha = 90 deg. b = 18.978(4) A beta = 117.17(3) deg. c = 10.602(2) A gamma = 90 deg.
Volume, Z	1975.7(7) A^3, 4
Density (calculated)	1.205 Mg/m^3
Absorption coefficient	0.068 mm^-1
F(000)	760
Crystal size	0.37 x 0.35 x 0.25 mm
Theta range for data collection	2.07 to 26.34 deg.
Limiting indices	-13<=h<=13, -23<=k<=23, -13<=l<=12
Reflections collected	20363
Independent reflections	4029 [R(int) = 0.0305]
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	4029 / 0 / 253
Goodness-of-fit on F^2	1.035
Final R indices [I>2sigma(I)]	R1 = 0.0419, wR2 = 0.1067
R indices (all data)	R1 = 0.0562, wR2 = 0.1157
Largest diff. peak and hole	0.269 and -0.237 e.A^-3

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for 1. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
C(1)	3359(2)	4461(1)	8718(2)	36(1)
C(2)	2933(1)	4820(1)	7307(1)	27(1)
C(3)	3031(1)	4457(1)	6218(2)	25(1)
C(4)	2645(1)	4751(1)	4880(1)	22(1)
C(5)	2123(1)	5440(1)	4623(1)	22(1)
C(6)	2053(1)	5811(1)	5727(2)	26(1)
C(7)	2456(1)	5520(1)	7067(2)	28(1)
C(8)	2412(2)	5959(1)	8231(2)	38(1)
C(9)	2868(1)	4341(1)	3800(1)	21(1)
C(10)	3725(1)	4599(1)	3292(1)	24(1)
C(11)	4027(1)	4210(1)	2343(2)	29(1)
C(12)	3497(2)	3554(1)	1924(2)	33(1)
C(13)	2618(2)	3257(1)	2425(2)	30(1)
C(14)	2070(2)	2569(1)	2023(2)	43(1)
C(15)	1173(2)	2304(1)	2449(2)	52(1)
C(16)	758(2)	2716(1)	3285(2)	46(1)
C(17)	1287(2)	3376(1)	3726(2)	33(1)
C(18)	2261(1)	3662(1)	3340(1)	24(1)
C(19)	1605(1)	5758(1)	3179(1)	22(1)
C(20)	409(1)	5511(1)	2103(2)	25(1)
C(21)	-108(1)	5774(1)	706(2)	26(1)
C(22)	591(1)	6280(1)	391(1)	24(1)
C(23)	1832(1)	6552(1)	1461(1)	23(1)
C(24)	2581(2)	7072(1)	1152(2)	29(1)
C(25)	3779(2)	7328(1)	2185(2)	37(1)
C(26)	4295(2)	7076(1)	3592(2)	33(1)
C(27)	3599(1)	6573(1)	3928(2)	26(1)
C(28)	2348(1)	6297(1)	2881(1)	22(1)

Table 3. Bond lengths [A] and angles [deg] for 1.

C(1)-C(2)	1.510(2)
C(2)-C(3)	1.391(2)
C(2)-C(7)	1.409(2)
C(3)-C(4)	1.3986(19)
C(4)-C(5)	1.4048(19)
C(4)-C(9)	1.4950(18)
C(5)-C(6)	1.3981(19)
C(5)-C(19)	1.4954(19)
C(6)-C(7)	1.394(2)
C(7)-C(8)	1.508(2)
C(9)-C(10)	1.3748(19)
C(9)-C(18)	1.4308(19)
C(10)-C(11)	1.406(2)
C(11)-C(12)	1.360(2)
C(12)-C(13)	1.418(2)
C(13)-C(14)	1.421(2)
C(13)-C(18)	1.427(2)
C(14)-C(15)	1.359(3)
C(15)-C(16)	1.406(3)
C(16)-C(17)	1.370(2)
C(17)-C(18)	1.421(2)
C(19)-C(20)	1.374(2)
C(19)-C(28)	1.4325(19)
C(20)-C(21)	1.413(2)
C(21)-C(22)	1.364(2)
C(22)-C(23)	1.419(2)
C(23)-C(24)	1.418(2)
C(23)-C(28)	1.4294(19)
C(24)-C(25)	1.364(2)
C(25)-C(26)	1.415(2)
C(26)-C(27)	1.370(2)
C(27)-C(28)	1.419(2)
C(3)-C(2)-C(7)	118.80(13)
C(3)-C(2)-C(1)	119.49(14)
C(7)-C(2)-C(1)	121.71(13)
C(2)-C(3)-C(4)	122.76(13)
C(3)-C(4)-C(5)	118.47(12)
C(3)-C(4)-C(9)	119.21(12)
C(5)-C(4)-C(9)	122.23(12)
C(6)-C(5)-C(4)	118.75(12)
C(6)-C(5)-C(19)	120.87(12)
C(4)-C(5)-C(19)	120.33(12)
C(7)-C(6)-C(5)	122.67(13)
C(6)-C(7)-C(2)	118.48(13)
C(6)-C(7)-C(8)	120.02(14)
C(2)-C(7)-C(8)	121.48(13)
C(10)-C(9)-C(18)	119.12(12)
C(10)-C(9)-C(4)	119.82(12)
C(18)-C(9)-C(4)	120.97(12)
C(9)-C(10)-C(11)	121.56(13)
C(12)-C(11)-C(10)	120.47(13)
C(11)-C(12)-C(13)	120.45(13)
C(12)-C(13)-C(14)	121.52(15)
C(12)-C(13)-C(18)	119.32(13)

C(14)-C(13)-C(18)		119.15(15)
C(15)-C(14)-C(13)		121.05(17)
C(14)-C(15)-C(16)		119.98(15)
C(17)-C(16)-C(15)		120.85(17)
C(16)-C(17)-C(18)		120.77(16)
C(17)-C(18)-C(13)		118.03(13)
C(17)-C(18)-C(9)		122.99(13)
C(13)-C(18)-C(9)		118.97(13)
C(20)-C(19)-C(28)		119.37(12)
C(20)-C(19)-C(5)	=	119.02(12)
C(28)-C(19)-C(5)		121.59(12)
C(19)-C(20)-C(21)		121.61(13)
C(22)-C(21)-C(20)		120.15(13)
C(21)-C(22)-C(23)		120.54(12)
C(24)-C(23)-C(22)		121.41(12)
C(24)-C(23)-C(28)		119.04(13)
C(22)-C(23)-C(28)		119.55(13)
C(25)-C(24)-C(23)		121.04(13)
C(24)-C(25)-C(26)		120.12(14)
C(27)-C(26)-C(25)		120.42(14)
C(26)-C(27)-C(28)		120.94(13)
C(27)-C(28)-C(23)		118.43(12)
C(27)-C(28)-C(19)		122.77(12)
C(23)-C(28)-C(19)		118.76(12)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters (A^2 x 10^3) for 1. The anisotropic displacement factor exponent takes the form: -2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
C(1)	35(1)	49(1)	22(1)	2(1)	13(1)	-8(1)
C(2)	23(1)	37(1)	21(1)	0(1)	10(1)	-8(1)
C(3)	26(1)	26(1)	25(1)	2(1)	11(1)	-3(1)
C(4)	21(1)	23(1)	21(1)	-1(1)	9(1)	-4(1)
C(5)	21(1)	23(1)	22(1)	-1(1)	9(1)	-4(1)
C(6)	25(1)	26(1)	28(1)	-3(1)	12(1)	-1(1)
C(7)	22(1)	38(1)	25(1)	-7(1)	12(1)	-7(1)
C(8)	37(1)	50(1)	30(1)	-11(1)	18(1)	-5(1)
C(9)	21(1)	21(1)	18(1)	3(1)	6(1)	3(1)
C(10)	22(1)	25(1)	21(1)	2(1)	7(1)	1(1)
C(11)	22(1)	43(1)	22(1)	5(1)	10(1)	8(1)
C(12)	33(1)	39(1)	21(1)	-1(1)	8(1)	16(1)
C(13)	34(1)	24(1)	19(1)	2(1)	1(1)	8(1)
C(14)	56(1)	24(1)	29(1)	-2(1)	2(1)	8(1)
C(15)	70(1)	22(1)	35(1)	1(1)	0(1)	-11(1)
C(16)	54(1)	38(1)	32(1)	9(1)	7(1)	-20(1)
C(17)	39(1)	30(1)	24(1)	5(1)	9(1)	-9(1)
C(18)	27(1)	21(1)	18(1)	5(1)	5(1)	3(1)
C(19)	23(1)	19(1)	22(1)	-1(1)	10(1)	4(1)
C(20)	24(1)	23(1)	28(1)	0(1)	10(1)	0(1)
C(21)	21(1)	28(1)	24(1)	-4(1)	5(1)	1(1)
C(22)	26(1)	24(1)	20(1)	1(1)	9(1)	7(1)
C(23)	26(1)	20(1)	23(1)	0(1)	11(1)	5(1)
C(24)	35(1)	27(1)	25(1)	5(1)	12(1)	0(1)
C(25)	39(1)	33(1)	36(1)	7(1)	14(1)	-10(1)
C(26)	31(1)	31(1)	30(1)	2(1)	7(1)	-9(1)
C(27)	28(1)	25(1)	22(1)	1(1)	8(1)	-1(1)
C(28)	24(1)	18(1)	23(1)	0(1)	10(1)	3(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for 1.

	x	y	z	U(eq)
H(1A)	3232	4778	9354	54
H(1B)	4302	4330	9113	54
H(1C)	2815	4047	8586	54
H(1D)	3667	3992	8681	54
H(1E)	2597	4440	8922	54
H(1F)	4085	4723	9449	54
H(3)	3368	3999	6387	30
H(6)	1724	6271	5561	31
H(8A)	2722	5682	9080	57
H(8B)	1494	6112	7947	57
H(8C)	2991	6363	8408	57
H(8D)	2082	6422	7877	57
H(8E)	3310	5993	9010	57
H(8F)	1814	5741	8548	57
H(10)	4113	5042	3582	28
H(11)	4594	4402	1999	35
H(12)	3713	3298	1305	39
H(14)	2330	2295	1460	52
H(15)	833	1850	2187	62
H(16)	116	2538	3541	55
H(17)	1005	3639	4284	39
H(20)	-73	5163	2300	30
H(21)	-925	5602	0	32
H(22)	250	6447	-533	29
H(24)	2249	7242	231	35
H(25)	4259	7668	1964	45
H(26)	5111	7253	4293	40
H(27)	3952	6410	4856	32

Compound 2

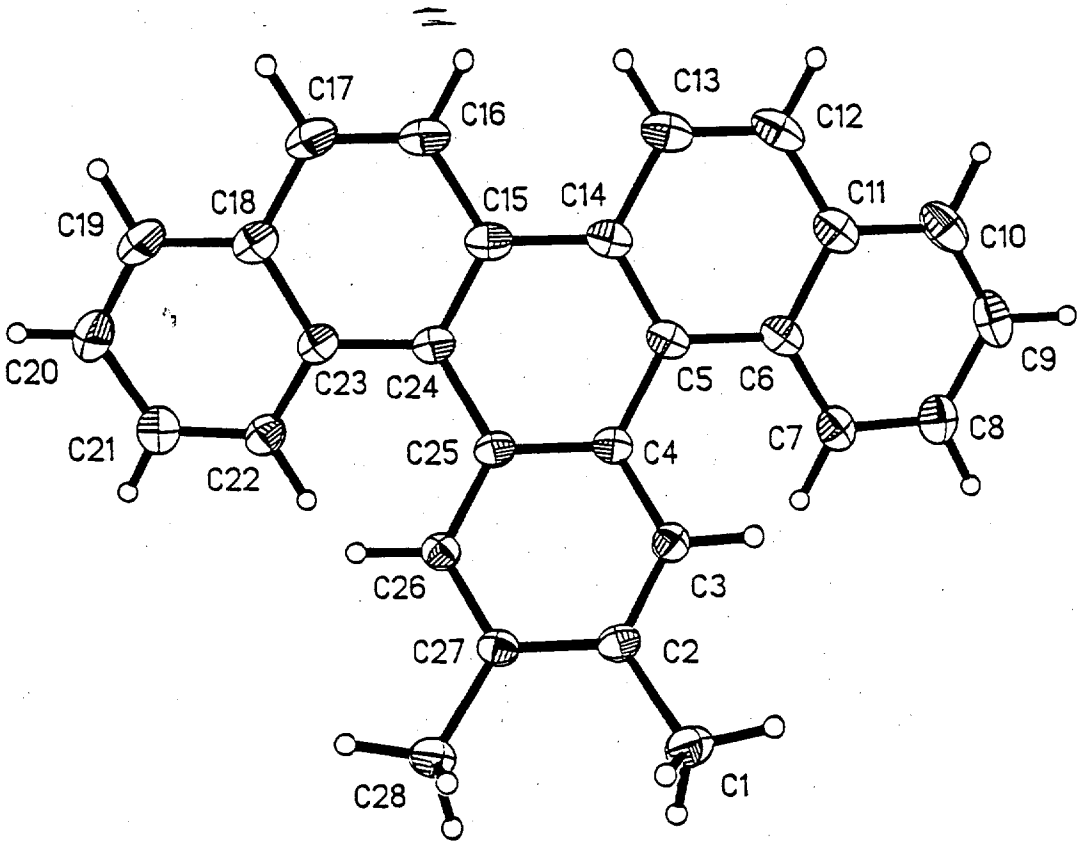

C17
C16
C13
C12
C18
C15
C14
C11
C19
C10
C20
C23
C24
C5
C6
C9
C21
C22
C25
C4
C7
C8
C26
C3
C27
C2
C28
C1

Table 6. Crystal data and structure refinement for 2.

Identification code	compound 2
Empirical formula	C28 H20
Formula weight	356.44
Temperature	120(2) K
Wavelength	0.71073 A
Crystal system	monoclinic
Space group	P2(1)/n
Unit cell dimensions	a = 12.024(2) A alpha = 90 deg. b = 7.5310(15) A beta = 99.62(3) deg. c = 19.962(4) A gamma = 90 deg.
Volume, Z	1782.2(6) A^3, 4
Density (calculated)	1.328 Mg/m^3
Absorption coefficient	0.075 mm^-1
F(000)	752
Crystal size	0.30 x 0.20 x 0.05 mm
Theta range for data collection	1.85 to 26.39 deg.
Limiting indices	-15<=h<=15, -9<=k<=9, -24<=l<=24
Reflections collected	18257
Independent reflections	3649 [R(int) = 0.0584]
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	3649 / 0 / 333
Goodness-of-fit on F^2	1.039
Final R indices [I>2sigma(I)]	R1 = 0.0484, wR2 = 0.1077
R indices (all data)	R1 = 0.0866, wR2 = 0.1278
Largest diff. peak and hole	0.200 and -0.236 e.A^-3

Table 7. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for 2. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
C(1)	6372(2)	1046(3)	564(1)	29(1)
C(2)	6450(2)	1568(2)	1294(1)	22(1)
C(3)	7488(2)	1783(2)	1698(1)	21(1)
C(4)	7625(1)	2161(2)	2397(1)	20(1)
C(5)	8731(1)	2140(2)	2826(1)	21(1)
C(6)	9766(1)	2534(2)	2575(1)	23(1)
C(7)	9803(2)	3469(2)	1966(1)	24(1)
C(8)	10809(2)	3874(3)	1760(1)	29(1)
C(9)	11835(2)	3320(3)	2147(1)	34(1)
C(10)	11833(2)	2455(3)	2747(1)	33(1)
C(11)	10818(2)	2091(2)	2988(1)	26(1)
C(12)	10819(2)	1372(3)	3642(1)	31(1)
C(13)	9852(2)	1207(3)	3901(1)	29(1)
C(14)	8780(2)	1631(2)	3504(1)	23(1)
C(15)	7764(2)	1644(2)	3810(1)	25(1)
C(16)	7774(2)	1076(3)	4494(1)	29(1)
C(17)	6856(2)	1234(3)	4800(1)	32(1)
C(18)	5870(2)	2128(2)	4472(1)	27(1)
C(19)	4950(2)	2463(3)	4812(1)	33(1)
C(20)	4054(2)	3460(3)	4513(1)	34(1)
C(21)	4058(2)	4215(3)	3874(1)	29(1)
C(22)	4919(2)	3855(2)	3522(1)	24(1)
C(23)	5833(2)	2743(2)	3794(1)	22(1)
C(24)	6750(1)	2298(2)	3436(1)	21(1)
C(25)	6642(1)	2305(2)	2698(1)	20(1)
C(26)	5585(2)	2119(2)	2275(1)	21(1)
C(27)	5469(1)	1752(2)	1588(1)	21(1)
C(28)	4318(2)	1430(3)	1179(1)	27(1)

Table 8. Bond lengths [A] and angles [deg] for 2.

C(1)-C(2)	1.497(3)
C(2)-C(3)	1.378(2)
C(2)-C(27)	1.410(2)
C(3)-C(4)	1.407(2)
C(4)-C(25)	1.417(2)
C(4)-C(5)	1.457(2)
C(5)-C(14)	1.399(3)
C(5)-C(6)	1.448(3)
C(6)-C(7)	1.412(3)
C(6)-C(11)	1.428(2)
C(7)-C(8)	1.376(3)
C(8)-C(9)	1.407(3)
C(9)-C(10)	1.364(3)
C(10)-C(11)	1.412(3)
C(11)-C(12)	1.413(3)
C(12)-C(13)	1.355(3)
C(13)-C(14)	1.431(2)
C(14)-C(15)	1.454(3)
C(15)-C(24)	1.407(2)
C(15)-C(16)	1.431(3)
C(16)-C(17)	1.351(3)
C(17)-C(18)	1.425(3)
C(18)-C(19)	1.414(3)
C(18)-C(23)	1.424(2)
C(19)-C(20)	1.365(3)
C(20)-C(21)	1.398(3)
C(21)-C(22)	1.372(3)
C(22)-C(23)	1.416(2)
C(23)-C(24)	1.449(2)
C(24)-C(25)	1.457(2)
C(25)-C(26)	1.411(2)
C(26)-C(27)	1.382(2)
C(27)-C(28)	1.505(3)
C(3)-C(2)-C(27)	118.94(16)
C(3)-C(2)-C(1)	120.25(17)
C(27)-C(2)-C(1)	120.72(16)
C(2)-C(3)-C(4)	123.22(17)
C(3)-C(4)-C(25)	118.02(16)
C(3)-C(4)-C(5)	121.59(16)
C(25)-C(4)-C(5)	119.73(15)
C(14)-C(5)-C(6)	119.40(16)
C(14)-C(5)-C(4)	117.26(16)
C(6)-C(5)-C(4)	123.27(16)
C(7)-C(6)-C(11)	117.48(17)
C(7)-C(6)-C(5)	123.48(16)
C(11)-C(6)-C(5)	118.84(17)
C(8)-C(7)-C(6)	121.59(18)
C(7)-C(8)-C(9)	120.3(2)
C(10)-C(9)-C(8)	119.67(19)
C(9)-C(10)-C(11)	121.32(19)
C(10)-C(11)-C(12)	121.38(17)
C(10)-C(11)-C(6)	119.43(18)
C(12)-C(11)-C(6)	119.12(17)
C(13)-C(12)-C(11)	121.24(18)

C(12)-C(13)-C(14)	121.32(19)
C(5)-C(14)-C(13)	118.97(18)
C(5)-C(14)-C(15)	120.12(16)
C(13)-C(14)-C(15)	120.79(17)
C(24)-C(15)-C(16)	118.60(17)
C(24)-C(15)-C(14)	119.66(16)
C(16)-C(15)-C(14)	121.69(17)
C(17)-C(16)-C(15)	121.83(18)
C(16)-C(17)-C(18)	120.91(18)
C(19)-C(18)-C(23)	119.68(18)
C(19)-C(18)-C(17)	121.46(18)
C(23)-C(18)-C(17)	118.83(17)
C(20)-C(19)-C(18)	120.84(19)
C(19)-C(20)-C(21)	119.9(2)
C(22)-C(21)-C(20)	120.3(2)
C(21)-C(22)-C(23)	121.68(18)
C(22)-C(23)-C(18)	117.10(17)
C(22)-C(23)-C(24)	123.65(16)
C(18)-C(23)-C(24)	119.14(16)
C(15)-C(24)-C(23)	118.91(16)
C(15)-C(24)-C(25)	117.35(16)
C(23)-C(24)-C(25)	123.39(16)
C(26)-C(25)-C(4)	118.00(16)
C(26)-C(25)-C(24)	121.65(16)
C(4)-C(25)-C(24)	119.30(15)
C(27)-C(26)-C(25)	123.04(17)
C(26)-C(27)-C(2)	118.73(16)
C(26)-C(27)-C(28)	120.11(17)
C(2)-C(27)-C(28)	121.02(16)

Symmetry transformations used to generate equivalent atoms:

Table 9. Anisotropic displacement parameters (A^2 x 10^3) for 2.
The anisotropic displacement factor exponent takes the form:
-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
C(1)	30(1)	38(1)	20(1)	-1(1)	2(1)	-4(1)
C(2)	27(1)	19(1)	20(1)	1(1)	2(1)	-1(1)
C(3)	22(1)	20(1)	21(1)	0(1)	4(1)	1(1)
C(4)	23(1)	15(1)	21(1)	0(1)	0(1)	0(1)
C(5)	23(1)	15(1)	24(1)	-5(1)	-2(1)	2(1)
C(6)	23(1)	17(1)	27(1)	-8(1)	-1(1)	1(1)
C(7)	24(1)	20(1)	29(1)	-6(1)	4(1)	1(1)
C(8)	31(1)	22(1)	34(1)	-8(1)	9(1)	-1(1)
C(9)	24(1)	27(1)	52(1)	-10(1)	12(1)	-1(1)
C(10)	22(1)	26(1)	48(1)	-8(1)	-2(1)	0(1)
C(11)	25(1)	19(1)	34(1)	-6(1)	-1(1)	1(1)
C(12)	25(1)	25(1)	37(1)	-3(1)	-10(1)	4(1)
C(13)	31(1)	24(1)	27(1)	-1(1)	-6(1)	2(1)
C(14)	27(1)	17(1)	24(1)	-4(1)	-3(1)	1(1)
C(15)	30(1)	19(1)	22(1)	-1(1)	-3(1)	-2(1)
C(16)	34(1)	28(1)	21(1)	3(1)	-5(1)	-2(1)
C(17)	41(1)	33(1)	19(1)	5(1)	0(1)	-8(1)
C(18)	34(1)	23(1)	23(1)	-1(1)	3(1)	-7(1)
C(19)	44(1)	35(1)	21(1)	1(1)	9(1)	-8(1)
C(20)	37(1)	38(1)	31(1)	-4(1)	16(1)	-4(1)
C(21)	31(1)	26(1)	33(1)	-3(1)	7(1)	-2(1)
C(22)	29(1)	21(1)	23(1)	1(1)	5(1)	-4(1)
C(23)	27(1)	19(1)	20(1)	-2(1)	3(1)	-6(1)
C(24)	26(1)	16(1)	20(1)	1(1)	1(1)	-4(1)
C(25)	25(1)	15(1)	18(1)	2(1)	1(1)	-1(1)
C(26)	21(1)	18(1)	22(1)	3(1)	3(1)	0(1)
C(27)	22(1)	17(1)	21(1)	3(1)	1(1)	-1(1)
C(28)	25(1)	31(1)	23(1)	0(1)	-1(1)	-1(1)

Table 10. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for 2.

	x	y	z	U(eq)
H(26)	4893(15)	2110(20)	2493(9)	19(5)
H(3)	8152(15)	1550(20)	1513(9)	15(4)
H(8)	10793(15)	4560(30)	1324(10)	30(5)
H(28B)	3714(18)	1590(30)	1474(12)	46(6)
H(22)	4915(15)	4420(30)	3085(10)	26(5)
H(21)	3457(17)	5030(30)	3674(10)	37(6)
H(7)	9104(16)	3900(30)	1688(10)	28(5)
H(28A)	4123(17)	2250(30)	792(11)	39(6)
H(9)	12559(18)	3580(30)	1980(11)	41(6)
H(19)	4993(16)	1970(30)	5277(11)	37(6)
H(16)	8472(18)	490(30)	4745(11)	44(6)
H(10)	12547(18)	2070(30)	3040(11)	39(6)
H(12)	11532(17)	1070(30)	3914(10)	36(6)
H(1B)	5980(20)	1930(30)	270(14)	64(8)
H(17)	6863(16)	790(30)	5266(11)	38(6)
H(1A)	7110(20)	830(30)	450(12)	58(7)
H(13)	9852(16)	790(30)	4370(11)	34(6)
H(20)	3439(17)	3690(30)	4756(11)	39(6)
H(1C)	5940(20)	-90(30)	462(12)	53(7)
H(28C)	4246(16)	250(30)	976(10)	39(6)