SUPPORTING INFORMATION

The Electrophilic Chemistry of Biologically Important α-Ketoacids.

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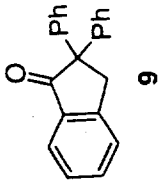

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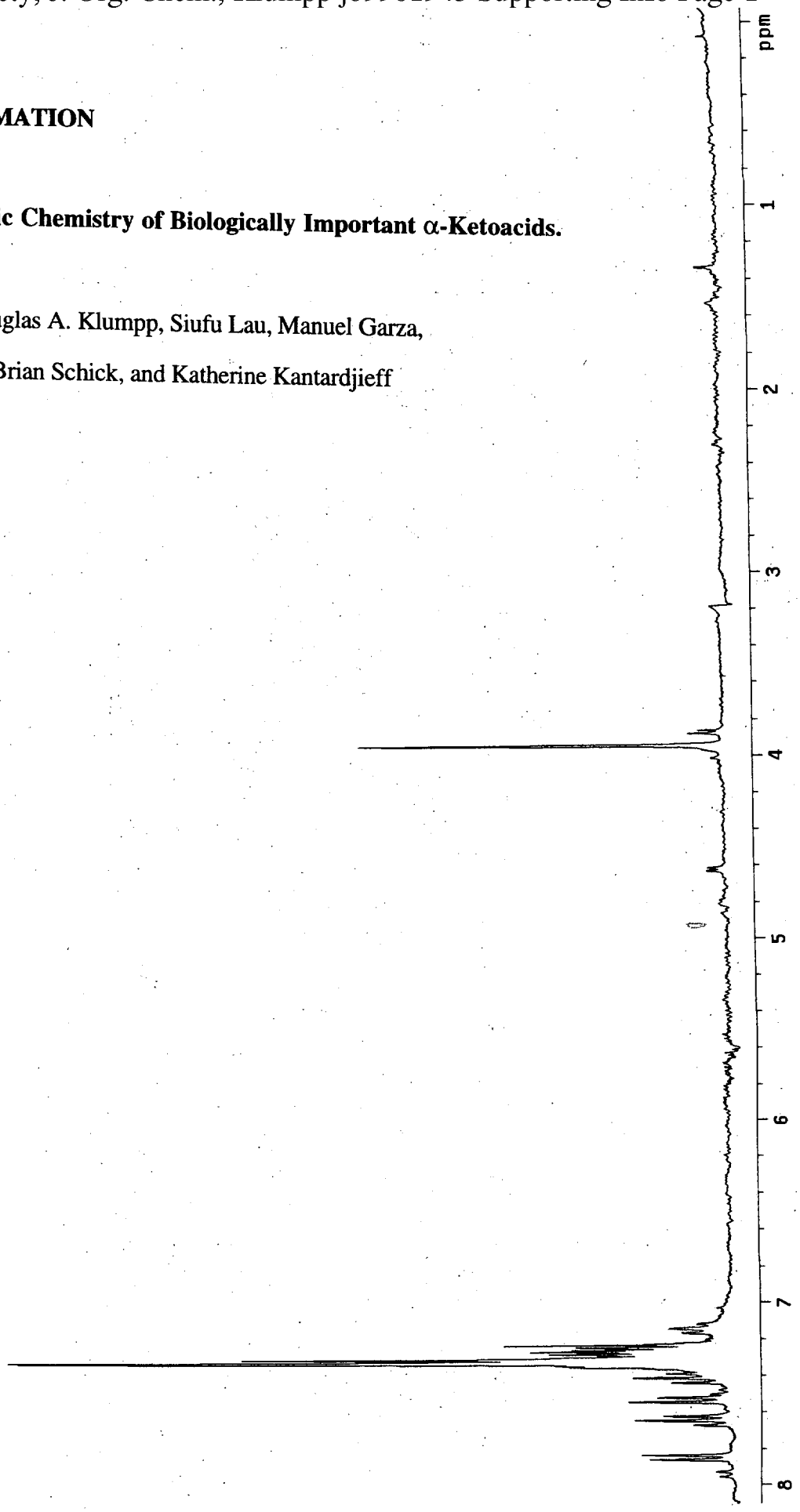

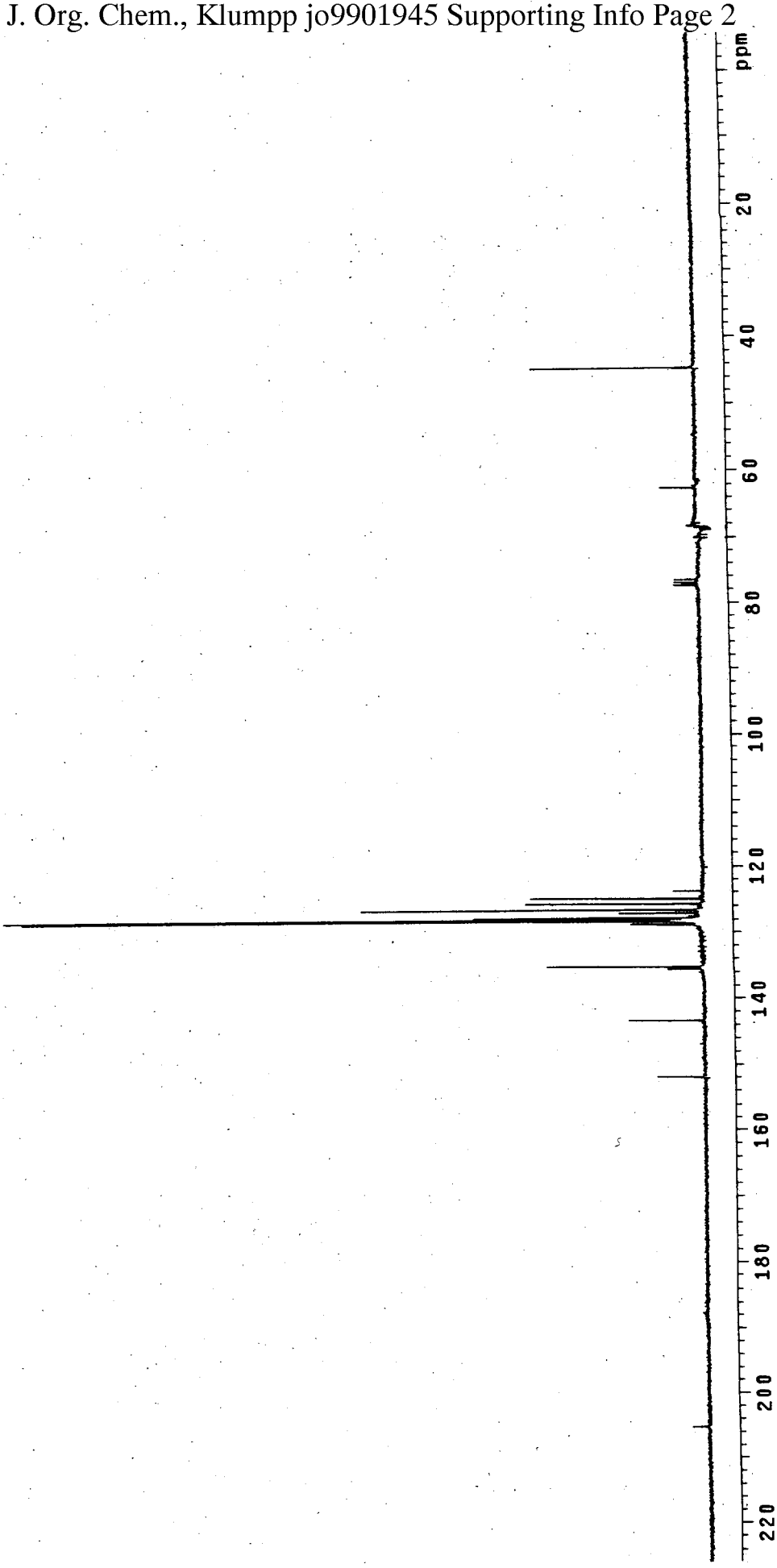

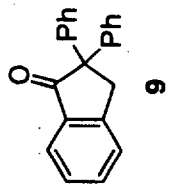

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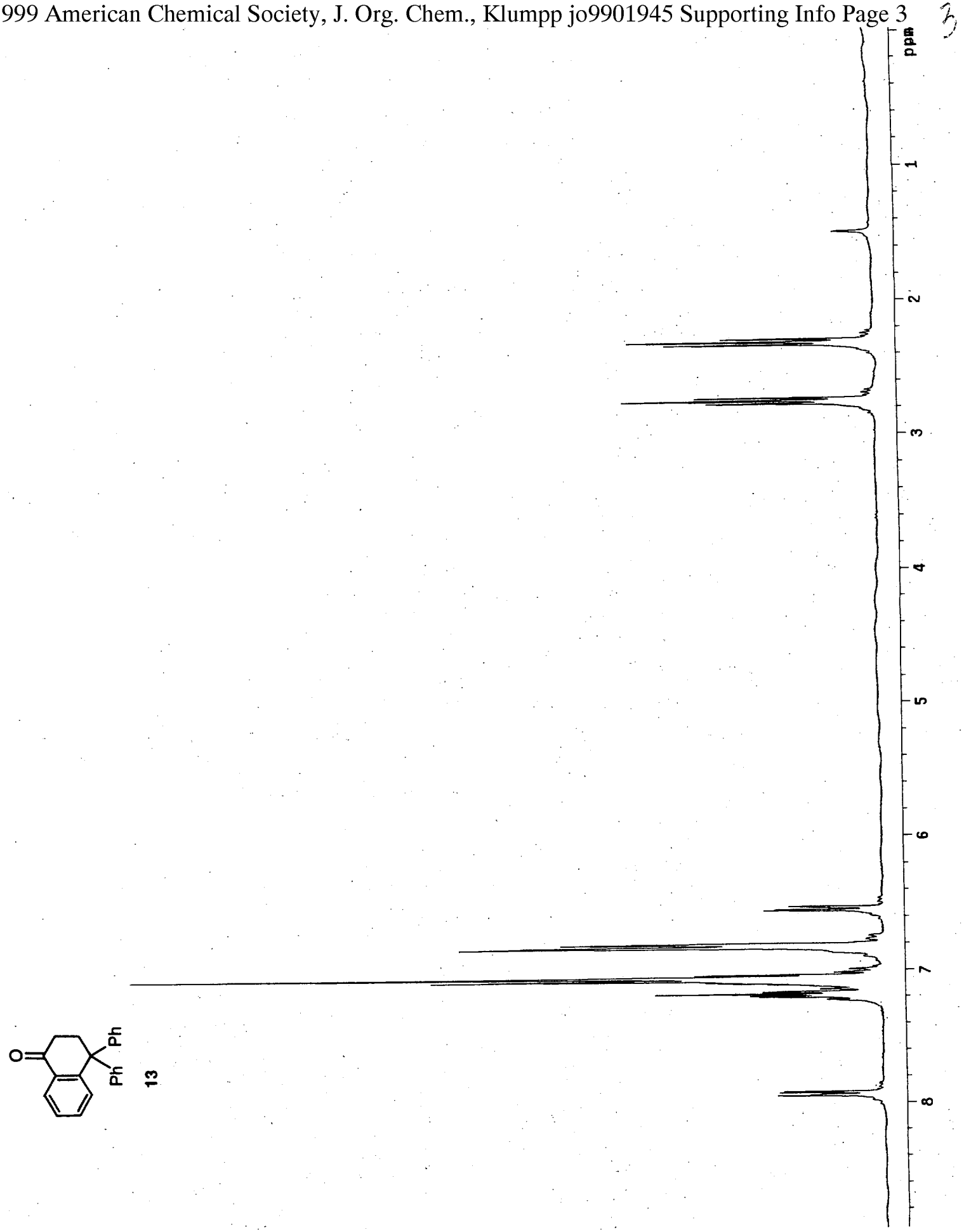

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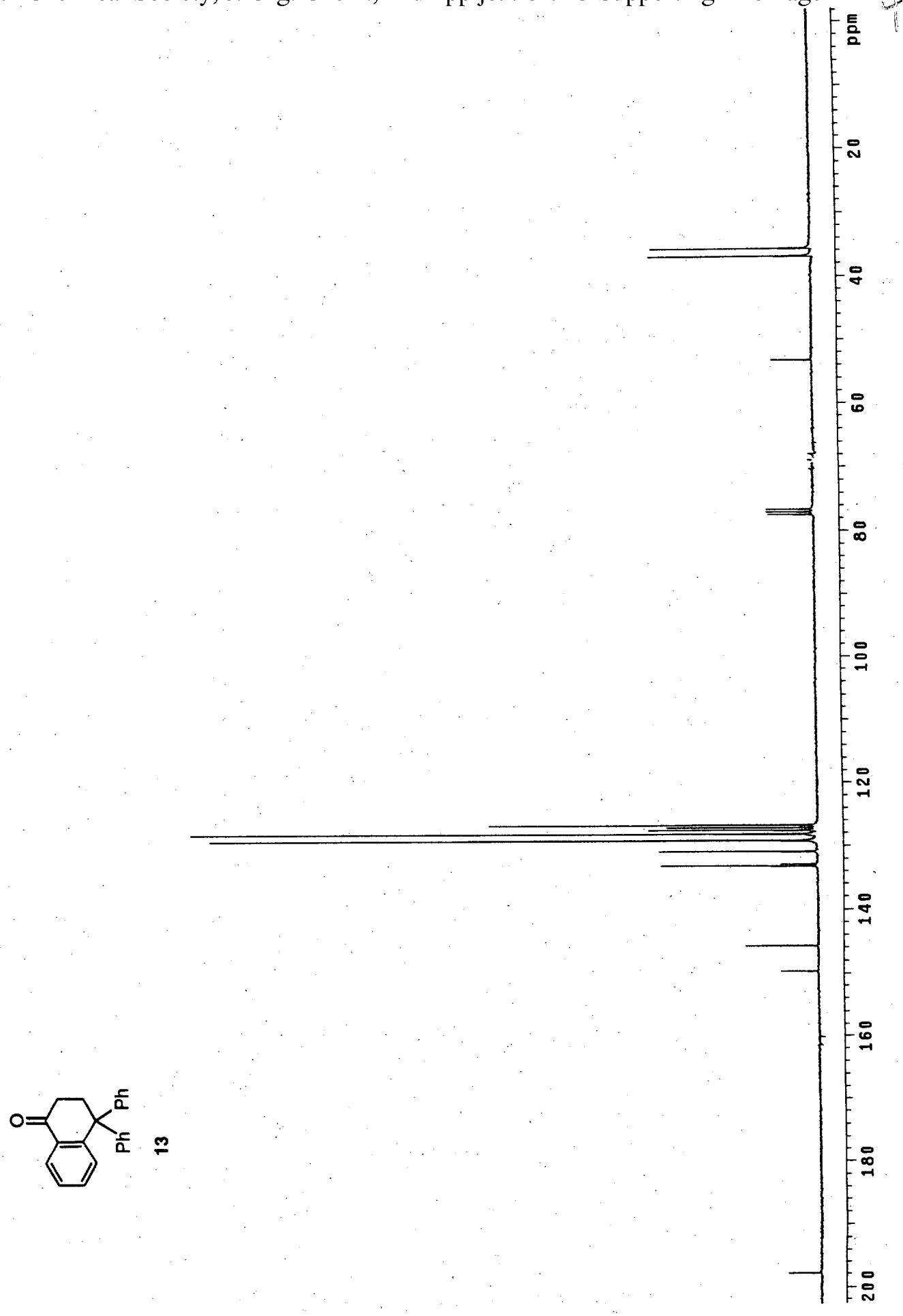

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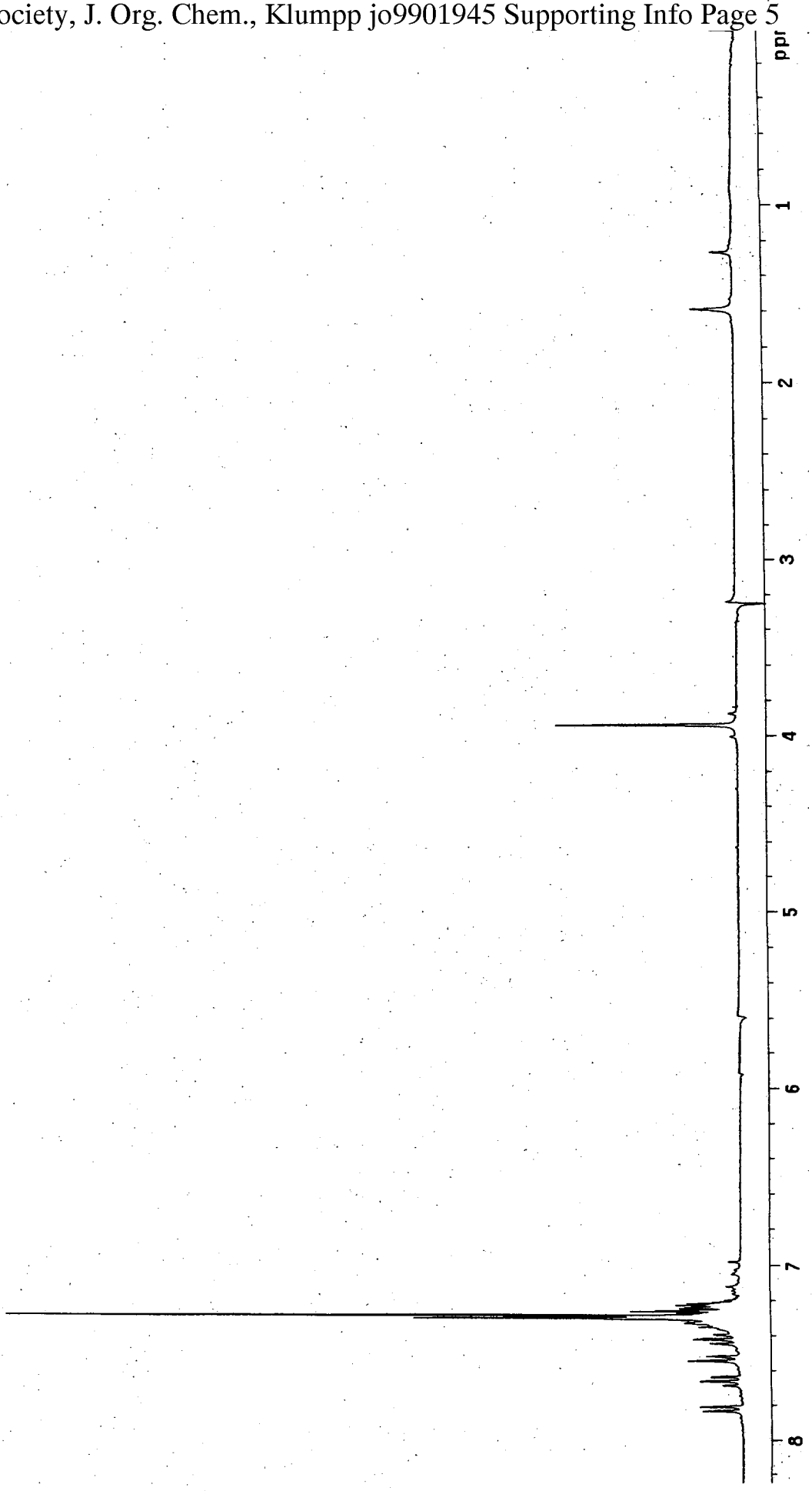

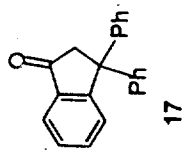

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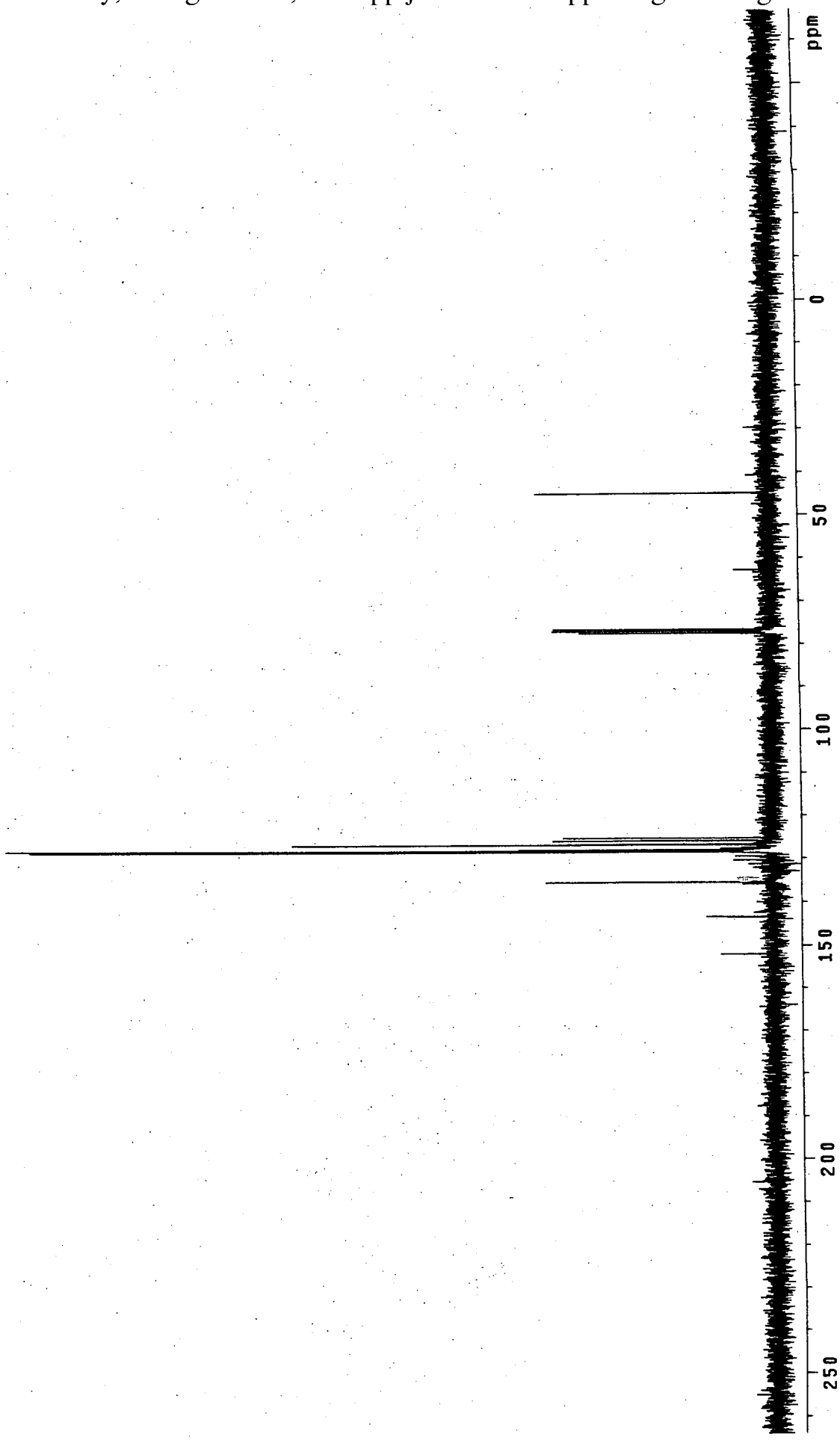

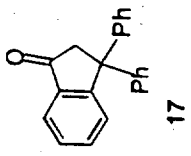

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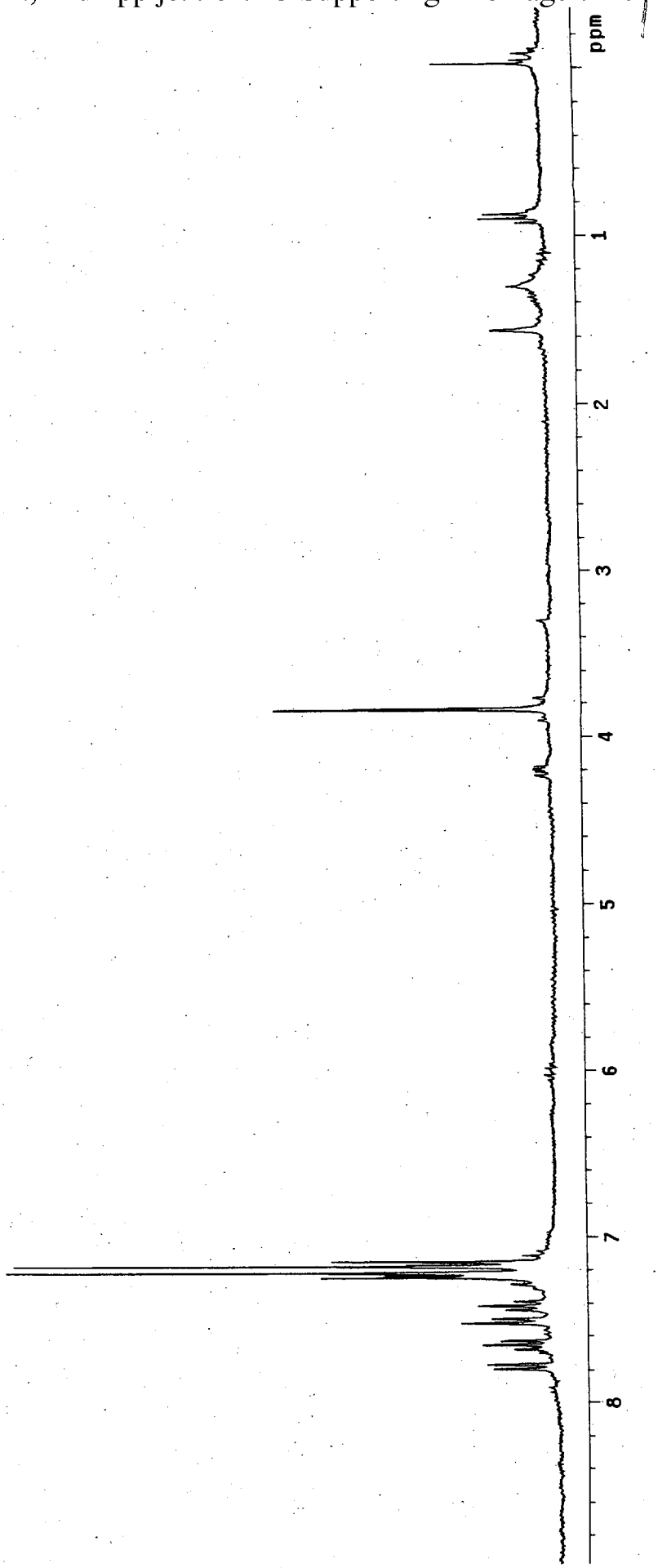

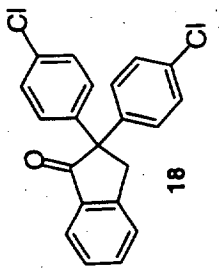

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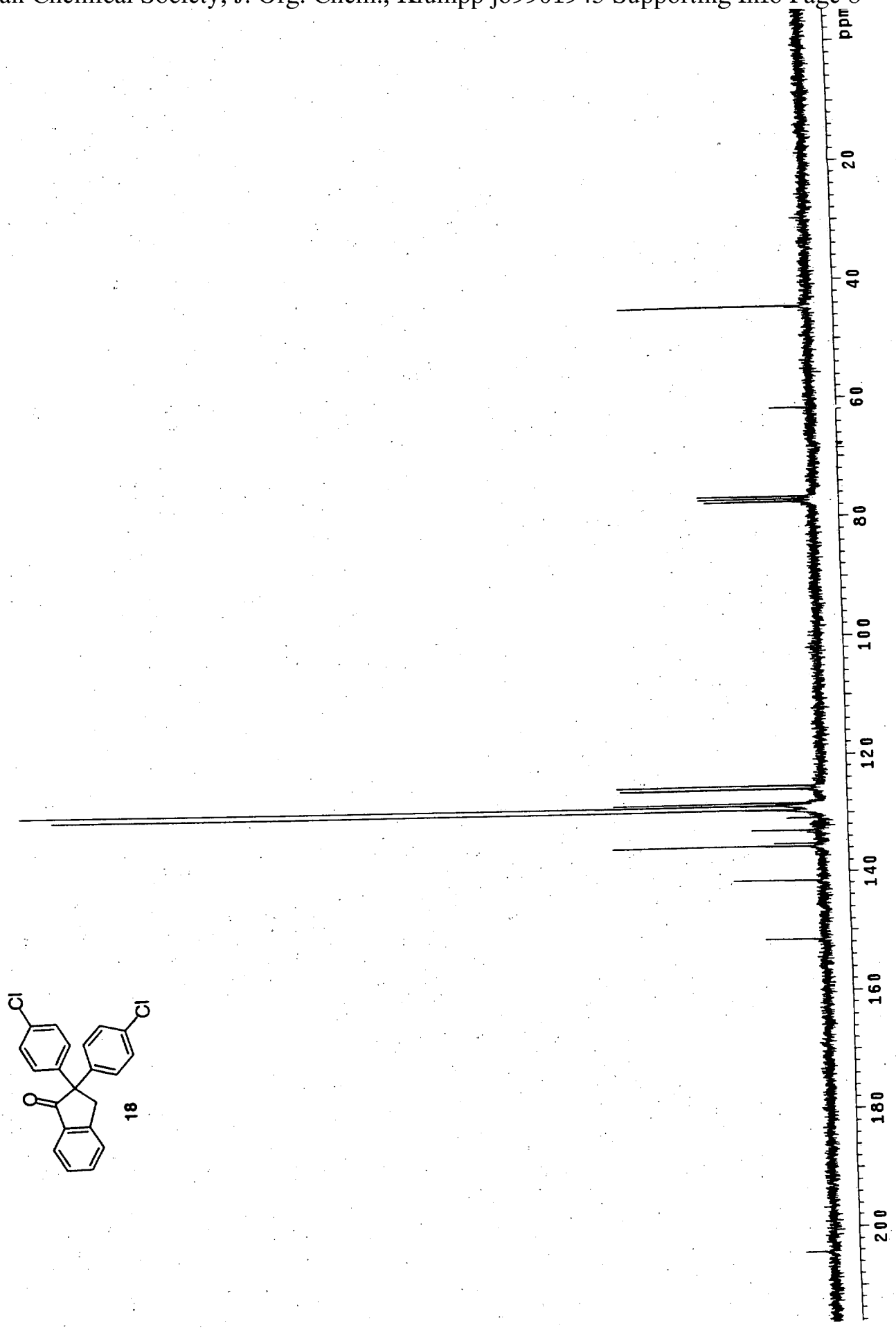

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Table 1. Crystal data and structure refinement for **4,4-diphenyl-1-tetralone (13)**

Identification code	d:\frames\frames\dk001\unknownm
Empirical formula	$C_{22}H_{18}O$
Formula weight	298.36
Temperature	293(2) K
Wavelength	0.71073 Å
Crystal system	Triclinic
Space group	$P\bar{1}$
Unit cell dimensions	a = 9.2401(10) Å alpha = 86.117(2)° b = 9.4511(10) Å beta = 69.114(2)° c = 11.2470(12) Å gamma = 61.266(2)°
Volume, Z	798.19(15) $Å^3$, 2
Density (calculated)	1.241 Mg/m^3
Absorption coefficient	0.074 mm^{-1}
F(000)	316
Crystal size	0.2 mm x 0.1 mm x 0.03 mm mm
θ range for data collection	1.95 to 28.13°
Limiting indices	$-12 \le h \le 11$, $-12 \le k \le 12$, $-14 \le l \le 14$
Reflections collected	8291
Independent reflections	3534 (R_{int} = 0.0385)
Completeness to θ = 28.13°	90.5 %
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	3534 / 0 / 209
Goodness-of-fit on F^2	2.257
Final R indices [I>2σ(I)]	R1 = 0.0443, wR2 = 0.0734
R indices (all data)	R1 = 0.0680, wR2 = 0.0757
Extinction coefficient	0.069(2)
Largest diff. peak and hole	0.194 and -0.135 $eÅ^{-3}$

Table 2. Atomic coordinates [x 10^4] and equivalent isotropic displacement parameters [$Å^2$ x 10^3] for C22. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
C(1)	3411(2)	6186(2)	4092(1)	54(1)
C(2)	2837(2)	7735(2)	4823(1)	60(1)
C(3)	4359(2)	8088(2)	4527(1)	52(1)
C(4)	5194(2)	8177(1)	3079(1)	42(1)
C(5)	5730(2)	6600(1)	2321(1)	44(1)
C(6)	4853(2)	5704(1)	2802(1)	50(1)
C(7)	5334(2)	4309(2)	2060(2)	68(1)
C(8)	6650(2)	3809(2)	868(2)	79(1)
C(9)	7533(2)	4674(2)	392(1)	70(1)
C(10)	7082(2)	6045(2)	1113(1)	56(1)
C(11)	6855(2)	8327(1)	2850(1)	42(1)
C(12)	8204(2)	7134(2)	3217(1)	53(1)
C(13)	9700(2)	7225(2)	3057(1)	63(1)
C(14)	9916(2)	8485(2)	2518(1)	65(1)
C(15)	8624(2)	9662(2)	2133(1)	64(1)
C(16)	7106(2)	9584(2)	2296(1)	52(1)
C(17)	3802(2)	9661(1)	2686(1)	43(1)
C(18)	3507(2)	9587(2)	1577(1)	54(1)
C(19)	2229(2)	10946(2)	1270(1)	68(1)
C(20)	1238(2)	12386(2)	2059(2)	73(1)
C(21)	1539(2)	12493(2)	3147(2)	78(1)
C(22)	2804(2)	11154(2)	3453(1)	67(1)
O	2740(1)	5332(1)	4524(1)	77(1)

Table 3. Bond lengths [Å] and angles [°] for C22.

C(1)-O	1.2194(13)	C(1)-C(2)	1.4955(18)
C(1)-C(6)	1.4882(18)	C(2)-C(3)	1.5179(16)
C(3)-C(4)	1.5507(15)	C(4)-C(5)	1.5340(15)
C(4)-C(11)	1.5380(15)	C(4)-C(17)	1.5500(14)
C(5)-C(10)	1.3925(17)	C(5)-C(6)	1.3979(16)
C(6)-C(7)	1.3976(17)	C(7)-C(8)	1.357(2)
C(8)-C(9)	1.3753(19)	C(9)-C(10)	1.3753(17)
C(11)-C(16)	1.3836(15)	C(11)-C(12)	1.3958(15)
C(12)-C(13)	1.3734(17)	C(13)-C(14)	1.3574(17)
C(14)-C(15)	1.3692(18)	C(15)-C(16)	1.3958(17)
C(17)-C(18)	1.3803(16)	C(17)-C(22)	1.3900(16)
C(18)-C(19)	1.3918(16)	C(20)-C(19)	1.355(2)
C(20)-C(21)	1.368(2)	C(21)-C(22)	1.3753(17)

O-C(1)-C(2)	121.77(13)	O-C(1)-C(6)	120.79(12)
C(2)-C(1)-C(6)	117.44(11)	C(1)-C(2)-C(3)	111.70(11)
C(2)-C(3)-C(4)	112.19(9)	C(5)-C(4)-C(11)	109.59(9)
C(5)-C(4)-C(17)	110.14(9)	C(11)-C(4)-C(17)	111.34(8)
C(5)-C(4)-C(3)	108.37(9)	C(11)-C(4)-C(3)	108.35(8)
C(17)-C(4)-C(3)	108.98(9)	C(10)-C(5)-C(6)	118.01(11)
C(10)-C(5)-C(4)	120.60(10)	C(6)-C(5)-C(4)	121.37(11)
C(5)-C(6)-C(7)	119.62(13)	C(5)-C(6)-C(1)	121.92(11)
C(7)-C(6)-C(1)	118.46(12)	C(8)-C(7)-C(6)	120.90(13)
C(7)-C(8)-C(9)	119.92(13)	C(10)-C(9)-C(8)	119.89(14)
C(9)-C(10)-C(5)	121.64(13)	C(16)-C(11)-C(12)	117.23(11)
C(16)-C(11)-C(4)	123.95(10)	C(12)-C(11)-C(4)	118.82(10)
C(13)-C(12)-C(11)	121.20(11)	C(14)-C(13)-C(12)	120.64(12)
C(15)-C(14)-C(13)	119.40(13)	C(14)-C(15)-C(16)	120.37(12)
C(15)-C(16)-C(11)	121.14(12)	C(18)-C(17)-C(22)	117.09(11)
C(18)-C(17)-C(4)	122.86(11)	C(22)-C(17)-C(4)	120.04(10)
C(17)-C(18)-C(19)	120.89(12)	C(20)-C(19)-C(18)	120.65(13)
C(19)-C(20)-C(21)	119.31(13)	C(20)-C(21)-C(22)	120.20(14)
C(21)-C(22)-C(17)	121.82(13)		

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters [$Å^2 \times 10^3$] for C22.

The anisotropic displacement factor exponent takes the form:

$$-2\pi^2 [(ha^*)^2 U_{11} + \ldots + 2hka^*b^* U_{12}]$$

	U11	U22	U33	U23	U13	U12
C(1)	51(1)	55(1)	63(1)	22(1)	-29(1)	-28(1)
C(2)	57(1)	70(1)	48(1)	10(1)	-12(1)	-33(1)
C(3)	54(1)	59(1)	41(1)	6(1)	-16(1)	-28(1)
C(4)	45(1)	45(1)	38(1)	4(1)	-16(1)	-21(1)
C(5)	49(1)	43(1)	42(1)	6(1)	-21(1)	-20(1)
C(6)	55(1)	43(1)	60(1)	12(1)	-29(1)	-24(1)
C(7)	82(1)	51(1)	84(1)	9(1)	-38(1)	-37(1)
C(8)	99(1)	54(1)	79(1)	-11(1)	-34(1)	-31(1)
C(9)	79(1)	62(1)	57(1)	-10(1)	-18(1)	-28(1)
C(10)	64(1)	55(1)	49(1)	0(1)	-18(1)	-30(1)
C(11)	44(1)	45(1)	34(1)	-1(1)	-12(1)	-20(1)
C(12)	52(1)	55(1)	52(1)	9(1)	-21(1)	-26(1)
C(13)	51(1)	75(1)	63(1)	8(1)	-25(1)	-28(1)
C(14)	54(1)	84(1)	64(1)	-1(1)	-19(1)	-40(1)
C(15)	70(1)	69(1)	62(1)	7(1)	-17(1)	-46(1)
C(16)	55(1)	51(1)	53(1)	7(1)	-20(1)	-27(1)
C(17)	42(1)	46(1)	41(1)	5(1)	-14(1)	-22(1)
C(18)	61(1)	53(1)	50(1)	9(1)	-24(1)	-28(1)
C(19)	79(1)	71(1)	64(1)	24(1)	-40(1)	-37(1)
C(20)	60(1)	65(1)	81(1)	25(1)	-31(1)	-20(1)
C(21)	68(1)	55(1)	76(1)	-1(1)	-22(1)	-7(1)
C(22)	66(1)	55(1)	60(1)	-6(1)	-27(1)	-11(1)
O	72(1)	75(1)	95(1)	32(1)	-31(1)	-48(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for 'C22.

	x	y	z	U(eq)
H(2A)	2370	7673	5735	72
H(2B)	1890	8621	4611	72
H(3A)	5267	7242	4799	62
H(3B)	3927	9114	5012	62
H(7)	4750	3712	2381	82
H(8)	6947	2886	380	94
H(9)	8435	4332	-416	84
H(10)	7695	6615	785	67
H(12)	8088	6260	3576	64
H(13)	10575	6422	3318	76
H(14)	10930	8542	2413	78
H(15)	8766	10518	1761	76
H(16)	6242	10390	2028	63
H(18)	4173	8616	1028	64
H(19)	2047	10873	520	81
H(20)	367	13284	1860	88
H(21)	887	13475	3682	93
H(22)	2998	11250	4193	81

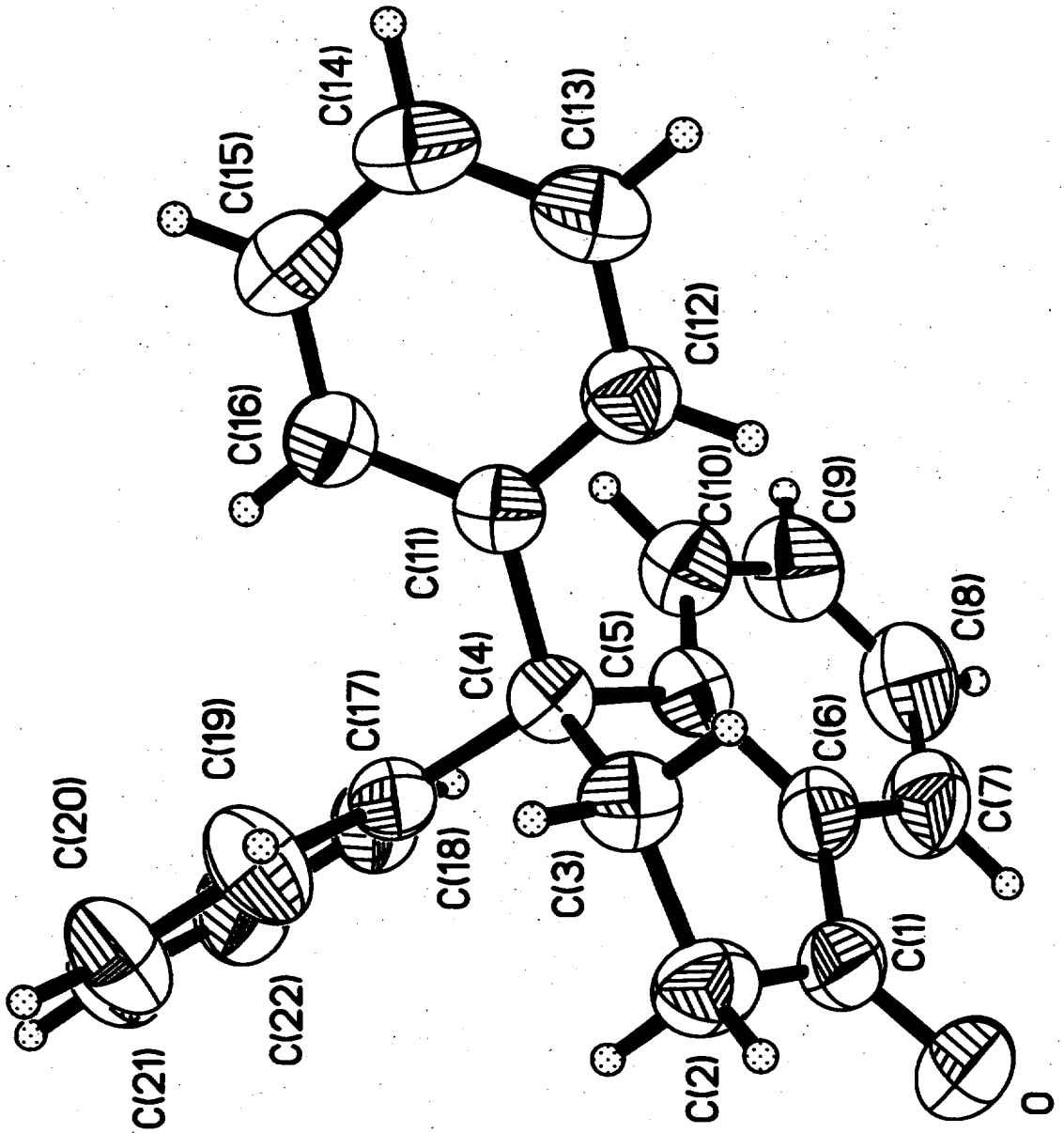

Figure 1. X-ray crystal structure of product **13**.