

Supporting Information (66 pages)

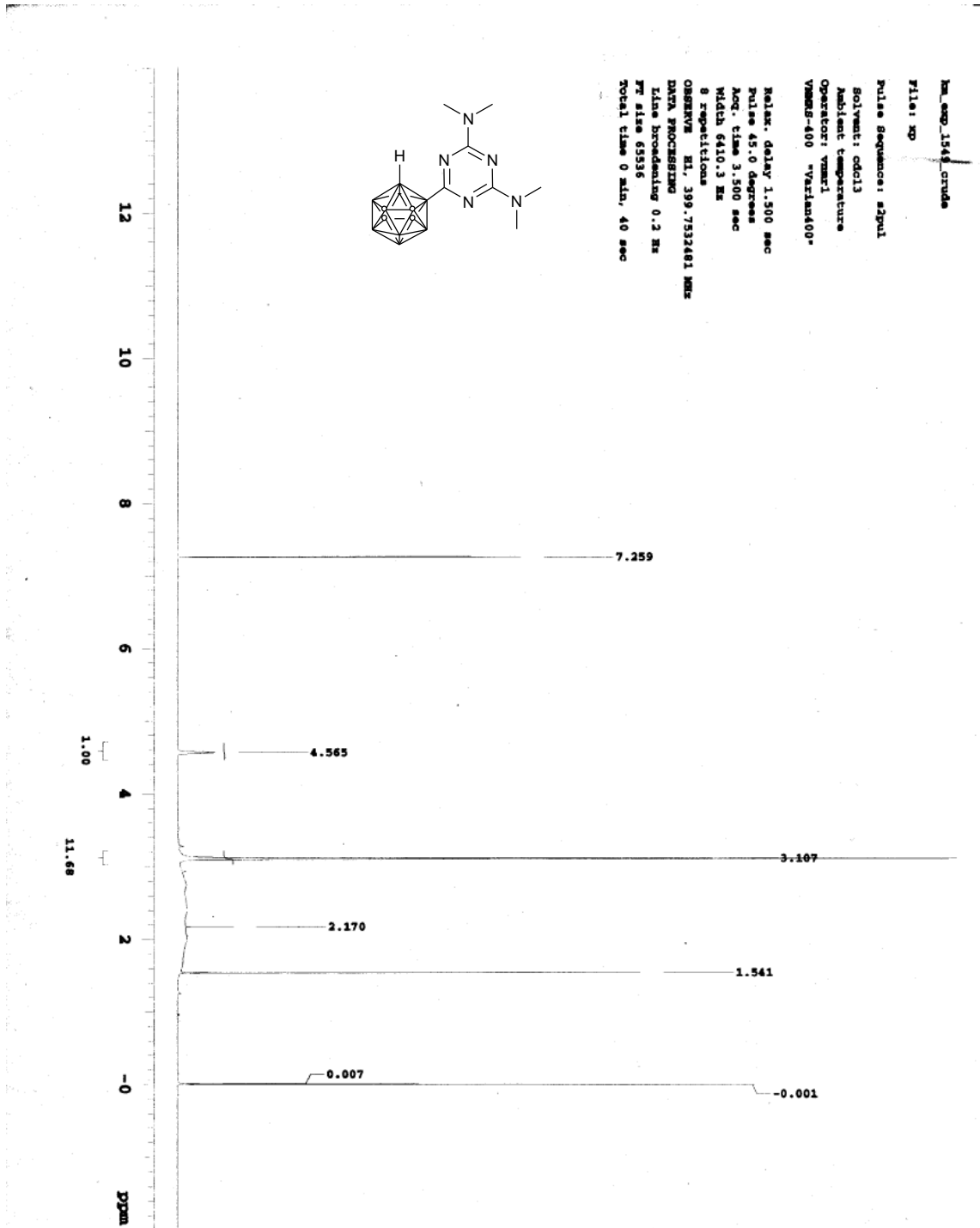
**Discovery of *ortho*-Carborane-Conjugated Triazines  
as Selective Topoisomerase I/II Inhibitors**Hiroyuki Nakamura,<sup>1,\*</sup> Atsushi Shoji,<sup>1</sup> Ayano Takeuchi,<sup>1</sup> Hyun Seung Ban,<sup>1</sup> Jong-Dae Lee,<sup>2</sup>  
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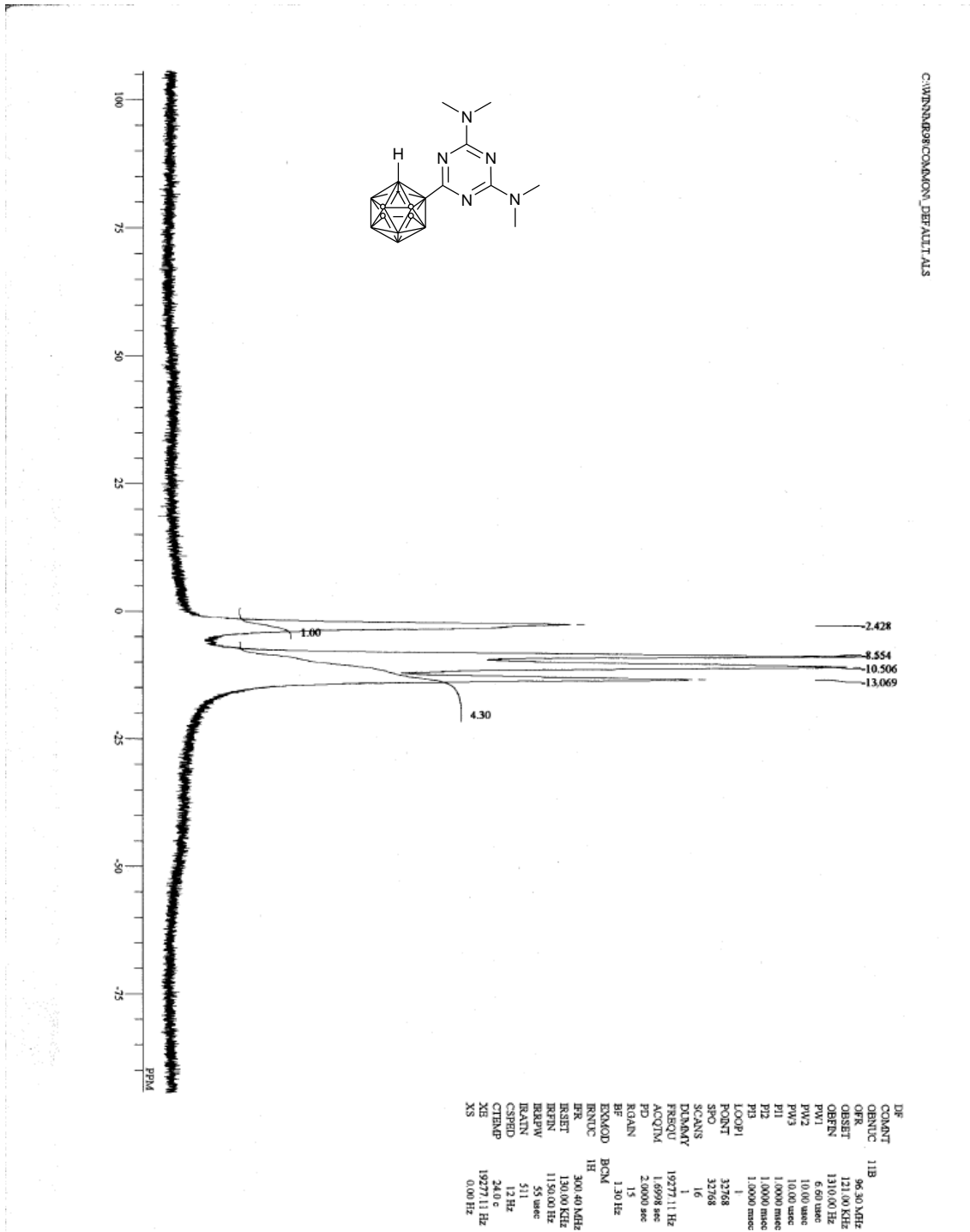
2,4-Bis(N,N-dimethylamino)-6-(o-carboran-1-yl)-1,3,5-triazine 3a

<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)



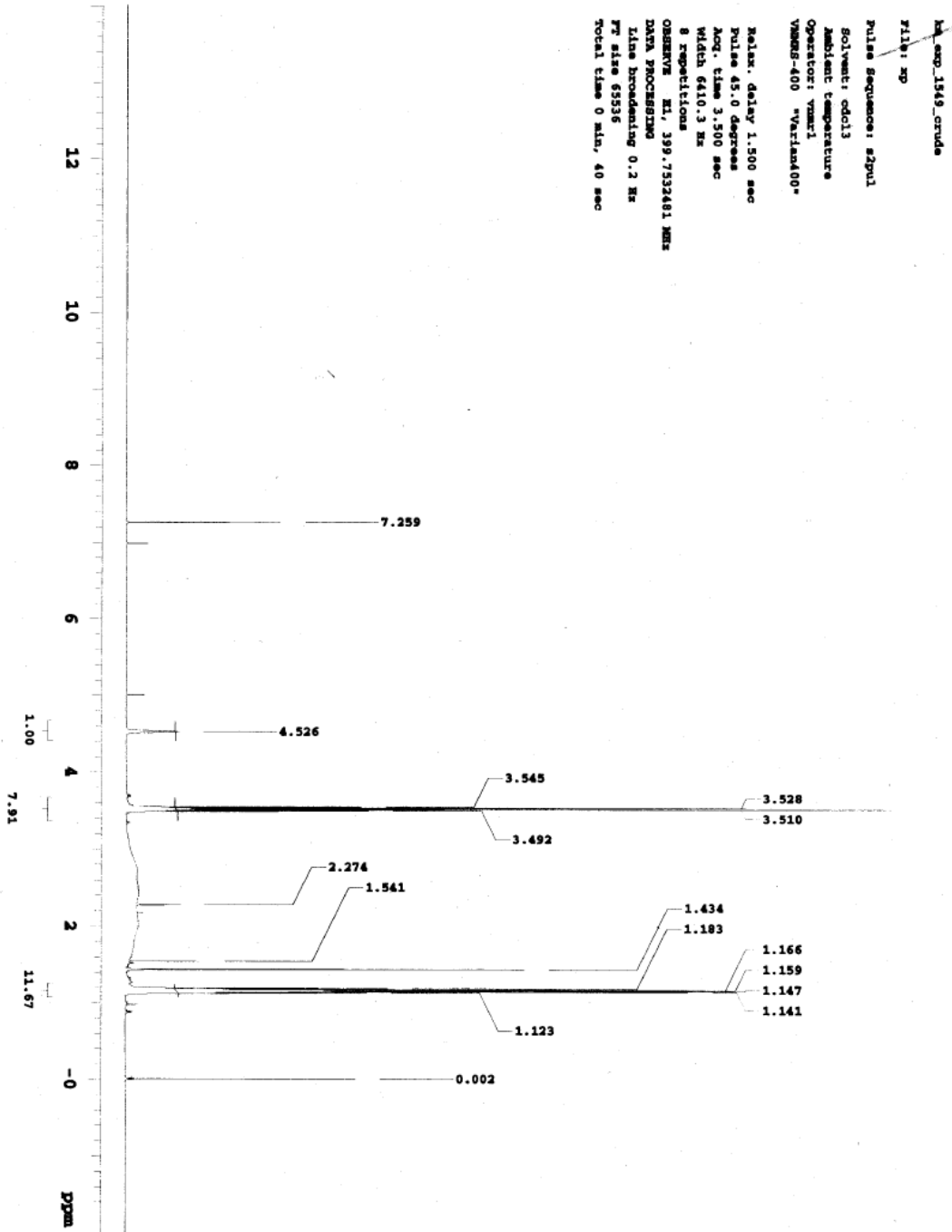
2,4-Bis(*N,N*-dimethylamino)-6-(*o*-carboran-1-yl)-1,3,5-triazine **3a**

$^{11}\text{B}$  NMR (96.3 MHz, MHz,  $\text{CDCl}_3$ )



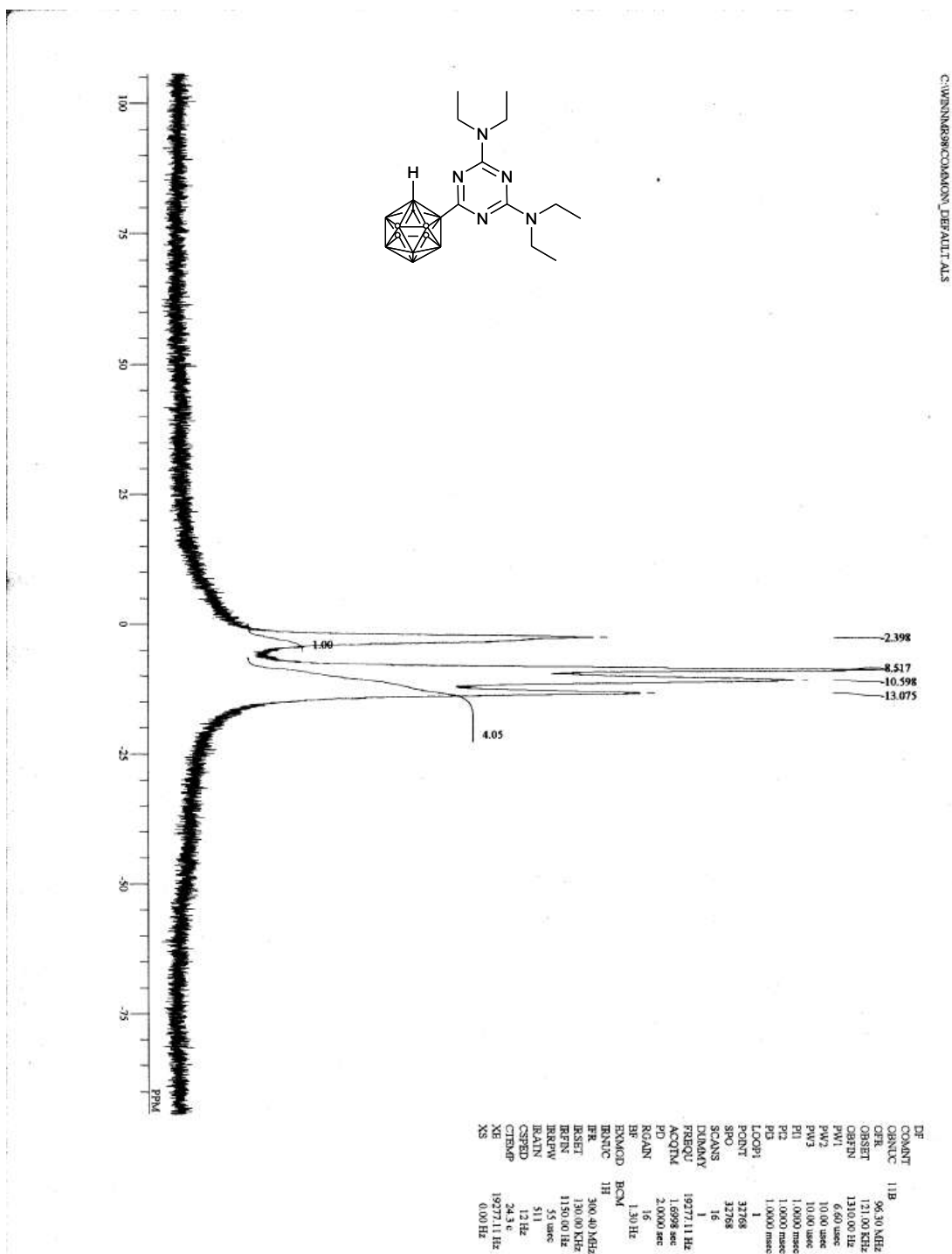
2,4-Bis(N,N-diethylamino)-6-(o-carboran-1-yl)-1,3,5-triazine 3b

<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)



2,4-Bis(N,N-diethylamino)-6-(o-carboran-1-yl)-1,3,5-triazine **3b**

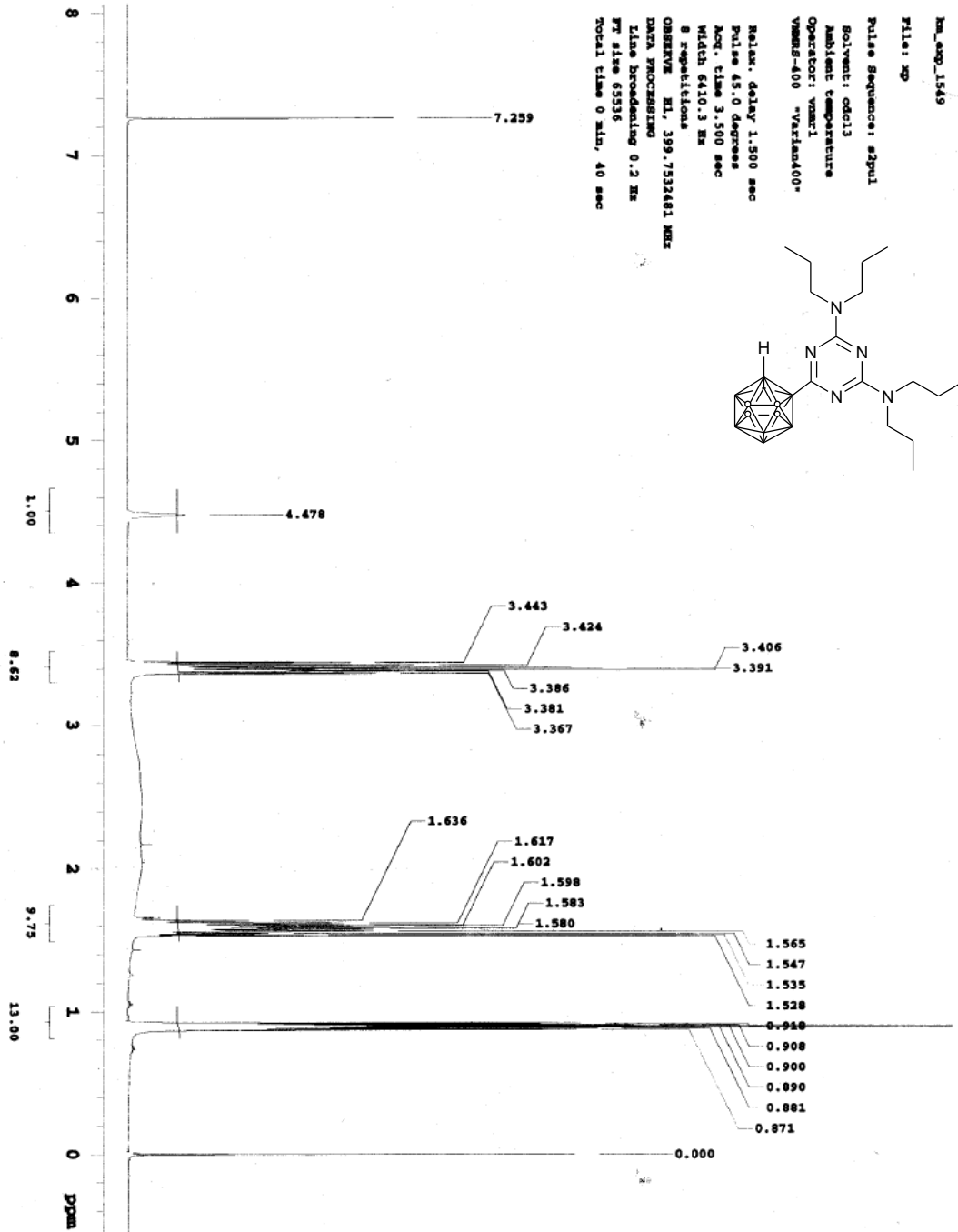
$^{11}\text{B}$  NMR (96.3 MHz, MHz,  $\text{CDCl}_3$ )



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CONT  
CONTC 11B  
OR 96.30 MHz  
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ORFTN 1310.00 Hz  
PWI 6.60 usec  
PW2 10.00 usec  
PW3 10.00 usec  
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PI2 1.0000 msec  
PI3 1.0000 msec  
LOOP1 1  
POINT 32768  
SPO 32768  
SCANS 16  
EXAMINY 1  
FREQY 19277.11 Hz  
ACQTM 1.6998 sec  
PD 2.0000 sec  
RGAIN 16  
HF 1.30 Hz  
EXMCO BOM  
RENIC 1H  
FR 300.40 MHz  
RSET 130.00 KHz  
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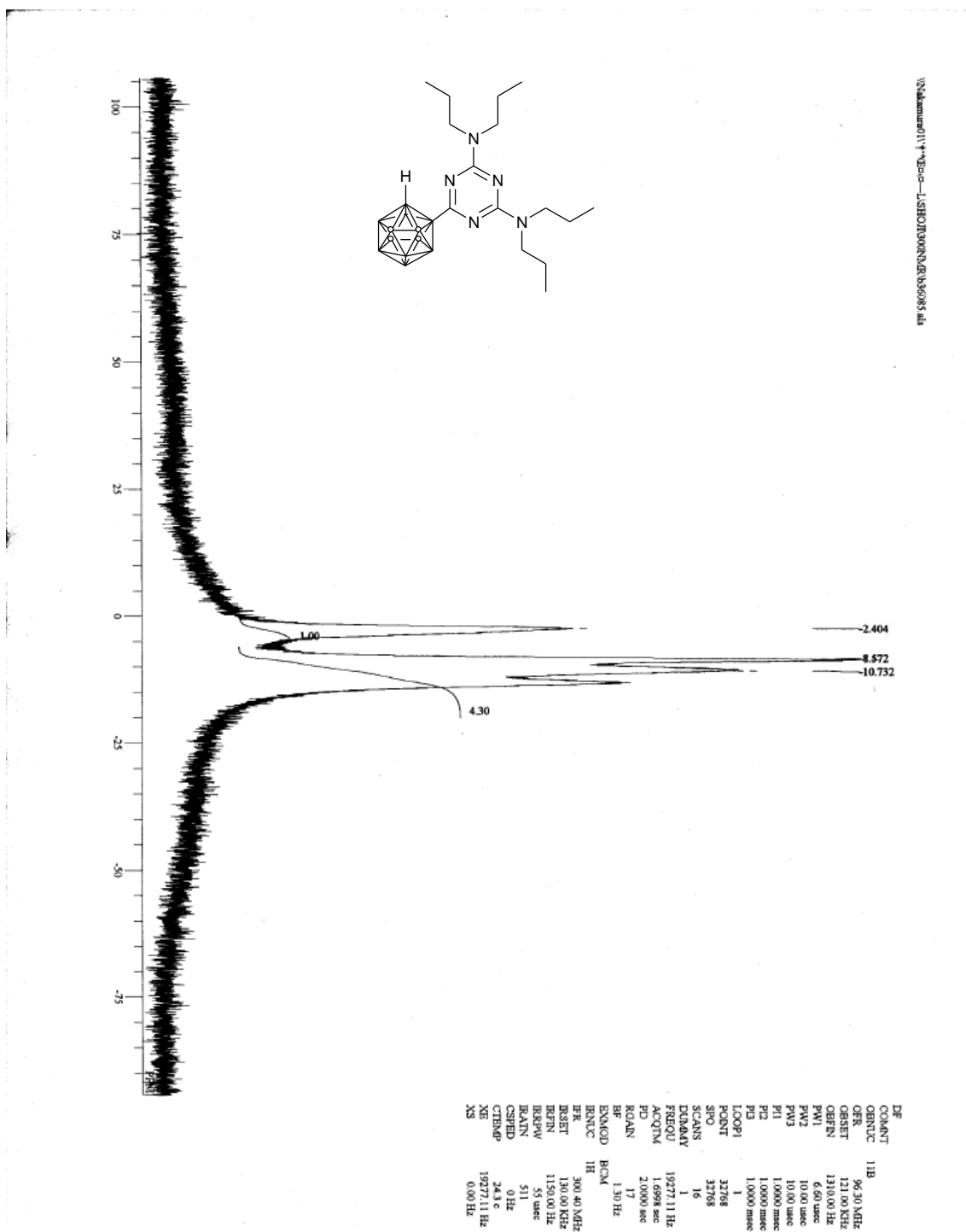
2,4-Bis(*N,N*-di-*n*-propylamino)-6-(*o*-carboran-1-yl)-1,3,5-triazine **3c**

<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)



2,4-Bis(*N,N*-di-*n*-propylamino)-6-(*o*-carboran-1-yl)-1,3,5-triazine **3c**

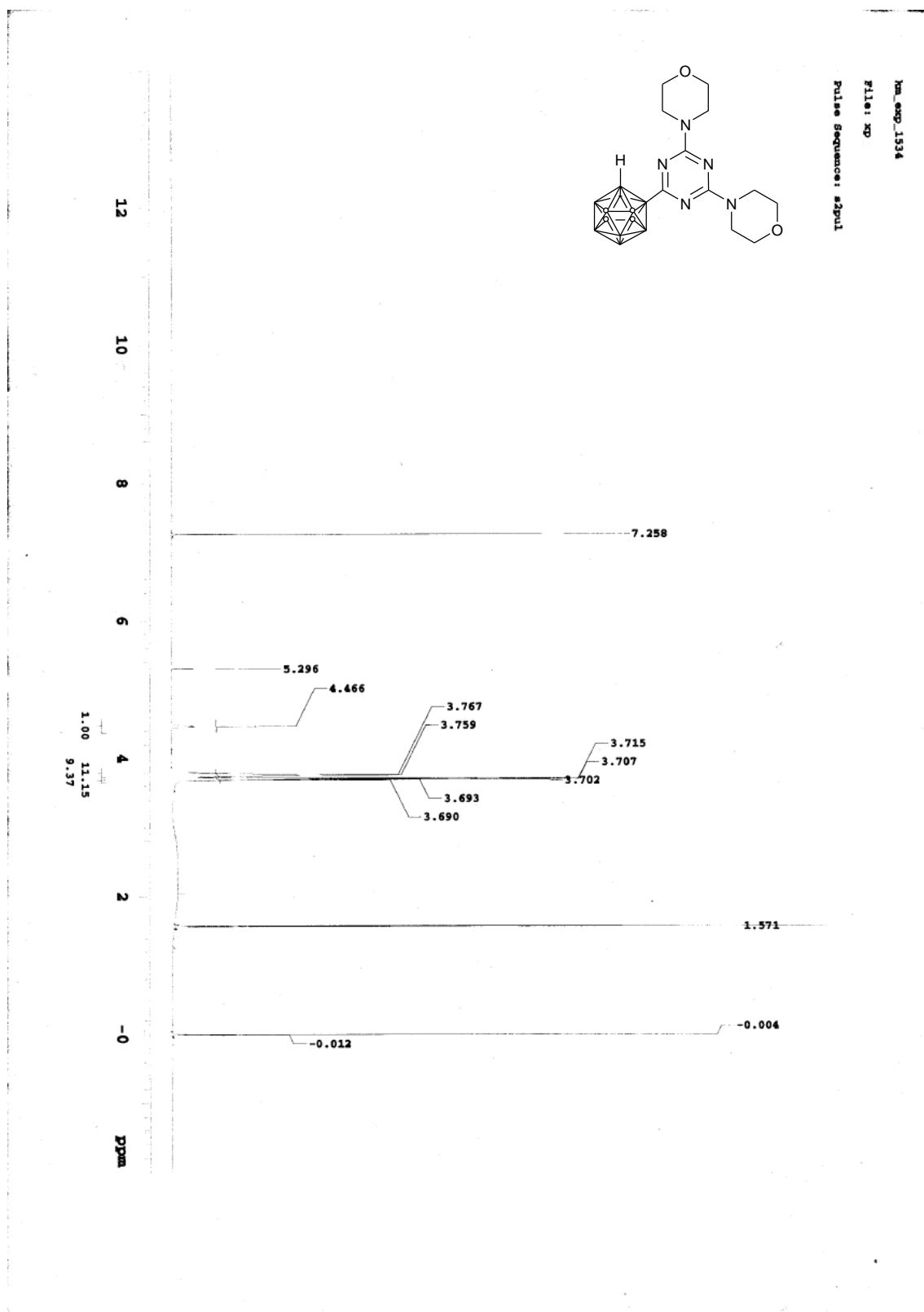
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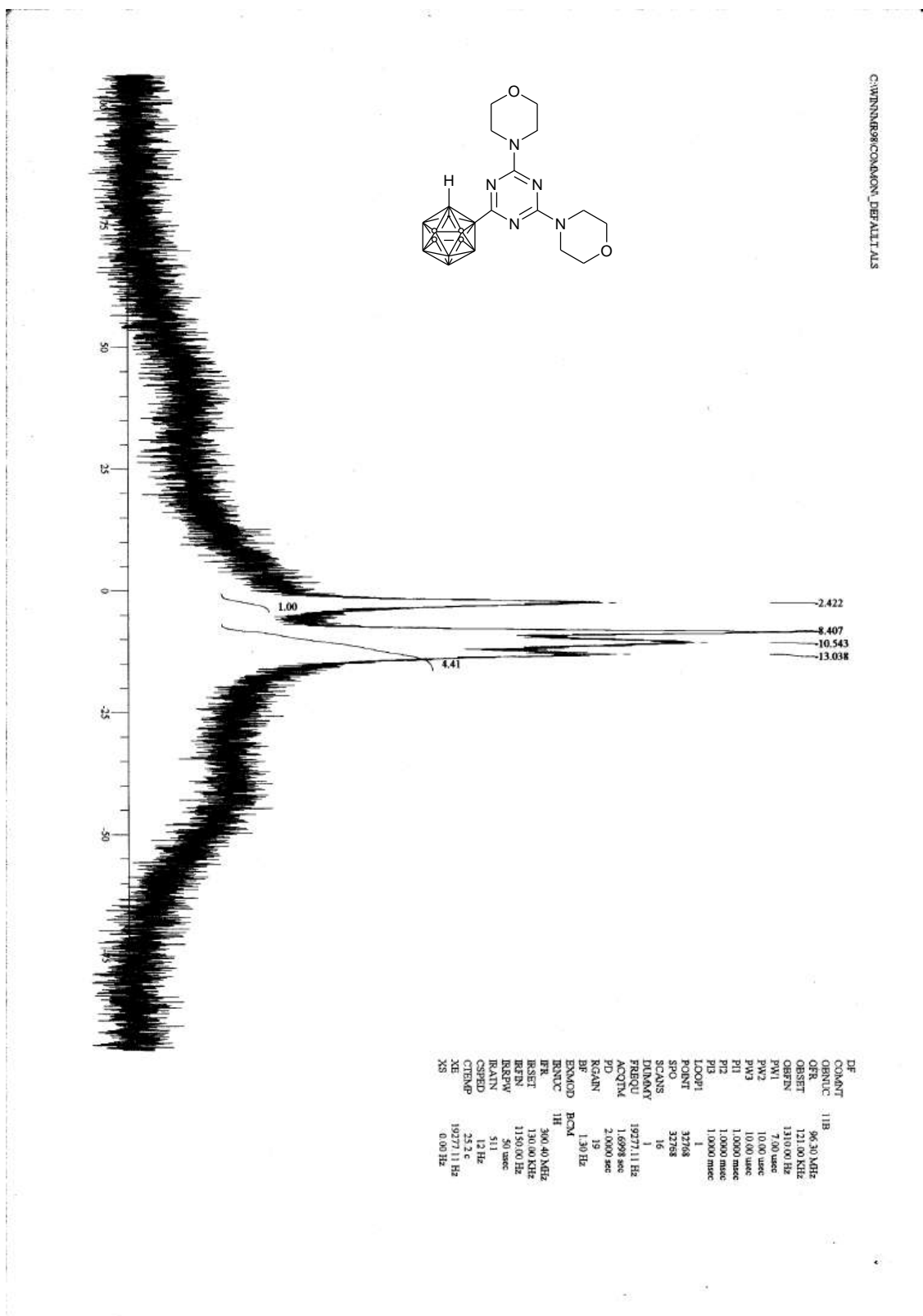
2,4-Bis-(N-morpholinyl)-6-(o-carboran-1-yl)-1,3,5-triazine **3d**

$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )



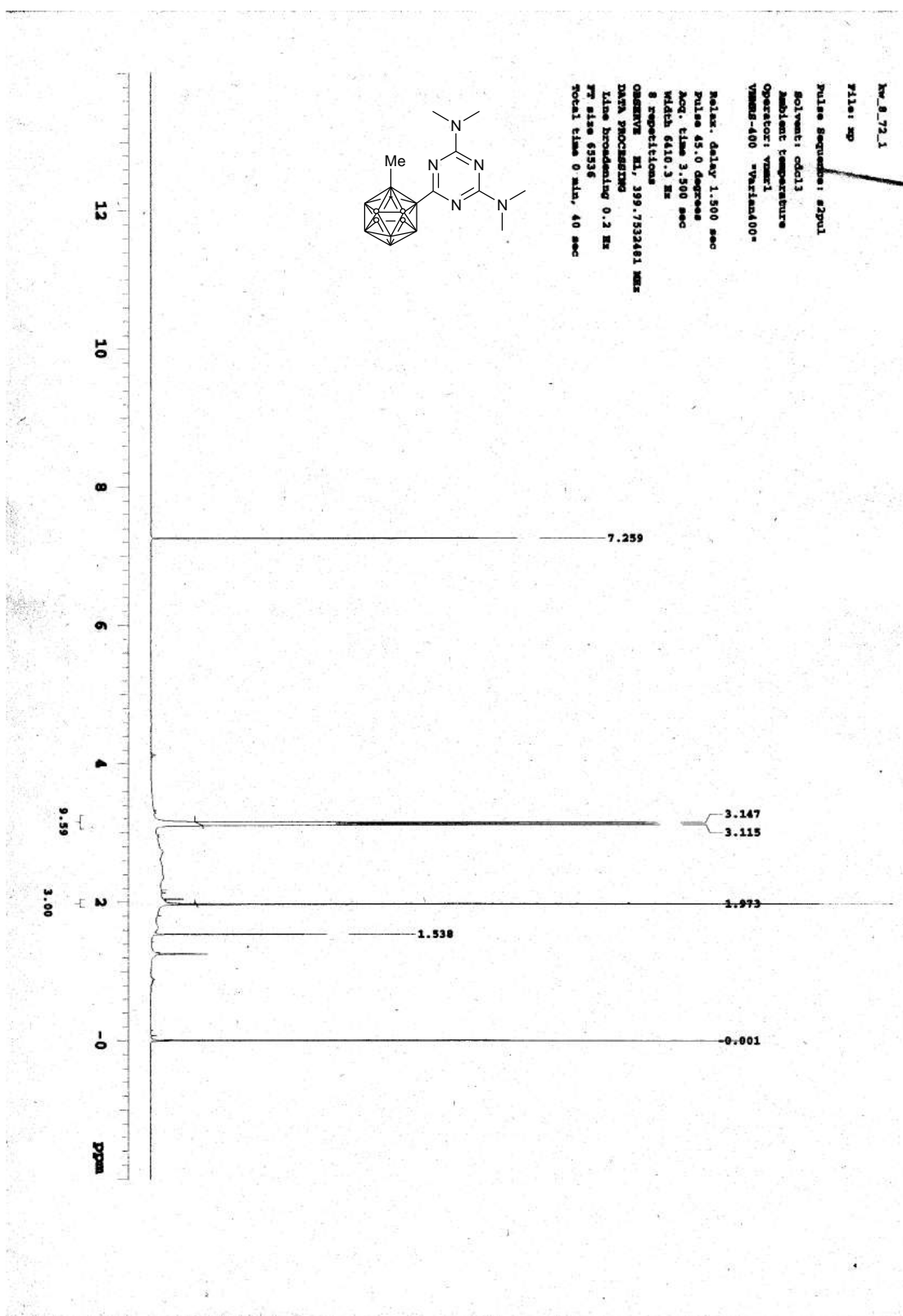
2,4-Bis-(N-morpholinyl)-6-(o-carboran-1-yl)-1,3,5-triazine **3d**

<sup>11</sup>B NMR (96.3 MHz, CDCl<sub>3</sub>)



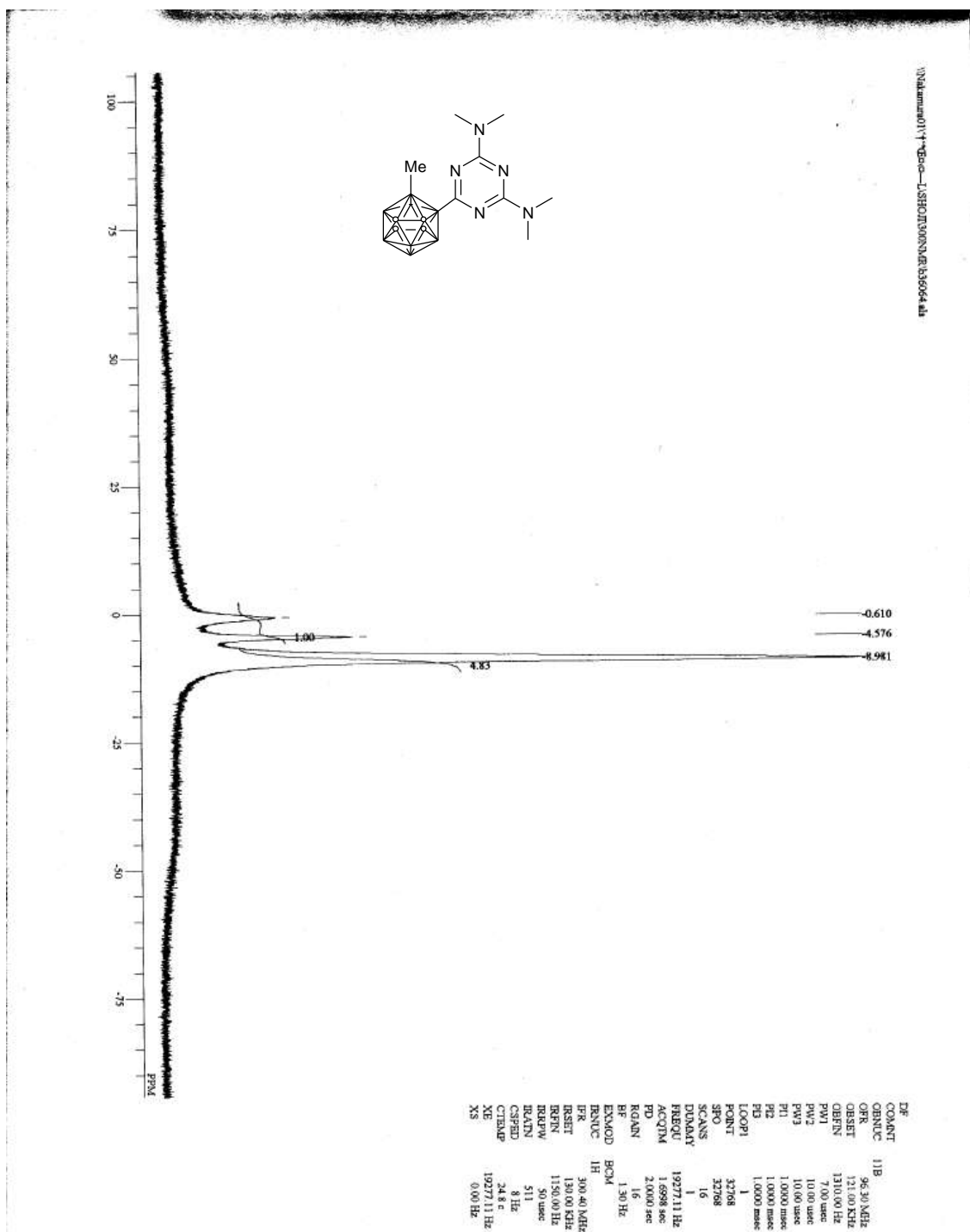
2,4-Bis(N,N-dimethylamino)-6-(2-methyl-o-carboran-1-yl)-1,3,5-triazine **4a**

$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )



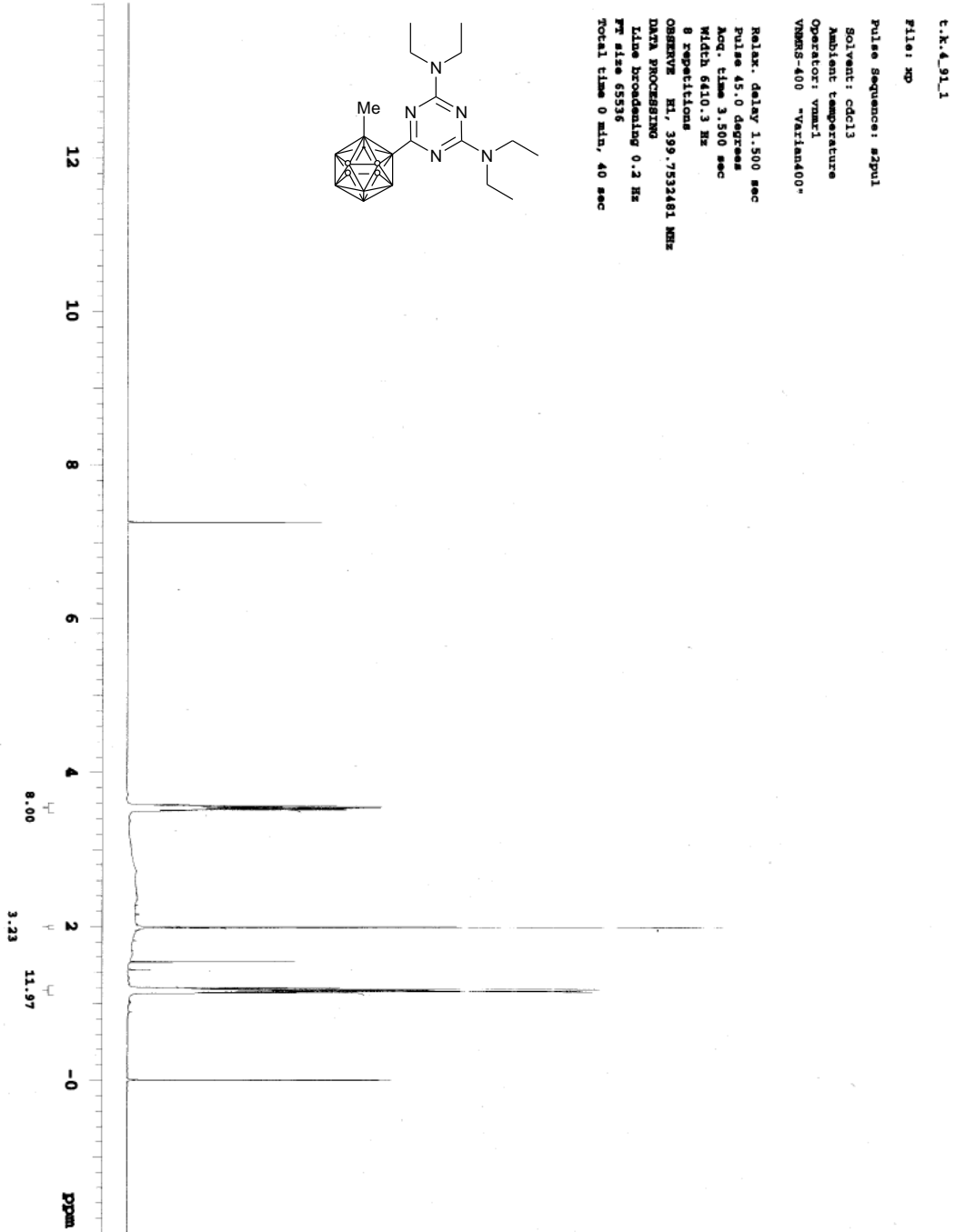
2,4-Bis(*N,N*-dimethylamino)-6-(2-methyl-*o*-carboran-1-yl)-1,3,5-triazine **4a**

$^{11}\text{B}$  NMR (96.3 MHz,  $\text{CDCl}_3$ )



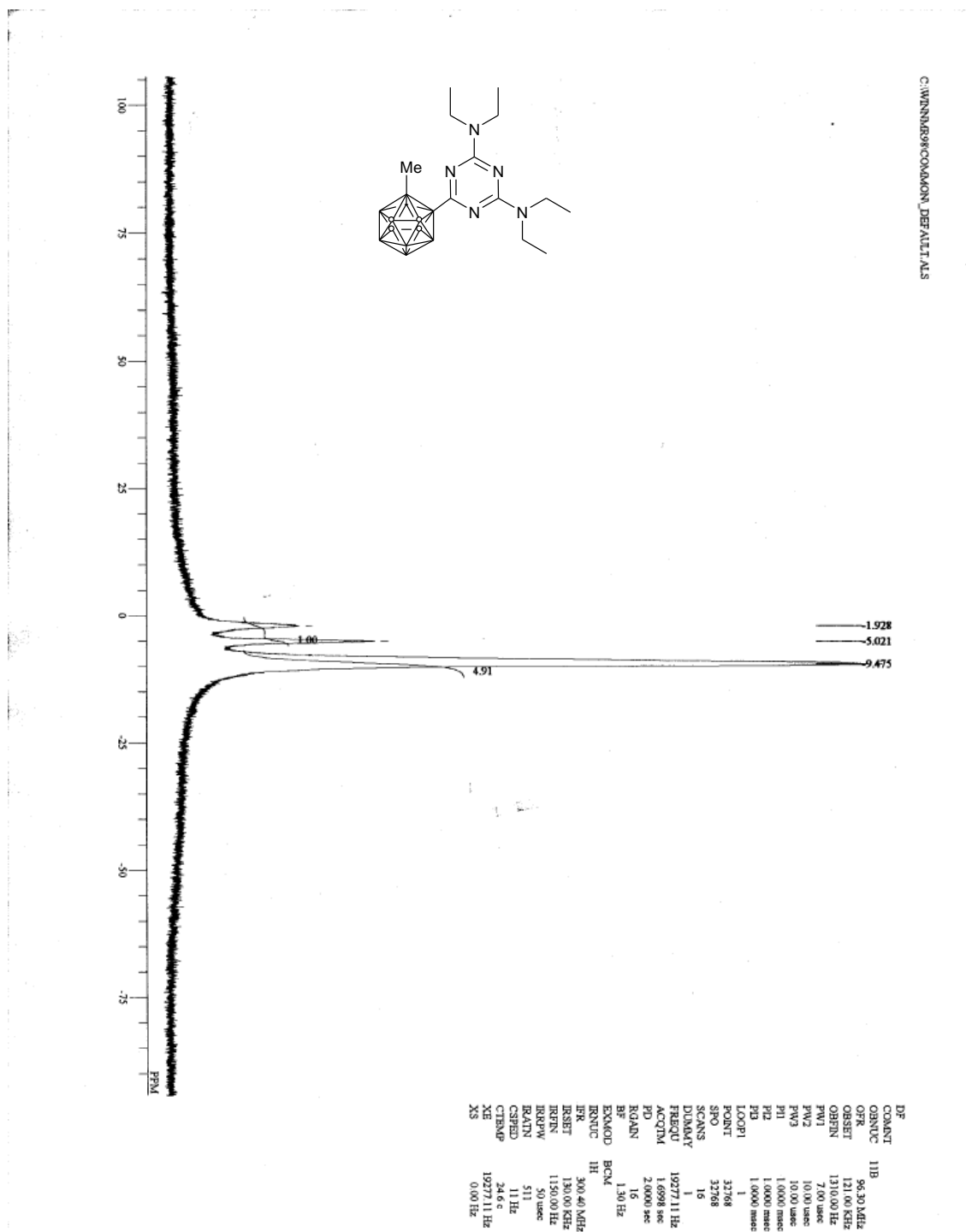
2,4-Bis(N,N-diethylamino)-6-(2-methyl-o-carboran-1-yl)-1,3,5-triazine **4b**

<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)



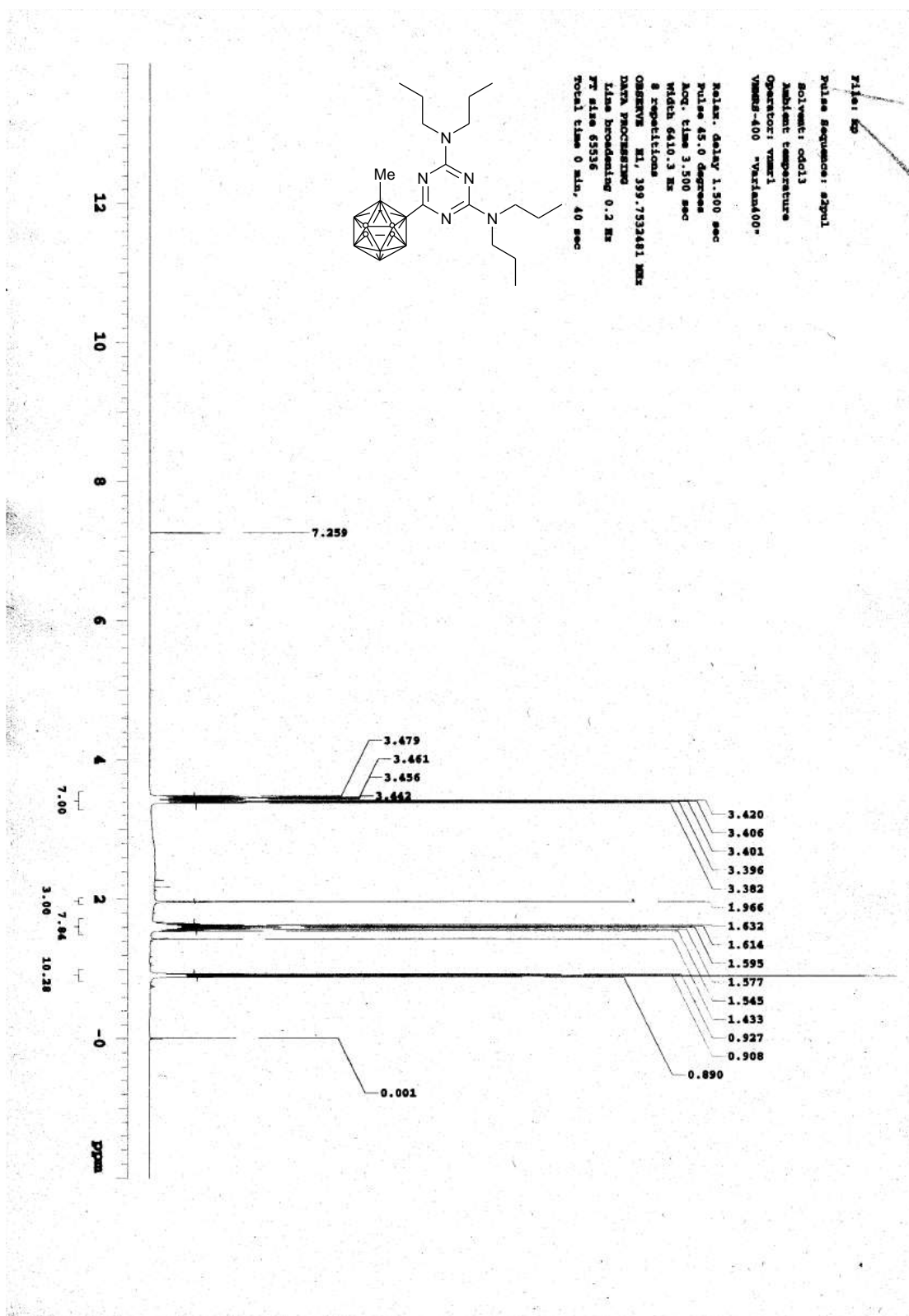
2,4-Bis(*N,N*-diethylamino)-6-(2-methyl-*o*-carboran-1-yl)-1,3,5-triazine **4b**

$^{11}\text{B}$  NMR (96.3 MHz,  $\text{CDCl}_3$ )



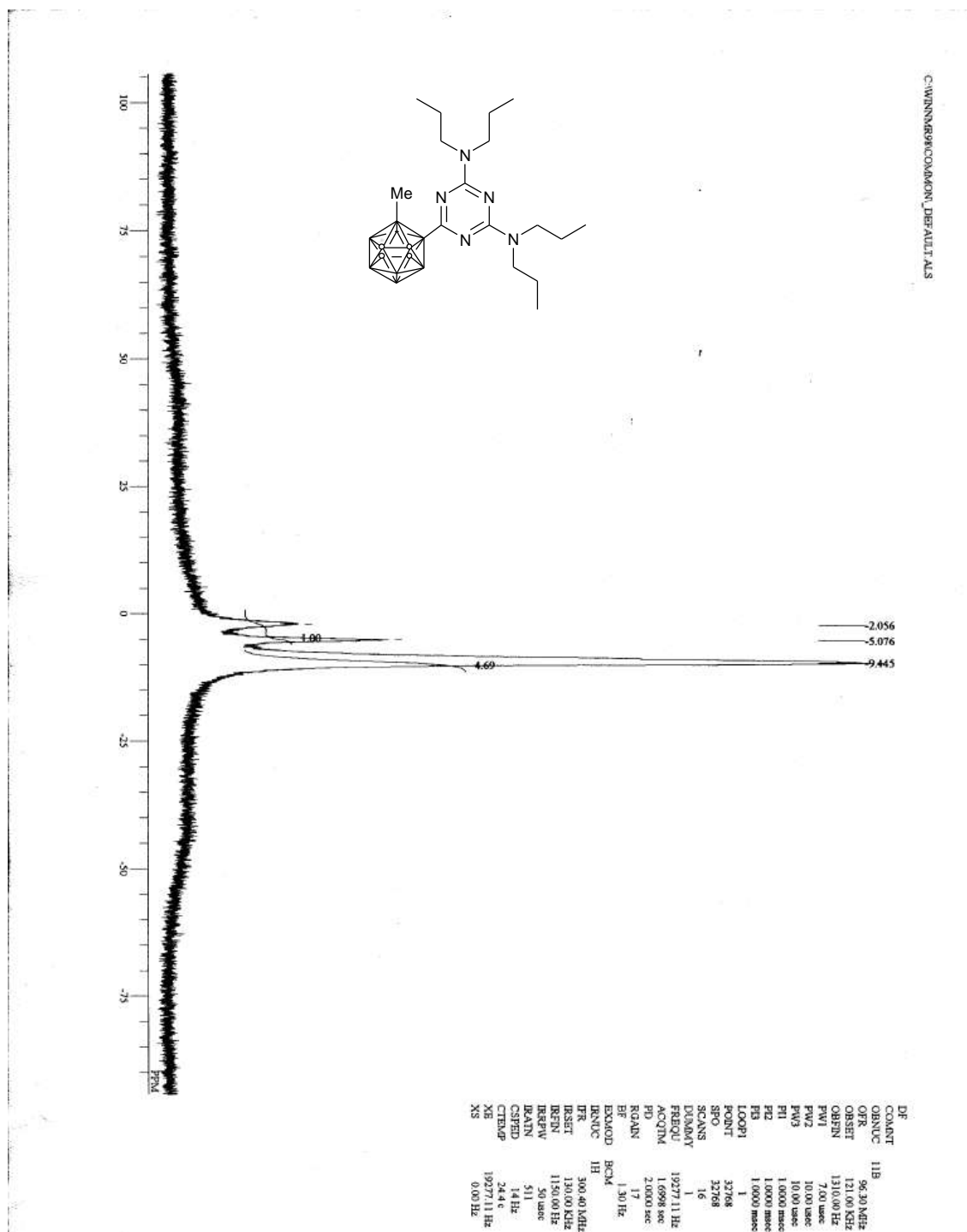
2,4-Bis(*N,N*-*n*-propylamino)-6-(2-methyl-*o*-carboran-1-yl)-1,3,5-triazine **4c**

<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)



2,4-Bis(*N,N*-*n*-propylamino)-6-(2-methyl-*o*-carboran-1-yl)-1,3,5-triazine **4c**

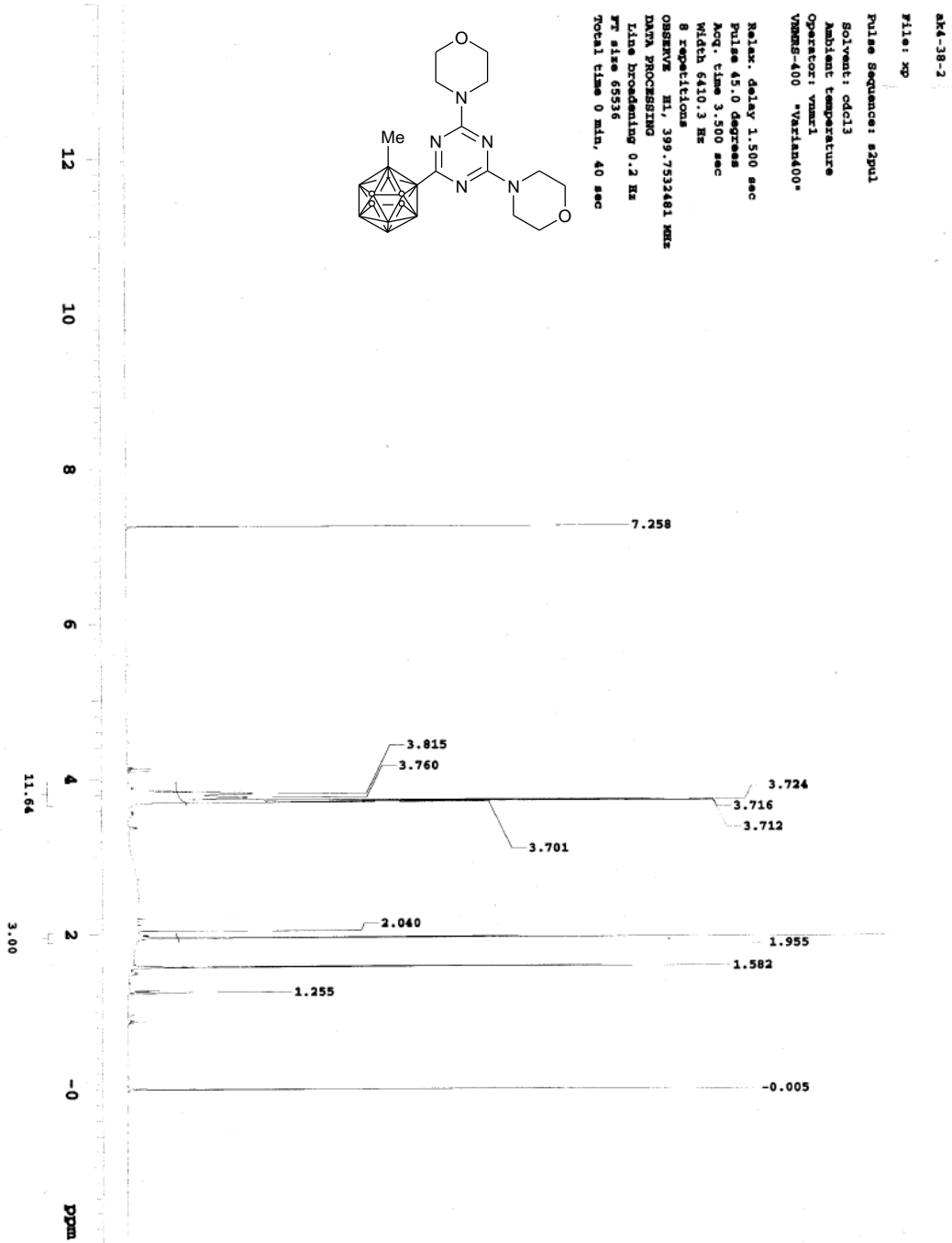
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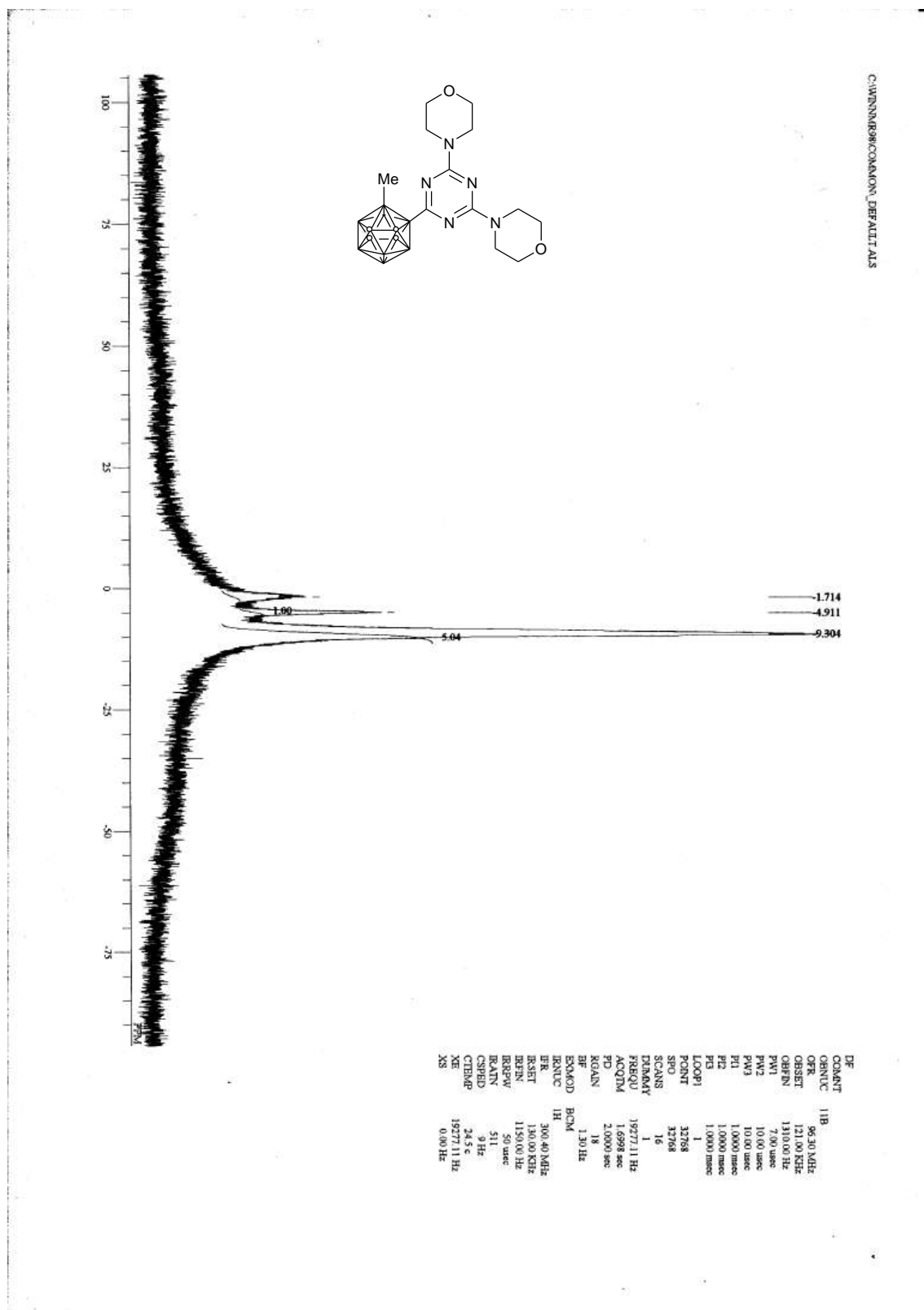
2,4-Bis-(N-morpholinyl)-6-(2-methyl-o-carboran-1-yl)-1,3,5-triazine **4d**

<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)



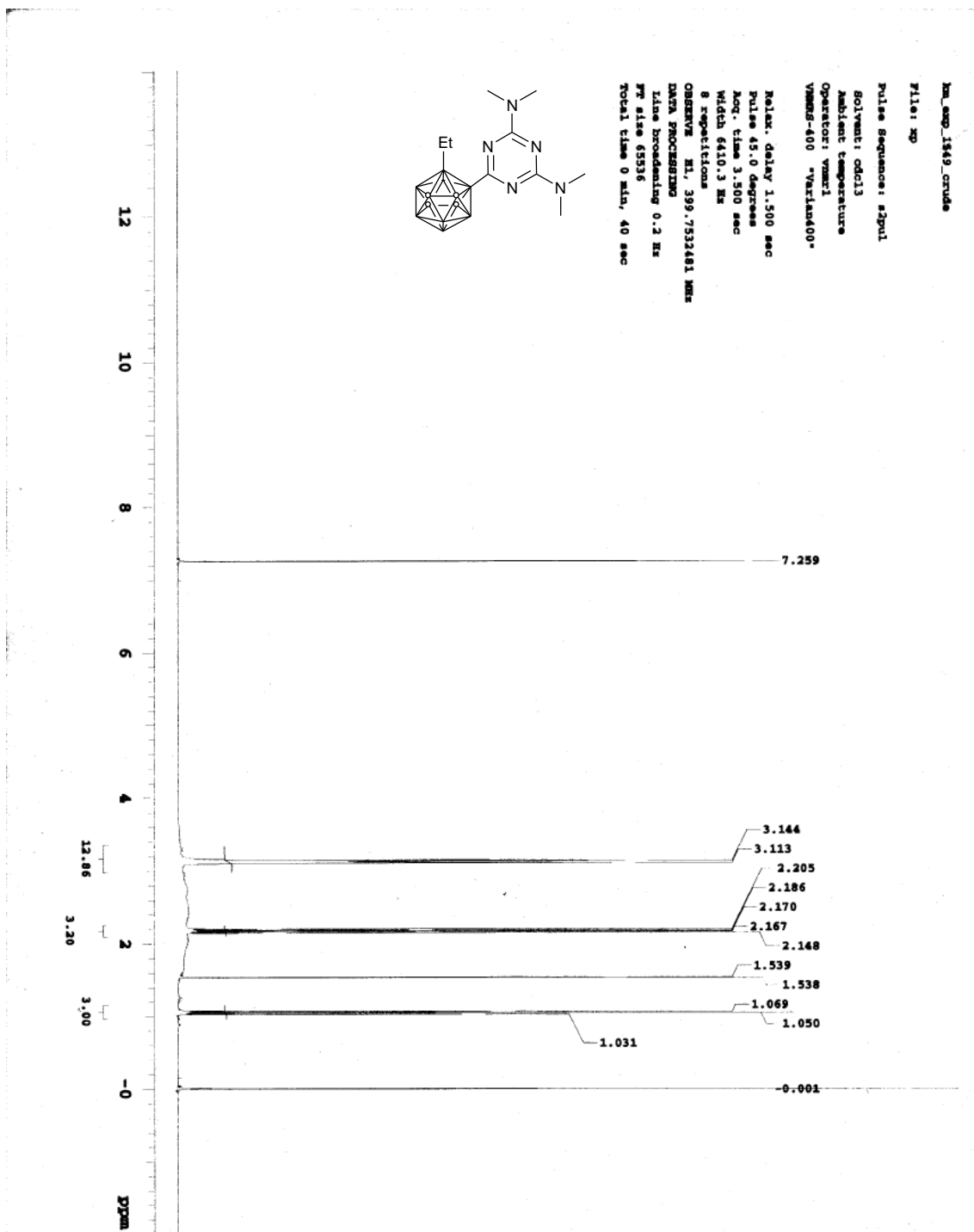
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$^{11}\text{B}$  NMR (96.3 MHz,  $\text{CDCl}_3$ )



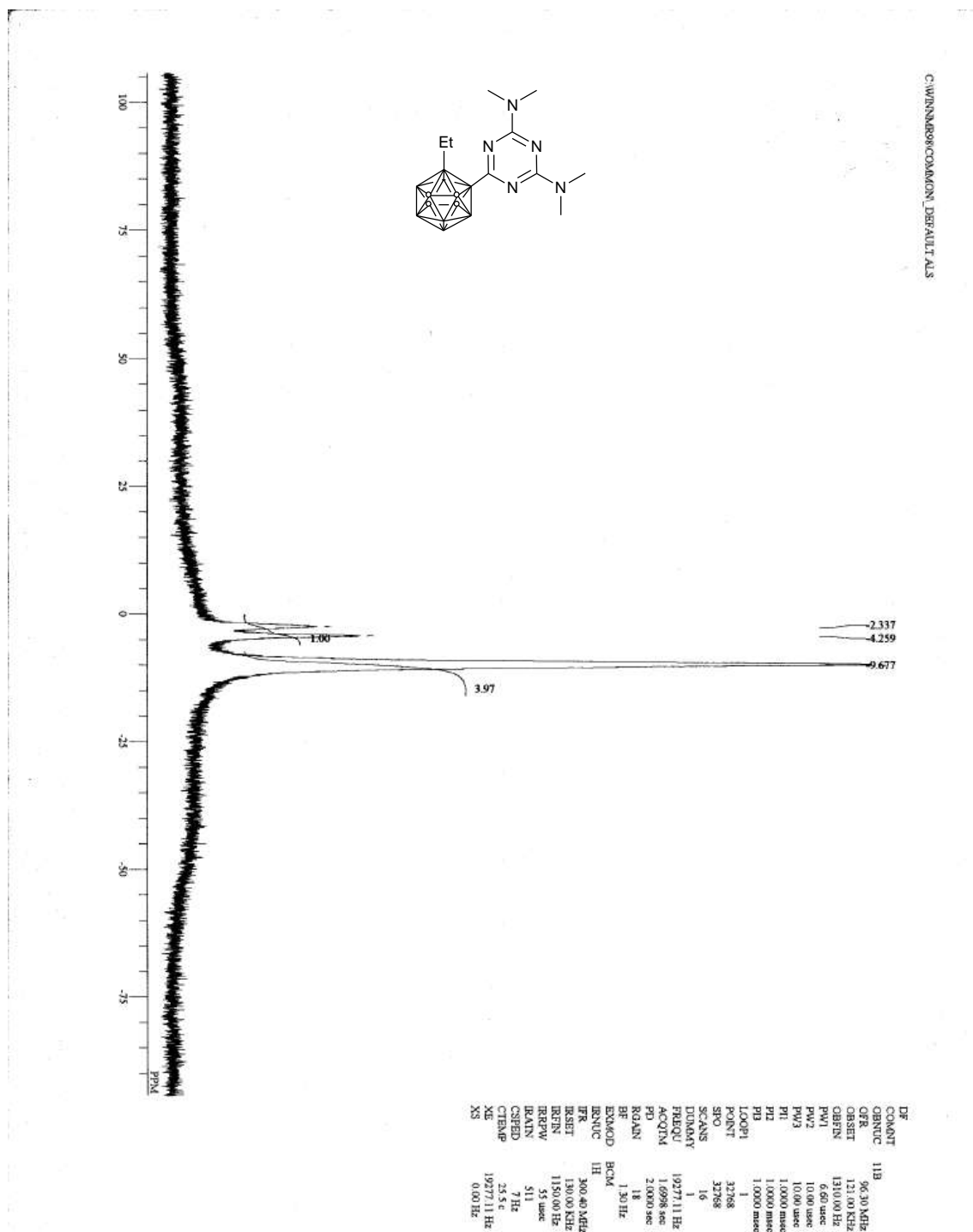
2,4-Bis(N,N-dimethylamino)-6-(2-ethyl-o-carboran-1-yl)-1,3,5-triazine 4e

<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)



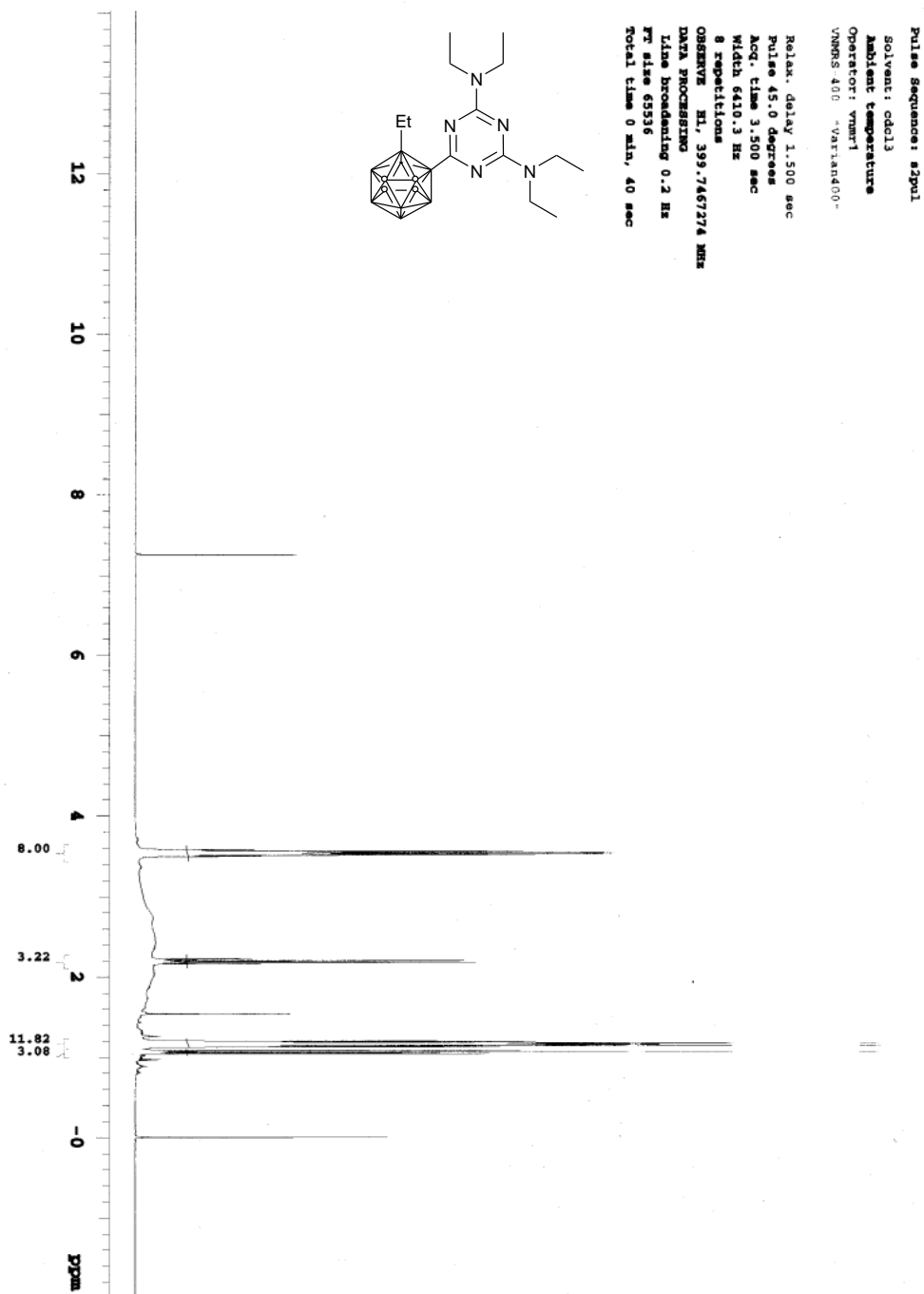
2,4-Bis(*N,N*-dimethylamino)-6-(2-ethyl-*o*-carboran-1-yl)-1,3,5-triazine **4e**

$^{11}\text{B}$  NMR (96.3 MHz,  $\text{CDCl}_3$ )



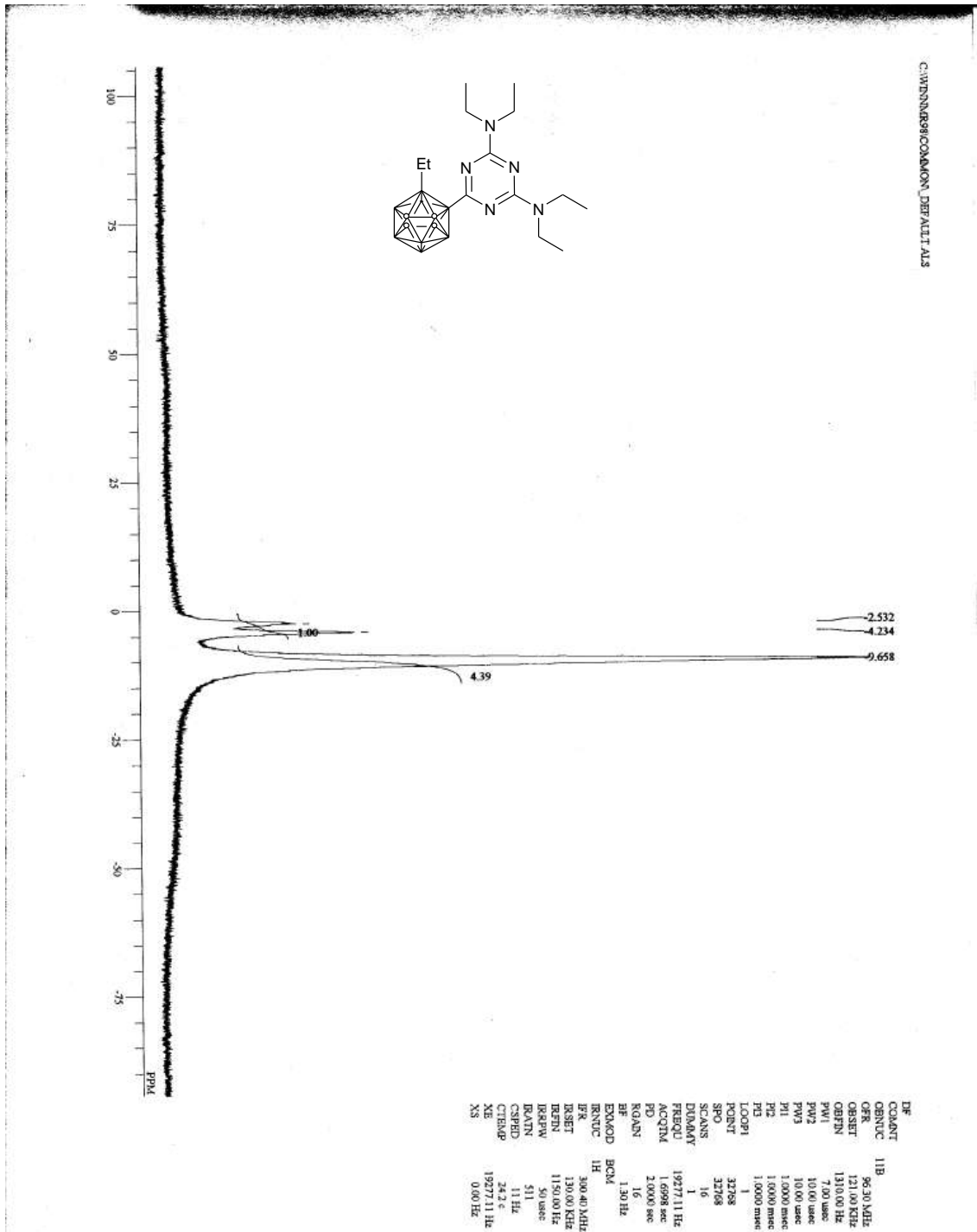
2,4-Bis(N,N-diethylamino)-6-(2-ethyl-o-carboran-1-yl)-1,3,5-triazine **4f**

<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)



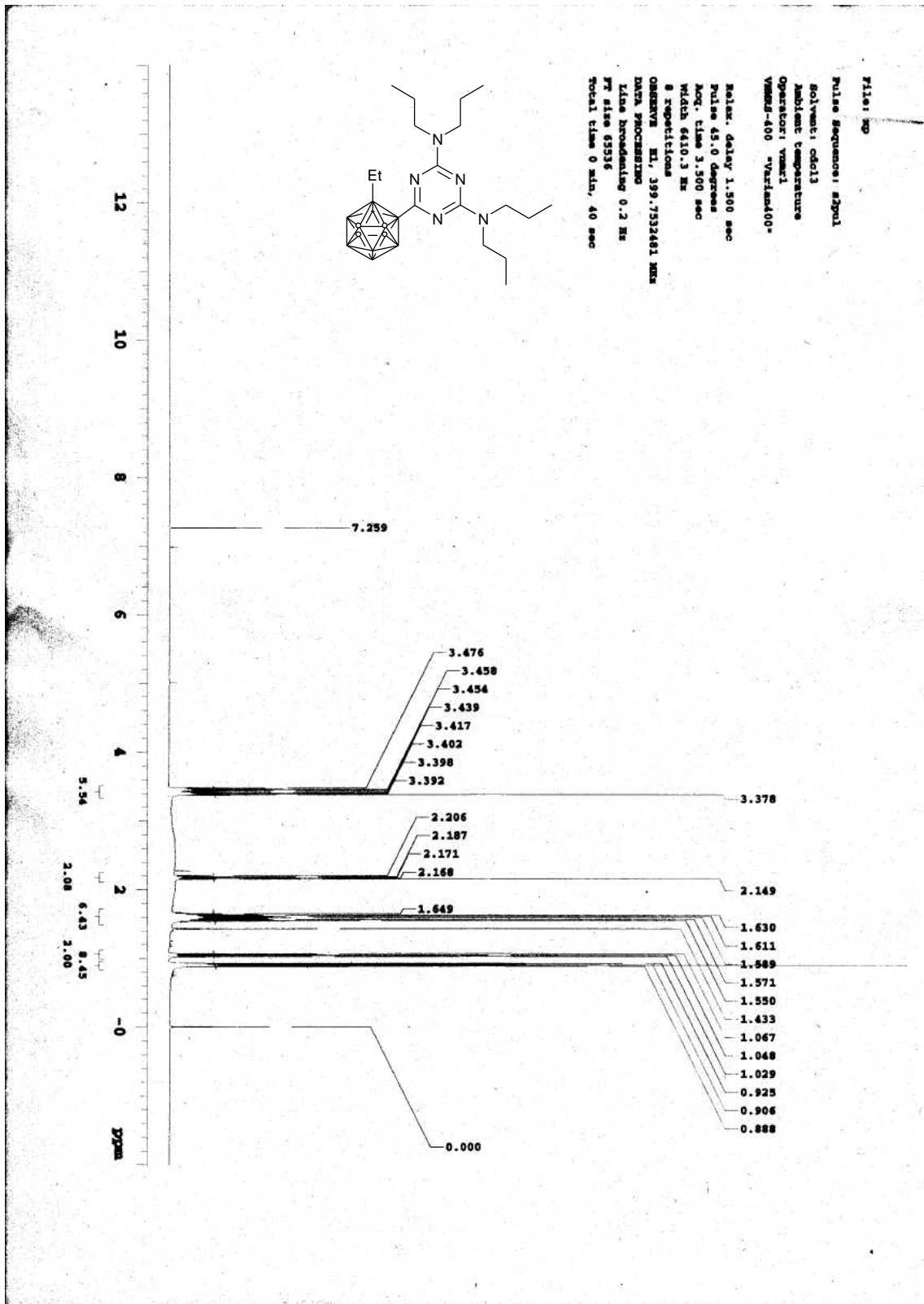
2,4-Bis(N,N-diethylamino)-6-(2-ethyl-o-carboran-1-yl)-1,3,5-triazine **4f**

$^{11}\text{B}$  NMR (96.3 MHz,  $\text{CDCl}_3$ )



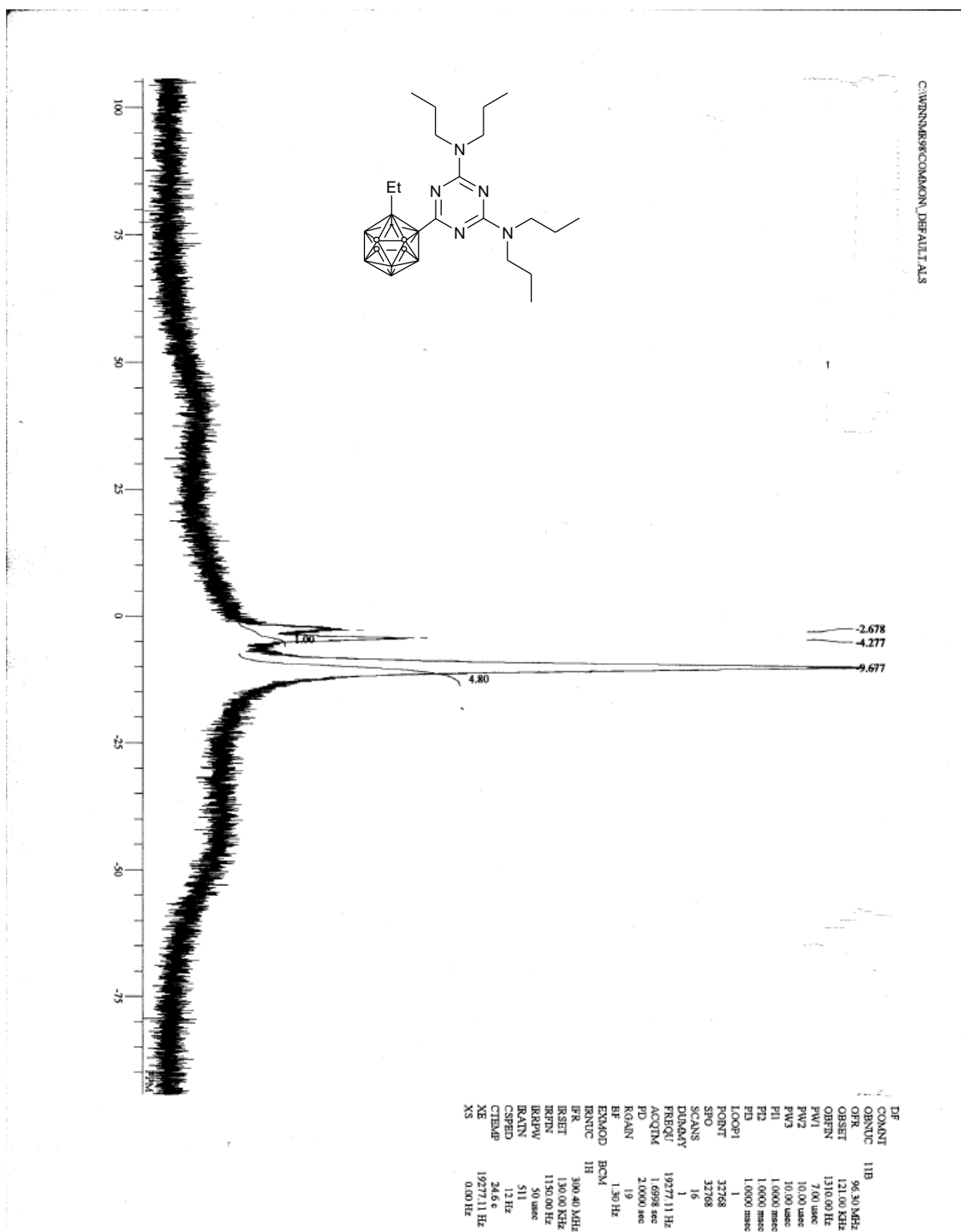
2,4-Bis(N,N-n-propylamino)-6-(2-ethyl-o-carboran-1-yl)-1,3,5-triazine 4g

<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)



2,4-Bis(*N,N*-*n*-propylamino)-6-(2-ethyl-*o*-carboran-1-yl)-1,3,5-triazine **4g**

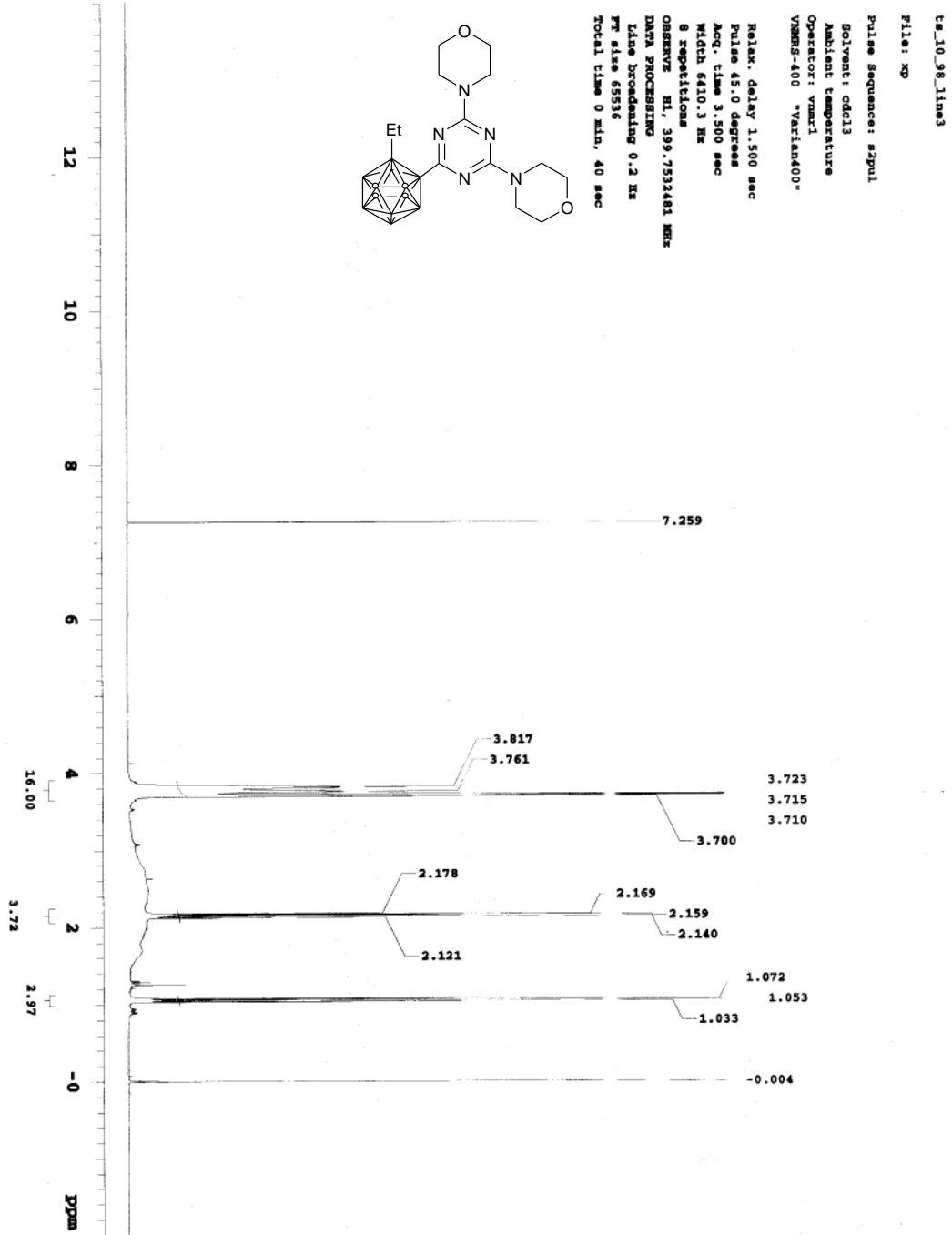
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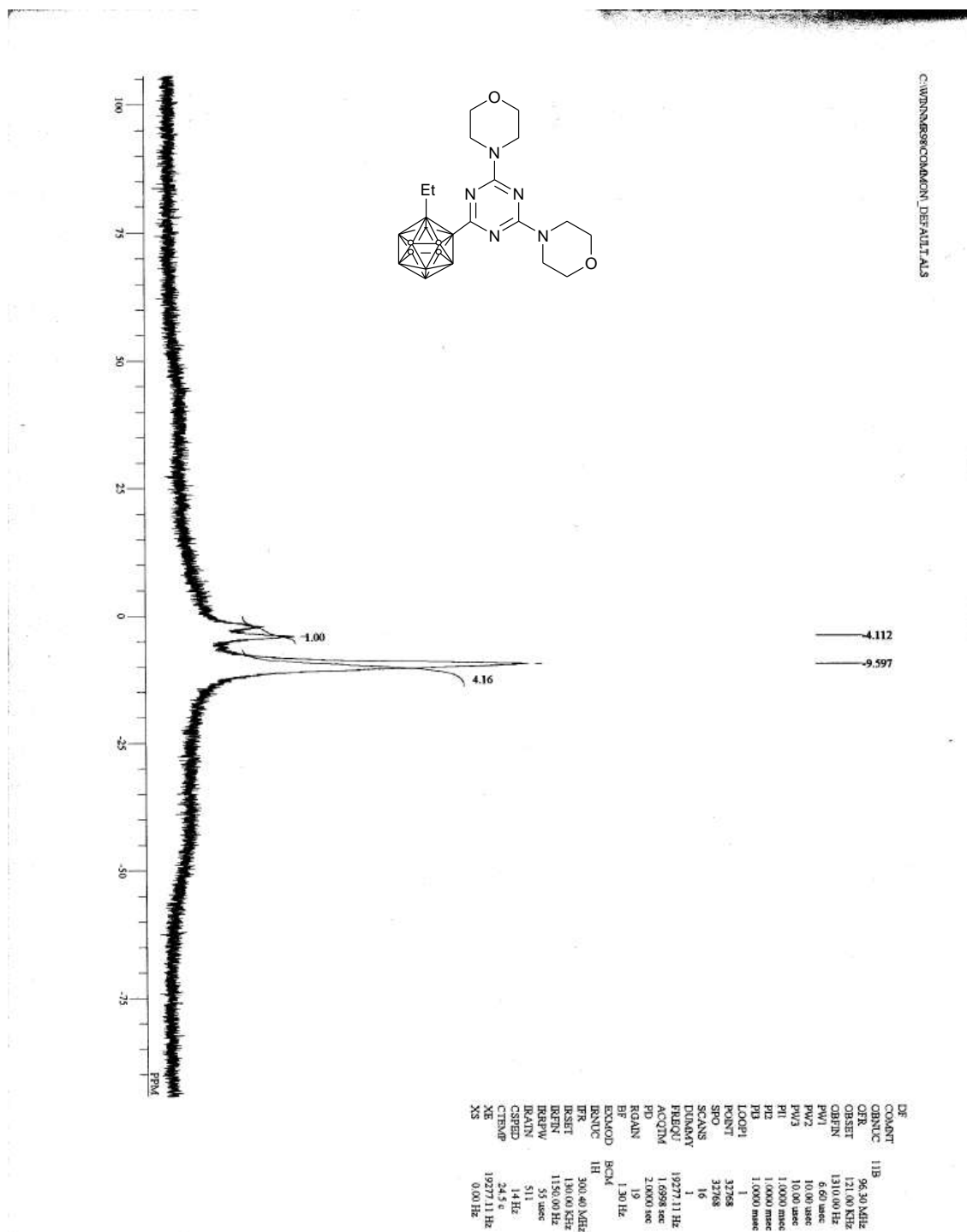
2,4-Bis-(N-morpholinyl)-6-(2-ethyl-o-carboran-1-yl)-1,3,5-triazine **4h**

<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)



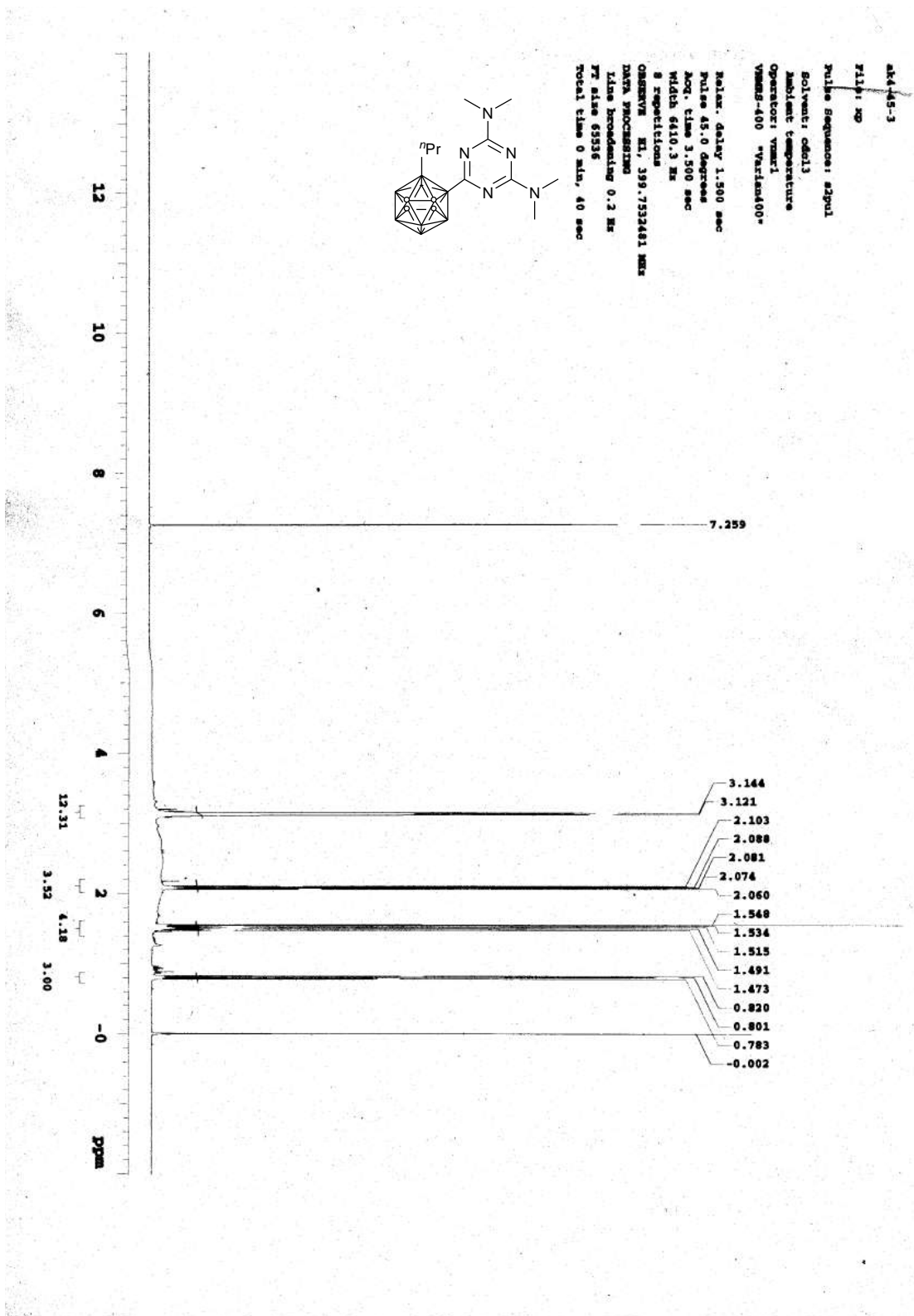
2,4-Bis-(N-morpholinyl)-6-(2-ethyl-o-carboran-1-yl)-1,3,5-triazine **4h**

$^{11}\text{B}$  NMR (96.3 MHz,  $\text{CDCl}_3$ )



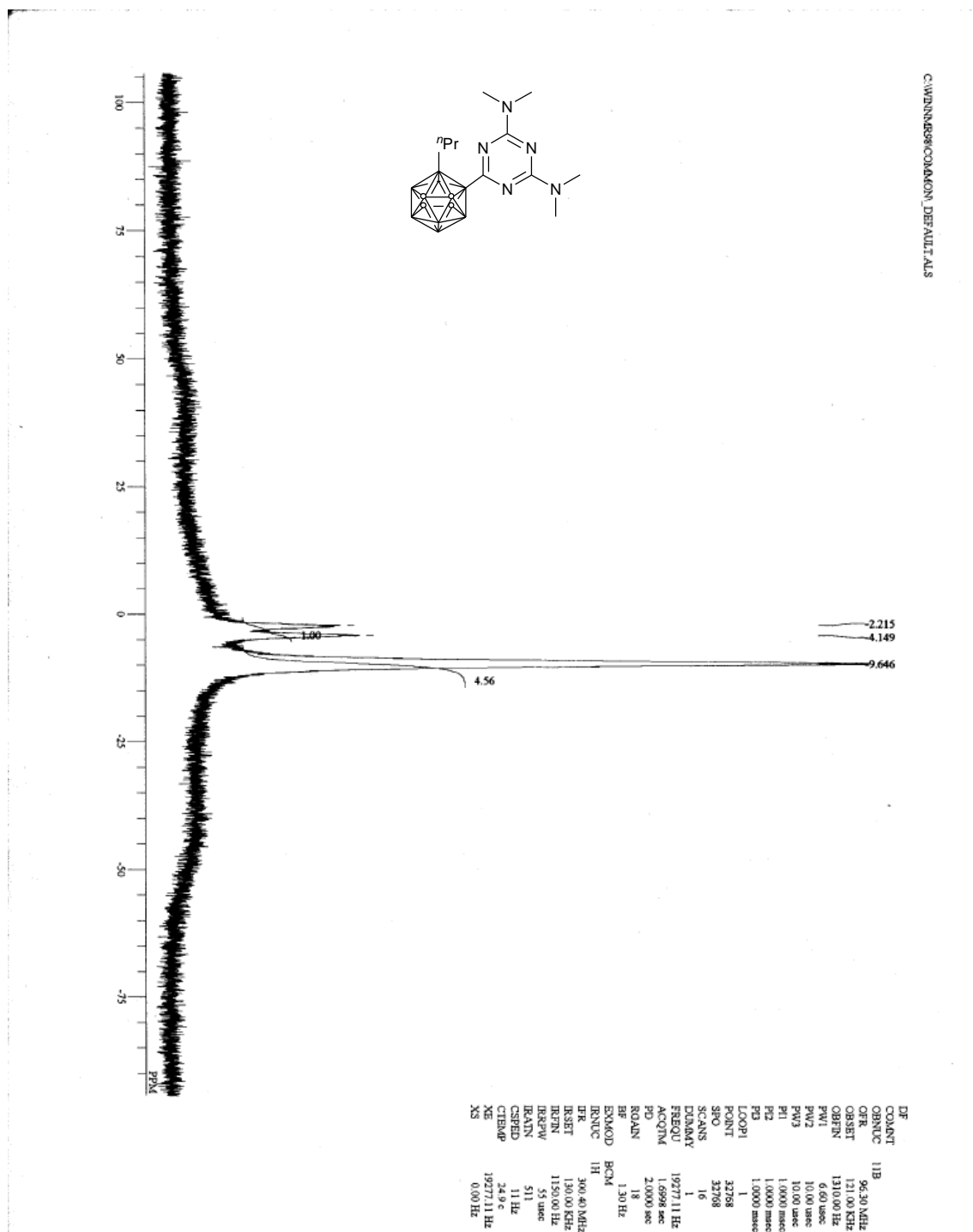
2,4-Bis(N,N-dimethylamino)-6-(2-n-propyl-o-carboran-1-yl)-1,3,5-triazine 4i

<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)



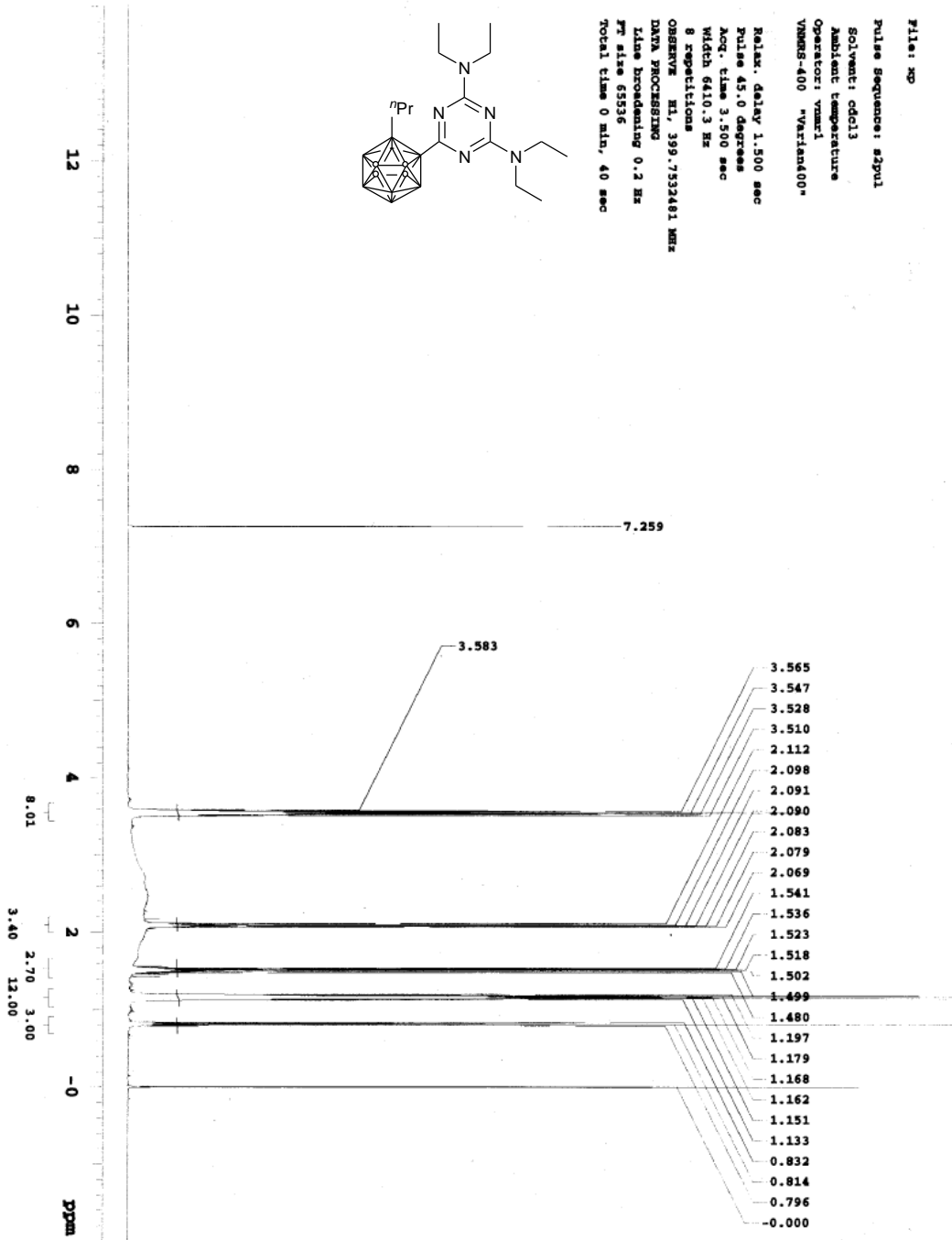
2,4-Bis(*N,N*-dimethylamino)-6-(2-*n*-propyl-*o*-carboran-1-yl)-1,3,5-triazine **4i**

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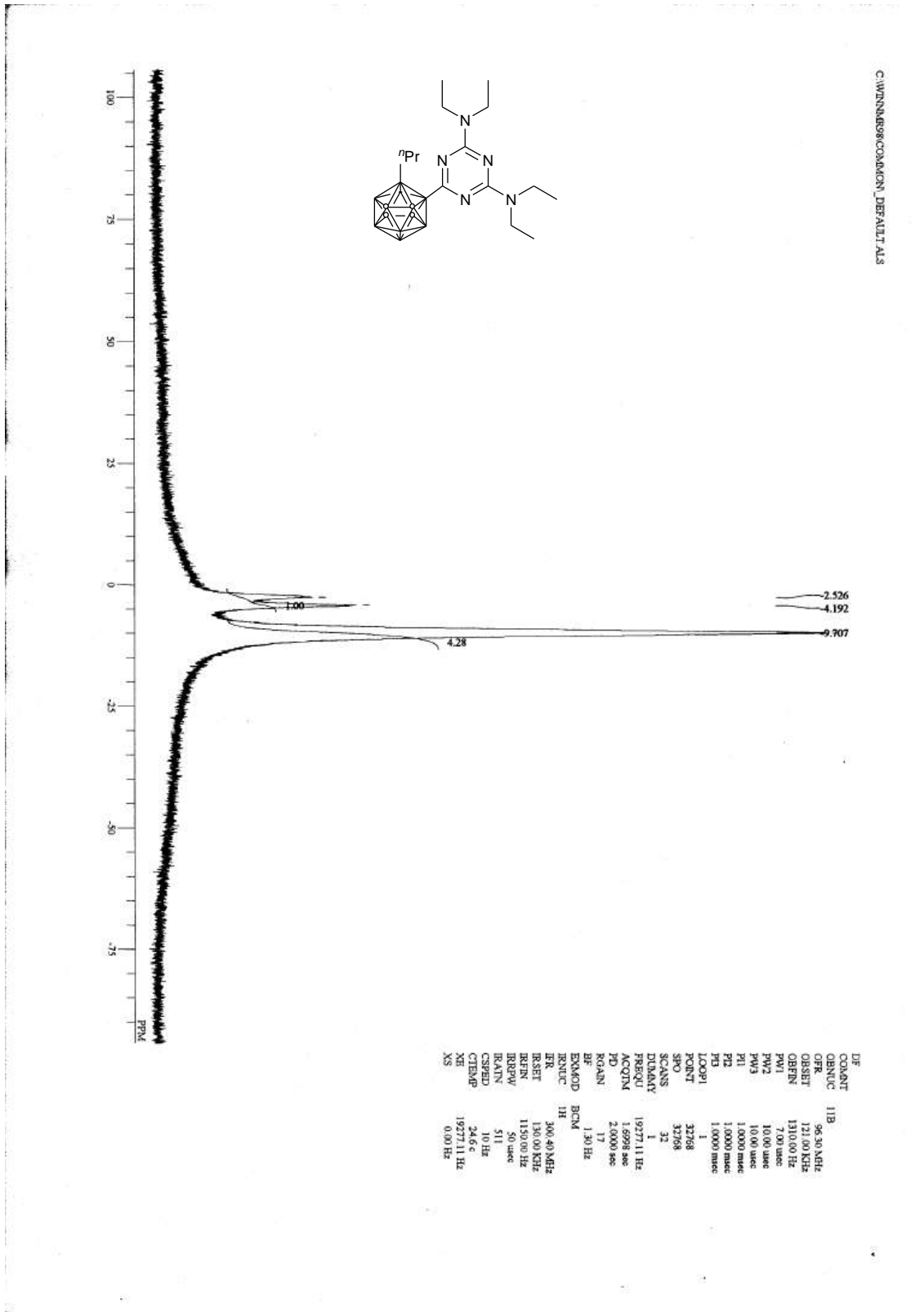
2, 4-Bis(N,N-diethylamino)-6-(2-n-propyl-o-carboran-1-yl)-1,3,5-triazine 4j

<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)



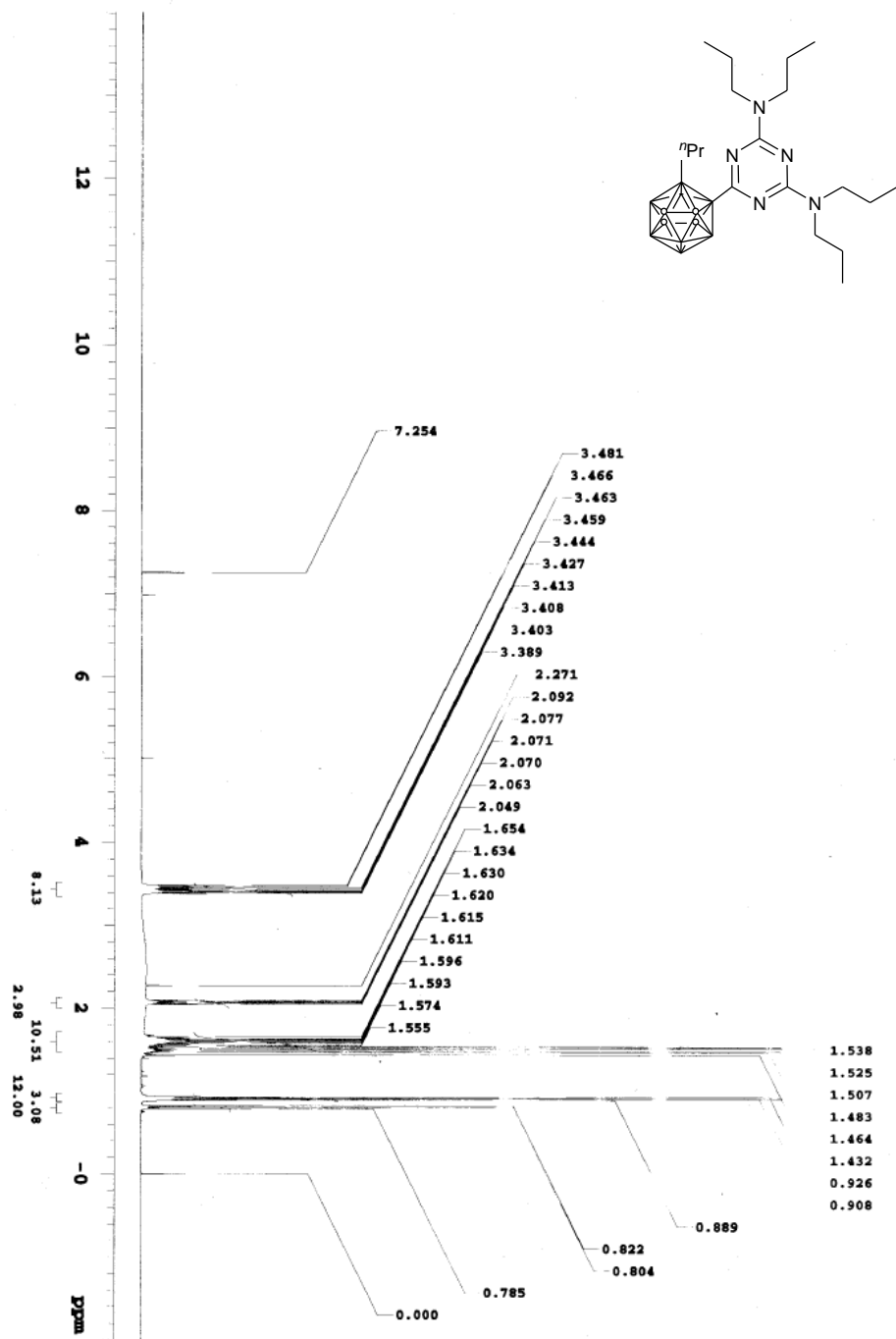
2, 4-Bis(N,N-diethylamino)-6-(2-n-propyl-o-carboran-1-yl)-1,3,5-triazine **4j**

$^{11}\text{B}$  NMR (96.3 MHz,  $\text{CDCl}_3$ )



2,4-Bis(N,N-n-propylamino)-6-(2-n-propyl-o-carboran-1-yl)-1,3,5-triazine **4k**

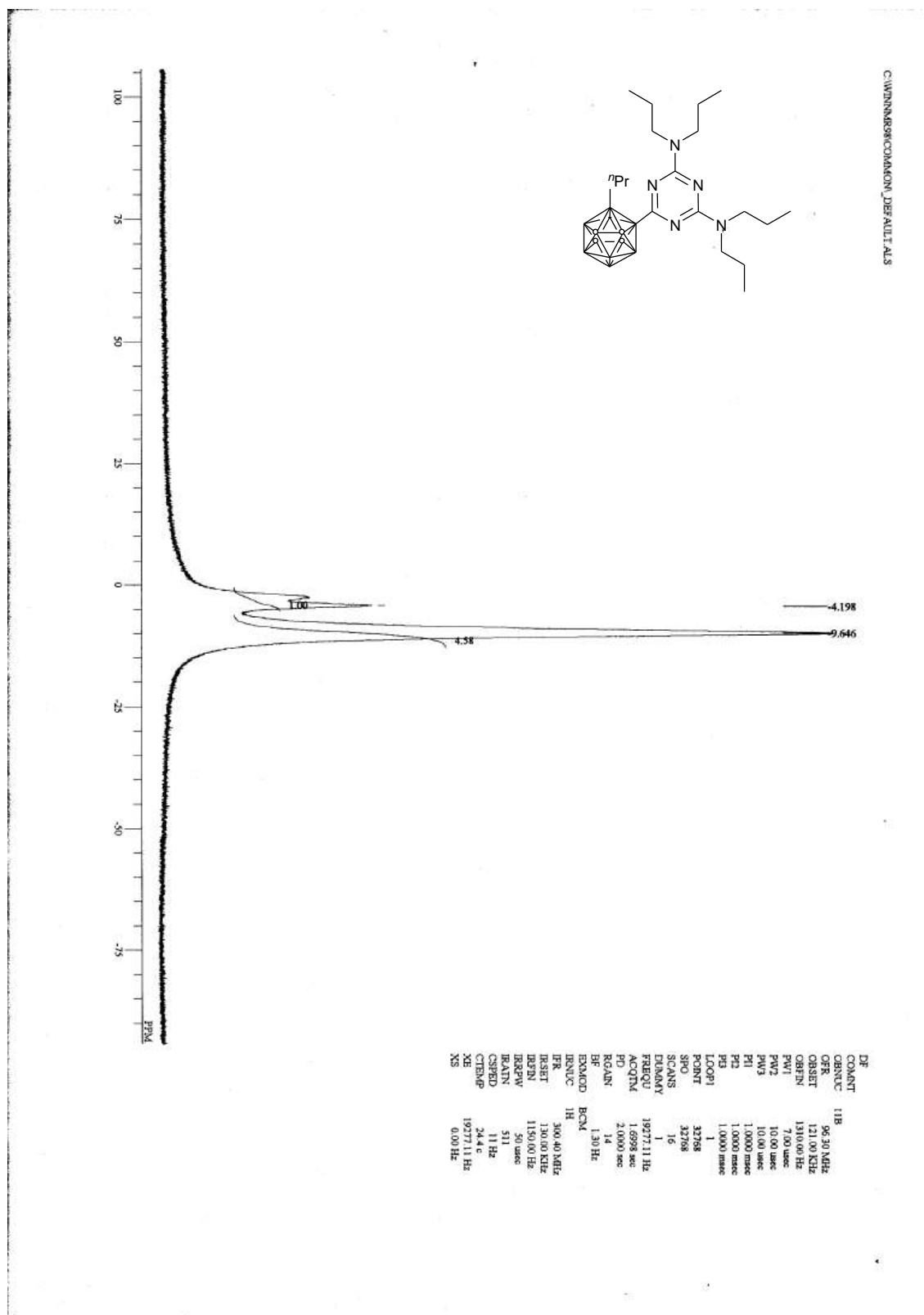
$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )



20110409\_14527\_13C  
File: xp  
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2,4-Bis(*N,N*-*n*-propylamino)-6-(2-*n*-propyl-*o*-carboran-1-yl)-1,3,5-triazine **4k**

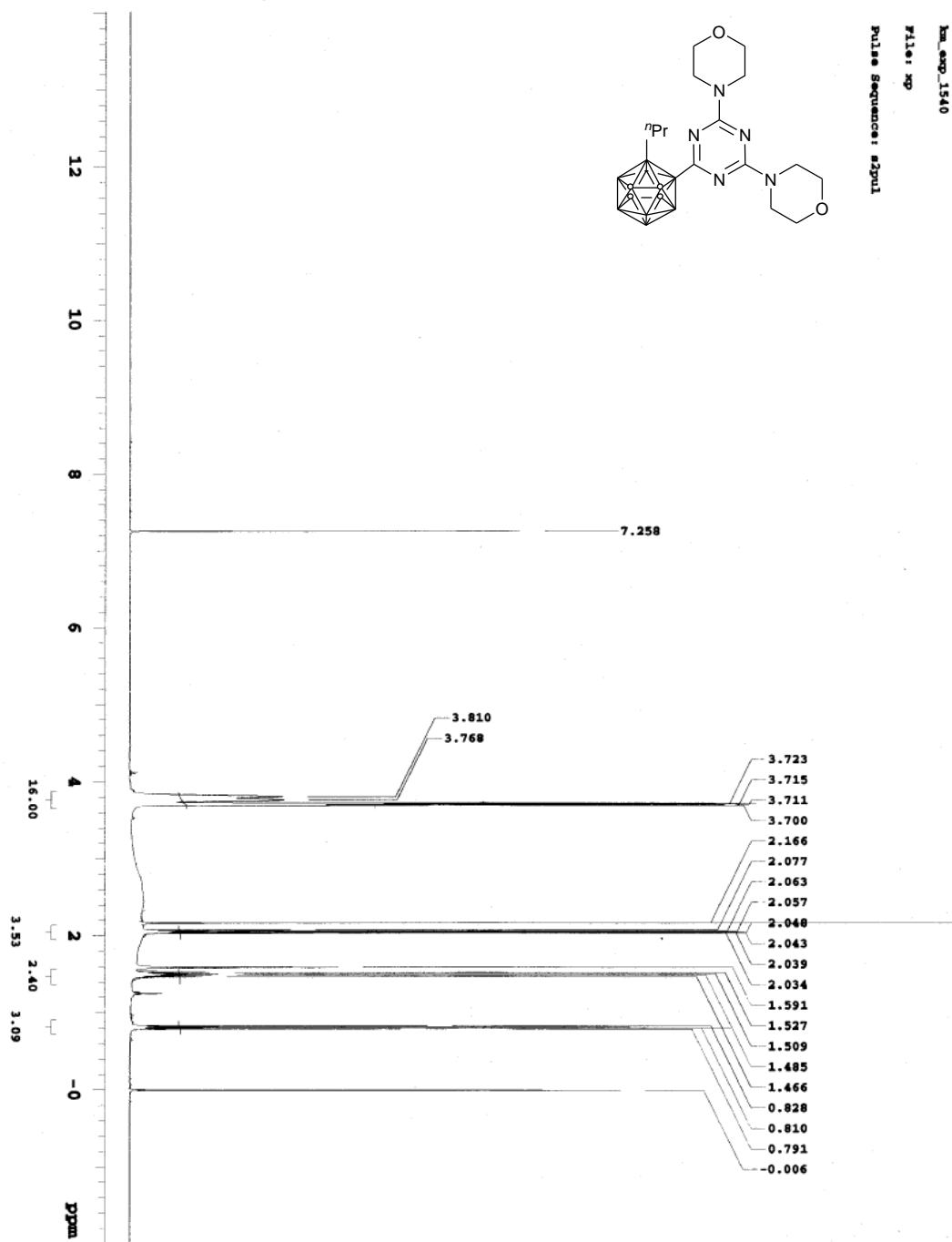
$^{11}\text{B}$  NMR (96.3 MHz,  $\text{CDCl}_3$ )





2,4-Bis-(N-morpholinyl)-6-(2-n-propyl-o-carboran-1-yl)-1,3,5-triazine **4l**

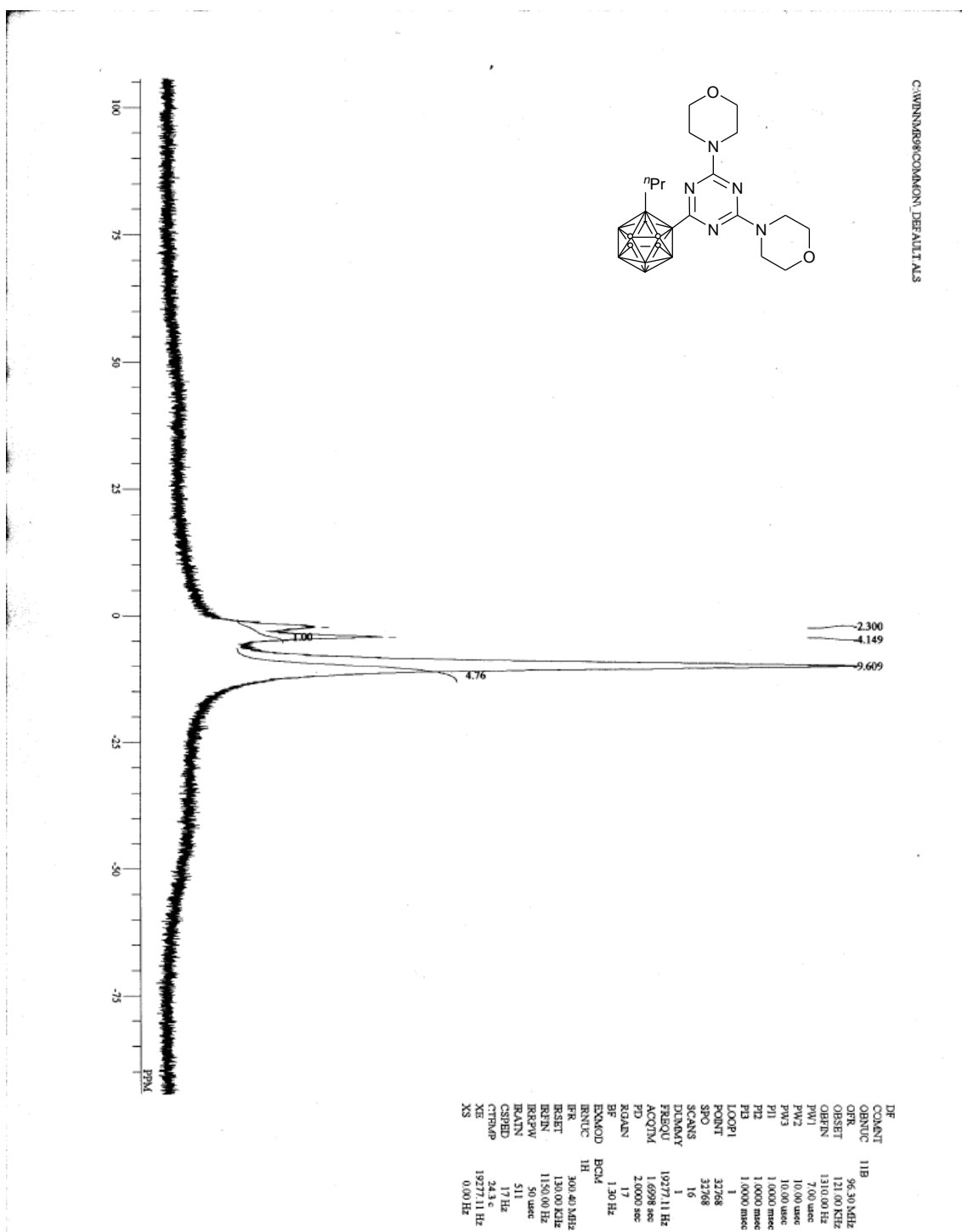
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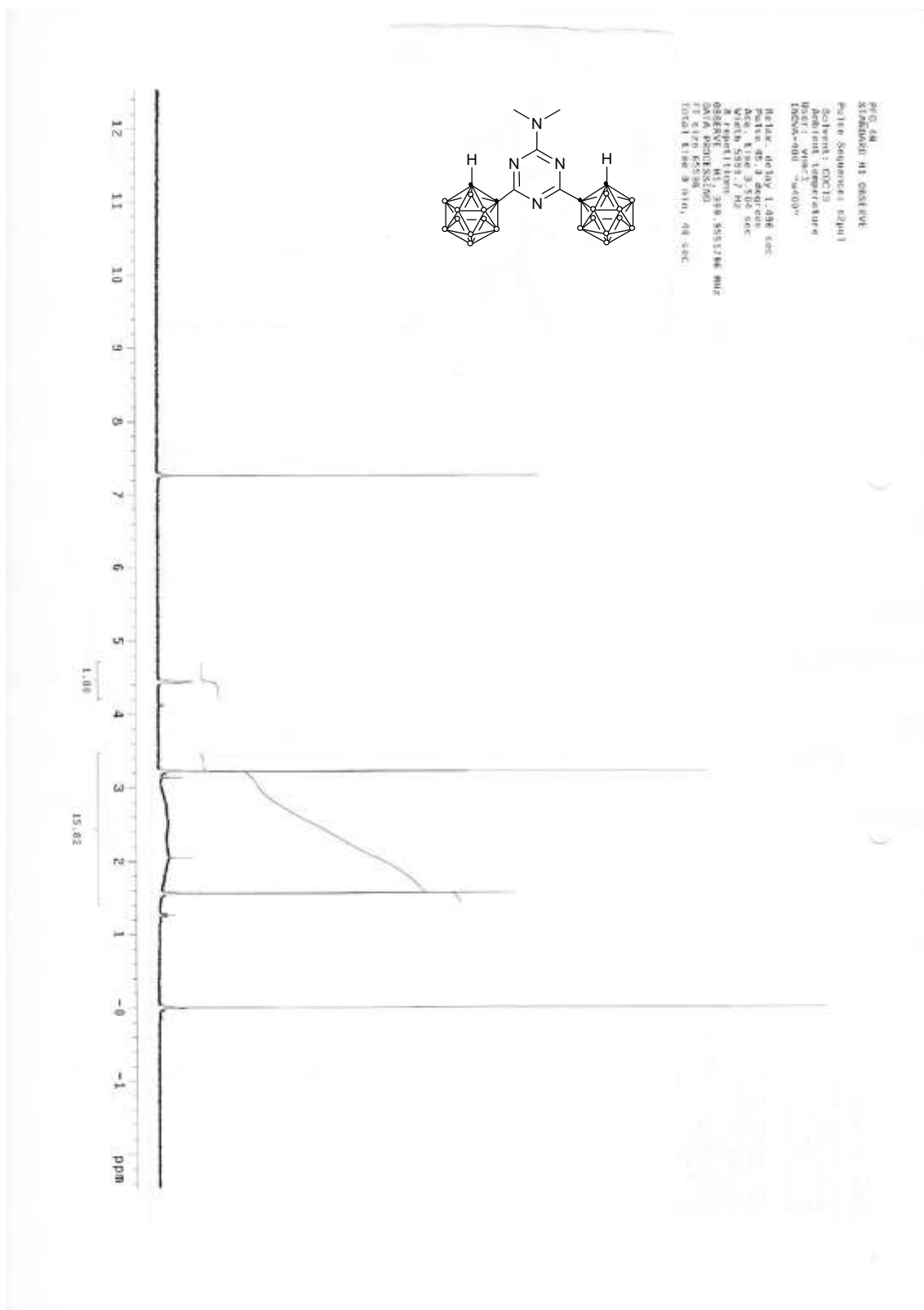
2,4-Bis-(N-morpholinyl)-6-(2-n-propyl-o-carboran-1-yl)-1,3,5-triazine **4l**

$^{11}\text{B}$  NMR (96.3 MHz,  $\text{CDCl}_3$ )



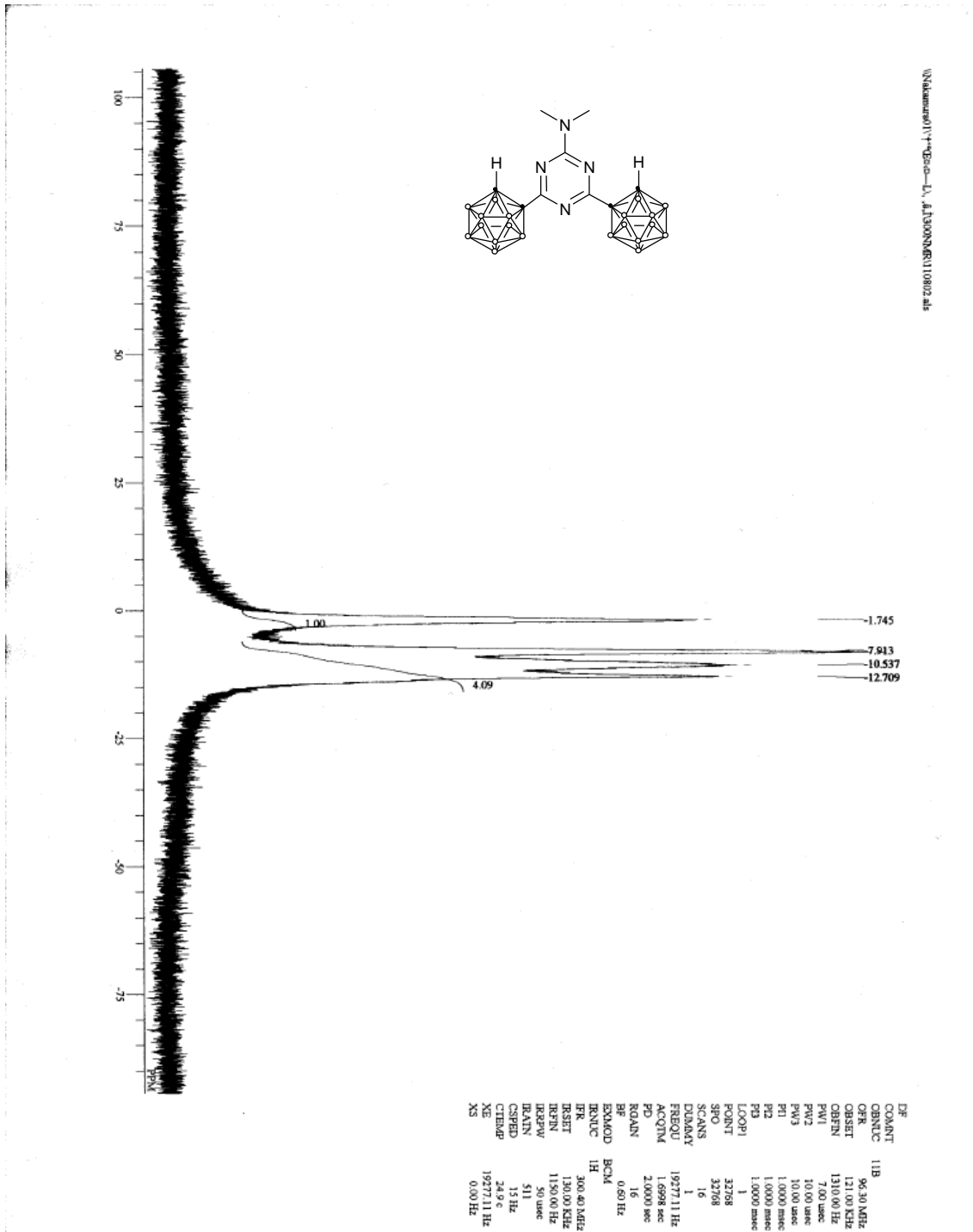
2,4-Bis(*o*-carboran-1-yl)-6-(*N,N*-dimethylamino)-1,3,5-triazine **6a**

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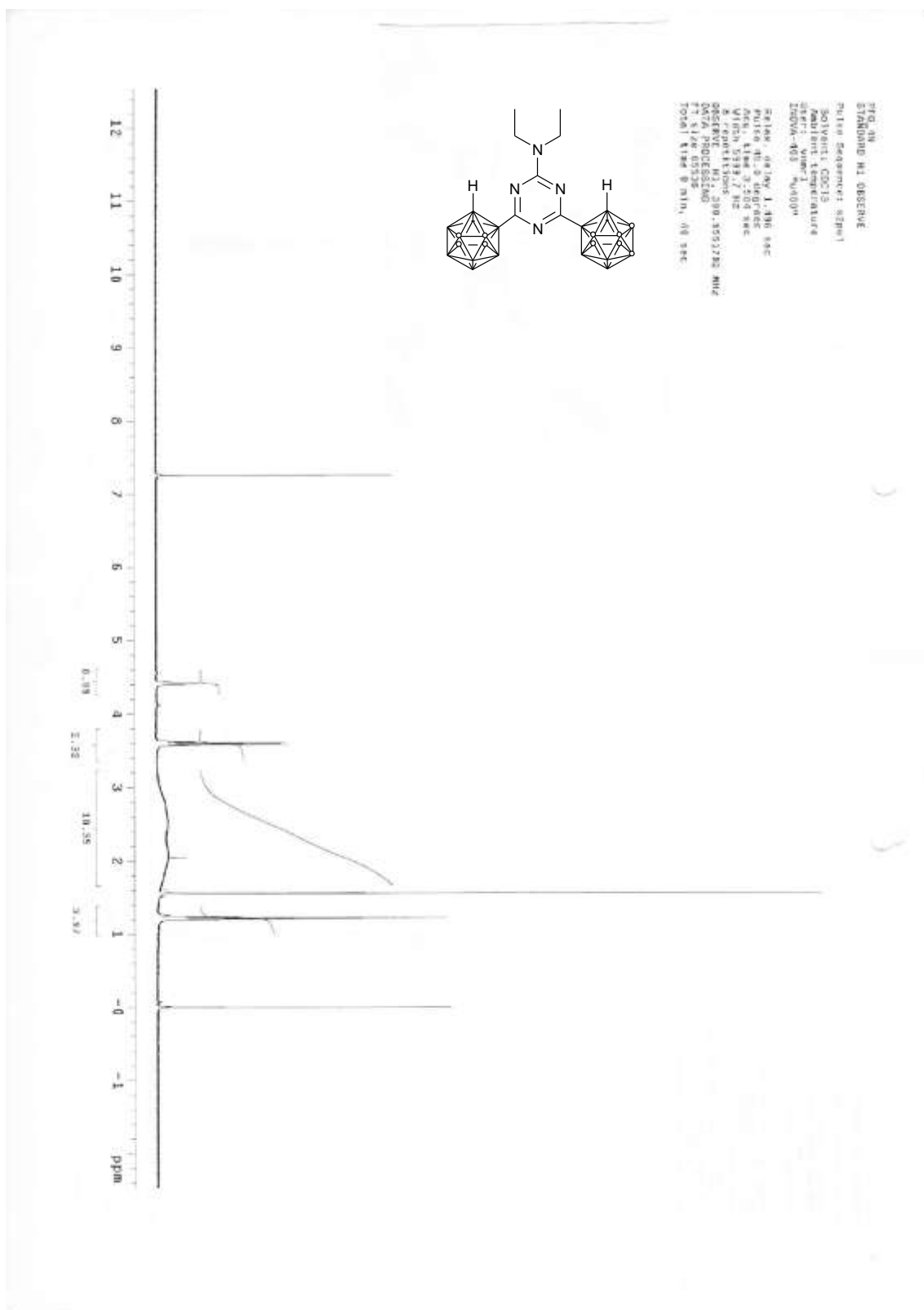
2,4-Bis(*o*-carboran-1-yl)-6-(*N,N*-dimethylamino)-1,3,5-triazine **6a**

$^{11}\text{B}$  NMR (96.3 MHz,  $\text{CDCl}_3$ )



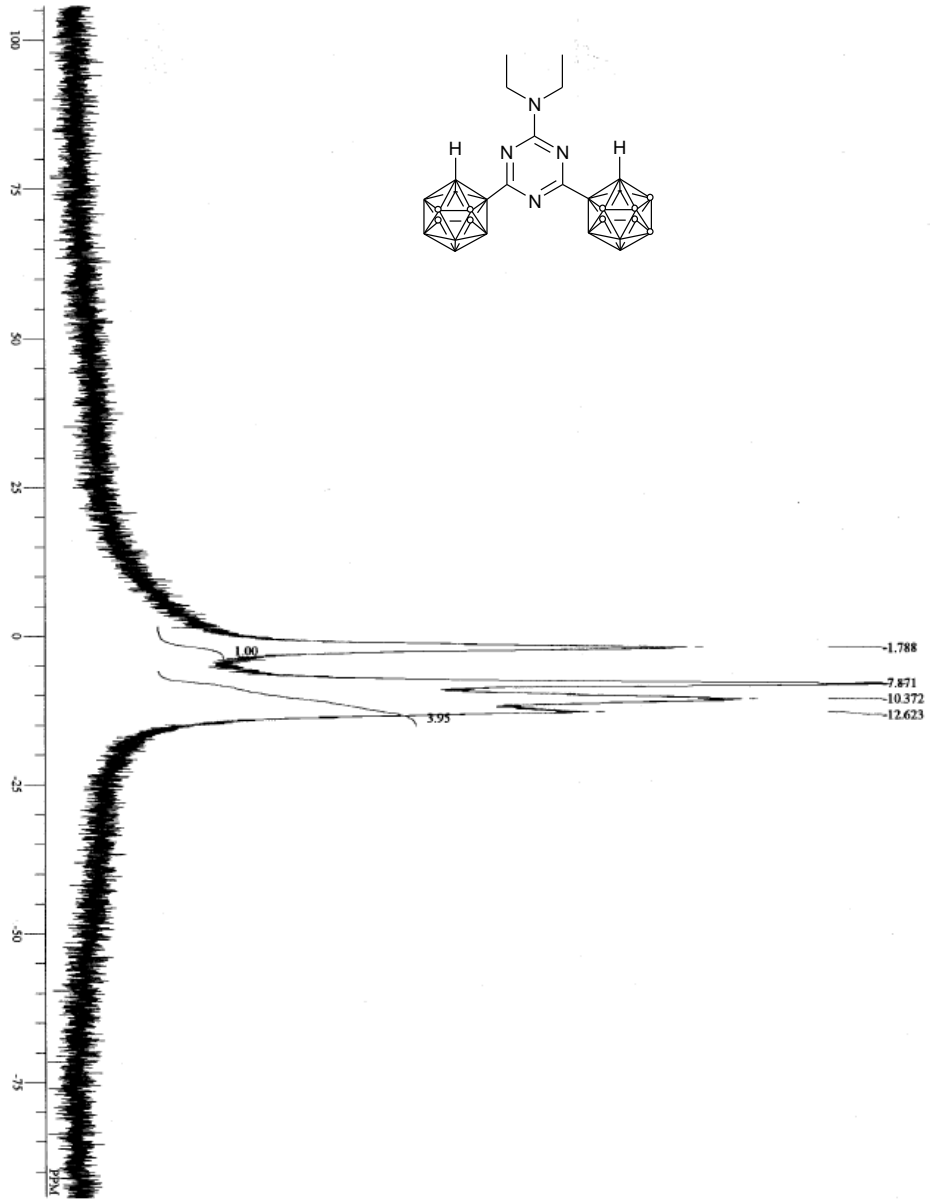
2, 4-Bis(o-Carboran-1-yl)-6-(N, N-diethylamino) -1, 3, 5-triazine **6b**

<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)



2, 4-Bis(*o*-Carboran-1-yl)-6-(*N,N*-diethylamino)-1, 3, 5-triazine **6b**

$^{11}\text{B}$  NMR (96.3 MHz,  $\text{CDCl}_3$ )



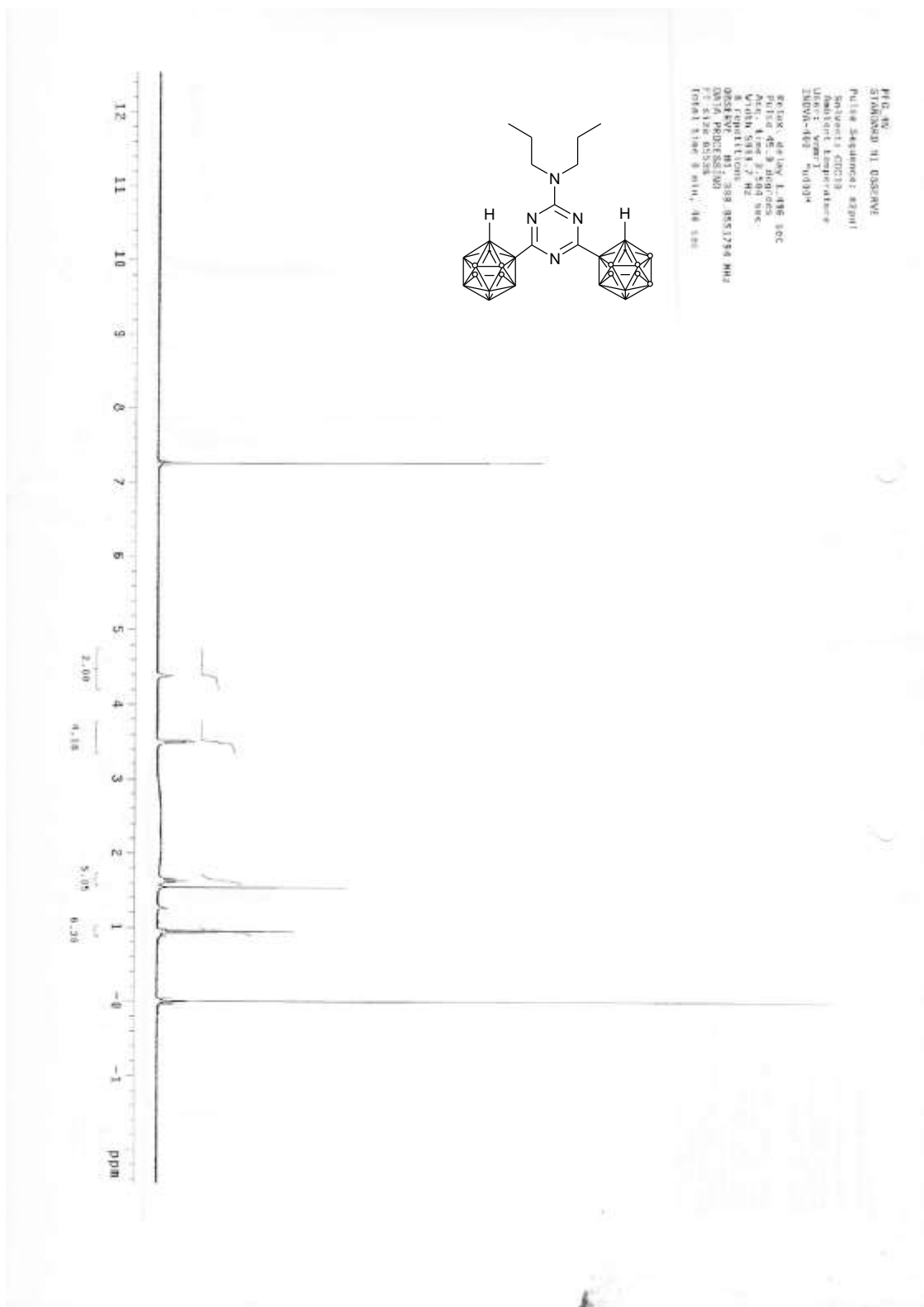
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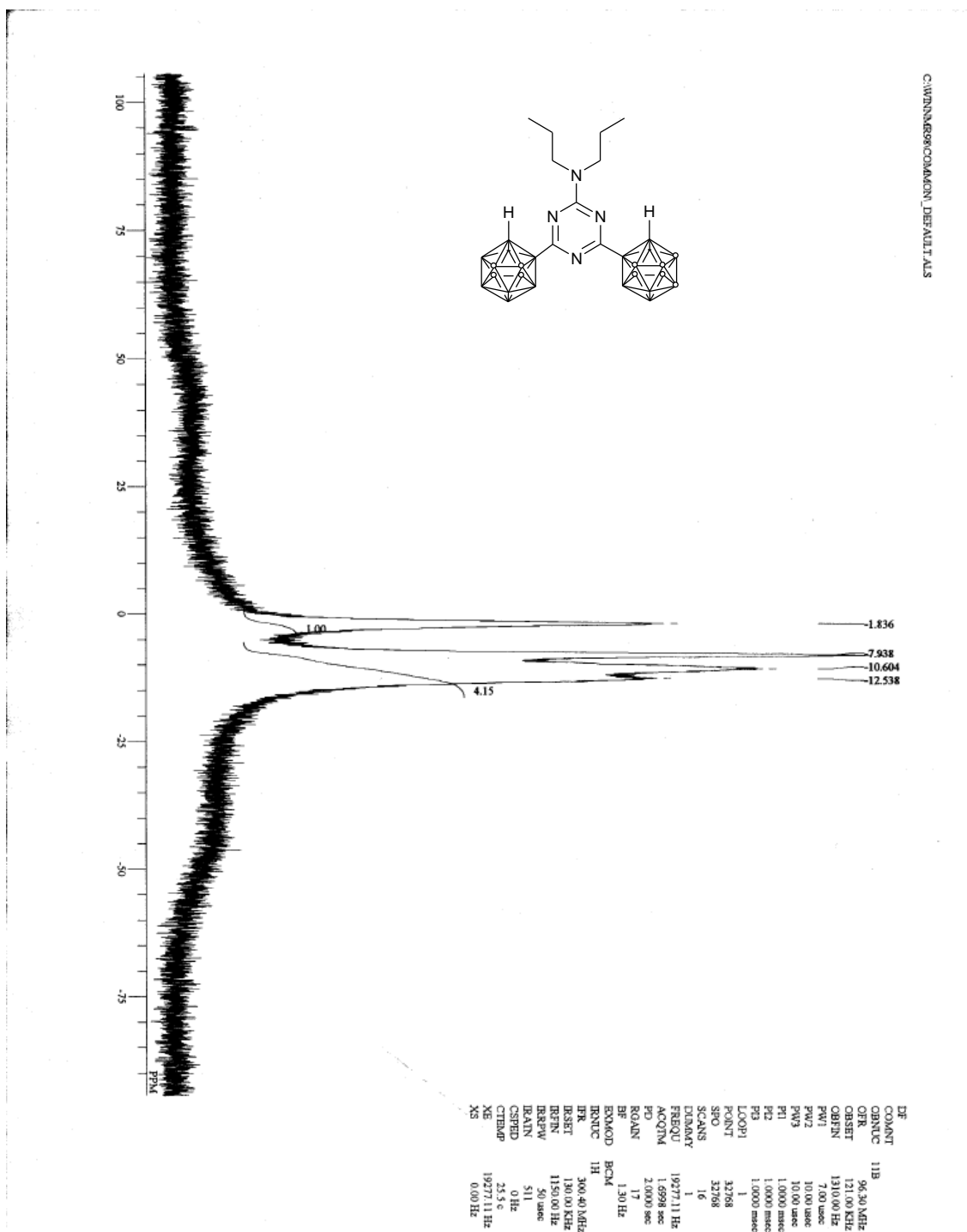
2, 4-Bis(*o*-Carboran-1-yl)-6-(*N,N*-di-*n*-propylamino) -1, 3, 5-triazine **6c**

$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )



2, 4-Bis(*o*-Carboran-1-yl)-6-(*N,N*-di-*n*-propylamino)-1, 3, 5-triazine **6c**

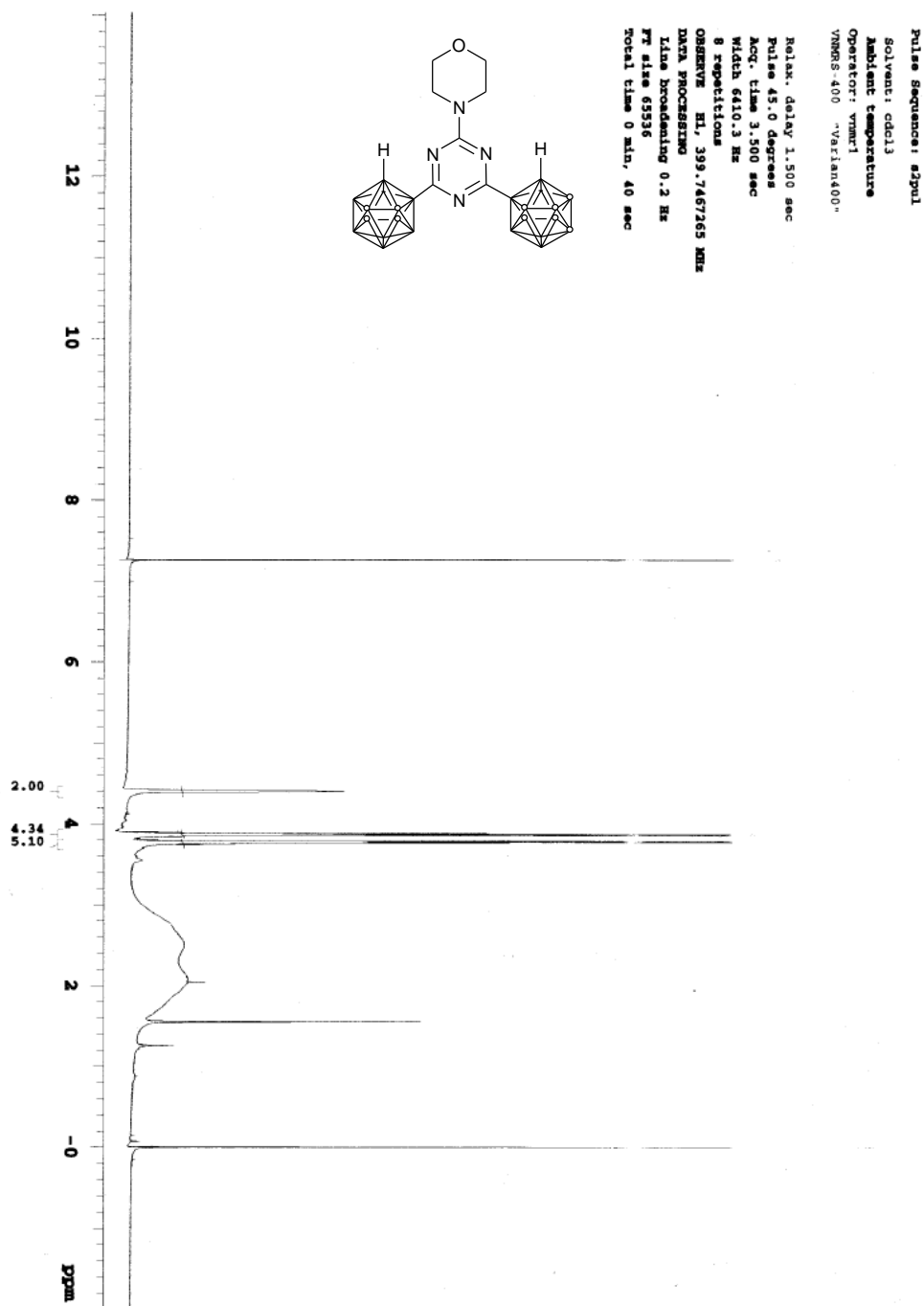
$^{11}\text{B}$  NMR (96.3 MHz,  $\text{CDCl}_3$ )





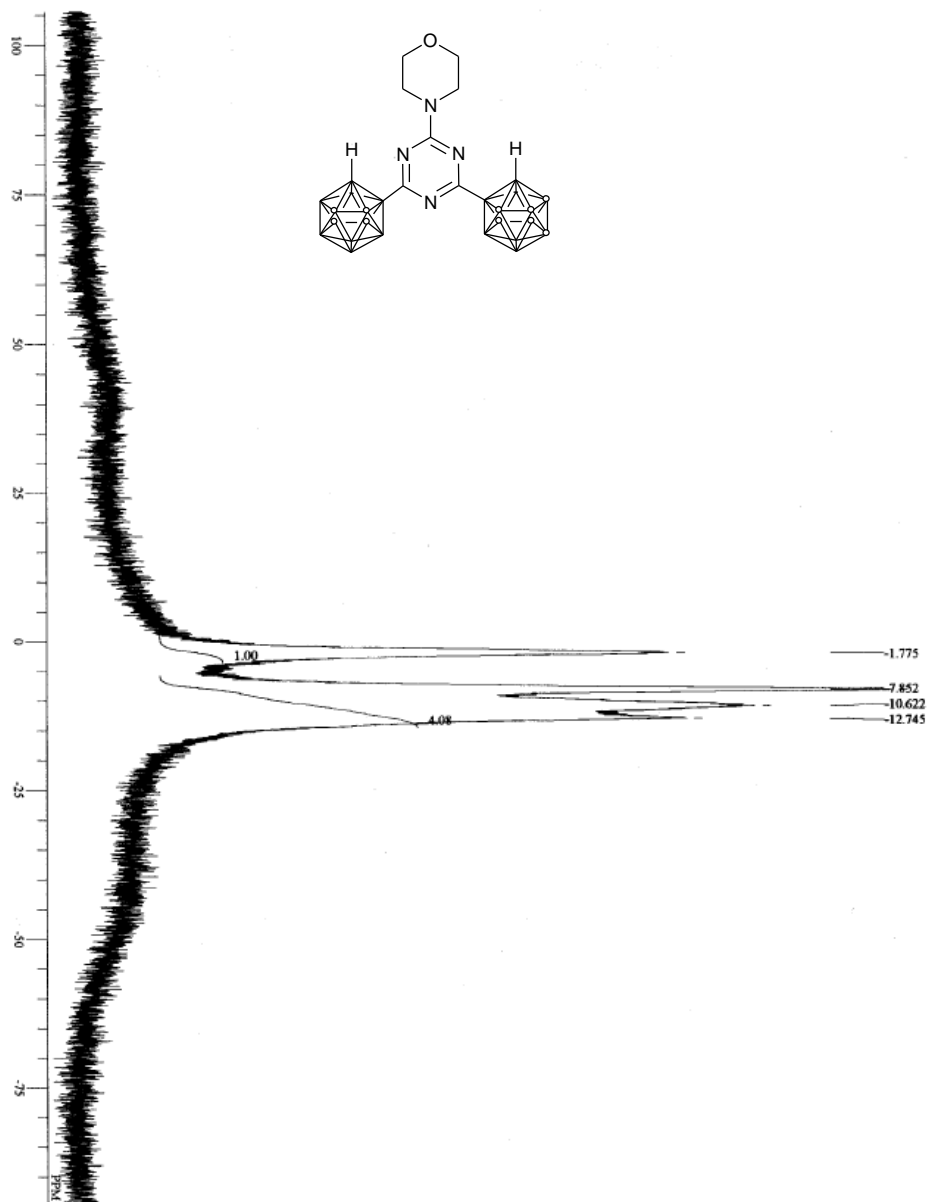
2, 4-Bis(o-Carboran-1-yl)-6-(N-morpholinyl) -1, 3, 5-triazine **6d**

$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )



2, 4-Bis(o-Carboran-1-yl)-6-(N-morpholinyl)-1, 3, 5-triazine **6d**

$^{11}\text{B}$  NMR (96.3 MHz,  $\text{CDCl}_3$ )

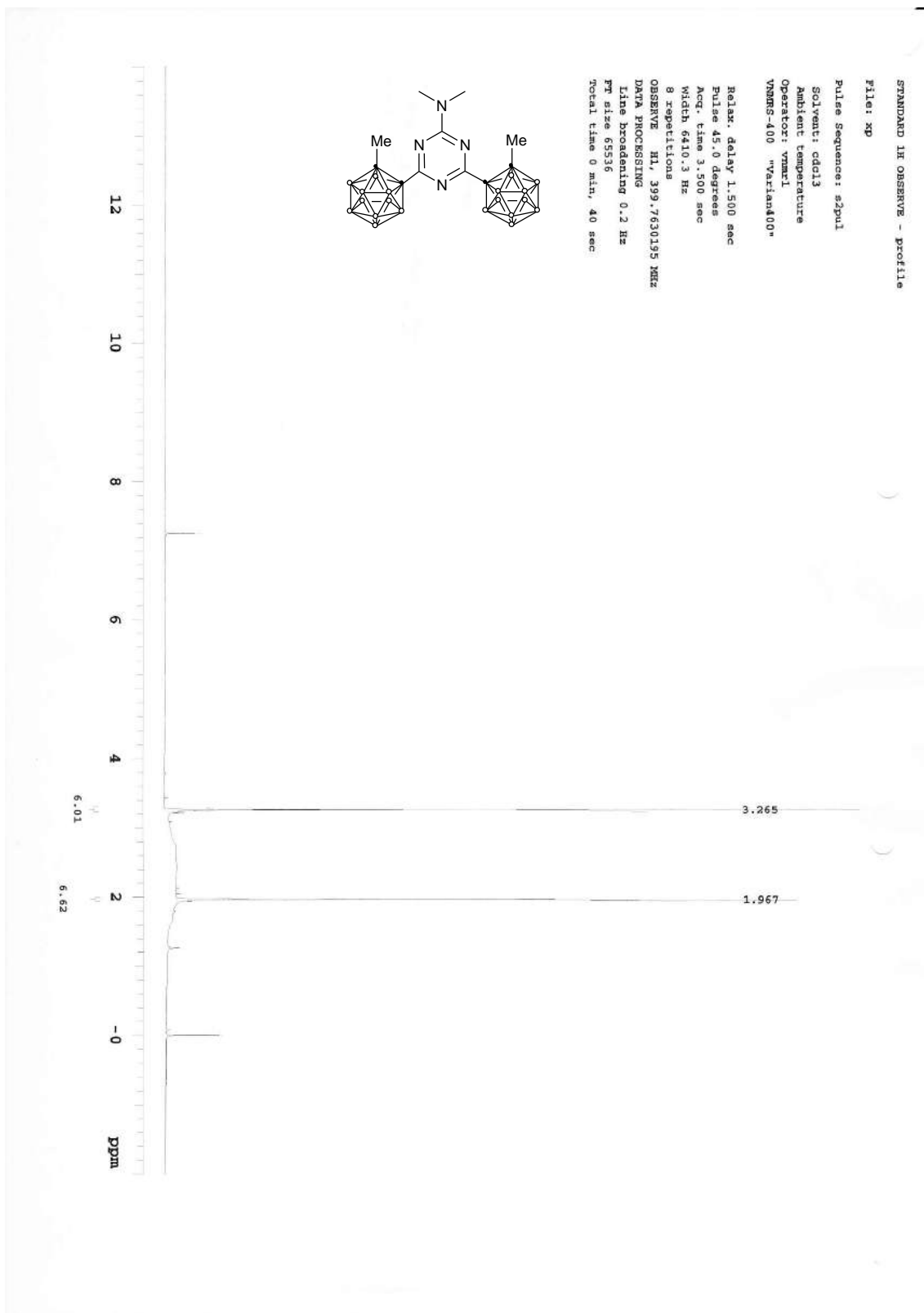


\\slchem001\1\96303-11\_113001\NMR\37075.dls

DE	CONT	11B
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OPR	121.00 KHz	
ORSET	1310.00 Hz	
CBFIN	7.00 usec	
PW1	10.00 usec	
PW2	10.00 usec	
PW3	10.00 usec	
P1	1.0000 msec	
P2	1.0000 msec	
P3	1.0000 msec	
LOOP1	1	
POINT	32768	
SFO	32768	
SCANS	16	
DUNAVY		
FREQ1	19277111 Hz	
PRGCU	1.6598 sec	
ACQTM	2.0000 sec	
PD	17	
RGAIN	1.30 Hz	
HF		
EXMOD	BCM	
IRNUC	HF	
IFR	300.40 MHz	
RSET	130.00 KHz	
IRFIN	1150.00 Hz	
RRPW	50 usec	
RATN	511	
CPED	13 Hz	
CTEMP	24.9 c	
XE	19277111 Hz	
XS	0.00 Hz	

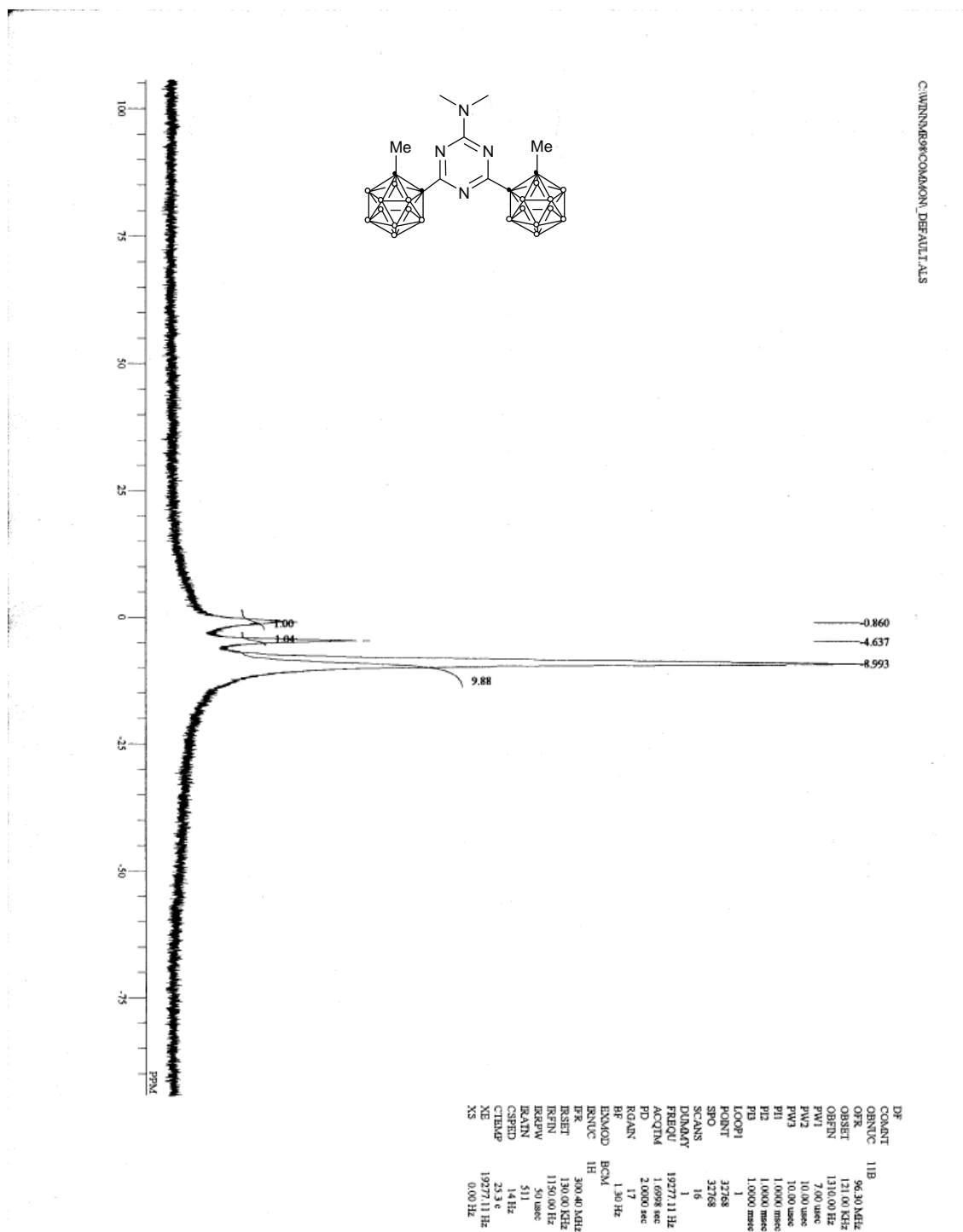
2, 4-Bis (2-methyl-o-carboran-1-yl) -6-(N,N-dimethylamino)- 1, 3, 5-triazine 7a

<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)



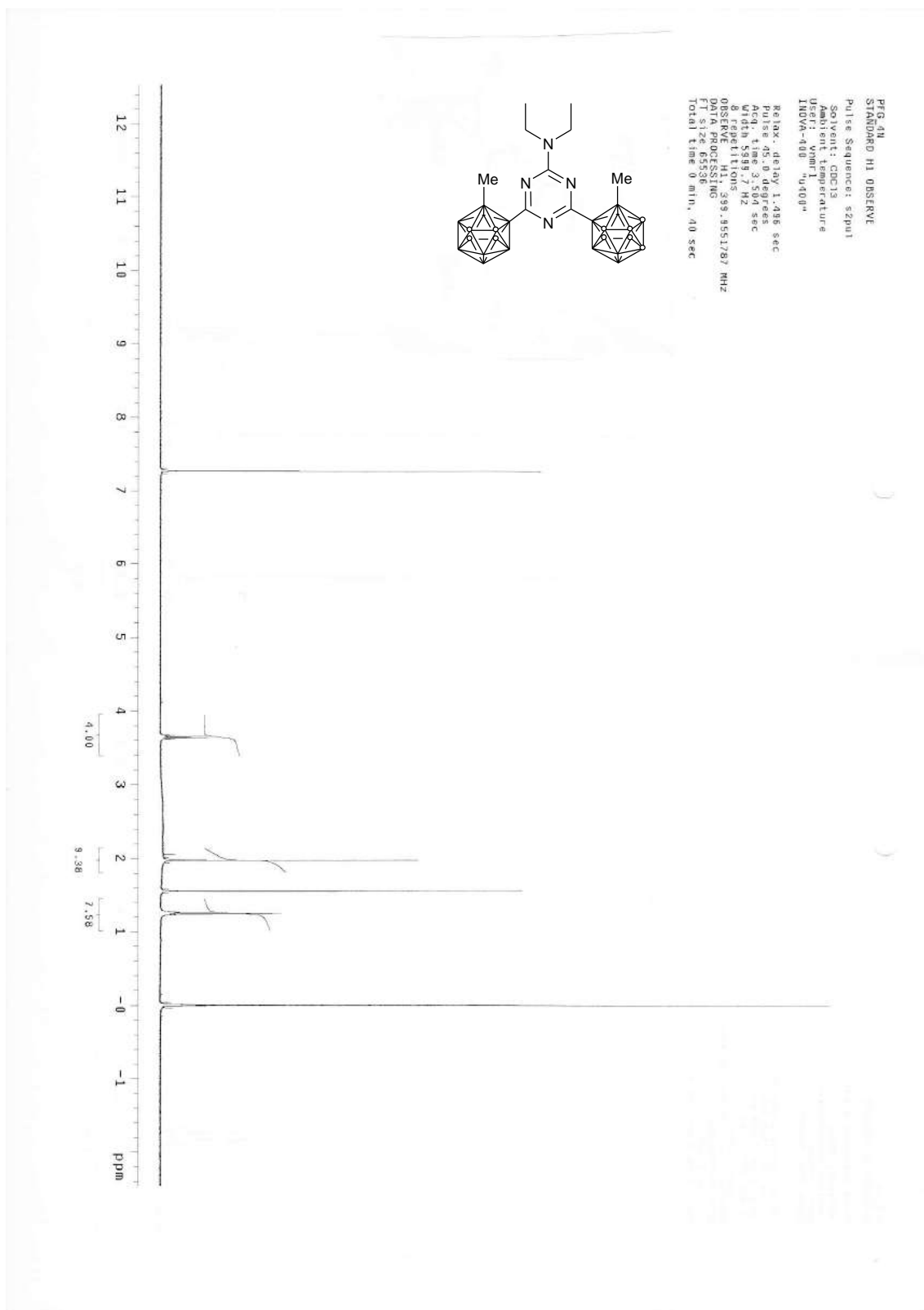
2, 4-Bis (2-methyl-o-carboran-1-yl) -6-(N,N-dimethylamino)- 1, 3, 5-triazine **7a**

$^{11}\text{B}$  NMR (96.3 MHz,  $\text{CDCl}_3$ )



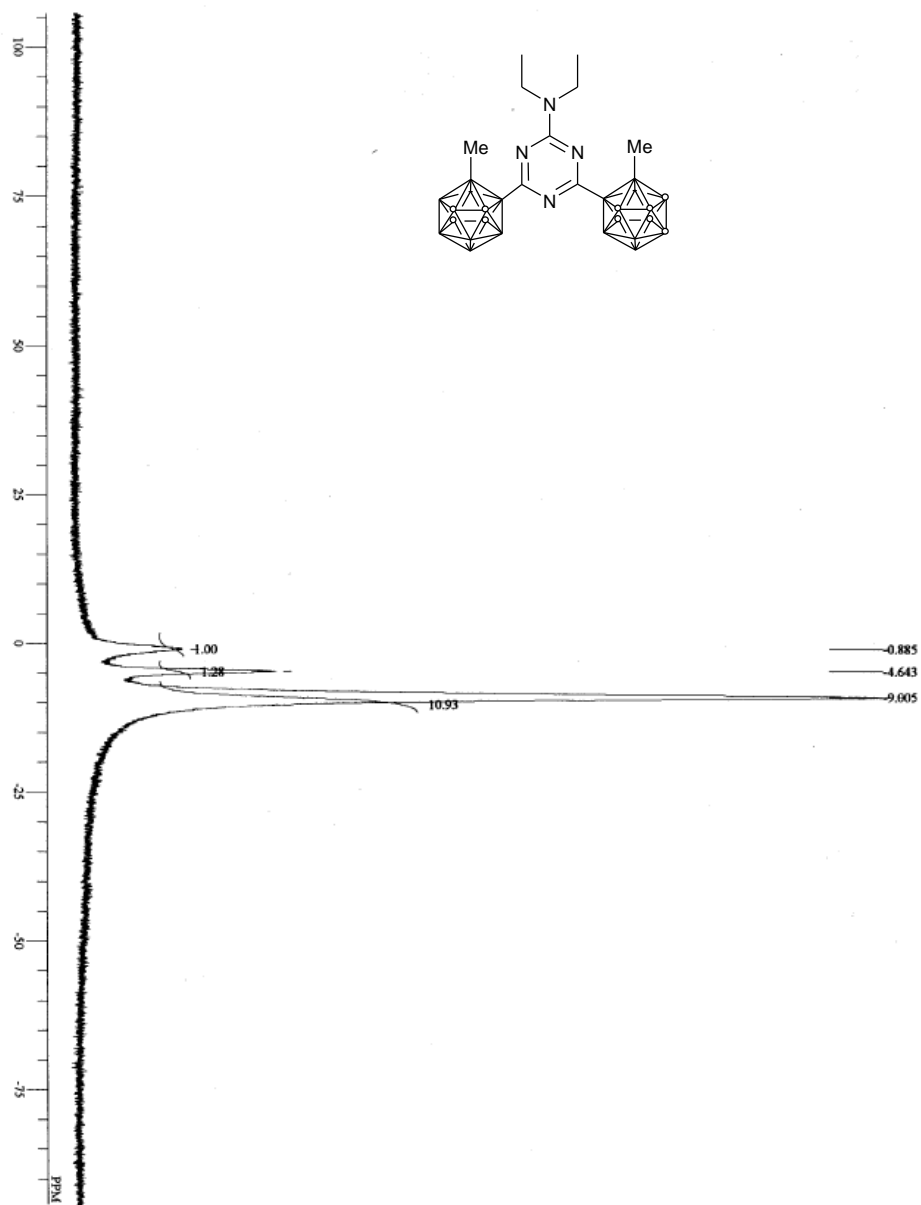
2, 4-Bis (2-methyl-o-carboran-1-yl) -6-(N,N-diethylamino)- 1, 3, 5-triazine **7b**

$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )



2, 4-Bis (2-methyl-o-carboran-1-yl) -6-(N,N-diethylamino)- 1, 3, 5-triazine **7b**

$^{11}\text{B}$  NMR (96.3 MHz,  $\text{CDCl}_3$ )

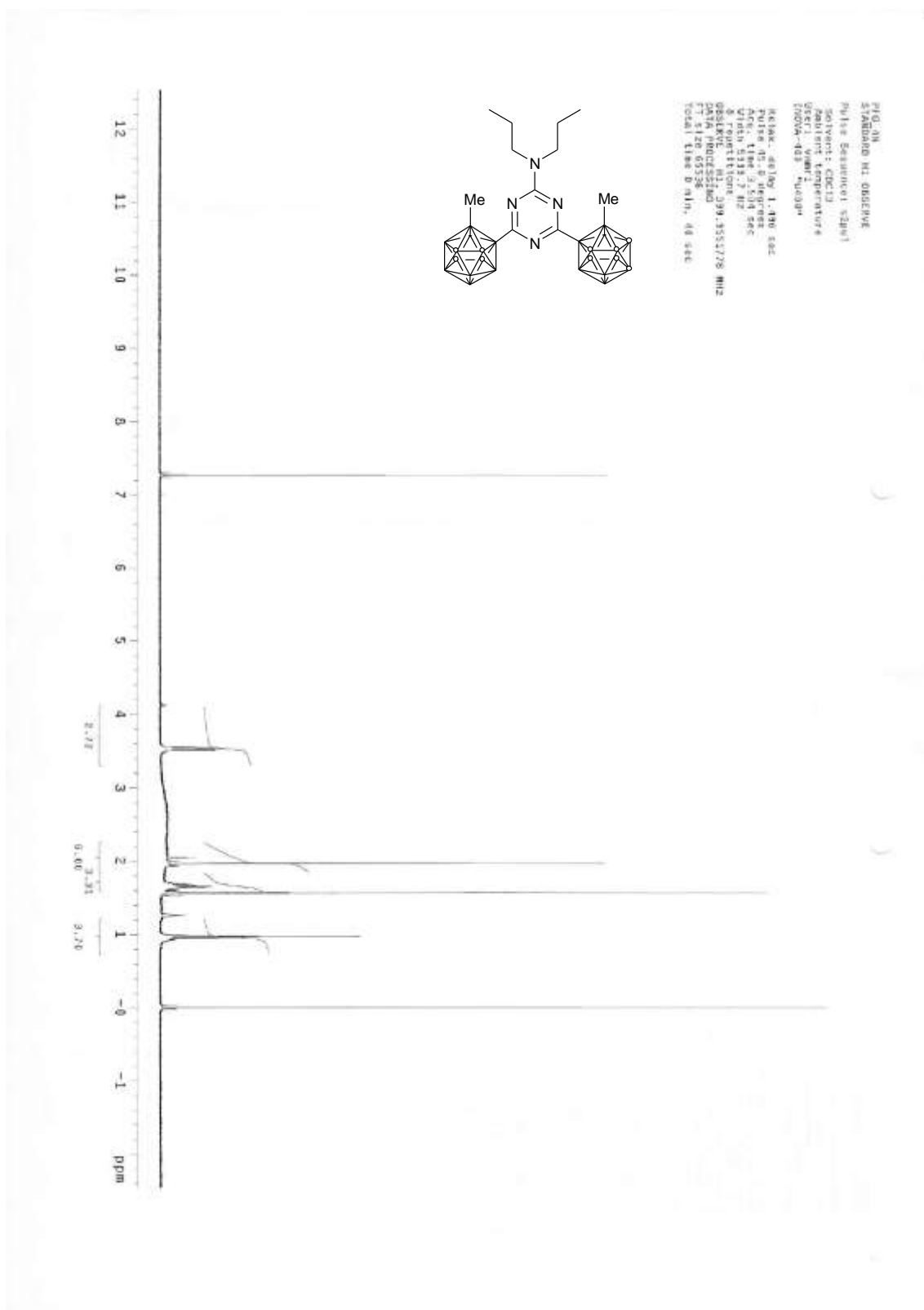


CHINNERS@COMACON\_DEFAULT.ILS

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OBNUC 96.30 MHz  
OPR 121.00 KHz  
OBSET 1310.00 Hz  
OBFIN 7.00 usec  
PWI 10.00 usec  
PW2 10.00 usec  
PWI 10.00 usec  
PPI 1.0000 msec  
PPI 1.0000 msec  
PPI 1.0000 msec  
LOOP1 1  
POINT 32768  
SFO 32768  
SCANS 16  
DUMAY 1  
FREQU 19777.11 Hz  
PREG 1.6698 sec  
ACQTM 2.0000 sec  
PD 16  
RGAIN 1.30 Hz  
BF  
EXMOD BCM  
ENVC IH  
FIR 300.40 MHz  
IRSET 130.00 KHz  
IRFIR 1150.00 Hz  
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XE 19777.11 Hz  
XS 0.00 Hz

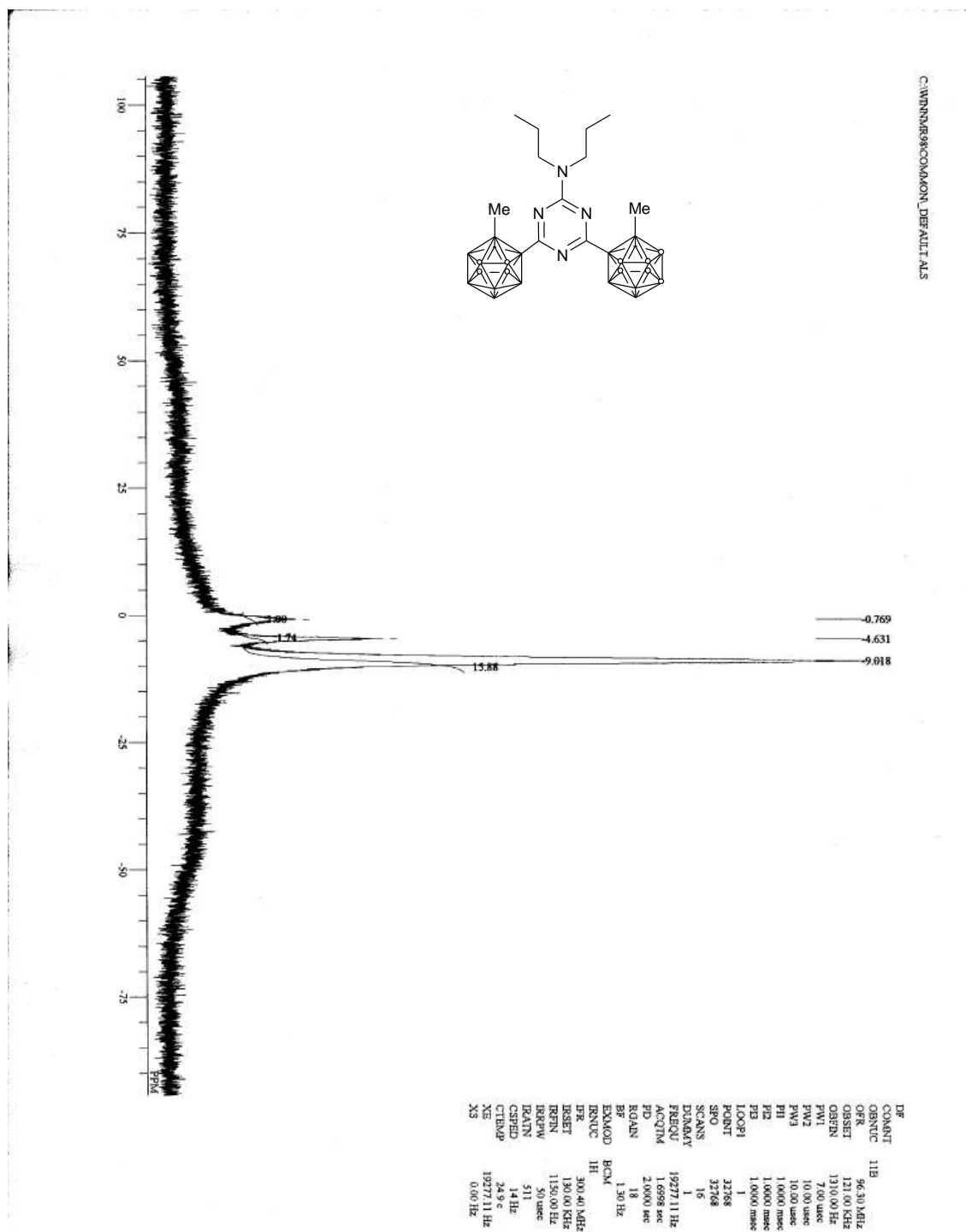
2, 4-Bis(2-methyl-o-carboran-1-yl) -6-(N,N-di-n-propylamino)- 1, 3, 5-triazine 7c

$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )



2, 4-Bis(2-methyl-o-carboran-1-yl) -6-(N,N-di-n-propylamino)- 1, 3, 5-triazine 7c

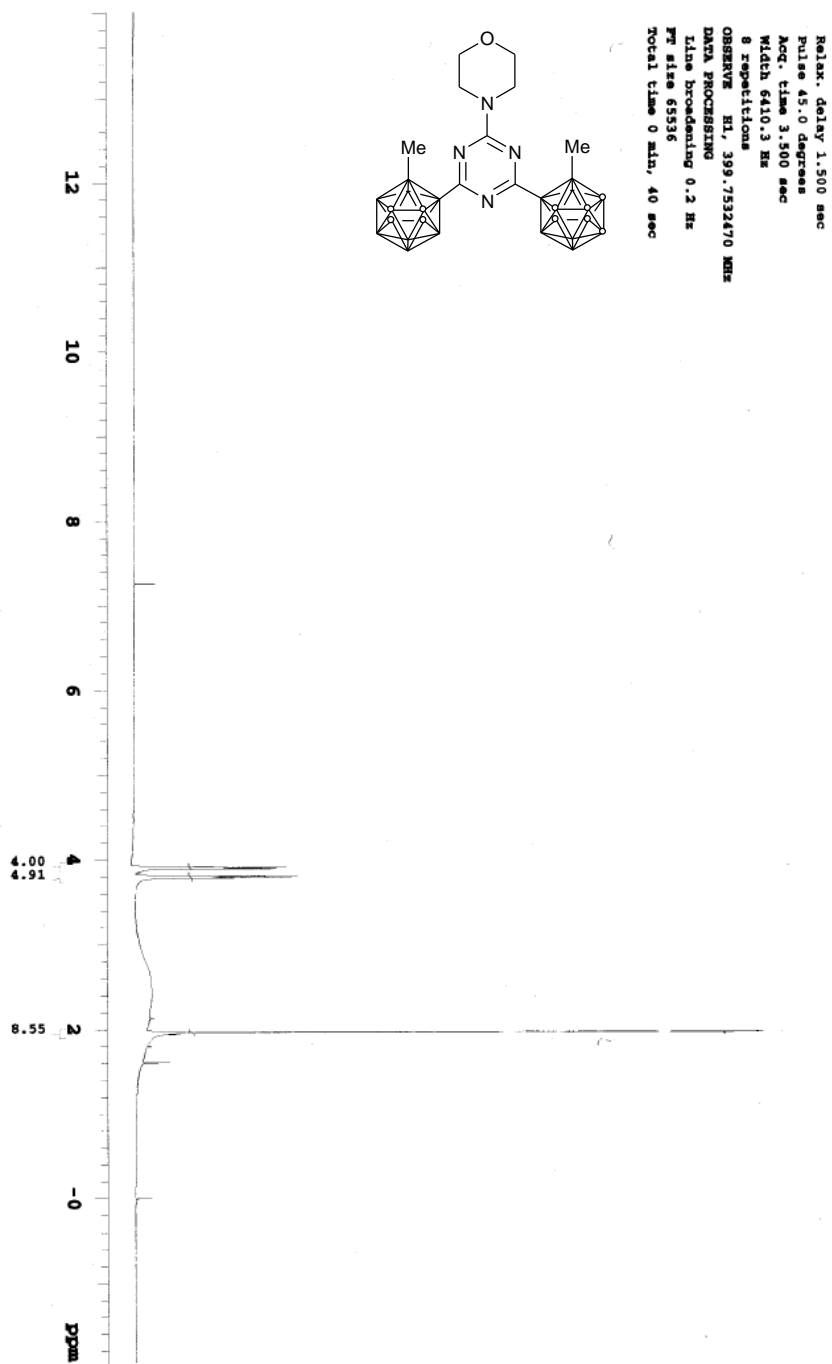
$^{11}\text{B}$  NMR (96.3 MHz,  $\text{CDCl}_3$ )





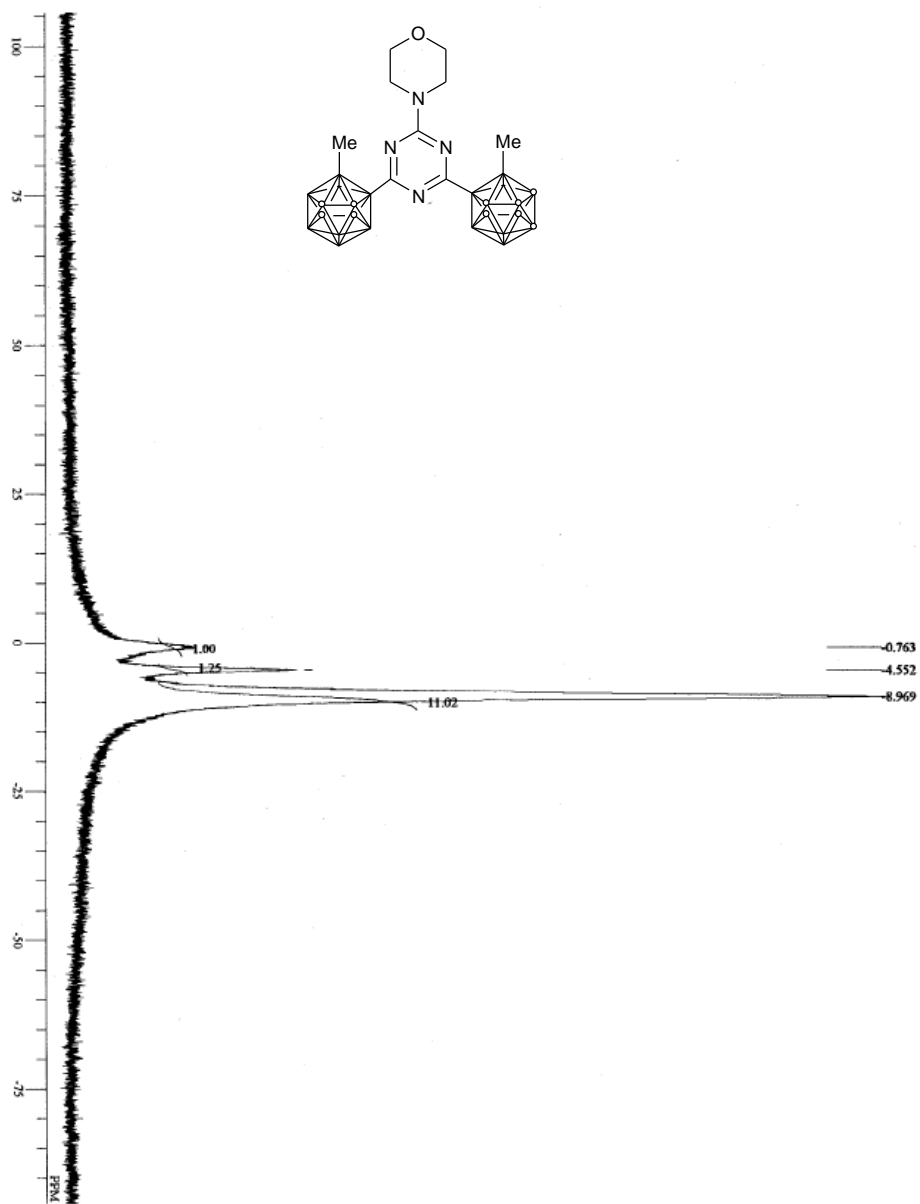
2, 4-Bis(2-methyl-o-carboran-1-yl) -6-(N-morpholinyl)- 1, 3, 5-triazine 7d

$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )



2, 4-Bis(2-methyl-o-carboran-1-yl)-6-(N-morpholinyl)-1, 3, 5-triazine **7d**

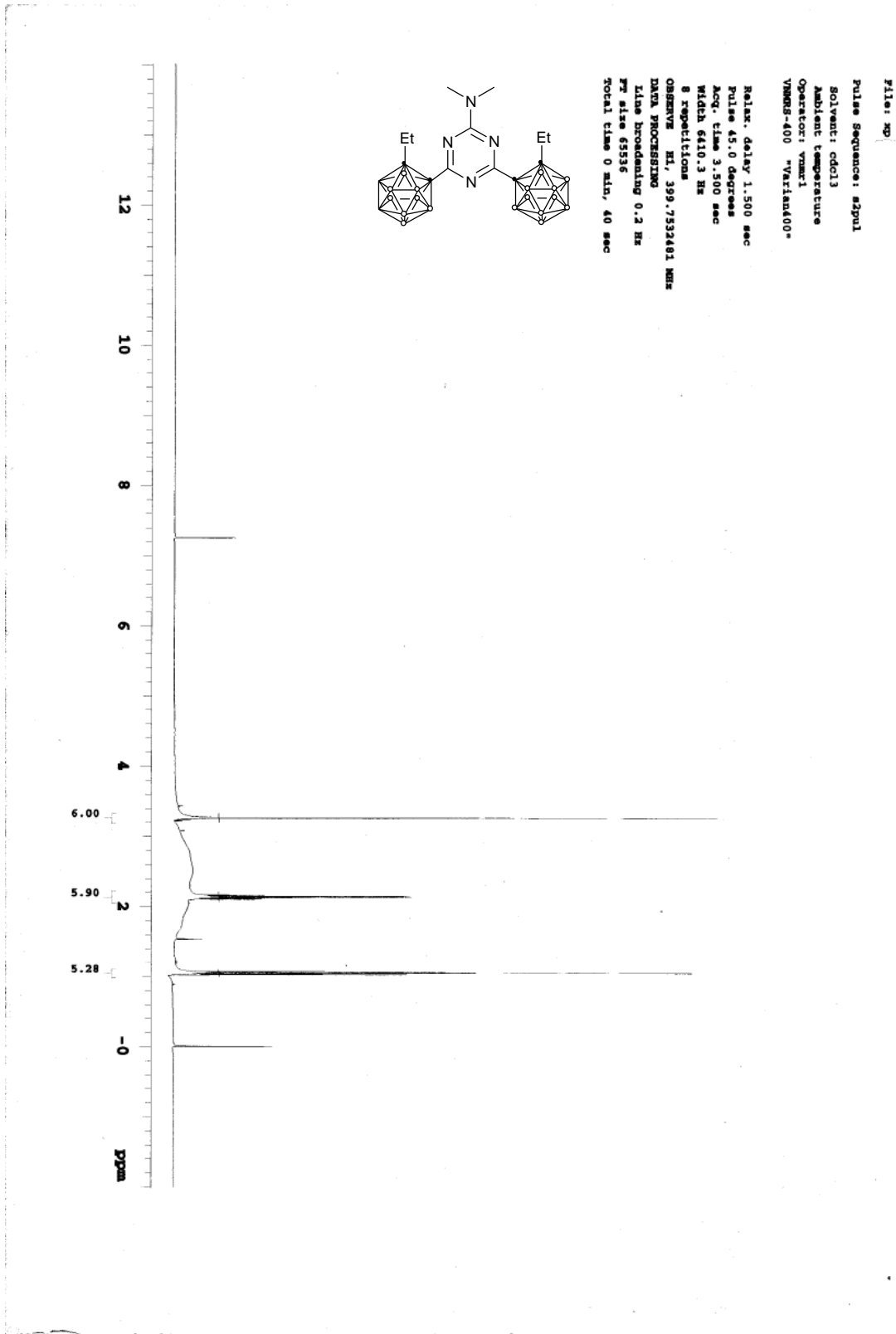
$^{11}\text{B}$  NMR (96.3 MHz,  $\text{CDCl}_3$ )



DE  
 CONAT 11B  
 CQINCC 96.30 MHz  
 ORN 121.00 XHz  
 OBSFET 1310.00 Hz  
 OBSFN 7.00 usec  
 PWT 10.00 usec  
 PWA 10.00 usec  
 PI 1.0000 msec  
 P2 1.0000 msec  
 P3 1.0000 msec  
 LOOP1 1  
 POINT 32768  
 SFO 32768  
 SCANS 16  
 DYNAM1 1  
 PRGOU 19277.11 Hz  
 ACQTM 1.6598 sec  
 PD 2.0000 sec  
 RGAIN 17  
 BF 1.30 Hz  
 EXXKOD BCM  
 IRNKC HH  
 FFR 300.40 MHz  
 RSET 130.00 KHz  
 RFRN 1150.00 Hz  
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 CSPED 10 Hz  
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 XS 0.00 Hz

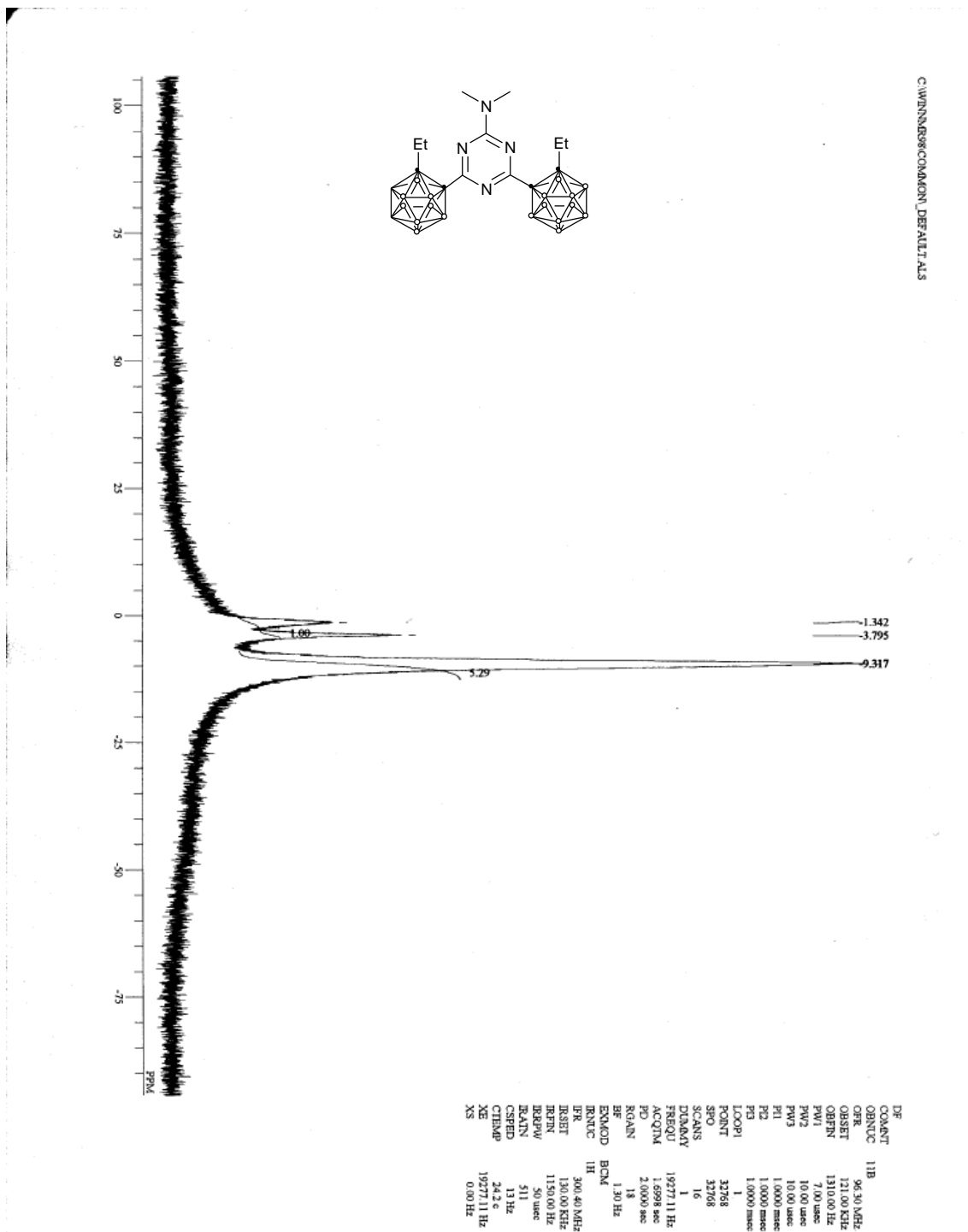
2, 4-Bis(2-ethyl-o-carboran-1-yl) -6-(N, N-dimethylamino)- 1, 3, 5-triazine 7e

<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)



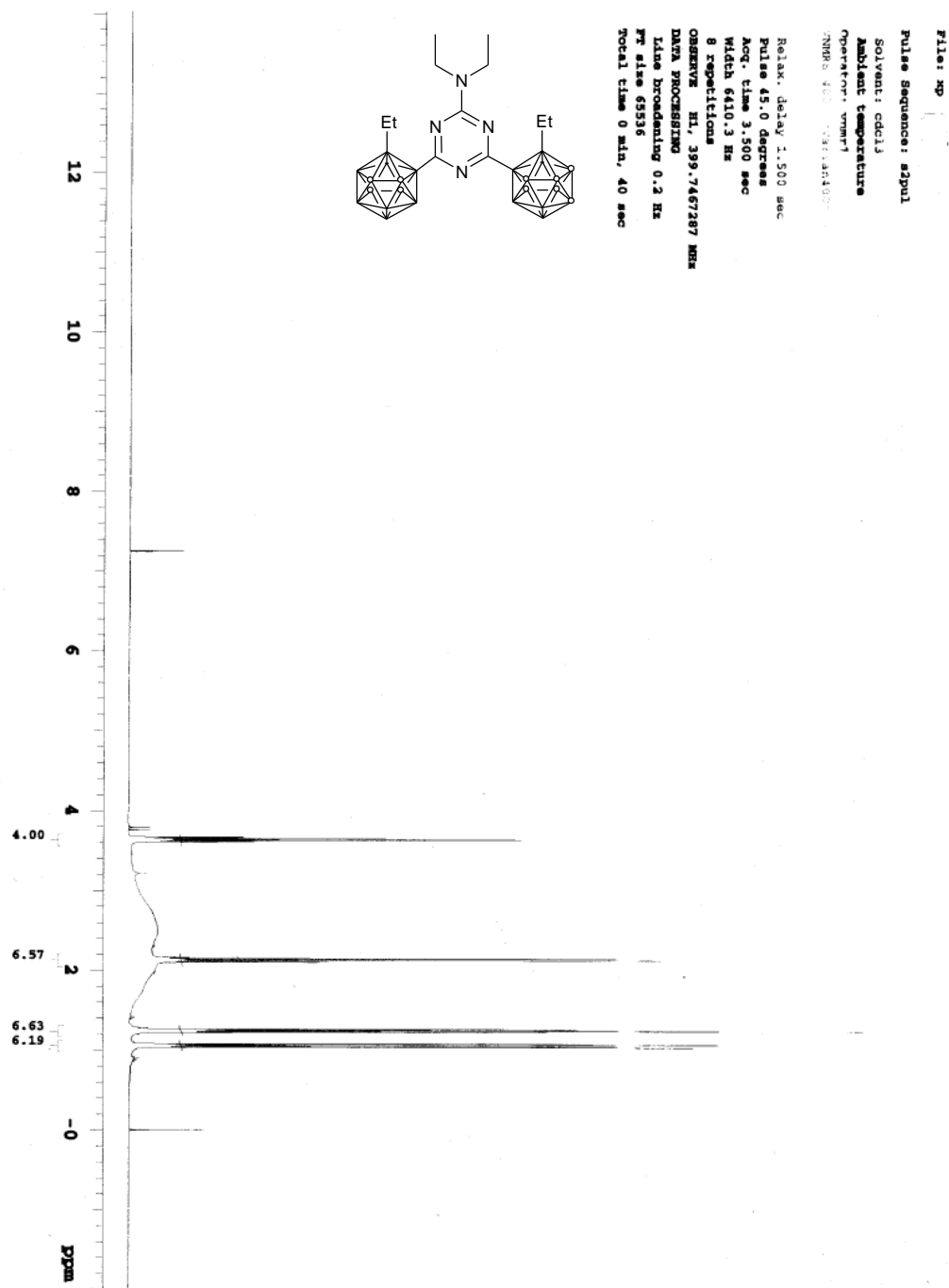
2, 4-Bis(2-ethyl-o-carboran-1-yl) -6-(N, N-dimethylamino)- 1, 3, 5-triazine 7e

<sup>11</sup>B NMR (96.3 MHz, CDCl<sub>3</sub>)



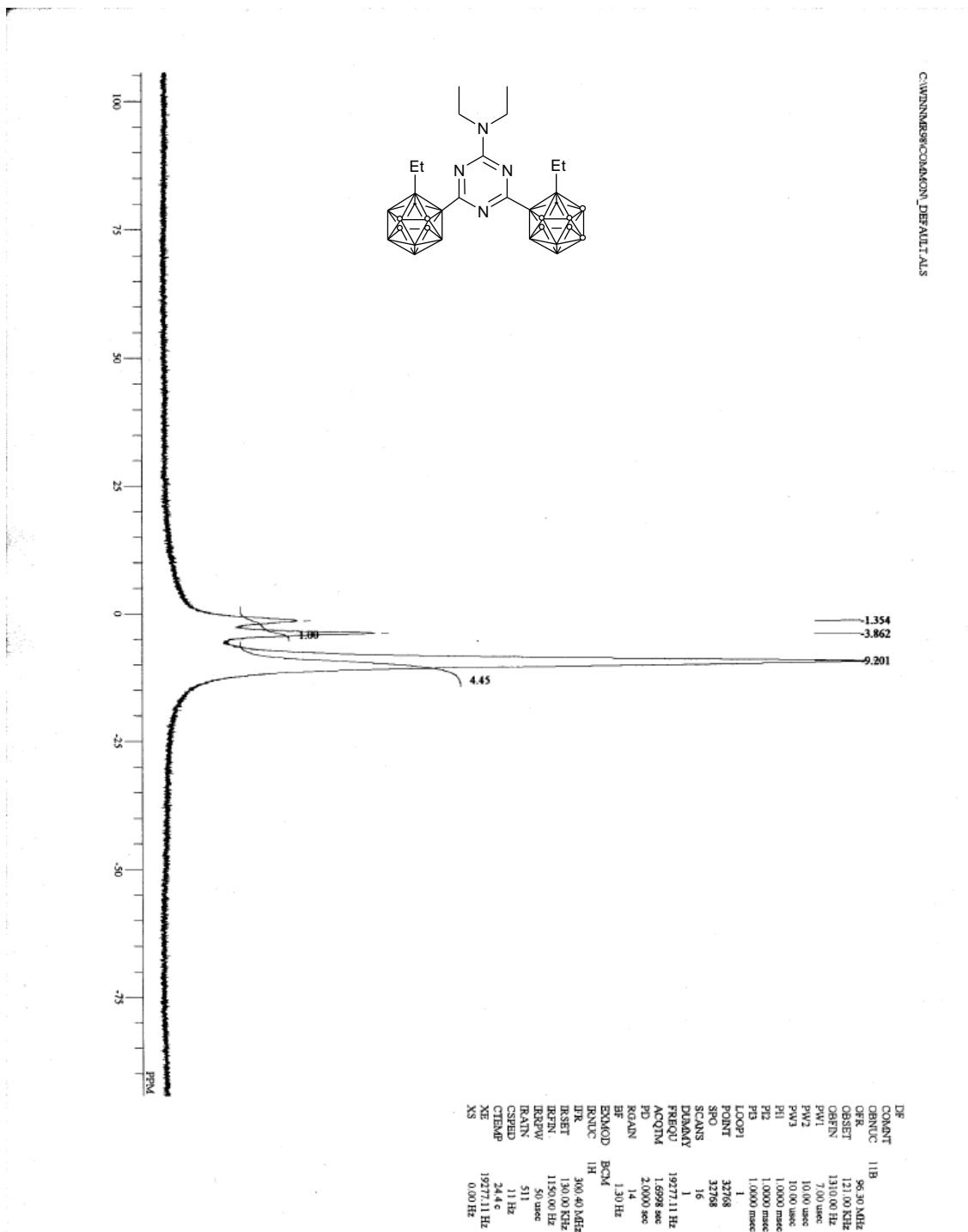
2, 4-Bis(2-ethyl-o-carboran-1-yl) -6-(N,N-diethylamino)- 1, 3, 5-triazine 7f

<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)



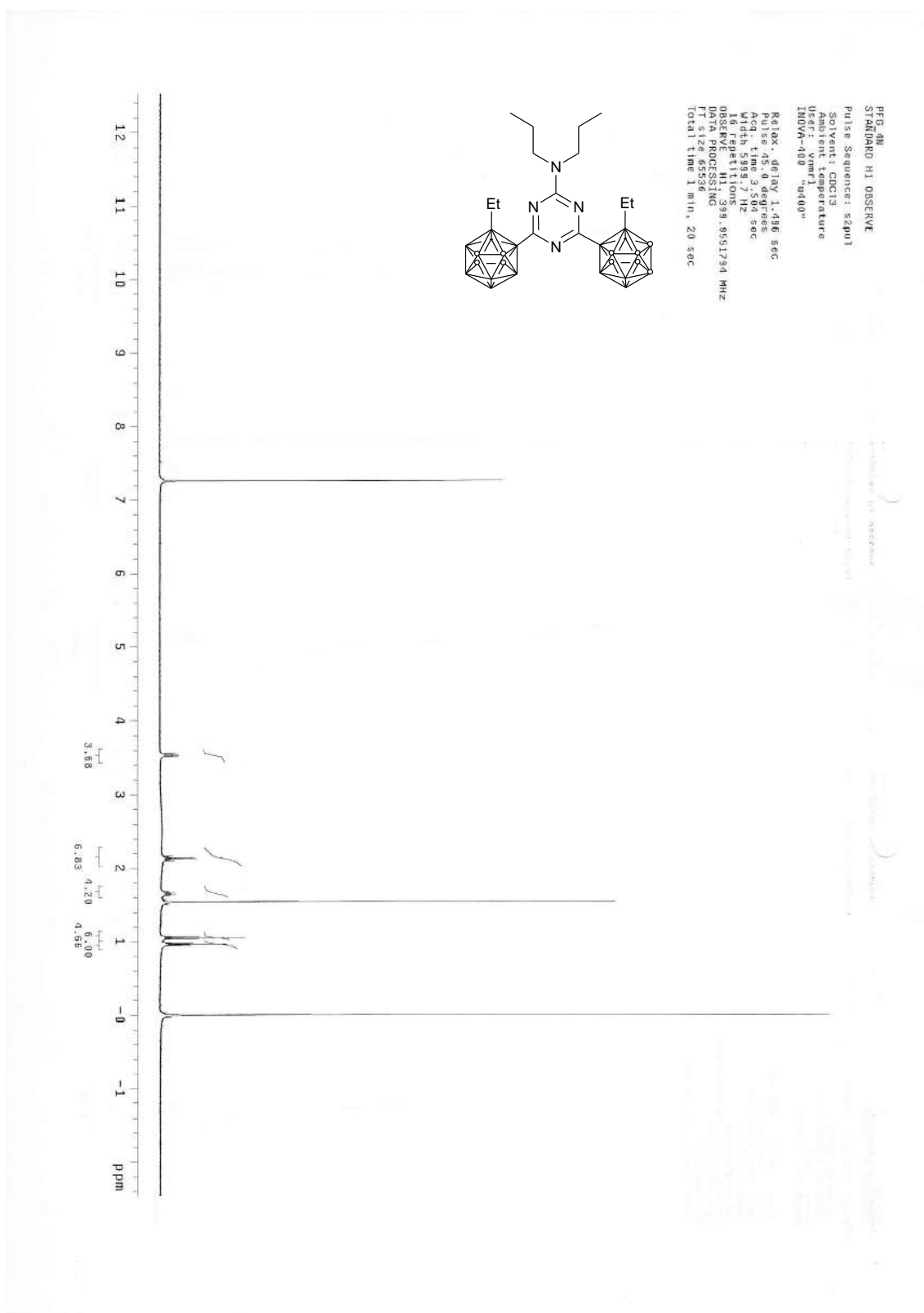
2, 4-Bis(2-ethyl-o-carboran-1-yl) -6-(N,N-diethylamino)- 1, 3, 5-triazine 7f

<sup>11</sup>B NMR (96.3 MHz, CDCl<sub>3</sub>)



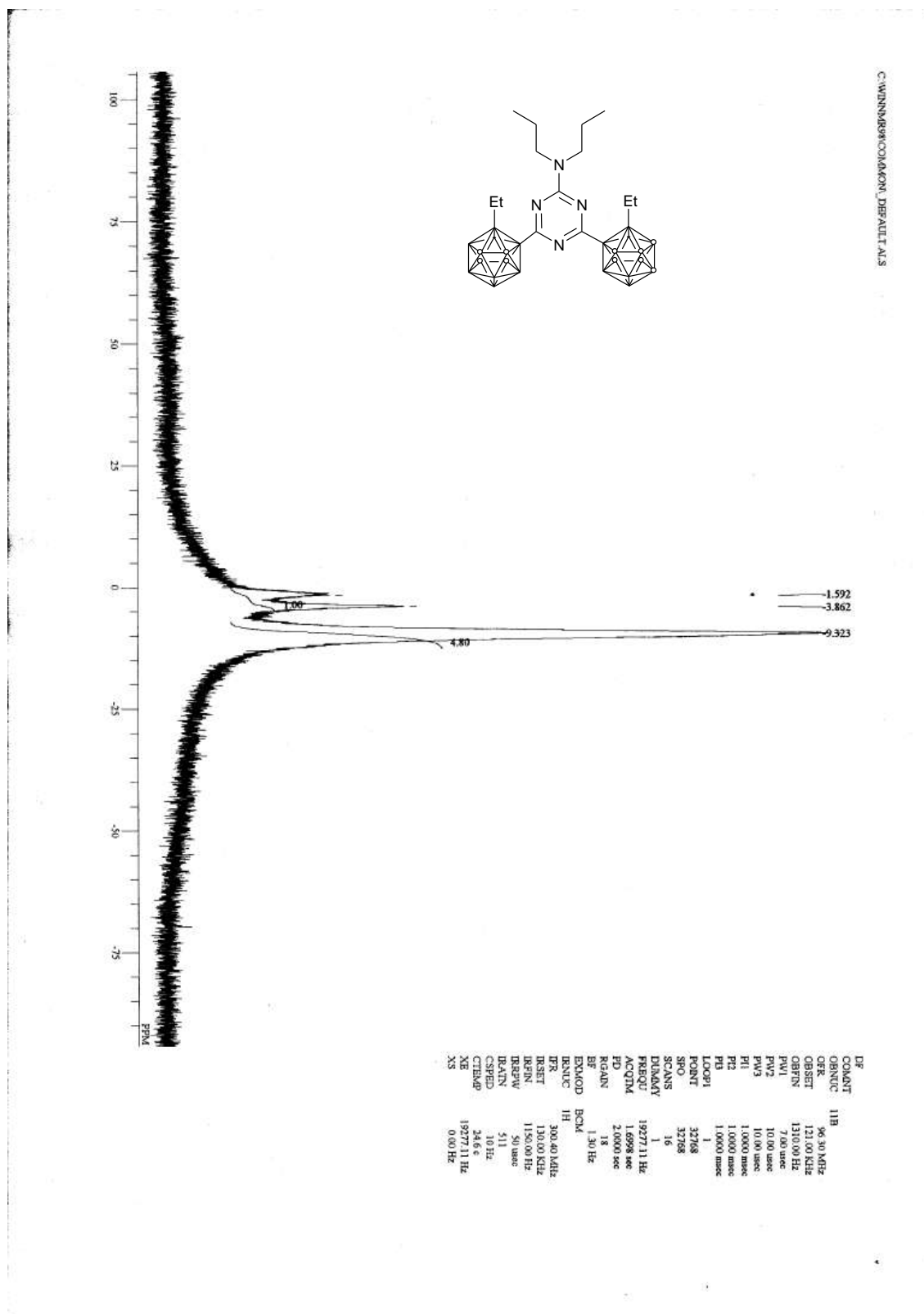
2, 4-Bis(2-ethyl-o-carboran-1-yl) -6-(N,N-di-n-propylamino)- 1, 3, 5-triazine **7g**

<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)



2, 4-Bis(2-ethyl-o-carboran-1-yl) -6-(N,N-di-n-propylamino)- 1, 3, 5-triazine 7g

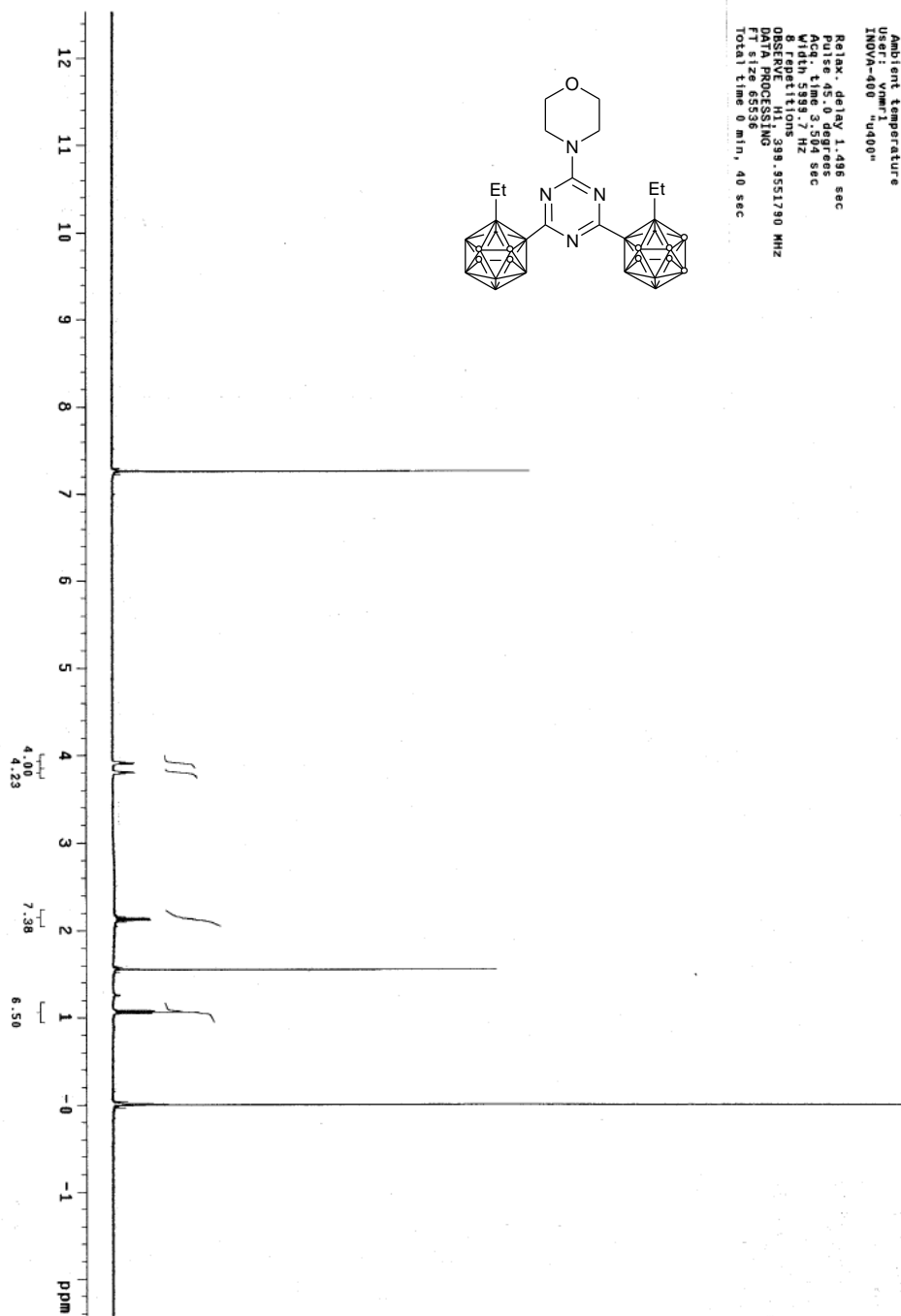
<sup>11</sup>B NMR (96.3 MHz, CDCl<sub>3</sub>)





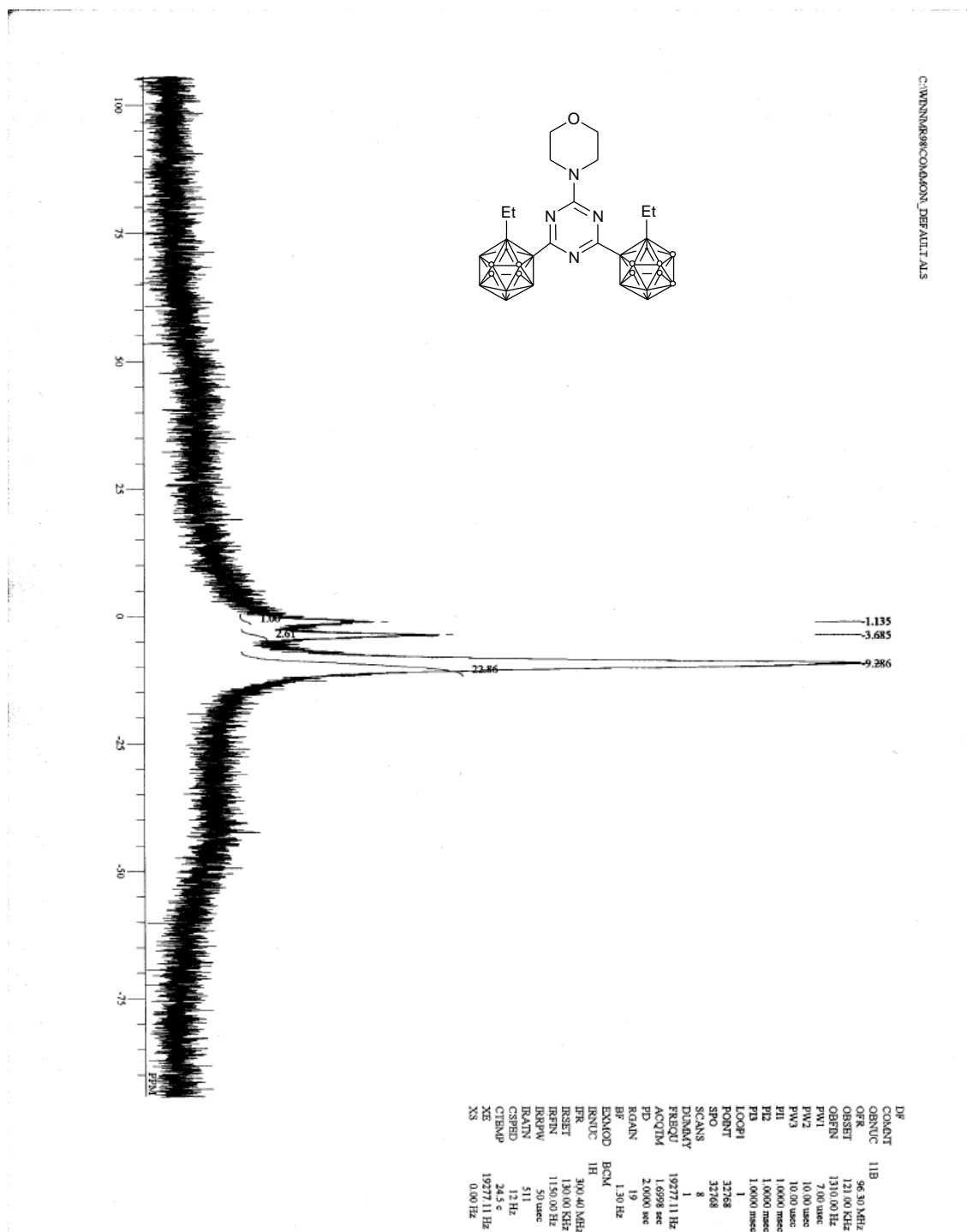
2, 4-Bis(2-ethyl-o-carboran-1-yl) -6-(N-morpholinyl)- 1, 3, 5-triazine 7h

<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)



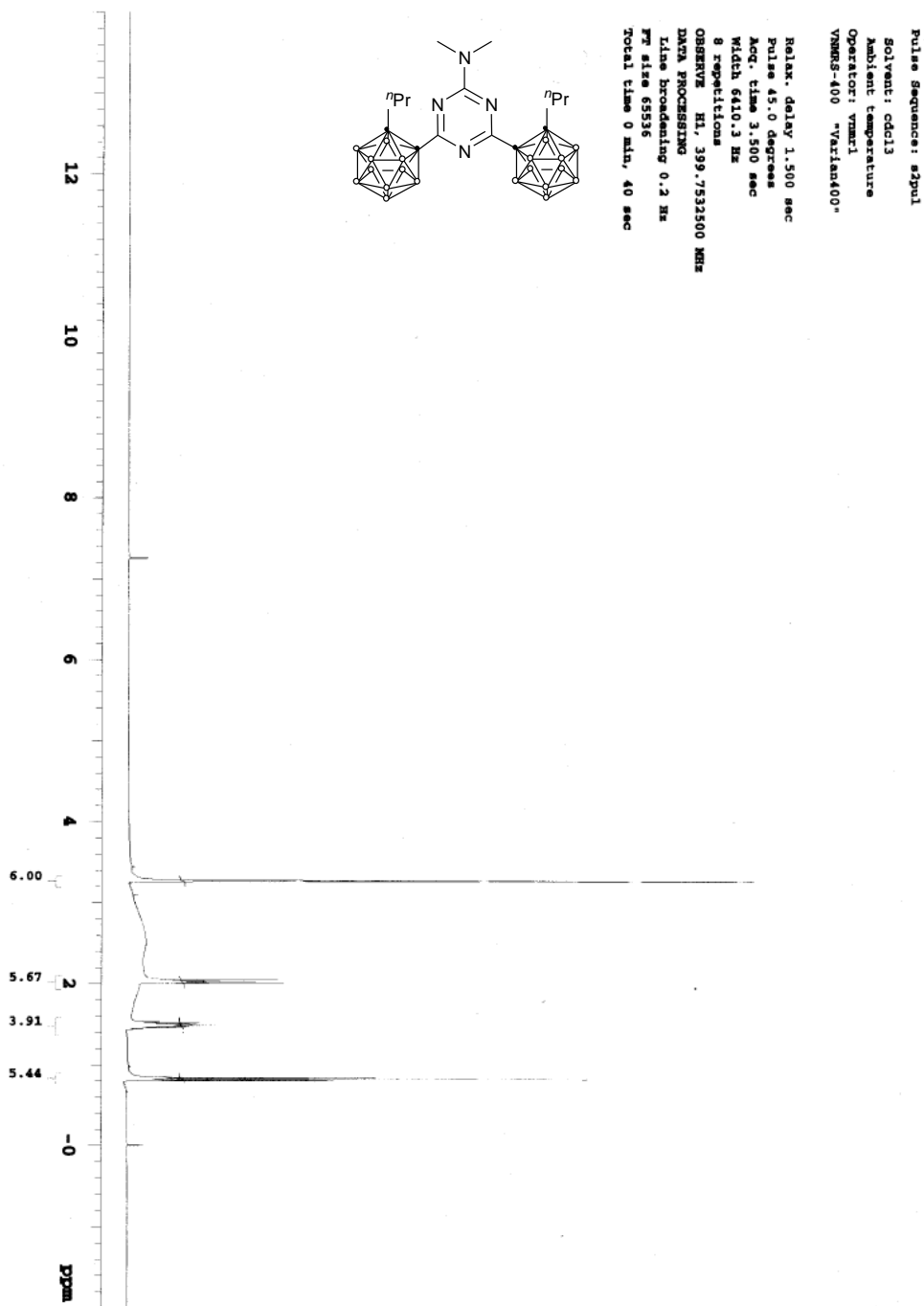
2, 4-Bis(2-ethyl-o-carboran-1-yl) -6-(N-morpholinyl)- 1, 3, 5-triazine **7h**

$^{11}\text{B}$  NMR (96.3 MHz,  $\text{CDCl}_3$ )



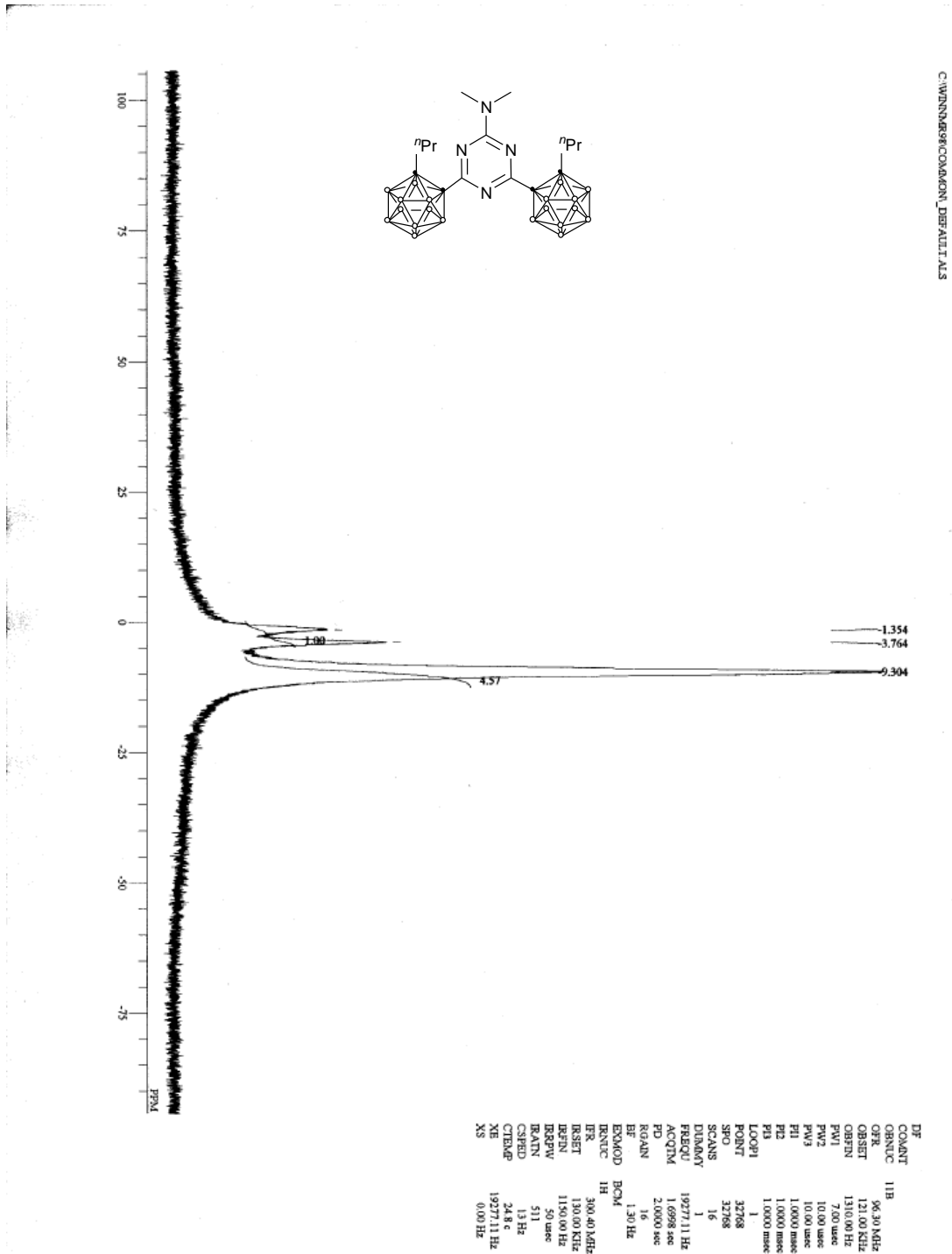
2, 4-Bis(2-n-propyl-o-carboran-1-yl) -6-(N, N-dimethylamino)- 1, 3, 5-triazine 7i

<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)



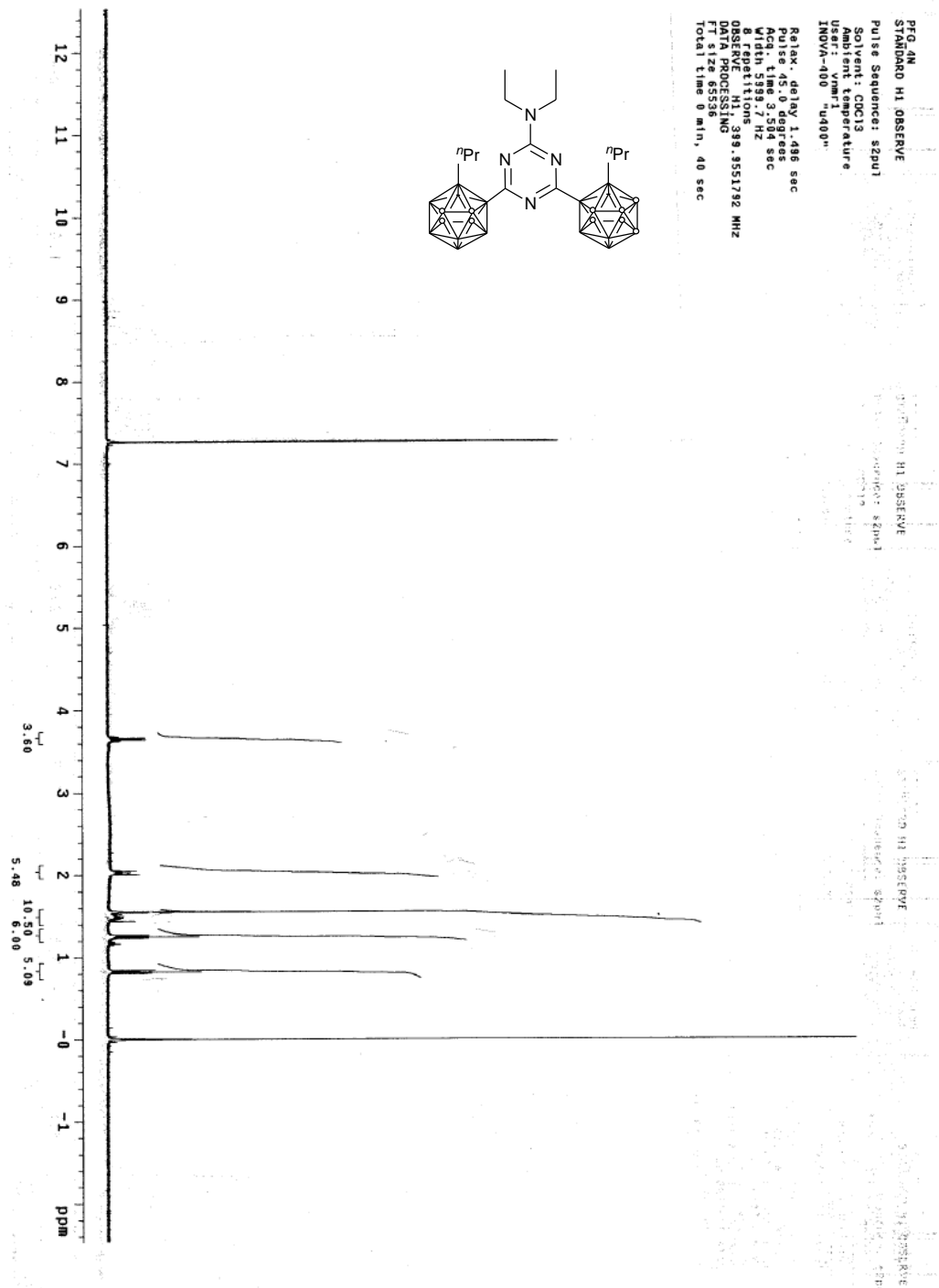
2, 4-Bis(2-n-propyl-o-carboran-1-yl) -6-(N, N-dimethylamino)- 1, 3, 5-triazine 7i

<sup>11</sup>B NMR (96.3 MHz, CDCl<sub>3</sub>)



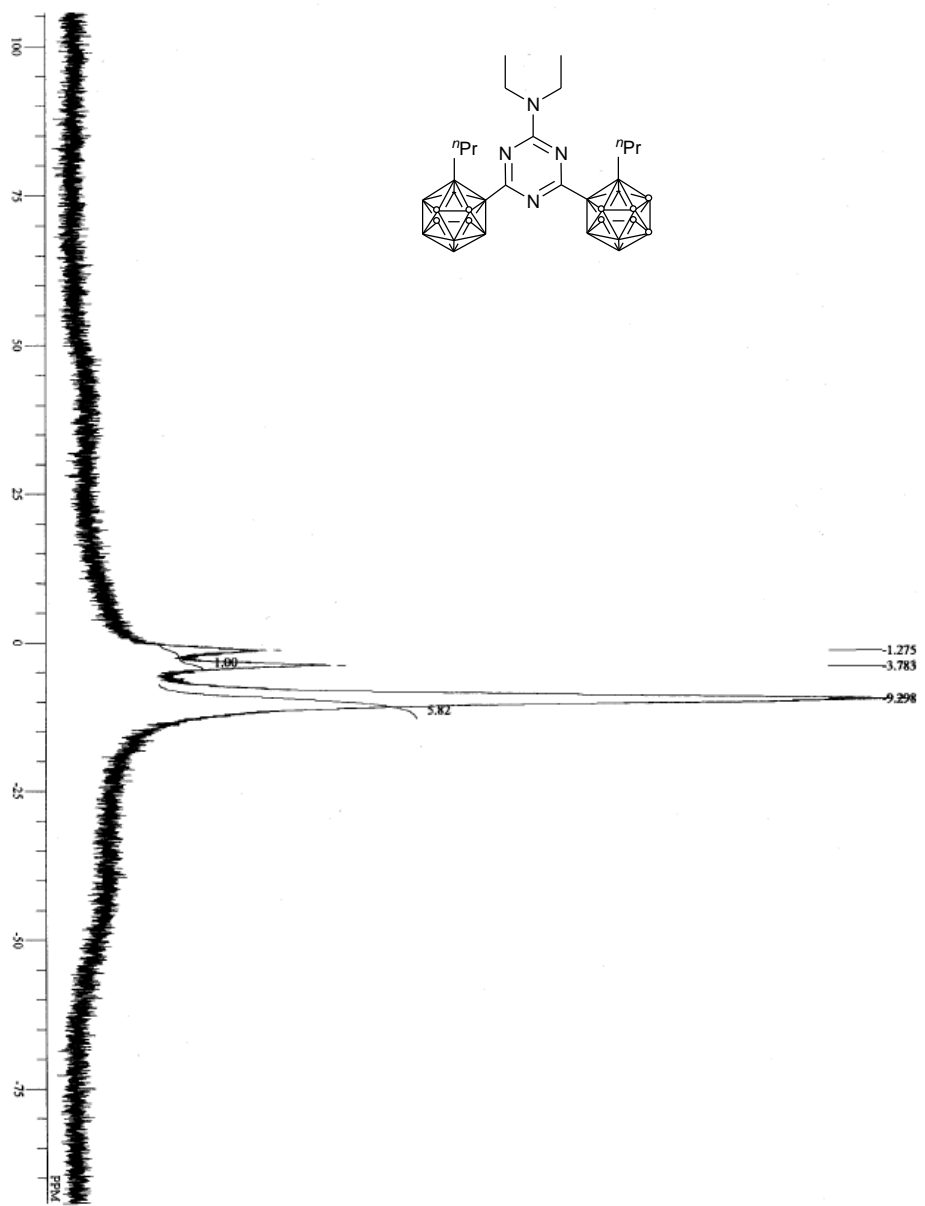
2, 4-Bis(2-n-propyl-o-carboran-1-yl) -6-(N,N-diethylamino)- 1, 3, 5-triazine 7j

$^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ )



2, 4-Bis(2-n-propyl-o-carboran-1-yl)-6-(N,N-diethylamino)-1, 3, 5-triazine 7j

$^{11}\text{B}$  NMR (96.3 MHz,  $\text{CDCl}_3$ )



C:\WINNMR\COMMON\_DEFAULT.ALS

DE  
 COMPT 11B  
 OBSNUC 96.30 MHz  
 OFR 121.00 KHz  
 OBSRT 1310.00 Hz  
 OBSFN 7.00 usec  
 PW1 10.00 usec  
 PW2 10.00 usec  
 PW3 10.00 usec  
 P1 1.0000 msec  
 P2 1.0000 msec  
 P3 1.0000 msec  
 LOOP1 1  
 POINT 32768  
 SFO 32768  
 SCANS 16  
 DIAMAT 1  
 FREQ1 19277.11 Hz  
 FREQ2 16598 usec  
 ACQTM 2.0000 sec  
 PD 18  
 RGAIN 1.30 Hz  
 BF  
 EXMOD BCM  
 H  
 RNUC 300.00 MHz  
 FR 130.00 KHz  
 RSET 1150.00 Hz  
 RFRN 50 usec  
 RRPRW 511  
 RATTN 511  
 CSPED 24.4 e  
 CTMPP 10 Hz  
 XE 19277.11 Hz  
 XS 0.00 Hz

2, 4-Bis(2-n-propyl-o-carboran-1-yl) -6-(N,N-di-n-propylamino)- 1, 3, 5-triazine 7k

<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)

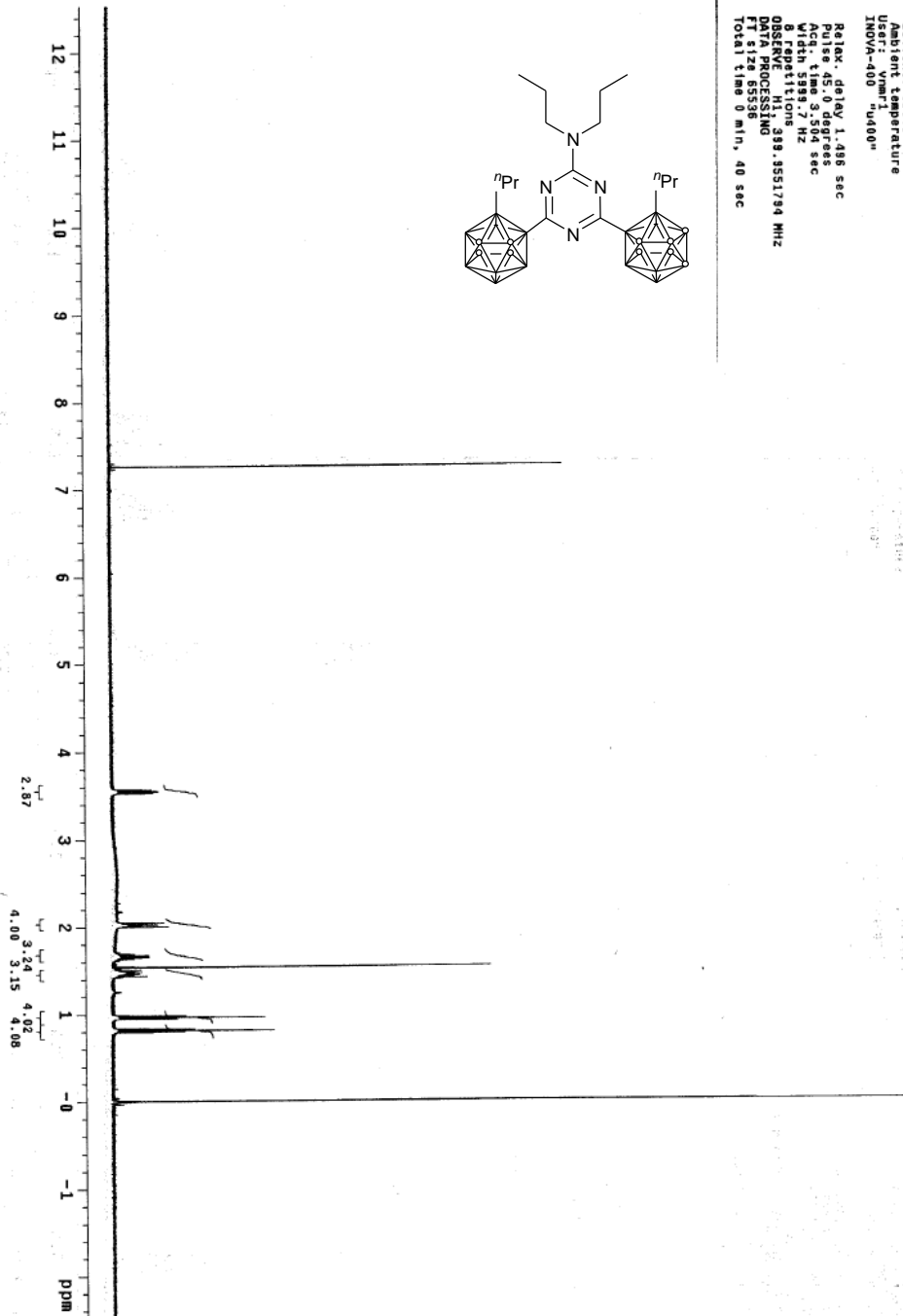
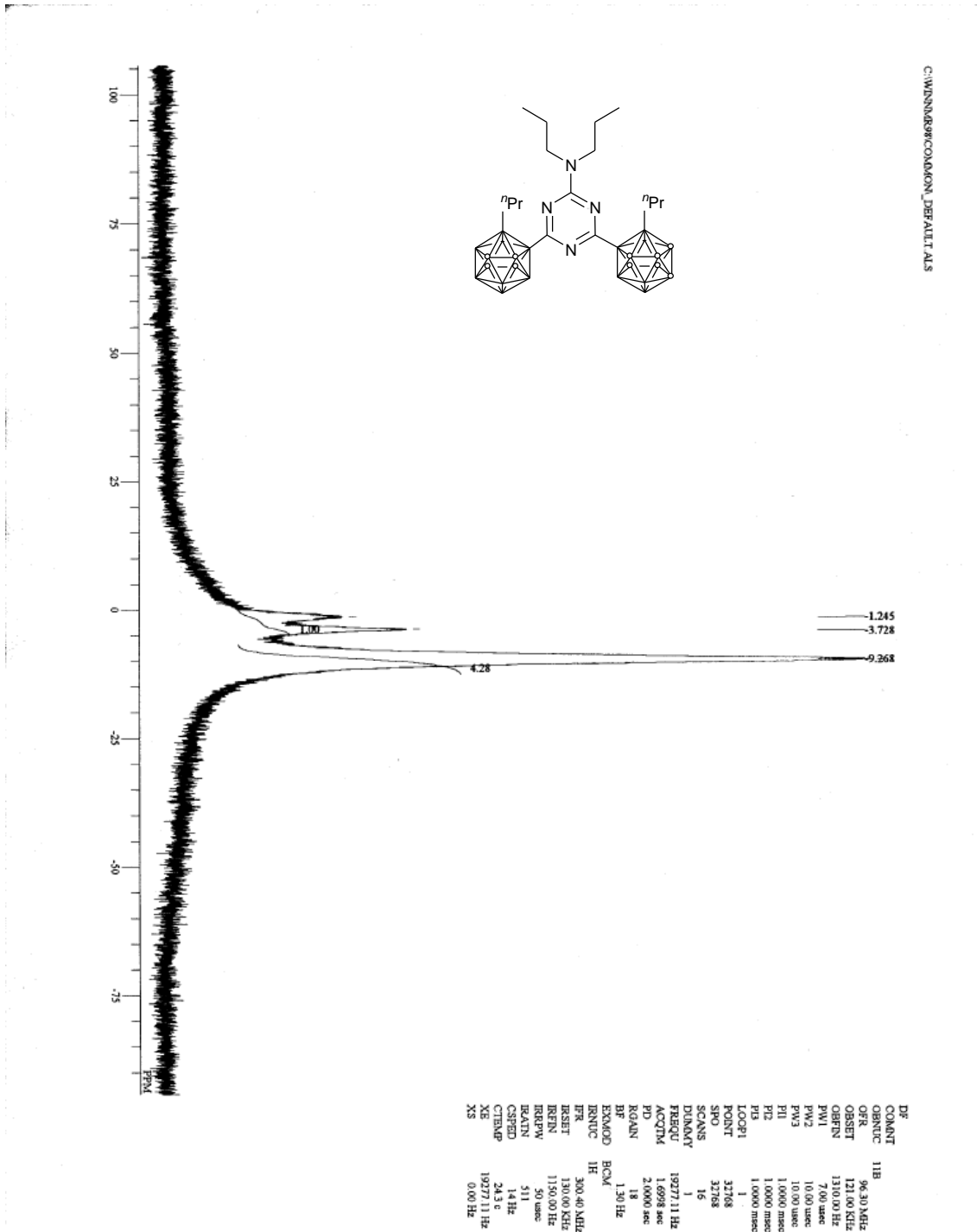


FIG. 4M  
STANDARD H1 OBSERVE  
Pulse Sequence: s2p1  
Solvent: CDCl3  
Ambient temperature  
User: vmm1 1/6/00  
INOVA-400 14000°  
Pulse delay: 1.488 sec  
Pulse: 45.0 degrees  
Acq. time: 3.504 sec  
Width: 5999.7 Hz  
# Repetitions: 389.9551794 MHz  
DATE ACQUIRED: 1/16/00  
FT size: 65536  
Total time: 0 min, 40 sec

2, 4-Bis(2-n-propyl-o-carboran-1-yl) -6-(N,N-di-n-propylamino)- 1, 3, 5-triazine 7k

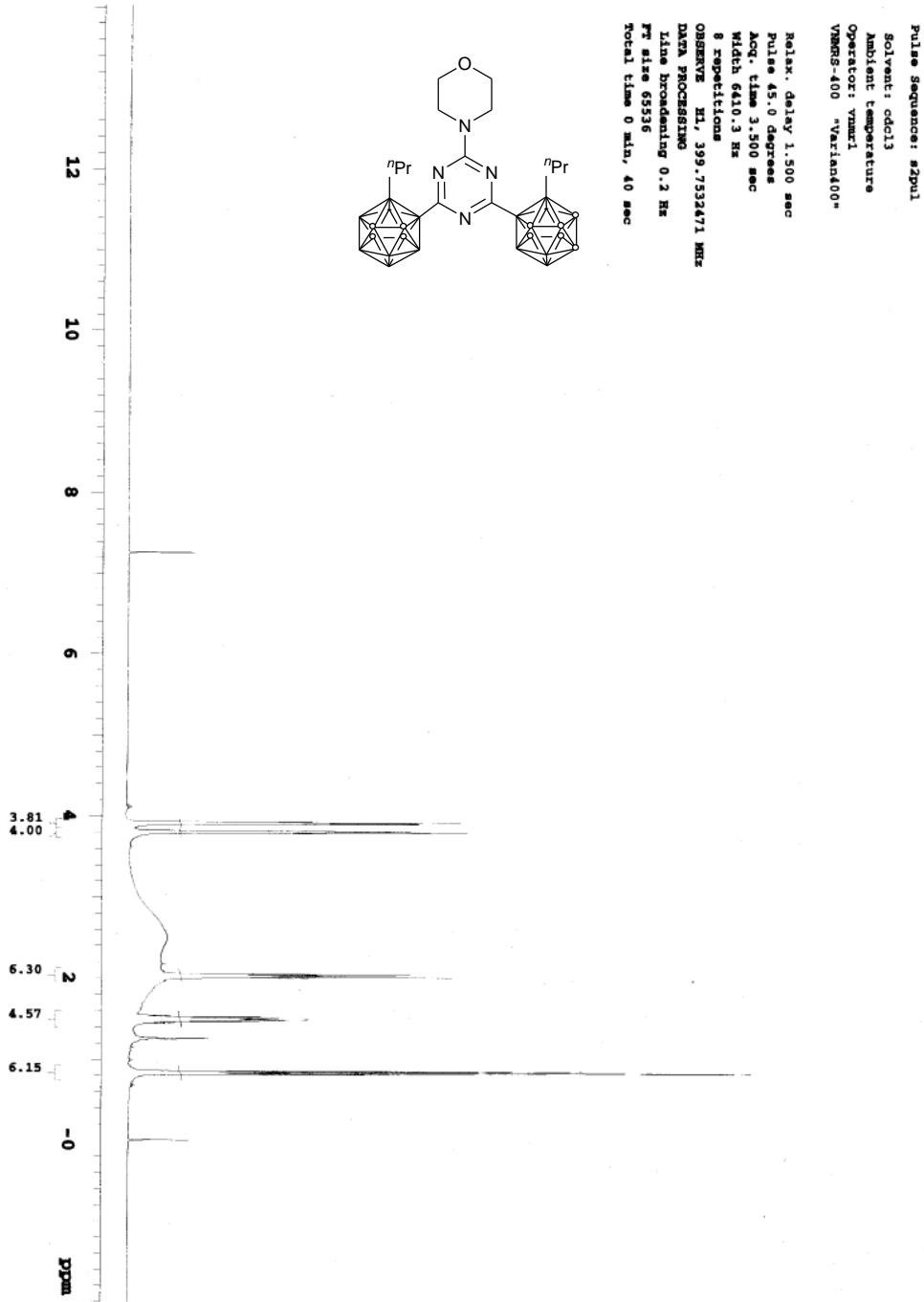
$^{11}\text{B}$  NMR (96.3 MHz,  $\text{CDCl}_3$ )





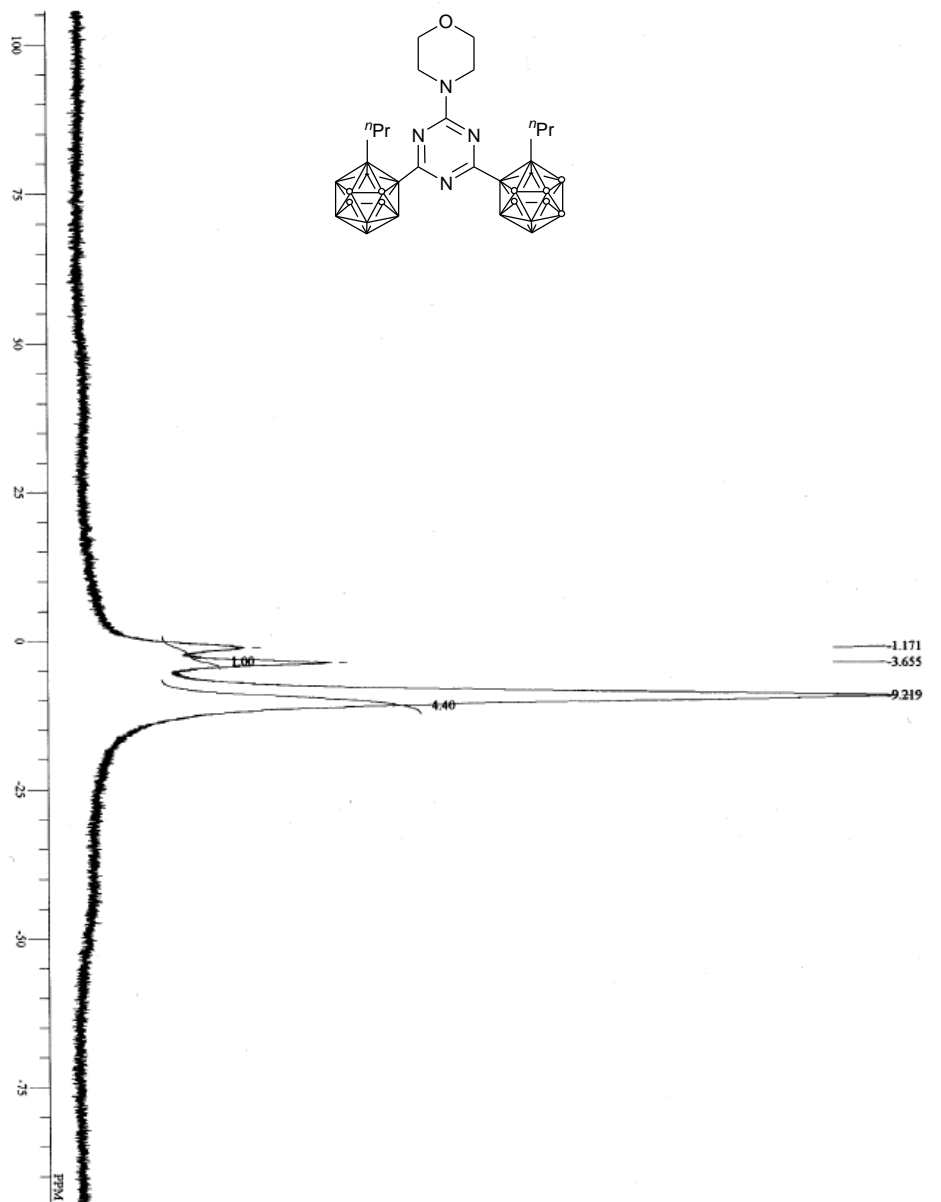
2, 4-Bis(2-n-propyl-o-carboran-1-yl) -6-( N-morpholinyl)- 1, 3, 5-triazine 7I

<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)



2, 4-Bis(2-n-propyl-o-carboran-1-yl)-6-(N-morpholinyl)-1, 3, 5-triazine **7l**

$^{11}\text{B}$  NMR (96.3 MHz,  $\text{CDCl}_3$ )



C:\WINNMR\9630\AKON1\_DEFAULT.ALS

```

DE
CONT 11B
CONTC 96.30 MHz
ORNT 121.00 KHz
OBSET 1310.00 Hz
OBSFN 710.000
PNU1 10.000 usec
PNU2 10.000 usec
PNU3 10.000 usec
PI1 1.0000 msec
PI2 1.0000 msec
PI3 1.0000 msec
LOOP1 1
POINT 32768
SPO 32768
SCANS 16
DUMPAV 1
FREQ1 192771.1 Hz
FREQ2 1.6598 sec
ACQTM 2.0000 sec
RGAIN 15
BF 1.50 Hz
EXMOD BCM
IH 11
IRNTC 300.40 MHz
IRSET 130.00 KHz
IRFTN 1150.00 Hz
IRRFW 50.000 usec
IRATN 511
CSFHD 11 Hz
CTHRP 24.2 g
XE 192771.1 Hz
XS 0.00 Hz
    
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