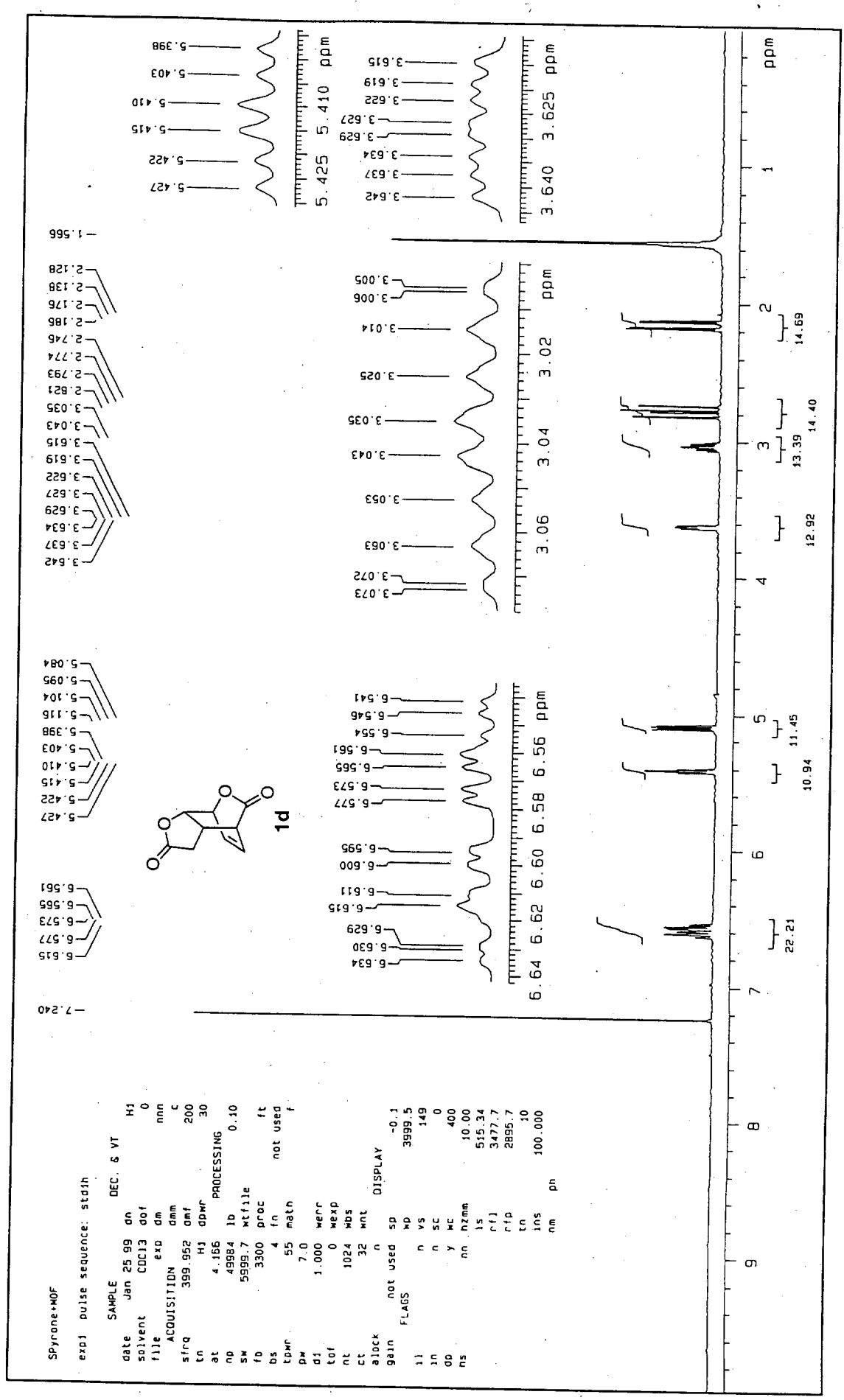

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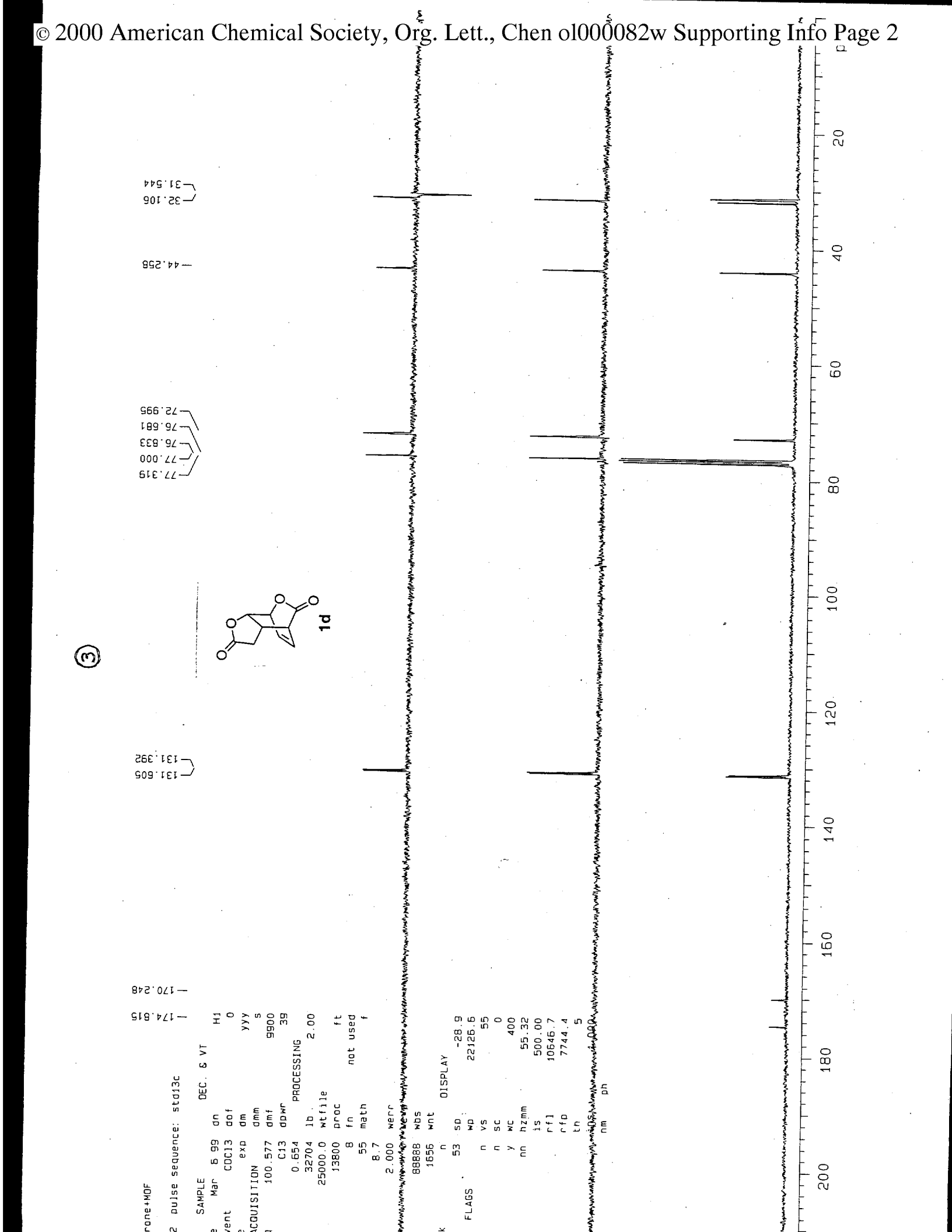

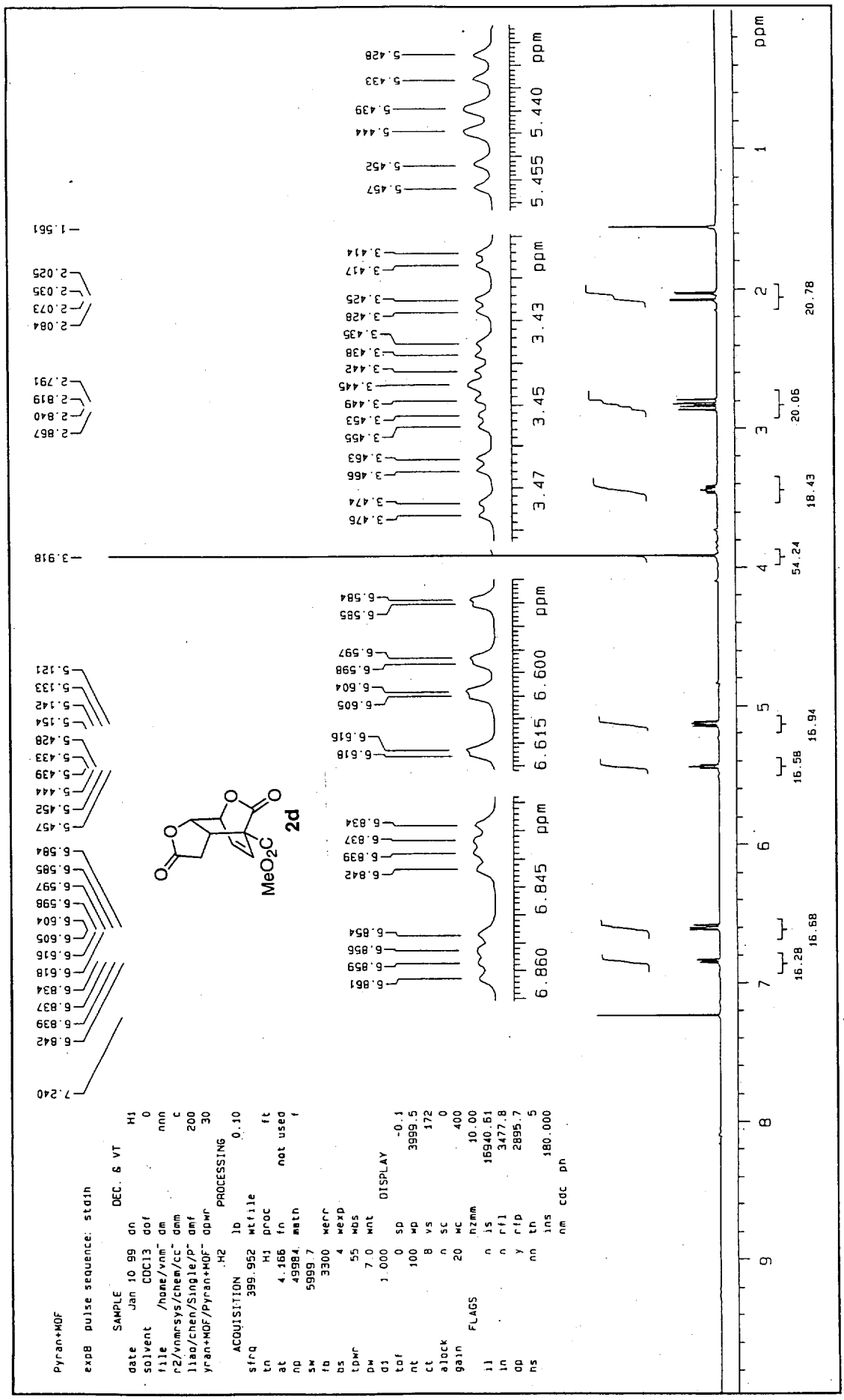

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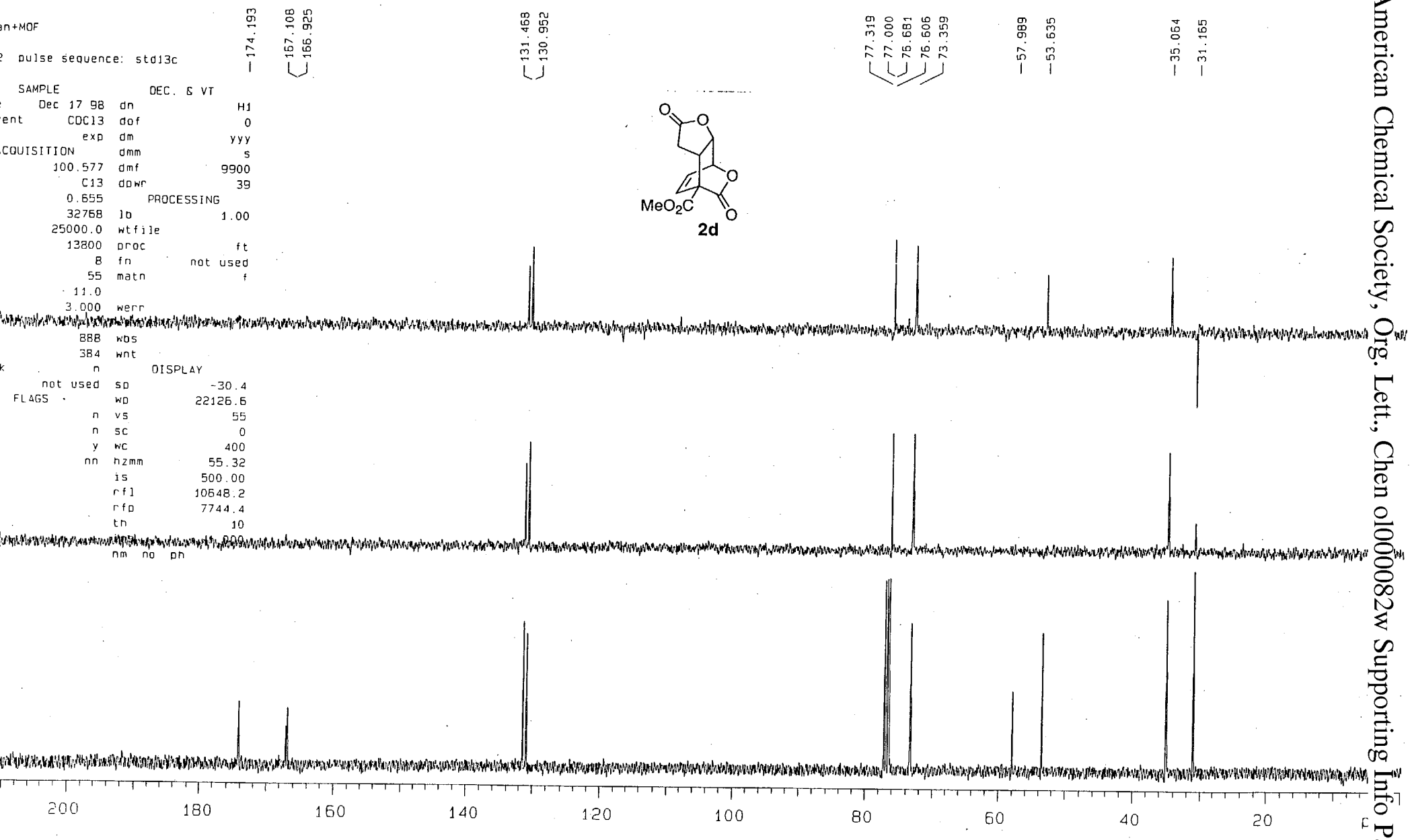
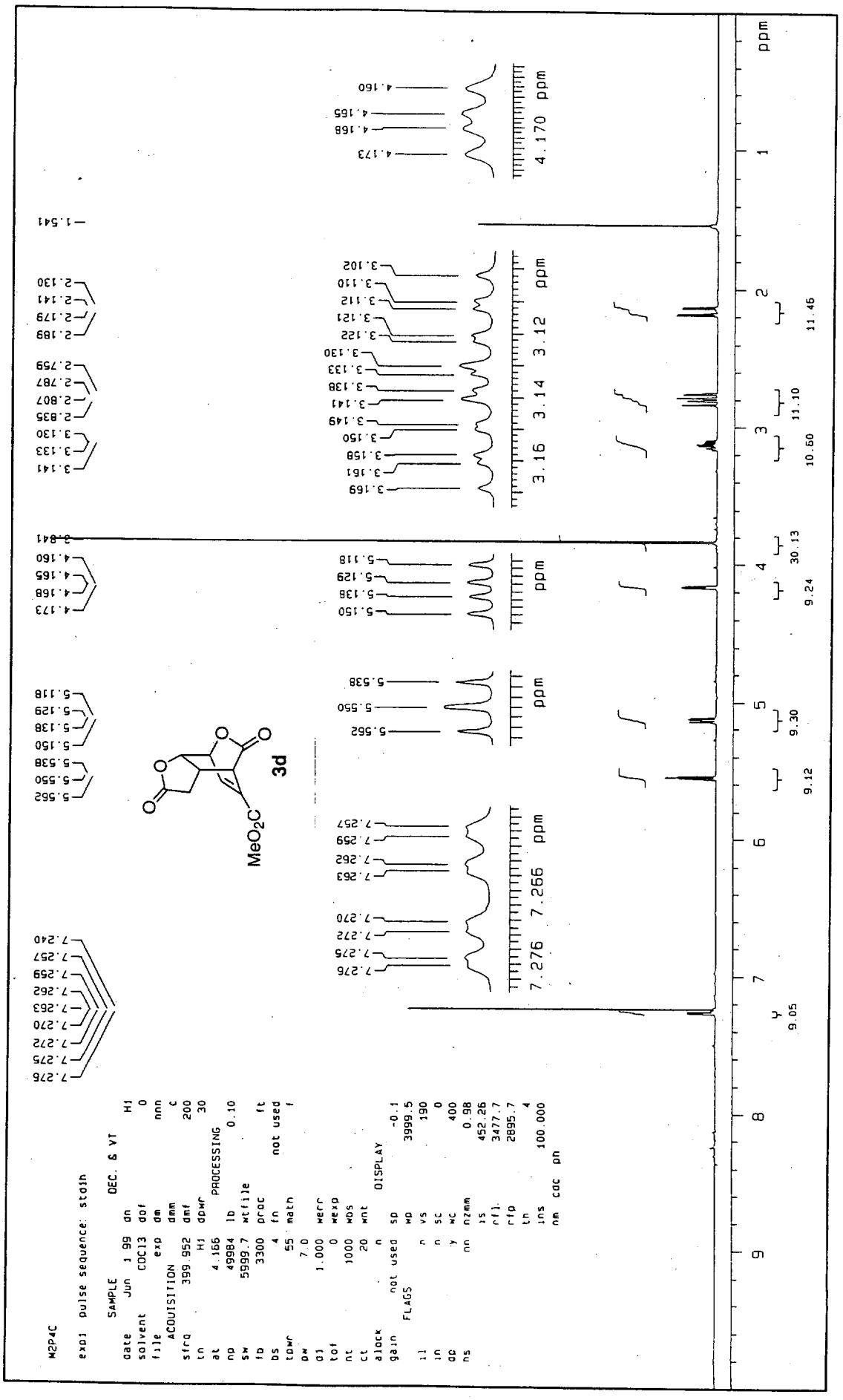


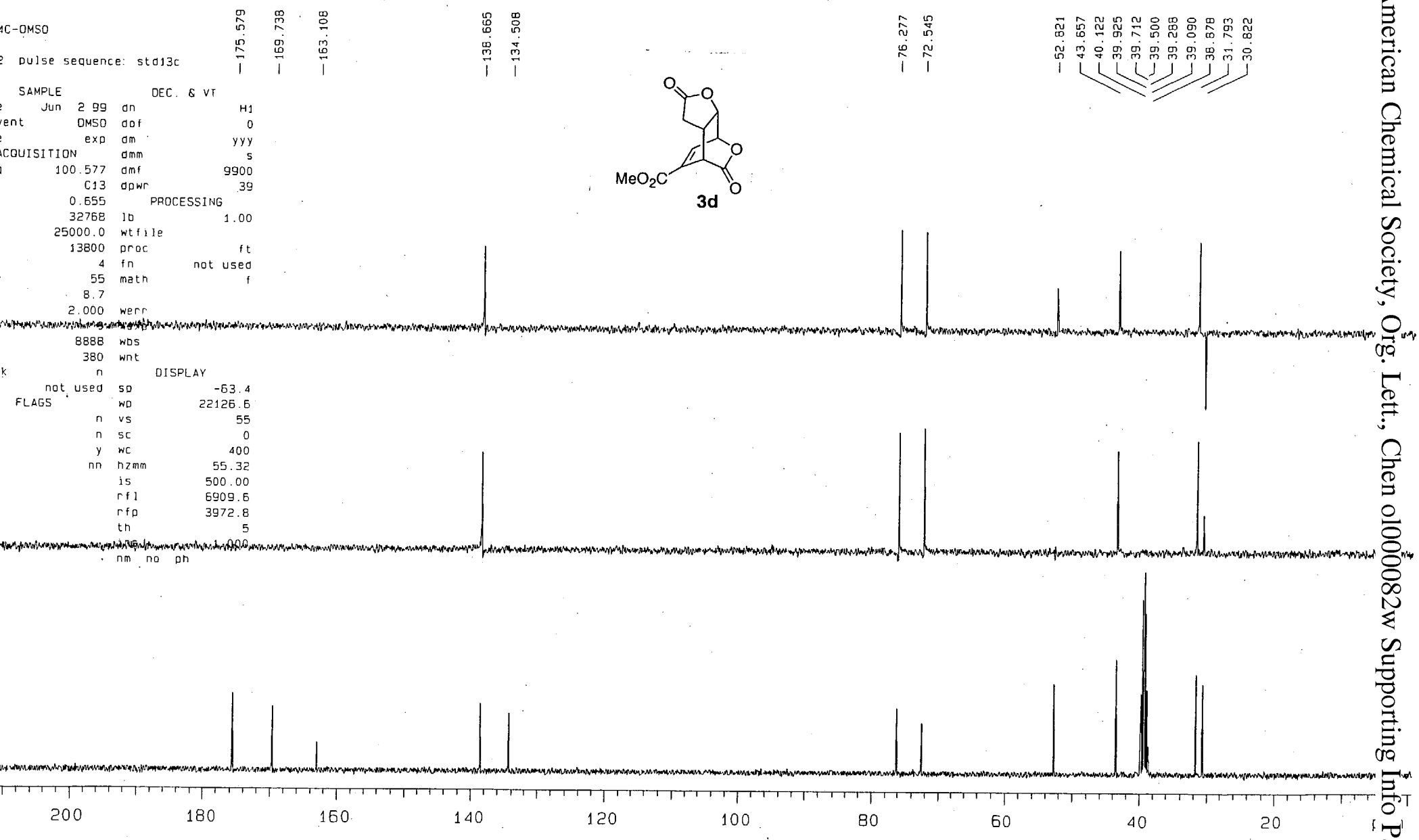
an+MOF

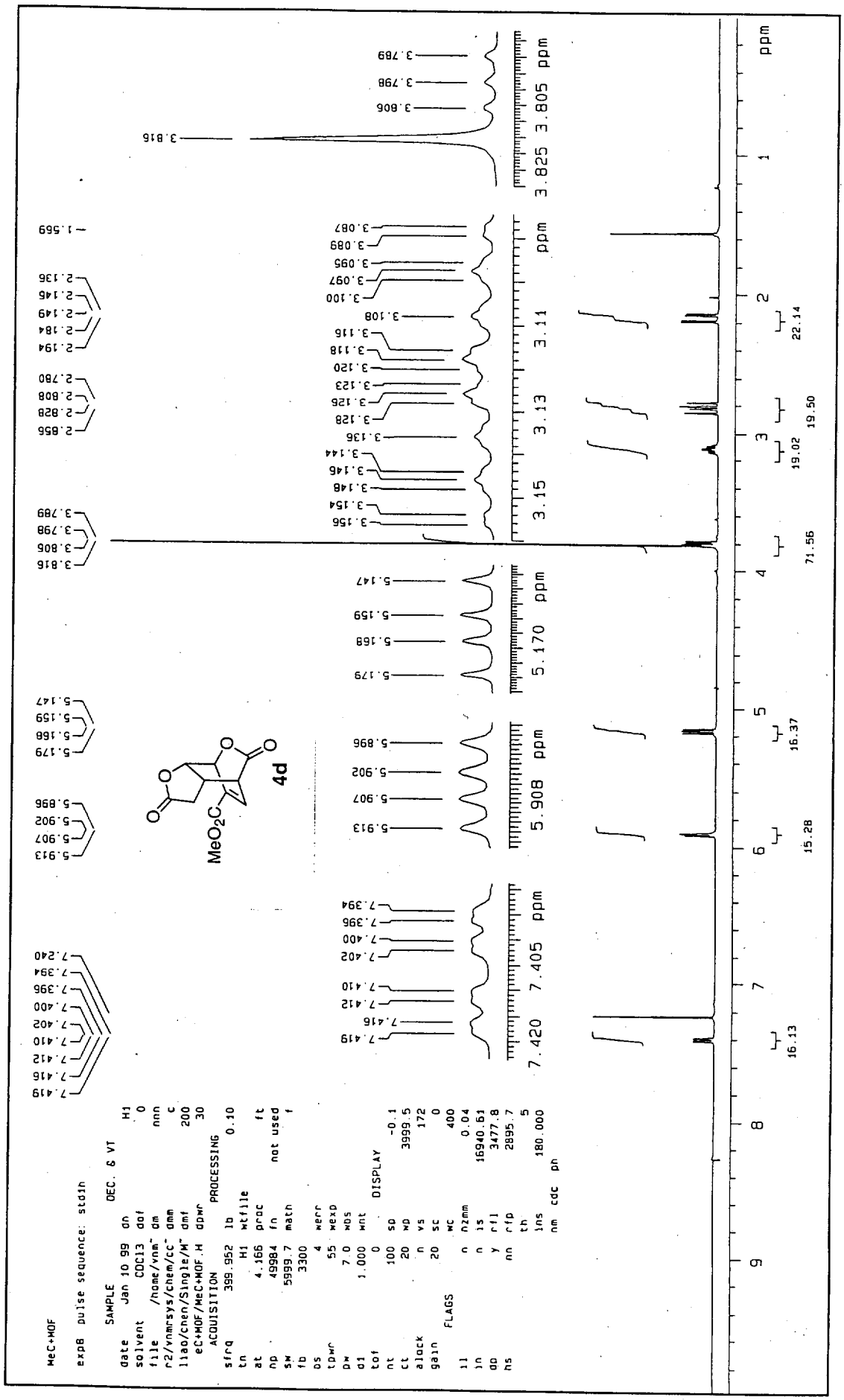
2 pulse sequence: std13c

SAMPLE	DEC. & VT	
Dec 17 98	dn	H1
CDCl3	dof	0
exp	dm	yyy
ACQUISITION	dmm	s
100.577	dmf	9900
C13	dpwr	39
0.655	PROCESSING	
32768	lb	1.00
25000.0	wtfile	
13800	proc	ft
8	fn	not used
55	math	f
11.0		
3.000	werr	
888	wbs	
384	wnt	
n	DISPLAY	
not used	sp	-30.4
FLAGS	wp	22126.6
n	vs	55
n	sc	0
y	wc	400
nn	hzmm	55.32
	is	500.00
	rfl	10648.2
	rfp	7744.4
	th	10
	nm no ph	



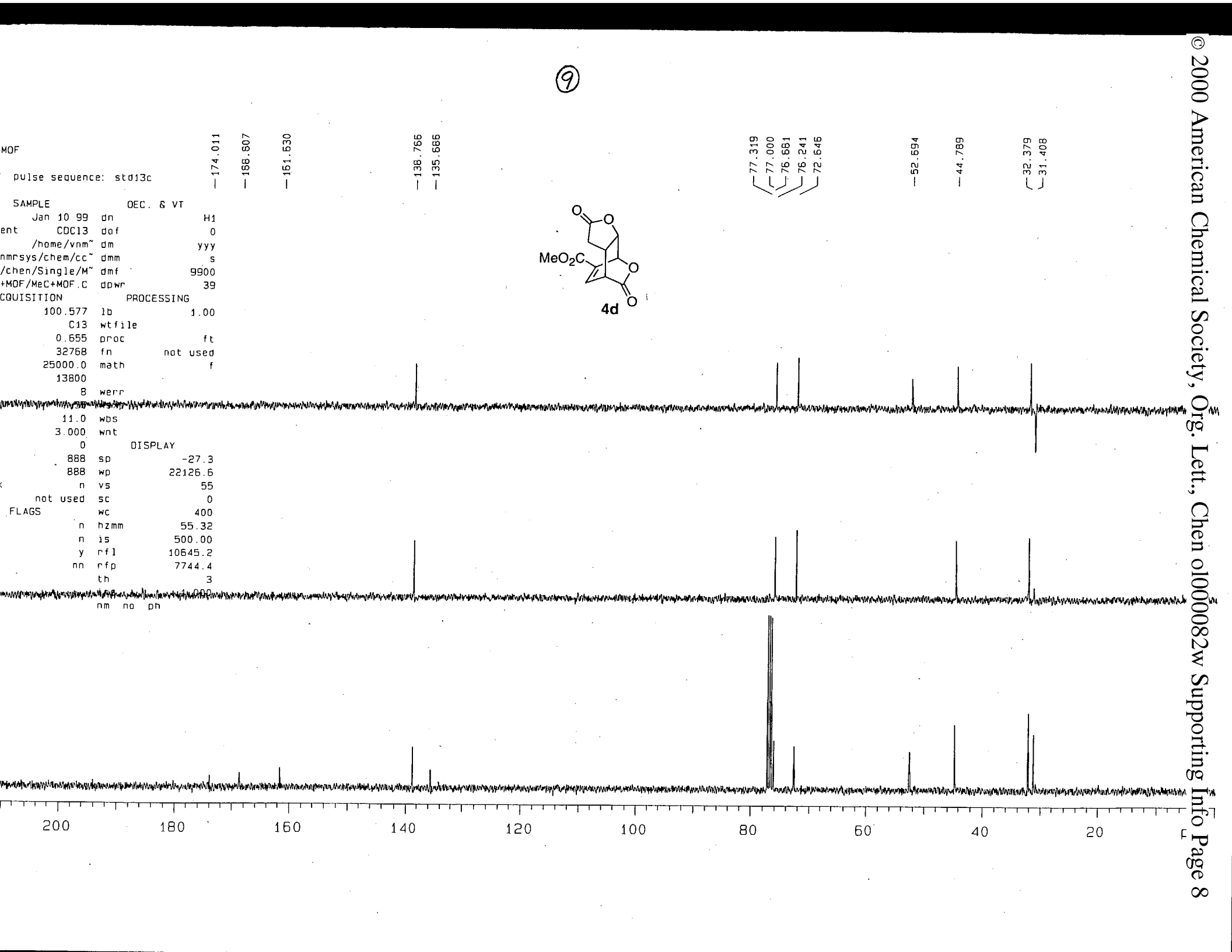
⑦

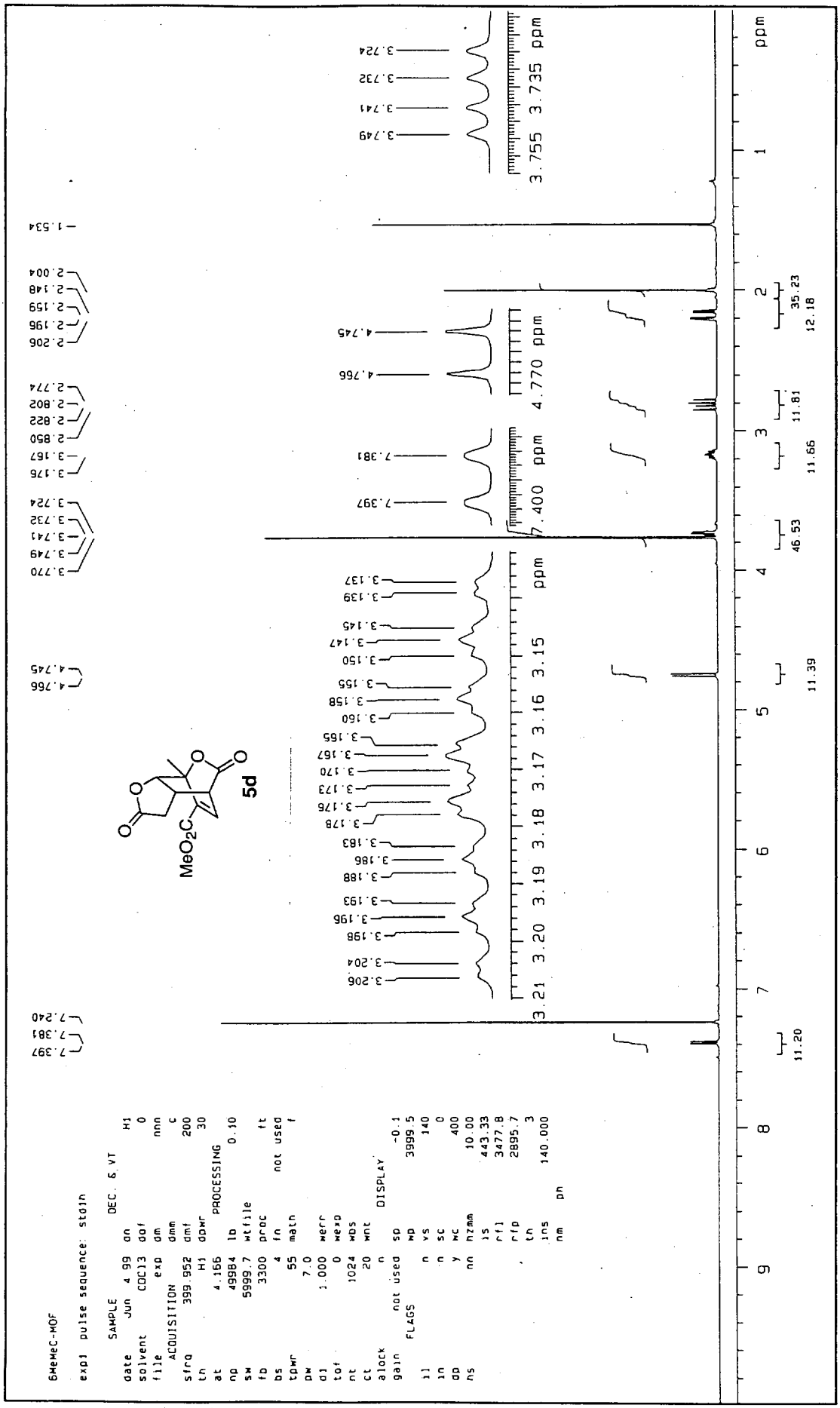




(8)

(9)





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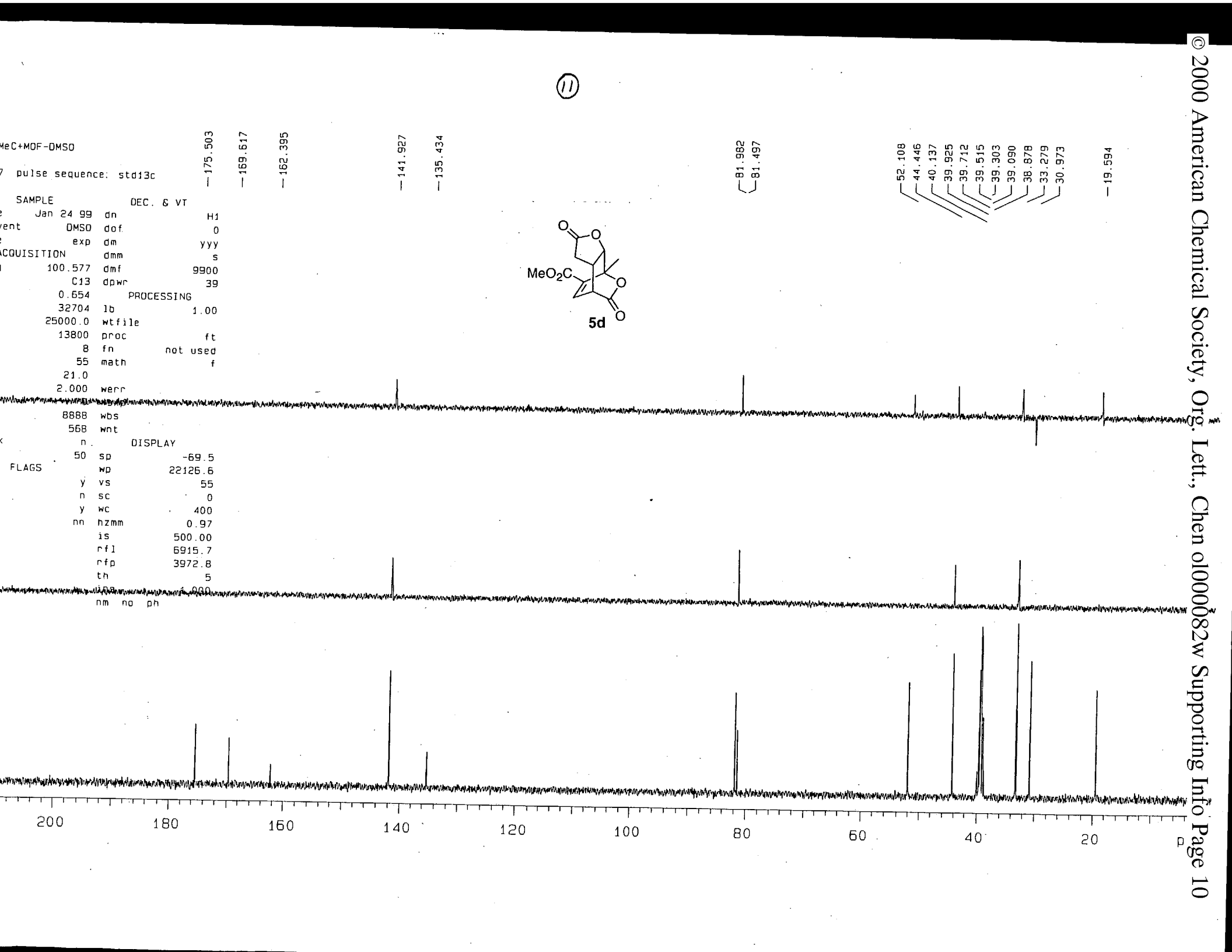
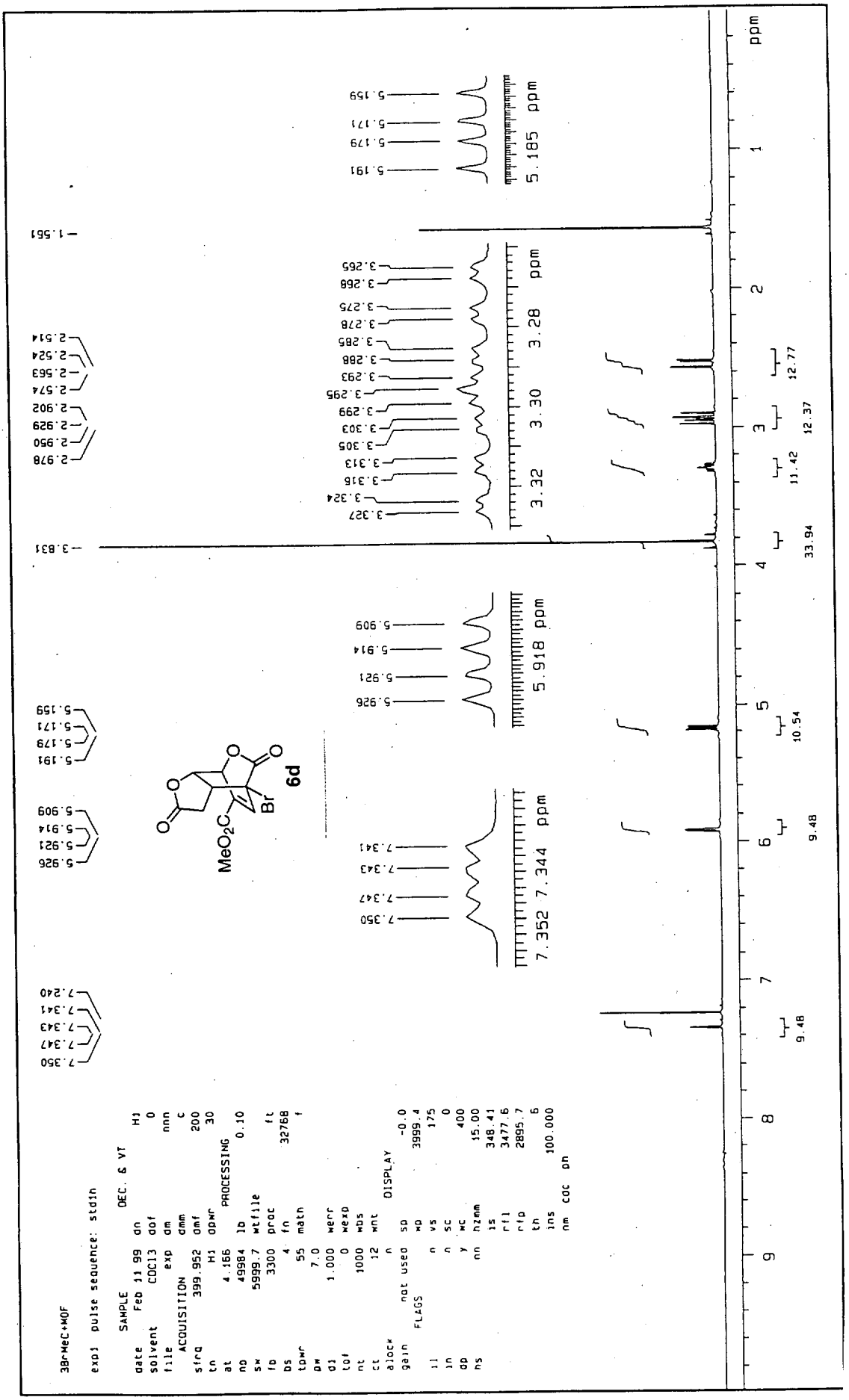
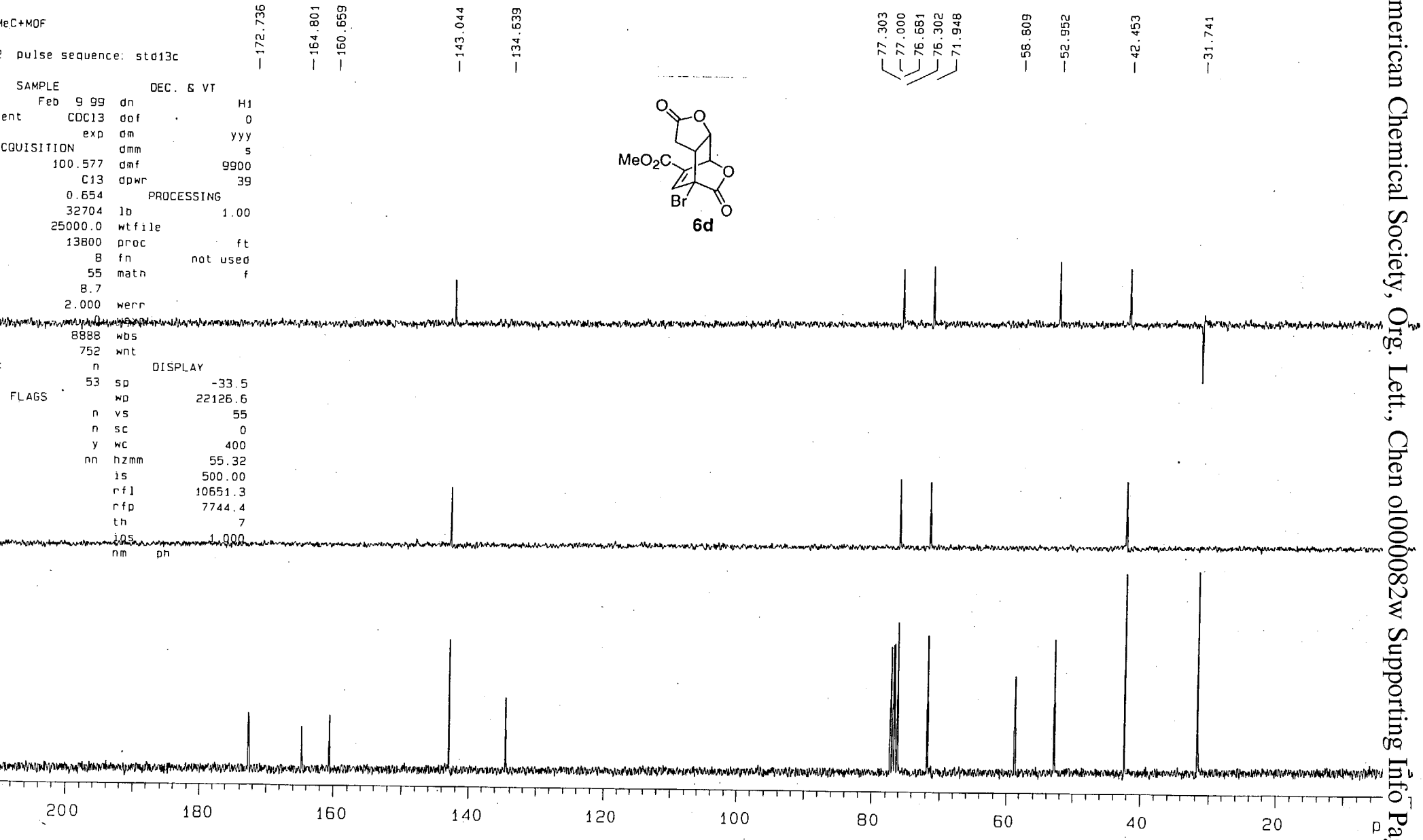
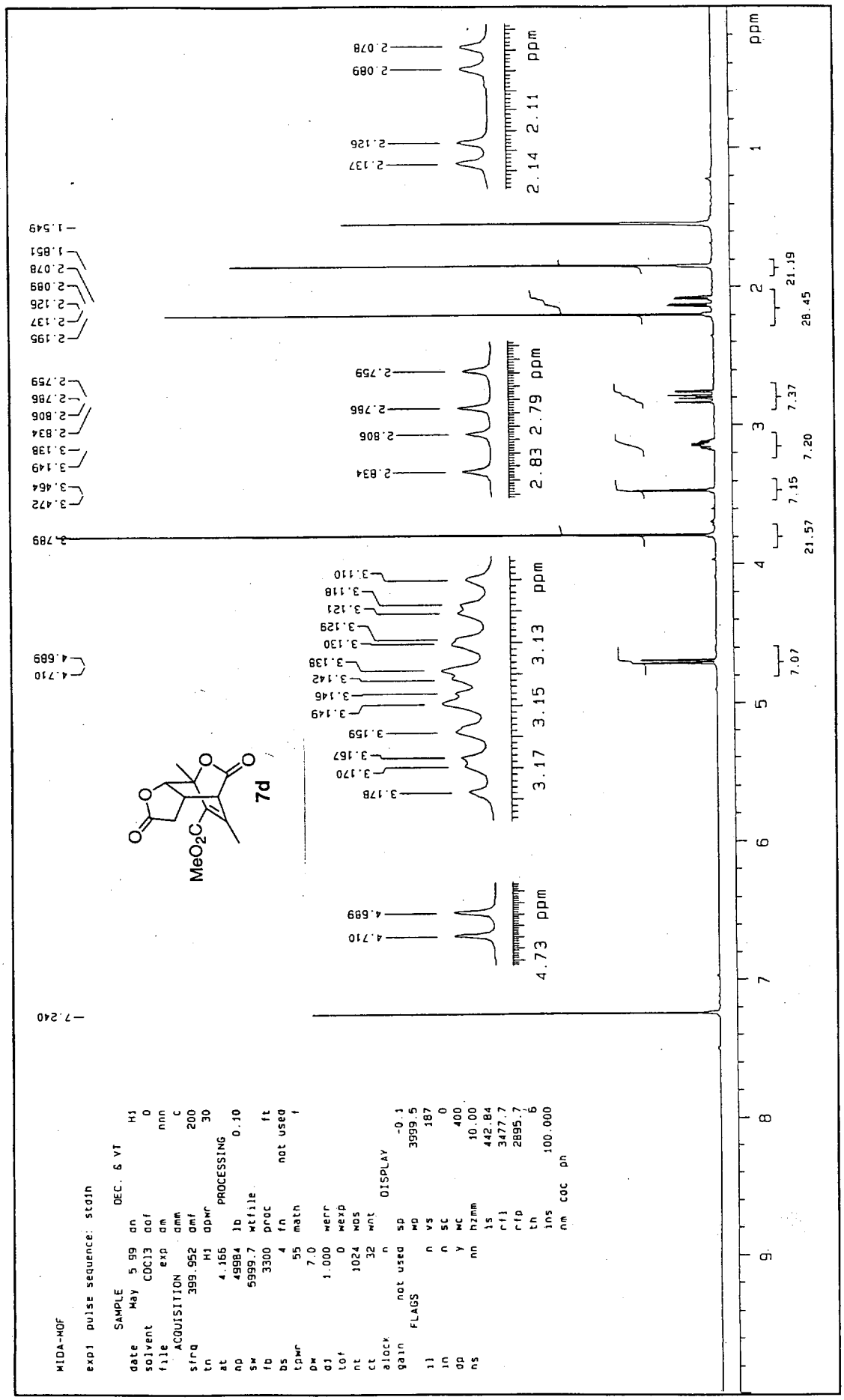
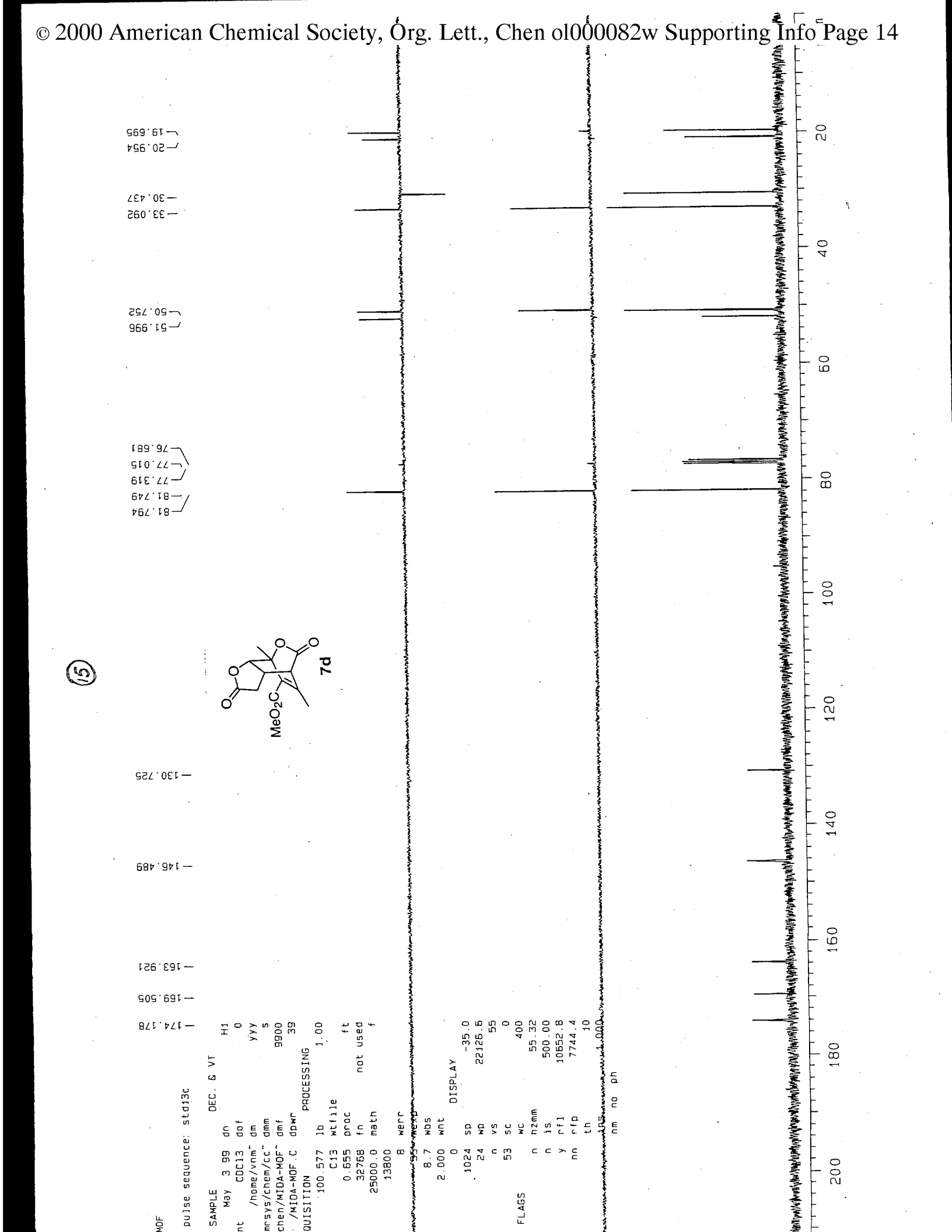


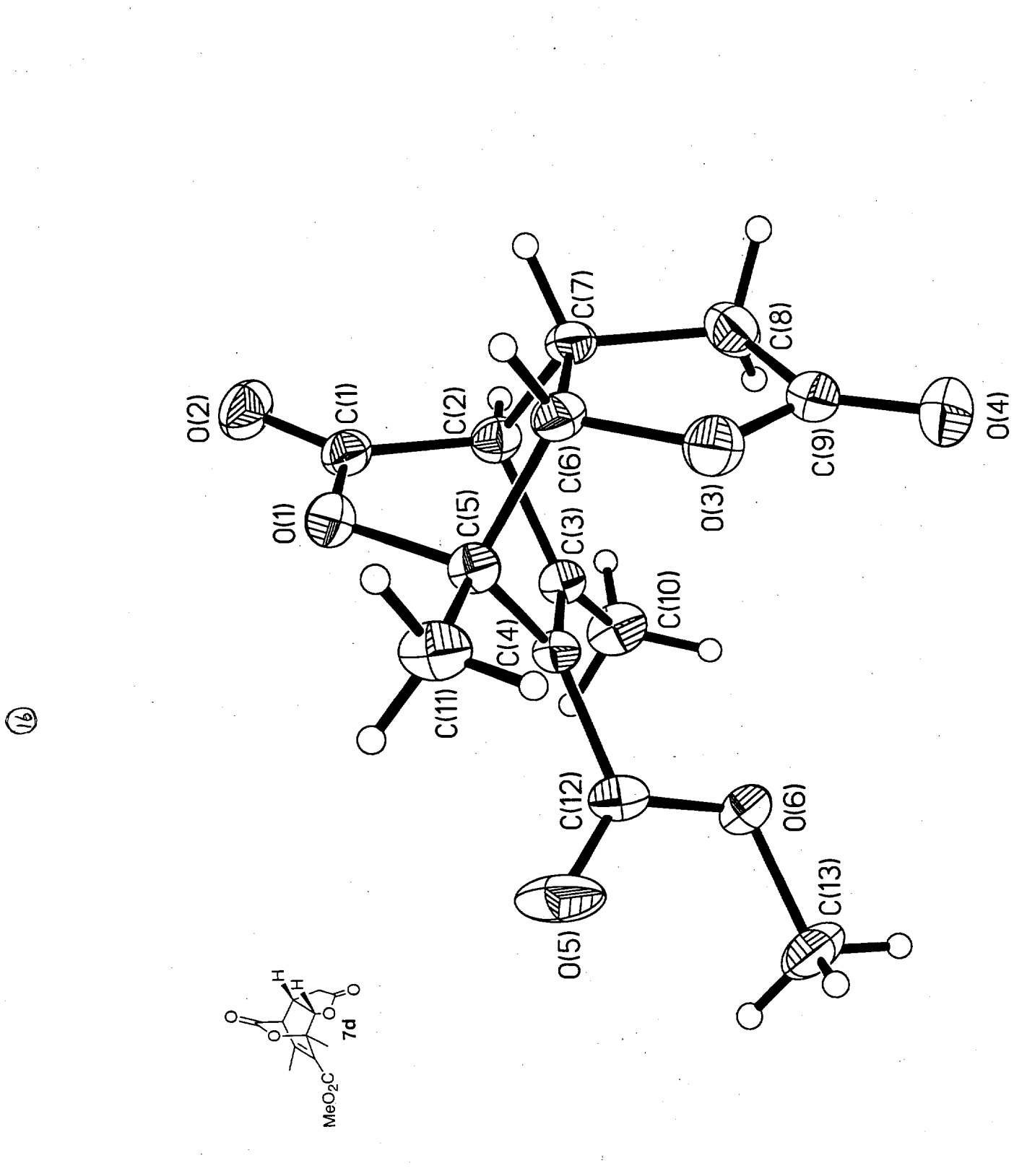
(12)











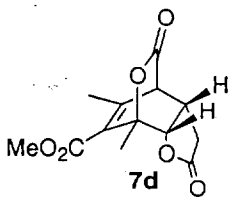
(16)

The molecular structure of IC6673, thermal ellipsoids drawn at the 30% probabilty level.

Table 1. Crystal data and structure refinement for 6673.

Identification code	ic6673
Empirical formula	$C_{13}H_{14}O_6$
Formula weight	266.24
Temperature	295(2) K
Wavelength	0.71073 Å
Crystal system	Monoclinic
Space group	$P2_1/n$
Unit cell dimensions	a = 12.612(3) Å alpha = 90° b = 7.429(2) Å beta = 105.69(2)° c = 13.834(3) Å gamma = 90°
Volume, Z	1247.8(4) $Å^3$, 4
Density (calculated)	1.417 Mg/m^3
Absorption coefficient	0.113 mm^{-1}
F(000)	560
Crystal size	0.65 x 0.45 x 0.20 mm
θ range for data collection	1.94 to 27.46°
Limiting indices	$-16 \le h \le 15$, $0 \le k \le 9$, $0 \le l \le 17$
Reflections collected	2857
Independent reflections	2857 (R_{int} = 0.0000)
Absorption correction	None
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	2857 / 0 / 173
Goodness-of-fit on F^2	1.111
Final R indices [I>2σ(I)]	R1 = 0.0502, wR2 = 0.1502
R indices (all data)	R1 = 0.0746, wR2 = 0.1671
Extinction coefficient	0.002(3)
Largest diff. peak and hole	0.374 and -0.301 $eÅ^{-3}$

(7)



7d

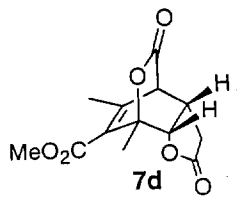
Table 2. Bond lengths [Å] and angles [°] for 6673.

O(1)-C(1)	1.345(3)	O(1)-C(5)	1.472(2)
O(2)-C(1)	1.201(2)	O(3)-C(9)	1.356(3)
O(3)-C(6)	1.435(2)	O(4)-C(9)	1.190(3)
O(5)-C(12)	1.198(3)	O(6)-C(12)	1.328(3)
O(6)-C(13)	1.450(3)	C(1)-C(2)	1.497(3)
C(2)-C(3)	1.514(3)	C(2)-C(7)	1.555(3)
C(3)-C(4)	1.335(3)	C(3)-C(10)	1.489(3)
C(4)-C(12)	1.489(3)	C(4)-C(5)	1.518(3)
C(5)-C(11)	1.499(3)	C(5)-C(6)	1.543(3)
C(6)-C(7)	1.531(3)	C(7)-C(8)	1.522(3)
C(8)-C(9)	1.489(3)		

C(1)-O(1)-C(5)	114.3(2)	C(9)-O(3)-C(6)	111.7(2)
C(12)-O(6)-C(13)	115.7(2)	O(2)-C(1)-O(1)	120.2(2)
O(2)-C(1)-C(2)	126.8(2)	O(1)-C(1)-C(2)	113.0(2)
C(1)-C(2)-C(3)	108.1(2)	C(1)-C(2)-C(7)	104.6(2)
C(3)-C(2)-C(7)	108.8(2)	C(4)-C(3)-C(10)	128.6(2)
C(4)-C(3)-C(2)	112.6(2)	C(10)-C(3)-C(2)	118.8(2)
C(3)-C(4)-C(12)	125.2(2)	C(3)-C(4)-C(5)	114.0(2)
C(12)-C(4)-C(5)	120.9(2)	O(1)-C(5)-C(11)	105.7(2)
O(1)-C(5)-C(4)	108.62(14)	C(11)-C(5)-C(4)	118.5(2)
O(1)-C(5)-C(6)	103.4(2)	C(11)-C(5)-C(6)	112.1(2)
C(4)-C(5)-C(6)	107.5(2)	O(3)-C(6)-C(7)	107.4(2)
O(3)-C(6)-C(5)	109.4(2)	C(7)-C(6)-C(5)	110.3(2)
C(8)-C(7)-C(6)	104.4(2)	C(8)-C(7)-C(2)	114.3(2)
C(6)-C(7)-C(2)	107.5(2)	C(9)-C(8)-C(7)	105.8(2)
O(4)-C(9)-O(3)	120.0(2)	O(4)-C(9)-C(8)	129.4(2)
O(3)-C(9)-C(8)	110.6(2)	O(5)-C(12)-O(6)	123.5(2)
O(5)-C(12)-C(4)	124.6(2)	O(6)-C(12)-C(4)	111.9(2)

(18)

Symmetry transformations used to generate equivalent atoms:



7d