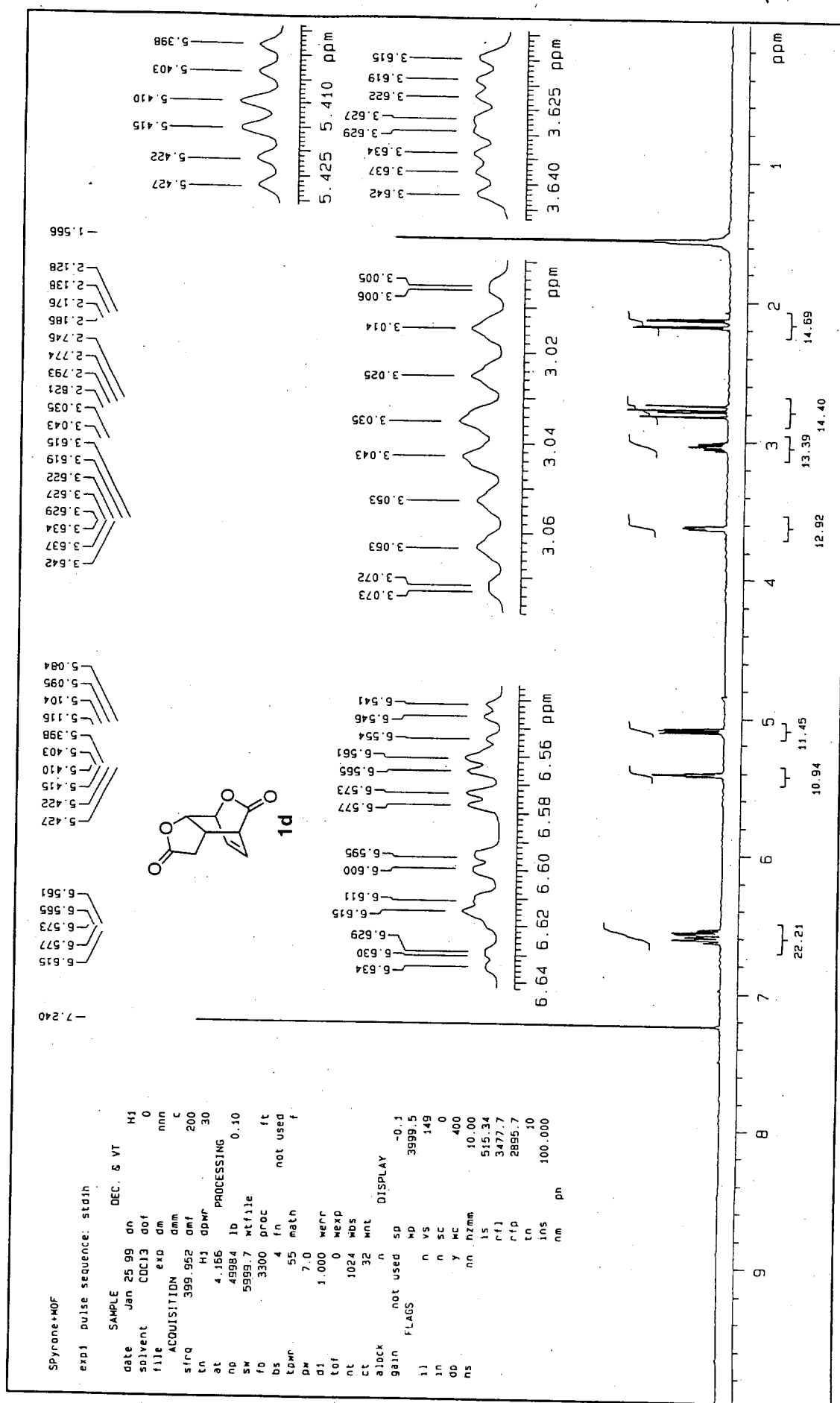




rone+wf
2 pulse sequence: std13c

174.815
170.248

131.605
131.392

32.106
31.544

72.995
76.681
76.833
77.000
77.319

44.258

SAMPLE DEC. & VT

Mar 5.99 dn H1

vent CDC13 dof 0

exp dm yyy

ACQUISITION dmm s

100.577 dmf 9900

C13 dnmr 39

0.654 PROCESSING

32704 lb 2.00

25000.0 wtfile

13800 proc ft

8 fn not used

55 math f

2.000 werr

88888 wds

1656 wnt

53 n

50 -28.9

WD 22126.6

n VS 55

n SC 0

y WC 400

nn hzmm 55.32

is 500.00

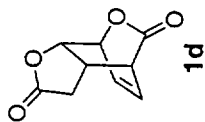
rfl 10646.7

rfd 7744.4

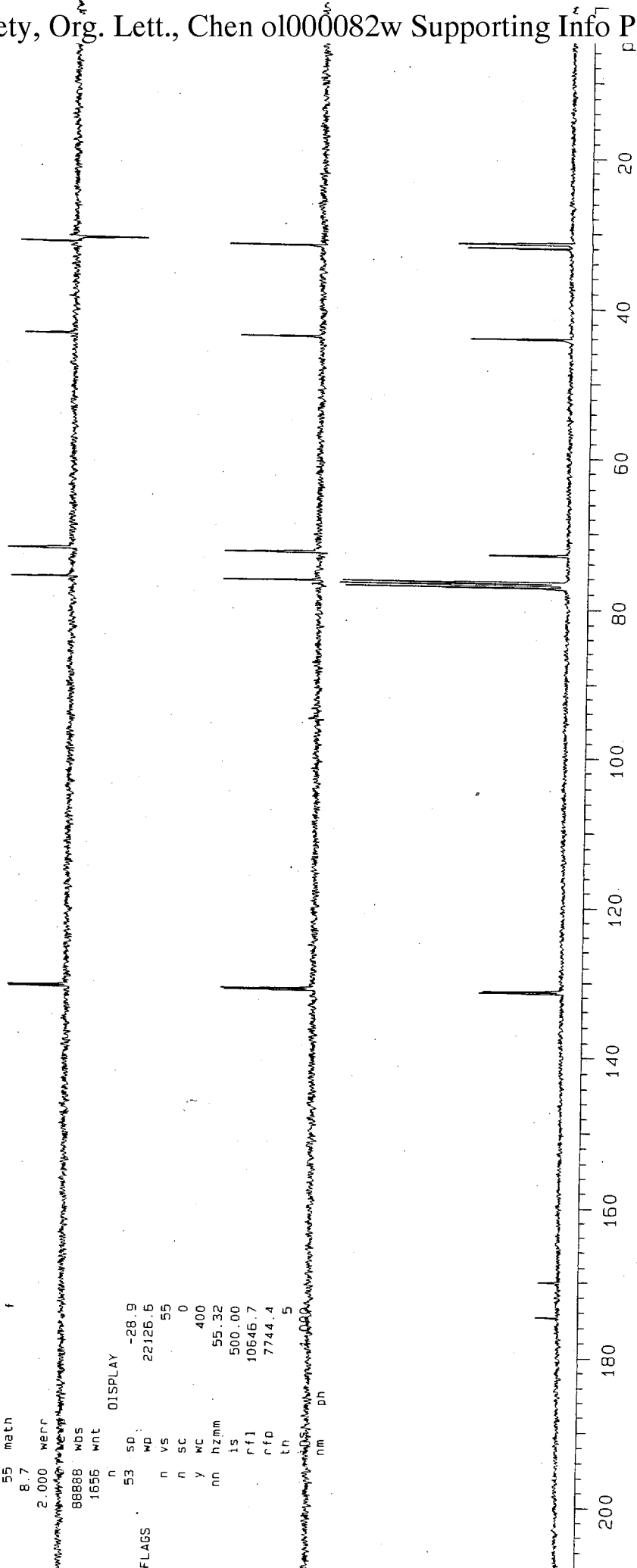
tn 5

nm ph

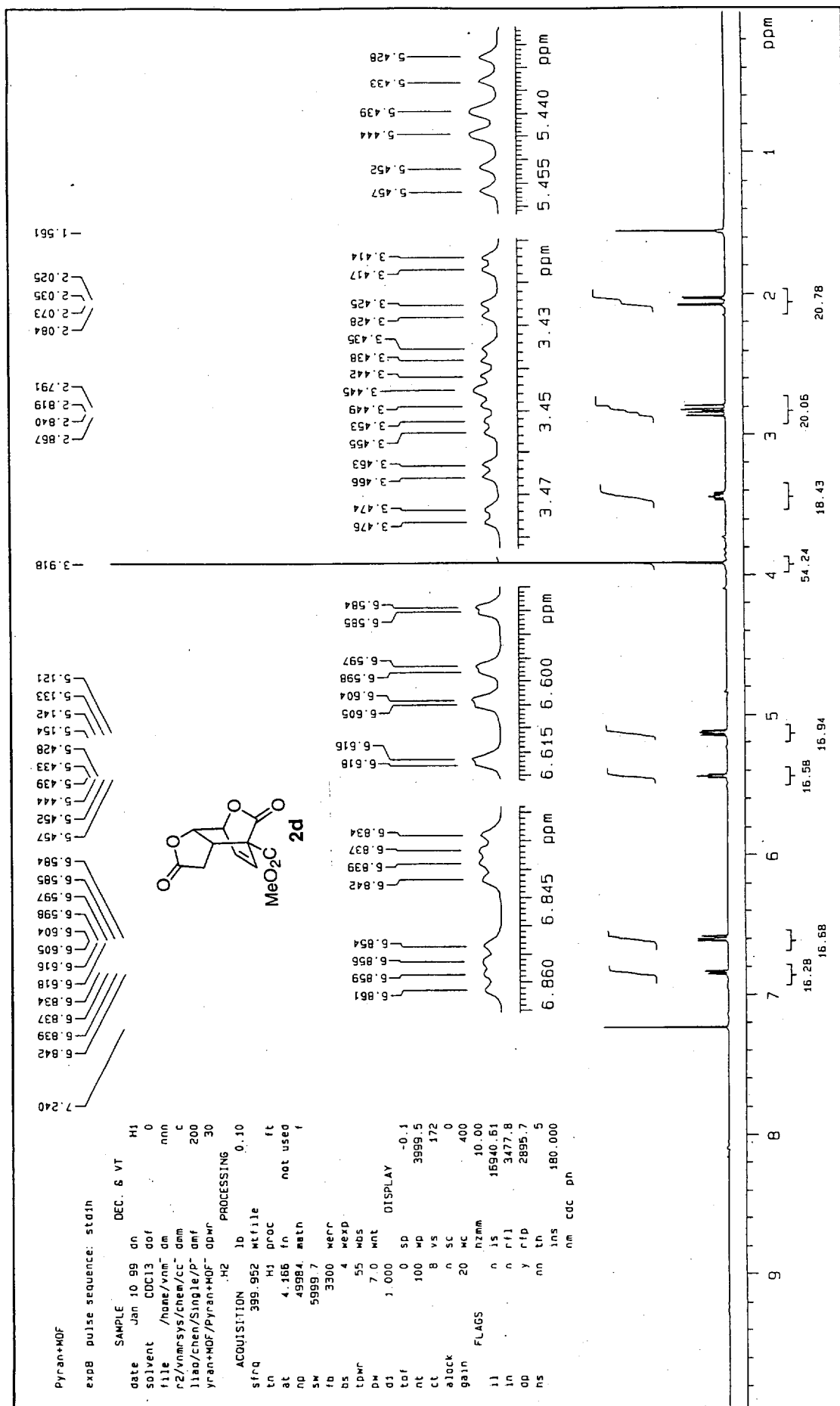
DISPLAY



③



4



⑤

nm+NOF
 pulse sequence: std13c

DEC. & VT

SAMPLE

Dec 17 98 dn H1

ent COC13 dof 0

exp dm yyy

COUSSION

100.577 dm S

C13 dm 9900

0.655 39

PROCESSING

32768 lb 1.00

25000.0 wfile

13800 proc ft

8 fn not used

55 matn f

11.0

3.000 werr

888 w05

384 wnt

not used

SD

22126.6

55

0

400

55.32

500.00

10648.2

7744.4

10

th

nm no dn

DISPLAY

not used

SD

22126.6

55

0

400

55.32

500.00

10648.2

7744.4

10

th

nm no dn

DISPLAY

not used

SD

22126.6

55

0

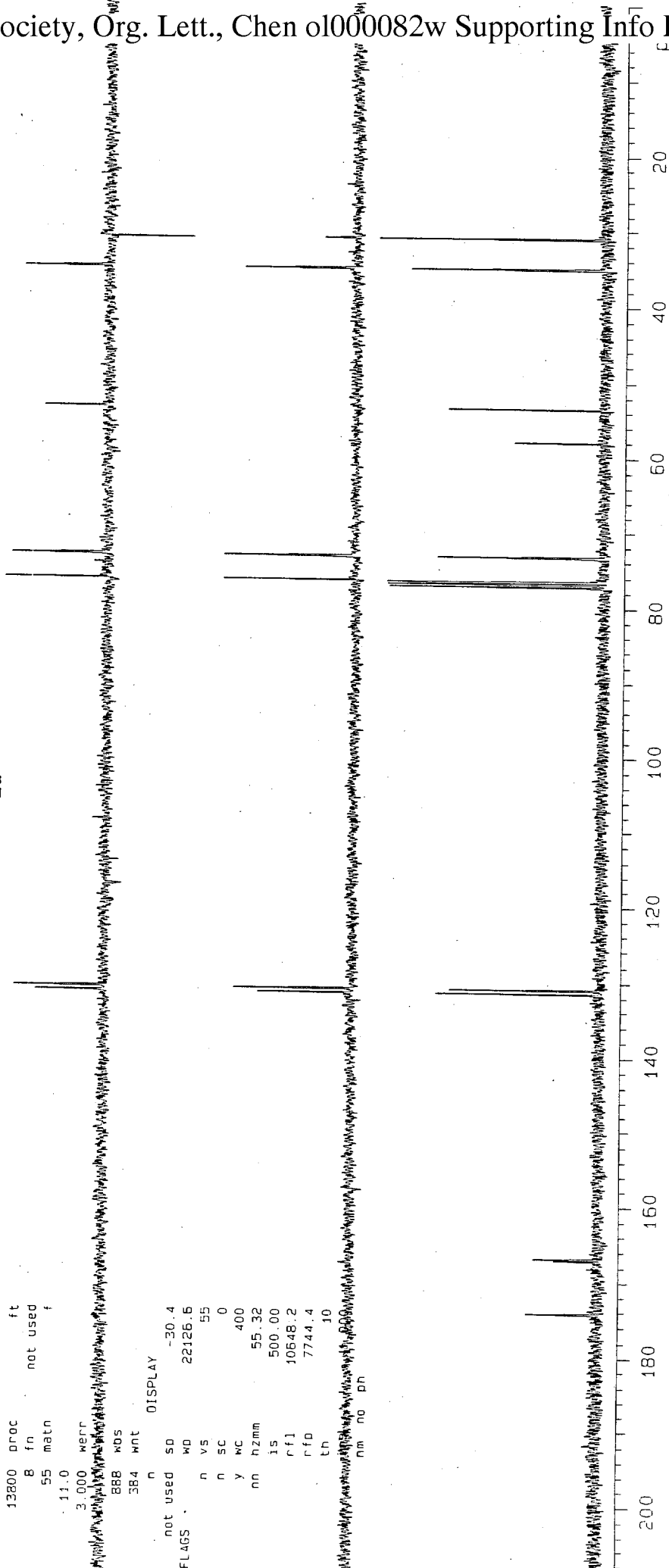
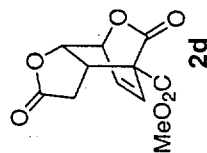
400

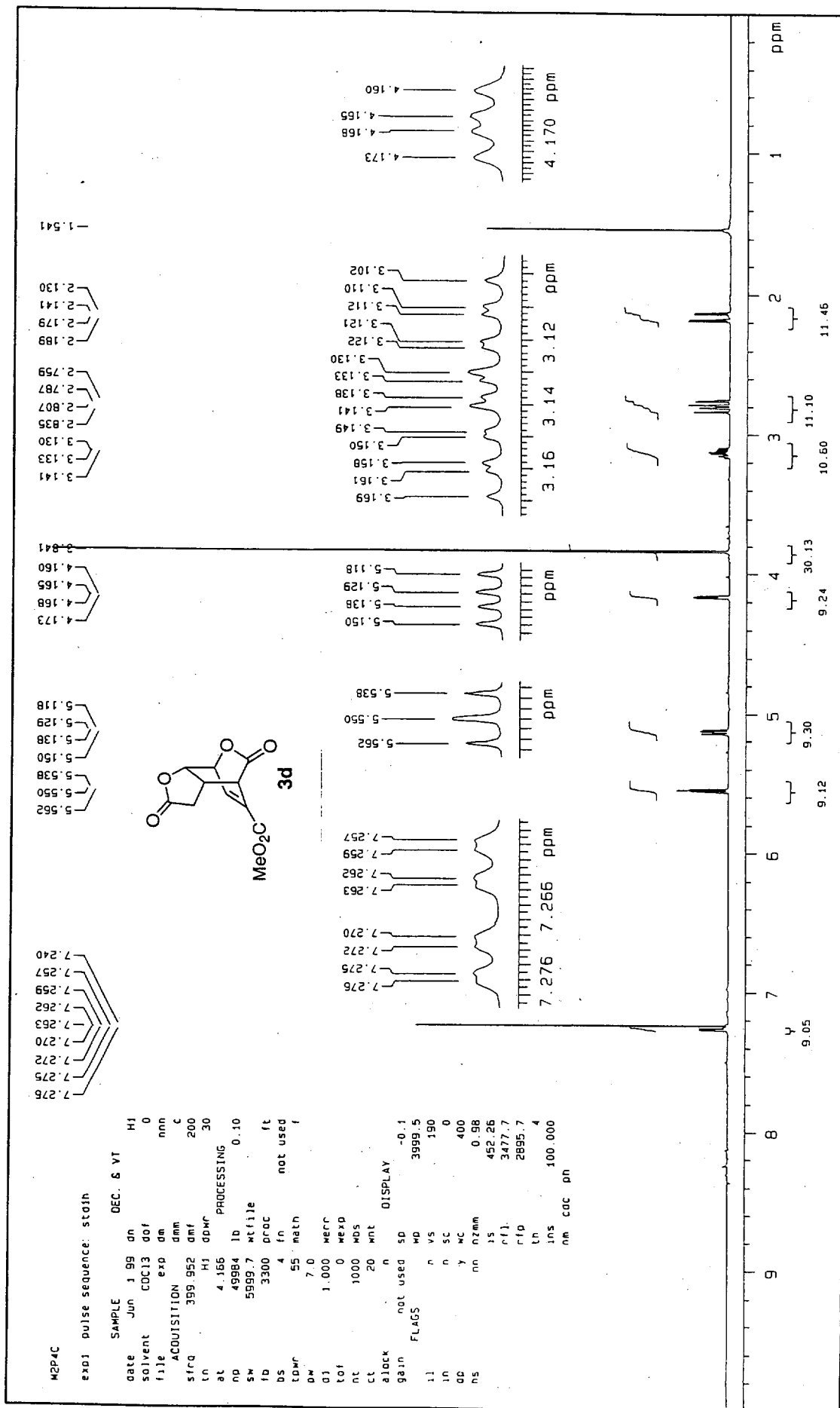
55.32

174.199
 167.108
 166.925

77.319
 77.000
 76.681
 76.606
 73.359

57.989
 53.635
 35.064
 31.165





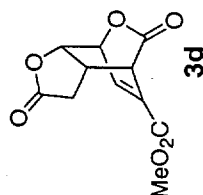
(6)

⑦

30.822
31.793
38.878
39.090
39.288
39.500
39.712
39.925
40.122
43.657
52.821

-72.545
-76.277

-134.508
-138.665
-163.108
-169.738
-175.979



4C-QM50

2 pulse sequence: std13c

SAMPLE DEC. & VT

2 Jun 2.99 dn H1

2 DMSO dof 0

2 exp dm yyy

2 ACQUISITION dm s

2 100.577 dmf 9900

2 C13 dmr 39

PROCESSING

0.655

32768 lb 1.00

25000.0 wfile

13800 proc ft

4 fn not used

55 math f

8.7

2.000 werr

8888 wds

380 wnt

not used

sp -63.4

wd 22126.6

n vs 55

n sc 0

y xc 400

nn hzmm 55.32

ls 500.00

rfl 6909.6

rfd 3972.8

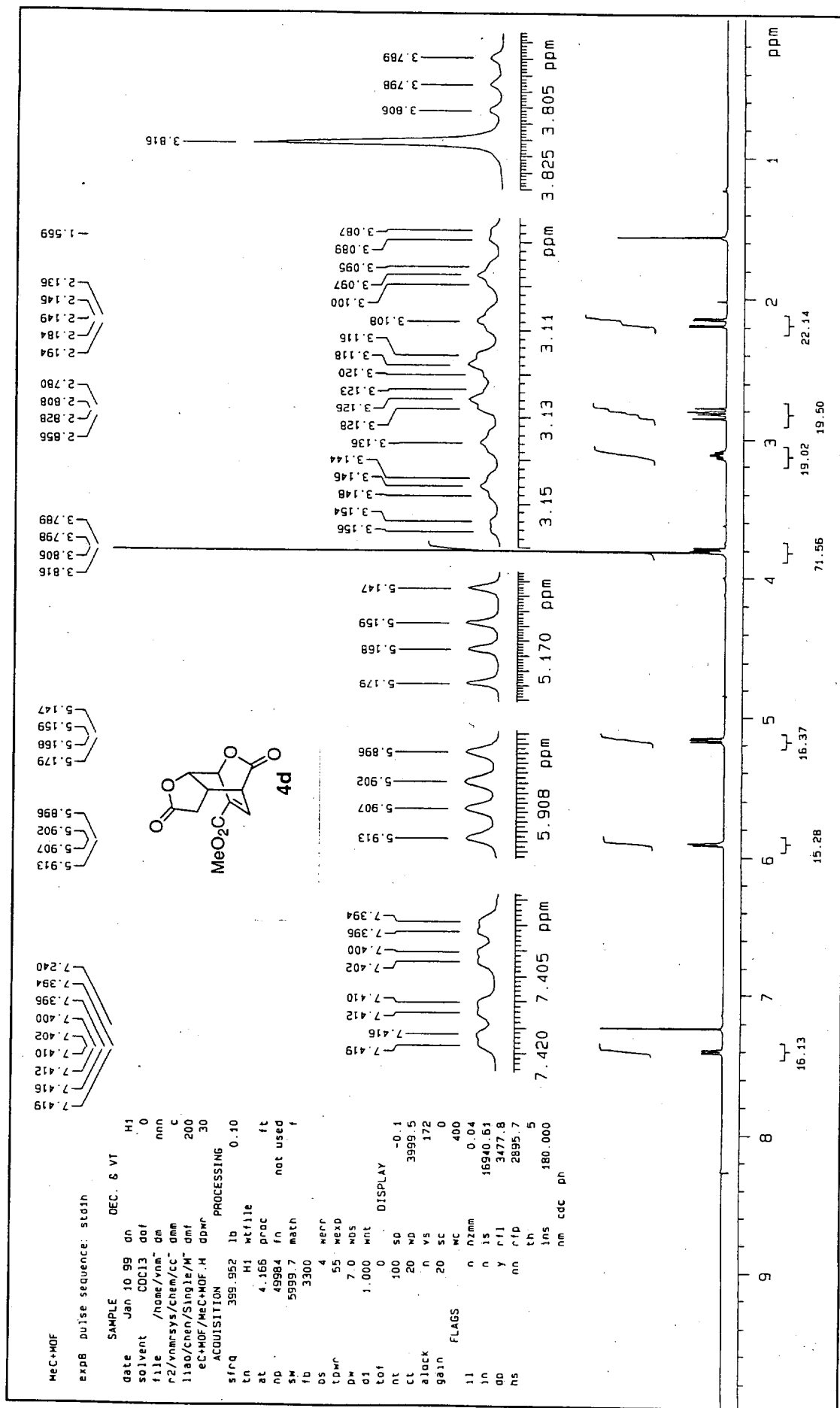
th 5

nm no ph

DISPLAY

FLAGS

200 180 160 140 120 100 80 60 40 20



9

MOF
pulse sequence: std13c

SAMPLE DEC. & VT

Jan 10 99 dn H1
ent CDC13 dof 0
/home/vnm~ dm yyy
nmrsys/chem/cc~ dmm s
/chen/Singlet/M~ dmf 9900
+MOF/Mec+MOF.C ddw 39

COUSITION PROCESSING

100.577 lb 1.00
C13 wfile
0.655 proc ft
32768 fn not used f
25000.0 math
13800

8 werr

11.0 wds

3.000 wnt

0 DISPLAY

888 sd -27.3
888 wd 22126.6
n v5 55

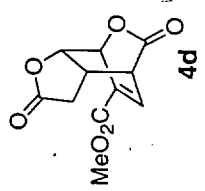
not used sc 0
wc 400

h2mm 55.32
n l5 500.00

y rfl 10645.2
nn rfp 7744.4

th 3

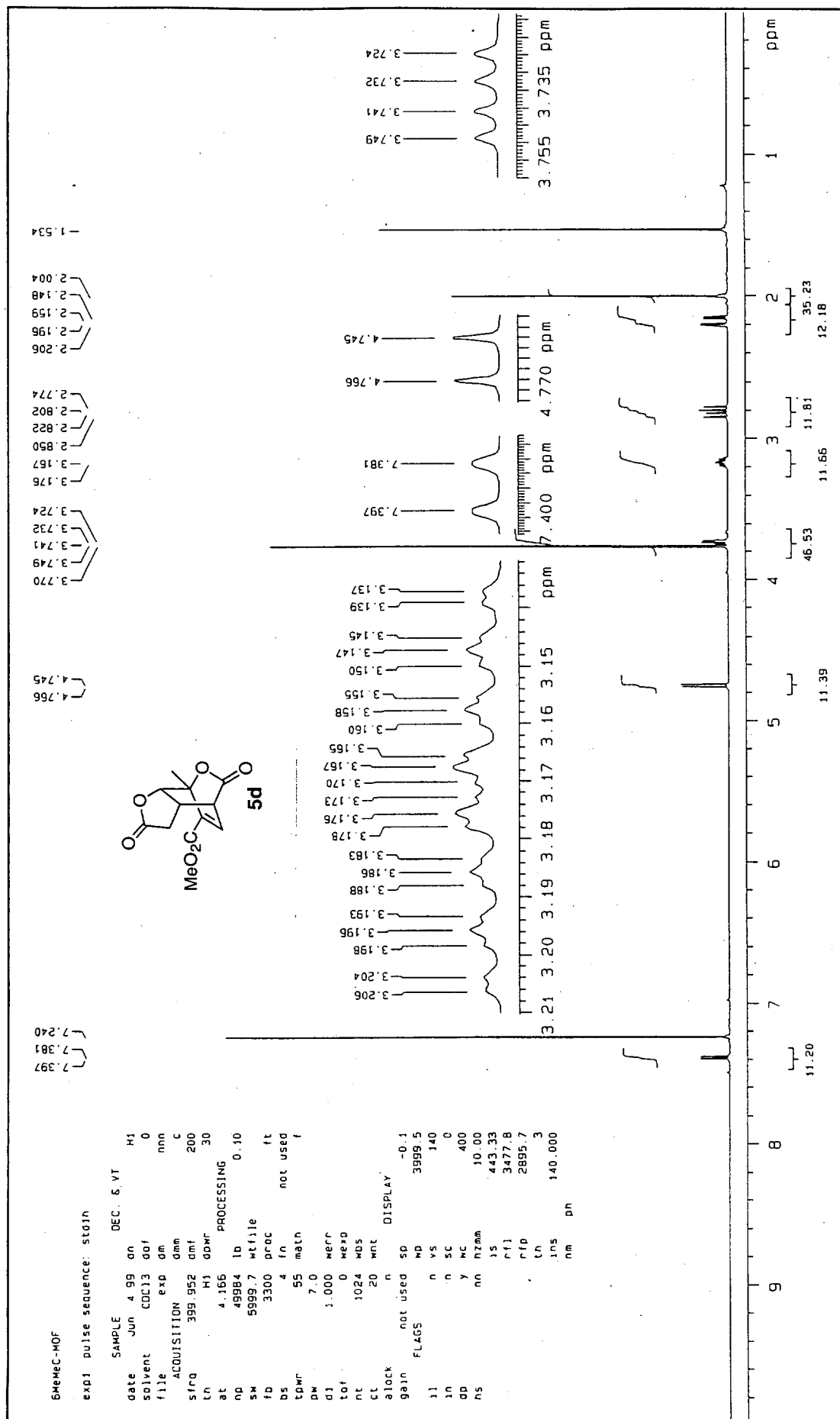
nm no dn



77.319
77.000
76.681
76.241
72.646
-52.694
-44.789
-32.379
-31.408

-174.011
-168.807
-161.630
-138.766
-135.686

200 180 160 140 120 100 80 60 40 20



MeC+MOF-DMSO

7 pulse sequence: std13c

SAMPLE DEC. & VT

2 Jan 24 99 dn H1

3 DMSO dof 0

4 exp dm YYY

5 ACQUISITION s

6 100.577 dmf 9900

7 C13 dpr 39

8 0.654 PROCESSING

9 32704 lb 1.00

10 25000.0 wfile

11 13800 proc ft

12 B fn not used f

13 55 math

14 21.0

15 2.000 werr

16 8888 wds

17 568 wnt

18 n .

19 DISPLAY

20 50 SP -69.5

21 WD 22125.6

22 Y VS 55

23 N SC 0

24 Y WC 400

25 NN HZMM 0.97

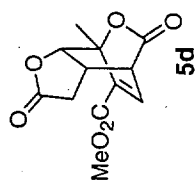
26 IS 500.00

27 RF1 5915.7

28 RFP 3972.8

29 TH 5

30 nm ng ph



-175.903

-169.617

-162.395

-141.927

-135.434

81.982

81.497

-19.594

30.973

33.279

38.878

39.090

39.303

39.515

39.712

39.925

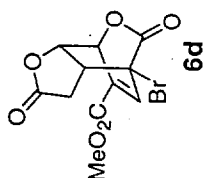
40.137

44.446

52.108



77.303
77.000
76.681
76.302
71.948
-58.809
-52.952
-42.453
-31.741



-172.736
-164.801
-160.659
-143.044
-134.639

1eC+MOF

2 pulse sequence: std13c

SAMPLE DEC. & VT

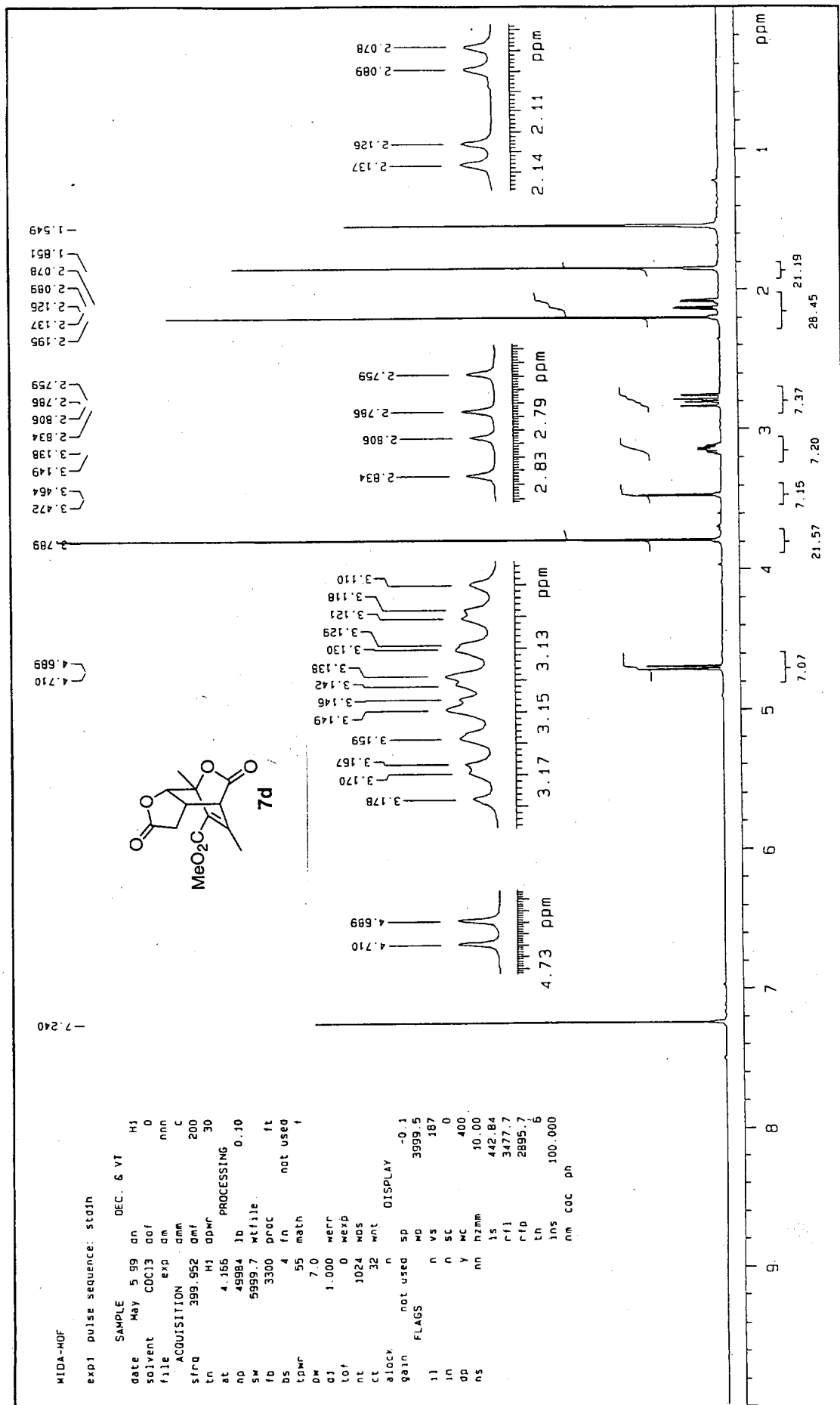
Feb 9.99 dn H1
ent COC13 0 of 0
exp dm yyy
COUSSION s
100.577 dmf 9900
C13 ddwr 39
0.654 PROCESSING
32704 lb 1.00
25000.0 wfile
13800 proc ft
8 fn not used
55 math f
8.7
2.000 werr
8888 wds
752 wnt

DISPLAY

53 sp -33.5
WD 22126.6
n VS 55
n SC 0
y WC 400
nn hzmm 55.32
ls 500.00
rf1 10651.3
rfd 7744.4
th 7
1.000
nm ph

FLAGS

200 180 160 140 120 100 80 60 40 20



(14)

(15)

19.695
20.954
30.437
33.092

50.752
51.996

76.681
77.015
77.319
81.749
81.794

130.725
146.489
163.921
169.505
174.178

MOF

pulse sequence: std13c

SAMPLE DEC. & VT

May 3 99 dn H1

nt CDC13 dof 0

/home/vnm~ dm yyy

mrsys/chem/cc~ dnm s

chen/MIDA-MOF~ dmf 9900

/MIDA-MOF.C dmr 39

QUISITION PROCESSING

100.577 lb 1.00

C13 wfile

0.555 proc ft

32768 fn not used

25000.0 math f

13800

8 werr

8.7 mbs

2.000 mnt

0

1024 sp

24 wp

n vs

53 sc

0

wc 400

n hzmm

55.32

n is

500.00

y rfl

10652.8

nn rfp

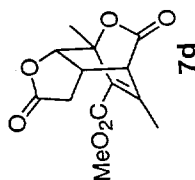
7744.4

th 10

nm no ph

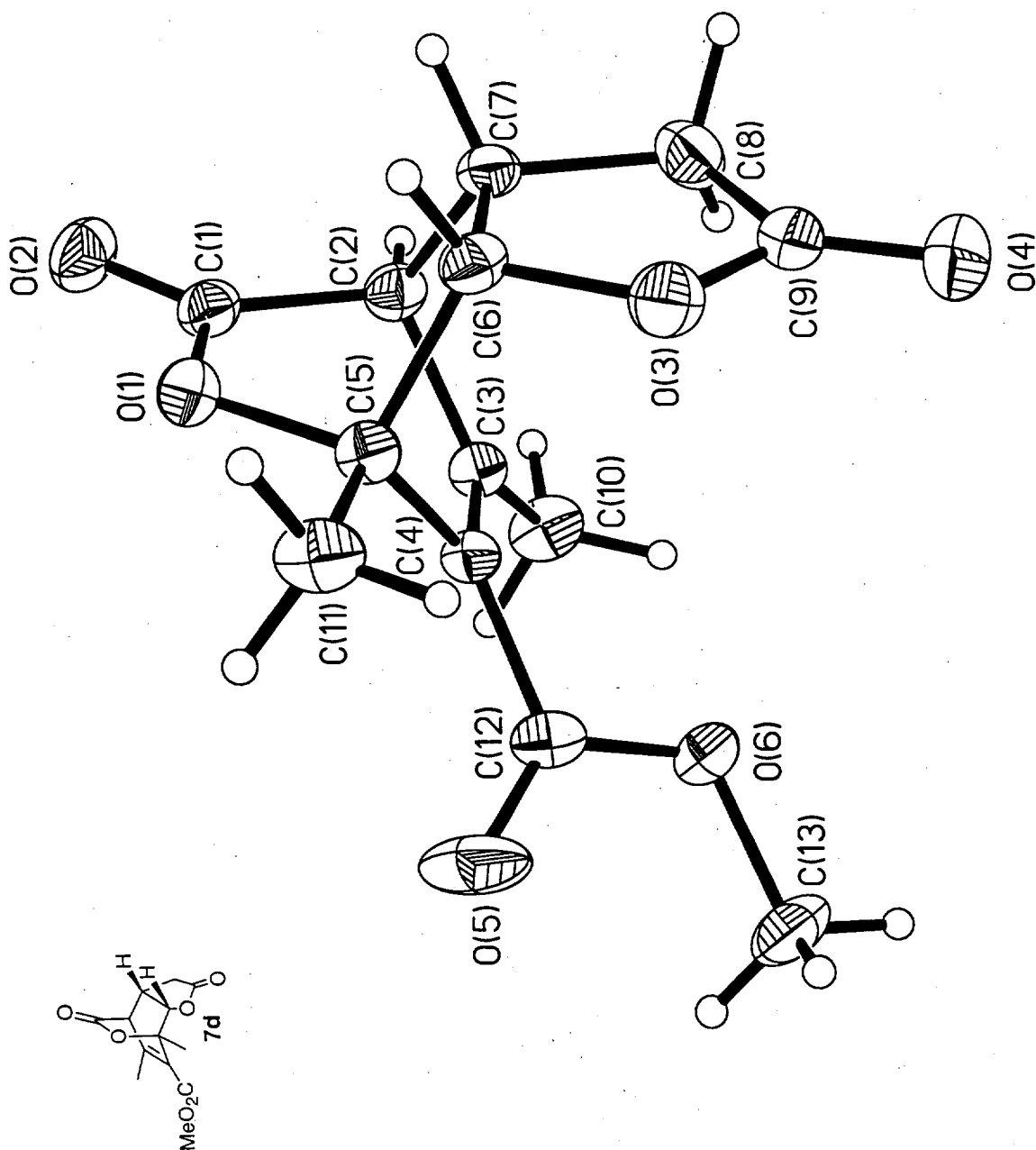
1.000

FLAGS



200 180 160 140 120 100 80 60 40 20

16



The molecular structure of IC6673, thermal ellipsoids drawn at the 30% probability 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 $\alpha = 90^\circ$ $b = 7.429(2)$ Å $\beta = 105.69(2)^\circ$ $c = 13.834(3)$ Å $\gamma = 90^\circ$
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	$-16 \leq h \leq 15$, $0 \leq k \leq 9$, $0 \leq l \leq 17$
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 [$I > 2\sigma(I)$]	$R1 = 0.0502$, $wR2 = 0.1502$
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

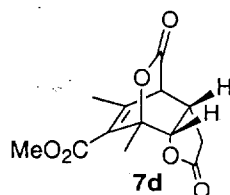


Table 2. Bond lengths [Å] and angles [°] for 6673.

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)

Symmetry transformations used to generate equivalent atoms:

