

Supplementary Data

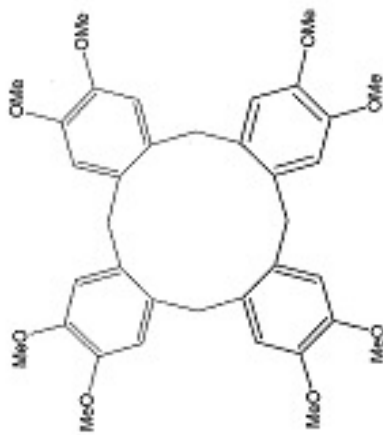
Synthesis, Crystal Structure, and Rearrangements of *ortho*-Cyclophane Cyclotetraveratrylene (CTTV) Tetraketone

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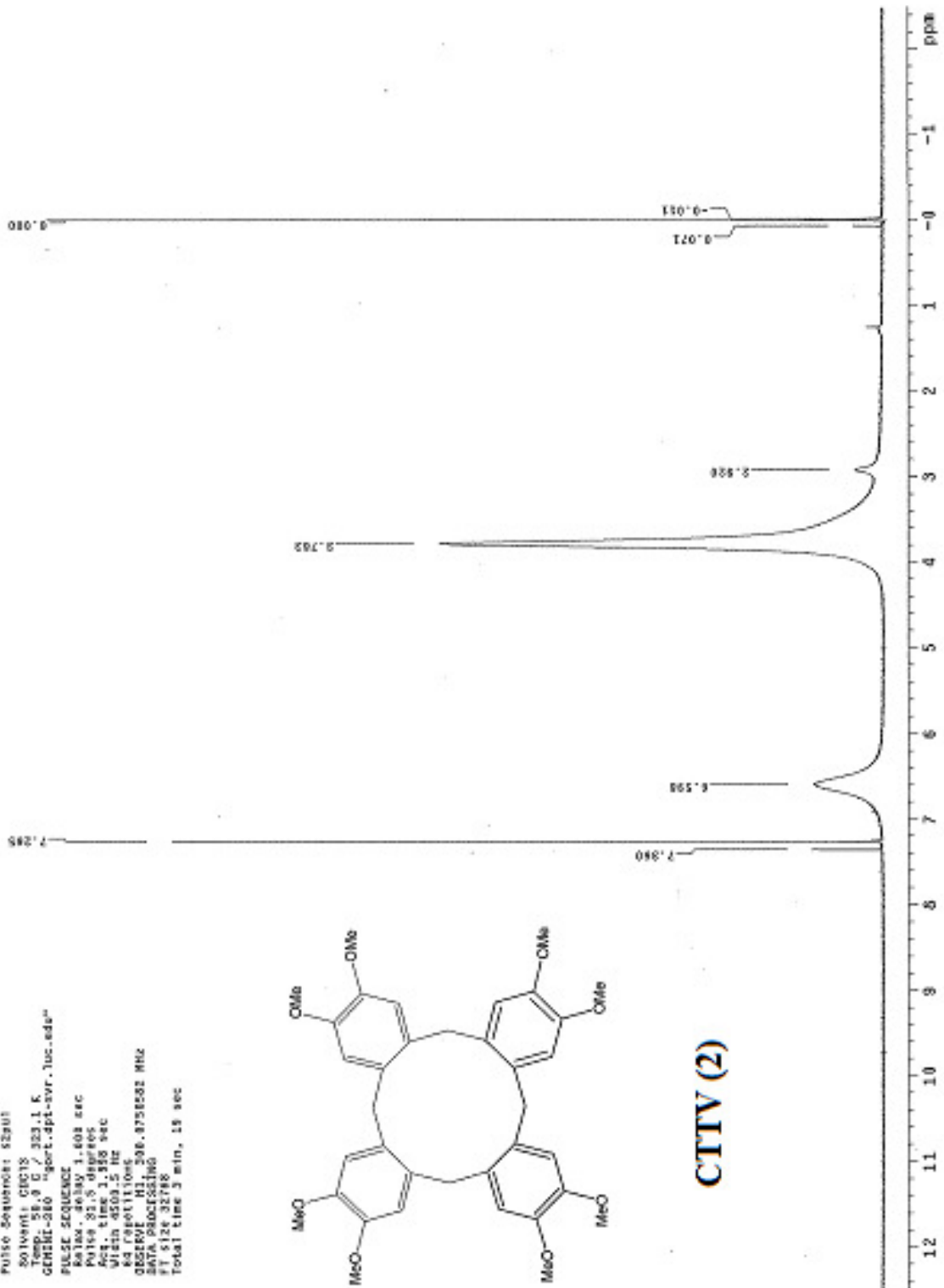
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ML7-057-2
 Pulse Sequence: zgpg30
 Solvent: CDCl3
 Temp: 29.9 C / 323.1 K
 GENIUM-360 -gort.dpt-svr.1uc.edg
 F1 F2 F3
 F4 F5 F6 F7 F8 F9
 F10 F11 F12 F13 F14 F15
 F16 F17 F18 F19 F20 F21
 F22 F23 F24 F25 F26 F27
 F28 F29 F30 F31 F32 F33
 F34 F35 F36 F37 F38 F39
 F40 F41 F42 F43 F44 F45
 F46 F47 F48 F49 F50 F51
 F52 F53 F54 F55 F56 F57
 F58 F59 F60 F61 F62 F63
 F64 F65 F66 F67 F68 F69
 F70 F71 F72 F73 F74 F75
 F76 F77 F78 F79 F80 F81
 F82 F83 F84 F85 F86 F87
 F88 F89 F90 F91 F92 F93
 F94 F95 F96 F97 F98 F99
 F100
 Kaim. delay 1.608 sec
 Pulse 92.0 degrees
 Acq. time 2.350 sec
 MTC: MEQ 2.000 sec
 64 (160111)000
 OBSERVE H1 300.8758582 MHz
 DATA PROCESSING
 FT SIZE 32788
 Total time 3 min. 19 sec

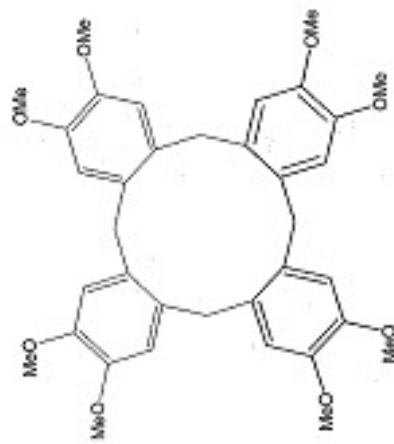


CTTV (2)

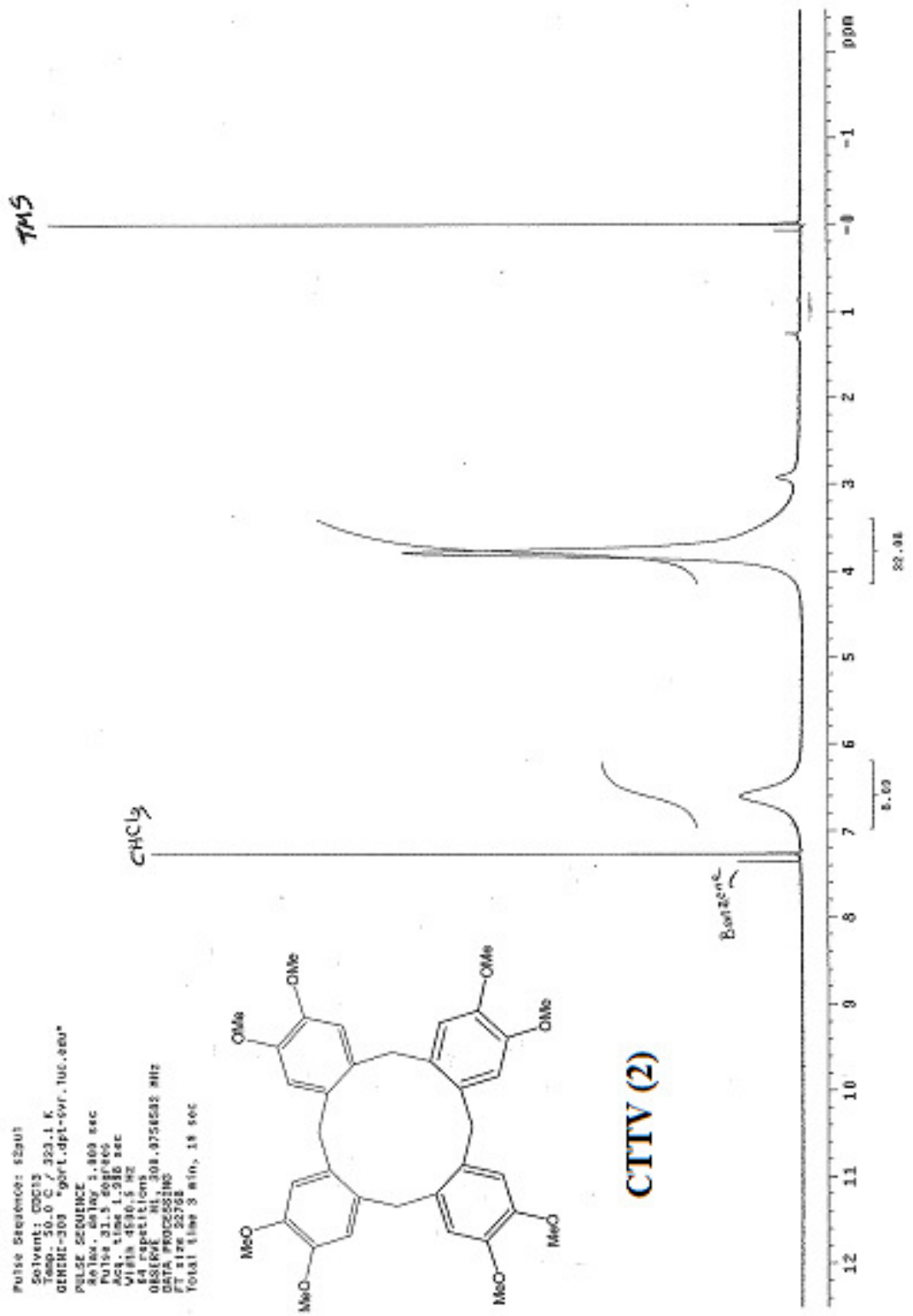


HL7-957-2

Pulse Sequence: s2au5
Solvent: CDCl3
Temp: 50.0 C / 323.1 K
GEMPR-303 *gprt.dpt-cvt.1uc.80u*
PULSE SEQUENCE
NOISE MEASURING 1.800 sec
PULSE 122.1 1.000 sec
PULSE 122.1 1.000 sec
WALTZ 4530.5 Hz
EA repetitions
OBSERVE HL 308.8754532 MHz
DATA PROCESSING
FT size 32768
Total time 3 min, 18 sec

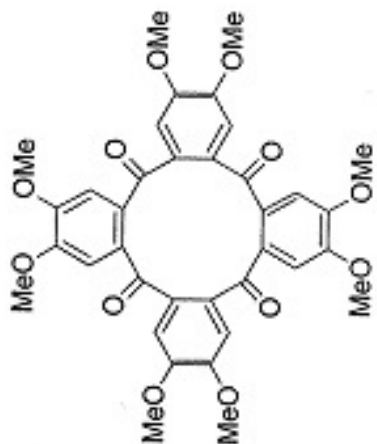


CTIV (2)

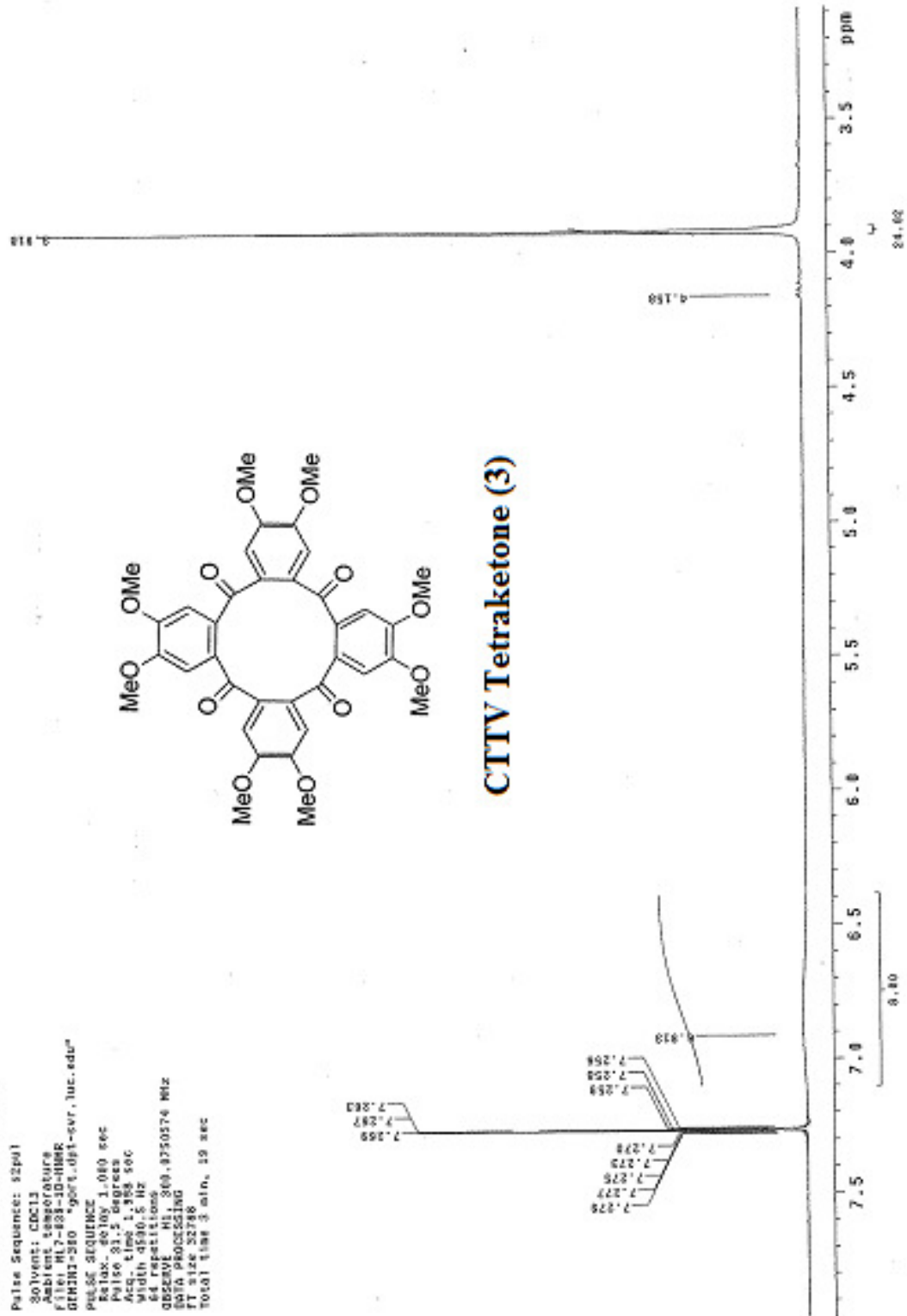


CTTV Tetraketone, Compound 13

Pulse Sequence: zgpg30
Solvent: CDCl3
Solute: sample
File: HL7-828-1D-HMR
GPM301-250 "90pt.dft-svt.luc.edu"
PULSE SEQUENCE: zgpg30
Pulse: 9.45 microseconds
Pulse 2: 9.45 microseconds
Acq time: 1.958 sec
Width: 4530.5 Hz
64 repetitions
QBS2AVE HL 369.9750574 MHz
DATA PROCESSING
FT size 32786
Total time 3 min, 19 sec



CTTV Tetraketone (3)

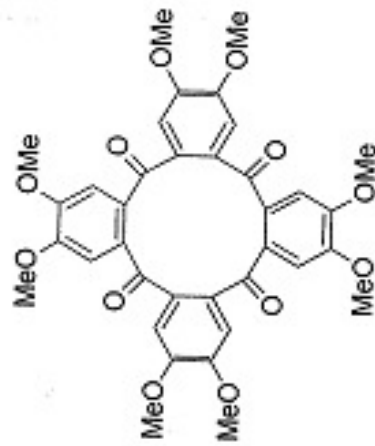


CTTV Tetraketone, Compound 19

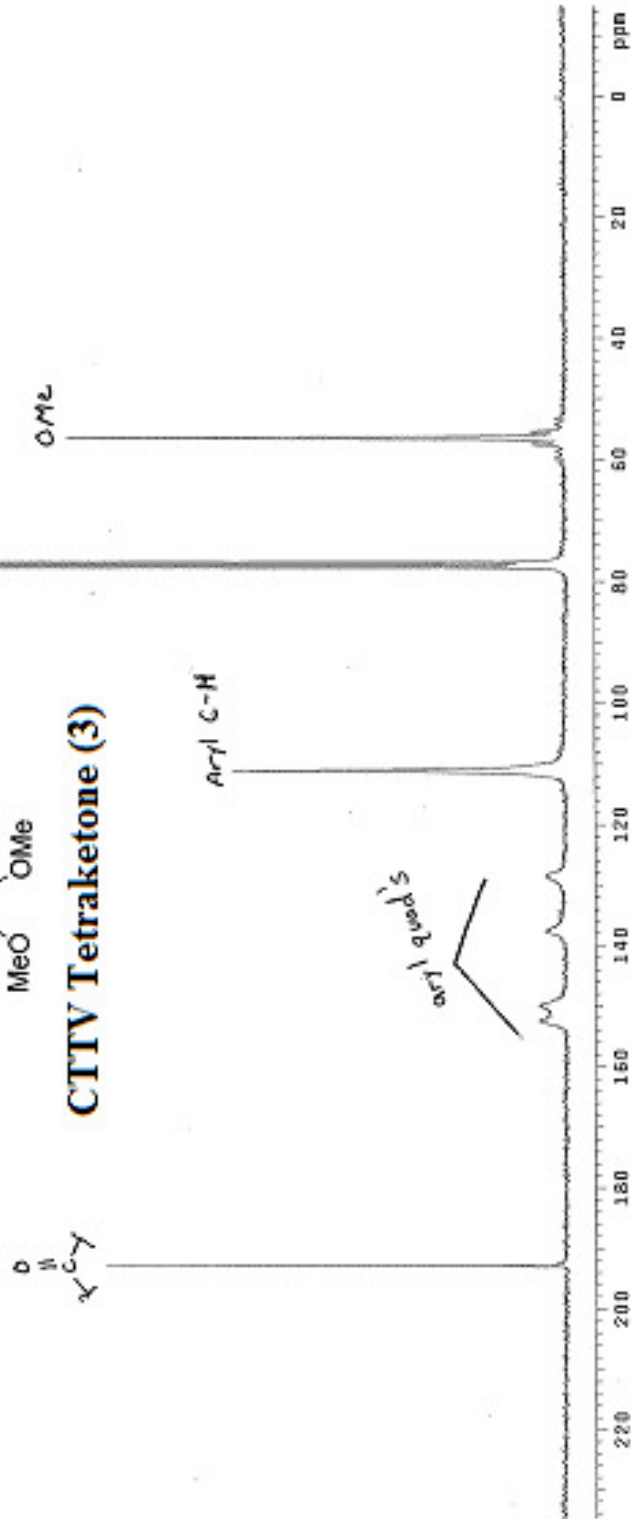
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Sample directory:

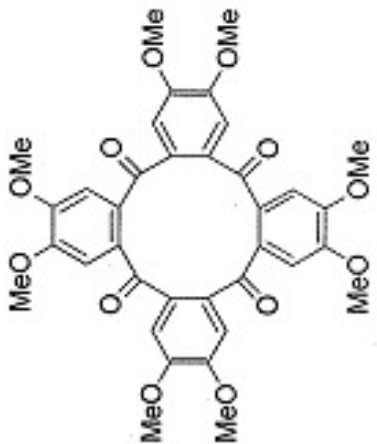
Pulse Sequence: gzgsl
Solvent: CDCl3
Ambient temperature
File: M3-835-10-CHMR
3MVA-038 "Proba.dpt-svr.3uc.edu"

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.269 sec
Width 18845.7 Hz
31256 repetitions
DSSRSE CL2 75.3828134 MHz
DC00P4 64 299.7828162 MHz
CompuProc: 0
ConvProc: 0
MUL2-18 Modulated
DATA PROCESSING
Line broadening 3.0 Hz
FT 5120 85508
Total time 257 hr. 7 min. 56 sec



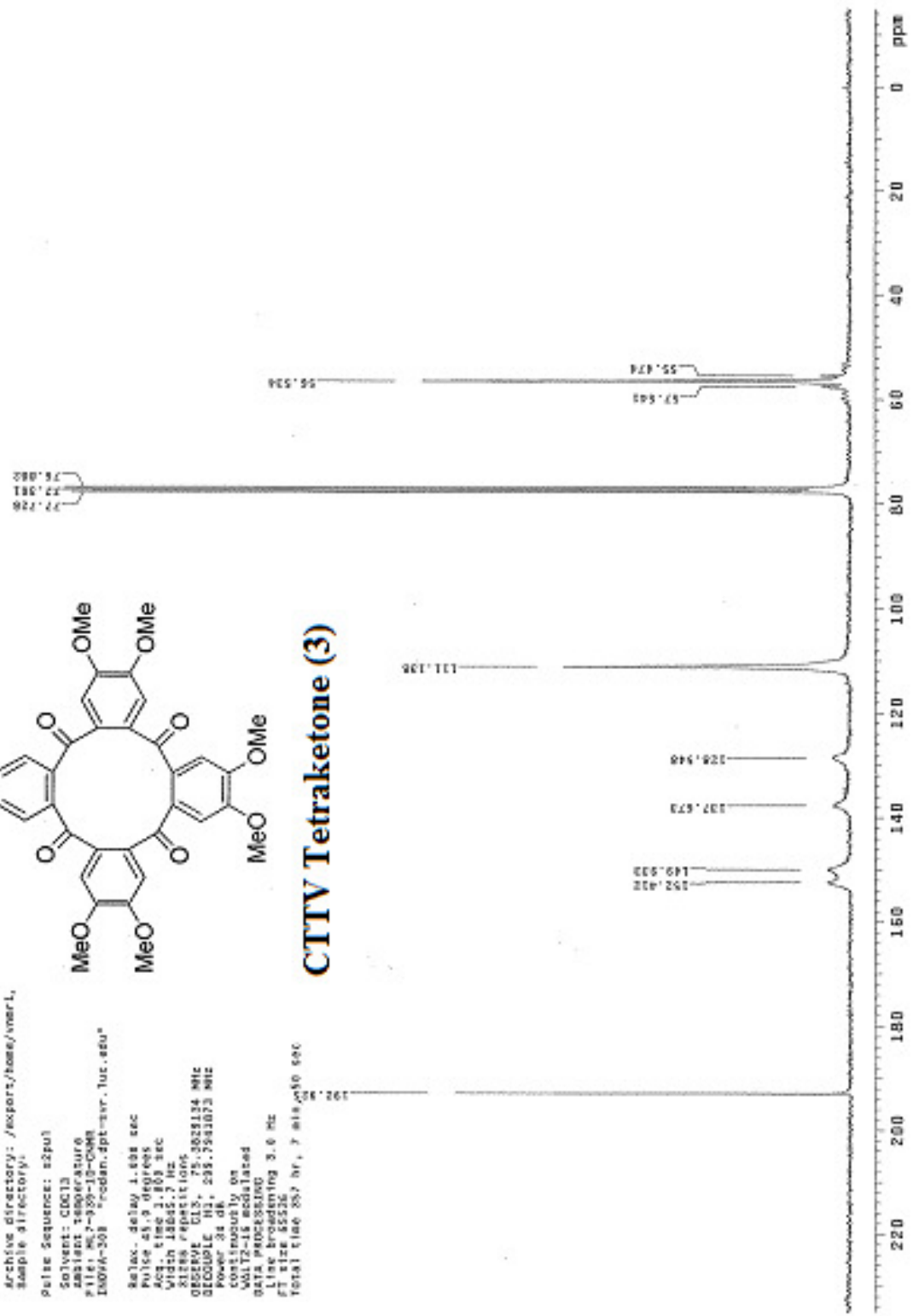
CTTV Tetraketone (3)

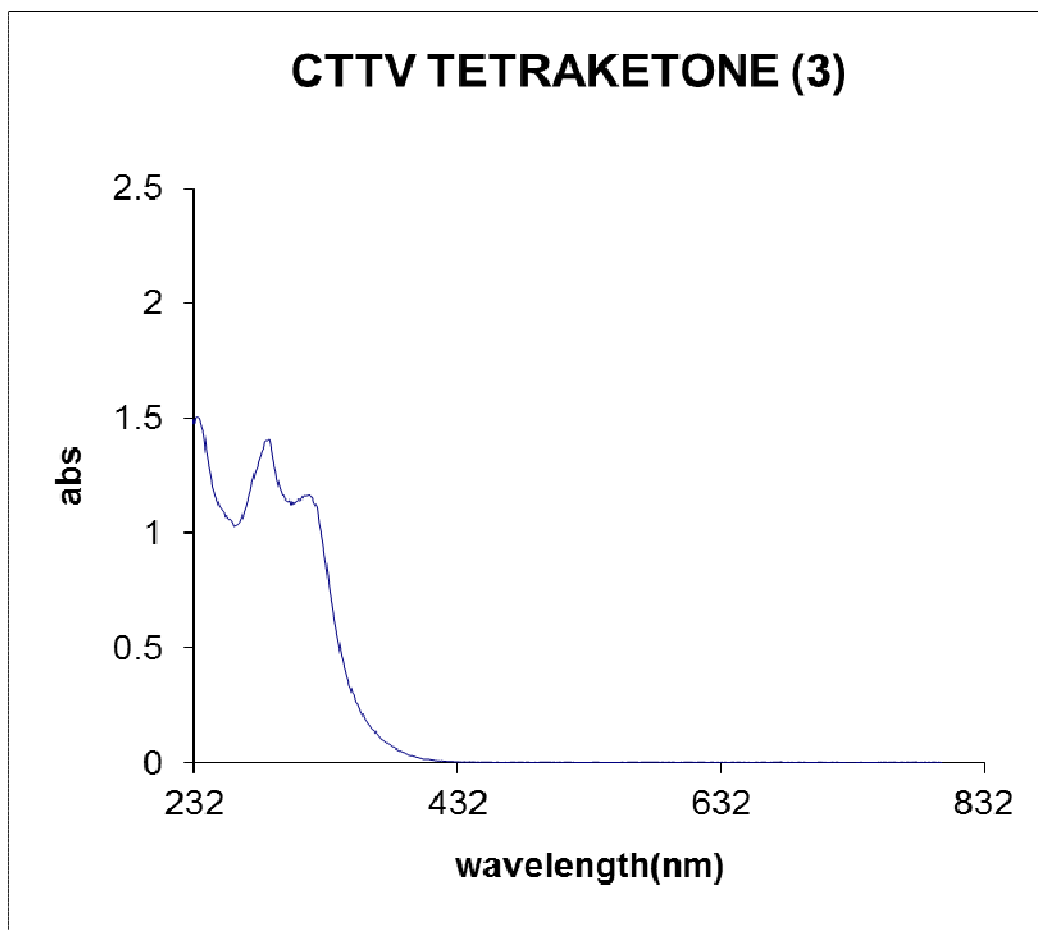




CTTV Tetraketone (3)

CTTV Tetraketone, Compound 13
 Archive directory: /exports/home/vmarL/
 Sample directory:
 Pulse Sequence: szpu1
 Solvent: CDCl3
 Acquisition temperature: 300.2 K
 File: 13-930-10-0508
 INOVA-300 /redan.dpt-mar.1uc.edu
 Relax delay: 1.000 sec
 No. of scans: 1000
 Acq time: 3.000 sec
 F2: 125.761 MHz
 Width: 13645.7 Hz
 Size: 8198 repetitions
 OBSERVE CH: 75.302134 MHz
 DECOUPLE H1: 231.7541073 MHz
 Power: 34 dB
 Continuously on
 VOLTAGE: 150.000 V
 DATA PROCESSING
 File: PROCESS100
 List: Processing 3.0 Hz
 Size: 182528
 Total time: 05.7 hr, 7 min, 00 sec



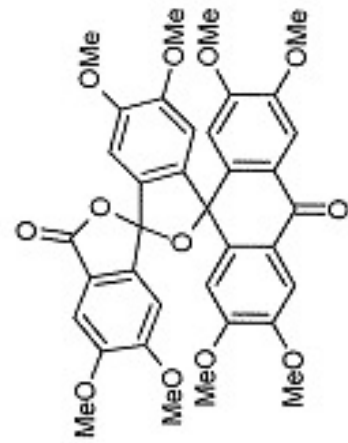


UV –absorption of CTTV-Tetraketone

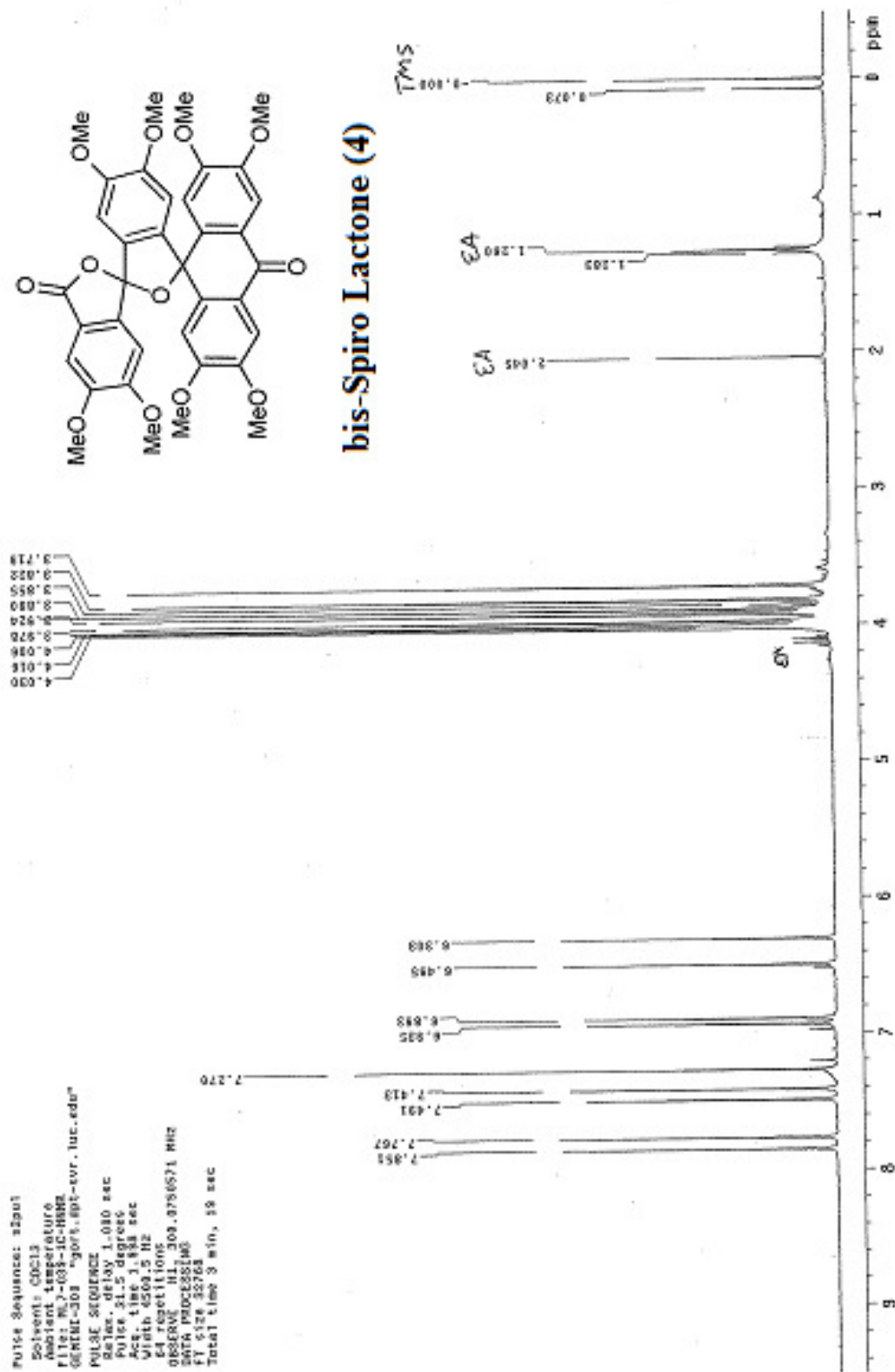
CTTV-TK (2.4mg, 0.037mmol) dissolved in 10ml Dichloromethane. 1.0ml was taken and diluted to 10ml with dichloromethane to make $3.7 \times 10^{-5} \text{M}$ solution

λ_{max} /absorbance	molar absorptivity (ϵ)
289nm (1.4081)	$3.81 \times 10^{-4} \text{M}$
320nm (1.1637)	$3.15 \times 10^{-4} \text{M}$

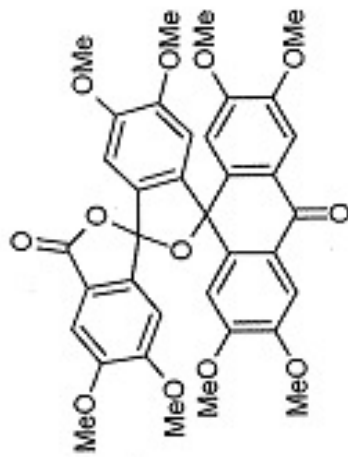
CTTV 81c-84inolactone
 Pulse Sequence: about
 Solvent: CDCl3
 Ambient Temperature
 File: WLJ-035-1C-NMR
 GEMV-308 %gvt-8pt-avr-1uc.edu
 PULSE SEQUENCE 1.080 sec
 Relax. 2.750 sec
 Solvent 2.750 sec
 Time 3.888 sec
 Width 4500.5 Hz
 EA repetitions
 OBSERVE H1 300.0750571 MHz
 DATA PROCESSING
 FT size 32768
 Total time 3 min, 19 sec



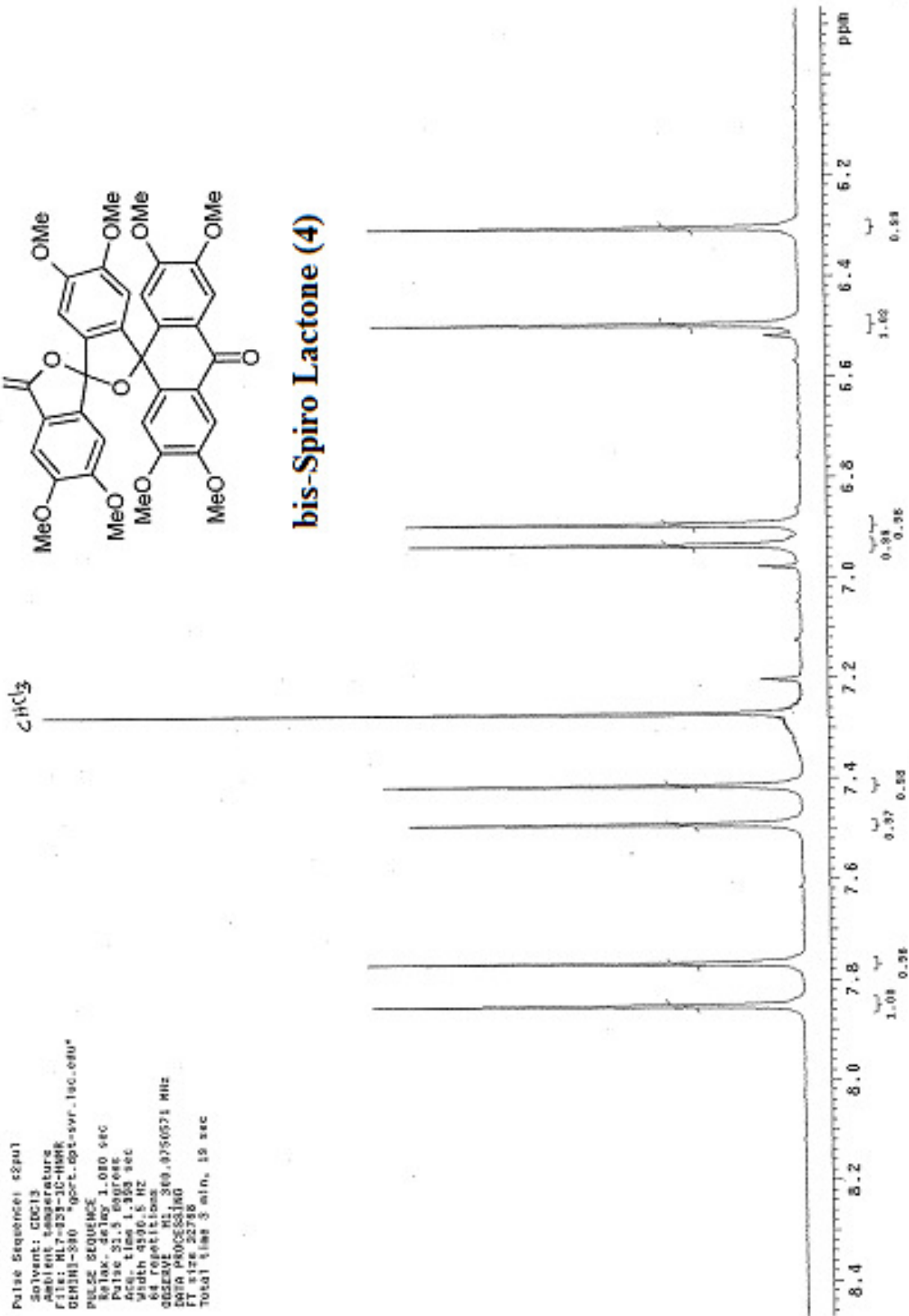
bis-Spiro Lactone (4)



CTVV 315-Spirolectons
 Pulse Sequence: e2p1
 Solvent: CDCl3
 Ambient Temperature
 File: NL7-229-1C-HMR
 GMIN1-890 *gpc1.dpt-svr-1sc.e90*
 PULSE SEQUENCE
 Relax delay: 1.000 sec
 Pulse: 21.5 1900 sec
 Width: 4996.5 Hz
 Gain: 64000
 QRESOLVE: 300.975071 MHz
 DATA F403E53180
 FT size: 23788
 Total time: 3 min, 19 sec



bis-Spiro Lactone (4)



OTTV Bis-Spirolactone, Compound 20

Pulse sequence: e2p1

solvent: CDCl3

acquisition: 10/25/04

file: 030510100

GEMINI-300 "gert.ept-ver.1nc.edg"

PULSE PROGRAM

Relax. delay 1.000 sec

Pulse SL 5 degrees

Acq. time 1.938 sec

Width 4280.3 Hz

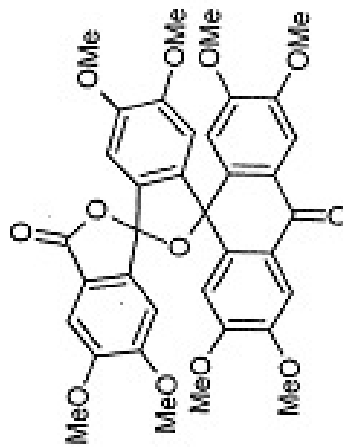
vs. resolution

030510100.HL: 300.0766671 MHz

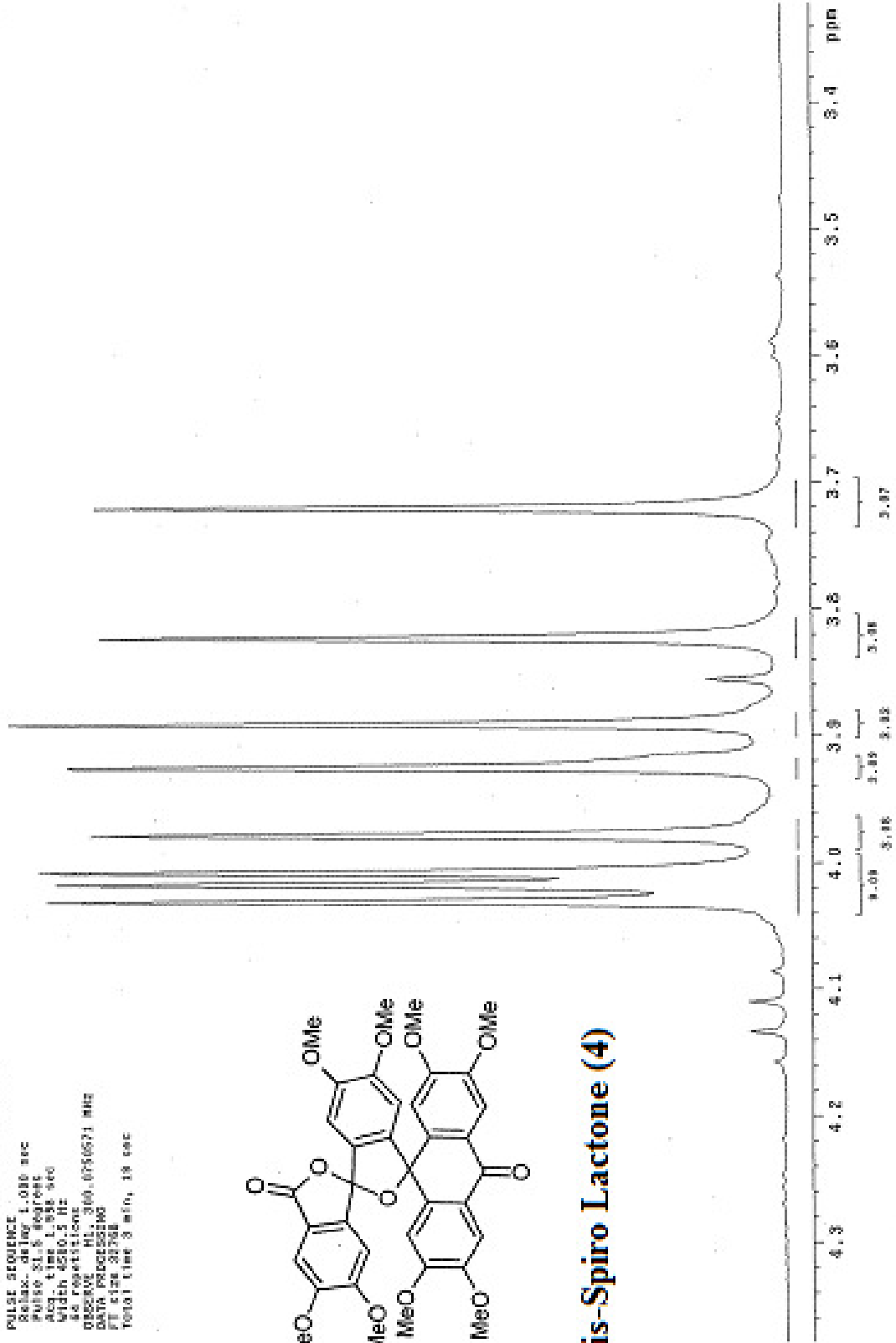
DATA PROCESSING

F1 size 32736

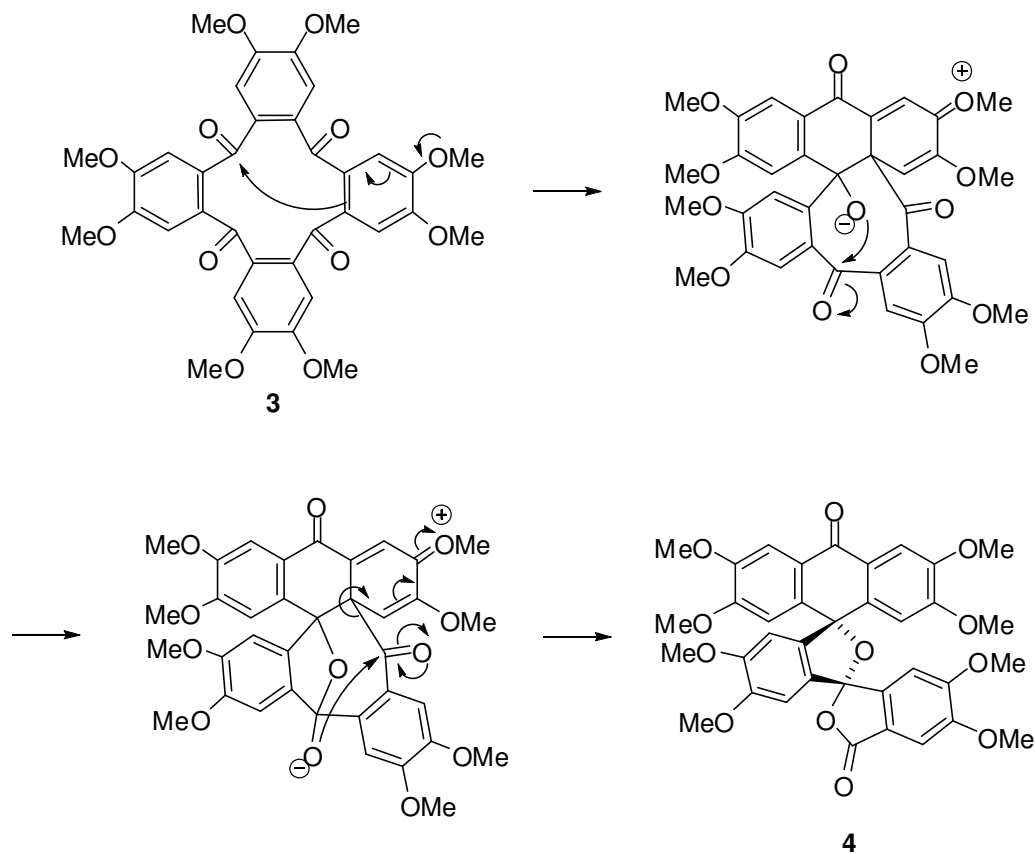
Total time 3 min, 18 sec



bis-Spiro Lactone (4)



Scheme S1. Proposed Mechanism of formation of the bis-spirolactone **4** from CTTV Tetraketone **3** in *basic* conditions



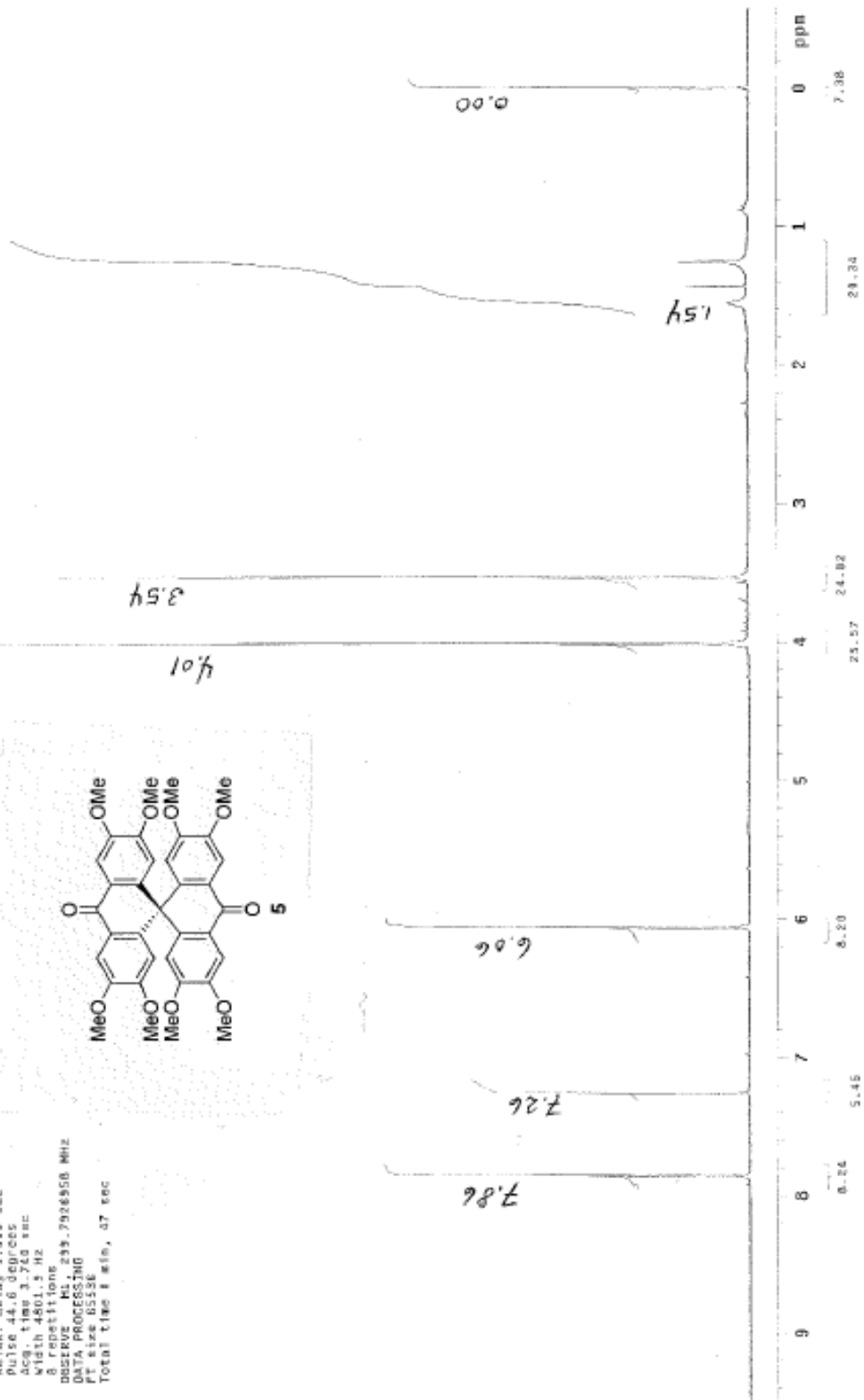
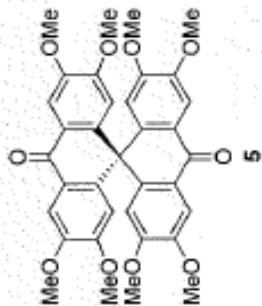
hrs-ii-113

Archive directory: /export/home/vnhr1/vnhrSys/data
Sample directory:
File: PROTON

Pulse sequence: s2pul

Solvent: DMSO
Temp: 25.0 C / 298.1 K
INSTR: spect-rodan-spt-svr. luc.edu

Relax. delay: 1.000 sec
Pulse: 44.6 degrecs
Acq. time: 3.760 sec
Width: 4801.5 Hz
8 repetitions
DATE_UTC: 93.09.28.05.00
DATA: PROTON.D
PT: 416.0558
Total time: 4 min, 47 sec



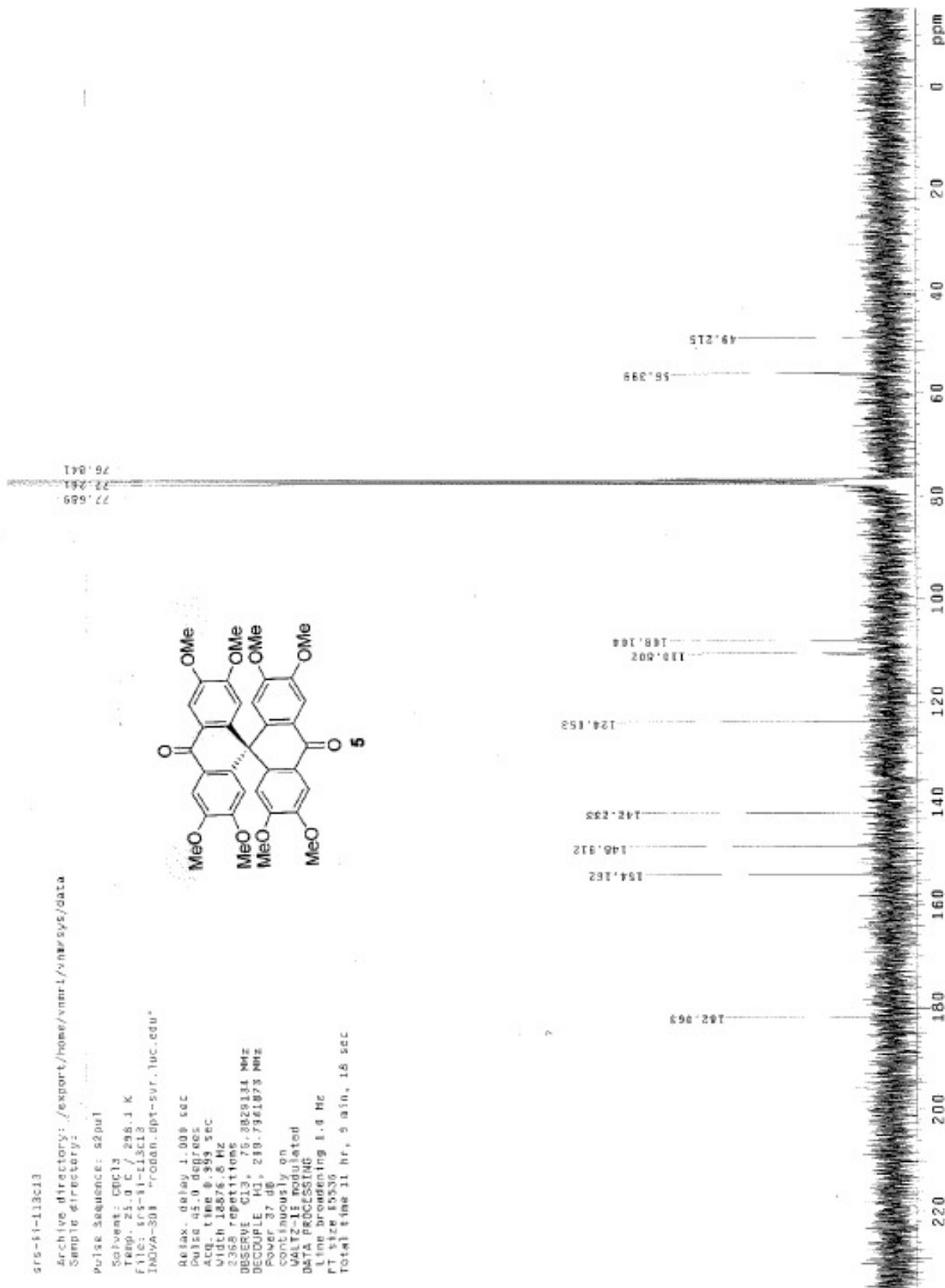
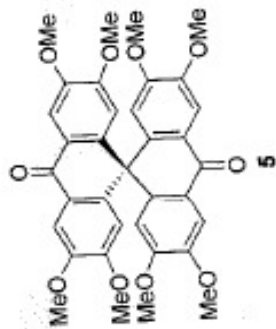
gms-ii-113c13

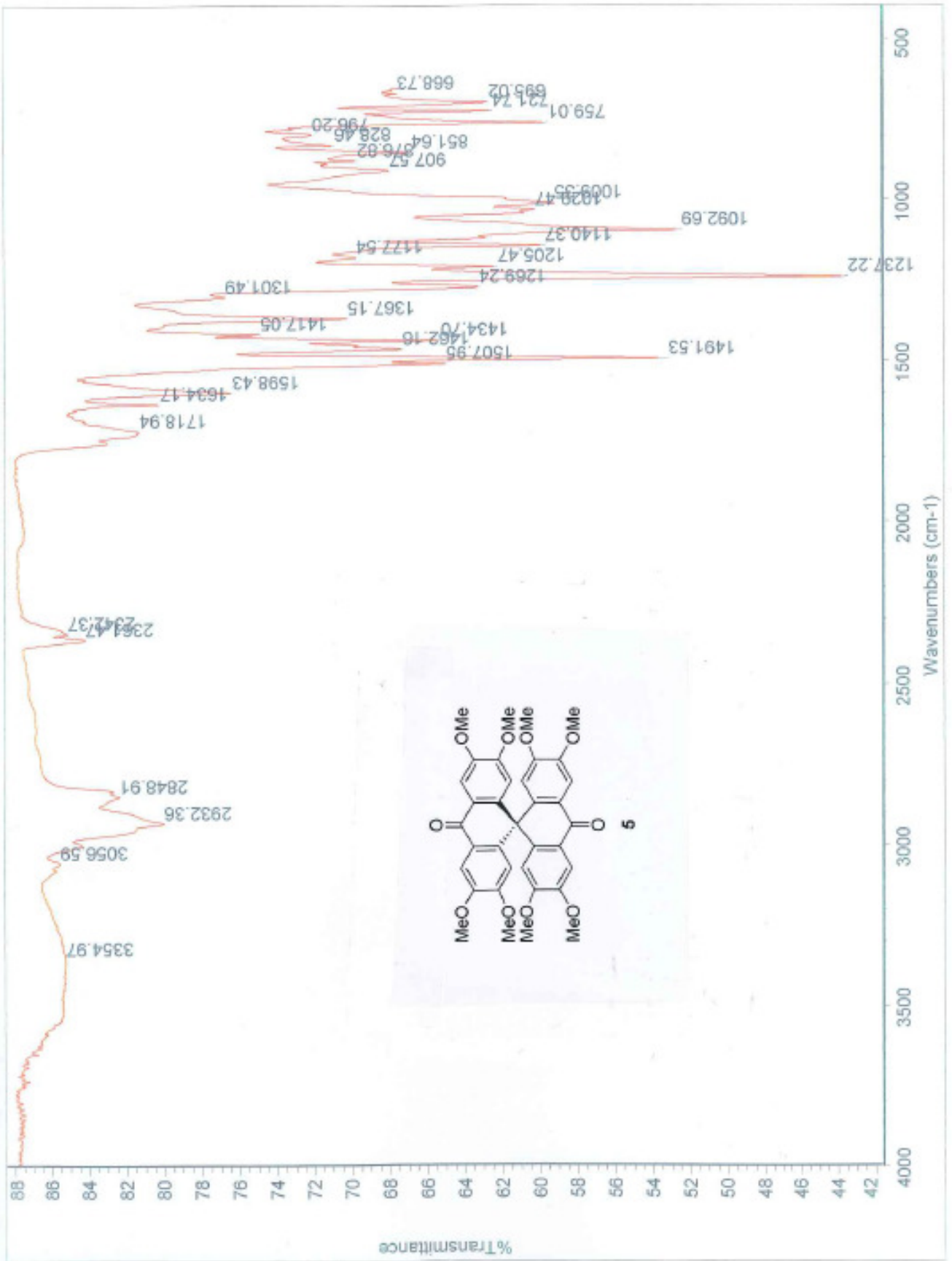
Archive directory: /export/home/vnari/vnarsys/data
Sample directory:

Pulse sequence: s2pul1

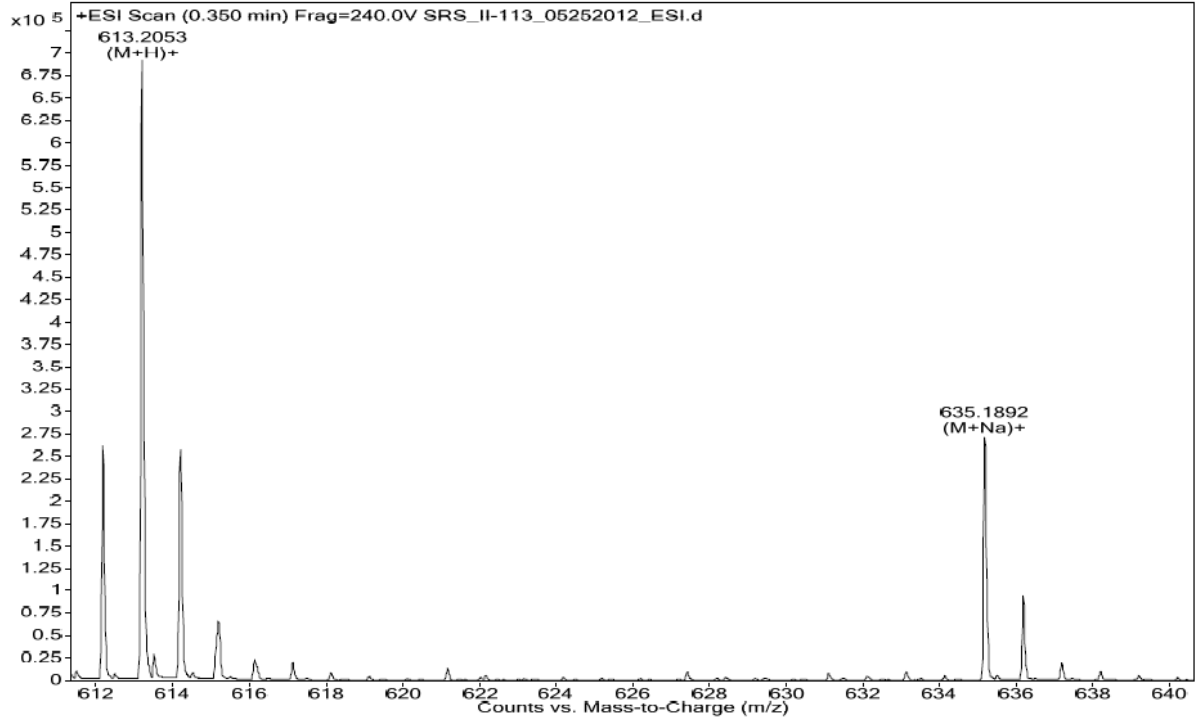
Solvent: CDCl3
Temp: 23.0 C / 298.1 K
F1: gms-ii-113c13
INSTR: spect-1000m-dpt-svr.luc.edu

Relax. delay: 1.000 sec
Pulse: 45.0 degrees
Acq. time: 9.959 sec
Width: 14876.6 Hz
2368 repetitions
OBSERVE: C13, 75.3829134 MHz
DECOUPLE: H1, 238.7361873 MHz
Power: 37 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening: 1.0 Hz
FT size: 65536
Total time: 11 hr, 5 min, 16 sec





Sample Name	SRS_II-113	Position	P1-E5	Instrument Name	Instrument 1	User Name	
Inj Vol	1	InjPosition		SampleType	Sample	IRM Calibration Status	Success
Data Filename	SRS_II-113_05252012_	ACQ Method	ESI_ASL_Pos_Main_051	Comment		Acquired Time	5/25/2012 2:36:11 PM



Scheme S2. Proposed Mechanism of formation of the 2,2',3,3',6,6',7,7'-octamethoxy-10H,10'H-9,9'-spirobi[anthracene]-10,10'-dione (**5**) from CTTV Tetraketone **3** in *acidic* conditions

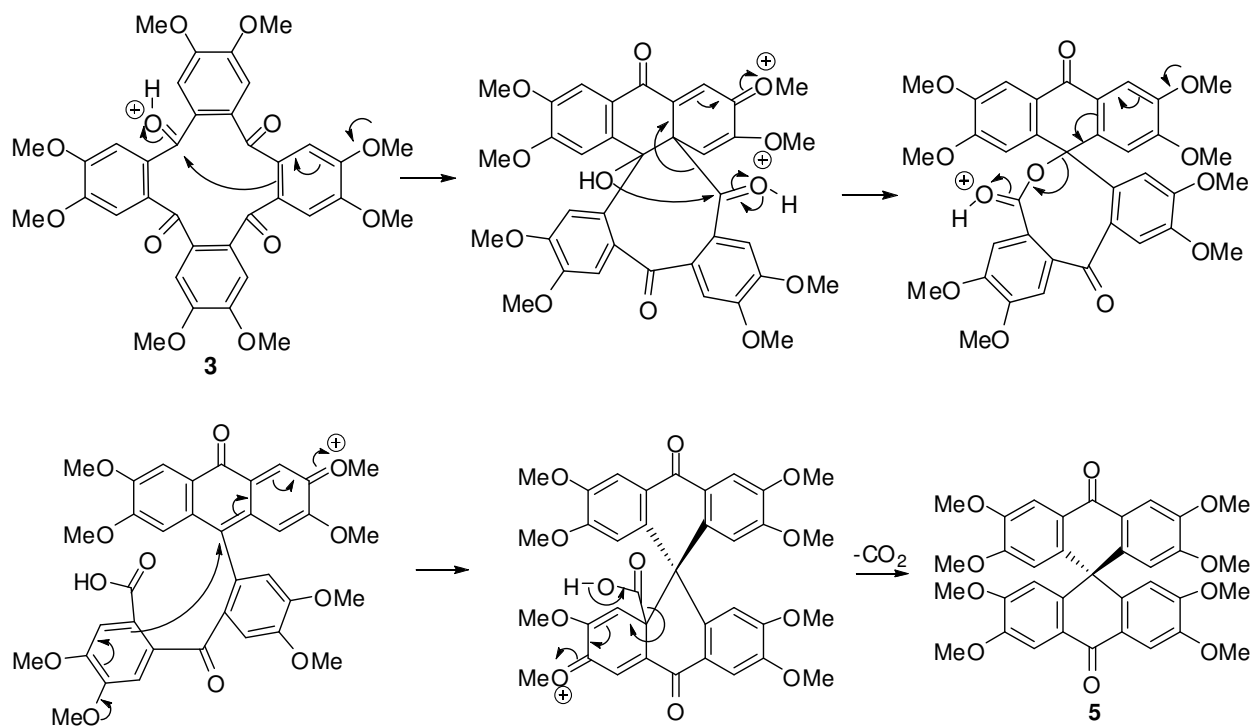


Table S1. Single Crystal Experimental details

For all structures: triclinic, $P\bar{1}$, $Z = 2$. Experiments were carried out using a Bruker AXS SMART APEX CCD diffractometer. Data collection used ω scans.

	3 ·3(CH ₂ Cl ₂)	4
Crystal data		
Chemical formula	C ₃₆ H ₃₂ O ₁₂ ·3(CH ₂ Cl ₂)	C ₃₆ H ₃₂ O ₁₂
M_r	911.39	656.62
Temperature (K)	100	100
a, b, c (Å)	11.9308 (7), 13.8064 (8), 14.0009 (7)	10.9038 (15), 10.9256 (15), 14.494 (2)
α, β, γ (°)	114.082 (3), 92.329 (3), 105.980 (3)	106.522 (2), 98.609 (2), 112.249 (2)
V (Å ³)	1993.17 (19)	1466.3 (3)
$F(000)$	940	688
D_x (Mg m ⁻³)	1.519	1.487
No. of reflections for cell measurement	2777	5210
θ range (°) for cell measurement	2.2–30.2	2.2–30.5
μ (mm ⁻¹)	0.50	0.11
Crystal shape	Plate	Block
Colour	Colourless	Colourless
Crystal size (mm)	0.2 × 0.16 × 0.08	0.39 × 0.38 × 0.32
Data collection		
Radiation type / source	Mo $K\alpha$, fine-focus sealed tube	Mo $K\alpha$, fine-focus sealed tube
Monochromator	Graphite	Graphite
Absorption correction	multi-scan (Apex2, Bruker, 2008)	multi-scan (Apex2, Bruker, 2008)
T_{\min}, T_{\max}	0.612, 0.746	0.861, 0.965
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	17017, 7022, 3759	14705, 7157, 4964
R_{int}	0.061	0.027
θ values (°)	$\theta_{\max} = 25.0, \theta_{\min} = 1.6$	$\theta_{\max} = 28.3, \theta_{\min} = 1.5$
Range of h, k, l	$h = -14 \rightarrow 14, k = -16 \rightarrow 16, l = -16 \rightarrow 16$	$h = -14 \rightarrow 14, k = -14 \rightarrow 14, l = -19 \rightarrow 19$
Refinement		
$R[F^2 > 2\sigma(F^2)], wR(F^2), S$	0.083, 0.244, 1.06	0.043, 0.126, 1.03
reflections/restraints/parameters	7022/0/441	7157/0/441
$\Delta\rho_{\max}, \Delta\rho_{\min}$ (e Å ⁻³)	0.33, -0.35	0.45, -0.27

Computer programs: Apex2 v2008.2-4 (Bruker, 2008), *SHELXTL* 6.14 (Bruker, 2000-2003), *SHELXTL* 6.14.

Table S2. Selected geometric parameters (Å, °)

3			
C1–O1	1.222 (5)	C18–H18C	0.9800
C1–C30	1.487 (6)	C19–O7	1.247 (5)
C1–C2	1.500 (6)	C19–C20	1.467 (6)
C2–C3	1.385 (6)	C20–C21	1.413 (6)
C2–C7	1.405 (6)	C20–C25	1.416 (6)
C3–C4	1.401 (6)	C21–C22	1.363 (6)
C3–H3	0.9500	C21–H21	0.9500
C4–O2	1.357 (5)	C22–O8	1.364 (5)
C4–C5	1.380 (6)	C22–C23	1.436 (6)
C5–O3	1.372 (5)	C23–C24	1.361 (6)
C5–C6	1.392 (6)	C23–O9	1.378 (5)
C6–C7	1.389 (6)	C24–C25	1.400 (6)
C6–H6	0.9500	C24–H24	0.9500
C7–C10	1.528 (6)	C25–C28	1.527 (6)
C8–O2	1.398 (6)	C26–O8	1.425 (5)
C8–H8A	0.9800	C26–H26A	0.9800
C8–H8B	0.9800	C26–H26B	0.9800
C8–H8C	0.9800	C26–H26C	0.9800
C9–O3	1.448 (6)	C27–O9	1.430 (5)
C9–H9A	0.9800	C27–H27A	0.9800
C9–H9B	0.9800	C27–H27B	0.9800
C9–H9C	0.9800	C27–H27C	0.9800
C10–O4	1.196 (5)	C28–O10	1.224 (5)
C10–C11	1.501 (6)	C28–C29	1.482 (6)
C11–C12	1.388 (6)	C29–C34	1.379 (6)
C11–C16	1.390 (5)	C29–C30	1.422 (6)
C12–C13	1.397 (6)	C30–C31	1.410 (6)
C12–H12	0.9500	C31–C32	1.379 (6)
C13–O5	1.337 (5)	C31–H31	0.9500
C13–C14	1.398 (6)	C32–O12	1.356 (5)
C14–O6	1.375 (5)	C32–C33	1.375 (6)
C14–C15	1.400 (6)	C33–O11	1.382 (5)
C15–C16	1.356 (6)	C33–C34	1.405 (6)

C15-H15	0.9500	C34-H34	0.9500
C16-C19	1.517 (6)	C35-O12	1.424 (6)
C17-O5	1.441 (5)	C35-H35A	0.9800
C17-H17A	0.9800	C35-H35B	0.9800
C17-H17B	0.9800	C35-H35C	0.9800
C17-H17C	0.9800	C36-O11	1.434 (6)
C18-O6	1.450 (6)	C36-H36A	0.9800
C18-H18A	0.9800	C36-H36B	0.9800
C18-H18B	0.9800	C36-H36C	0.9800
O1-C1-C30	120.1 (4)	C21-C20-C19	117.3 (4)
O1-C1-C2	119.8 (4)	C25-C20-C19	123.6 (4)
C30-C1-C2	119.4 (4)	C22-C21-C20	120.5 (4)
C3-C2-C7	120.1 (4)	C22-C21-H21	119.8
C3-C2-C1	115.9 (4)	C20-C21-H21	119.8
C7-C2-C1	124.0 (4)	C21-C22-O8	126.0 (4)
C2-C3-C4	120.2 (4)	C21-C22-C23	120.1 (4)
C2-C3-H3	119.9	O8-C22-C23	113.9 (4)
C4-C3-H3	119.9	C24-C23-O9	124.4 (4)
O2-C4-C5	116.9 (4)	C24-C23-C22	119.9 (4)
O2-C4-C3	123.1 (4)	O9-C23-C22	115.7 (4)
C5-C4-C3	120.0 (4)	C23-C24-C25	120.6 (4)
O3-C5-C4	114.2 (4)	C23-C24-H24	119.7
O3-C5-C6	126.1 (4)	C25-C24-H24	119.7
C4-C5-C6	119.7 (4)	C24-C25-C20	120.0 (4)
C7-C6-C5	121.1 (4)	C24-C25-C28	113.9 (3)
C7-C6-H6	119.4	C20-C25-C28	126.0 (4)
C5-C6-H6	119.4	O8-C26-H26A	109.5
C6-C7-C2	118.9 (4)	O8-C26-H26B	109.5
C6-C7-C10	113.0 (4)	H26A-C26-H26B	109.5
C2-C7-C10	128.2 (4)	O8-C26-H26C	109.5
O2-C8-H8A	109.5	H26A-C26-H26C	109.5
O2-C8-H8B	109.5	H26B-C26-H26C	109.5
H8A-C8-H8B	109.5	O9-C27-H27A	109.5
O2-C8-H8C	109.5	O9-C27-H27B	109.5
H8A-C8-H8C	109.5	H27A-C27-H27B	109.5
H8B-C8-H8C	109.5	O9-C27-H27C	109.5

O3-C9-H9A	109.5	H27A-C27-H27C	109.5
O3-C9-H9B	109.5	H27B-C27-H27C	109.5
H9A-C9-H9B	109.5	O10-C28-C29	120.4 (4)
O3-C9-H9C	109.5	O10-C28-C25	117.7 (4)
H9A-C9-H9C	109.5	C29-C28-C25	121.3 (4)
H9B-C9-H9C	109.5	C34-C29-C30	119.6 (4)
O4-C10-C11	121.1 (4)	C34-C29-C28	116.2 (4)
O4-C10-C7	120.9 (4)	C30-C29-C28	124.0 (4)
C11-C10-C7	117.7 (3)	C31-C30-C29	118.1 (4)
C12-C11-C16	118.6 (4)	C31-C30-C1	115.2 (4)
C12-C11-C10	115.5 (3)	C29-C30-C1	126.6 (4)
C16-C11-C10	125.9 (4)	C32-C31-C30	120.7 (4)
C11-C12-C13	122.2 (4)	C32-C31-H31	119.7
C11-C12-H12	118.9	C30-C31-H31	119.7
C13-C12-H12	118.9	O12-C32-C33	116.0 (4)
O5-C13-C12	125.6 (4)	O12-C32-C31	122.7 (4)
O5-C13-C14	117.3 (4)	C33-C32-C31	121.2 (4)
C12-C13-C14	117.1 (4)	C32-C33-O11	117.4 (3)
O6-C14-C13	114.7 (4)	C32-C33-C34	118.7 (4)
O6-C14-C15	124.3 (4)	O11-C33-C34	123.5 (4)
C13-C14-C15	120.9 (4)	C29-C34-C33	121.1 (4)
C16-C15-C14	120.1 (4)	C29-C34-H34	119.4
C16-C15-H15	119.9	C33-C34-H34	119.4
C14-C15-H15	119.9	O12-C35-H35A	109.5
C15-C16-C11	121.0 (4)	O12-C35-H35B	109.5
C15-C16-C19	111.2 (4)	H35A-C35-H35B	109.5
C11-C16-C19	127.6 (4)	O12-C35-H35C	109.5
O5-C17-H17A	109.5	H35A-C35-H35C	109.5
O5-C17-H17B	109.5	H35B-C35-H35C	109.5
H17A-C17-H17B	109.5	O11-C36-H36A	109.5
O5-C17-H17C	109.5	O11-C36-H36B	109.5
H17A-C17-H17C	109.5	H36A-C36-H36B	109.5
H17B-C17-H17C	109.5	O11-C36-H36C	109.5
O6-C18-H18A	109.5	H36A-C36-H36C	109.5
O6-C18-H18B	109.5	H36B-C36-H36C	109.5
H18A-C18-H18B	109.5	C4-O2-C8	118.7 (3)
O6-C18-H18C	109.5	C5-O3-C9	114.7 (4)

H18A-C18-H18C	109.5	C13-O5-C17	118.5 (3)
H18B-C18-H18C	109.5	C14-O6-C18	117.3 (3)
O7-C19-C20	119.8 (4)	C22-O8-C26	116.0 (3)
O7-C19-C16	118.1 (4)	C23-O9-C27	117.3 (4)
C20-C19-C16	122.0 (3)	C33-O11-C36	115.4 (3)
C21-C20-C25	118.9 (4)	C32-O12-C35	116.9 (3)
O1-C1-C2-C3	-0.8 (6)	C21-C22-C23-C24	4.2 (7)
C30-C1-C2-C3	-170.9 (4)	O8-C22-C23-C24	-178.1 (4)
O1-C1-C2-C7	178.2 (4)	C21-C22-C23-O9	-175.4 (4)
C30-C1-C2-C7	8.1 (6)	O8-C22-C23-O9	2.3 (6)
C7-C2-C3-C4	-0.1 (6)	O9-C23-C24-C25	176.4 (4)
C1-C2-C3-C4	179.0 (4)	C22-C23-C24-C25	-3.1 (7)
C2-C3-C4-O2	176.4 (4)	C23-C24-C25-C20	1.0 (7)
C2-C3-C4-C5	-2.7 (6)	C23-C24-C25-C28	177.7 (4)
O2-C4-C5-O3	2.0 (6)	C21-C20-C25-C24	0.1 (6)
C3-C4-C5-O3	-178.9 (4)	C19-C20-C25-C24	-175.5 (4)
O2-C4-C5-C6	-176.4 (4)	C21-C20-C25-C28	-176.1 (4)
C3-C4-C5-C6	2.7 (6)	C19-C20-C25-C28	8.3 (7)
O3-C5-C6-C7	-178.3 (4)	C24-C25-C28-O10	82.1 (5)
C4-C5-C6-C7	-0.1 (6)	C20-C25-C28-O10	-101.5 (5)
C5-C6-C7-C2	-2.6 (6)	C24-C25-C28-C29	-89.1 (5)
C5-C6-C7-C10	176.0 (4)	C20-C25-C28-C29	87.3 (6)
C3-C2-C7-C6	2.6 (6)	O10-C28-C29-C34	-2.6 (6)
C1-C2-C7-C6	-176.3 (4)	C25-C28-C29-C34	168.4 (4)
C3-C2-C7-C10	-175.7 (4)	O10-C28-C29-C30	-178.2 (4)
C1-C2-C7-C10	5.3 (7)	C25-C28-C29-C30	-7.2 (6)
C6-C7-C10-O4	84.4 (5)	C34-C29-C30-C31	-0.9 (6)
C2-C7-C10-O4	-97.1 (5)	C28-C29-C30-C31	174.6 (4)
C6-C7-C10-C11	-89.2 (5)	C34-C29-C30-C1	178.1 (4)
C2-C7-C10-C11	89.3 (5)	C28-C29-C30-C1	-6.5 (7)
O4-C10-C11-C12	-3.1 (6)	O1-C1-C30-C31	-80.2 (5)
C7-C10-C11-C12	170.4 (4)	C2-C1-C30-C31	89.9 (5)
O4-C10-C11-C16	177.5 (4)	O1-C1-C30-C29	100.9 (6)
C7-C10-C11-C16	-9.0 (6)	C2-C1-C30-C29	-89.0 (5)
C16-C11-C12-C13	0.2 (6)	C29-C30-C31-C32	1.2 (6)
C10-C11-C12-C13	-179.2 (4)	C1-C30-C31-C32	-177.9 (4)

C11-C12-C13-O5	179.2 (4)	C30-C31-C32-O12	179.0 (4)
C11-C12-C13-C14	-0.3 (6)	C30-C31-C32-C33	3.5 (6)
O5-C13-C14-O6	-0.6 (6)	O12-C32-C33-O11	2.1 (6)
C12-C13-C14-O6	178.9 (4)	C31-C32-C33-O11	177.9 (4)
O5-C13-C14-C15	-179.7 (4)	O12-C32-C33-C34	175.9 (4)
C12-C13-C14-C15	-0.1 (6)	C31-C32-C33-C34	-8.3 (6)
O6-C14-C15-C16	-178.2 (4)	C30-C29-C34-C33	-4.0 (6)
C13-C14-C15-C16	0.7 (7)	C28-C29-C34-C33	-179.9 (4)
C14-C15-C16-C11	-0.9 (7)	C32-C33-C34-C29	8.6 (6)
C14-C15-C16-C19	-177.3 (4)	O11-C33-C34-C29	-177.9 (4)
C12-C11-C16-C15	0.4 (6)	C5-C4-O2-C8	174.6 (4)
C10-C11-C16-C15	179.8 (4)	C3-C4-O2-C8	-4.5 (6)
C12-C11-C16-C19	176.2 (4)	C4-C5-O3-C9	178.0 (4)
C10-C11-C16-C19	-4.5 (7)	C6-C5-O3-C9	-3.8 (6)
C15-C16-C19-O7	-89.3 (5)	C12-C13-O5-C17	2.6 (6)
C11-C16-C19-O7	94.6 (5)	C14-C13-O5-C17	-177.9 (4)
C15-C16-C19-C20	86.8 (5)	C13-C14-O6-C18	-177.0 (4)
C11-C16-C19-C20	-89.3 (5)	C15-C14-O6-C18	2.0 (6)
O7-C19-C20-C21	6.5 (6)	C21-C22-O8-C26	-1.4 (6)
C16-C19-C20-C21	-169.5 (4)	C23-C22-O8-C26	-179.0 (4)
O7-C19-C20-C25	-177.9 (4)	C24-C23-O9-C27	-2.0 (6)
C16-C19-C20-C25	6.2 (6)	C22-C23-O9-C27	177.5 (4)
C25-C20-C21-C22	1.0 (6)	C32-C33-O11-C36	-179.2 (4)
C19-C20-C21-C22	176.9 (4)	C34-C33-O11-C36	7.3 (6)
C20-C21-C22-O8	179.5 (4)	C33-C32-O12-C35	-175.1 (4)
C20-C21-C22-C23	-3.1 (7)	C31-C32-O12-C35	9.2 (6)
4			
C1-O8	1.4752 (19)	C19-C24	1.373 (2)
C1-C19	1.522 (2)	C19-C20	1.395 (2)
C1-C14	1.523 (2)	C20-C21	1.389 (2)
C1-C2	1.526 (2)	C20-H20	0.9500
C2-C7	1.389 (2)	C21-O6	1.367 (2)
C2-C3	1.400 (2)	C21-C22	1.421 (2)
C3-C4	1.385 (2)	C22-O7	1.359 (2)
C3-H3	0.9500	C22-C23	1.388 (2)
C4-O1	1.361 (2)	C23-C24	1.396 (2)

C4-C5	1.412 (2)	C23-H23	0.9500
C5-O2	1.362 (2)	C24-C25	1.500 (2)
C5-C6	1.375 (2)	C25-O8	1.405 (2)
C6-C7	1.409 (2)	C25-O12	1.4876 (19)
C6-H6	0.9500	C25-C26	1.511 (2)
C7-C8	1.474 (2)	C26-C31	1.375 (2)
C8-O3	1.228 (2)	C26-C27	1.393 (2)
C8-C9	1.480 (2)	C27-C28	1.386 (2)
C9-C14	1.386 (2)	C27-H27	0.9500
C9-C10	1.407 (2)	C28-O9	1.357 (2)
C10-C11	1.370 (2)	C28-C29	1.423 (2)
C10-H10	0.9500	C29-O10	1.355 (2)
C11-O4	1.3707 (19)	C29-C30	1.380 (2)
C11-C12	1.414 (2)	C30-C31	1.394 (2)
C12-O5	1.3578 (19)	C30-H30	0.9500
C12-C13	1.389 (2)	C31-C32	1.460 (2)
C13-C14	1.398 (2)	C32-O11	1.203 (2)
C13-H13	0.9500	C32-O12	1.374 (2)
C15-O1	1.424 (2)	C33-O6	1.425 (2)
C15-H15A	0.9800	C33-H33A	0.9800
C15-H15B	0.9800	C33-H33B	0.9800
C15-H15C	0.9800	C33-H33C	0.9800
C16-O2	1.426 (2)	C34-O7	1.433 (2)
C16-H16A	0.9800	C34-H34A	0.9800
C16-H16B	0.9800	C34-H34B	0.9800
C16-H16C	0.9800	C34-H34C	0.9800
C17-O4	1.427 (2)	C35-O9	1.426 (2)
C17-H17A	0.9800	C35-H35A	0.9800
C17-H17B	0.9800	C35-H35B	0.9800
C17-H17C	0.9800	C35-H35C	0.9800
C18-O5	1.429 (2)	C36-O10	1.421 (2)
C18-H18A	0.9800	C36-H36A	0.9800
C18-H18B	0.9800	C36-H36B	0.9800
C18-H18C	0.9800	C36-H36C	0.9800
O8-C1-C19	101.93 (12)	C19-C20-H20	121.0
O8-C1-C14	109.27 (12)	O6-C21-C20	124.36 (15)

C19-C1-C14	109.61 (13)	O6-C21-C22	114.57 (15)
O8-C1-C2	111.22 (13)	C20-C21-C22	121.04 (15)
C19-C1-C2	111.03 (13)	O7-C22-C23	124.80 (15)
C14-C1-C2	113.18 (14)	O7-C22-C21	114.99 (15)
C7-C2-C3	118.92 (15)	C23-C22-C21	120.15 (15)
C7-C2-C1	121.25 (15)	C22-C23-C24	117.56 (15)
C3-C2-C1	119.56 (14)	C22-C23-H23	121.2
C4-C3-C2	120.51 (15)	C24-C23-H23	121.2
C4-C3-H3	119.7	C19-C24-C23	122.57 (15)
C2-C3-H3	119.7	C19-C24-C25	109.04 (14)
O1-C4-C3	124.86 (15)	C23-C24-C25	128.38 (15)
O1-C4-C5	114.78 (14)	O8-C25-O12	108.97 (12)
C3-C4-C5	120.30 (15)	O8-C25-C24	105.16 (13)
O2-C5-C6	125.51 (15)	O12-C25-C24	108.29 (13)
O2-C5-C4	115.17 (14)	O8-C25-C26	115.02 (14)
C6-C5-C4	119.32 (15)	O12-C25-C26	102.03 (13)
C5-C6-C7	120.18 (15)	C24-C25-C26	117.06 (14)
C5-C6-H6	119.9	C31-C26-C27	120.20 (16)
C7-C6-H6	119.9	C31-C26-C25	109.30 (15)
C2-C7-C6	120.65 (15)	C27-C26-C25	130.24 (15)
C2-C7-C8	121.89 (15)	C28-C27-C26	118.10 (16)
C6-C7-C8	117.42 (15)	C28-C27-H27	120.9
O3-C8-C7	121.53 (15)	C26-C27-H27	120.9
O3-C8-C9	121.51 (16)	O9-C28-C27	125.07 (16)
C7-C8-C9	116.95 (14)	O9-C28-C29	113.89 (15)
C14-C9-C10	120.40 (15)	C27-C28-C29	121.02 (16)
C14-C9-C8	122.27 (15)	O10-C29-C30	125.13 (16)
C10-C9-C8	117.32 (15)	O10-C29-C28	114.66 (15)
C11-C10-C9	120.85 (16)	C30-C29-C28	120.20 (16)
C11-C10-H10	119.6	C29-C30-C31	117.36 (15)
C9-C10-H10	119.6	C29-C30-H30	121.3
C10-C11-O4	124.98 (15)	C31-C30-H30	121.3
C10-C11-C12	119.20 (15)	C26-C31-C30	122.89 (16)
O4-C11-C12	115.81 (14)	C26-C31-C32	109.06 (15)
O5-C12-C13	125.09 (15)	C30-C31-C32	128.05 (16)
O5-C12-C11	115.20 (14)	O11-C32-O12	121.74 (16)
C13-C12-C11	119.71 (15)	O11-C32-C31	130.45 (16)

C12-C13-C14	121.04 (15)	O12-C32-C31	107.80 (14)
C12-C13-H13	119.5	O6-C33-H33A	109.5
C14-C13-H13	119.5	O6-C33-H33B	109.5
C9-C14-C13	118.80 (15)	H33A-C33-H33B	109.5
C9-C14-C1	121.20 (14)	O6-C33-H33C	109.5
C13-C14-C1	119.66 (14)	H33A-C33-H33C	109.5
O1-C15-H15A	109.5	H33B-C33-H33C	109.5
O1-C15-H15B	109.5	O7-C34-H34A	109.5
H15A-C15-H15B	109.5	O7-C34-H34B	109.5
O1-C15-H15C	109.5	H34A-C34-H34B	109.5
H15A-C15-H15C	109.5	O7-C34-H34C	109.5
H15B-C15-H15C	109.5	H34A-C34-H34C	109.5
O2-C16-H16A	109.5	H34B-C34-H34C	109.5
O2-C16-H16B	109.5	O9-C35-H35A	109.5
H16A-C16-H16B	109.5	O9-C35-H35B	109.5
O2-C16-H16C	109.5	H35A-C35-H35B	109.5
H16A-C16-H16C	109.5	O9-C35-H35C	109.5
H16B-C16-H16C	109.5	H35A-C35-H35C	109.5
O4-C17-H17A	109.5	H35B-C35-H35C	109.5
O4-C17-H17B	109.5	O10-C36-H36A	109.5
H17A-C17-H17B	109.5	O10-C36-H36B	109.5
O4-C17-H17C	109.5	H36A-C36-H36B	109.5
H17A-C17-H17C	109.5	O10-C36-H36C	109.5
H17B-C17-H17C	109.5	H36A-C36-H36C	109.5
O5-C18-H18A	109.5	H36B-C36-H36C	109.5
O5-C18-H18B	109.5	C4-O1-C15	117.40 (13)
H18A-C18-H18B	109.5	C5-O2-C16	116.87 (13)
O5-C18-H18C	109.5	C11-O4-C17	115.36 (13)
H18A-C18-H18C	109.5	C12-O5-C18	116.36 (13)
H18B-C18-H18C	109.5	C21-O6-C33	116.52 (14)
C24-C19-C20	120.59 (15)	C22-O7-C34	116.43 (13)
C24-C19-C1	110.17 (14)	C25-O8-C1	112.09 (12)
C20-C19-C1	129.20 (15)	C28-O9-C35	116.50 (14)
C21-C20-C19	118.06 (15)	C29-O10-C36	116.50 (14)
C21-C20-H20	121.0	C32-O12-C25	111.06 (12)
O8-C1-C2-C7	-144.20 (15)	C21-C22-C23-C24	1.4 (2)

C19-C1-C2-C7	103.04 (17)	C20-C19-C24-C23	-0.4 (2)
C14-C1-C2-C7	-20.7 (2)	C1-C19-C24-C23	177.51 (15)
O8-C1-C2-C3	41.9 (2)	C20-C19-C24-C25	178.54 (14)
C19-C1-C2-C3	-70.87 (19)	C1-C19-C24-C25	-3.56 (18)
C14-C1-C2-C3	165.36 (14)	C22-C23-C24-C19	-1.2 (2)
C7-C2-C3-C4	-1.5 (2)	C22-C23-C24-C25	-179.87 (15)
C1-C2-C3-C4	172.51 (15)	C19-C24-C25-O8	10.27 (17)
C2-C3-C4-O1	-178.92 (15)	C23-C24-C25-O8	-170.89 (15)
C2-C3-C4-C5	-1.7 (2)	C19-C24-C25-O12	-106.11 (15)
O1-C4-C5-O2	1.0 (2)	C23-C24-C25-O12	72.7 (2)
C3-C4-C5-O2	-176.50 (15)	C19-C24-C25-C26	139.35 (15)
O1-C4-C5-C6	-179.10 (15)	C23-C24-C25-C26	-41.8 (2)
C3-C4-C5-C6	3.4 (2)	O8-C25-C26-C31	-126.51 (15)
O2-C5-C6-C7	178.02 (15)	O12-C25-C26-C31	-8.72 (17)
C4-C5-C6-C7	-1.9 (2)	C24-C25-C26-C31	109.26 (16)
C3-C2-C7-C6	3.1 (2)	O8-C25-C26-C27	59.4 (2)
C1-C2-C7-C6	-170.86 (15)	O12-C25-C26-C27	177.23 (17)
C3-C2-C7-C8	-174.49 (15)	C24-C25-C26-C27	-64.8 (2)
C1-C2-C7-C8	11.6 (2)	C31-C26-C27-C28	-1.2 (2)
C5-C6-C7-C2	-1.4 (2)	C25-C26-C27-C28	172.34 (17)
C5-C6-C7-C8	176.30 (16)	C26-C27-C28-O9	178.50 (16)
C2-C7-C8-O3	179.10 (17)	C26-C27-C28-C29	-2.9 (3)
C6-C7-C8-O3	1.4 (3)	O9-C28-C29-O10	3.5 (2)
C2-C7-C8-C9	0.8 (2)	C27-C28-C29-O10	-175.23 (16)
C6-C7-C8-C9	-176.86 (15)	O9-C28-C29-C30	-175.76 (15)
O3-C8-C9-C14	179.27 (17)	C27-C28-C29-C30	5.5 (3)
C7-C8-C9-C14	-2.4 (2)	O10-C29-C30-C31	177.01 (16)
O3-C8-C9-C10	-2.3 (3)	C28-C29-C30-C31	-3.8 (3)
C7-C8-C9-C10	175.97 (15)	C27-C26-C31-C30	2.8 (3)
C14-C9-C10-C11	-0.3 (2)	C25-C26-C31-C30	-171.93 (16)
C8-C9-C10-C11	-178.76 (15)	C27-C26-C31-C32	-177.33 (15)
C9-C10-C11-O4	-178.78 (15)	C25-C26-C31-C32	7.92 (19)
C9-C10-C11-C12	0.7 (2)	C29-C30-C31-C26	-0.3 (3)
C10-C11-C12-O5	179.45 (15)	C29-C30-C31-C32	179.92 (16)
O4-C11-C12-O5	-1.1 (2)	C26-C31-C32-O11	175.35 (18)
C10-C11-C12-C13	-0.7 (2)	C30-C31-C32-O11	-4.8 (3)
O4-C11-C12-C13	178.76 (14)	C26-C31-C32-O12	-3.67 (19)

O5-C12-C13-C14	-179.72 (15)	C30-C31-C32-O12	176.17 (16)
C11-C12-C13-C14	0.5 (2)	C3-C4-O1-C15	-0.2 (2)
C10-C9-C14-C13	0.1 (2)	C5-C4-O1-C15	-177.54 (14)
C8-C9-C14-C13	178.41 (15)	C6-C5-O2-C16	-0.9 (2)
C10-C9-C14-C1	173.28 (15)	C4-C5-O2-C16	178.96 (15)
C8-C9-C14-C1	-8.4 (2)	C10-C11-O4-C17	-3.3 (2)
C12-C13-C14-C9	-0.1 (2)	C12-C11-O4-C17	177.28 (14)
C12-C13-C14-C1	-173.47 (15)	C13-C12-O5-C18	0.6 (2)
O8-C1-C14-C9	143.63 (15)	C11-C12-O5-C18	-179.63 (14)
C19-C1-C14-C9	-105.45 (17)	C20-C21-O6-C33	-12.8 (2)
C2-C1-C14-C9	19.1 (2)	C22-C21-O6-C33	165.53 (14)
O8-C1-C14-C13	-43.21 (19)	C23-C22-O7-C34	-3.5 (2)
C19-C1-C14-C13	67.71 (18)	C21-C22-O7-C34	179.40 (14)
C2-C1-C14-C13	-167.75 (14)	O12-C25-O8-C1	102.57 (14)
O8-C1-C19-C24	-4.15 (16)	C24-C25-O8-C1	-13.34 (16)
C14-C1-C19-C24	-119.84 (15)	C26-C25-O8-C1	-143.63 (14)
C2-C1-C19-C24	114.38 (15)	C19-C1-O8-C25	11.06 (16)
O8-C1-C19-C20	173.51 (15)	C14-C1-O8-C25	126.99 (14)
C14-C1-C19-C20	57.8 (2)	C2-C1-O8-C25	-107.33 (15)
C2-C1-C19-C20	-68.0 (2)	C27-C28-O9-C35	-13.0 (3)
C24-C19-C20-C21	1.6 (2)	C29-C28-O9-C35	168.28 (16)
C1-C19-C20-C21	-175.83 (15)	C30-C29-O10-C36	-5.1 (2)
C19-C20-C21-O6	176.85 (14)	C28-C29-O10-C36	175.69 (15)
C19-C20-C21-C22	-1.3 (2)	O11-C32-O12-C25	178.68 (16)
O6-C21-C22-O7	-1.3 (2)	C31-C32-O12-C25	-2.19 (18)
C20-C21-C22-O7	177.04 (14)	O8-C25-O12-C32	128.56 (14)
O6-C21-C22-C23	-178.56 (14)	C24-C25-O12-C32	-117.56 (14)
C20-C21-C22-C23	-0.2 (2)	C26-C25-O12-C32	6.52 (17)
O7-C22-C23-C24	-175.53 (15)		