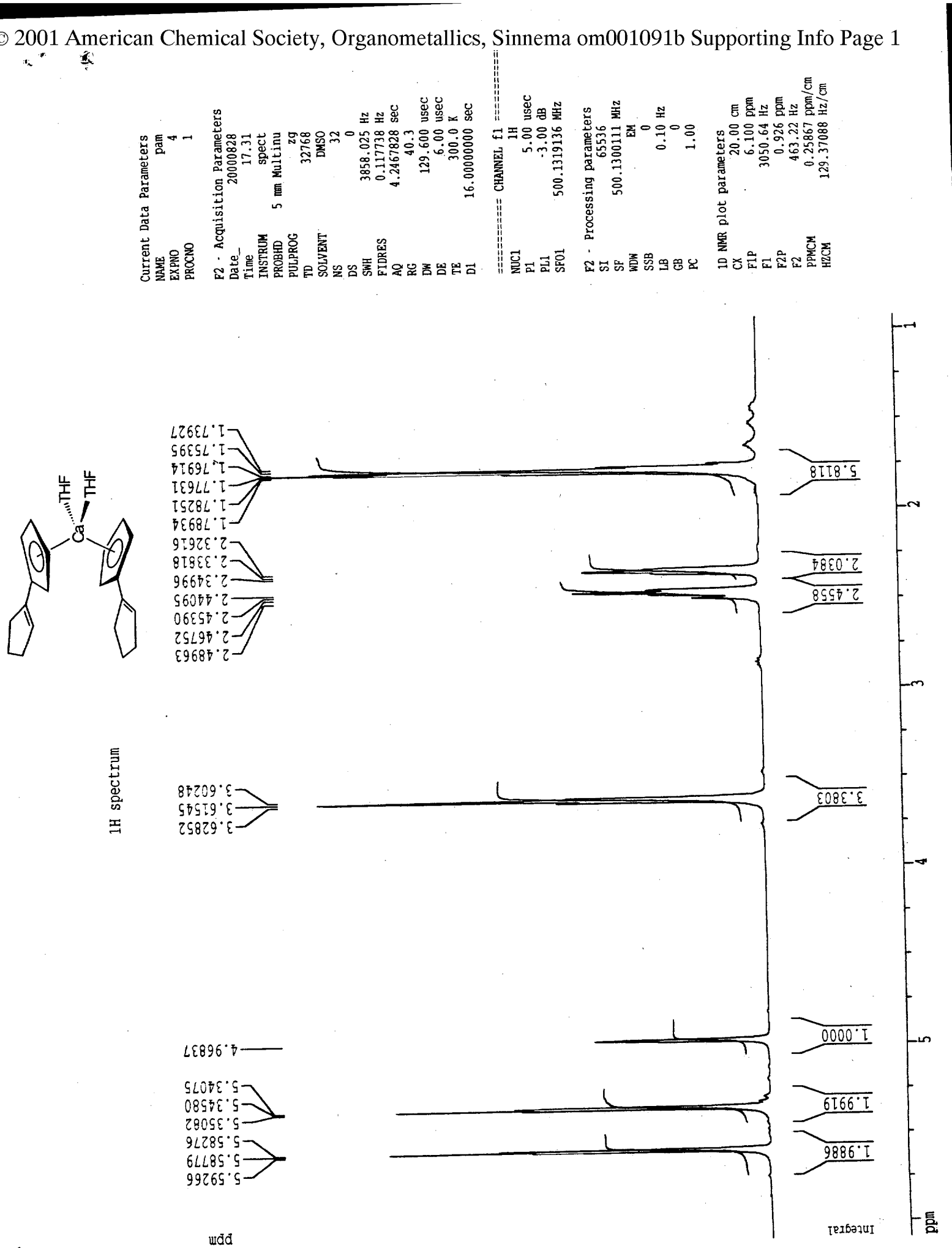
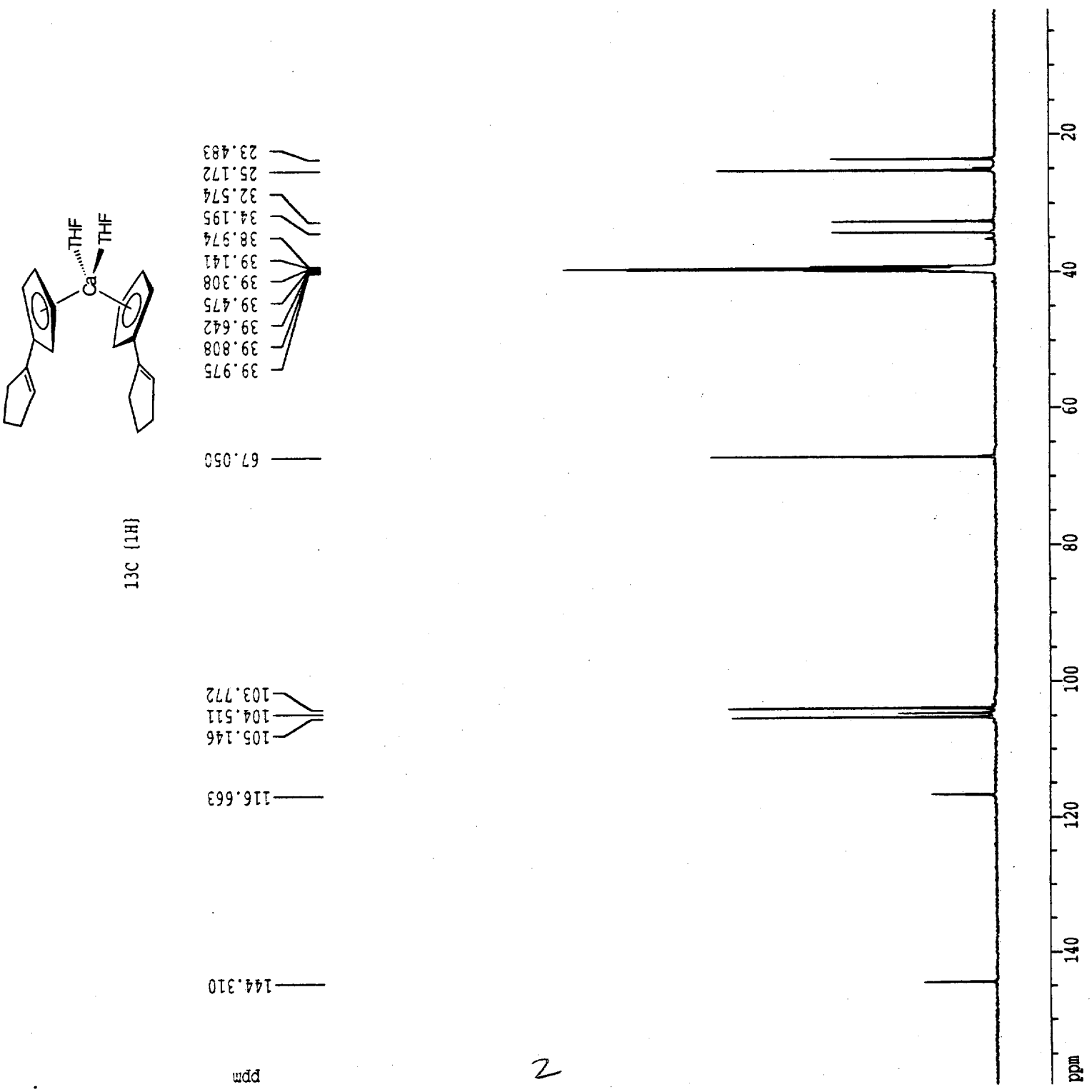
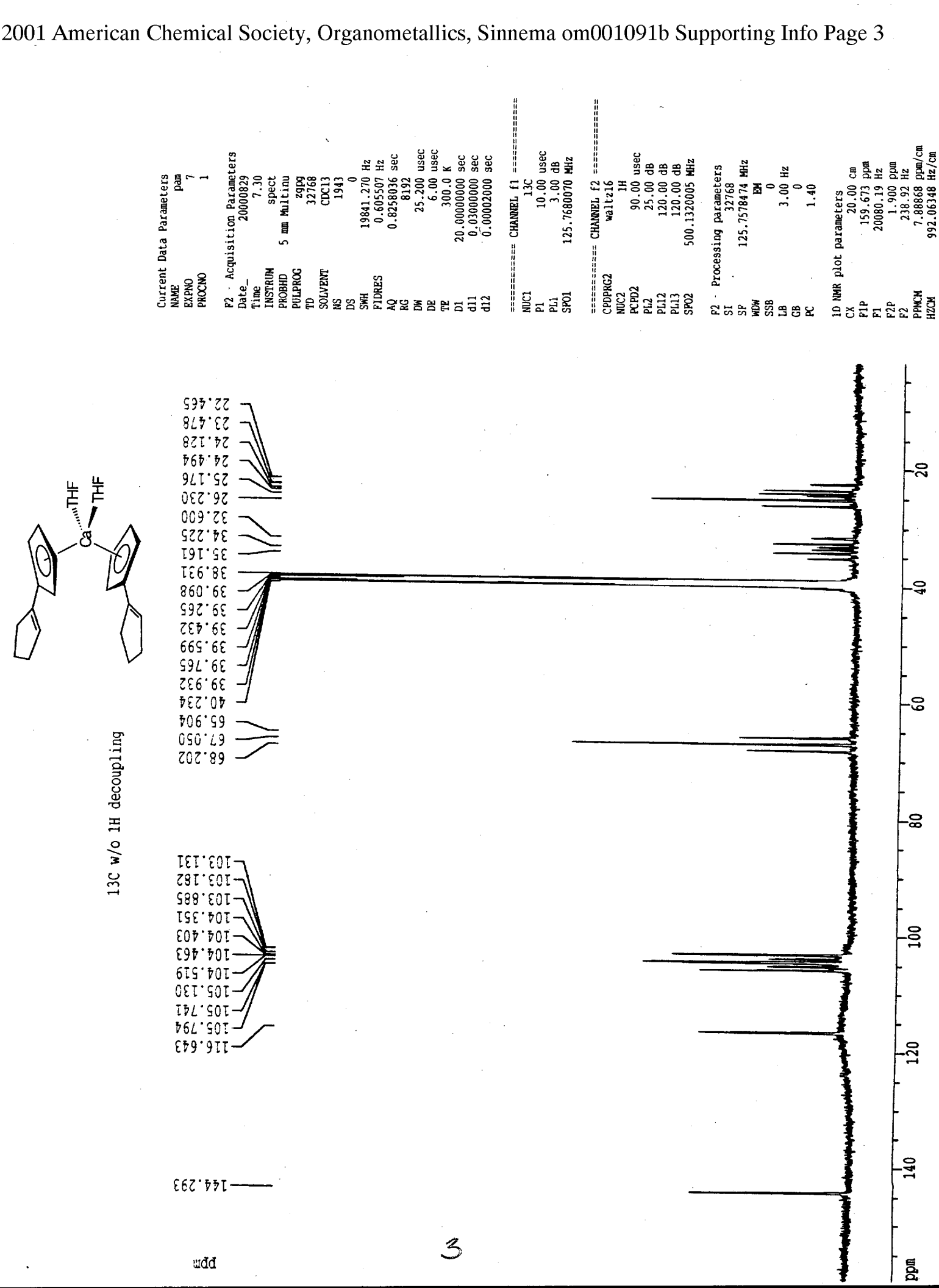
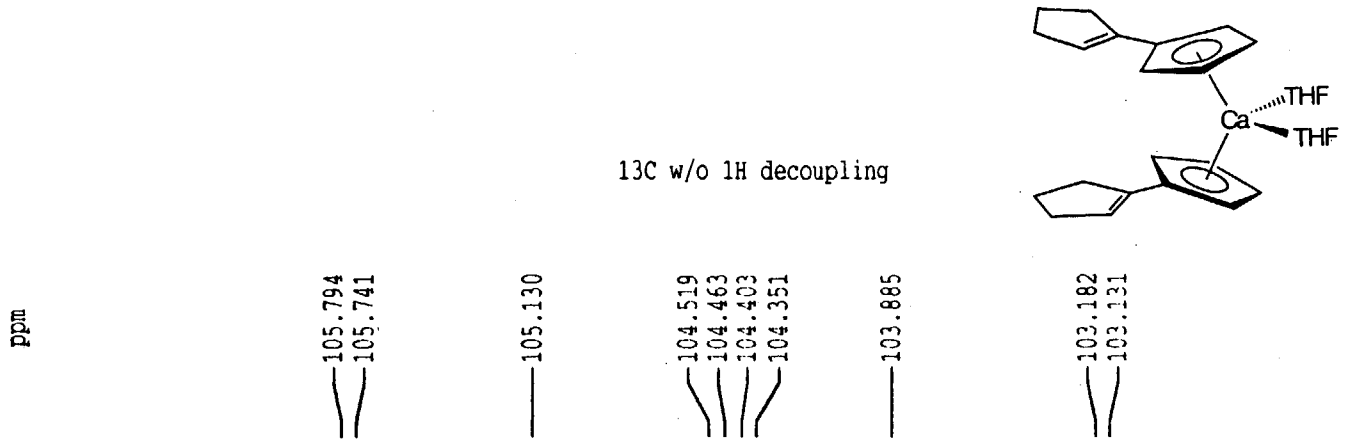




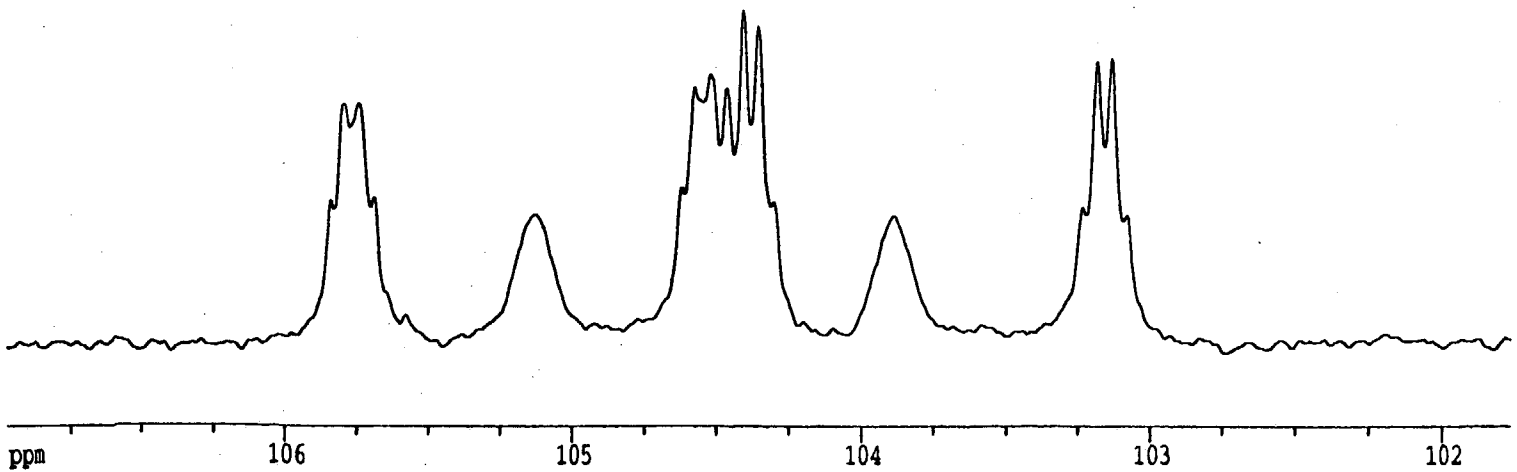




13C w/o 1H decoupling

ppm

105.794
105.741
105.130
104.519
104.463
104.403
104.351
103.885
103.182
103.131



Current Data Parameters
NAME pam
EXPNO 7
PROCNO 1

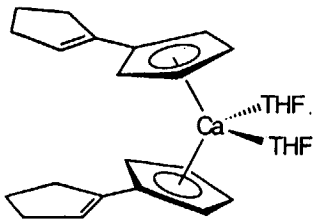
F2 - Acquisition Parameters
Date_ 20000829
Time 7.30
INSTRUM spect
PROBHD 5 mm Multinu
PULPROG zgpg
TD 32768
SOLVENT CDCl3
NS 1943
DS 0
SWH 19841.270 Hz
FIDRES 0.605507 Hz
AQ 0.8258036 sec
RG 8192
DW 25.200 usec
DE 6.00 usec
TE 300.0 K
D1 20.00000000 sec
d11 0.03000000 sec
d12 0.00002000 sec

========== CHANNEL f1 ==========
NUC1 13C
P1 10.00 usec
PL1 3.00 dB
SFO1 125.7680070 MHz

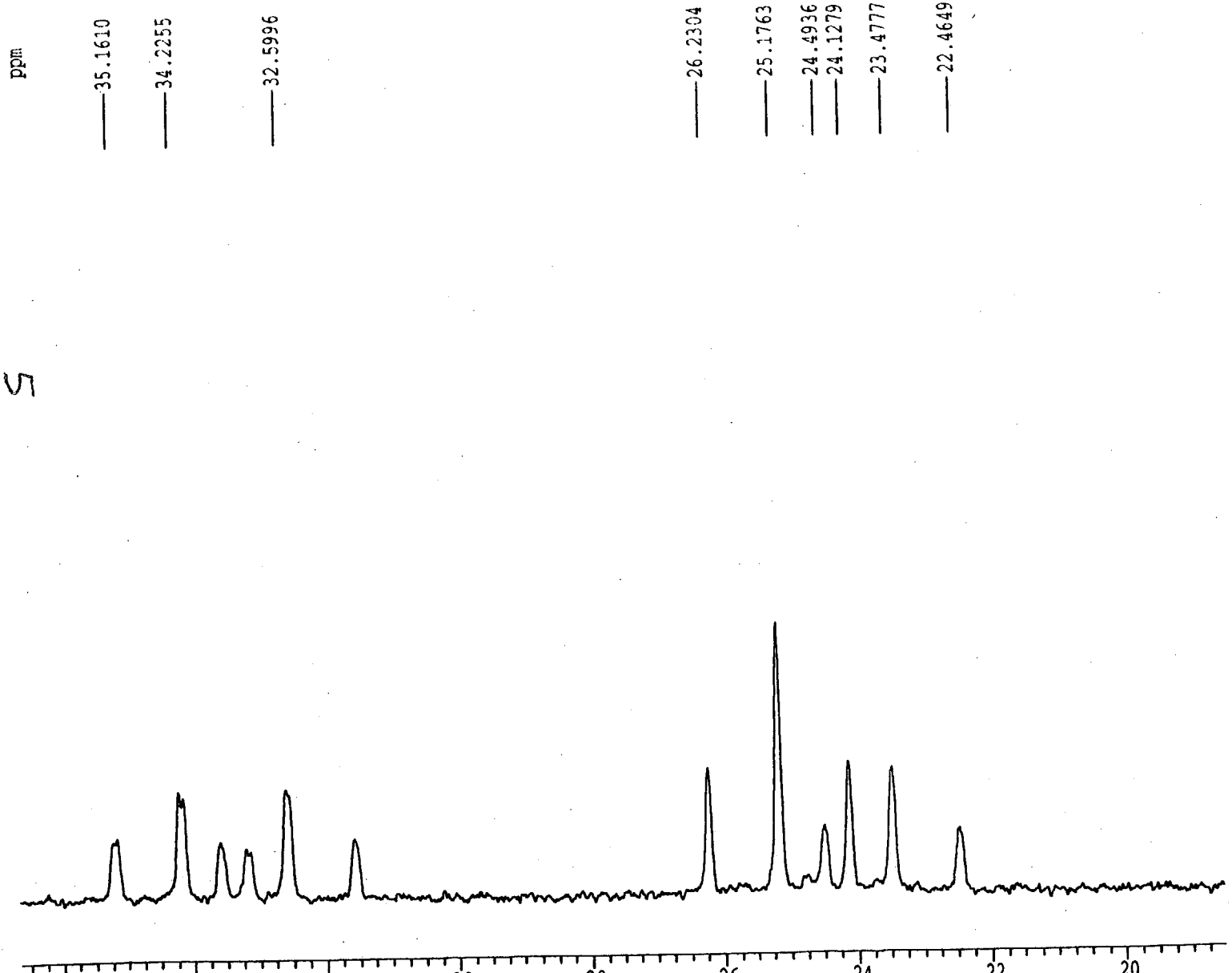
========== CHANNEL f2 ==========
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 25.00 dB
PL12 120.00 dB
PL13 120.00 dB
SFO2 500.1320005 MHz

F2 - Processing parameters
SI 32768
SF 125.7578474 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.40

1D NMR plot parameters
CX 20.00 cm
F1P 106.978 ppm
F1 13453.33 Hz
F2P 101.759 ppm
F2 12796.98 Hz
PPMCM 0.26096 ppm/cm
HZCM 32.81719 Hz/cm



13C w/o 1H decoupling



Current Data Parameters

NAME	pam
EXPNO	7
PROCNO	1

F2 - Acquisition Parameters

Date_	20000829
Time	7.30
INSTRUM	spect
PROBHD	5 mm Multinu
PULPROG	zgpg
TD	32768
SOLVENT	CDCl3
NS	1943
DS	0
SWH	19841.270 Hz
FIDRES	0.605507 Hz
AQ	0.8258036 sec
RG	8192
DW	25.200 usec
DE	6.00 usec
TE	300.0 K
D1	20.00000000 sec
d11	0.03000000 sec
d12	0.00002000 sec

========== CHANNEL f1 ==========

NUC1	13C
P1	10.00 usec
PL1	3.00 dB
SFO1	125.7680070 MHz

========== CHANNEL f2 ==========

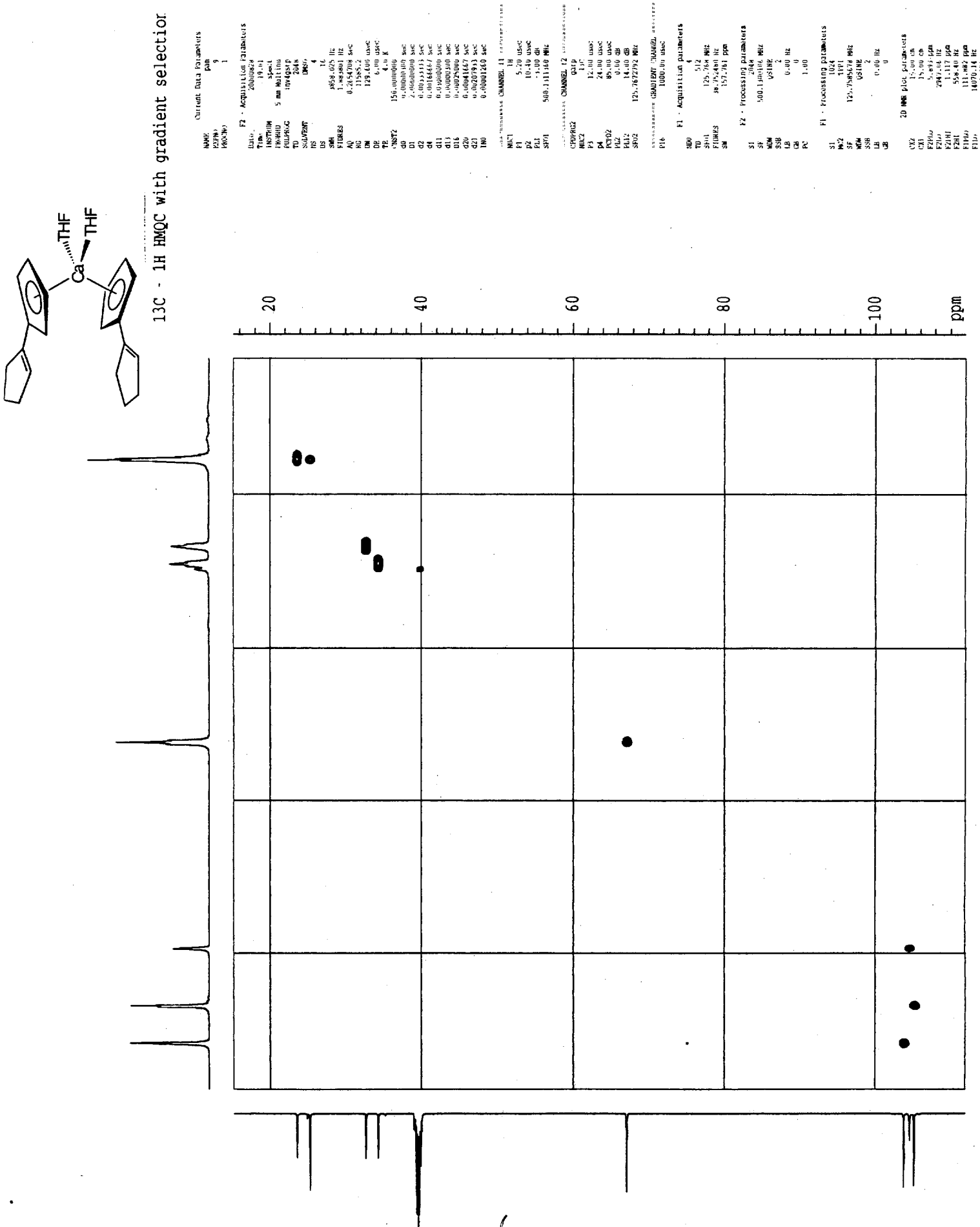
CPDPRG2	waltz16
NUC2	1H
PCPD2	90.00 usec
PL2	25.00 dB
PL12	120.00 dB
PL13	120.00 dB
SFO2	500.1320005 MHz

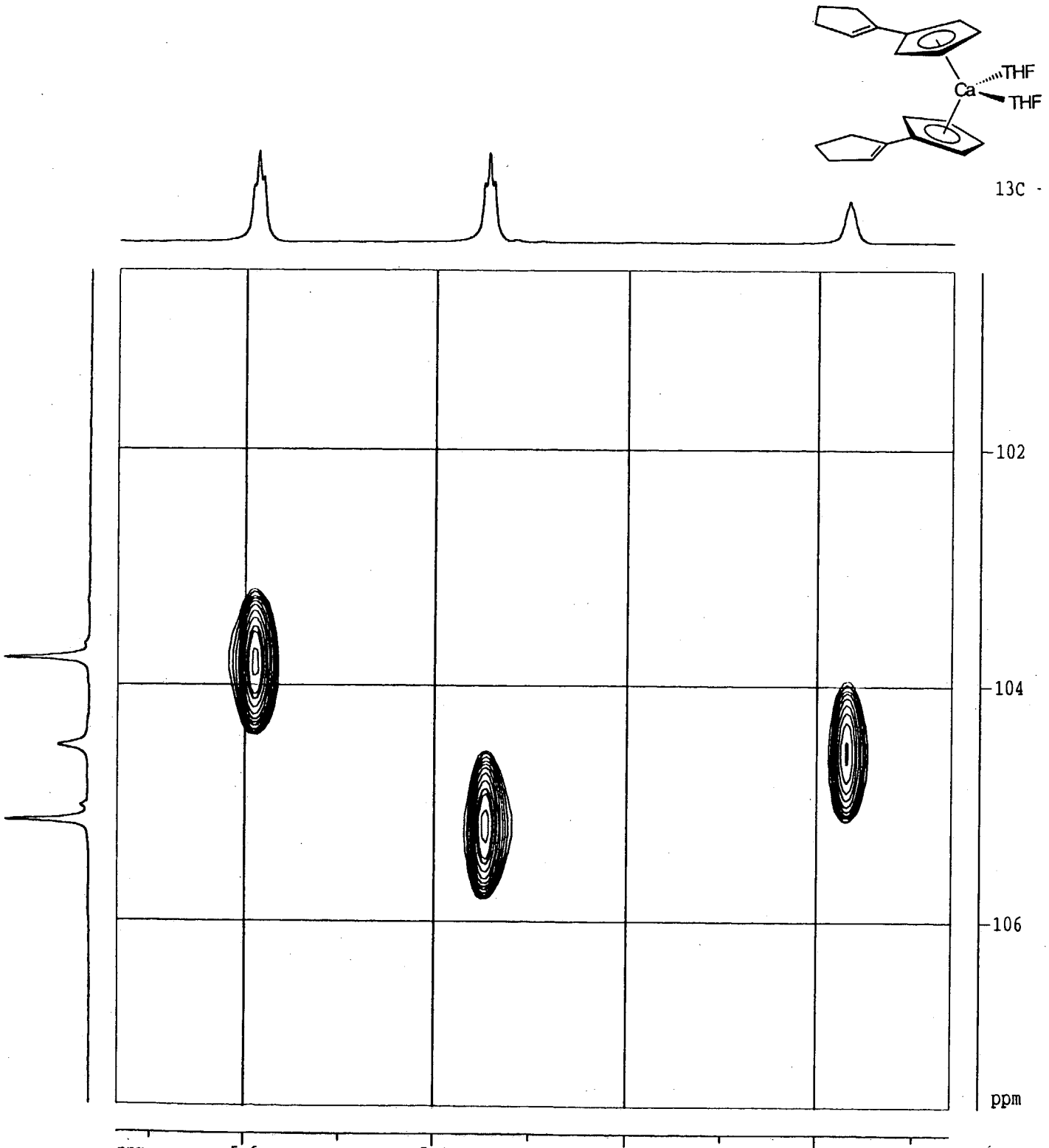
F2 - Processing parameters

SI	32768
SF	125.7578474 MHz
WDW	EM
SSB	0
LB	3.00 Hz
GB	0
PC	1.40

1D NMR plot parameters

CX	20.00 cm
F1P	36.667 ppm
F1	4611.13 Hz
F2P	18.528 ppm
F2	2329.98 Hz
PPMCM	0.90696 ppm/cm
HZCM	114.05762 Hz/cm





Current Data Parameters

NAME	pam
EXPNO	9
PROCNO	1

F2 - Acquisition Parameters

Date	20000826
Time	19.01
INSTRUM	spect
PROBHD	5 mm Multinu
PULPROG	inv4gs1.p
TD	2048
SOLVENT	DMSO
NS	4
DS	16
SWH	8000.025 Hz
FIDRES	1.953801 Hz
AQ	0.2654704 sec
RG	11585.2
DW	129.600 usec
DE	6.00 usec
TE	4.0 K
CNST2	150.0000000
d0	0.0000030 sec
D1	2.0000000 sec
d2	0.0033333 sec
d4	0.0016667 sec
d11	0.0500000 sec
d13	0.0000080 sec
D16	0.0002500 sec
d20	0.0041667 sec
d21	0.0020793 sec
ING	0.0000126 sec

CHANNEL f1

NUC1	1H
P1	5.20 usec
p2	10.40 usec
PL1	-3.00 dB
SFO1	500.1311360 MHz

CHANNEL f2

CPDPRG2	garp
NUC2	13C
P3	12.00 usec
p4	24.00 usec
PCPD2	85.00 usec
PL2	0.00 dB
PL12	14.00 dB
SFO2	125.7672792 MHz

GRADIENT CHANNEL

P16	1000.00 usec

F1 - Acquisition parameters

NDO	4
TD	512
SFO1	125.768 MHz
FIDRES	38.7528x0 Hz
SW	157.761 ppm

F2 - Processing parameters

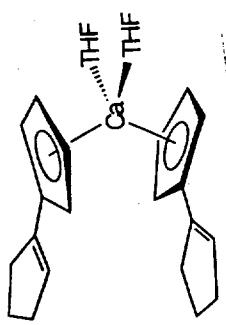
SI	2048
SF	500.1400106 MHz
WDW	QSINE
SSB	2
LB	0.00 Hz
GB	0
PC	1.00

F1 - Processing parameters

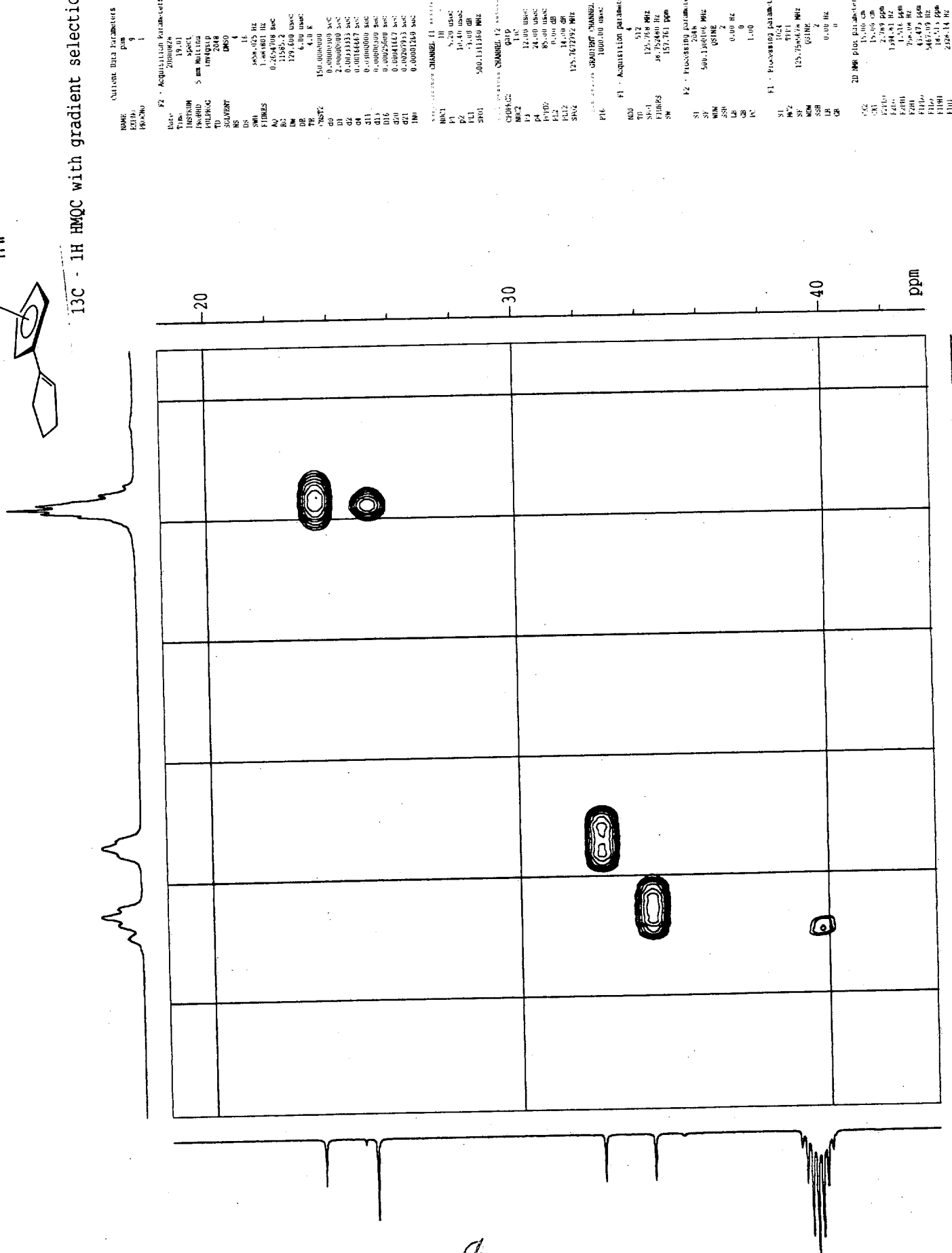
SI	1024
MC2	TPPI
SF	125.7585678 MHz
WDW	QSINE
SSB	2
LB	0.00 Hz
GB	0

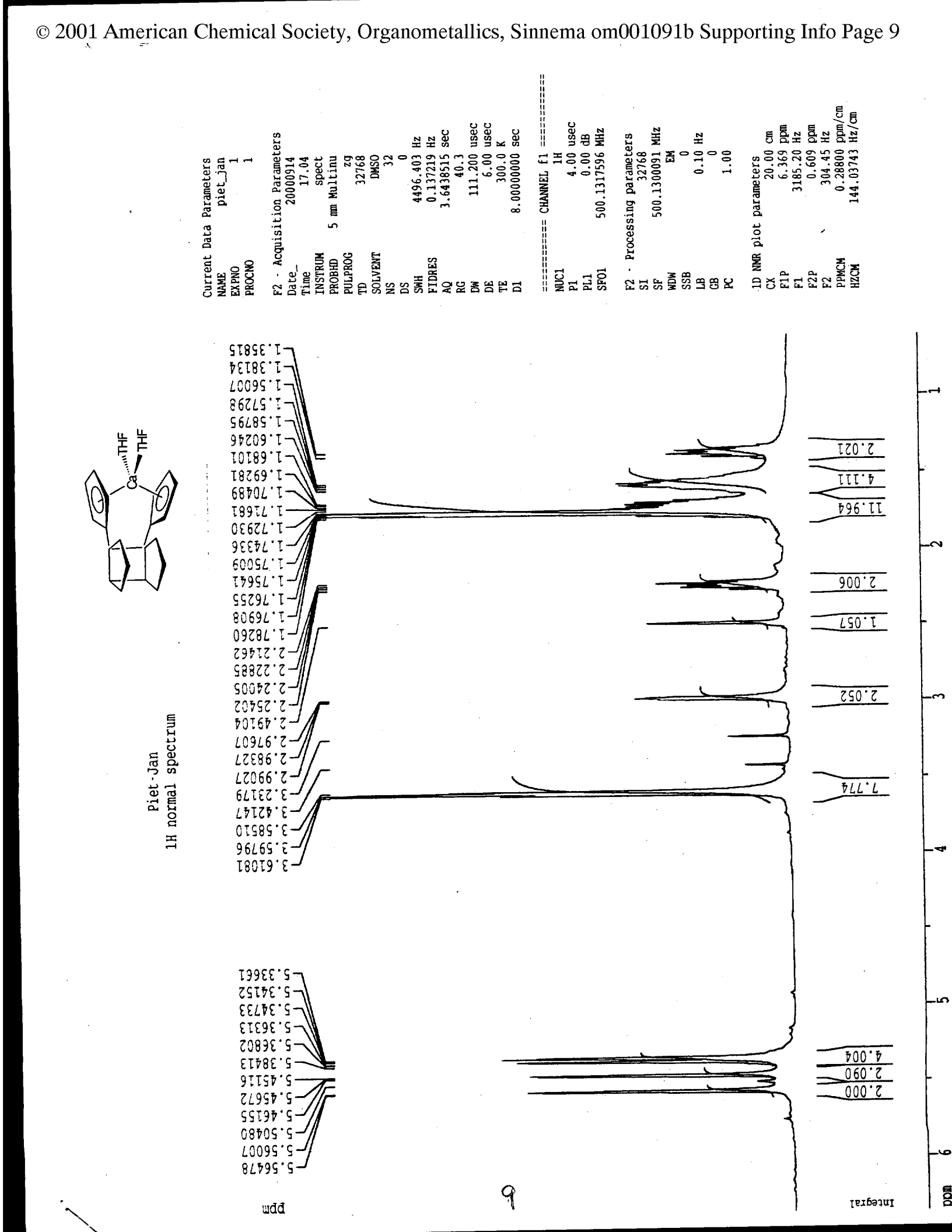
2D NMR plot parameters

CX2	15.00 cm
CX1	15.00 cm
F2PLO	5.734 ppm
F2LO	2867.94 Hz
F2PH1	4.861 ppm
F2H1	2430.90 Hz
F1PLO	107.566 ppm
F1LO	13527.80 Hz
F1PH1	100.481 ppm
F1H1	12636.30 Hz

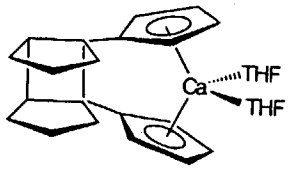


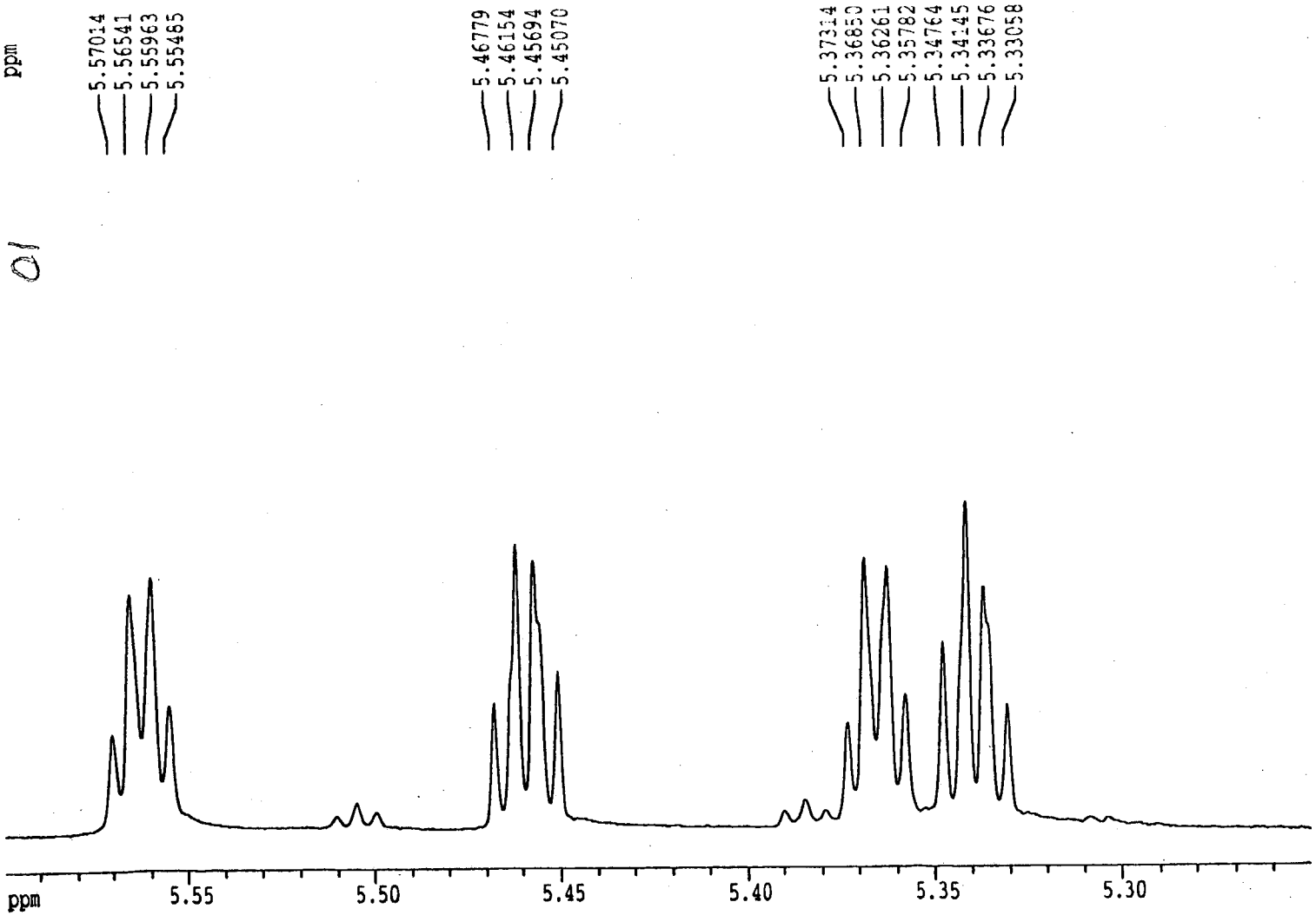
13C - 1H HMQC with gradient selection





Piet-Jan
1H gaussian line narrowing





Current Data Parameters

NAME	piet_jan
EXPNO	1
PROCNO	1

F2 - Acquisition Parameters

Date_	20000914
Time	17.04
INSTRUM	spect
PROBHD	5 mm Multinu
PULPROG	zg
TD	32768
SOLVENT	DMSO
NS	32
DS	0
SWH	4496.403 Hz
FIDRES	0.137219 Hz
AQ	3.6438515 sec
RG	40.3
DW	111.200 usec
DE	6.00 usec
TE	300.0 K
D1	8.00000000 sec

========== CHANNEL f1 ==========

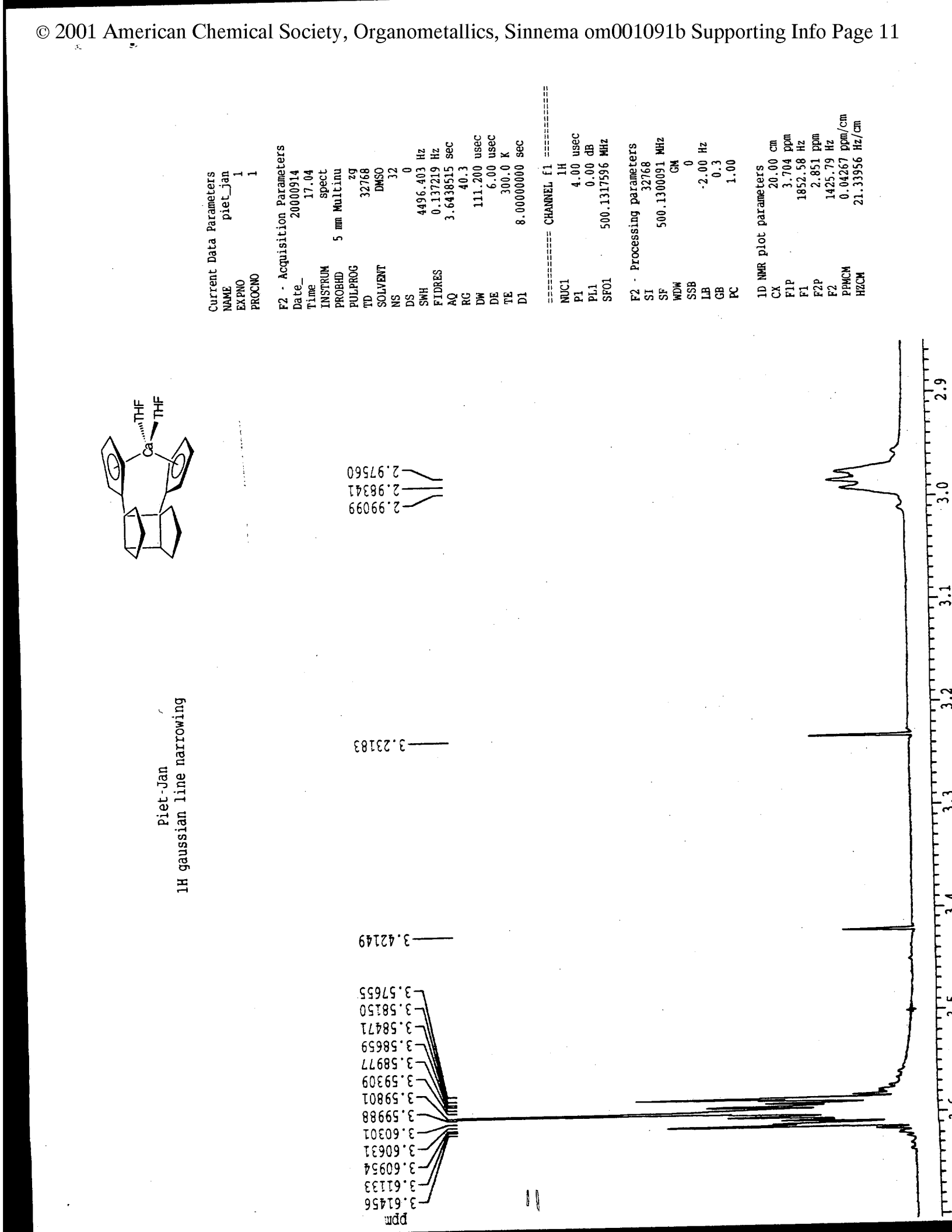
NUC1	1H
P1	4.00 usec
PL1	0.00 dB
SFO1	500.1317596 MHz

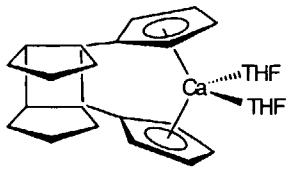
F2 - Processing parameters

SI	32768
SF	500.1300091 MHz
WDW	GM
SSB	0
LB	-2.00 Hz
GB	0.3
PC	1.00

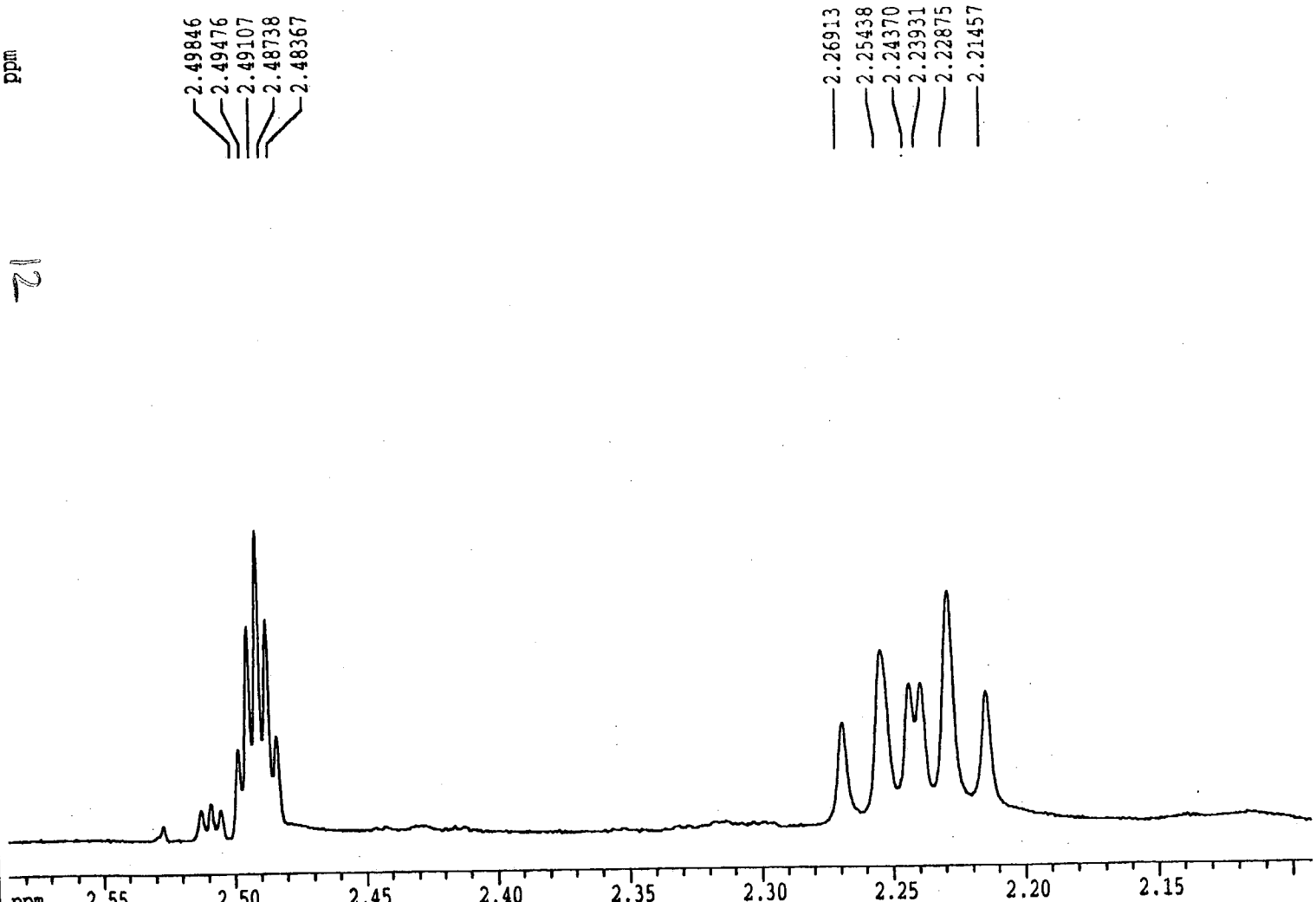
1D NMR plot parameters

CX	20.00 cm
F1P	5.600 ppm
F1	2800.62 Hz
F2P	5.250 ppm
F2	2625.74 Hz
PPMCM	0.01748 ppm/cm
HZCM	8.74390 Hz/cm





Piet-Jan
1H gaussian line narrowing



Current Data Parameters

NAME	piet_jan
EXPNO	1
PROCNO	1

F2 - Acquisition Parameters

Date_	20000914
Time	17.04
INSTRUM	spect
PROBHD	5 mm Multinu
PULPROG	zg
TD	32768
SOLVENT	DMSO
NS	32
DS	0
SWH	4496.403 Hz
FIDRES	0.137219 Hz
AQ	3.6438515 sec
RG	40.3
DW	111.200 usec
DE	6.00 usec
TE	300.0 K
D1	8.00000000 sec

========== CHANNEL f1 ==========

NUC1	1H
P1	4.00 usec
PL1	0.00 dB
SFO1	500.1317596 MHz

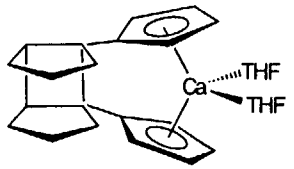
F2 - Processing parameters

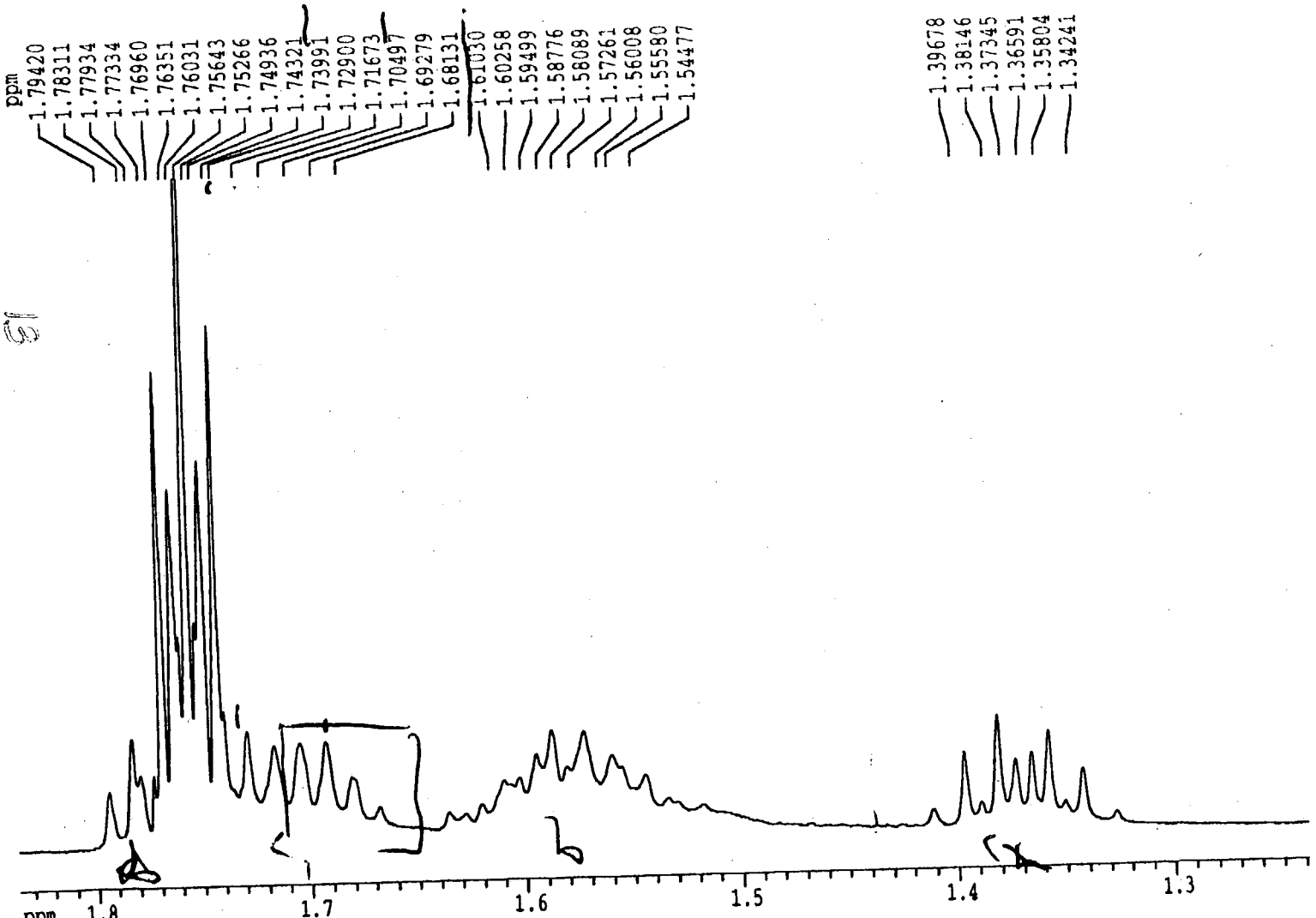
SI	32768
SF	500.1300091 MHz
WDW	GM
SSB	0
LB	-2.00 Hz
GB	0.3
PC	1.00

1D NMR plot parameters

CX	20.00 cm
F1P	2.587 ppm
F1	1293.76 Hz
F2P	2.093 ppm
F2	1046.69 Hz
PPMCM	0.02470 ppm/cm
HZCM	12.35351 Hz/cm

Piet-Jan
1H gaussian line narrowing





Current Data Parameters

NAME	piet_jan
EXPNO	1
PROCNO	1

F2 - Acquisition Parameters

Date_	20000914
Time	17.04
INSTRUM	spect
PROBHD	5 mm Multinu
PULPROG	zg
TD	32768
SOLVENT	DMSO
NS	32
DS	0
SWH	4496.403 Hz
FIDRES	0.137219 Hz
AQ	3.6438515 sec
RG	40.3
DW	111.200 usec
DE	6.00 usec
TE	300.0 K
D1	8.00000000 sec

========== CHANNEL f1 ==========

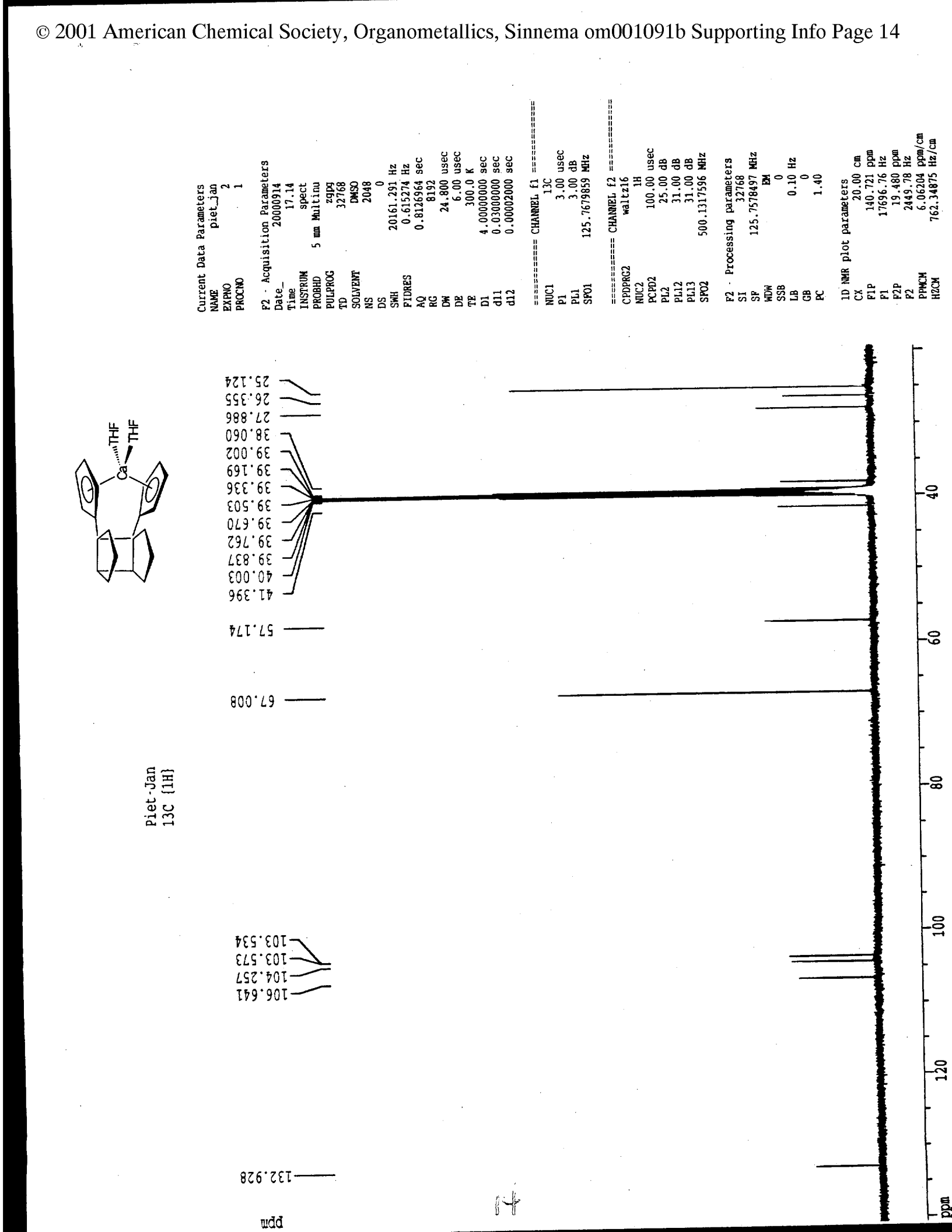
NUC1	1H
P1	4.00 usec
PL1	0.00 dB
SFO1	500.1317596 MHz

F2 - Processing parameters

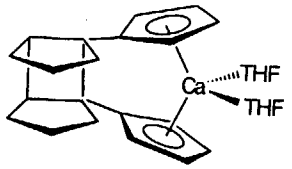
SI	32768
SF	500.1300091 MHz
WDW	GM
SSB	0
LB	-2.00 Hz
GB	0.3
PC	1.00

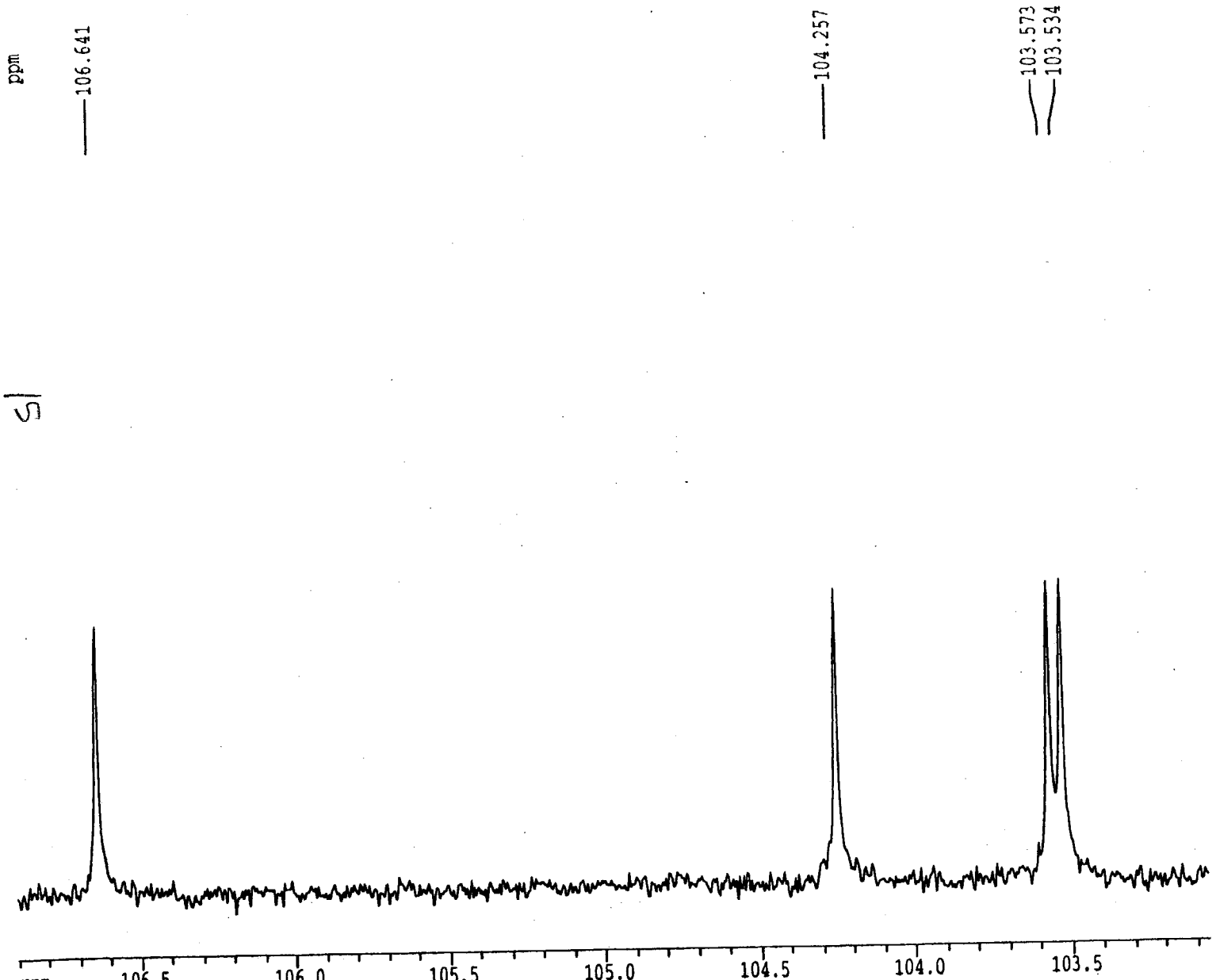
1D NMR plot parameters

CX	20.00 cm
F1P	1.837 ppm
F1	918.85 Hz
F2P	1.239 ppm
F2	619.58 Hz
PPMCM	0.02992 ppm/cm
HZCM	14.96318 Hz/cm



Piet-Jan
13C {1H}





Current Data Parameters

NAME	piet_jan
EXPNO	2
PROCNO	1

F2 - Acquisition Parameters

Date_	20000914
Time	17.14
INSTRUM	spect
PROBHD	5 mm Multinu
PULPROG	zgpg
TD	32768
SOLVENT	DMSO
NS	2048
DS	0
SWH	20161.291 Hz
FIDRES	0.615274 Hz
AQ	0.8126964 sec
RG	8192
DW	24.800 usec
DE	6.00 usec
TE	300.0 K
D1	4.00000000 sec
d11	0.03000000 sec
d12	0.00002000 sec

========== CHANNEL f1 ==========

NUC1	13C
P1	3.00 usec
PL1	3.00 dB
SFO1	125.7679859 MHz

========== CHANNEL f2 ==========

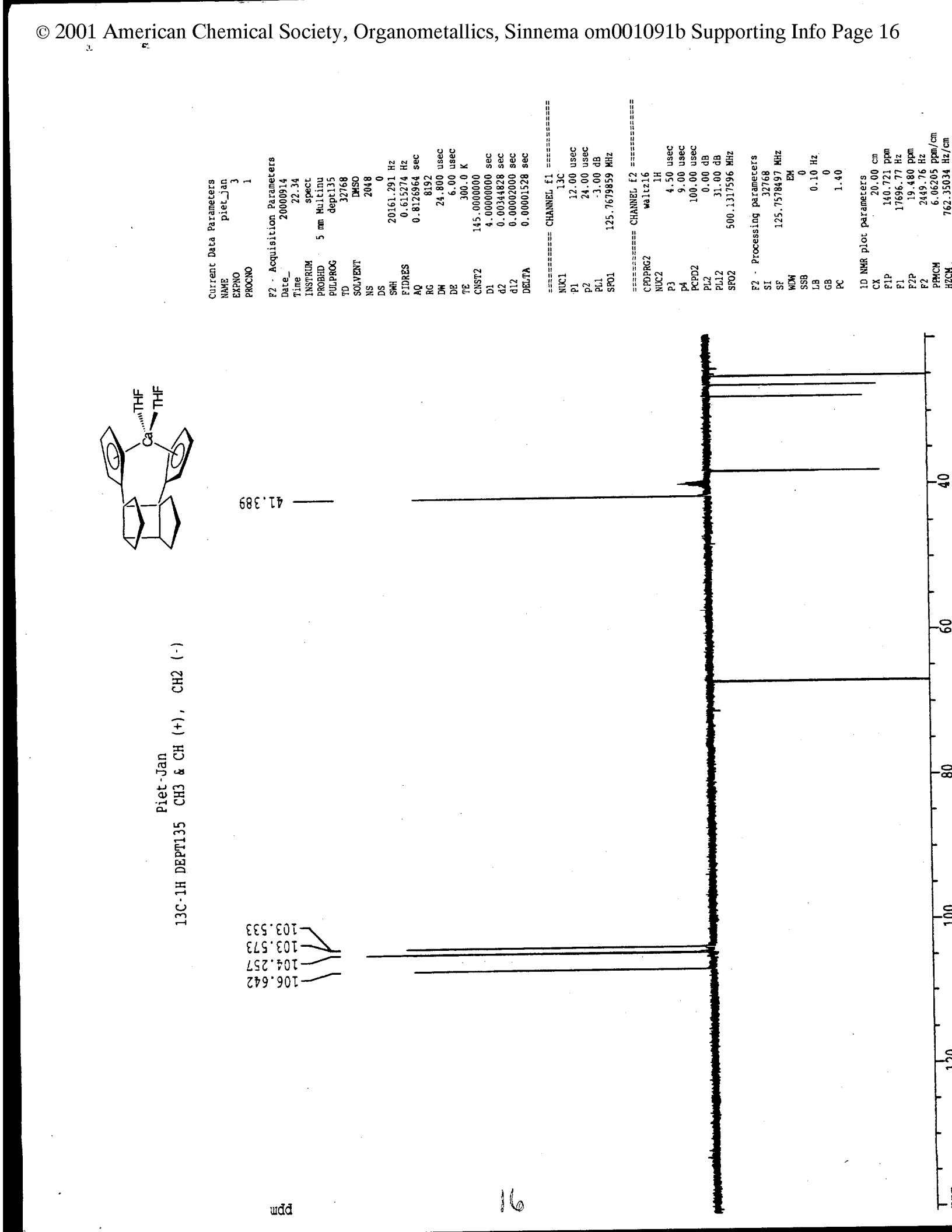
CPDPRG2	waltz16
NUC2	1H
PCPD2	100.00 usec
PL2	25.00 dB
PL12	31.00 dB
PL13	31.00 dB
SFO2	500.1317596 MHz

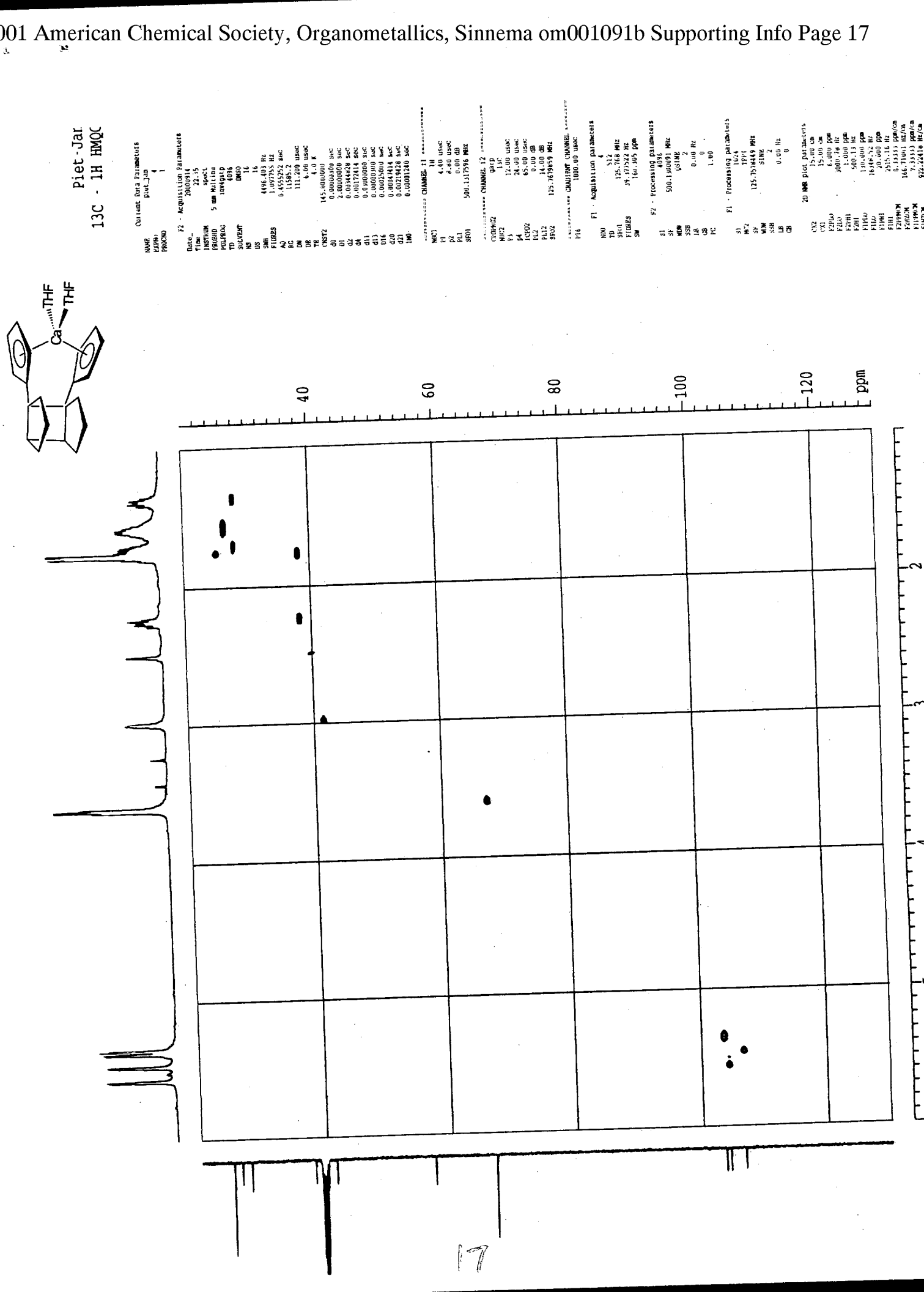
F2 - Processing parameters

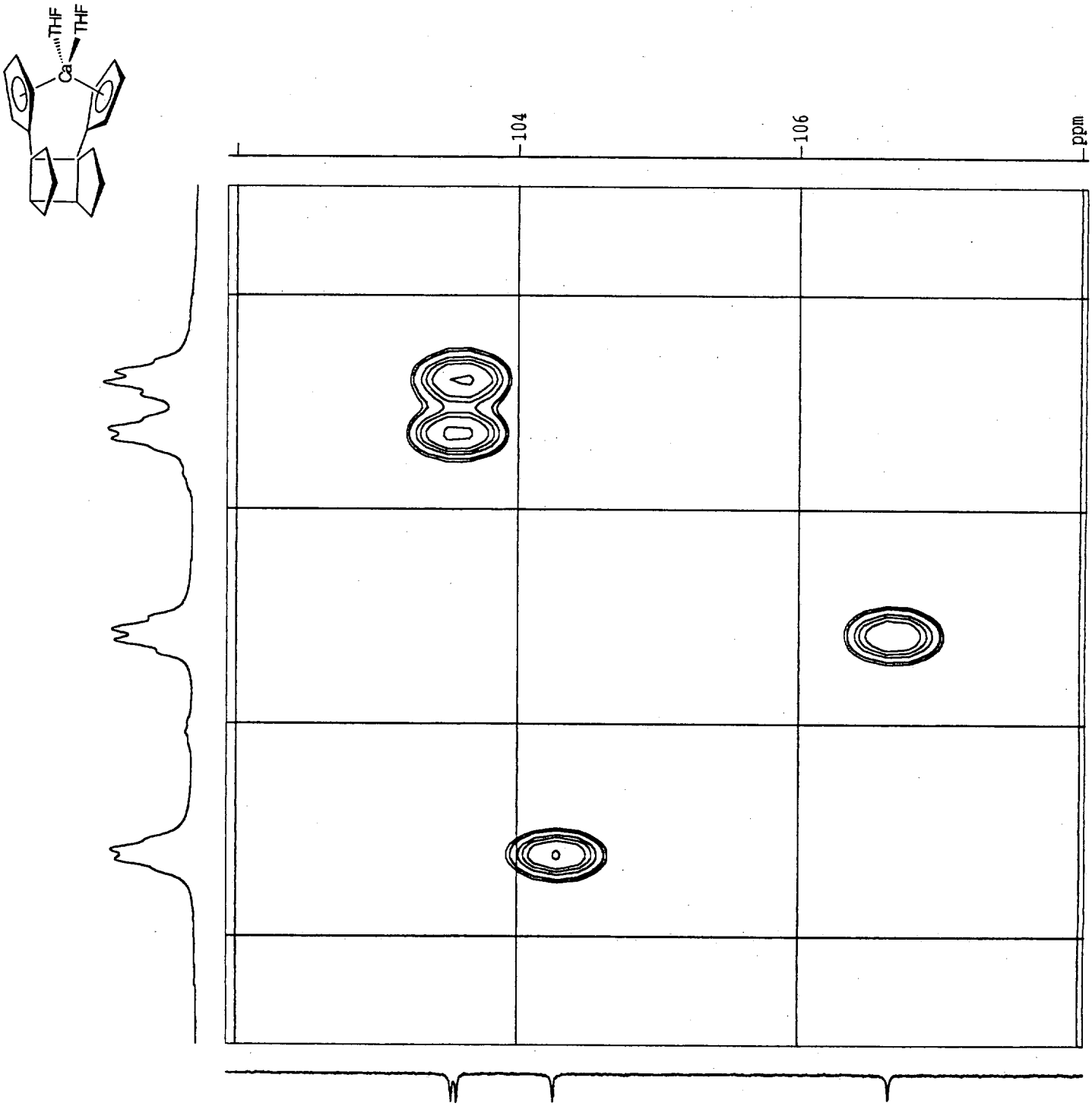
SI	32768
SF	125.7578497 MHz
WDW	EM
SSB	0
LB	0.10 Hz
GB	0
PC	1.40

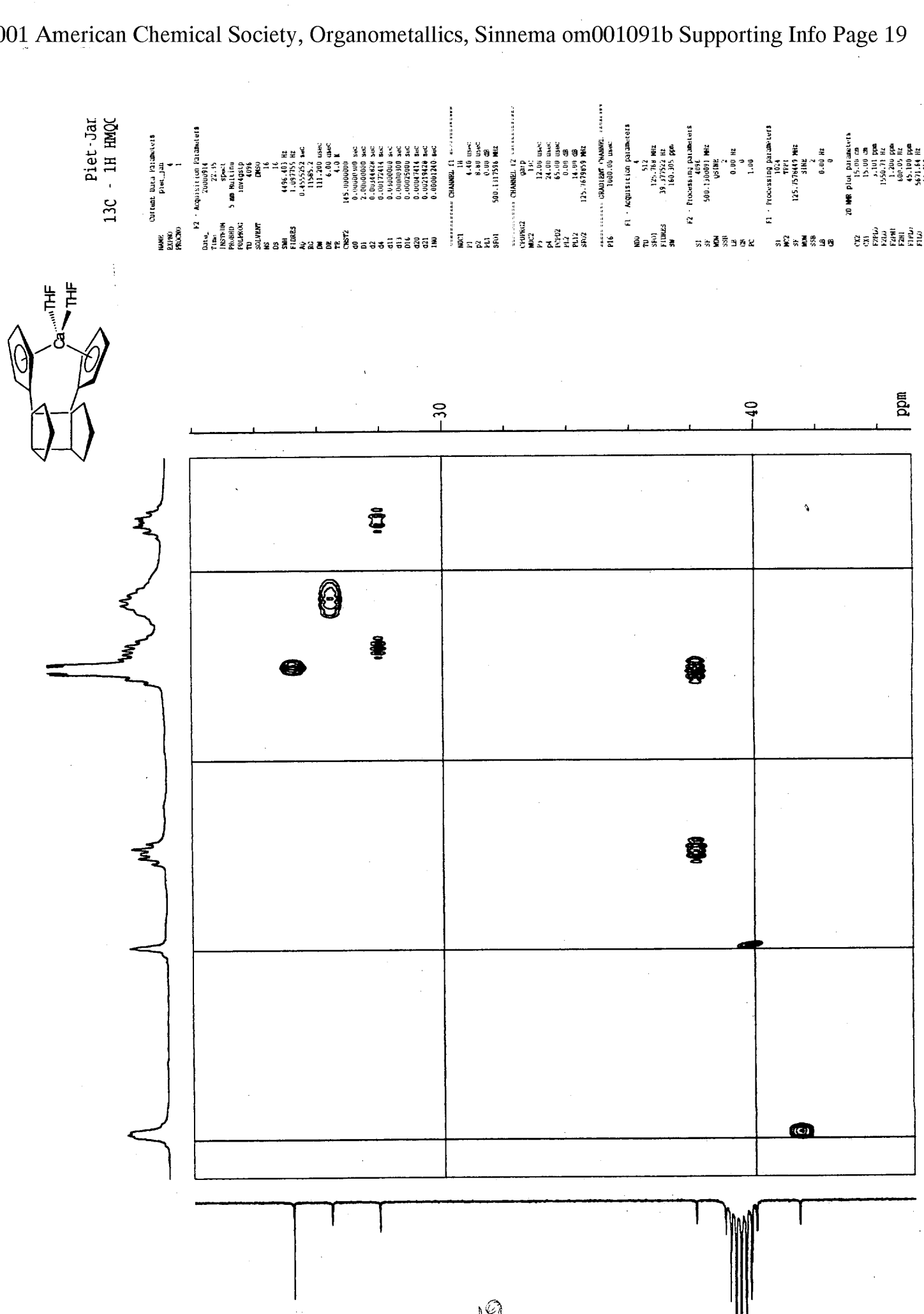
1D NMR plot parameters

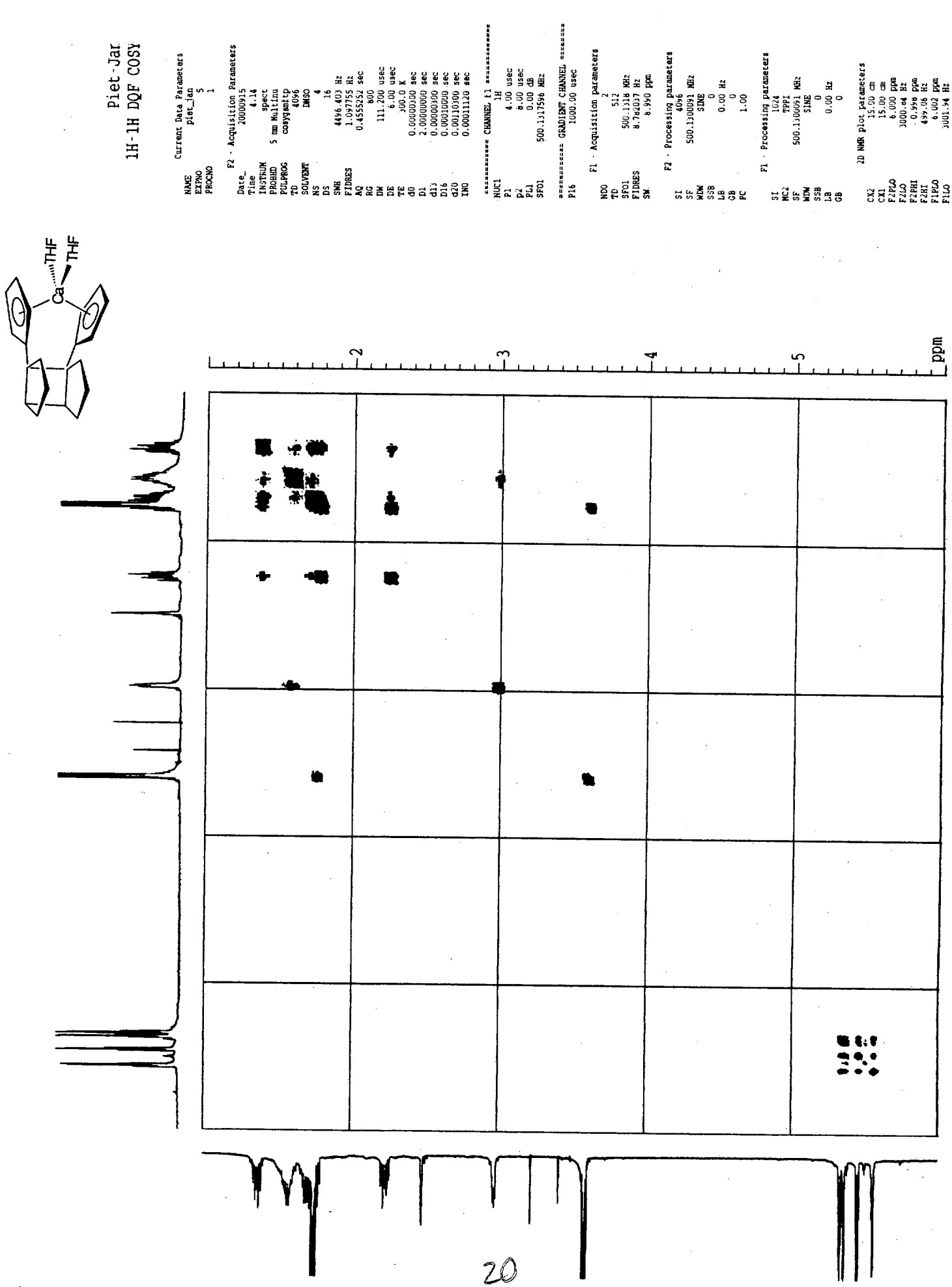
CX	20.00 cm
F1P	106.906 ppm
F1	13444.21 Hz
F2P	103.065 ppm
F2	12961.19 Hz
PPMCM	0.19204 ppm/cm
HZCM	24.15100 Hz/cm

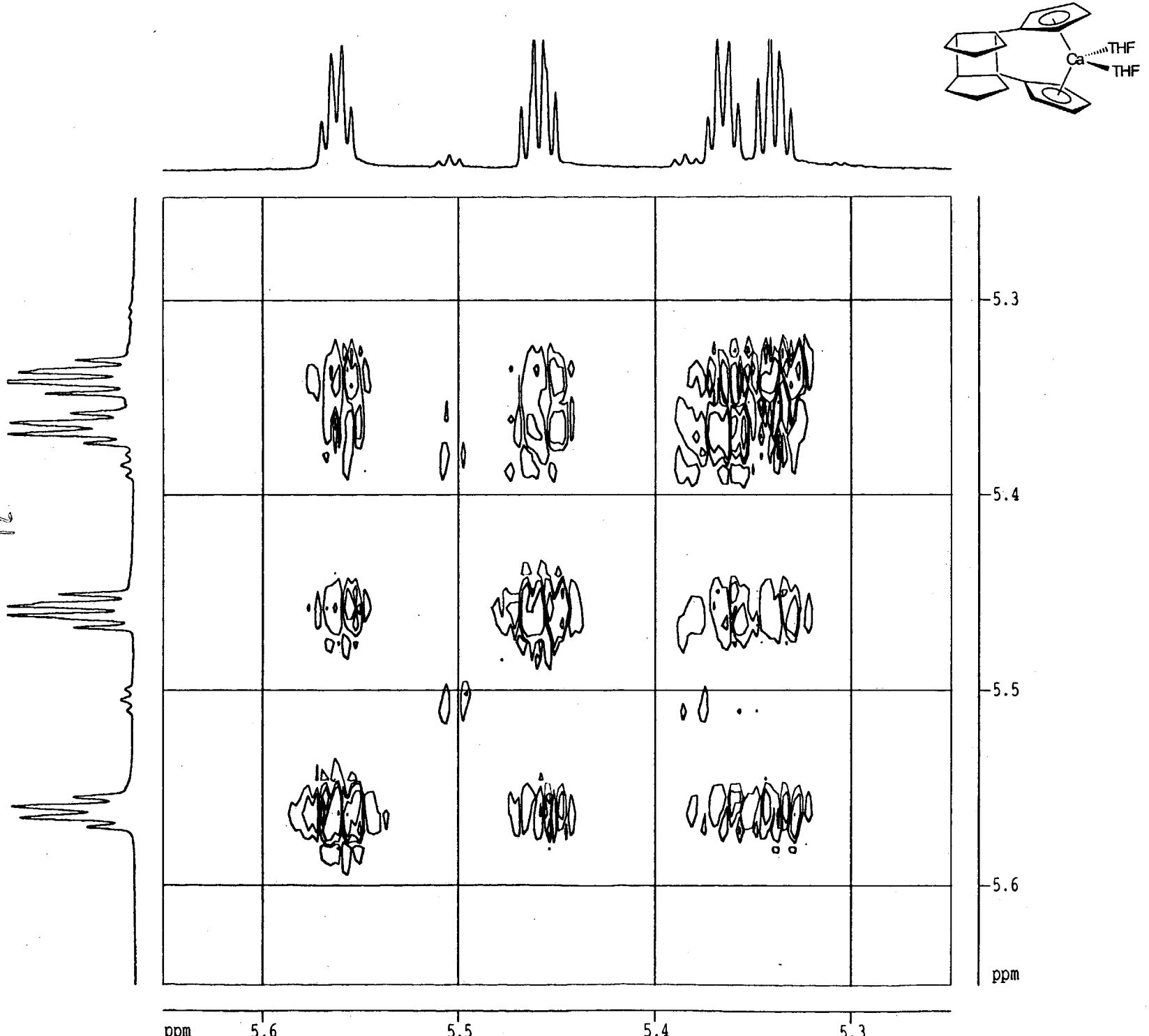












Piet-Jar
1H-1H DQF COSY

Current Data Parameters

NAME	piet_jan
EXPNO	5
PROCNO	1

F2 - Acquisition Parameters

Date_	20000915
Time	4.14
INSTRUM	spect
PROBHD	5 mm Multinu
PULPROG	cosygsmftp
TD	4096
SOLVENT	DMSO
NS	4
DS	16
SWH	4496.403 Hz
FIDRES	1.097755 Hz
AQ	0.4555252 sec
RG	800
DW	111.200 usec
DE	6.00 usec
TE	300.0 K
d0	0.00000300 sec
D1	2.00000000 sec
d13	0.00000300 sec
D16	0.00010000 sec
d20	0.00110300 sec
INO	0.00011120 sec

========== CHANNEL f1 ==========

NUC1	1H
P1	4.00 usec
p2	8.00 usec
PL1	0.00 dB
SFO1	500.1317598 MHz

========== GRADIENT CHANNEL ========

P16	1000.00 usec

F1 - Acquisition parameters

NDO	2
TD	512
SFO1	500.1318 MHz
FIDRES	8.782037 Hz
SW	8.990 ppm

F2 - Processing parameters

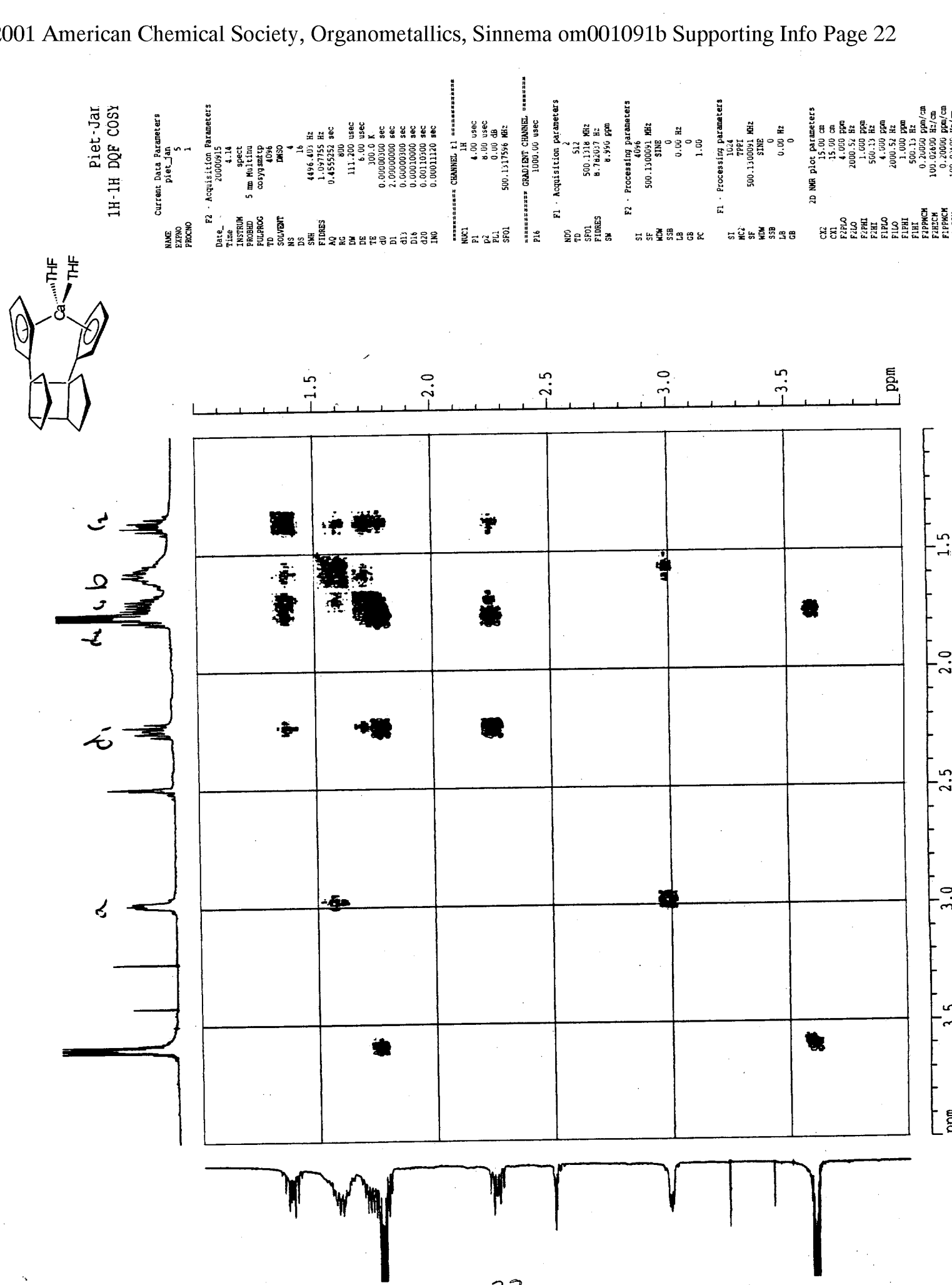
SI	4096
SF	500.1300091 MHz
WDW	SINE
SSB	0
LB	0.00 Hz
GB	0
PC	1.00

F1 - Processing parameters

SI	1024
MC2	TPPI
SF	500.1300091 MHz
WDW	SINE
SSB	0
LB	0.00 Hz
GB	0

2D NMR plot parameters

CX2	15.00 cm
CX1	15.00 cm
F2PLO	5.651 ppm
F2LO	2826.30 Hz
F2PHI	5.249 ppm
F2HI	2625.41 Hz
F1PLO	5.651 ppm
F1LO	2826.30 Hz
F1PHI	5.247 ppm
F1HI	2624.31 Hz
F2PPMCM	0.02678 ppm/cm
F2HZCM	13.39261 Hz/cm
F1PPMCM	0.02662 ppm/cm



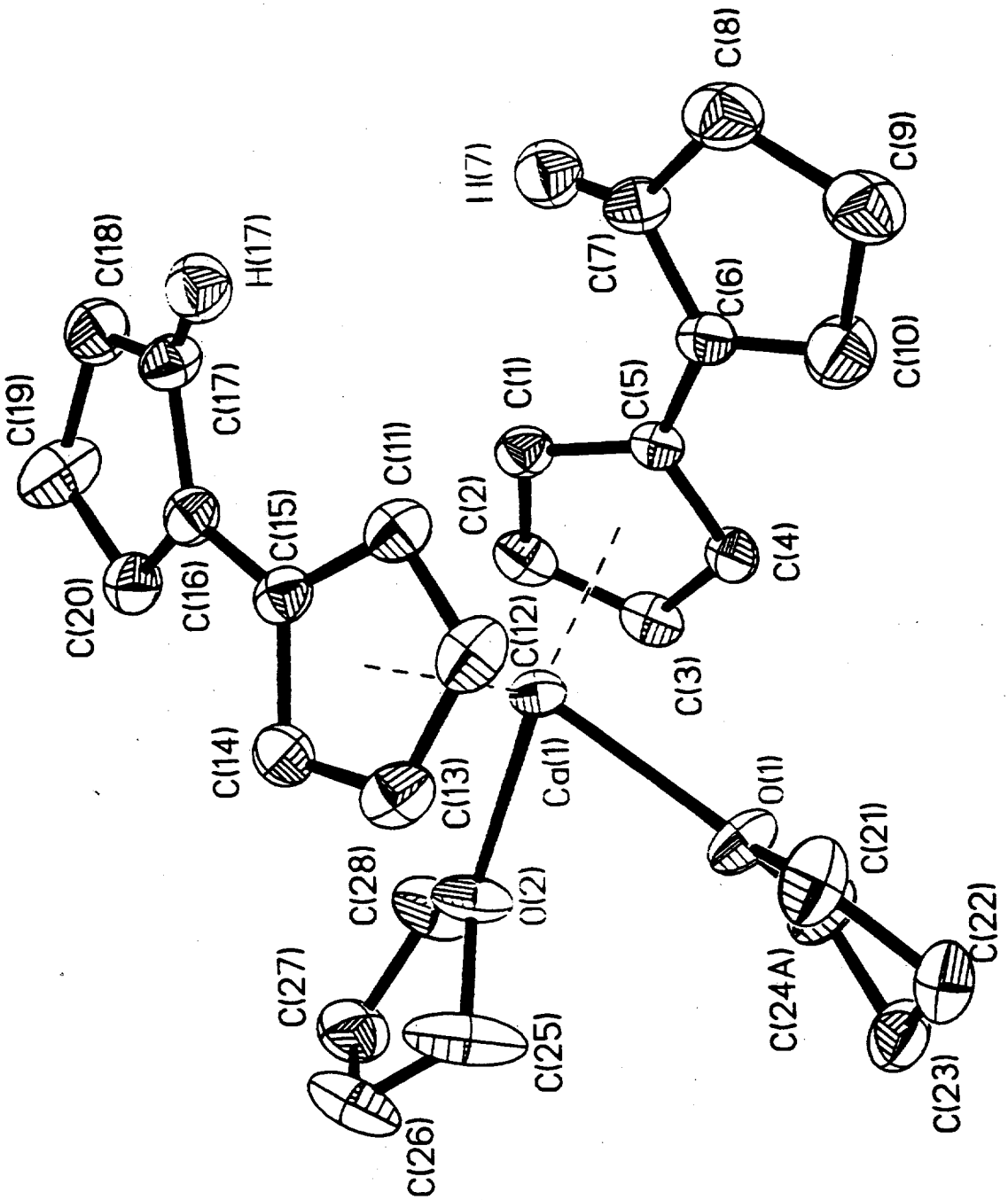

C(8)
C(9)
I(7)
C(7)
C(6)
C(10)
C(1)
C(5)
C(2)
C(4)
C(3)
C(12)
C(18)
H(17)
C(19)
C(17)
C(11)
C(15)
C(20)
C(16)
C(14)
C(13)
Ca(1)
O(1)
C(21)
C(28)
O(2)
C(22)
C(24A)
C(27)
C(25)
C(23)
C(26)

Table 1. Crystal data and structure refinement for Calcocene derivative.2THF.

Identification code	bt120	
Empirical formula	C28 H38 Ca O2	
Formula weight	446.66	
Temperature	203(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	C2/c	
Unit cell dimensions	a = 38.3350(2) Å	α= 90°.
	b = 8.26430(10) Å	β= 98.4790(10)°.
	c = 16.1604(3) Å	γ = 90°.
Volume	5063.85(12) Å^3	
Z	8	
Density (calculated)	1.172 Mg/m^3	
Absorption coefficient	0.269 mm^{-1}	
F(000)	1936	
Crystal size	0.40 x 0.40 x 0.13 mm^3	
Crystal color and habit	colorless block	
Diffractometer	Siemens SMART 1000	
Theta range for data collection	1.07 to 25.00°.	
Index ranges	-45<=h<=45, -9<=k<=9, -14<=l<=19	
Reflections collected	29162	
Independent reflections	4396 [R(int) = 0.0456]	
Completeness to theta = 25.00°	98.5 %	
Absorption correction†	Empirical	
Max. and min. transmission	0.9659 and 0.9001	
Solution method	XS, Bruker SHELXTL v. 5.10	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	4396 / 0 / 292	
Goodness-of-fit on F^2	1.067	
Final R indices [I>2sigma(I)]	R1 = 0.0703, wR2 = 0.1495	
R indices (all data)	R1 = 0.0979, wR2 = 0.1647	
Largest diff. peak and hole	0.323 and -0.273 e.Å^{-3}	

† SADABS: an empirical absorption program by G. M. Sheldrick using the method described by Blessing, R. H.; *Acta Cryst.*, A51, **1995**, 33.

Refinement Note: a THF moiety is disordered in one carbon position (C24a, C24b) with refined occupancy of 83 and 17%.

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for BT120. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Ca(1)	1253(1)	2016(1)	3022(1)	37(1)
C(1)	1245(1)	5287(4)	3093(2)	48(1)
C(2)	1107(1)	4915(4)	2265(3)	53(1)
C(3)	1381(1)	4271(5)	1881(2)	55(1)
C(4)	1688(1)	4235(5)	2466(2)	50(1)
C(5)	1607(1)	4862(4)	3235(2)	43(1)
C(6)	1853(1)	5059(4)	4008(2)	47(1)
C(7)	1793(1)	5930(5)	4716(2)	54(1)
C(8)	2105(1)	5758(7)	5390(3)	78(1)
C(9)	2375(1)	4858(7)	5001(3)	80(2)
C(10)	2197(1)	4375(7)	4138(3)	79(2)
C(11)	1204(1)	2166(5)	4682(2)	48(1)
C(12)	1356(1)	650(5)	4570(2)	55(1)
C(13)	1100(1)	-325(5)	4096(3)	58(1)
C(14)	790(1)	585(5)	3904(3)	55(1)
C(15)	852(1)	2146(4)	4269(2)	45(1)
C(16)	598(1)	3490(5)	4205(2)	49(1)
C(17)	631(1)	4905(5)	4706(2)	55(1)
C(18)	348(1)	6094(5)	4362(3)	68(1)
C(19)	112(1)	5187(7)	3691(3)	86(2)
C(20)	302(1)	3628(5)	3558(3)	61(1)
O(1)	1686(1)	240(3)	2611(2)	58(1)
C(21)	1909(1)	-866(6)	3098(3)	73(1)
C(22)	2134(1)	-1673(6)	2524(3)	72(1)
C(23)	1926(1)	-1422(6)	1681(3)	74(1)
C(24A)	1771(2)	191(8)	1749(3)	65(2)
C(24B)	1582(6)	-950(40)	1872(16)	52(9)
O(2)	890(1)	763(3)	1882(2)	61(1)
C(25)	852(2)	-959(6)	1804(4)	117(3)
C(26)	501(2)	-1245(7)	1404(4)	106(2)
C(27)	392(1)	237(7)	877(4)	88(2)

C(28)	665(1)	1448(6)	1193(3)	78(2)

Table 3. Bond lengths [Å] and angles [°] for BT120.

Ca(1)-O(2)	2.377(2)	O(1)-C(21)	1.409(5)
Ca(1)-O(1)	2.383(3)	O(1)-C(24A)	1.477(5)
Ca(1)-C(14)	2.705(4)	O(1)-C(24B)	1.55(2)
Ca(1)-C(1)	2.707(4)	C(21)-C(22)	1.511(6)
Ca(1)-C(15)	2.710(3)	C(22)-C(23)	1.489(7)
Ca(1)-C(5)	2.711(3)	C(23)-C(24B)	1.45(2)
Ca(1)-C(2)	2.711(4)	C(23)-C(24A)	1.469(7)
Ca(1)-C(3)	2.718(4)	O(2)-C(28)	1.420(5)
Ca(1)-C(11)	2.718(3)	O(2)-C(25)	1.435(5)
Ca(1)-C(4)	2.718(4)	C(25)-C(26)	1.423(7)
Ca(1)-C(13)	2.719(4)	C(26)-C(27)	1.515(8)
Ca(1)-C(12)	2.720(4)	C(27)-C(28)	1.485(6)
C(1)-C(2)	1.398(5)		
C(1)-C(5)	1.417(5)	O(2)-Ca(1)-O(1)	82.44(10)
C(2)-C(3)	1.400(6)	O(2)-Ca(1)-C(14)	82.16(12)
C(3)-C(4)	1.396(5)	O(1)-Ca(1)-C(14)	114.56(11)
C(4)-C(5)	1.423(5)	O(2)-Ca(1)-C(1)	117.27(11)
C(5)-C(6)	1.458(5)	O(1)-Ca(1)-C(1)	129.79(12)
C(6)-C(7)	1.400(5)	C(14)-Ca(1)-C(1)	113.68(12)
C(6)-C(10)	1.423(6)	O(2)-Ca(1)-C(15)	105.20(11)
C(7)-C(8)	1.500(6)	O(1)-Ca(1)-C(15)	136.61(10)
C(8)-C(9)	1.488(7)	C(14)-Ca(1)-C(15)	30.49(11)
C(9)-C(10)	1.513(6)	C(1)-Ca(1)-C(15)	85.26(12)
C(11)-C(12)	1.404(5)	O(2)-Ca(1)-C(5)	134.49(10)
C(11)-C(15)	1.415(5)	O(1)-Ca(1)-C(5)	102.33(11)
C(12)-C(13)	1.405(6)	C(14)-Ca(1)-C(5)	131.81(12)
C(13)-C(14)	1.401(6)	C(1)-Ca(1)-C(5)	30.33(11)
C(14)-C(15)	1.424(5)	C(15)-Ca(1)-C(5)	101.47(11)
C(15)-C(16)	1.471(5)	O(2)-Ca(1)-C(2)	88.66(11)
C(16)-C(17)	1.417(5)	O(1)-Ca(1)-C(2)	121.59(12)
C(16)-C(20)	1.431(5)	C(14)-Ca(1)-C(2)	121.12(13)
C(17)-C(18)	1.508(6)	C(1)-Ca(1)-C(2)	29.90(11)
C(18)-C(19)	1.505(6)	C(15)-Ca(1)-C(2)	101.48(13)
C(19)-C(20)	1.510(6)	C(5)-Ca(1)-C(2)	49.93(11)

O(2)-Ca(1)-C(3)	85.17(11)	C(14)-Ca(1)-C(12)	49.56(13)
O(1)-Ca(1)-C(3)	91.72(12)	C(1)-Ca(1)-C(12)	112.14(13)
C(14)-Ca(1)-C(3)	148.79(13)	C(15)-Ca(1)-C(12)	49.75(12)
C(1)-Ca(1)-C(3)	49.30(12)	C(5)-Ca(1)-C(12)	103.97(12)
C(15)-Ca(1)-C(3)	131.01(13)	C(2)-Ca(1)-C(12)	140.75(13)
C(5)-Ca(1)-C(3)	49.78(11)	C(3)-Ca(1)-C(12)	153.25(13)
C(2)-Ca(1)-C(3)	29.89(13)	C(11)-Ca(1)-C(12)	29.92(11)
O(2)-Ca(1)-C(11)	131.87(12)	C(4)-Ca(1)-C(12)	124.88(13)
O(1)-Ca(1)-C(11)	117.08(10)	C(13)-Ca(1)-C(12)	29.94(13)
C(14)-Ca(1)-C(11)	49.82(13)	C(2)-C(1)-C(5)	108.8(4)
C(1)-Ca(1)-C(11)	84.83(12)	C(2)-C(1)-Ca(1)	75.2(2)
C(15)-Ca(1)-C(11)	30.23(11)	C(5)-C(1)-Ca(1)	75.0(2)
C(5)-Ca(1)-C(11)	86.61(12)	C(1)-C(2)-C(3)	107.9(4)
C(2)-Ca(1)-C(11)	111.44(13)	C(1)-C(2)-Ca(1)	74.9(2)
C(3)-Ca(1)-C(11)	133.15(12)	C(3)-C(2)-Ca(1)	75.3(2)
O(2)-Ca(1)-C(4)	110.76(11)	C(4)-C(3)-C(2)	108.6(3)
O(1)-Ca(1)-C(4)	80.62(11)	C(4)-C(3)-Ca(1)	75.1(2)
C(14)-Ca(1)-C(4)	161.89(12)	C(2)-C(3)-Ca(1)	74.8(2)
C(1)-Ca(1)-C(4)	49.57(12)	C(3)-C(4)-C(5)	108.3(4)
C(15)-Ca(1)-C(4)	131.41(12)	C(3)-C(4)-Ca(1)	75.1(2)
C(5)-Ca(1)-C(4)	30.39(11)	C(5)-C(4)-Ca(1)	74.5(2)
C(2)-Ca(1)-C(4)	49.42(13)	C(1)-C(5)-C(4)	106.4(3)
C(3)-Ca(1)-C(4)	29.76(11)	C(1)-C(5)-C(6)	127.3(3)
C(11)-Ca(1)-C(4)	115.48(12)	C(4)-C(5)-C(6)	126.3(3)
O(2)-Ca(1)-C(13)	91.64(12)	C(1)-C(5)-Ca(1)	74.7(2)
O(1)-Ca(1)-C(13)	87.97(11)	C(4)-C(5)-Ca(1)	75.1(2)
C(14)-Ca(1)-C(13)	29.94(12)	C(6)-C(5)-Ca(1)	117.0(2)
C(1)-Ca(1)-C(13)	132.74(13)	C(7)-C(6)-C(10)	110.0(4)
C(15)-Ca(1)-C(13)	49.82(12)	C(7)-C(6)-C(5)	126.5(4)
C(5)-Ca(1)-C(13)	133.37(12)	C(10)-C(6)-C(5)	123.5(4)
C(2)-Ca(1)-C(13)	150.16(14)	C(6)-C(7)-C(8)	109.7(4)
C(3)-Ca(1)-C(13)	176.80(13)	C(9)-C(8)-C(7)	105.7(4)
C(11)-Ca(1)-C(13)	49.49(12)	C(8)-C(9)-C(10)	105.9(4)
C(4)-Ca(1)-C(13)	153.03(13)	C(6)-C(10)-C(9)	108.4(4)
O(2)-Ca(1)-C(12)	121.43(12)	C(12)-C(11)-C(15)	108.2(4)
O(1)-Ca(1)-C(12)	89.35(11)	C(12)-C(11)-Ca(1)	75.1(2)

C(15)-C(11)-Ca(1)	74.6(2)	C(16)-C(20)-C(19)	108.1(4)
C(11)-C(12)-C(13)	108.3(4)	C(21)-O(1)-C(24A)	108.0(3)
C(11)-C(12)-Ca(1)	75.0(2)	C(21)-O(1)-C(24B)	95.0(11)
C(13)-C(12)-Ca(1)	75.0(2)	C(24A)-O(1)-C(24B)	47.5(10)
C(14)-C(13)-C(12)	108.3(4)	C(21)-O(1)-Ca(1)	129.3(2)
C(14)-C(13)-Ca(1)	74.5(2)	C(24A)-O(1)-Ca(1)	122.6(2)
C(12)-C(13)-Ca(1)	75.1(2)	C(24B)-O(1)-Ca(1)	119.4(9)
C(13)-C(14)-C(15)	108.1(4)	O(1)-C(21)-C(22)	107.3(3)
C(13)-C(14)-Ca(1)	75.6(2)	C(23)-C(22)-C(21)	102.9(4)
C(15)-C(14)-Ca(1)	75.0(2)	C(24B)-C(23)-C(24A)	49.4(12)
C(11)-C(15)-C(14)	107.1(3)	C(24B)-C(23)-C(22)	103.0(11)
C(11)-C(15)-C(16)	126.9(3)	C(24A)-C(23)-C(22)	103.0(4)
C(14)-C(15)-C(16)	126.0(4)	C(23)-C(24A)-O(1)	104.1(4)
C(11)-C(15)-Ca(1)	75.2(2)	C(23)-C(24B)-O(1)	101.2(15)
C(14)-C(15)-Ca(1)	74.6(2)	C(28)-O(2)-C(25)	106.6(3)
C(16)-C(15)-Ca(1)	114.9(2)	C(28)-O(2)-Ca(1)	130.7(2)
C(17)-C(16)-C(20)	110.3(4)	C(25)-O(2)-Ca(1)	122.7(3)
C(17)-C(16)-C(15)	125.5(4)	C(26)-C(25)-O(2)	106.3(5)
C(20)-C(16)-C(15)	123.9(4)	C(25)-C(26)-C(27)	106.6(4)
C(16)-C(17)-C(18)	109.2(4)	C(28)-C(27)-C(26)	103.2(4)
C(19)-C(18)-C(17)	105.3(4)	O(2)-C(28)-C(27)	108.4(4)
C(18)-C(19)-C(20)	106.1(4)		

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for BT120. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Ca(1)	46(1)	33(1)	30(1)	0(1)	1(1)	2(1)
C(1)	56(2)	36(2)	53(2)	0(2)	9(2)	1(2)
C(2)	57(2)	37(2)	60(3)	12(2)	-7(2)	-1(2)
C(3)	74(3)	53(2)	35(2)	6(2)	3(2)	-16(2)
C(4)	56(2)	57(2)	40(2)	-1(2)	16(2)	-12(2)
C(5)	49(2)	39(2)	41(2)	-2(2)	5(2)	-6(2)
C(6)	58(2)	42(2)	43(2)	-3(2)	8(2)	-9(2)
C(7)	66(3)	55(2)	40(2)	-7(2)	2(2)	0(2)
C(8)	96(4)	89(4)	48(3)	-12(2)	8(3)	-15(3)
C(9)	79(3)	95(4)	59(3)	-9(3)	-15(3)	-1(3)
C(10)	67(3)	104(4)	60(3)	-18(3)	-5(2)	15(3)
C(11)	59(2)	56(2)	28(2)	2(2)	3(2)	6(2)
C(12)	68(3)	64(3)	33(2)	12(2)	9(2)	17(2)
C(13)	85(3)	39(2)	55(3)	11(2)	21(2)	8(2)
C(14)	61(3)	44(2)	63(3)	3(2)	19(2)	-7(2)
C(15)	57(2)	42(2)	38(2)	3(2)	15(2)	1(2)
C(16)	53(2)	49(2)	44(2)	2(2)	10(2)	2(2)
C(17)	62(3)	58(2)	45(2)	-9(2)	3(2)	6(2)
C(18)	64(3)	57(3)	84(3)	-3(2)	14(3)	8(2)
C(19)	92(4)	99(4)	60(3)	-13(3)	-10(3)	42(3)
C(20)	52(2)	64(3)	68(3)	-8(2)	9(2)	4(2)
O(1)	80(2)	59(2)	34(1)	2(1)	7(1)	28(2)
C(21)	68(3)	94(4)	57(3)	18(3)	9(2)	28(3)
C(22)	55(3)	83(3)	80(3)	8(3)	17(2)	13(2)
C(23)	64(3)	90(4)	69(3)	-17(3)	16(2)	11(3)
C(24A)	87(4)	73(4)	38(3)	5(3)	18(3)	23(4)
C(24B)	40(14)	70(20)	48(15)	-12(13)	10(11)	-6(13)
O(2)	84(2)	37(1)	51(2)	-1(1)	-23(2)	-4(1)
C(25)	186(7)	43(3)	98(4)	-5(3)	-65(4)	-11(3)
C(26)	120(5)	80(4)	112(5)	-7(4)	-6(4)	-54(4)
C(27)	61(3)	86(4)	108(5)	-22(3)	-16(3)	-3(3)

C(28)	75(3)	68(3)	75(3)	9(2)	-40(3)	-3(2)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for BT120.

	x	y	z	U(eq)
H(1A)	1122	5934	3478	58
H(2A)	874	5258	1972	64
H(3A)	1370	4077	1273	65
H(4A)	1928	4014	2338	60
H(7)	1589	6533	4763	65
H(8A)	2195	6824	5585	93
H(8B)	2040	5156	5868	93
H(9A)	2454	3898	5332	96
H(9B)	2580	5548	4962	96
H(10A)	2333	4774	3713	94
H(10B)	2182	3194	4095	94
H(11A)	1309	3018	5071	57
H(12A)	1585	265	4868	66
H(13A)	1121	-1504	4008	70
H(14A)	557	147	3664	66
H(17)	803	5075	5177	66
H(18A)	216	6455	4802	82
H(18B)	452	7041	4126	82
H(19A)	72	5819	3173	103
H(19B)	-116	4962	3870	103
H(20A)	142	2705	3580	74
H(20B)	381	3636	3009	74
H(21A)	1769	-1676	3345	87
H(21B)	2059	-299	3551	87
H(22A)	2366	-1158	2565	86
H(22B)	2165	-2827	2652	86
H(24A)	1558	325	1339	78
H(24B)	1940	1042	1662	78
H(23A)	1740	-2234	1549	60
H(23B)	2073	-1489	1237	60

H(24C)	1450	-1876	2040	62
H(24D)	1441	-404	1395	62
H(23C)	1872	-2472	1401	60
H(23D)	2058	-817	1322	60
H(25A)	1022	-1401	1468	141
H(25B)	891	-1472	2357	141
H(26A)	343	-1406	1822	128
H(26B)	492	-2211	1051	128
H(27A)	392	15	282	220(40)
H(27B)	156	609	960	180(30)
H(28A)	803	1737	749	94
H(28B)	554	2431	1369	94

Table 6. Torsion angles [°] for BT120.

O(2)-Ca(1)-C(1)-C(2)	-18.3(3)	O(1)-Ca(1)-C(2)-C(3)	-2.4(3)
O(1)-Ca(1)-C(1)-C(2)	85.4(3)	C(14)-Ca(1)-C(2)-C(3)	-162.6(2)
C(14)-Ca(1)-C(1)-C(2)	-111.7(3)	C(1)-Ca(1)-C(2)-C(3)	113.6(3)
C(15)-Ca(1)-C(1)-C(2)	-123.0(3)	C(15)-Ca(1)-C(2)-C(3)	172.1(2)
C(5)-Ca(1)-C(1)-C(2)	114.5(3)	C(5)-Ca(1)-C(2)-C(3)	76.7(2)
C(3)-Ca(1)-C(1)-C(2)	37.0(2)	C(11)-Ca(1)-C(2)-C(3)	142.3(2)
C(11)-Ca(1)-C(1)-C(2)	-153.3(3)	C(4)-Ca(1)-C(2)-C(3)	36.5(2)
C(4)-Ca(1)-C(1)-C(2)	76.5(3)	C(13)-Ca(1)-C(2)-C(3)	-173.6(3)
C(13)-Ca(1)-C(1)-C(2)	-139.7(3)	C(12)-Ca(1)-C(2)-C(3)	134.7(3)
C(12)-Ca(1)-C(1)-C(2)	-165.8(2)	C(1)-C(2)-C(3)-C(4)	0.2(4)
O(2)-Ca(1)-C(1)-C(5)	-132.9(2)	Ca(1)-C(2)-C(3)-C(4)	-68.2(3)
O(1)-Ca(1)-C(1)-C(5)	-29.2(3)	C(1)-C(2)-C(3)-Ca(1)	68.4(3)
C(14)-Ca(1)-C(1)-C(5)	133.8(2)	O(2)-Ca(1)-C(3)-C(4)	-149.9(3)
C(15)-Ca(1)-C(1)-C(5)	122.5(2)	O(1)-Ca(1)-C(3)-C(4)	-67.6(2)
C(2)-Ca(1)-C(1)-C(5)	-114.5(3)	C(14)-Ca(1)-C(3)-C(4)	144.0(3)
C(3)-Ca(1)-C(1)-C(5)	-77.5(2)	C(1)-Ca(1)-C(3)-C(4)	77.4(3)
C(11)-Ca(1)-C(1)-C(5)	92.1(2)	C(15)-Ca(1)-C(3)-C(4)	104.2(3)
C(4)-Ca(1)-C(1)-C(5)	-38.0(2)	C(5)-Ca(1)-C(3)-C(4)	37.1(2)
C(13)-Ca(1)-C(1)-C(5)	105.8(2)	C(2)-Ca(1)-C(3)-C(4)	114.4(3)
C(12)-Ca(1)-C(1)-C(5)	79.7(2)	C(11)-Ca(1)-C(3)-C(4)	63.1(3)
C(5)-C(1)-C(2)-C(3)	-0.5(4)	C(13)-Ca(1)-C(3)-C(4)	-152(2)
Ca(1)-C(1)-C(2)-C(3)	-68.7(3)	C(12)-Ca(1)-C(3)-C(4)	24.4(4)
C(5)-C(1)-C(2)-Ca(1)	68.2(3)	O(2)-Ca(1)-C(3)-C(2)	95.7(2)
O(2)-Ca(1)-C(2)-C(1)	163.8(3)	O(1)-Ca(1)-C(3)-C(2)	178.0(2)
O(1)-Ca(1)-C(2)-C(1)	-116.0(2)	C(14)-Ca(1)-C(3)-C(2)	29.5(4)
C(14)-Ca(1)-C(2)-C(1)	83.8(3)	C(1)-Ca(1)-C(3)-C(2)	-37.1(2)
C(15)-Ca(1)-C(2)-C(1)	58.5(3)	C(15)-Ca(1)-C(3)-C(2)	-10.2(3)
C(5)-Ca(1)-C(2)-C(1)	-36.9(2)	C(5)-Ca(1)-C(3)-C(2)	-77.3(2)
C(3)-Ca(1)-C(2)-C(1)	-113.6(3)	C(11)-Ca(1)-C(3)-C(2)	-51.3(3)
C(11)-Ca(1)-C(2)-C(1)	28.7(3)	C(4)-Ca(1)-C(3)-C(2)	-114.4(3)
C(4)-Ca(1)-C(2)-C(1)	-77.1(3)	C(13)-Ca(1)-C(3)-C(2)	94(2)
C(13)-Ca(1)-C(2)-C(1)	72.8(4)	C(12)-Ca(1)-C(3)-C(2)	-90.0(4)
C(12)-Ca(1)-C(2)-C(1)	21.1(4)	C(2)-C(3)-C(4)-C(5)	0.2(4)
O(2)-Ca(1)-C(2)-C(3)	-82.6(2)	Ca(1)-C(3)-C(4)-C(5)	-67.7(3)

C(2)-C(3)-C(4)-Ca(1)	68.0(3)
O(2)-Ca(1)-C(4)-C(3)	32.4(3)
O(1)-Ca(1)-C(4)-C(3)	110.5(3)
C(14)-Ca(1)-C(4)-C(3)	-101.3(4)
C(1)-Ca(1)-C(4)-C(3)	-76.4(3)
C(15)-Ca(1)-C(4)-C(3)	-102.7(3)
C(5)-Ca(1)-C(4)-C(3)	-114.3(4)
C(2)-Ca(1)-C(4)-C(3)	-36.7(2)
C(11)-Ca(1)-C(4)-C(3)	-133.9(2)
C(13)-Ca(1)-C(4)-C(3)	176.7(3)
C(12)-Ca(1)-C(4)-C(3)	-166.9(2)
O(2)-Ca(1)-C(4)-C(5)	146.6(2)
O(1)-Ca(1)-C(4)-C(5)	-135.2(2)
C(14)-Ca(1)-C(4)-C(5)	13.0(5)
C(1)-Ca(1)-C(4)-C(5)	37.9(2)
C(15)-Ca(1)-C(4)-C(5)	11.5(3)
C(2)-Ca(1)-C(4)-C(5)	77.6(2)
C(3)-Ca(1)-C(4)-C(5)	114.3(4)
C(11)-Ca(1)-C(4)-C(5)	-19.6(3)
C(13)-Ca(1)-C(4)-C(5)	-69.0(4)
C(12)-Ca(1)-C(4)-C(5)	-52.6(3)
C(2)-C(1)-C(5)-C(4)	0.7(4)
Ca(1)-C(1)-C(5)-C(4)	69.0(2)
C(2)-C(1)-C(5)-C(6)	179.2(3)
Ca(1)-C(1)-C(5)-C(6)	-112.5(4)
C(2)-C(1)-C(5)-Ca(1)	-68.3(3)
C(3)-C(4)-C(5)-C(1)	-0.5(4)
Ca(1)-C(4)-C(5)-C(1)	-68.7(2)
C(3)-C(4)-C(5)-C(6)	-179.1(3)
Ca(1)-C(4)-C(5)-C(6)	112.7(4)
C(3)-C(4)-C(5)-Ca(1)	68.1(3)
O(2)-Ca(1)-C(5)-C(1)	66.0(3)
O(1)-Ca(1)-C(5)-C(1)	157.5(2)
C(14)-Ca(1)-C(5)-C(1)	-62.5(3)
C(15)-Ca(1)-C(5)-C(1)	-59.1(2)
C(2)-Ca(1)-C(5)-C(1)	36.3(2)
C(3)-Ca(1)-C(5)-C(1)	75.8(2)
C(11)-Ca(1)-C(5)-C(1)	-85.6(2)
C(4)-Ca(1)-C(5)-C(1)	112.1(3)
C(13)-Ca(1)-C(5)-C(1)	-103.5(2)
C(12)-Ca(1)-C(5)-C(1)	-110.1(2)
O(2)-Ca(1)-C(5)-C(4)	-46.1(3)
O(1)-Ca(1)-C(5)-C(4)	45.4(2)
C(14)-Ca(1)-C(5)-C(4)	-174.6(2)
C(1)-Ca(1)-C(5)-C(4)	-112.1(3)
C(15)-Ca(1)-C(5)-C(4)	-171.2(2)
C(2)-Ca(1)-C(5)-C(4)	-75.8(2)
C(3)-Ca(1)-C(5)-C(4)	-36.3(2)
C(11)-Ca(1)-C(5)-C(4)	162.3(2)
C(13)-Ca(1)-C(5)-C(4)	144.4(2)
C(12)-Ca(1)-C(5)-C(4)	137.8(2)
O(2)-Ca(1)-C(5)-C(6)	-169.6(2)
O(1)-Ca(1)-C(5)-C(6)	-78.1(3)
C(14)-Ca(1)-C(5)-C(6)	61.9(3)
C(1)-Ca(1)-C(5)-C(6)	124.4(4)
C(15)-Ca(1)-C(5)-C(6)	65.3(3)
C(2)-Ca(1)-C(5)-C(6)	160.8(3)
C(3)-Ca(1)-C(5)-C(6)	-159.8(3)
C(11)-Ca(1)-C(5)-C(6)	38.9(3)
C(4)-Ca(1)-C(5)-C(6)	-123.5(4)
C(13)-Ca(1)-C(5)-C(6)	20.9(4)
C(12)-Ca(1)-C(5)-C(6)	14.3(3)
C(1)-C(5)-C(6)-C(7)	-10.6(6)
C(4)-C(5)-C(6)-C(7)	167.7(4)
Ca(1)-C(5)-C(6)-C(7)	-101.4(4)
C(1)-C(5)-C(6)-C(10)	170.0(4)
C(4)-C(5)-C(6)-C(10)	-11.7(6)
Ca(1)-C(5)-C(6)-C(10)	79.1(5)
C(10)-C(6)-C(7)-C(8)	-3.5(5)
C(5)-C(6)-C(7)-C(8)	177.0(4)
C(6)-C(7)-C(8)-C(9)	6.0(5)
C(7)-C(8)-C(9)-C(10)	-6.0(6)

C(7)-C(6)-C(10)-C(9)	-0.4(6)	O(2)-Ca(1)-C(12)-C(13)	-6.3(3)
C(5)-C(6)-C(10)-C(9)	179.1(4)	O(1)-Ca(1)-C(12)-C(13)	-87.1(2)
C(8)-C(9)-C(10)-C(6)	4.2(6)	C(14)-Ca(1)-C(12)-C(13)	36.7(2)
O(2)-Ca(1)-C(11)-C(12)	81.2(3)	C(1)-Ca(1)-C(12)-C(13)	139.6(2)
O(1)-Ca(1)-C(11)-C(12)	-23.9(3)	C(15)-Ca(1)-C(12)-C(13)	77.1(3)
C(14)-Ca(1)-C(11)-C(12)	76.4(3)	C(5)-Ca(1)-C(12)-C(13)	170.4(2)
C(1)-Ca(1)-C(11)-C(12)	-156.4(3)	C(2)-Ca(1)-C(12)-C(13)	128.4(3)
C(15)-Ca(1)-C(11)-C(12)	114.2(4)	C(3)-Ca(1)-C(12)-C(13)	-179.6(3)
C(5)-Ca(1)-C(11)-C(12)	-126.0(3)	C(11)-Ca(1)-C(12)-C(13)	114.1(4)
C(2)-Ca(1)-C(11)-C(12)	-170.3(2)	C(4)-Ca(1)-C(12)-C(13)	-165.1(2)
C(3)-Ca(1)-C(11)-C(12)	-145.6(3)	C(11)-C(12)-C(13)-C(14)	0.6(4)
C(4)-Ca(1)-C(11)-C(12)	-116.2(3)	Ca(1)-C(12)-C(13)-C(14)	-67.7(3)
C(13)-Ca(1)-C(11)-C(12)	36.8(2)	C(11)-C(12)-C(13)-Ca(1)	68.2(3)
O(2)-Ca(1)-C(11)-C(15)	-33.0(3)	O(2)-Ca(1)-C(13)-C(14)	-71.2(3)
O(1)-Ca(1)-C(11)-C(15)	-138.0(2)	O(1)-Ca(1)-C(13)-C(14)	-153.5(3)
C(14)-Ca(1)-C(11)-C(15)	-37.7(2)	C(1)-Ca(1)-C(13)-C(14)	59.4(3)
C(1)-Ca(1)-C(11)-C(15)	89.5(2)	C(15)-Ca(1)-C(13)-C(14)	37.5(2)
C(5)-Ca(1)-C(11)-C(15)	119.8(2)	C(5)-Ca(1)-C(13)-C(14)	101.4(3)
C(2)-Ca(1)-C(11)-C(15)	75.6(2)	C(2)-Ca(1)-C(13)-C(14)	19.0(4)
C(3)-Ca(1)-C(11)-C(15)	100.2(3)	C(3)-Ca(1)-C(13)-C(14)	-69(2)
C(4)-Ca(1)-C(11)-C(15)	129.6(2)	C(11)-Ca(1)-C(13)-C(14)	77.5(3)
C(13)-Ca(1)-C(11)-C(15)	-77.3(2)	C(4)-Ca(1)-C(13)-C(14)	141.9(3)
C(12)-Ca(1)-C(11)-C(15)	-114.2(4)	C(12)-Ca(1)-C(13)-C(14)	114.3(4)
C(15)-C(11)-C(12)-C(13)	-0.4(4)	O(2)-Ca(1)-C(13)-C(12)	174.6(2)
Ca(1)-C(11)-C(12)-C(13)	-68.2(3)	O(1)-Ca(1)-C(13)-C(12)	92.2(2)
C(15)-C(11)-C(12)-Ca(1)	67.8(2)	C(14)-Ca(1)-C(13)-C(12)	-114.3(4)
O(2)-Ca(1)-C(12)-C(11)	-120.4(2)	C(1)-Ca(1)-C(13)-C(12)	-54.8(3)
O(1)-Ca(1)-C(12)-C(11)	158.9(3)	C(15)-Ca(1)-C(13)-C(12)	-76.8(3)
C(14)-Ca(1)-C(12)-C(11)	-77.4(3)	C(5)-Ca(1)-C(13)-C(12)	-12.9(3)
C(1)-Ca(1)-C(12)-C(11)	25.5(3)	C(2)-Ca(1)-C(13)-C(12)	-95.3(3)
C(15)-Ca(1)-C(12)-C(11)	-37.0(2)	C(3)-Ca(1)-C(13)-C(12)	177(27)
C(5)-Ca(1)-C(12)-C(11)	56.3(3)	C(11)-Ca(1)-C(13)-C(12)	-36.8(2)
C(2)-Ca(1)-C(12)-C(11)	14.4(4)	C(4)-Ca(1)-C(13)-C(12)	27.6(4)
C(3)-Ca(1)-C(12)-C(11)	66.3(4)	C(12)-C(13)-C(14)-C(15)	-0.5(4)
C(4)-Ca(1)-C(12)-C(11)	80.8(3)	Ca(1)-C(13)-C(14)-C(15)	-68.5(3)
C(13)-Ca(1)-C(12)-C(11)	-114.1(4)	C(12)-C(13)-C(14)-Ca(1)	68.1(3)

O(2)-Ca(1)-C(14)-C(13)	107.3(3)	C(3)-Ca(1)-C(15)-C(11)	-107.9(2)
O(1)-Ca(1)-C(14)-C(13)	29.3(3)	C(4)-Ca(1)-C(15)-C(11)	-68.0(3)
C(1)-Ca(1)-C(14)-C(13)	-136.3(2)	C(13)-Ca(1)-C(15)-C(11)	76.1(2)
C(15)-Ca(1)-C(14)-C(13)	-113.7(4)	C(12)-Ca(1)-C(15)-C(11)	36.6(2)
C(5)-Ca(1)-C(14)-C(13)	-107.0(3)	O(2)-Ca(1)-C(15)-C(14)	42.3(2)
C(2)-Ca(1)-C(14)-C(13)	-169.1(2)	O(1)-Ca(1)-C(15)-C(14)	-52.8(3)
C(3)-Ca(1)-C(14)-C(13)	174.2(3)	C(1)-Ca(1)-C(15)-C(14)	159.3(2)
C(11)-Ca(1)-C(14)-C(13)	-76.3(3)	C(5)-Ca(1)-C(15)-C(14)	-175.0(2)
C(4)-Ca(1)-C(14)-C(13)	-115.8(4)	C(2)-Ca(1)-C(15)-C(14)	134.0(2)
C(12)-Ca(1)-C(14)-C(13)	-36.7(2)	C(3)-Ca(1)-C(15)-C(14)	139.2(2)
O(2)-Ca(1)-C(14)-C(15)	-139.1(2)	C(11)-Ca(1)-C(15)-C(14)	-112.9(3)
O(1)-Ca(1)-C(14)-C(15)	143.0(2)	C(4)-Ca(1)-C(15)-C(14)	179.1(2)
C(1)-Ca(1)-C(14)-C(15)	-22.7(3)	C(13)-Ca(1)-C(15)-C(14)	-36.7(2)
C(5)-Ca(1)-C(14)-C(15)	6.6(3)	C(12)-Ca(1)-C(15)-C(14)	-76.3(3)
C(2)-Ca(1)-C(14)-C(15)	-55.4(3)	O(2)-Ca(1)-C(15)-C(16)	-80.7(3)
C(3)-Ca(1)-C(14)-C(15)	-72.1(3)	O(1)-Ca(1)-C(15)-C(16)	-175.8(2)
C(11)-Ca(1)-C(14)-C(15)	37.4(2)	C(14)-Ca(1)-C(15)-C(16)	-123.0(4)
C(4)-Ca(1)-C(14)-C(15)	-2.2(5)	C(1)-Ca(1)-C(15)-C(16)	36.3(3)
C(13)-Ca(1)-C(14)-C(15)	113.7(4)	C(5)-Ca(1)-C(15)-C(16)	62.1(3)
C(12)-Ca(1)-C(14)-C(15)	76.9(3)	C(2)-Ca(1)-C(15)-C(16)	11.0(3)
C(12)-C(11)-C(15)-C(14)	0.1(4)	C(3)-Ca(1)-C(15)-C(16)	16.2(3)
Ca(1)-C(11)-C(15)-C(14)	68.3(3)	C(11)-Ca(1)-C(15)-C(16)	124.1(4)
C(12)-C(11)-C(15)-C(16)	-178.4(3)	C(4)-Ca(1)-C(15)-C(16)	56.1(3)
Ca(1)-C(11)-C(15)-C(16)	-110.2(4)	C(13)-Ca(1)-C(15)-C(16)	-159.7(3)
C(12)-C(11)-C(15)-Ca(1)	-68.2(3)	C(12)-Ca(1)-C(15)-C(16)	160.7(3)
C(13)-C(14)-C(15)-C(11)	0.2(4)	C(11)-C(15)-C(16)-C(17)	-15.9(6)
Ca(1)-C(14)-C(15)-C(11)	-68.8(2)	C(14)-C(15)-C(16)-C(17)	165.8(4)
C(13)-C(14)-C(15)-C(16)	178.7(4)	Ca(1)-C(15)-C(16)-C(17)	-105.7(4)
Ca(1)-C(14)-C(15)-C(16)	109.8(4)	C(11)-C(15)-C(16)-C(20)	156.4(4)
C(13)-C(14)-C(15)-Ca(1)	69.0(3)	C(14)-C(15)-C(16)-C(20)	-21.8(6)
O(2)-Ca(1)-C(15)-C(11)	155.2(2)	Ca(1)-C(15)-C(16)-C(20)	66.7(4)
O(1)-Ca(1)-C(15)-C(11)	60.1(3)	C(20)-C(16)-C(17)-C(18)	-1.9(5)
C(14)-Ca(1)-C(15)-C(11)	112.9(3)	C(15)-C(16)-C(17)-C(18)	171.4(4)
C(1)-Ca(1)-C(15)-C(11)	-87.8(2)	C(16)-C(17)-C(18)-C(19)	7.8(5)
C(5)-Ca(1)-C(15)-C(11)	-62.1(2)	C(17)-C(18)-C(19)-C(20)	-10.3(5)
C(2)-Ca(1)-C(15)-C(11)	-113.1(2)	C(17)-C(16)-C(20)-C(19)	-4.8(5)

C(15)-C(16)-C(20)-C(19)	-178.2(4)	C(24B)-O(1)-C(21)-C(22)	45.2(11)
C(18)-C(19)-C(20)-C(16)	9.6(6)	Ca(1)-O(1)-C(21)-C(22)	-179.7(3)
O(2)-Ca(1)-O(1)-C(21)	-128.0(4)	O(1)-C(21)-C(22)-C(23)	-21.4(5)
C(14)-Ca(1)-O(1)-C(21)	-50.2(4)	C(21)-C(22)-C(23)-C(24B)	-14.9(14)
C(1)-Ca(1)-O(1)-C(21)	112.6(4)	C(21)-C(22)-C(23)-C(24A)	35.9(5)
C(15)-Ca(1)-O(1)-C(21)	-23.8(4)	C(24B)-C(23)-C(24A)-O(1)	58.7(13)
C(5)-Ca(1)-O(1)-C(21)	98.1(4)	C(22)-C(23)-C(24A)-O(1)	-37.3(6)
C(2)-Ca(1)-O(1)-C(21)	148.3(4)	C(21)-O(1)-C(24A)-C(23)	24.5(6)
C(3)-Ca(1)-O(1)-C(21)	147.2(4)	C(24B)-O(1)-C(24A)-C(23)	-55.5(13)
C(11)-Ca(1)-O(1)-C(21)	5.5(4)	Ca(1)-O(1)-C(24A)-C(23)	-157.3(3)
C(4)-Ca(1)-O(1)-C(21)	119.4(4)	C(24A)-C(23)-C(24B)-O(1)	-53.6(12)
C(13)-Ca(1)-O(1)-C(21)	-36.0(4)	C(22)-C(23)-C(24B)-O(1)	42.6(17)
C(12)-Ca(1)-O(1)-C(21)	-6.1(4)	C(21)-O(1)-C(24B)-C(23)	-54.4(16)
O(2)-Ca(1)-O(1)-C(24A)	54.3(4)	C(24A)-O(1)-C(24B)-C(23)	55.6(12)
C(14)-Ca(1)-O(1)-C(24A)	132.0(4)	Ca(1)-O(1)-C(24B)-C(23)	164.3(9)
C(1)-Ca(1)-O(1)-C(24A)	-65.2(4)	O(1)-Ca(1)-O(2)-C(28)	-129.6(4)
C(15)-Ca(1)-O(1)-C(24A)	158.4(4)	C(14)-Ca(1)-O(2)-C(28)	114.2(4)
C(5)-Ca(1)-O(1)-C(24A)	-79.7(4)	C(1)-Ca(1)-O(2)-C(28)	1.5(4)
C(2)-Ca(1)-O(1)-C(24A)	-29.5(4)	C(15)-Ca(1)-O(2)-C(28)	94.0(4)
C(3)-Ca(1)-O(1)-C(24A)	-30.6(4)	C(5)-Ca(1)-O(2)-C(28)	-29.7(5)
C(11)-Ca(1)-O(1)-C(24A)	-172.3(4)	C(2)-Ca(1)-O(2)-C(28)	-7.5(4)
C(4)-Ca(1)-O(1)-C(24A)	-58.4(4)	C(3)-Ca(1)-O(2)-C(28)	-37.2(4)
C(13)-Ca(1)-O(1)-C(24A)	146.2(4)	C(11)-Ca(1)-O(2)-C(28)	110.5(4)
C(12)-Ca(1)-O(1)-C(24A)	176.1(4)	C(4)-Ca(1)-O(2)-C(28)	-52.7(4)
O(2)-Ca(1)-O(1)-C(24B)	-1.7(14)	C(13)-Ca(1)-O(2)-C(28)	142.6(4)
C(14)-Ca(1)-O(1)-C(24B)	76.1(14)	C(12)-Ca(1)-O(2)-C(28)	145.8(4)
C(1)-Ca(1)-O(1)-C(24B)	-121.1(14)	O(1)-Ca(1)-O(2)-C(25)	53.4(5)
C(15)-Ca(1)-O(1)-C(24B)	102.5(14)	C(14)-Ca(1)-O(2)-C(25)	-62.8(5)
C(5)-Ca(1)-O(1)-C(24B)	-135.7(14)	C(1)-Ca(1)-O(2)-C(25)	-175.5(4)
C(2)-Ca(1)-O(1)-C(24B)	-85.4(14)	C(15)-Ca(1)-O(2)-C(25)	-83.0(5)
C(3)-Ca(1)-O(1)-C(24B)	-86.5(14)	C(5)-Ca(1)-O(2)-C(25)	153.3(4)
C(11)-Ca(1)-O(1)-C(24B)	131.8(14)	C(2)-Ca(1)-O(2)-C(25)	175.5(5)
C(4)-Ca(1)-O(1)-C(24B)	-114.3(14)	C(3)-Ca(1)-O(2)-C(25)	145.8(5)
C(13)-Ca(1)-O(1)-C(24B)	90.3(14)	C(11)-Ca(1)-O(2)-C(25)	-66.5(5)
C(12)-Ca(1)-O(1)-C(24B)	120.2(14)	C(4)-Ca(1)-O(2)-C(25)	130.3(4)
C(24A)-O(1)-C(21)-C(22)	-1.6(6)	C(13)-Ca(1)-O(2)-C(25)	-34.4(5)

C(12)-Ca(1)-O(2)-C(25)	-31.2(5)	C(25)-C(26)-C(27)-C(28)	-13.8(7)
C(28)-O(2)-C(25)-C(26)	-30.5(7)	C(25)-O(2)-C(28)-C(27)	21.4(6)
Ca(1)-O(2)-C(25)-C(26)	147.2(4)	Ca(1)-O(2)-C(28)-C(27)	-155.9(4)
O(2)-C(25)-C(26)-C(27)	27.2(7)	C(26)-C(27)-C(28)-O(2)	-4.7(7)