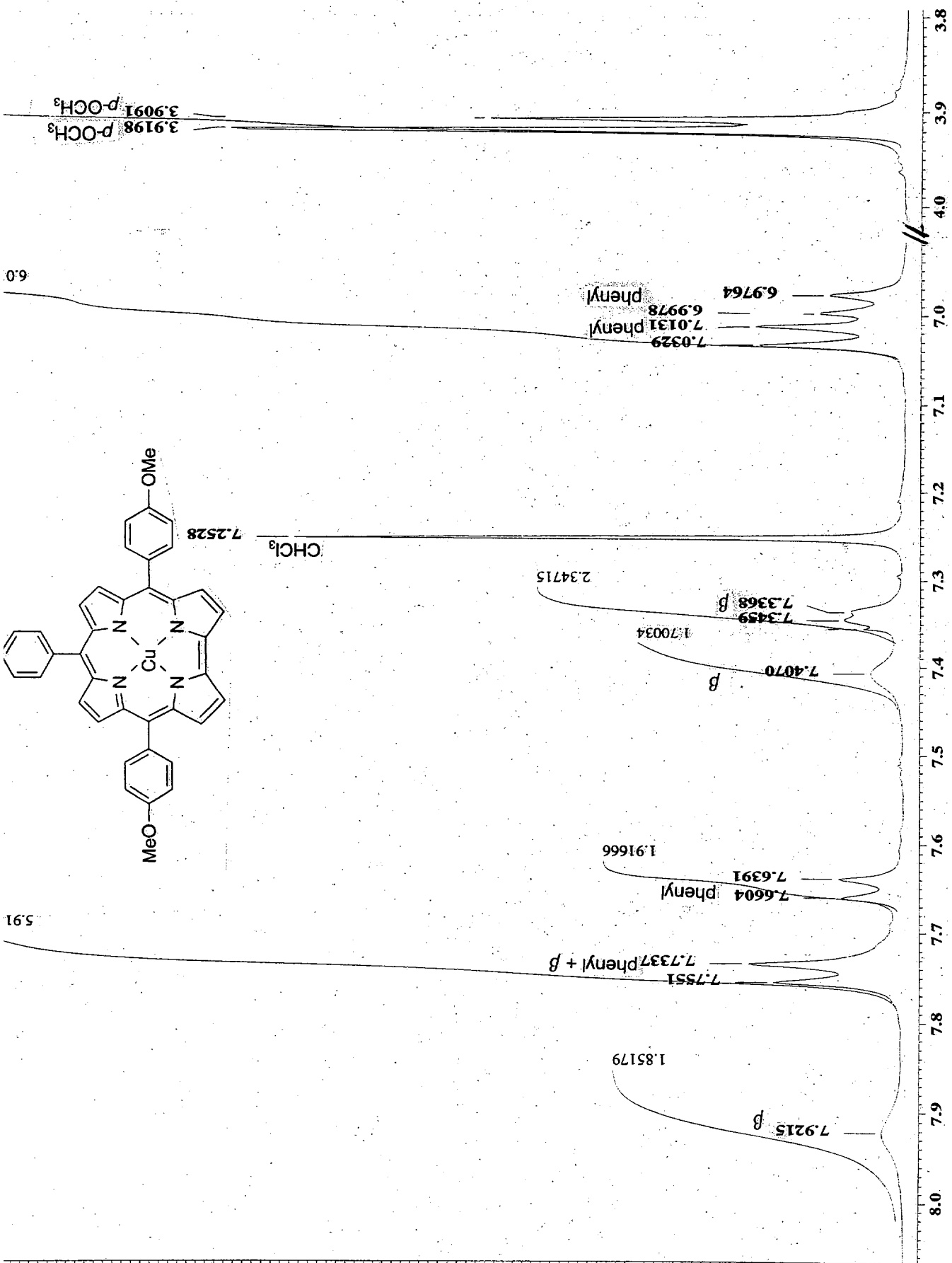


JA 112697

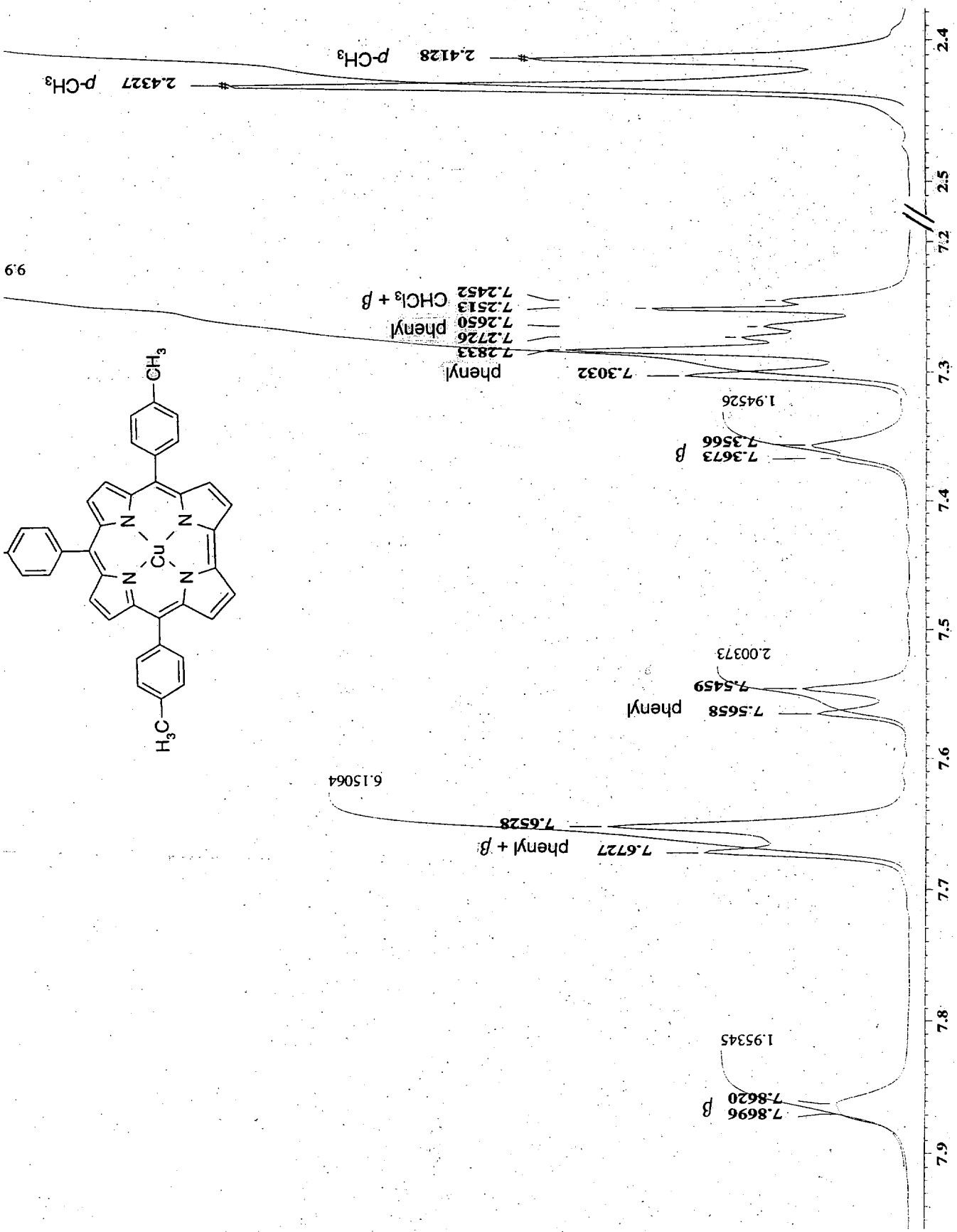
Supporting Information

IR spectra and ^1H NMR spectra of various Cu(III) triarylcorroles studied and plausible assignments are shown in the following pages.



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----- ACQUISITION PARAMETERS -----
 File Name = 1d_Cu(III)_TFC.24
 Author = Ingar Halvorsen
 Sample ID = CuTriphenylCorrole
 Content = Single Pulse Experiment
 Creation Date = 27-OCT-2000 17:50:58
 Revision Date = 22-MAY-2001 13:44:11

Spec Site = Eclipse.400
 Spec Type = DELTA_NMR

Data Format = 1D COMPLEX
 Dimensions = X
 Dim Title = 1H
 Dim Size = 16384
 Dim Units = (ppm)
 Scans = 86

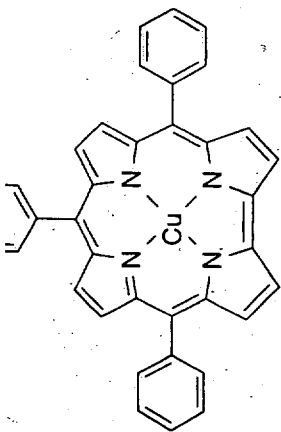
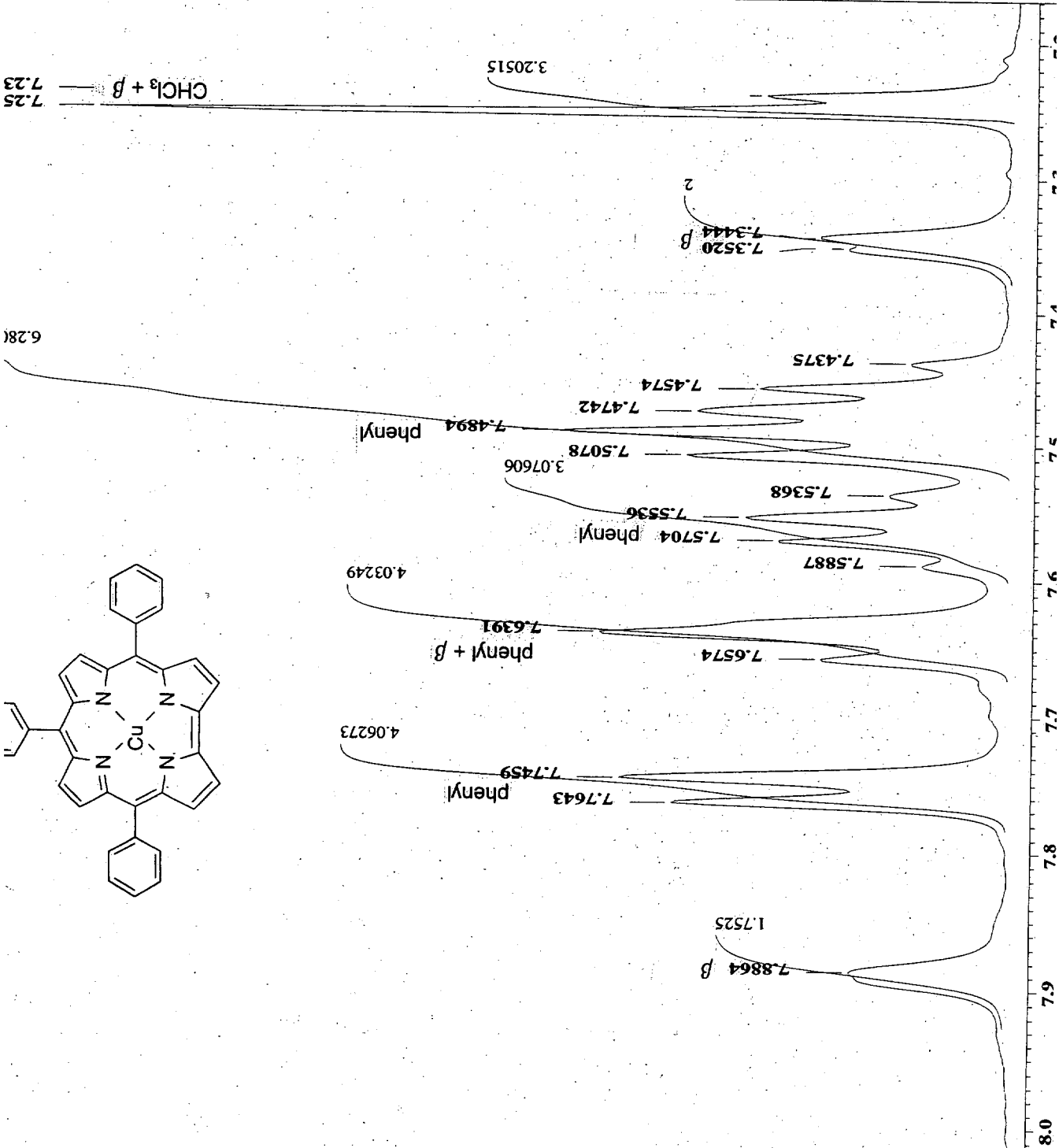
Mod_return = 1
 X_points = 16384
 X_prescans = 4
 X_domain = 1H
 X_offset = 5 (ppm)
 X_freq = 399.7841973 [MHz]
 X_sweep = 0.61038882 [Hz]
 X_resolution = 1.6384 [s]
 X_acq_duration = FALSE
 Digital_filter = 1

Delay_of_start = 1 [s]
 Actual_start_time = 27-OCT-2000 17:42:
 Acq_delay = 97.2 [us]
 X90 = 11.3 [us]
 Irr90 = 11.3 [us]

Tri90 = 10 [us]
 Qua90 = 10 [us]
 Irr90_hi = 20 [us]
 Tri90_hi = 20 [us]
 Qua90_hi = 10 [us]
 X90_lo = 10 [us]
 Irr90_lo = 50 [us]
 Tri90_lo = 10 [us]
 Qua90_lo = 10 [us]
 Spin_lock_90 = 72.3 [us]
 Spin_lock_attn = 15 [dB]
 Deut_grad_shim_90 = 1 [us]
 Deut_grad_shim_attn = 10 [dB]
 Acc_card = 16/1MHz/20
 Field_strength = 9.389766 [T]
 Filter_mode = BUTTERWORTH
 Filter_width = 4.99727748 [kHz]
 Recvr_gain = 19
 Irr_code = 146
 Obs_pwidth = 1 [us]
 Irr_pwidth = WAUGH
 Tri_noise = 50 [us]
 Qua_noise = WAUGH
 Qua_pwidth = 1 [us]
 Qua_noise = WAUGH

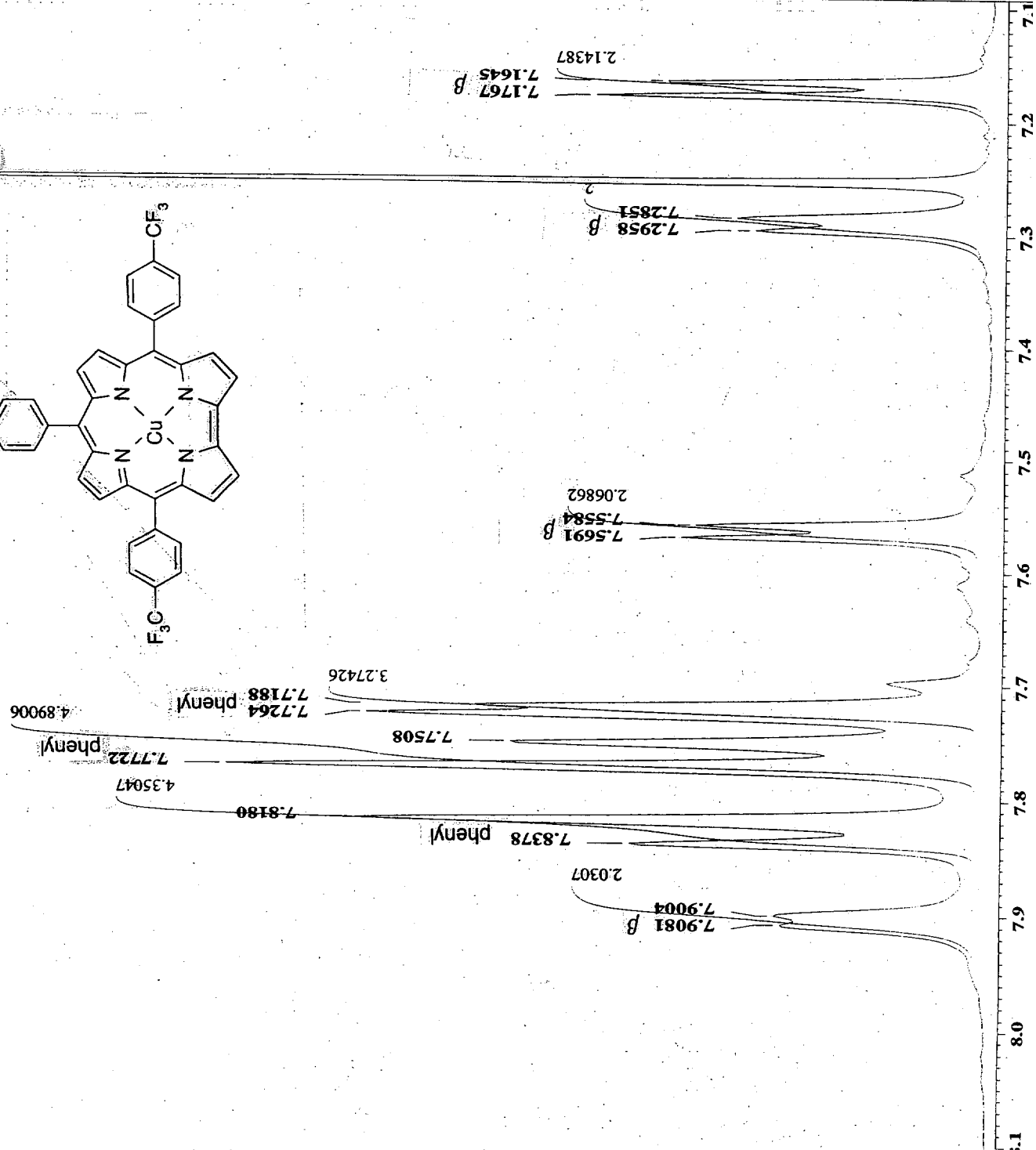
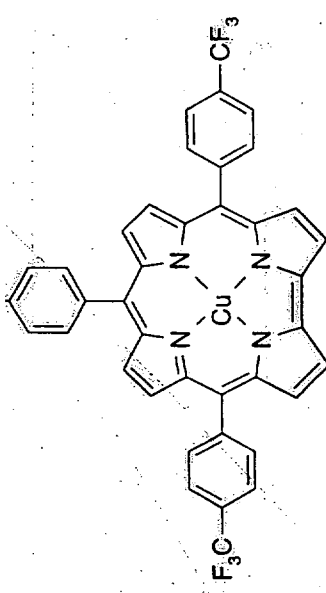
Solvent = CHLOROFORM-D
 Lock_strength = 585
 Lock_level = 180
 Lock_gain = 21
 Lock_osc_offset = 61.6311 [kHz]

6.281
 7.23
 7.25
 CHCl₃ + β





C



ACQUISITION PARAMETERS
 File name: 131_T(4-CF3-Ph)Cu(II)
 Author: Ingar Halvorsen
 Sample ID: 131_T(4-CF3-Ph)Cu(II)
 Content: Corion@ingar
 Creation Date: 21-Sep-2000 10:49:17
 Revision Date: 16-May-2001 08:09:20
 Spec Name: Eclips-400
 Date Formatted: DELTAUMR
 Dimensions: 1D, COMPLEX
 Dim 1: 1H
 Dim 2: 16384
 Dim 3: 16384
 Dim Units: (ppm)
 Scans: 190
 Mod Return: 1
 X Points: 16384
 X Prescans: 4
 X Domain: 1H
 X Offset: 0 (ppm)
 X Sweep: 199.78219838 (MHz)
 X Resolution: 10 (kHz)
 X Acq Duration: 0.61038882 (Hz)
 Digital Filter: F, 1.6384 (s)
 Filter Factor: FALSE
 Delay of Start: 1 (s)
 Actual Start Time: 24-SEP-2000 10:30:
 Acq Delay: 97.2 (us)
 X90: 11.3 (us)
 Irr90: 11.3 (us)
 Tr190: 10 (us)
 Quc90: 19 (us)
 X90: 11.3 (us)
 Irr90: 11.3 (us)
 Tr190: 10 (us)
 Quc90: 19 (us)
 X90: 11.3 (us)
 Irr90: 11.3 (us)
 Tr190: 10 (us)
 Quc90: 19 (us)
 X90: 11.3 (us)
 Irr90: 11.3 (us)
 Tr190: 10 (us)
 Quc90: 19 (us)
 Spin Lock 90: 1 (us)
 Spin Lock Attn: 15 (dB)
 Deut Grad Spin 90: 1 (us)
 Deut Grad Spin Attn: 15 (dB)
 Acq Solvent: BUTTERWORTH
 Filter Width: 4.9972748 (kHz)
 Resol Gain: 19
 Irr: 146
 Obs Width: 1 (us)
 Obs Noise: WAUGH
 Irr Width: 50 (us)
 Irr Noise: WALTZ
 Tri Width: 1 (us)
 Tri Noise: WALTZ
 Qua Width: 1 (us)
 Qua Noise: WAUGH
 Solvent: CHLOROFORM-D
 Lock Strength: 1699
 Lock Level: 180
 Lock Gain: 24
 Lock Osc Offset: 63.6311 (kHz)

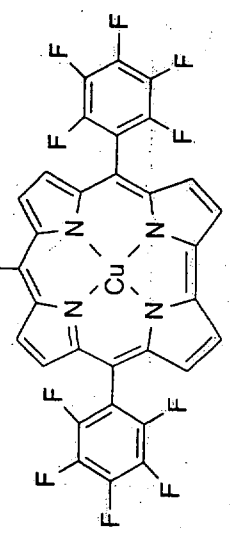


2.03

2.04

©

2.028



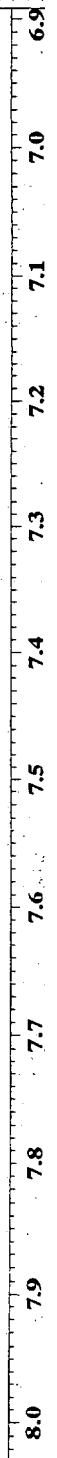
7.0241
7.0118

7.1996

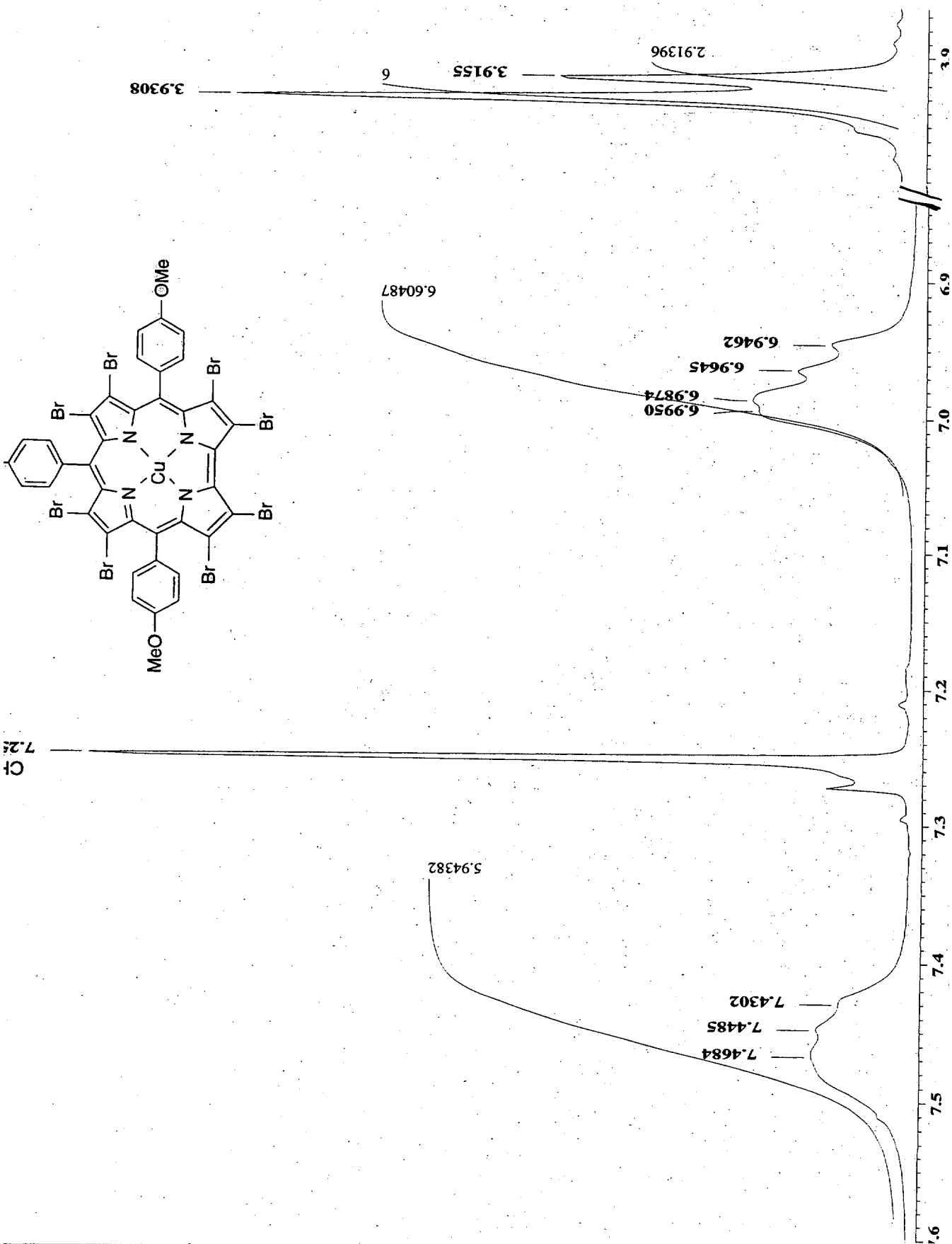
7.3859
7.3768

7.9722
7.9630

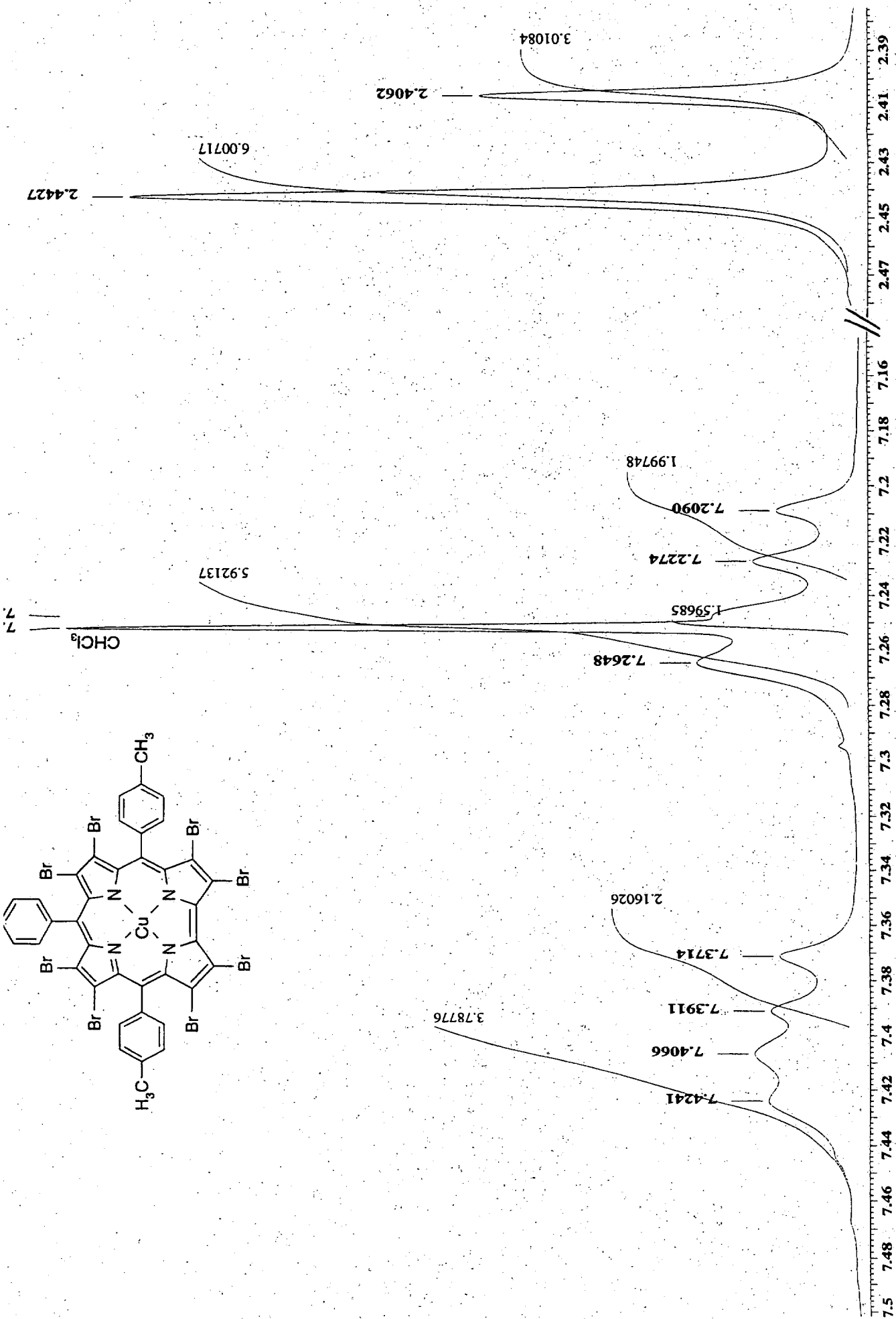
ACQUISITION PARAMETERS
 File Name = ID: C:\Pentastar\fluorCorr
 Author = Inga Halvorsen
 Sample ID = CUPFLUORIN
 Cont. Exp. = Single Pulse Experiment
 Creation Date = 22-AUG-2000 11:38:19
 Revision Date = 16-MAY-2001 08:28:53
 Spec File = Eclipse_270
 Spec Type = DELTA_NMR
 Data Format = 1D_COMPLEX
 Dimensions = X
 Dim Title = 1H
 Dim Size = 16384
 Dim Units = [ppm]
 Scans = 237
 Mod return = 1
 X_points = 16384
 X_prescans = 0
 X_domain = 1H
 X_offset = 0 [ppm]
 X_freq = 599.78219838 [MHz]
 X_sweep = 1
 X_resolution = 0.61038882 [Hz]
 X_acquisition = 6.3384 [s]
 Digital Filter = FALSE
 Filter Factor = 1
 Delay of start = 1 [ms]
 Active Start Time = 22-AUG-2000 11:15:
 Acquisition Time = 07:11 [us]
 X90 = 34.1 [us]
 T19 = 1.1 [us]
 T19 = 1.1 [us]
 T19 = 1.1 [us]
 X90 = 10 [us]
 X90 = 20 [us]
 T19 = 20 [us]
 T19 = 10 [us]
 X90 = 10 [us]
 X90 = 150 [us]
 T19 = 10 [us]
 T19 = 10 [us]
 X90 = 10 [us]
 Spin Speed [RPM] = 7200 [RPM]
 Spin Mod = 90
 Deut. Mod = 15 [dB]
 Deut. Grad. Gain = 16 [dB]
 Acc. Card = 9.389766 [Hz]
 Field Strength = BURBANK
 Filter Mode = 21
 Filter Width = 4.99727748 [kHz]
 Recv. Gain = 146
 Irr. Code = 1 [us]
 Obs. Width = WAUGH
 Irr. Width = 50 [us]
 Irr. Noise = WALTZ
 Tri. Width = 1 [us]
 Tri. Noise = WALTZ
 Qua. Width = 1 [us]
 Qua. Noise = WAUGH
 Solvent = CHLOROFORM-D
 Lock Strength = 346
 Lock Level = 100
 Lock Gain = 27
 Lock SPC Offset = 6.11 [kHz]
 Lock Phase = 26.1 [deg]



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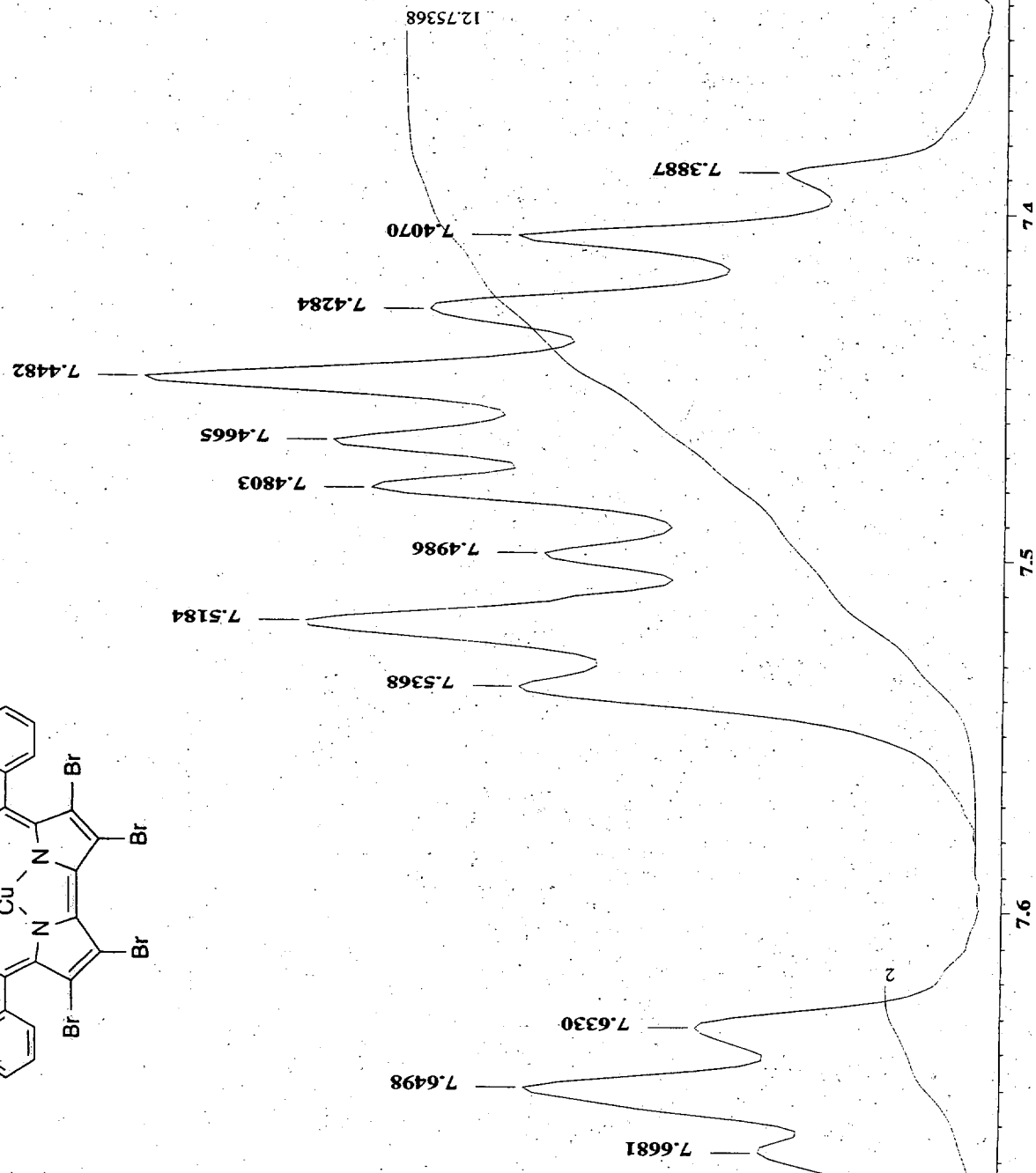
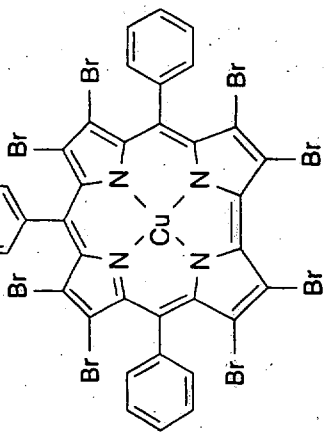


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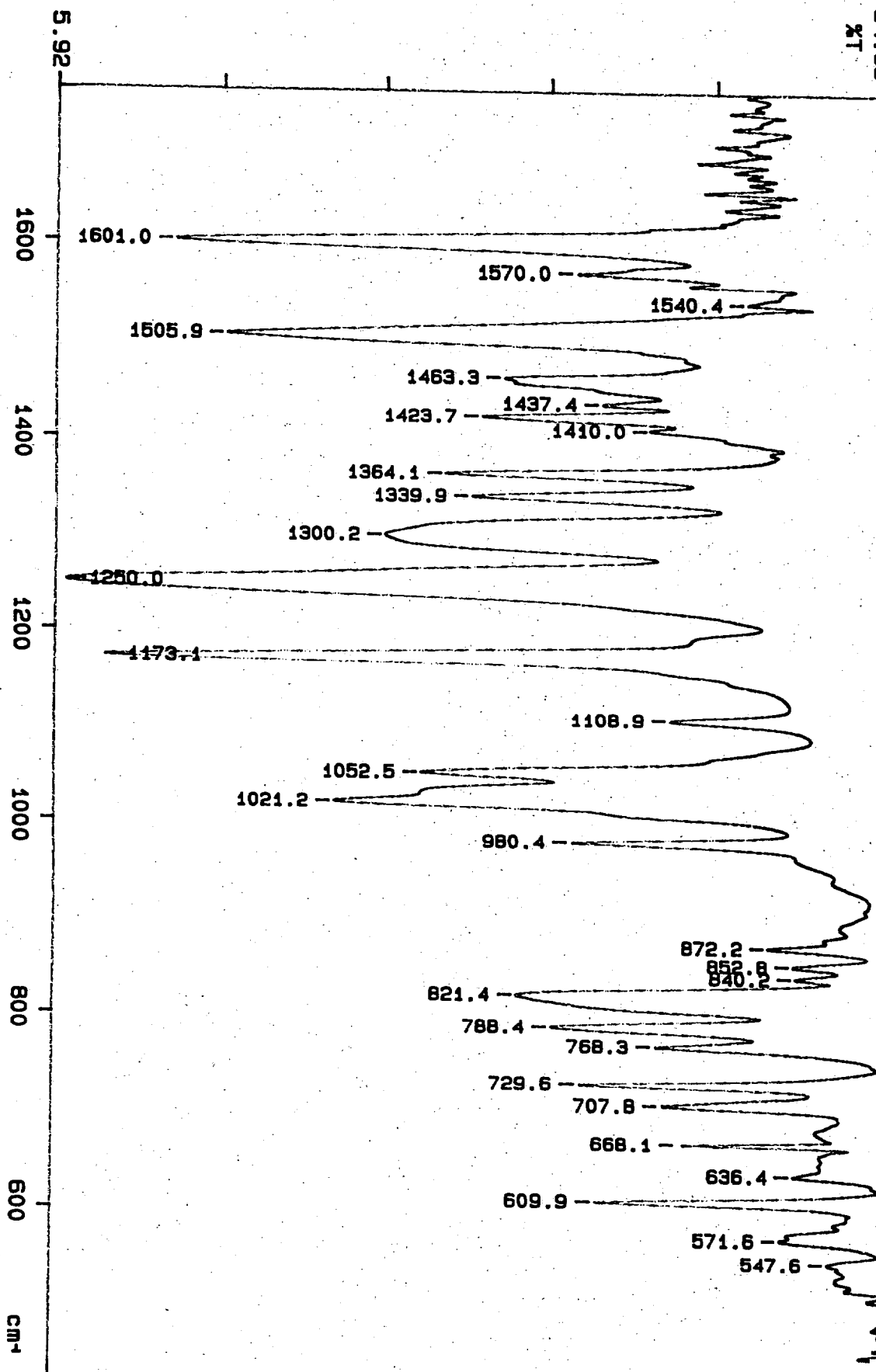


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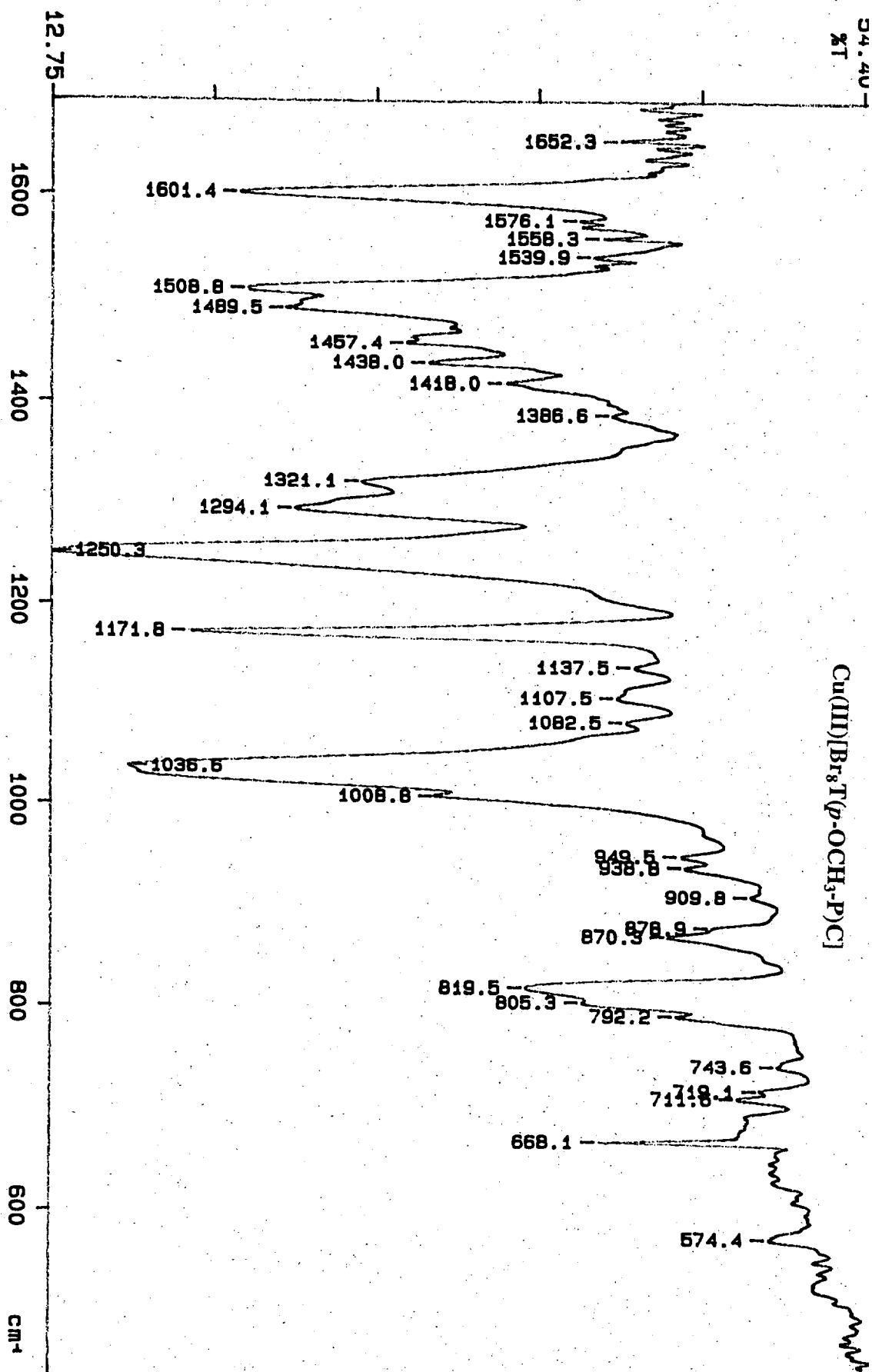
----- ACQUISITION PARAMETERS -----
File Name      = idBr8CutPC 25C.25ppm.
Author        = Univar Halvorsen
Sample ID     = 25C.25ppm
Content       = 7-MAX Pulse Experiment
Creation Date = 7-MAY-2001 11:10:33
Revision Date = 15-MAY-2001 11:08:29
SpecSite     = 201psc-400
SpecType     = DEPTMNMWB
DataDir      = 110000000
Dimensionless = 1
Dim X1       = 16384
Dim X2       = 16384
Dim Y1       = 16384
Dim Y2       = 16384
Scales       = [DPM]
Scales      = 256
Xpoints      = 16384
Xprescans    = 4
Xdomain      = 1
Xoffset      = 1
Xrange       = 39.7841973 [MHz]
Xsweep       = 10 [kHz]
Xresolution  = 0.61038882 [Hz]
Xacquisition = 1.6384 [s]
Xacceleration = FALSE
Digital filter =
Filter type   =
Filter cutoff =
Delay of start = 1 [s]
Actual_start_time = 7-MAY-2001 10:46:
Acq_delay     = 97.2 [us]
X90          = 11.3 [us]
Irr90        = 10 [us]
Tr190        = 10 [us]
Qza90        = 10 [us]
X90_hl       = 20 [us]
Irr90_hl     = 10 [us]
Qza90_hl     = 10 [us]
X90_lo       = 20 [us]
Irr90_lo     = 10 [us]
Tr190_lo     = 10 [us]
Qza90_lo     = 10 [us]
SpinLock_90  = 2.3 [us]
SpinLock_attn = 45 [dB]
Deut_solv    = H2O
Deut_solv    = 167 [MHz]
Acq_offset   = 9389766 [Hz]
P1           = 9389766 [Hz]
P2           = BUTTERWORTH
Filter width = 199727748 [kHz]
Recycle delay = 3.9
T1           = 146
T1_rho      = 1 [us]
Obsolwidth  = WAUGH
Obsolnoise  = 1 [us]
Irr_width   = WAUGH
Irr_noise   = 1 [us]
Tri_noise   = 1 [us]
Qza_noise   = 1 [us]
Solvnt      = CHLOROFORM-D
Lock_MW     = 754
Lock_Prob   = 180
Lock_start  = 22
Lock_offset = 61.6311 [MHz]
    
```



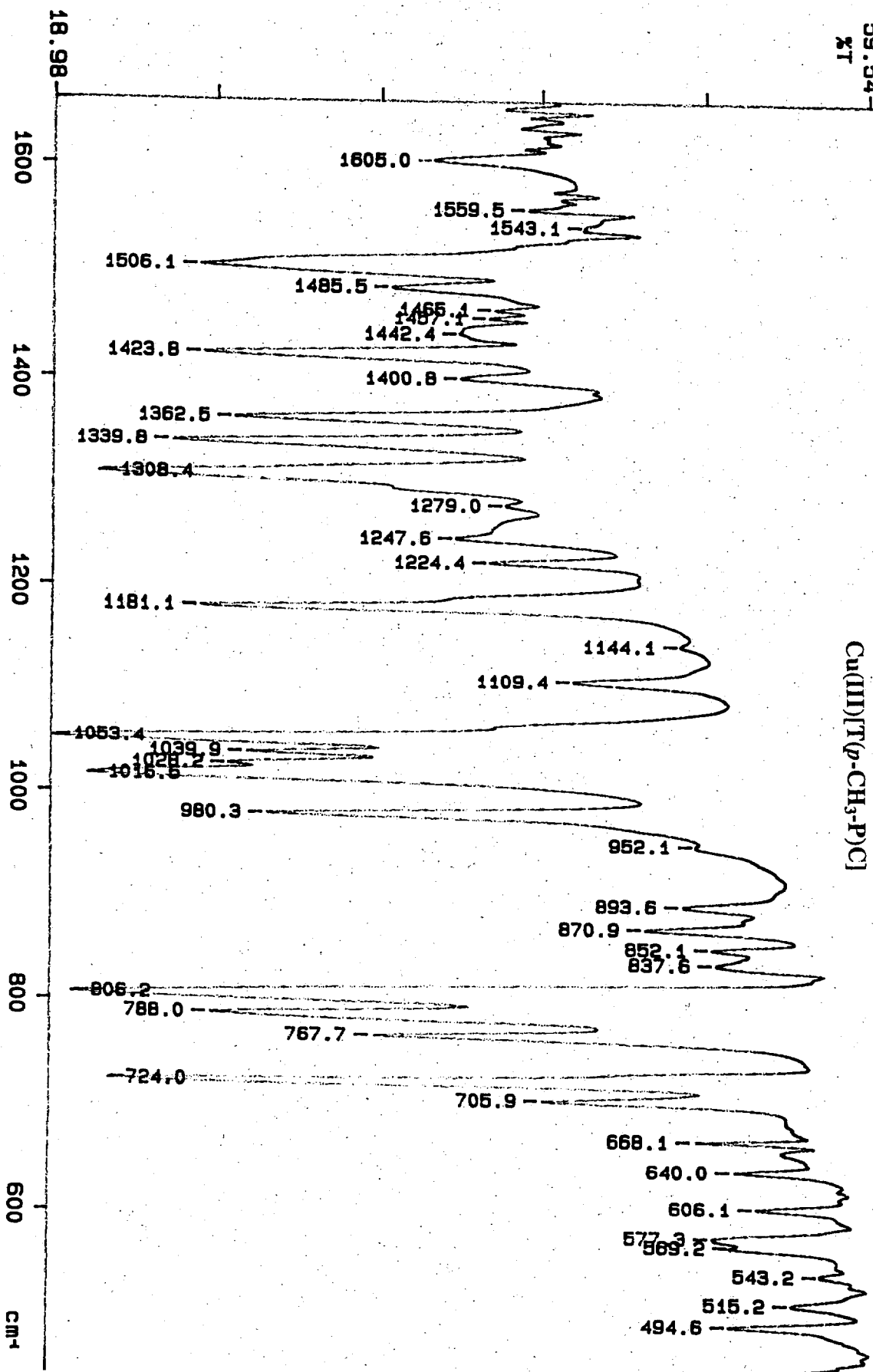
U11



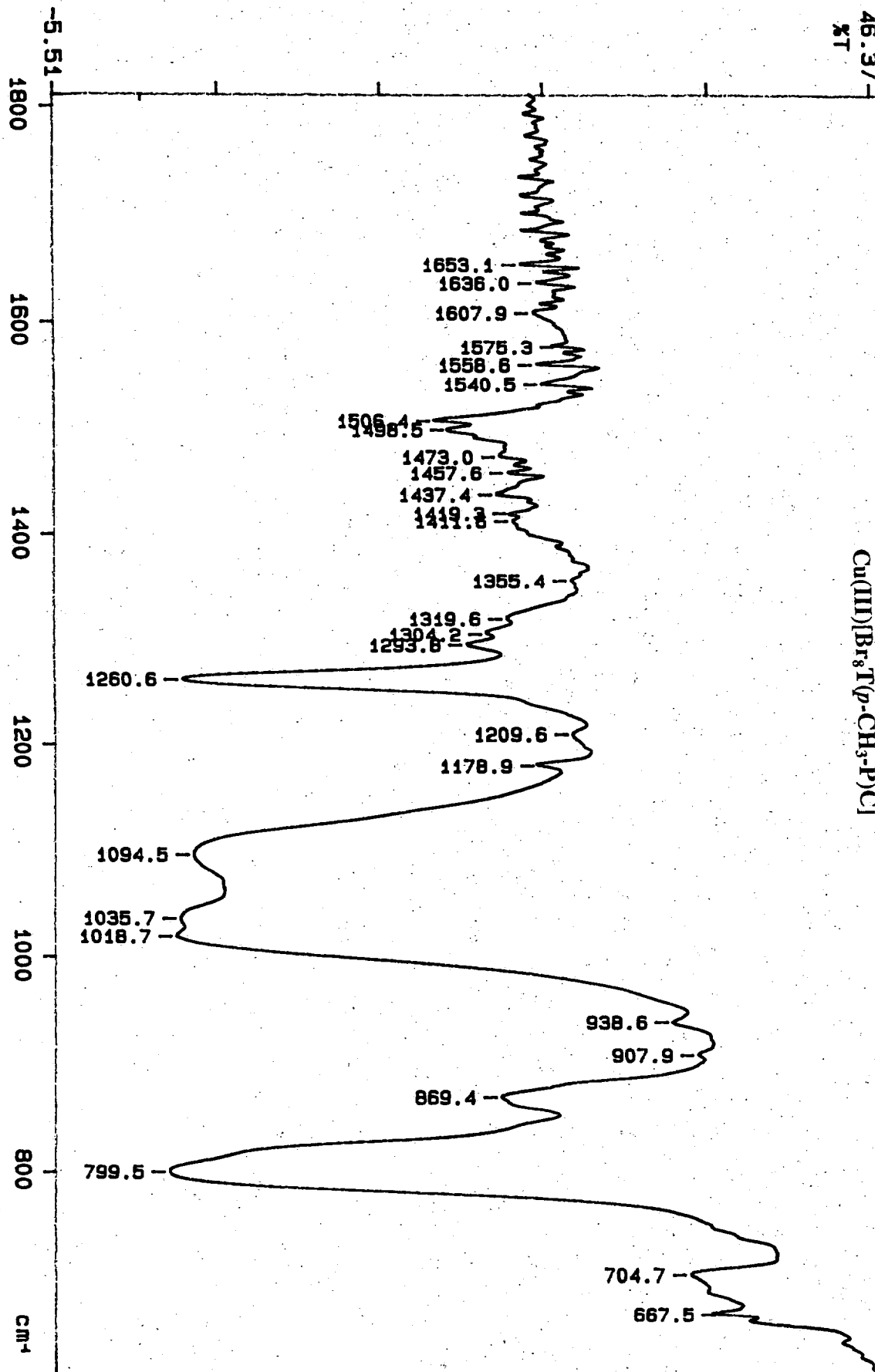
312



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S 14



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