

## Supporting Information (37 pages)

### Synthesis of triazolyl methyl-substituted amino- and oxy-undecahydrododecaborates for potential application in boron neutron capture therapy

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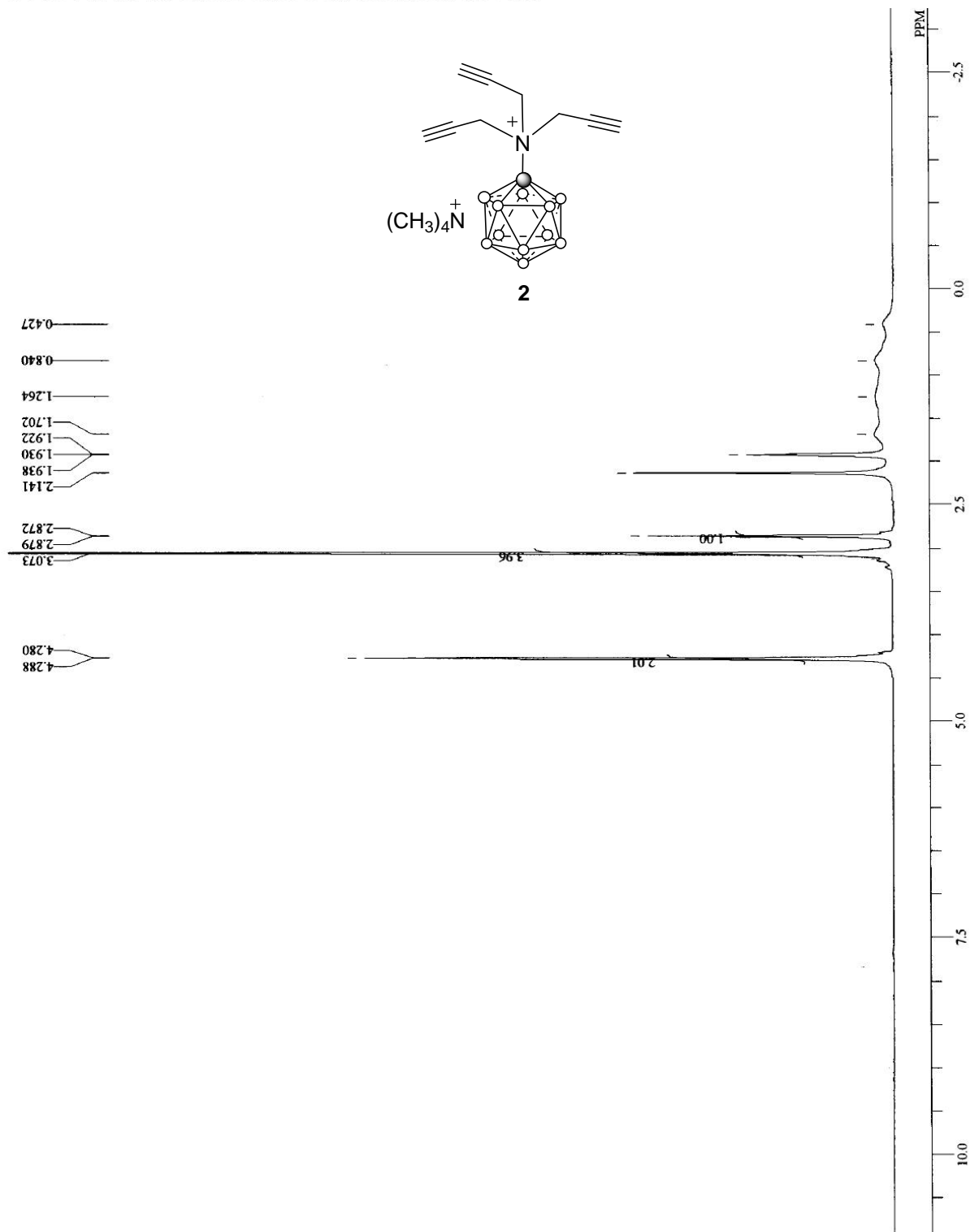
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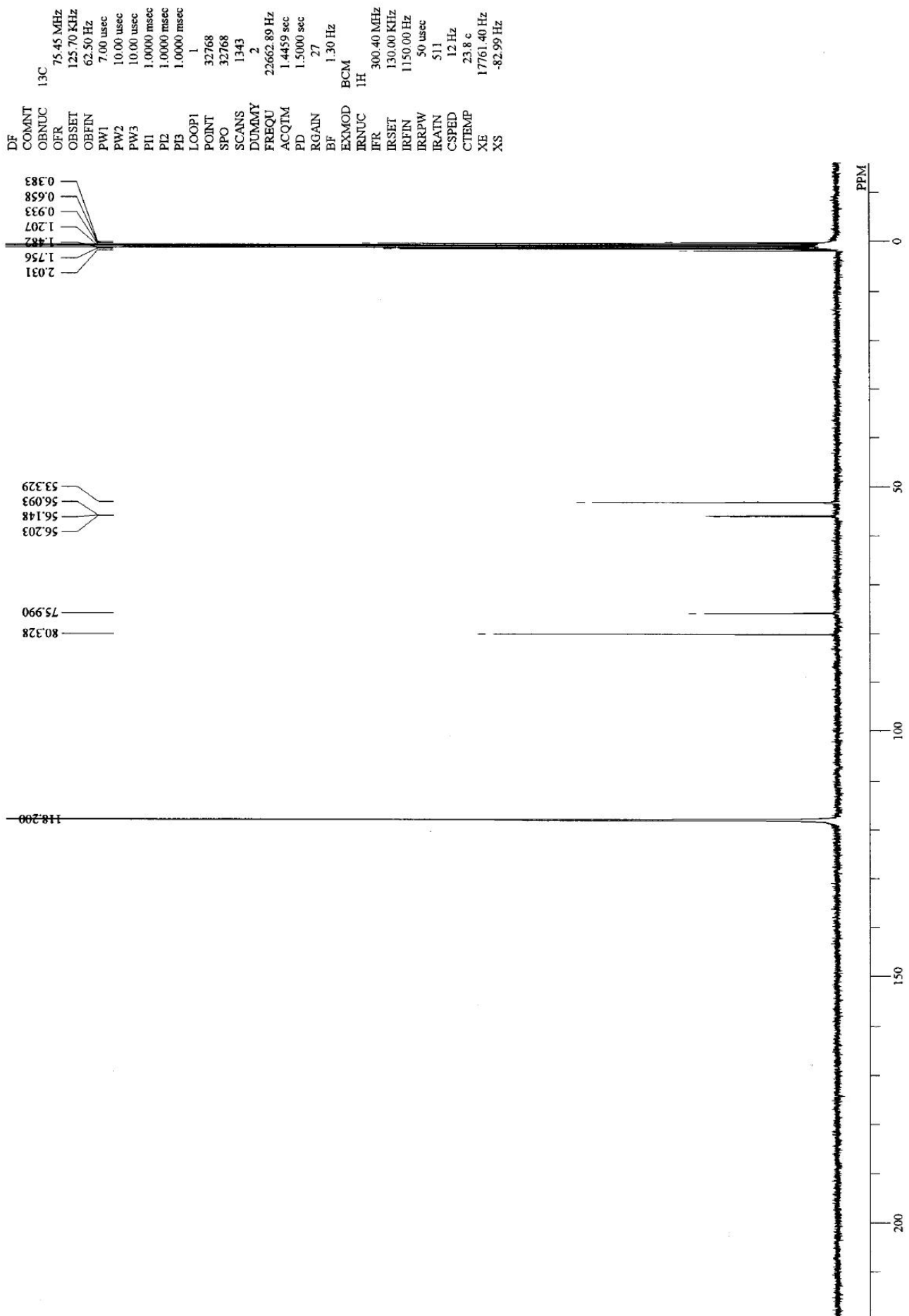
*N,N,N*-Tris-(prop-2-ynyl)amine-undecahydro-*closo*-dodecaborate (1-) tetramethylammonium salt (**2**)  
<sup>1</sup>H NMR (300 MHz, CD<sub>3</sub>CN)

DF 300.40 MHz  
 OBNUC 130.00 KHz  
 OFR 1150.00 Hz  
 OBFIN 5.40 usec  
 PW1 10.00 usec  
 PW2 10.00 usec  
 PW3 10.00 usec  
 P11 1.0000 msec  
 P12 1.0000 msec  
 P13 1.0000 msec  
 LOOP1 1  
 POINT 32768  
 SPO 32768  
 SCANS 8  
 DUMMAY 1  
 FREQU 6015.04 Hz  
 ACQTM 5.4477 sec  
 PD 1.5510 sec  
 RGAIN 15  
 BF 1.30 Hz  
 EXMOD NON  
 IRNUC 1H  
 IFR 300.40 MHz  
 IRSET 130.00 KHz  
 IRFIN 1150.00 Hz  
 IRRPW 50 usec  
 IRATN 511  
 CTEMP 22.5 C  
 XE 4255.94 Hz  
 XS 336.29 Hz

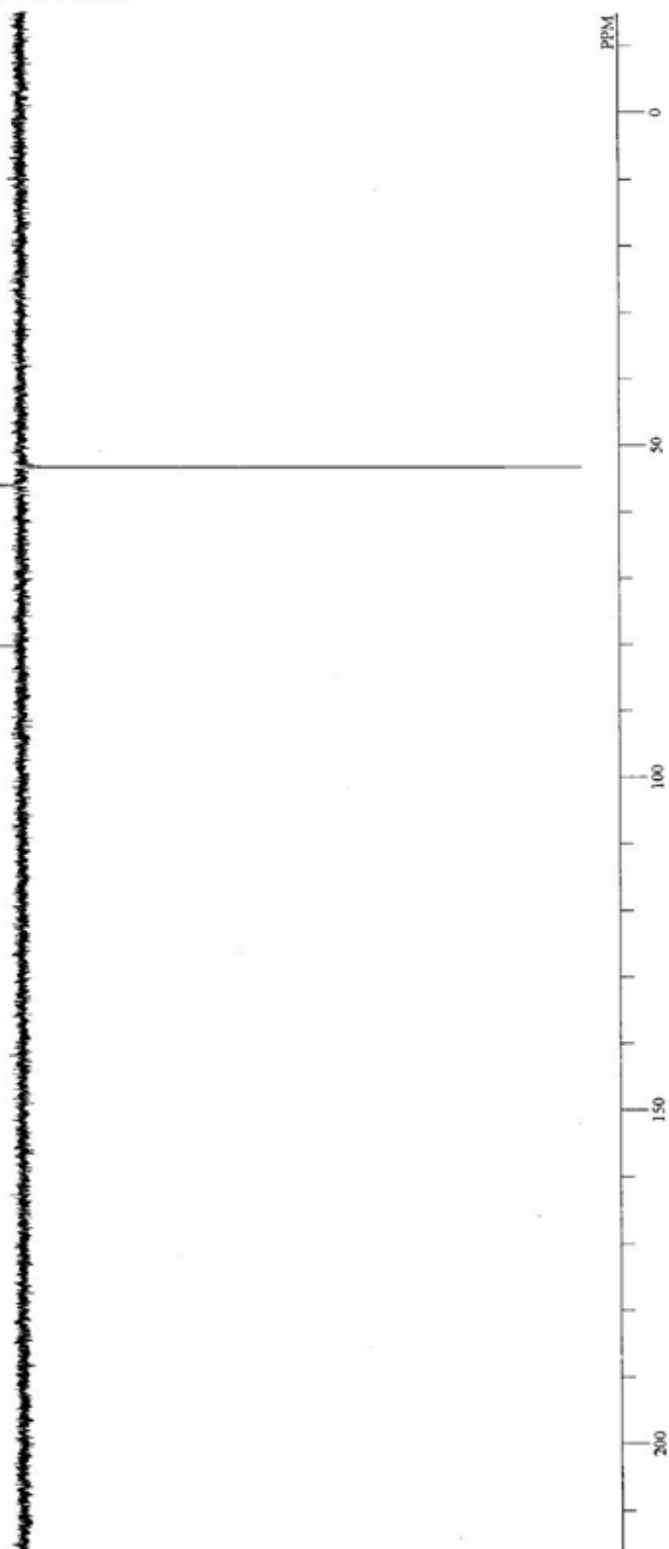


<sup>13</sup>C NMR (75 MHz, CD<sub>3</sub>CN)

<sup>13</sup>C NMR DEPT 135° (75 MHz, CD<sub>3</sub>CN)

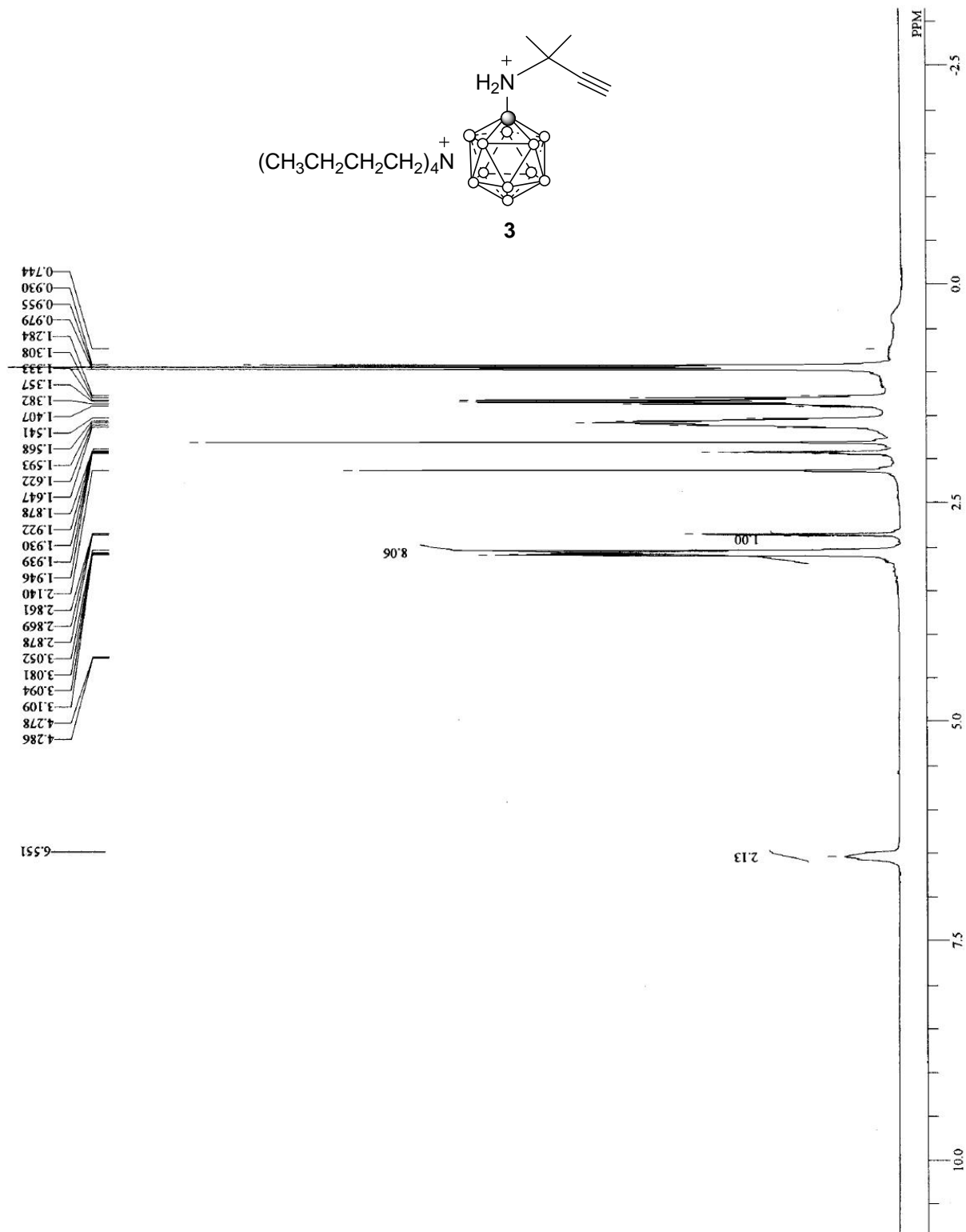


DF  
 COMENT  
 OBNUC 13C  
 OFR 75.45 MHz  
 OBSFET 125.70 KHz  
 OBSFIN 62.50 Hz  
 PW1 13.00 usec  
 PW2 20.60 usec  
 PW3 30.90 usec  
 P11 3.4480 msec  
 P12 1.0000 msec  
 P13 1.0000 msec  
 LOOP1 1  
 POINT 32768  
 SPO 32768  
 SCANS 949  
 DUNAMY 4  
 FREQU 22662.89 Hz  
 ACQTM 1.4459 sec  
 PD 1.5540 sec  
 RGAIN 27  
 BF 1.30 Hz  
 EXMOD DEPT  
 IRNUC 1H  
 IFR 300.40 MHz  
 IRSET 130.00 KHz  
 IREFN 1150.00 Hz  
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 XE 17451.56 Hz  
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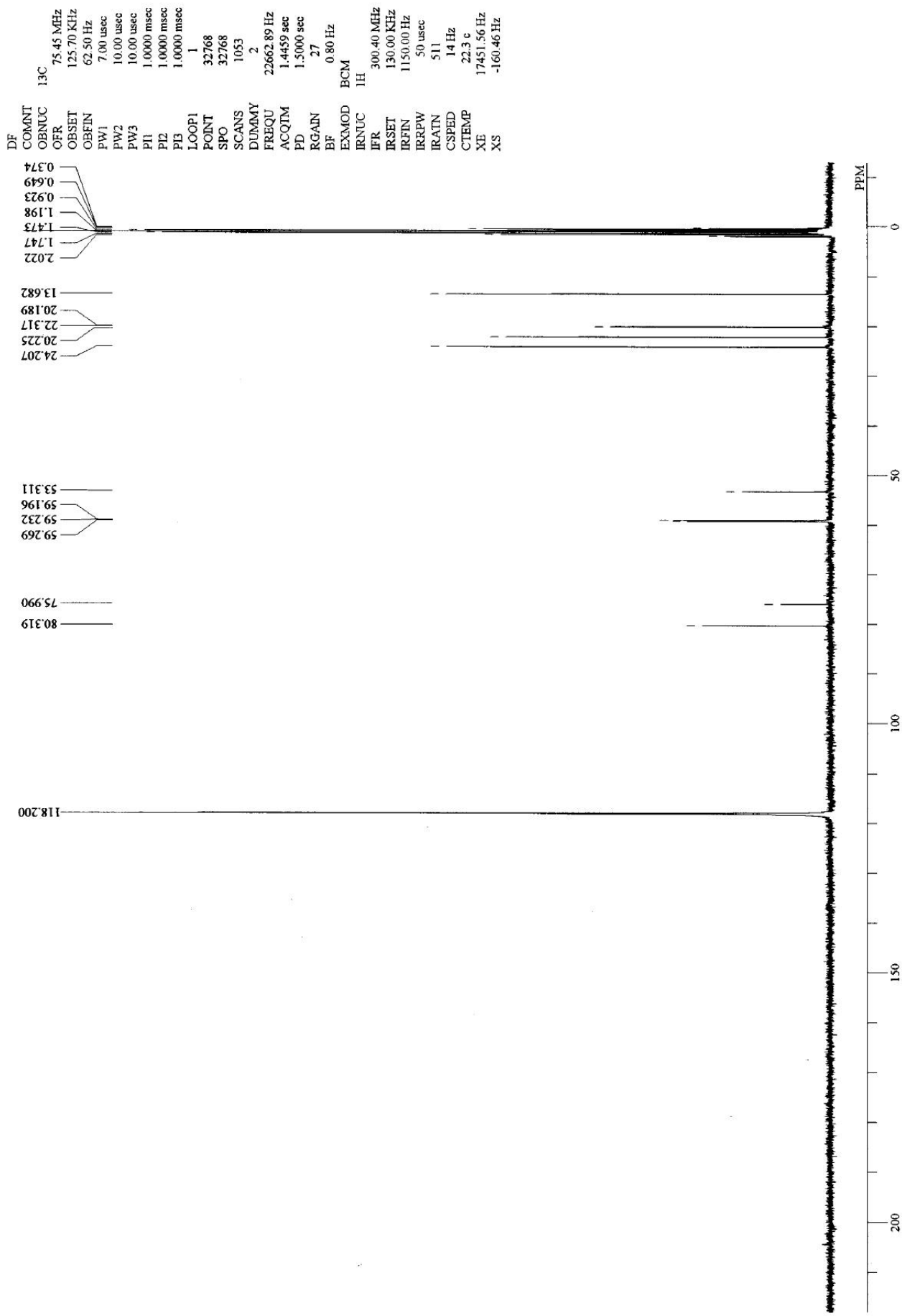
$N$ -(1,1-Dimethyl-prop-2-ynyl)amine-undecahydro-*closo*-dodecaborate (1-) tetrabutylammonium salt (**3**)  
<sup>1</sup>H NMR (300 MHz, CD<sub>3</sub>CN)

DF 300.40 MHz  
 OBNUC 130.00 KHz  
 OFR 1150.00 Hz  
 OBSET 5.40 usec  
 OBFIN 10.00 usec  
 PW1 10.00 usec  
 PW3 10.00 usec  
 P11 1.0000 msec  
 P12 1.0000 msec  
 P13 1.0000 msec  
 LOOP1 1  
 POINT 32768  
 SPO 32768  
 SCANS 8  
 DUMY 1  
 FREQU 6015.04 Hz  
 ACQTM 5.4477 sec  
 PD 1.5510 sec  
 RGAIN 11  
 BF 0.80 Hz  
 EXMOD NON  
 IRNUC 1H  
 IFR 300.40 MHz  
 IRSET 130.00 KHz  
 IRFIN 1150.00 Hz  
 IRRPW 50 usec  
 IRAIN 511  
 CSPED 14 Hz  
 CTEMP 23.5 c  
 XE 4200.14 Hz  
 XS 337.76 Hz

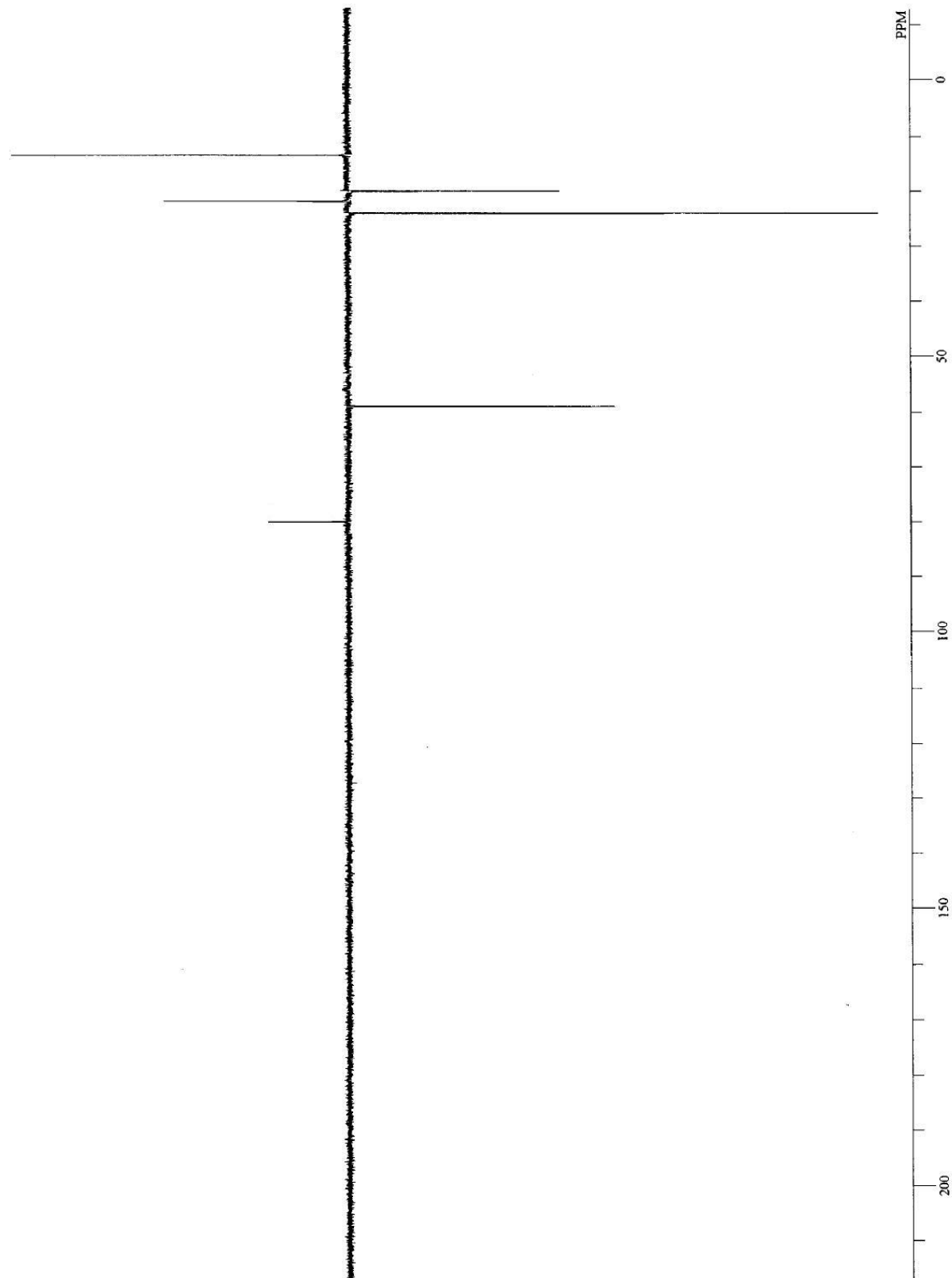


$^{13}\text{C}$  NMR (75 MHz,  $\text{CD}_3\text{CN}$ )

<sup>13</sup>C NMR DEPT 135° (75 MHz, CD<sub>3</sub>CN)

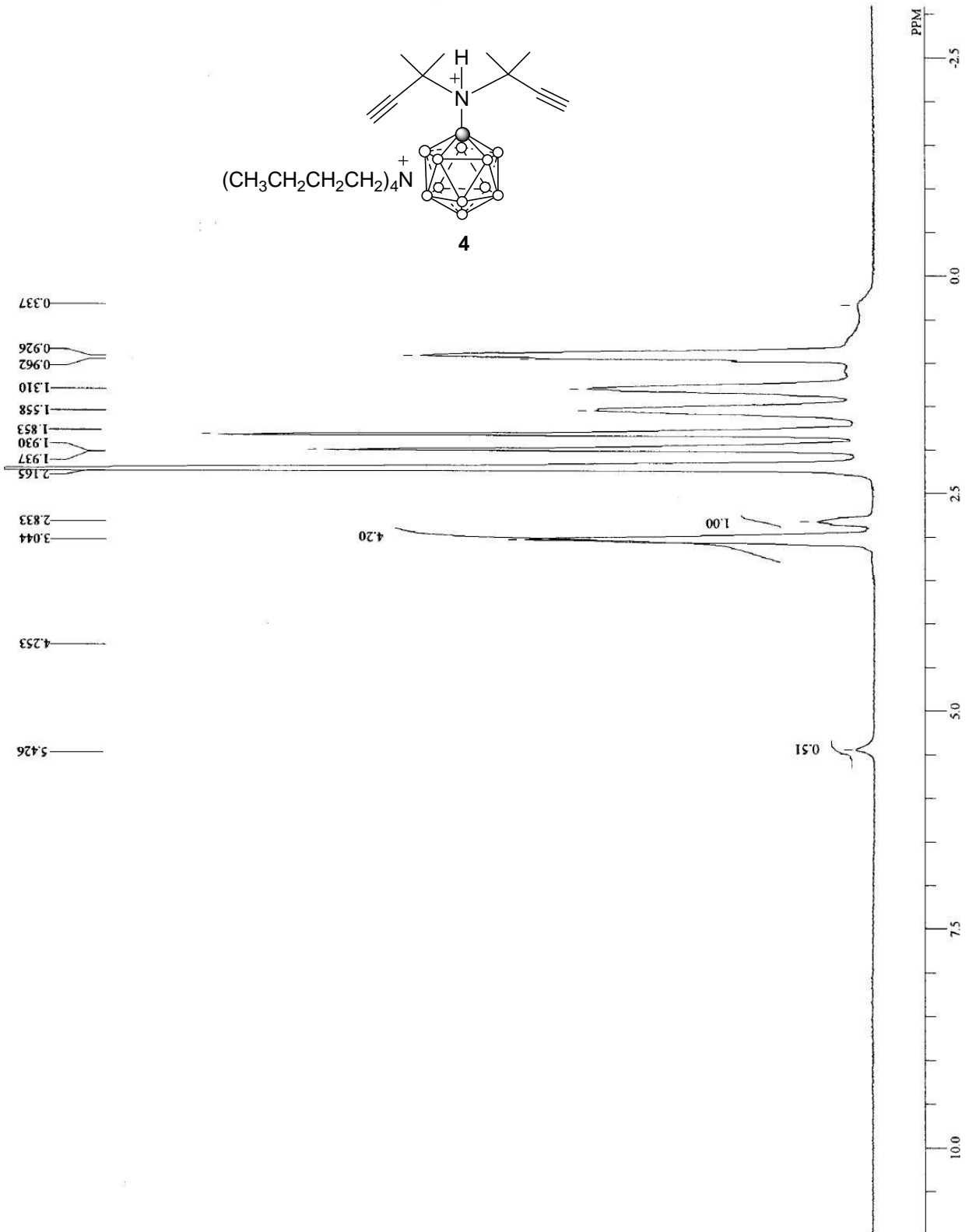


DF COMNT  
 OBNUC 13C  
 OFR 75.45 MHz  
 OBSET 125.70 KHz  
 OBFIN 62.50 Hz  
 PW1 14.00 usec  
 PW2 18.40 usec  
 PW3 27.60 usec  
 PI1 3.5000 msec  
 PI2 1.0000 msec  
 PI3 1.0000 msec  
 LOOP1 1  
 POINT 32768  
 SPO 32768  
 SCANS 1125  
 DUMMY 4  
 FREQU 22662.89 Hz  
 ACQTM 1.4459 sec  
 PD 2.0000 sec  
 RGAIN 27  
 BF 0.80 Hz  
 EXMOD DEPT  
 IRNUC 1H  
 IFR 300.40 MHz  
 IRSET 130.00 KHz  
 IRFIN 1150.00 Hz  
 IRRPW 50 usec  
 IRATN 511  
 CSPED 14 Hz  
 CTEMP 23.7 c  
 XE 17374.10 Hz  
 XS -121.72 Hz



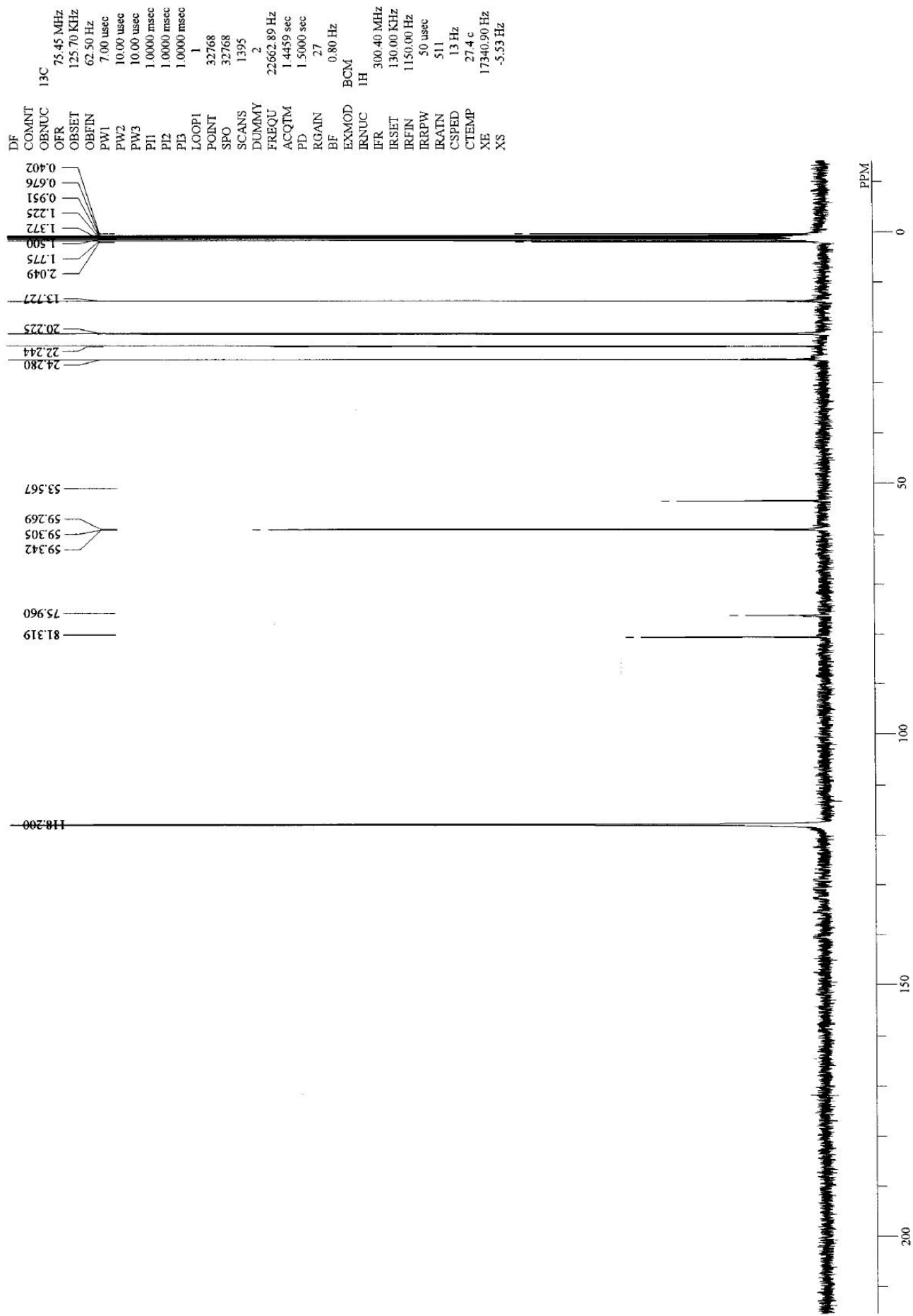
$N,N$ -bis-(1,1-dimethyl-prop-ynyl)amine-undecahydro-*closo*-dodecaborate (1-) tetrabutylammonium salt (**4**)  
<sup>1</sup>H NMR (300 MHz, CD<sub>3</sub>CN)

DF COMANT  
 OBNUC <sup>1</sup>H  
 OFR 300.40 MHz  
 OBSFET 130.00 KHz  
 OBFEN 1150.00 Hz  
 PW1 5.40 usec  
 PW2 10.00 usec  
 PW3 10.00 usec  
 P11 1.0000 msec  
 P12 1.0000 msec  
 P13 1.0000 msec  
 LOOP1 1  
 POINT 32768  
 SPO 32768  
 SCANS 8  
 DUMBY 1  
 FREQU 6015.04 Hz  
 ACQTM 5.4477 sec  
 PD 1.5510 sec  
 RGAIN 16  
 BF 1.30 Hz  
 EXMOD NON  
 IRNUC <sup>1</sup>H  
 IFR 300.40 MHz  
 IRSET 130.00 KHz  
 IRFIN 1150.00 Hz  
 IRRPW 50 usec  
 IRATN 511  
 CSPED 15 Hz  
 CTEMP 23.2 c  
 XE 4226.57 Hz  
 XS 309.86 Hz



<sup>13</sup>C NMR (75 MHz, CD<sub>3</sub>CN)

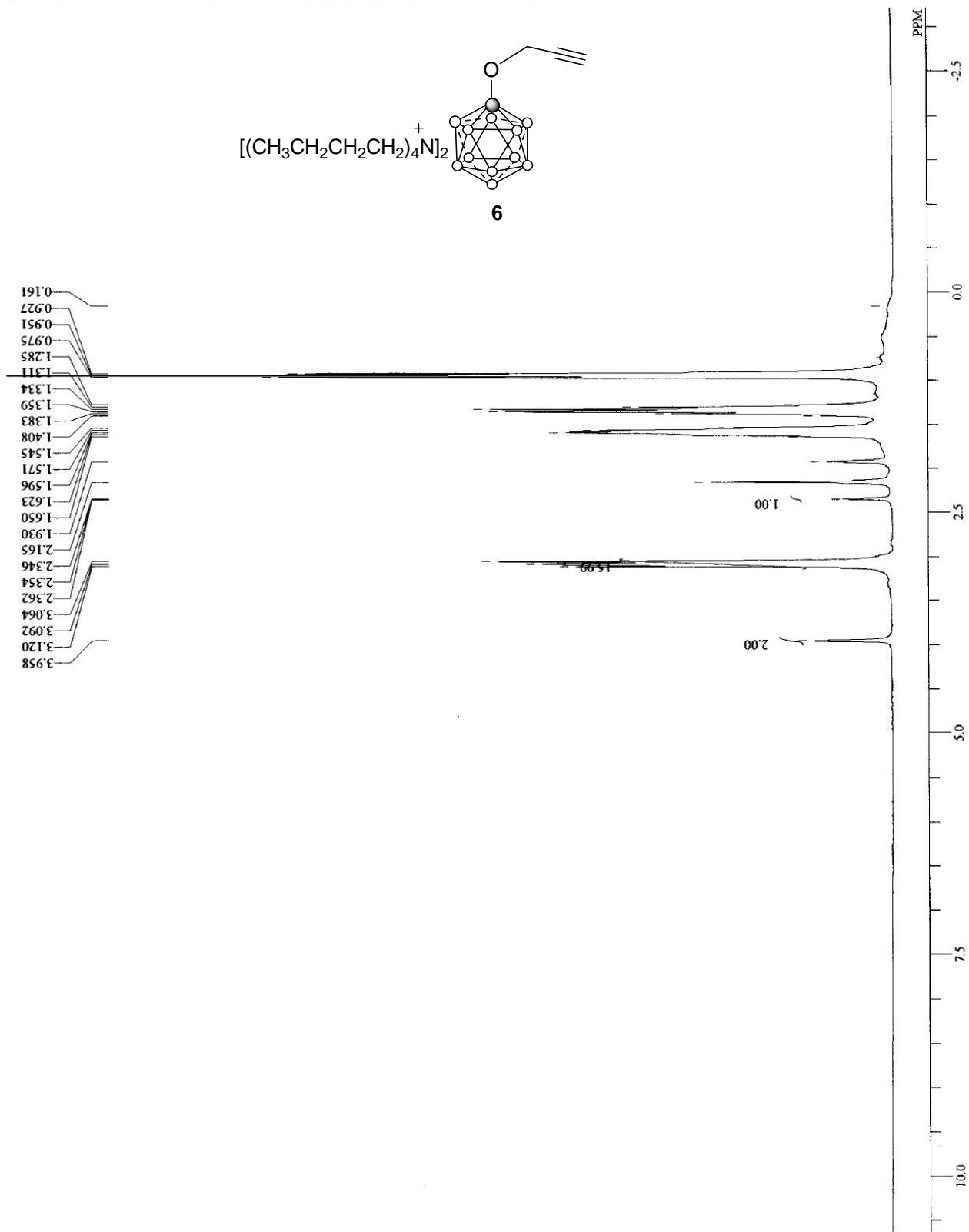
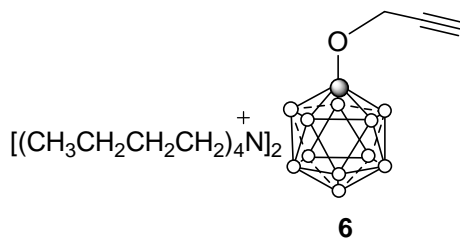




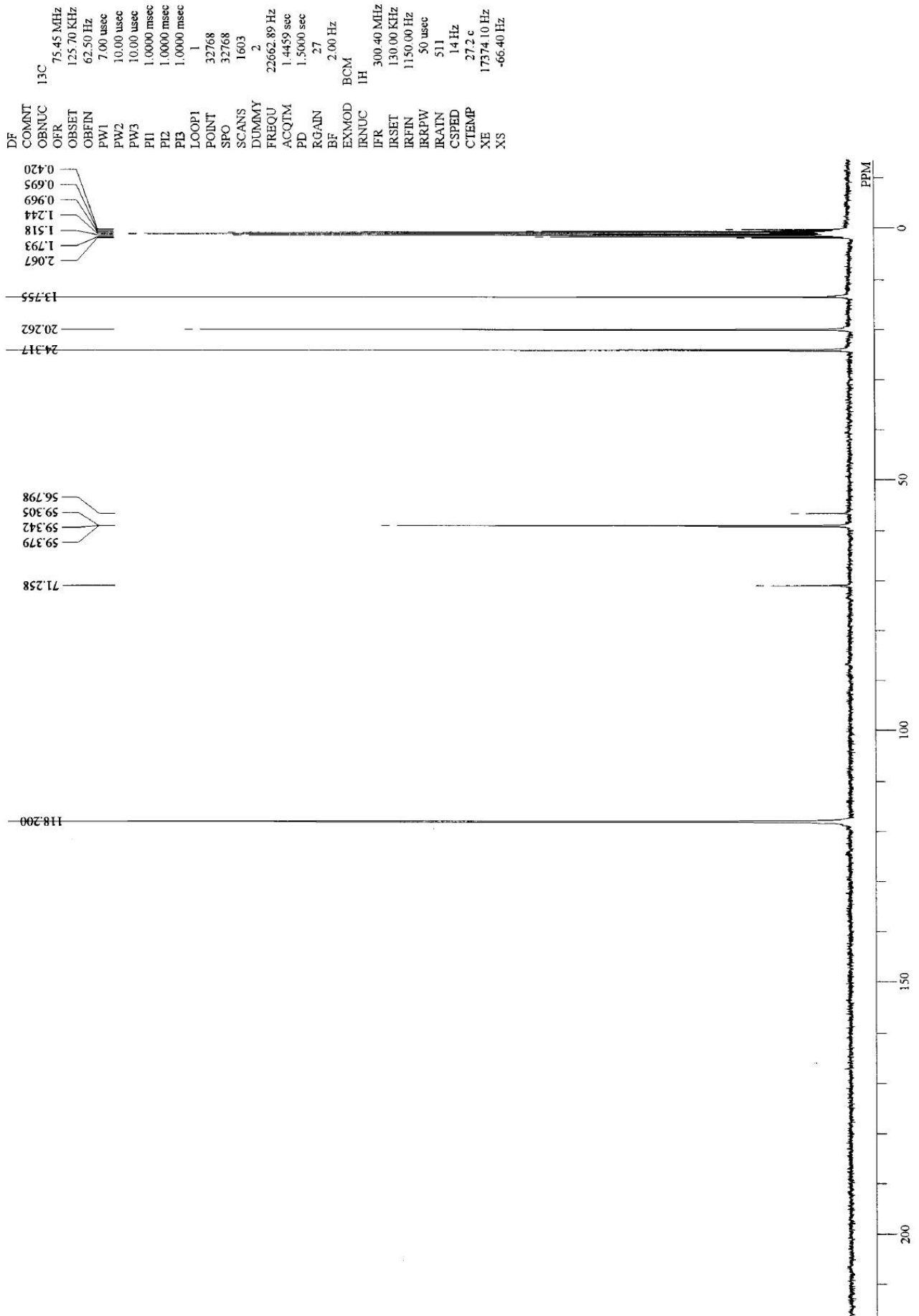
O-(Prop-2-ynyl)hydroxo-undecahydro-closo-dodecaborate (2-) ditetrabutylammonium salt (6)

<sup>1</sup>H NMR (300 MHz, CD<sub>3</sub>CN)

DF 300.40 MHz  
COMNT 130.00 KHz  
OBNUC 1150.00 Hz  
OFR 5.40 usec  
OBSET 10.00 usec  
OBFIN 10.00 usec  
PW1 1.0000 msec  
PW2 1.0000 msec  
PW3 1.0000 msec  
PI1 1.0000 msec  
PI2 1.0000 msec  
PI3 1.0000 msec  
LOOP1 1  
POINT 32768  
SPO 32768  
SCANS 8  
DUMMY 1  
FREQU 6015.04 Hz  
ACQIM 5.4477 sec  
PD 1.5510 sec  
RGAIN 9  
BF 0.80 Hz  
EXMOD NON  
IRNUC 1H  
IFR 300.40 MHz  
IRSET 130.00 KHz  
IRFIN 1150.00 Hz  
IRRPW 50 usec  
IRATN 511  
CSPED 11 Hz  
CTEMP 24.1 c  
XE 4167.83 Hz  
XS 374.47 Hz

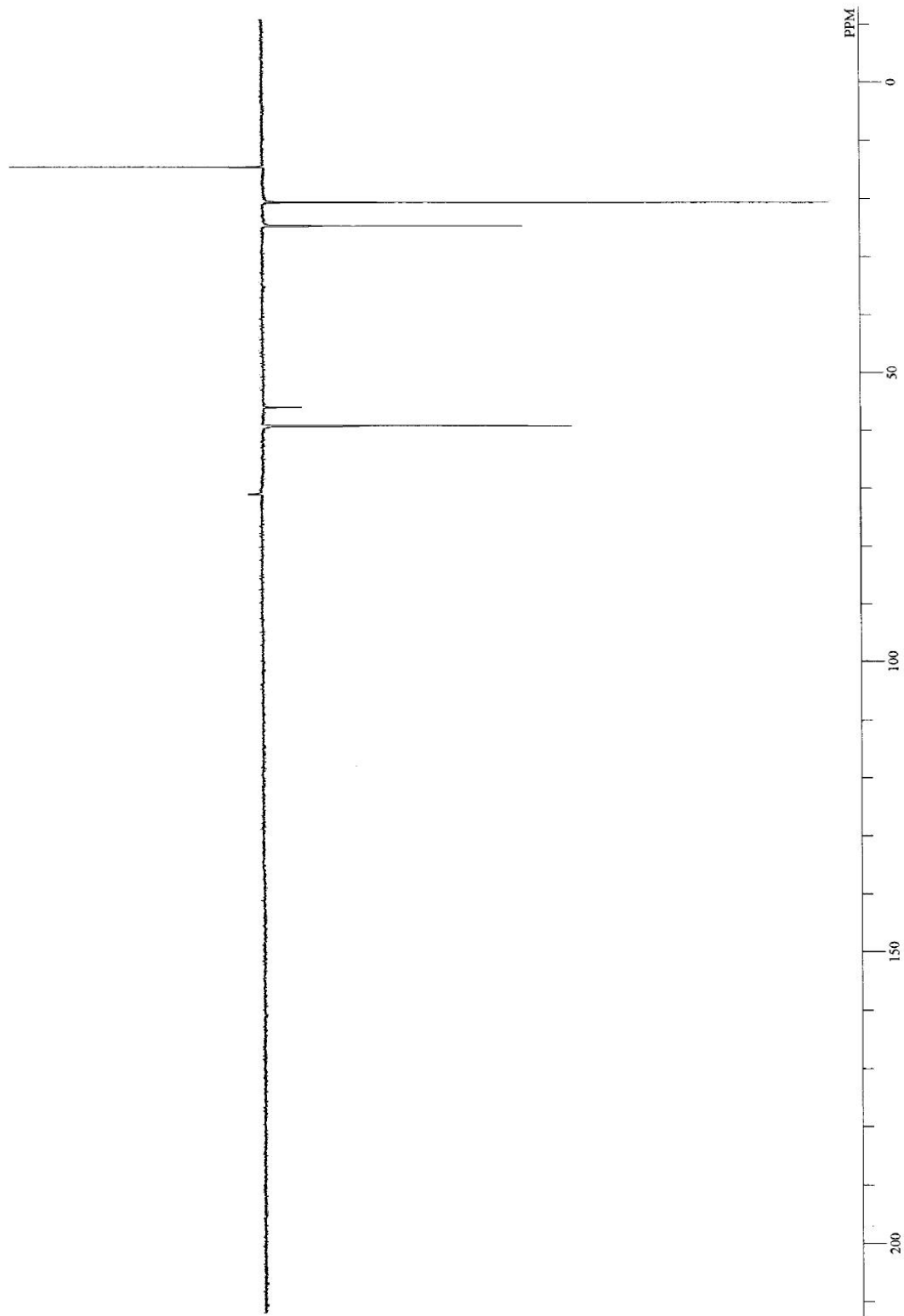


<sup>13</sup>C NMR (75 MHz, CD<sub>3</sub>CN)



<sup>13</sup>C NMR DEPT 135° (75 MHz, CD<sub>3</sub>CN)

DF COMNT  
 OBNUC 13C  
 OFR 75.45 MHz  
 OBSET 125.70 KHz  
 OBFIN 62.50 Hz  
 PW1 14.00 usec  
 PW2 18.40 usec  
 PW3 27.60 usec  
 PI 3.5000 msec  
 PI2 1.0000 msec  
 PI3 1.0000 msec  
 LOOP1 1  
 POINT 32768  
 SFO 32768  
 SCANS 894  
 DUMY 4  
 FREQU 22662.89 Hz  
 ACQTM 1.4459 sec  
 PD 2.0000 sec  
 RGAIN 28  
 BF 2.00 Hz  
 EXMCD DEPT  
 IRNUC 1H  
 IFR 300.40 MHz  
 IRSET 130.00 KHz  
 IRFIN 1150.00 Hz  
 IRRPW 50 usec  
 IRATN 511  
 CSPED 13 Hz  
 CTEMP 26.0 c  
 XE 17108.52 Hz  
 XS 33.20 Hz

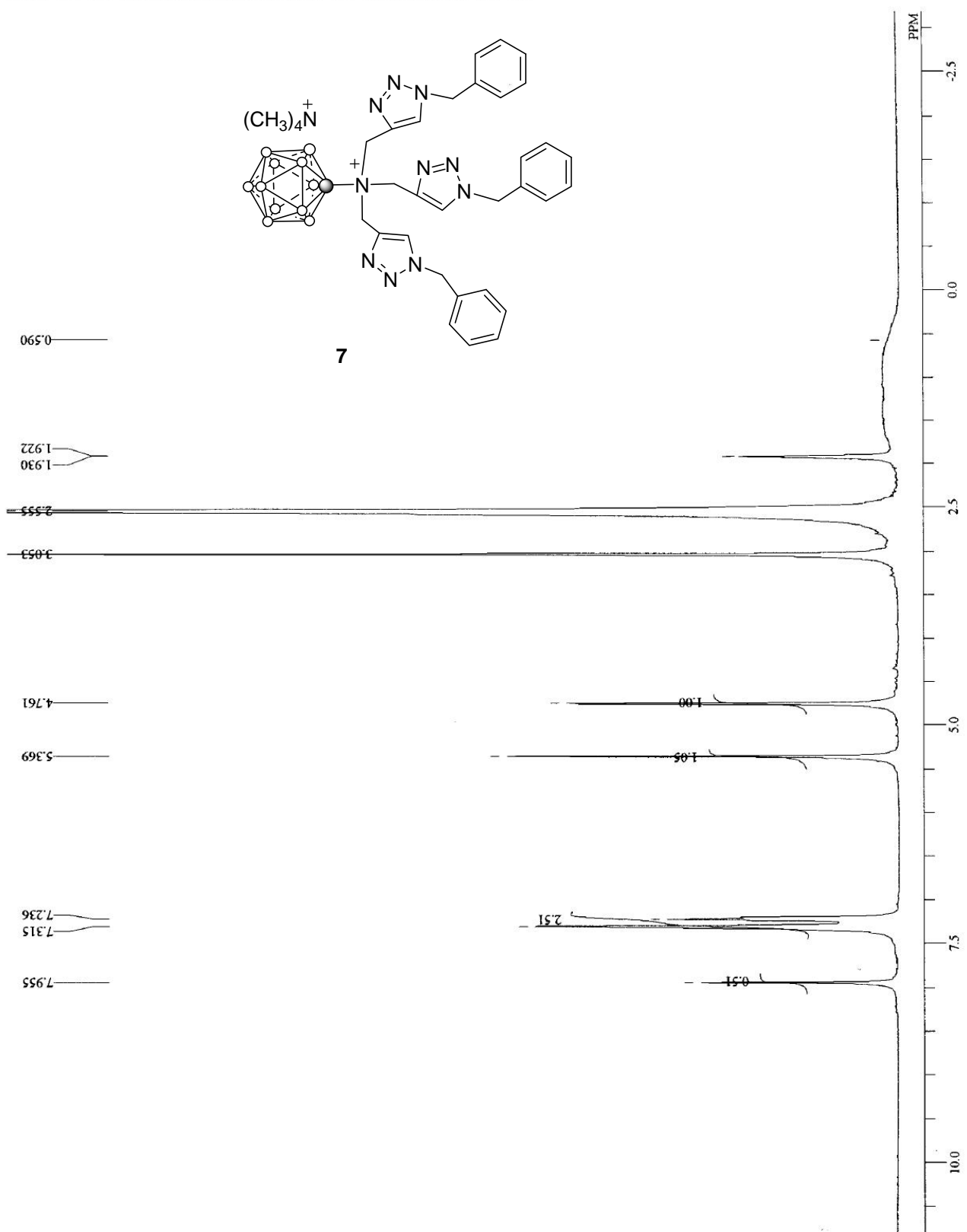


*N,N,N*-Tris[1-benzyl-(1,2,3-triazol-4-yl)methyl]aminoundecahydro-*closo*-dodecaborate tetramethylammonium salt (**7**)

(1-)

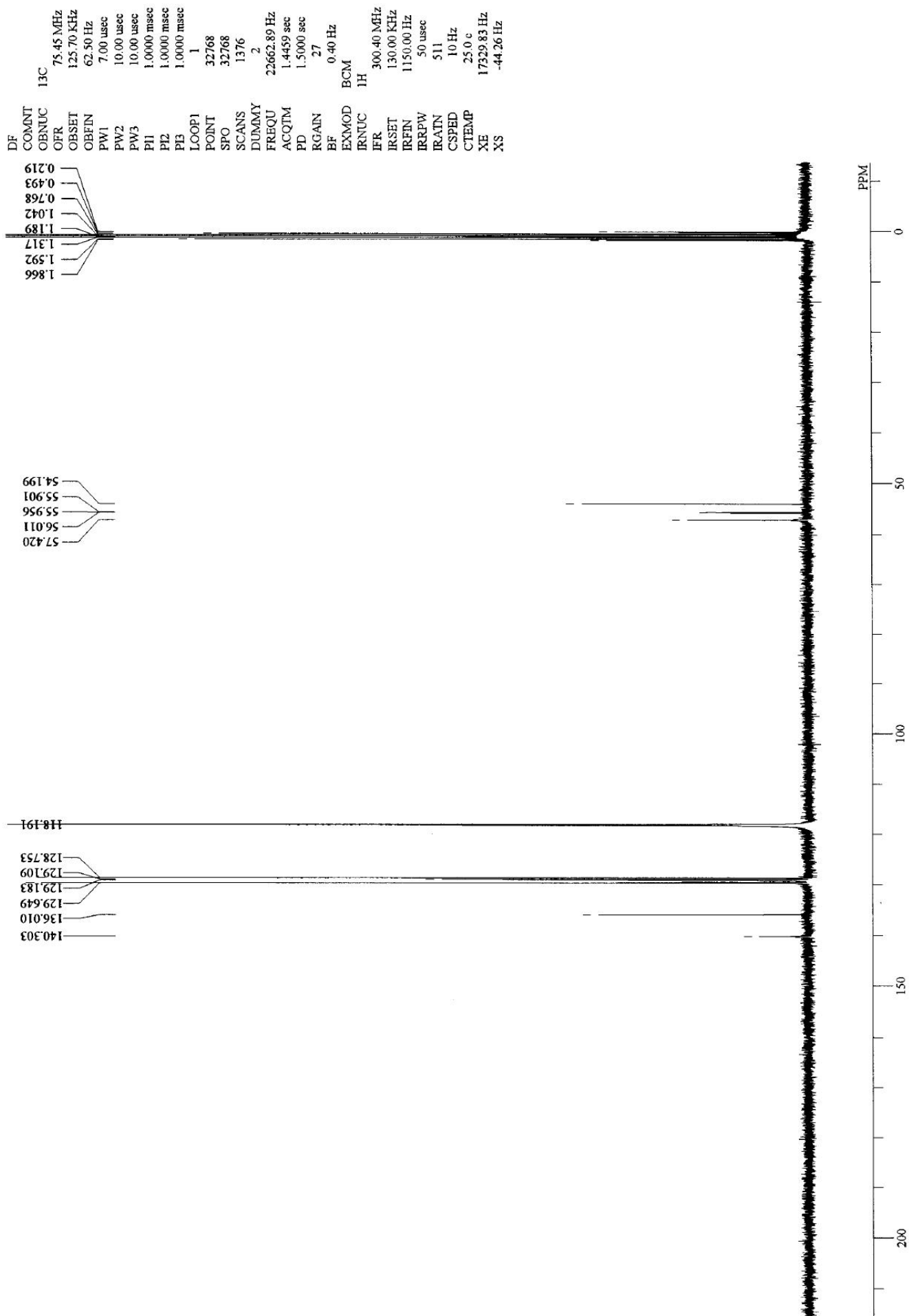
<sup>1</sup>H NMR (300 MHz, CD<sub>3</sub>CN)

DF COMNT  
OBNUC 300.40 MHz  
OFR 130.00 KHz  
OBSET 1150.00 Hz  
OBFIN 5.40 usec  
PW1 10.00 usec  
PW2 10.00 usec  
PW3 10.00 usec  
PI1 1.0000 msec  
PI2 1.0000 msec  
PI3 1.0000 msec  
LOOP1 1  
POINT 32768  
SPO 32768  
SCANS 8  
DUMMY 1  
FREQU 6015.04 Hz  
ACQTM 5.4477 sec  
PD 1.5510 sec  
RGAIN 12  
BF 0.40 Hz  
EXMOD NON  
IRNUC 300.40 MHz  
IFR 130.00 KHz  
IRSET 1150.00 Hz  
IRFIN 50 usec  
IRRPW 511  
IRATN 14 Hz  
CSPED 23.7 c  
CTEMP 4206.01 Hz  
XE 346.57 Hz  
XS



<sup>13</sup>C NMR (75 MHz, CD<sub>3</sub>CN)

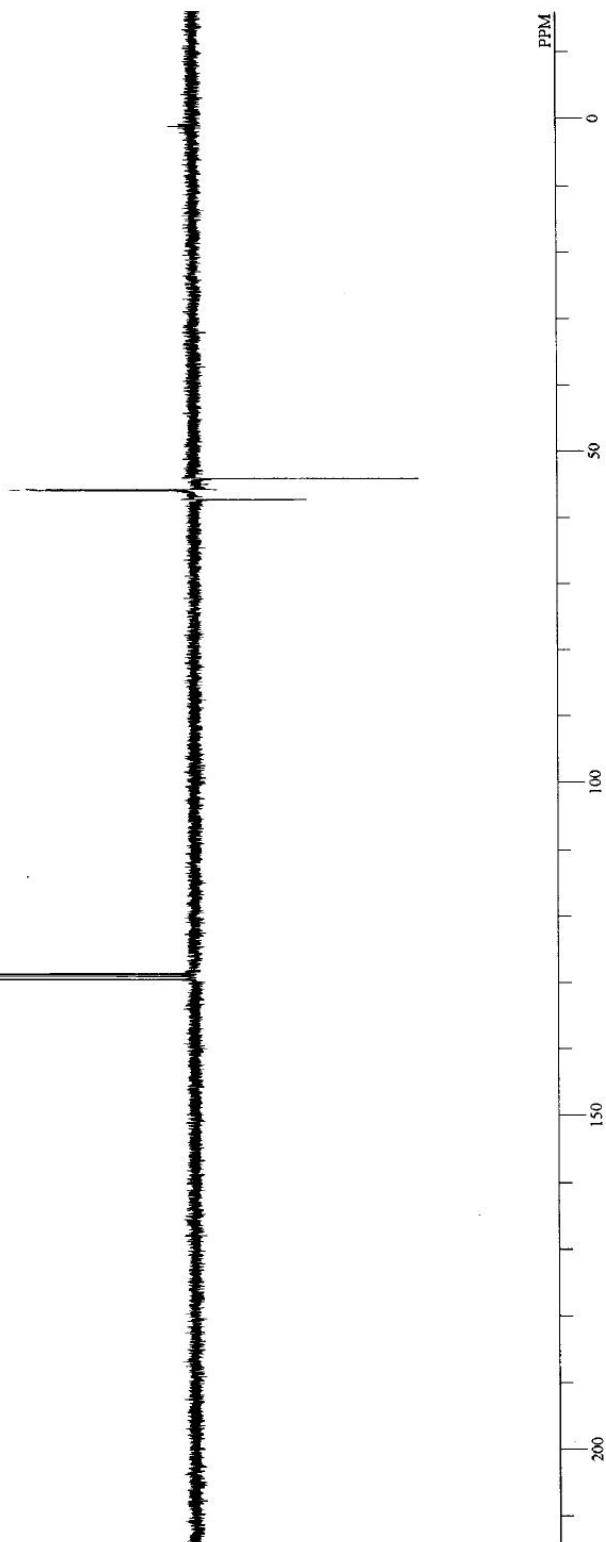
<sup>13</sup>C NMR DEPT 135° (75 MHz, CD<sub>3</sub>CN)



DF COMNT 13C  
 OBNUC 75.45 MHz  
 OFR 125.70 KHz  
 OBSET 62.50 Hz  
 OBFIN 14.00 usec  
 PW1 18.40 usec  
 PW3 27.60 usec  
 PH 3.5000 msec  
 PI2 1.0000 msec  
 PI3 1.0000 msec  
 LOOP1 1  
 POINT 32768  
 SPO 32768  
 SCANS 253  
 DUMMY 4  
 FREQU 22662.89 Hz  
 ACQTM 1.4459 sec  
 PD 2.0000 sec  
 RGAIN 28  
 BF 0.40 Hz  
 EXMOD DEPT  
 IRNUC 1H  
 IFR 300.40 MHz  
 IRSET 130.00 KHz  
 IRFIN 1150.00 Hz  
 IRRPW 50. usec  
 IRATN 511  
 CSPED 14 Hz  
 CTEMP 23.4 c  
 XE 17429.43 Hz  
 XS 82.99 Hz

57.420  
 56.002  
 55.947  
 55.892  
 54.189

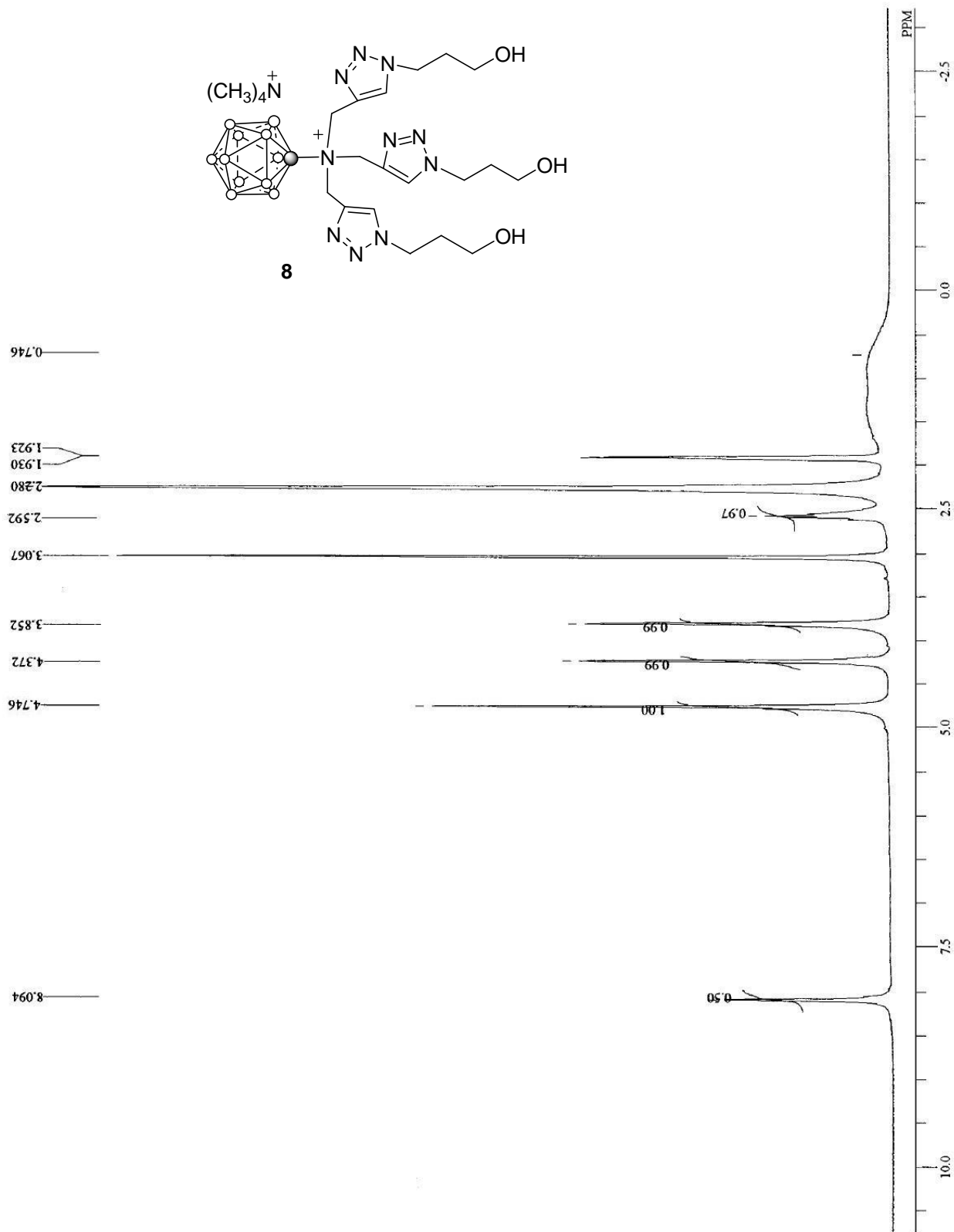
129.649  
 129.192  
 129.109  
 128.753



*N,N,N*-Tris-[1-(3-hydroxypropyl)-(1,2,3-triazol-4-yl)methyl]aminoundecahydro-*closo*-dodecaborate tetramethylammonium salt (**8**) (1-)

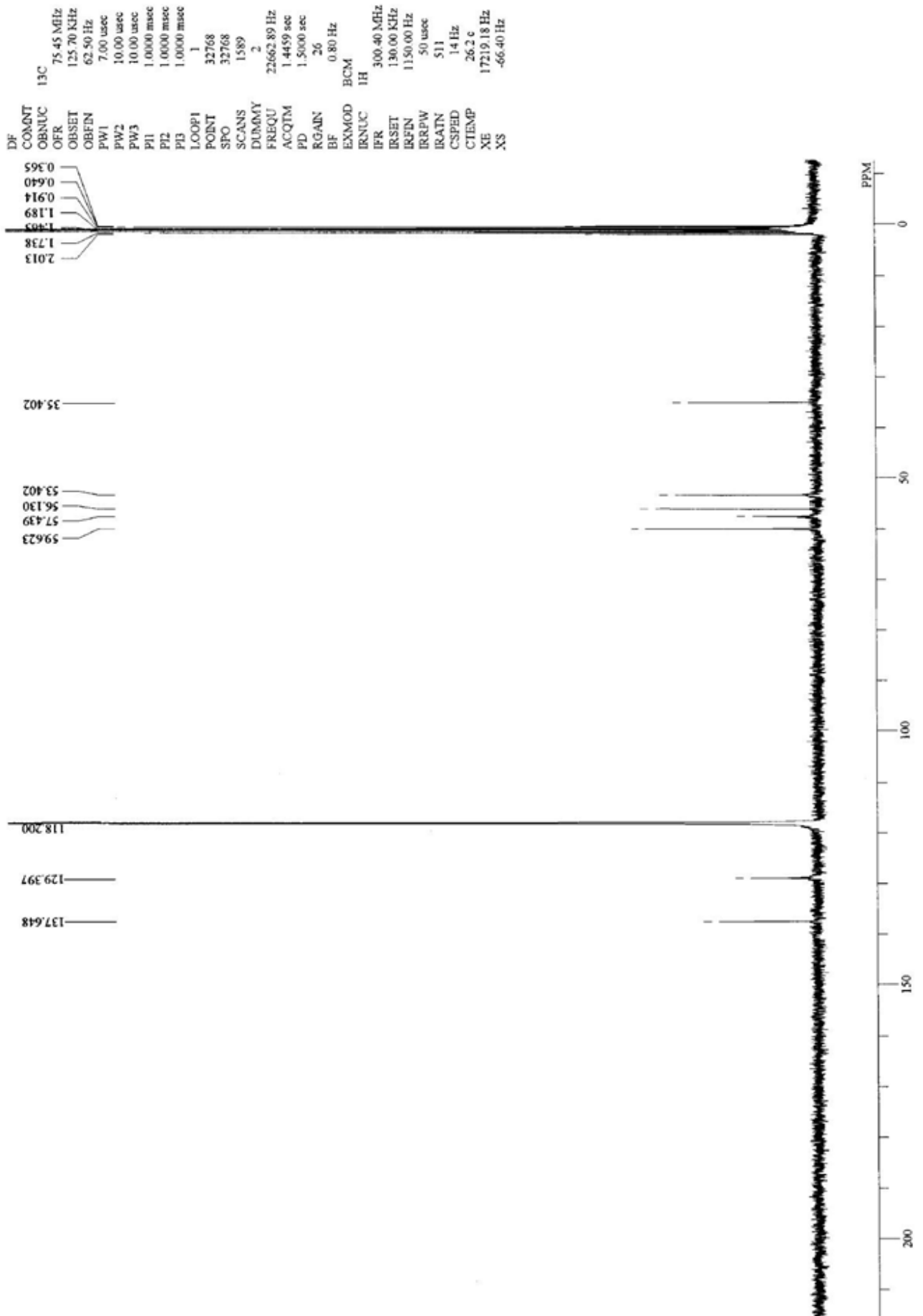
<sup>1</sup>H NMR (300 MHz, CD<sub>3</sub>CN)

DF COMNT  
OBNUC 300.40 MHz  
OFR 130.00 KHz  
OBSET 1150.00 Hz  
OBFIN 5.40 usec  
PW1 10.00 usec  
PW2 10.00 usec  
PW3 10.00 usec  
P11 1.0000 msec  
P12 1.0000 msec  
P13 1.0000 msec  
LOOP1 1  
POINT 32768  
SPO 32768  
SCANS 8  
DUMMY 1  
FREQU 6015.04 Hz  
ACQTM 5.4477 sec  
PD 1.5510 sec  
RGAIN 16  
BF 0.40 Hz  
NON  
IRNUC 300.40 MHz  
IFR 130.00 KHz  
IRSET 1150.00 Hz  
IRFIN 50 usec  
IRRPW 511  
IRATN 8 Hz  
CSPED 24.7 c  
CTEMP 4200.14 Hz  
XE 358.32 Hz  
XS



<sup>13</sup>C NMR (75 MHz, CD<sub>3</sub>CN)



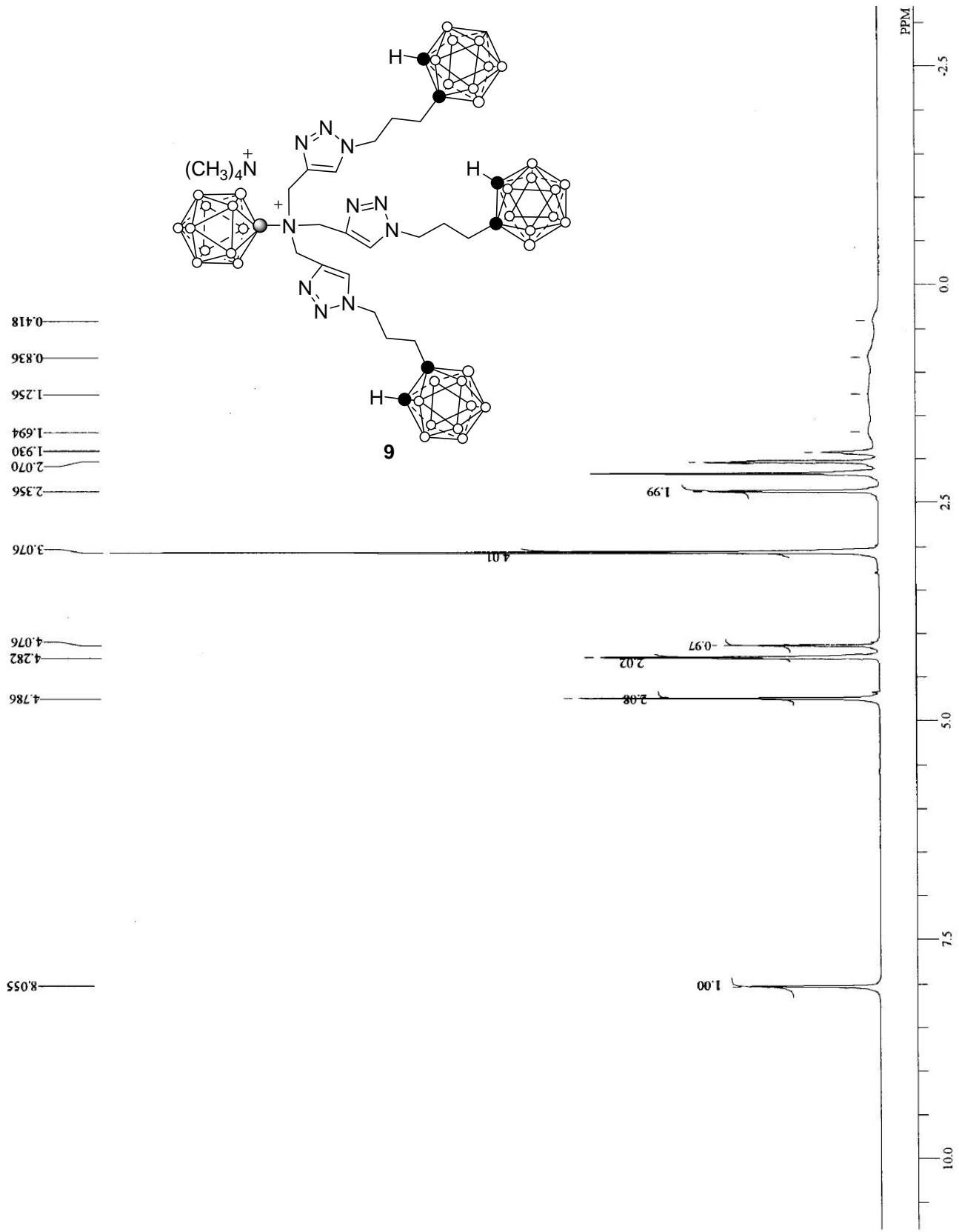


*N,N,N*-Tris-[1-(3-*o*-carboranylpropyl)-(1,2,3-triazol-4-yl)methyl]aminoundecahydro-*closo*-dodecaborate (1-)

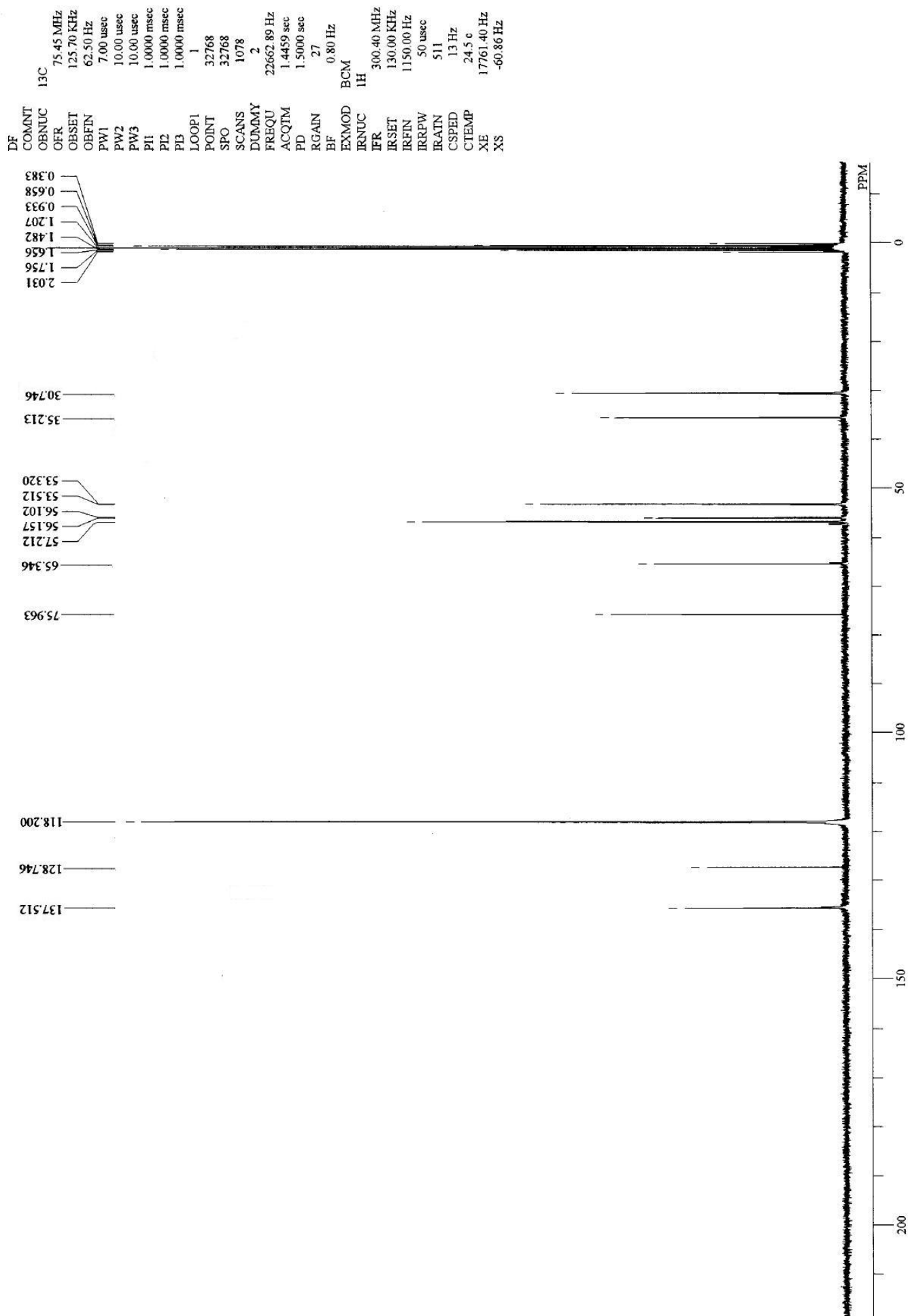
tetramethylammonium salt (**9**)

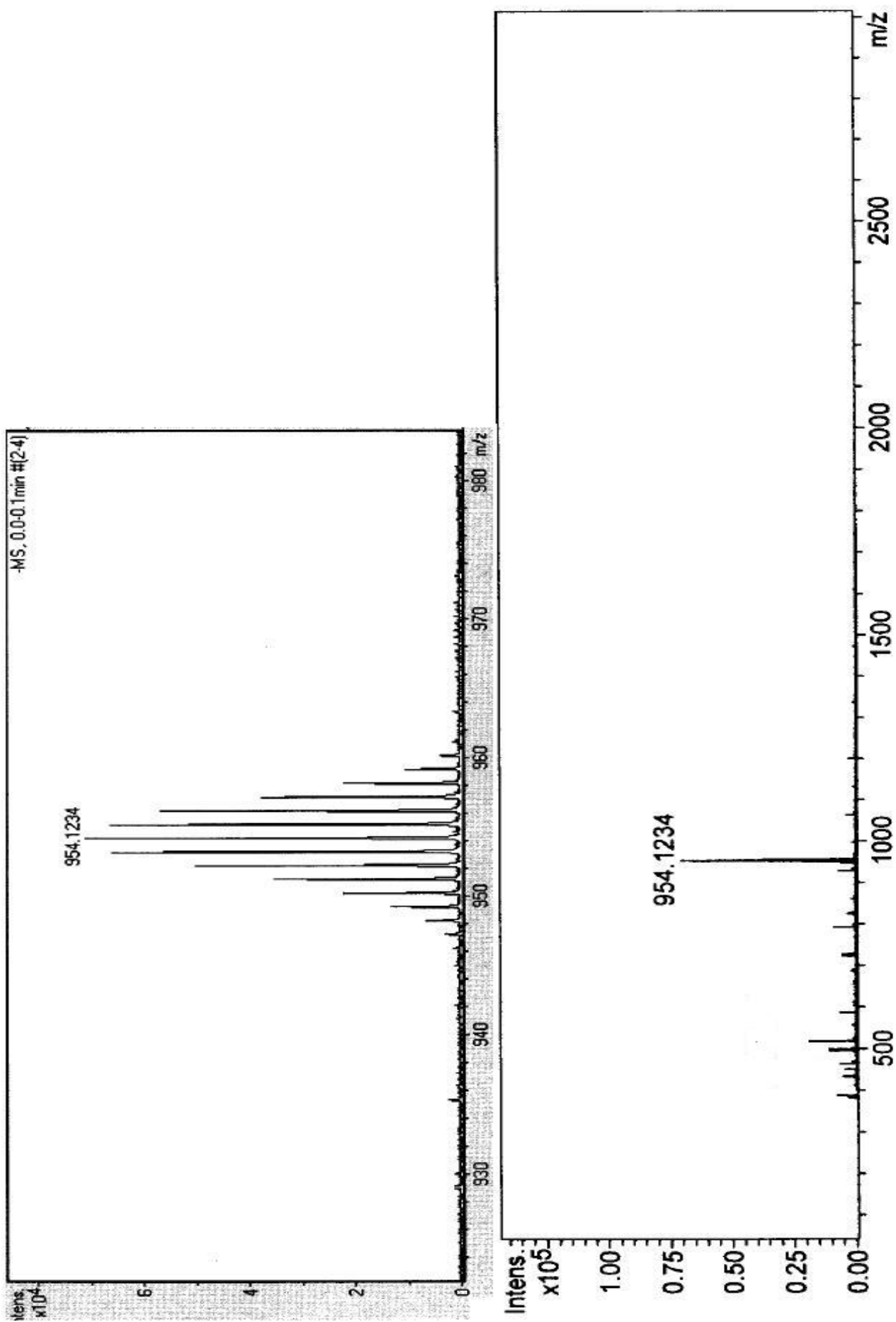
<sup>1</sup>H NMR (300 MHz, CD<sub>3</sub>CN)

DF 300.40 MHz  
 COMNT 130.00 KHz  
 OBNUC 1150.00 Hz  
 OFR 5.40 usec  
 OBSET 10.00 usec  
 OBFIN 10.00 usec  
 PW1 1.0000 msec  
 PW2 1.0000 msec  
 PW3 1.0000 msec  
 P11 1.0000 msec  
 P12 1.0000 msec  
 P13 1.0000 msec  
 LOOP1 1  
 POINT 32768  
 SPO 32768  
 SCANS 8  
 DUMMY 1  
 FREQU 6015.04 Hz  
 ACQTM 5.4477 sec  
 PD 1.5510 sec  
 RGAIN 12  
 BF 1.30 Hz  
 EXMOD NON  
 IRNUC 1H  
 IFR 300.40 MHz  
 IRSET 130.00 KHz  
 IRFIN 1150.00 Hz  
 IRRPW 50 usec  
 IRATN 511  
 CSPED 12 Hz  
 CTEMP 22.6 c  
 XE 4206.01 Hz  
 XS 346.57 Hz



<sup>13</sup>C NMR (75 MHz, CD<sub>3</sub>CN)

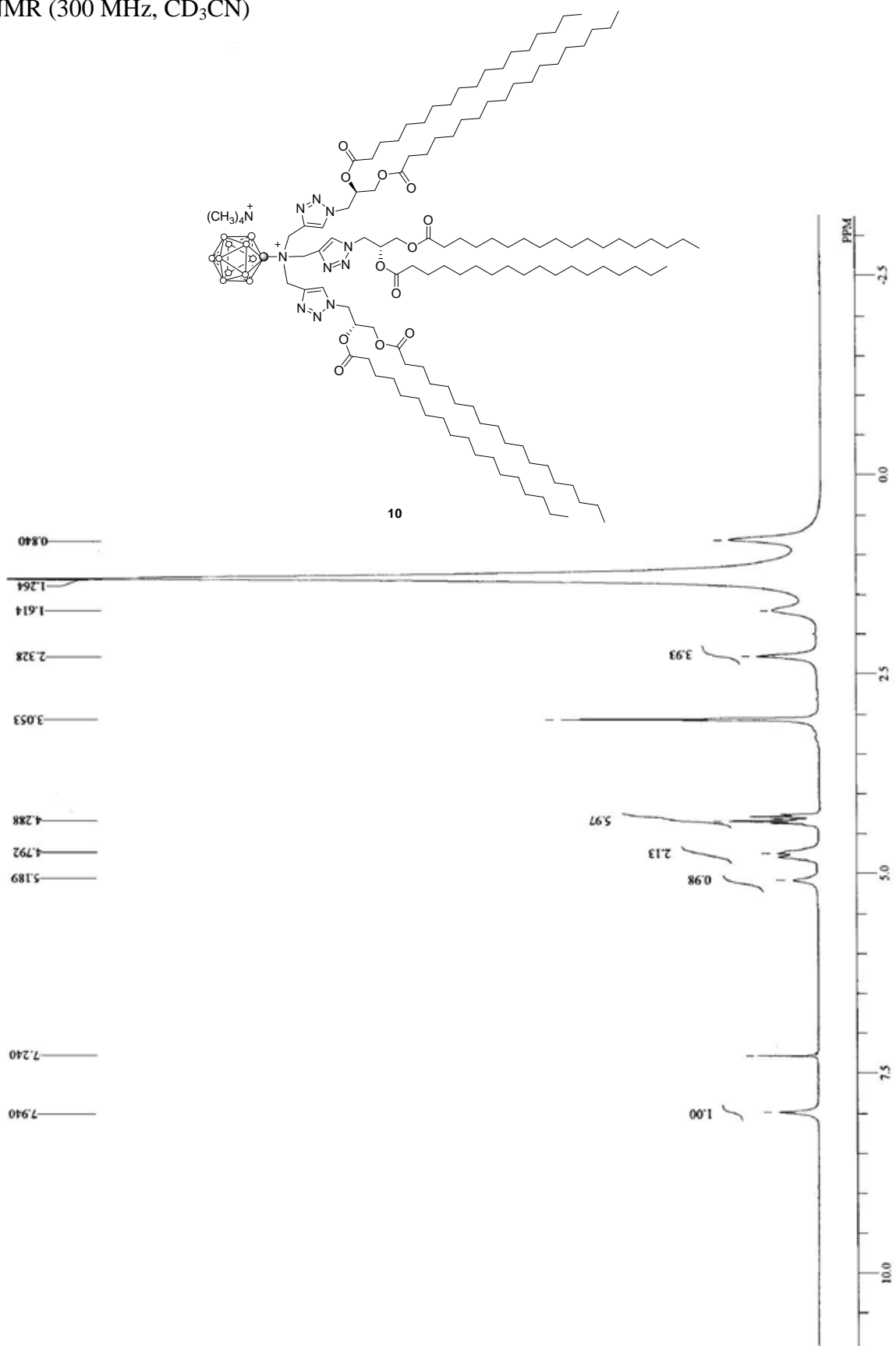




*N,N,N*-Tris-

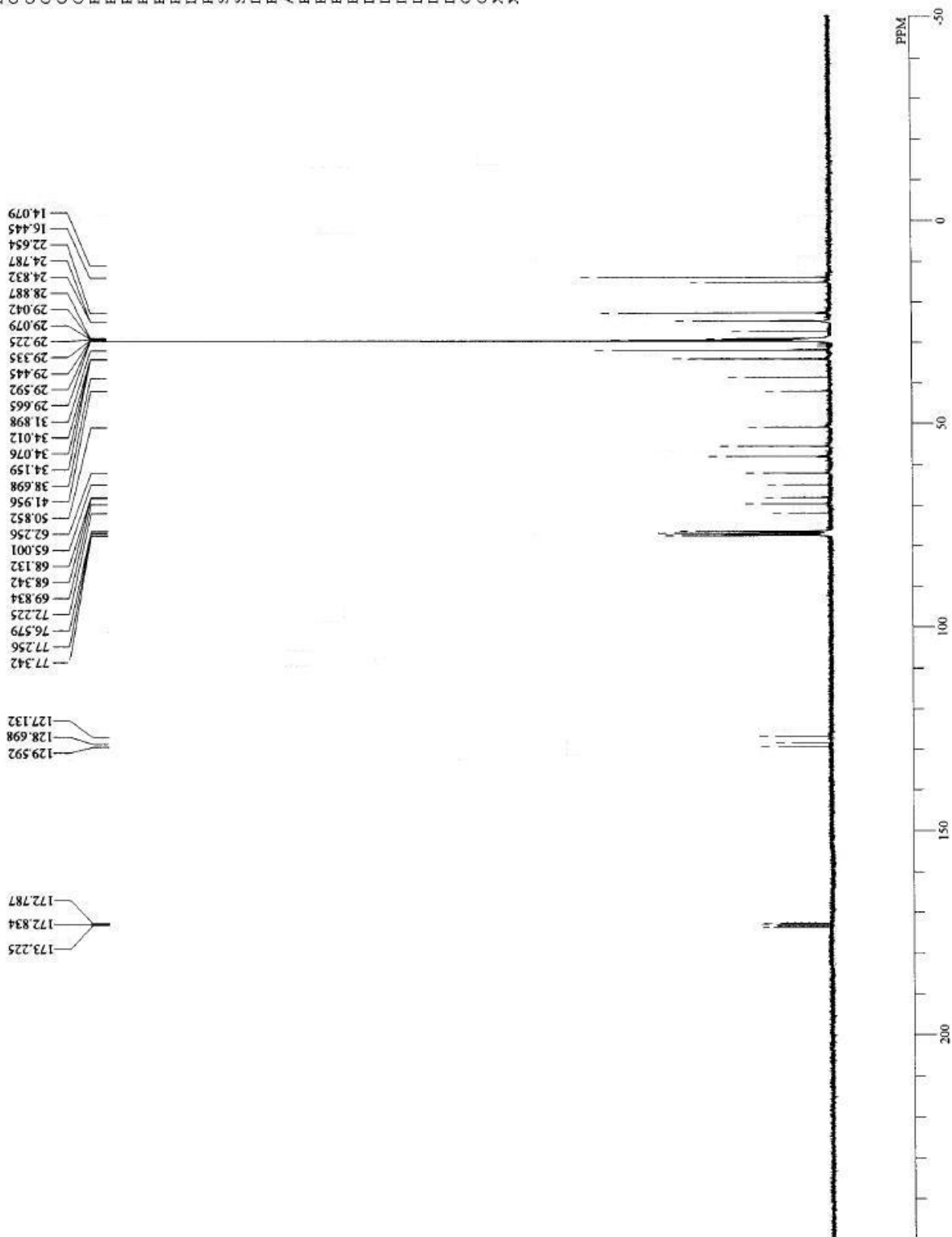
[1-(1,2-*O*-distearoyl-*sn*-3-glycerol)-(1',2',3'-triazol-4yl)methyl]aminoundecahydro-*closo*-dodecaborate (1-)  
tetramethylammonium salt (**10**)

<sup>1</sup>H NMR (300 MHz, CD<sub>3</sub>CN)

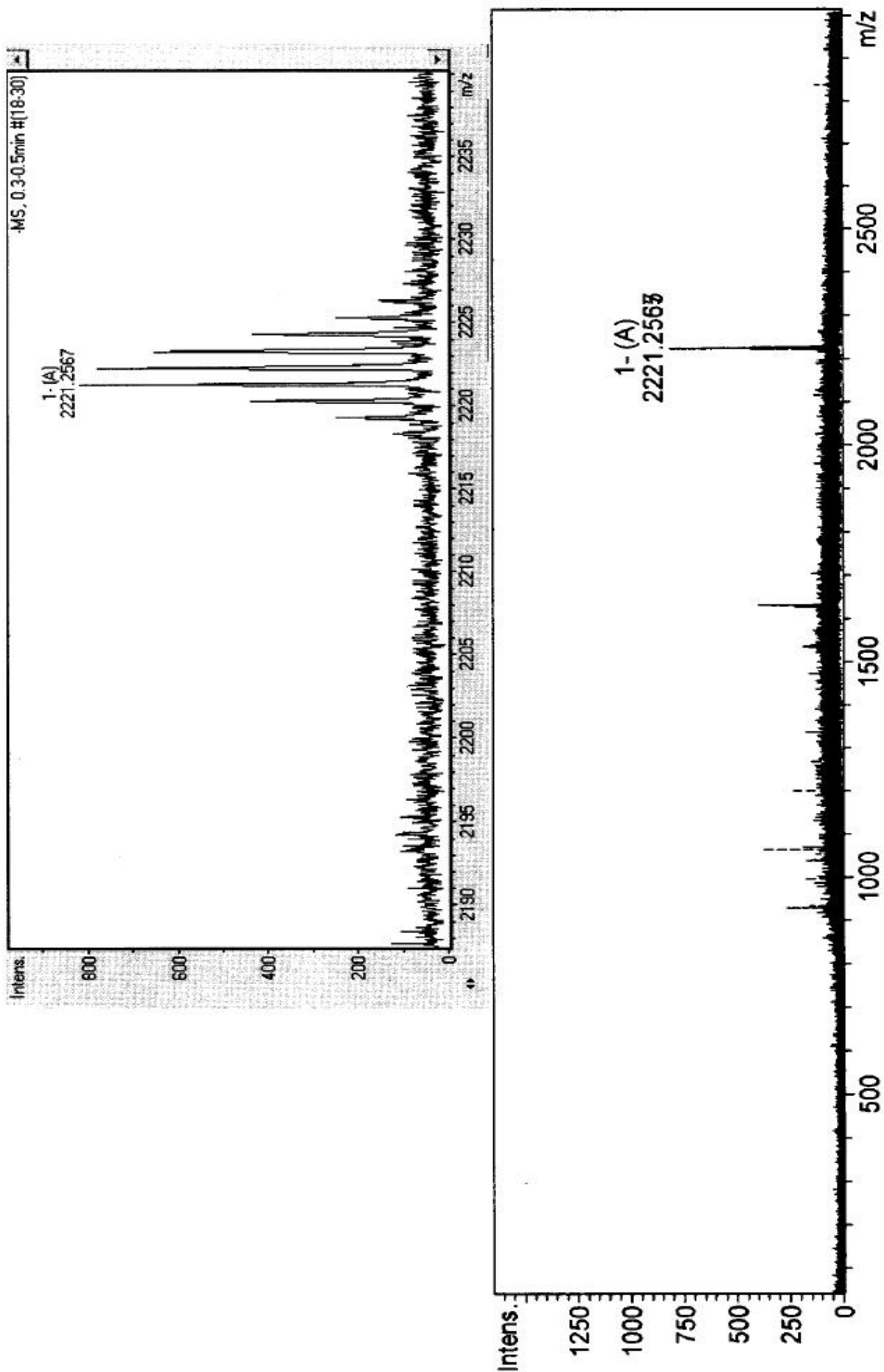


<sup>13</sup>C NMR (75 MHz, CD<sub>3</sub>CN)

<sup>13</sup>C  
 DF  
 COMNT  
 OBNUC  
 OFR  
 OBSSET  
 OBFIN  
 PW1  
 PW2  
 PW3  
 P1  
 P2  
 P3  
 LOOP1  
 POINT  
 SPO  
 SCANS  
 DUMY  
 FREQU  
 ACQTM  
 PD  
 RGAIN  
 BF  
 EXMOD  
 IRNUC  
 IFR  
 IRSET  
 IRFIN  
 IRRPW  
 IRAIN  
 CSPED  
 CTEMP  
 XE  
 XS  
 75.45 MHz  
 125.70 KHz  
 62.50 Hz  
 7.00 usec  
 10.00 usec  
 10.00 usec  
 1.0000 msec  
 1.0000 msec  
 1.0000 msec  
 1  
 32768  
 32768  
 2500  
 2  
 22662.89 Hz  
 1.4459 sec  
 1.5000 sec  
 27  
 0.80 Hz  
 BCM  
 1H  
 300.40 MHz  
 130.00 KHz  
 1150.00 Hz  
 50 usec  
 511  
 10 Hz  
 15.1 c  
 22662.89 Hz  
 0.00 Hz



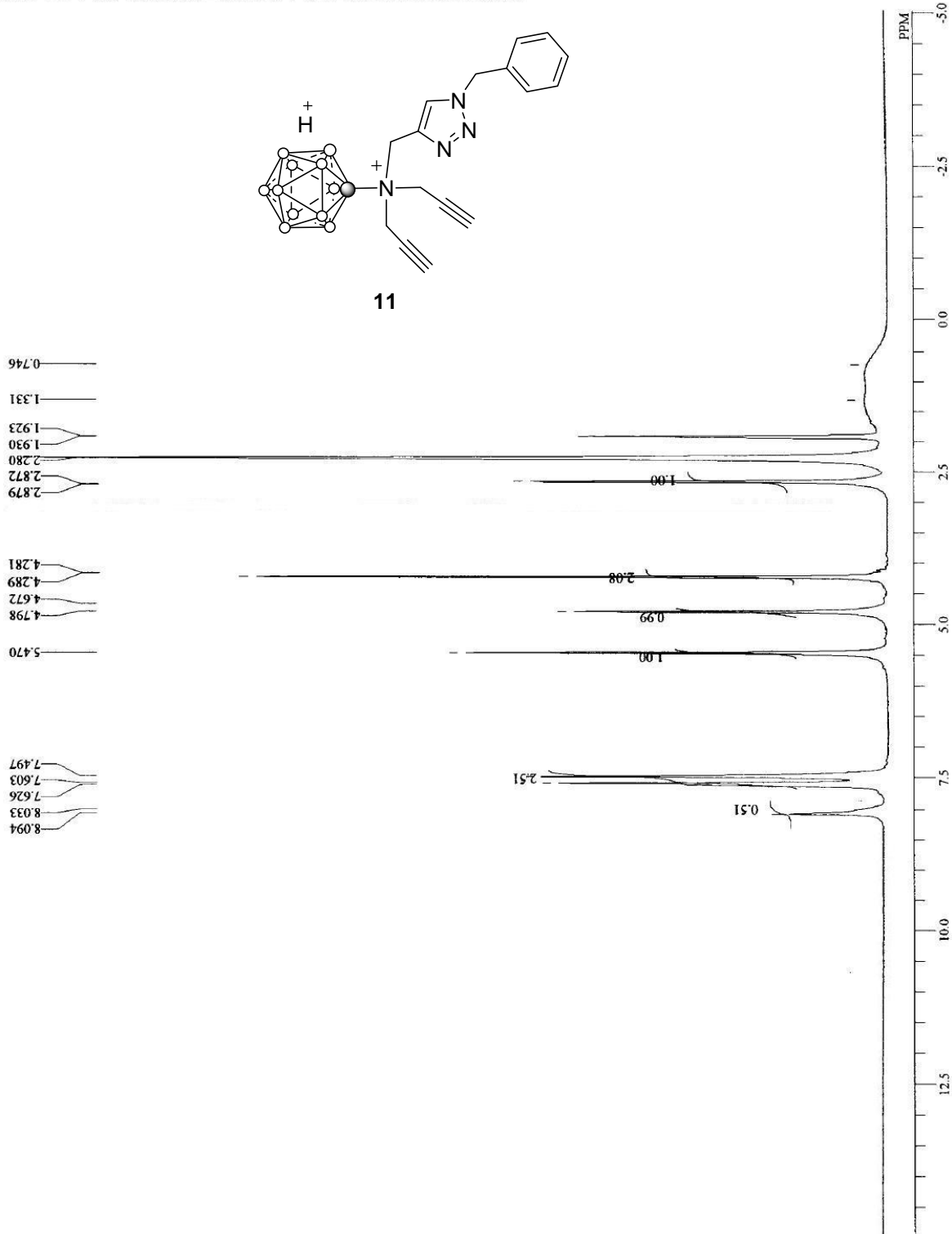
ESI negative-MS Spectrum (MicrOTOF 169)



*N,N,N*-Tris-*N,N*-Bis(Prop-2-ynyl)-*N*-[1-benzyl-(1,2,3-triazol-4-yl)methyl]aminoundecahydro-*closo*-dodecaborate (1-) (**11**)

<sup>1</sup>H NMR (300 MHz, CD<sub>3</sub>CN)

DF 300.40 MHz  
 CONTC 130.00 KHz  
 OBNUC 1150.00 Hz  
 OFR 5.40 usec  
 OBSET 10.00 usec  
 OBFIN 10.00 usec  
 PW1 1.0000 msec  
 PW2 1.0000 msec  
 PW3 1.0000 msec  
 PI1 1.0000 msec  
 PI2 1.0000 msec  
 PI3 1.0000 msec  
 LOOP1 1  
 POINT 32768  
 SFO 32768  
 SCANS 8  
 DUMMT 1  
 FREQU 6015.04 Hz  
 ACQTM 5.4477 sec  
 PD 1.5510 sec  
 RGAIN 16  
 BF 0.40 Hz  
 EXMOD NON  
 IRNUC 1H  
 IFR 300.40 MHz  
 IRSET 130.00 KHz  
 IRFIN 1150.00 Hz  
 IRRPW 50 usec  
 IRATN 511  
 CSPED 8 Hz  
 CTEMP 24.7 c  
 XE 6015.04 Hz  
 XS 0.00 Hz



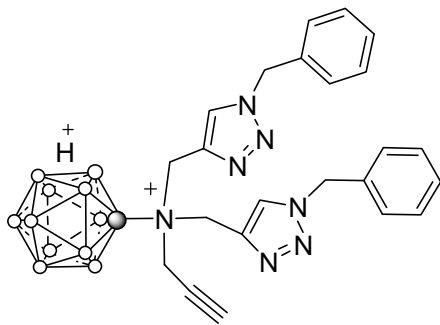


*N*-(Prop-2-ynyl)-*N,N*-bis[1-benzyl-(1,2,3-triazol-4-yl)methyl]aminoundecahydro-*closo*-dodecaborate (1-)

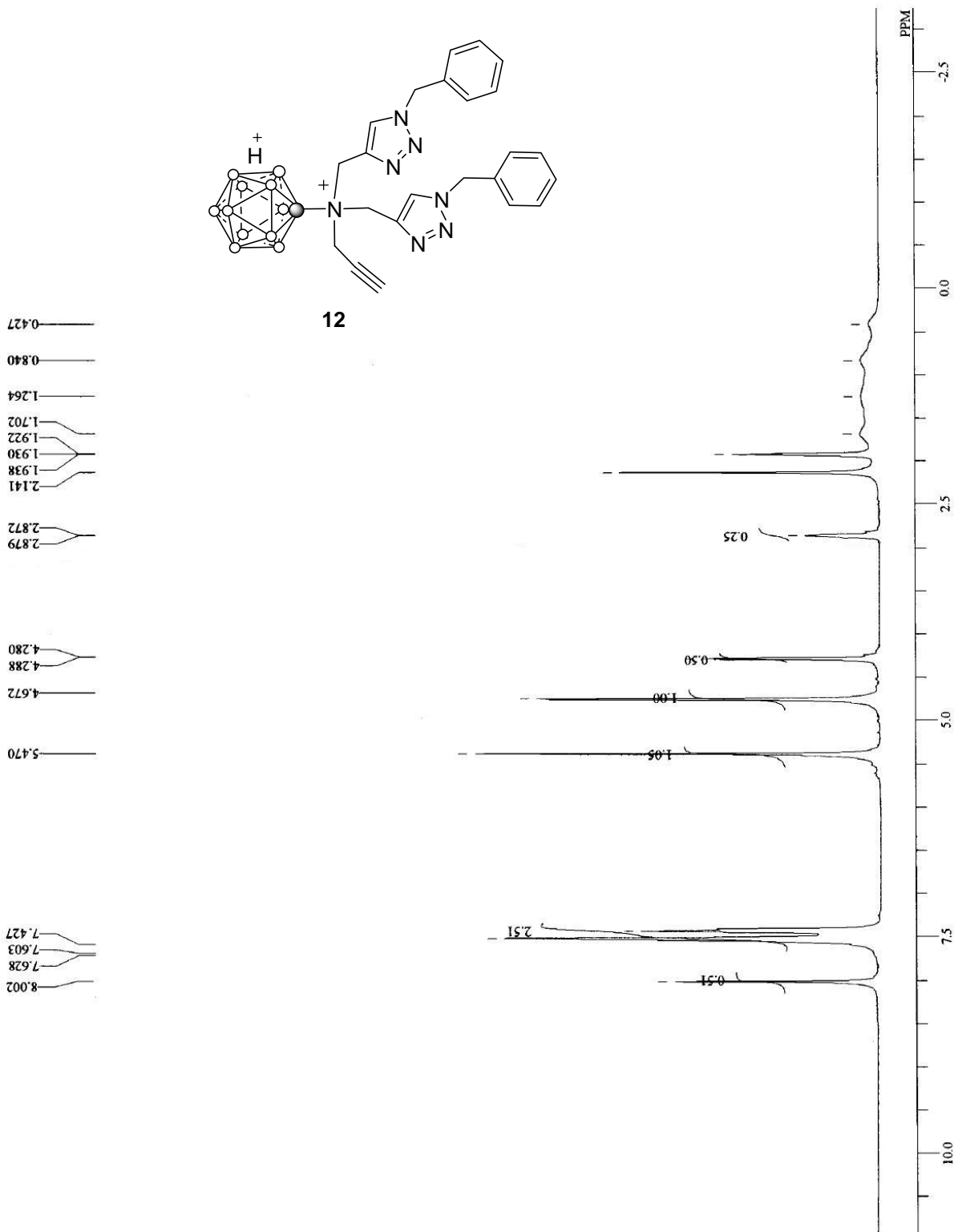
(12)

<sup>1</sup>H NMR (300 MHz, CD<sub>3</sub>CN)

DF 300.40 MHz  
 COMNT 130.00 KHz  
 OBNUC 1150.00 Hz  
 OFR 5.40 usec  
 OBSSET 10.00 usec  
 OBFEN 10.00 usec  
 PW1 1.0000 msec  
 PW2 1.0000 msec  
 PW3 1.0000 msec  
 P11 1.0000 msec  
 P12 1.0000 msec  
 P13 1.0000 msec  
 LOOP1 1  
 POINT 32768  
 SPO 32768  
 SCANS 8  
 DUMMY 1  
 FRBQU 6015.04 Hz  
 ACQTM 5.4477 sec  
 PD 1.5510 sec  
 RGAIN 15  
 BF 1.30 Hz  
 EXMOD NON  
 IRNUC 300.40 MHz  
 IFR 130.00 KHz  
 IRFN 1150.00 Hz  
 IRRPW 50 usec  
 IRATN 511  
 CSPIED 10 Hz  
 CTIEMP 22.5 c  
 XE 4255.94 Hz  
 XS 336.29 Hz



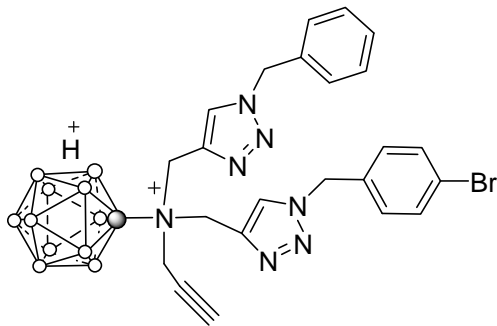
12



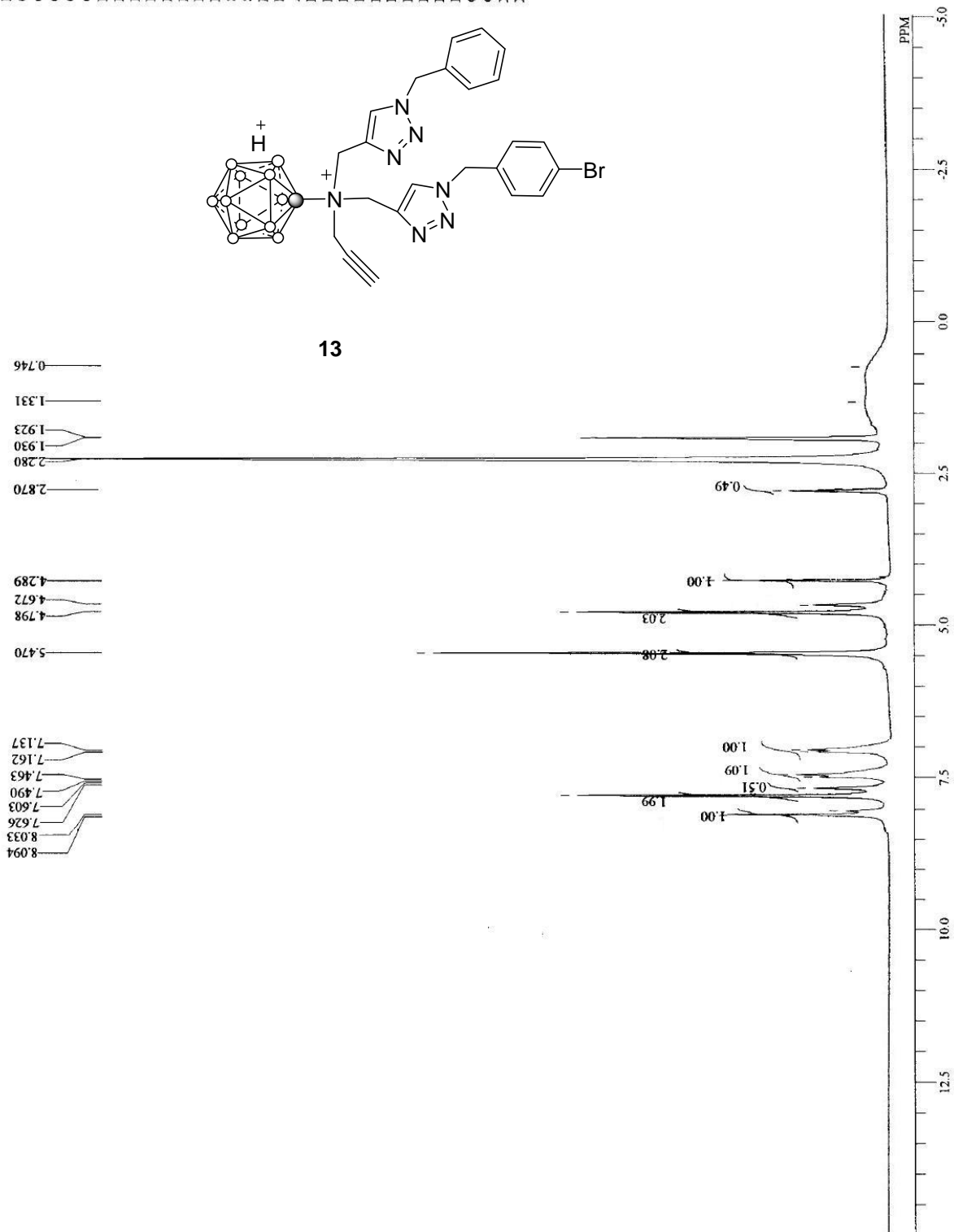
*N*-(Prop-2-ynyl)-*N*-[1-benzyl-(1,2,3-triazol-4-yl)methyl]-*N*-[1-(*p*-bromobenzyl-1,2,3-triazol-4yl)methyl]ammonium noundecahydro-*closo*-dodecaborate (1-) tetramethylammonium salt (**13**)

<sup>1</sup>H NMR (300 MHz, CD<sub>3</sub>CN)

DF COMNT 300.40 MHz  
 OBNUC 130.00 KHz  
 OFR 1150.00 Hz  
 OBSET 5.40 usec  
 OBFIN 10.00 usec  
 PW1 10.00 usec  
 PW2 10.00 usec  
 PW3 1.0000 msec  
 P1 1.0000 msec  
 P2 1.0000 msec  
 P3 1.0000 msec  
 LOOP1 1  
 POINT 32768  
 SPO 32768  
 SCANS 8  
 DUMMY 1  
 FREQU 6015.04 Hz  
 ACQTM 5.4477 sec  
 PD 1.5510 sec  
 RGAIN 16  
 BF 0.40 Hz  
 EXMOD NON  
 IRNUC 300.40 MHz  
 IRSET 130.00 KHz  
 IRFIN 1150.00 Hz  
 IRRPW 50 usec  
 IRATN 511  
 CSPED 8 Hz  
 CTEMP 24.7 c  
 XE 6015.04 Hz  
 XS 0.00 Hz



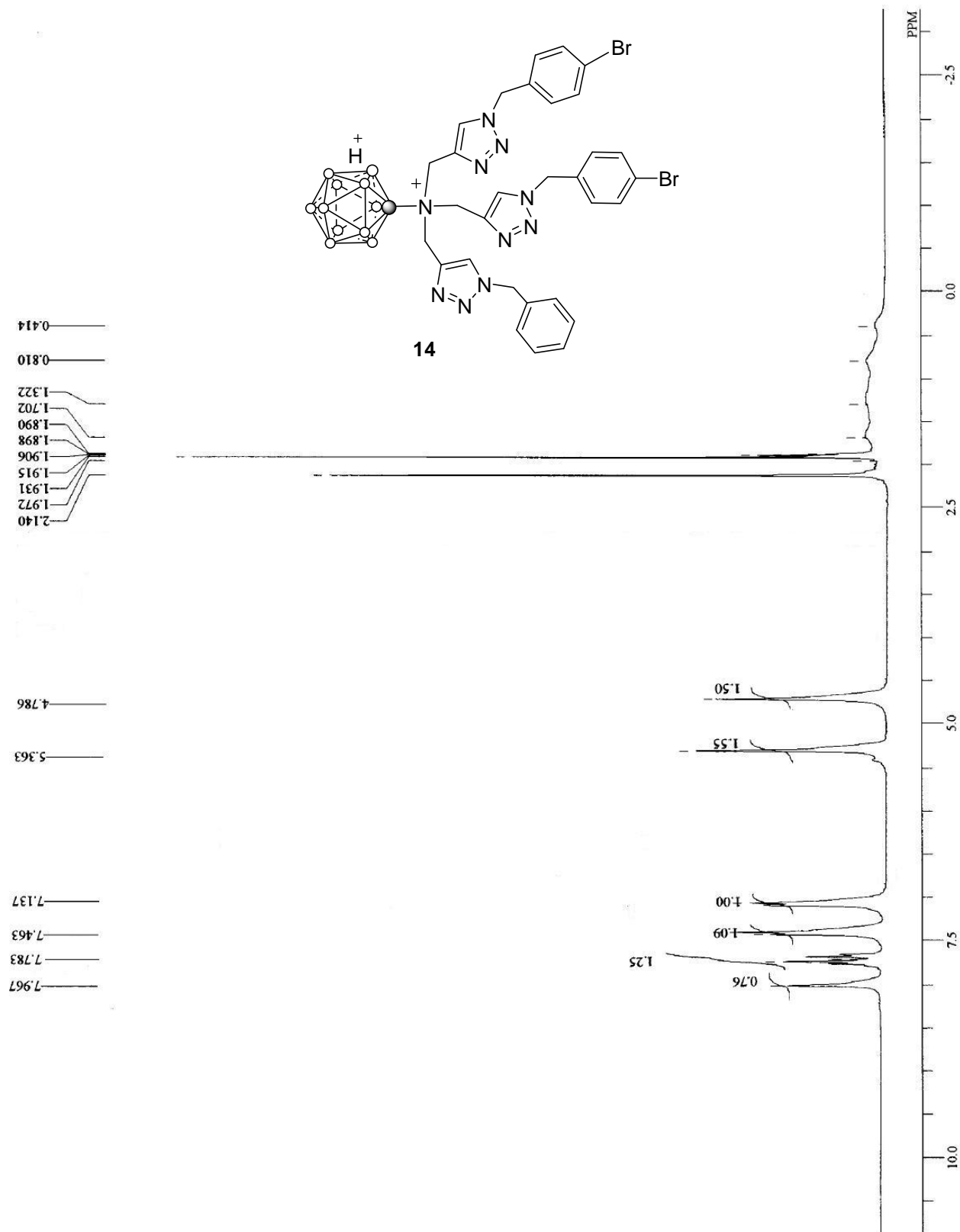
**13**



*N,N*-bis[1-(*p*-bromobenzyl-1,2,3-triazol-4-yl)methyl]-*N*-[1-benzyl-(1,2,3-triazol-4-yl)methyl]aminoundecahydro-*closo*-dodecaborate (1-) (**14**)

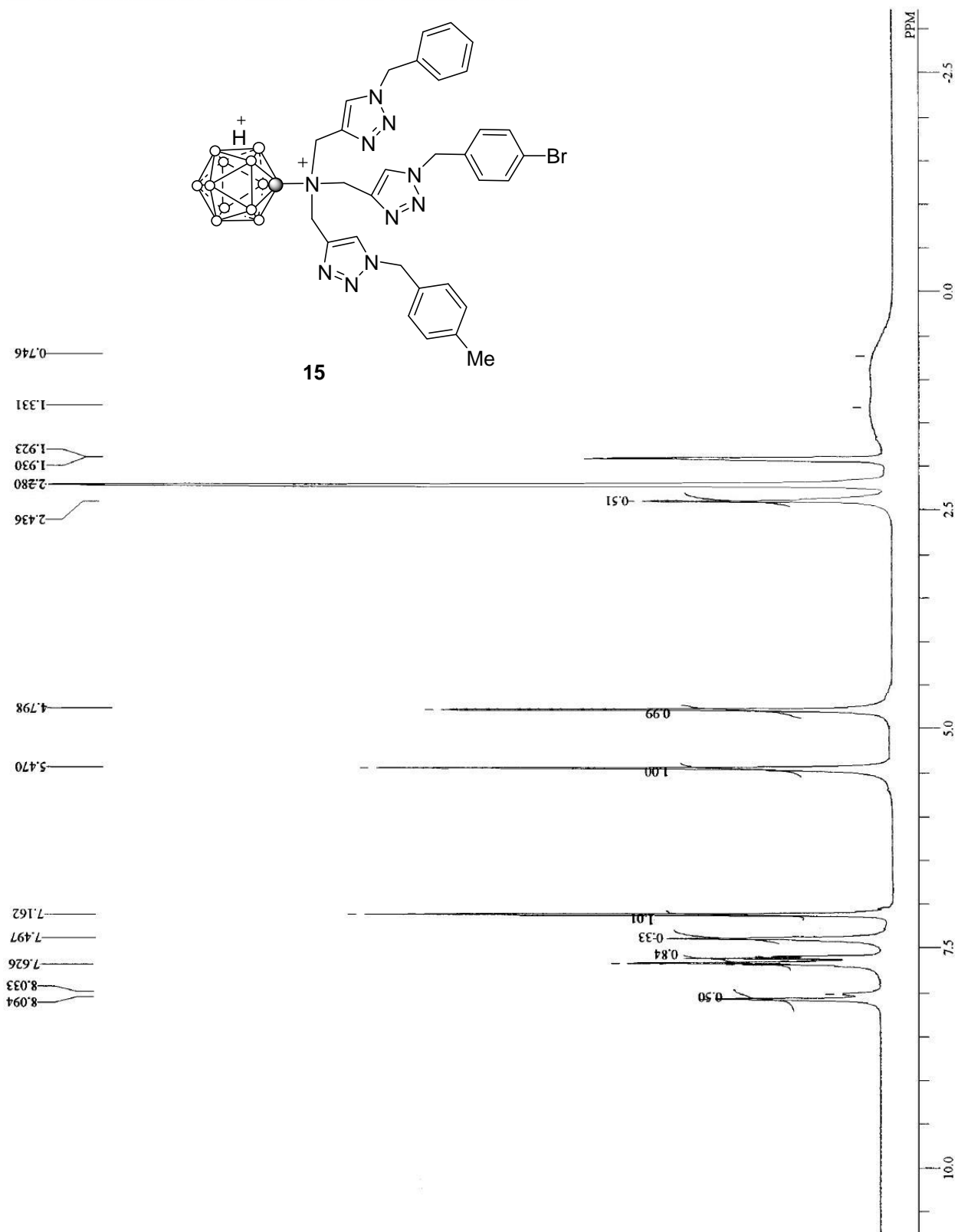
<sup>1</sup>H NMR (300 MHz, CD<sub>3</sub>CN)

DF 300.40 MHz  
 COMNT 130.00 KHz  
 OBNUC 1150.00 Hz  
 OFR 5.40 usec  
 OBSET 10.00 usec  
 OBFIN 10.00 usec  
 PW1 1.0000 msec  
 PW2 1.0000 msec  
 PW3 1.0000 msec  
 PH 1.0000 msec  
 PI2 1.0000 msec  
 PI3 1.0000 msec  
 LOOP1 1  
 POINT 32768  
 SPO 32768  
 SCANS 8  
 DUMMY 1  
 FREQU 6015.04 Hz  
 ACQTM 5.4477 sec  
 PD 1.5510 sec  
 RGAIN 13  
 BF 0.80 Hz  
 EXMOD NON  
 IRNUC 1H  
 IFR 300.40 MHz  
 IRSET 130.00 KHz  
 IRFIN 1150.00 Hz  
 IRPW 50 usec  
 IRATN 511  
 CSPED 12 Hz  
 CTEMP 24.2 C  
 XE 4247.13 Hz  
 XS 340.70 Hz



*N*-[1-benzyl-(1,2,3-triazol-4-yl)methyl]-*N*-[1-(*p*-bromobenzyl-1,2,3-triazol-4-yl)methyl]-*N*-[1-(*p*-methylbenzyl-1,2,3-triazol-4-yl)methyl]aminoundecahydro-*closo*-dodecaborate (1-) (**15**)  
<sup>1</sup>H NMR (300 MHz, CD<sub>3</sub>CN)

DF 300.40 MHz  
 COMNT 130.00 KHz  
 OBNUC 1150.00 Hz  
 OFR 5.40 usec  
 OBSSET 10.00 usec  
 OBFIN 10.00 usec  
 PW1 1.0000 msec  
 PW2 1.0000 msec  
 PW3 1.0000 msec  
 PL1 1.0000 msec  
 PL2 1.0000 msec  
 PL3 1.0000 msec  
 LOOP1 1  
 POINT 32768  
 SPO 32768  
 SCANS 8  
 DUNMY 1  
 FREQU 6015.04 Hz  
 ACQTM 5.4477 sec  
 PD 1.5510 sec  
 RGAIN 16  
 BF 0.40 Hz  
 EXMOD NON  
 IRNUC 1H  
 IFR 300.40 MHz  
 IRSET 130.00 KHz  
 IRFIN 1150.00 Hz  
 IRRPW 50 usec  
 IRATN 511  
 CSTEP 8 Hz  
 CTEMP 24.7 c  
 XE 4200.14 Hz  
 XS 358.32 Hz



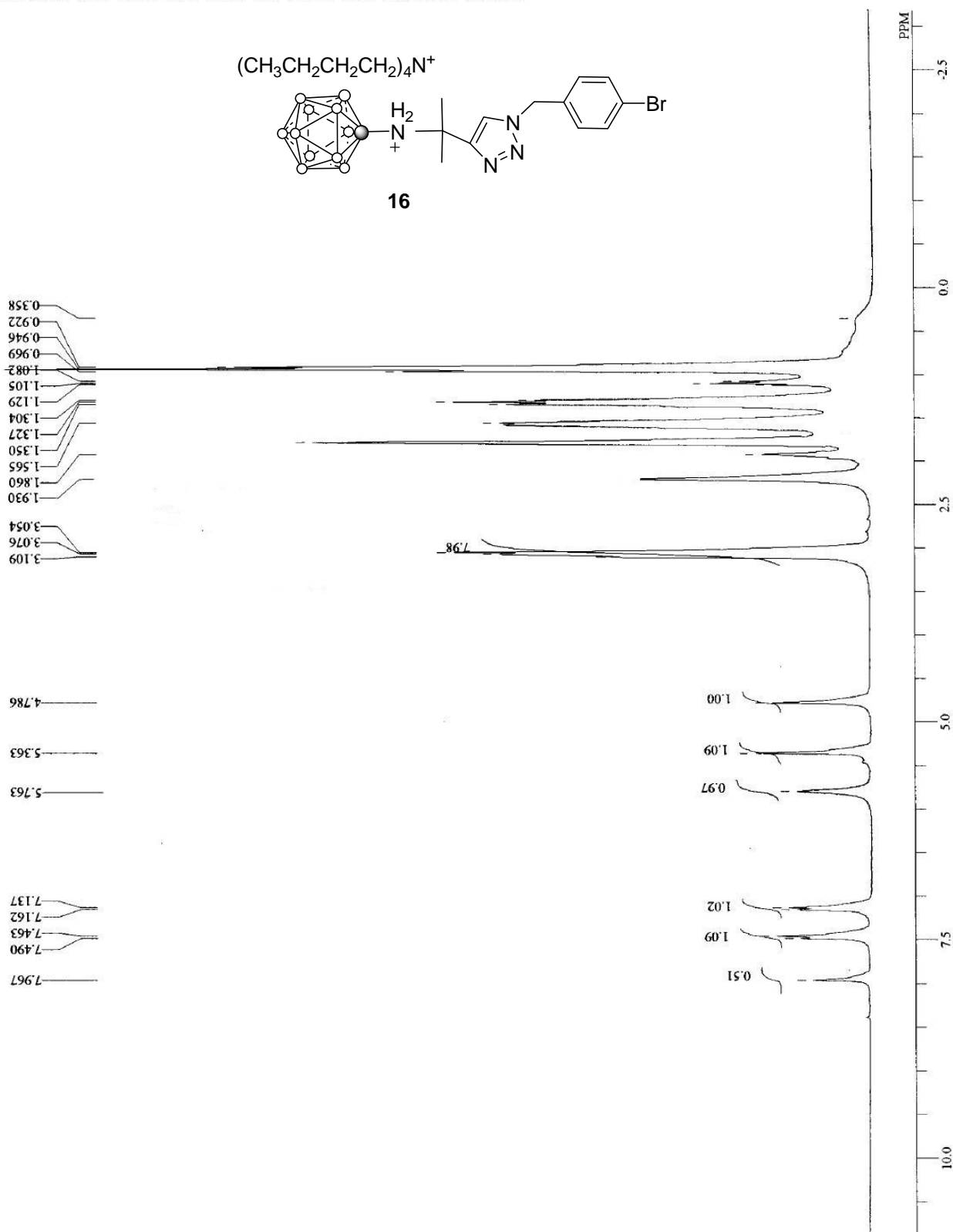
*N*-[1-(*p*-Bromobenzyl-1,2,3-triazol-4-yl)isopropyl]aminoundecahydro-*closo*-dodecaborate

(1-)

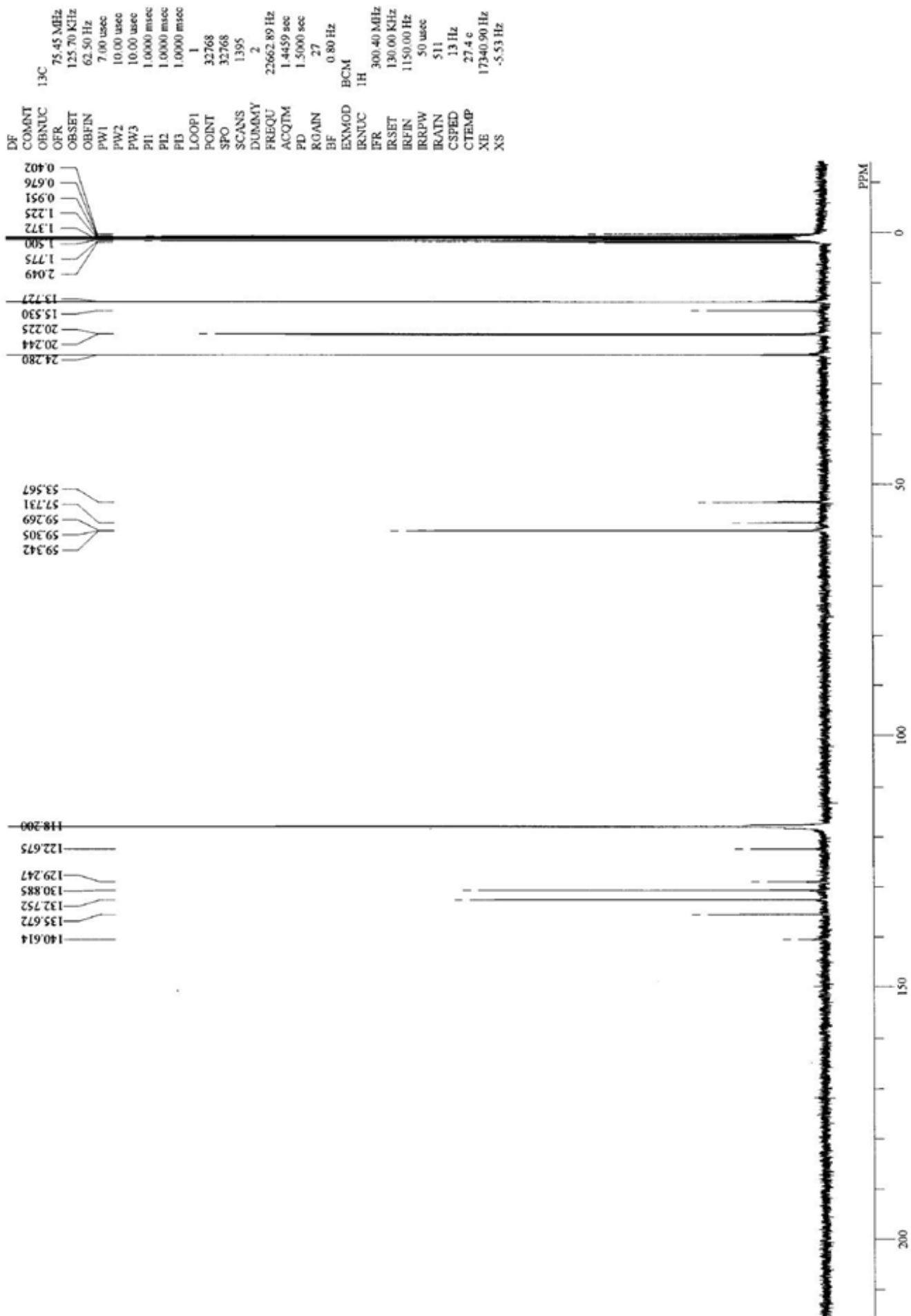
Tetrabutylammonium Salt (**16**)

<sup>1</sup>H NMR (300 MHz, CD<sub>3</sub>CN)

DF 300.40 MHz  
 COMNT 130.00 KHz  
 OBNUC 1150.00 Hz  
 OFR 5.40 usec  
 OBSET 10.00 usec  
 OBFEN 10.00 usec  
 PW1 1.0000 msec  
 PW2 1.0000 msec  
 PW3 1.0000 msec  
 PI 1.0000 msec  
 PI2 1.0000 msec  
 PI3 1.0000 msec  
 LOOP1 1  
 POINT 32768  
 SPO 32768  
 SCANS 8  
 DUMMY 1  
 FREQU 6015.04 Hz  
 ACQTM 5.4477 sec  
 PD 1.5510 sec  
 RGAIN 10  
 BF 0.80 Hz  
 EXMOD NON  
 IRNUC 1H  
 IFR 300.40 MHz  
 IRSET 130.00 KHz  
 IRFIN 1150.00 Hz  
 IRRPW 50 usec  
 IRATN 511  
 CSPED 14 Hz  
 CTEMP 24.2 c  
 XE 4226.57 Hz  
 XS 336.29 Hz



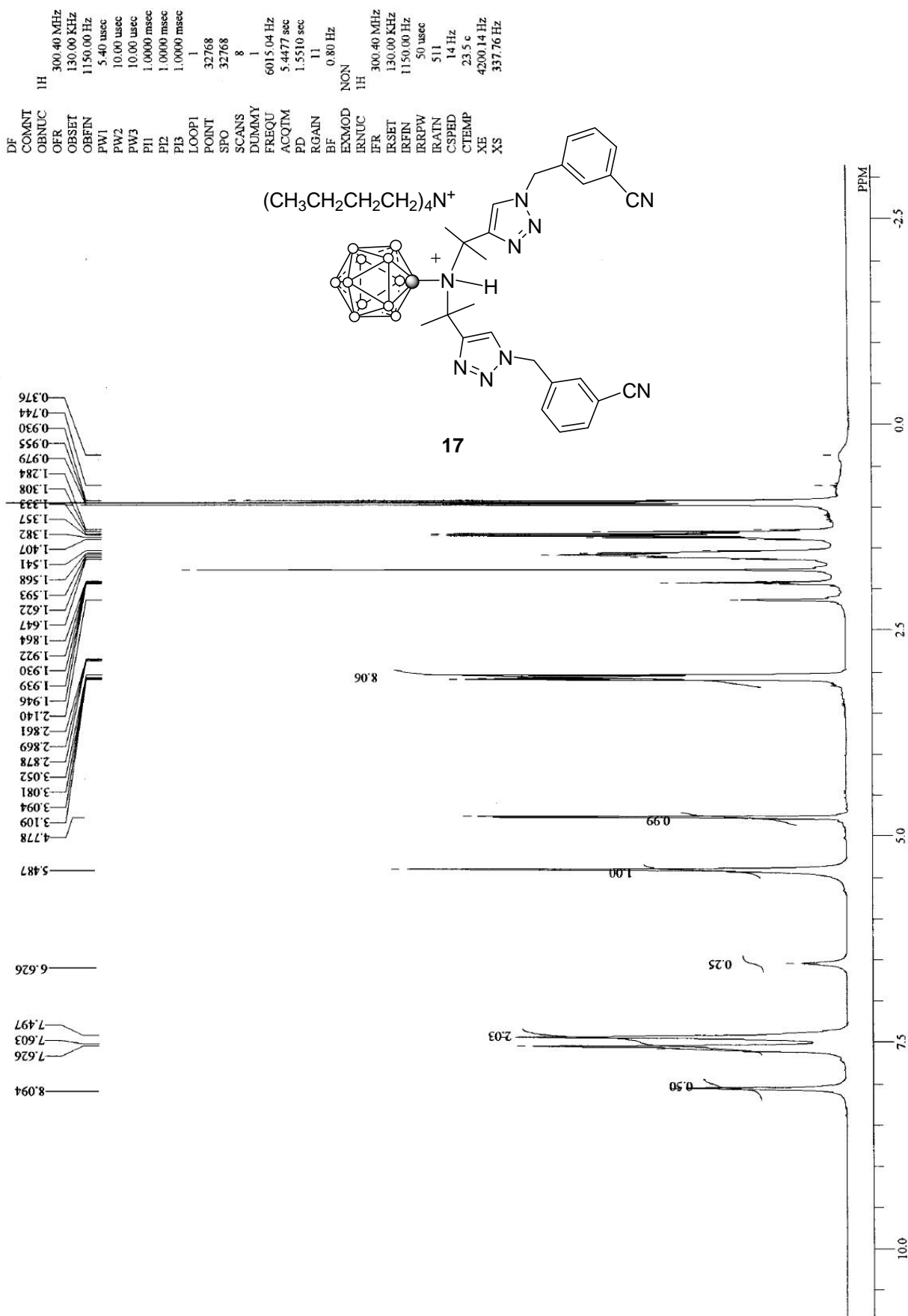
<sup>13</sup>C NMR (75 MHz, CD<sub>3</sub>CN)



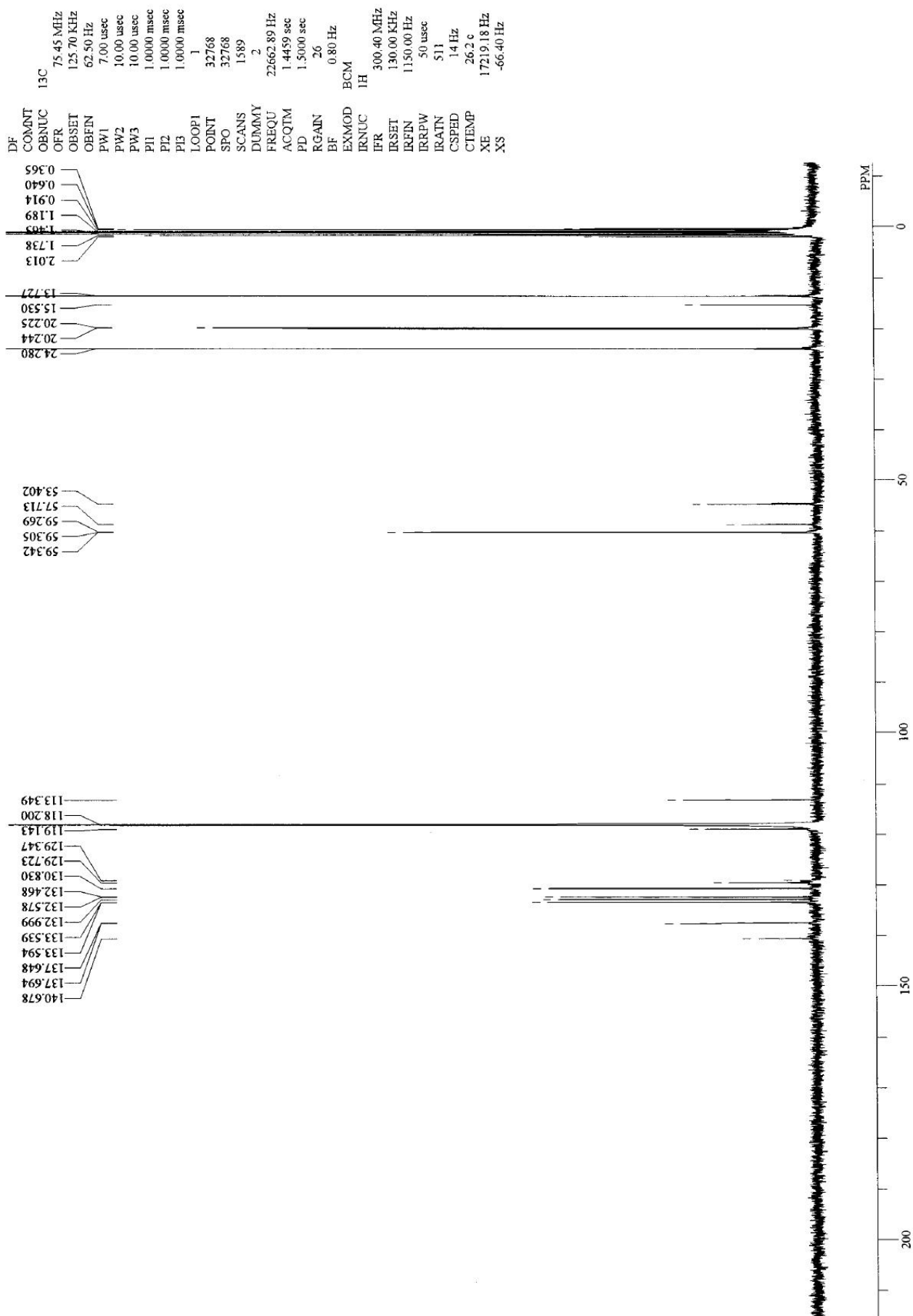
*N,N*-Bis-[1-(*m*-cyanobenzyl-1,2,3-triazol-4-yl)isopropyl]aminoundecahydro-*closo*-dodecaborate  
Tetrabutylammonium Salt (**17**)

(1-)

<sup>1</sup>H NMR (300 MHz, CD<sub>3</sub>CN)



<sup>13</sup>C NMR (75 MHz, CD<sub>3</sub>CN)





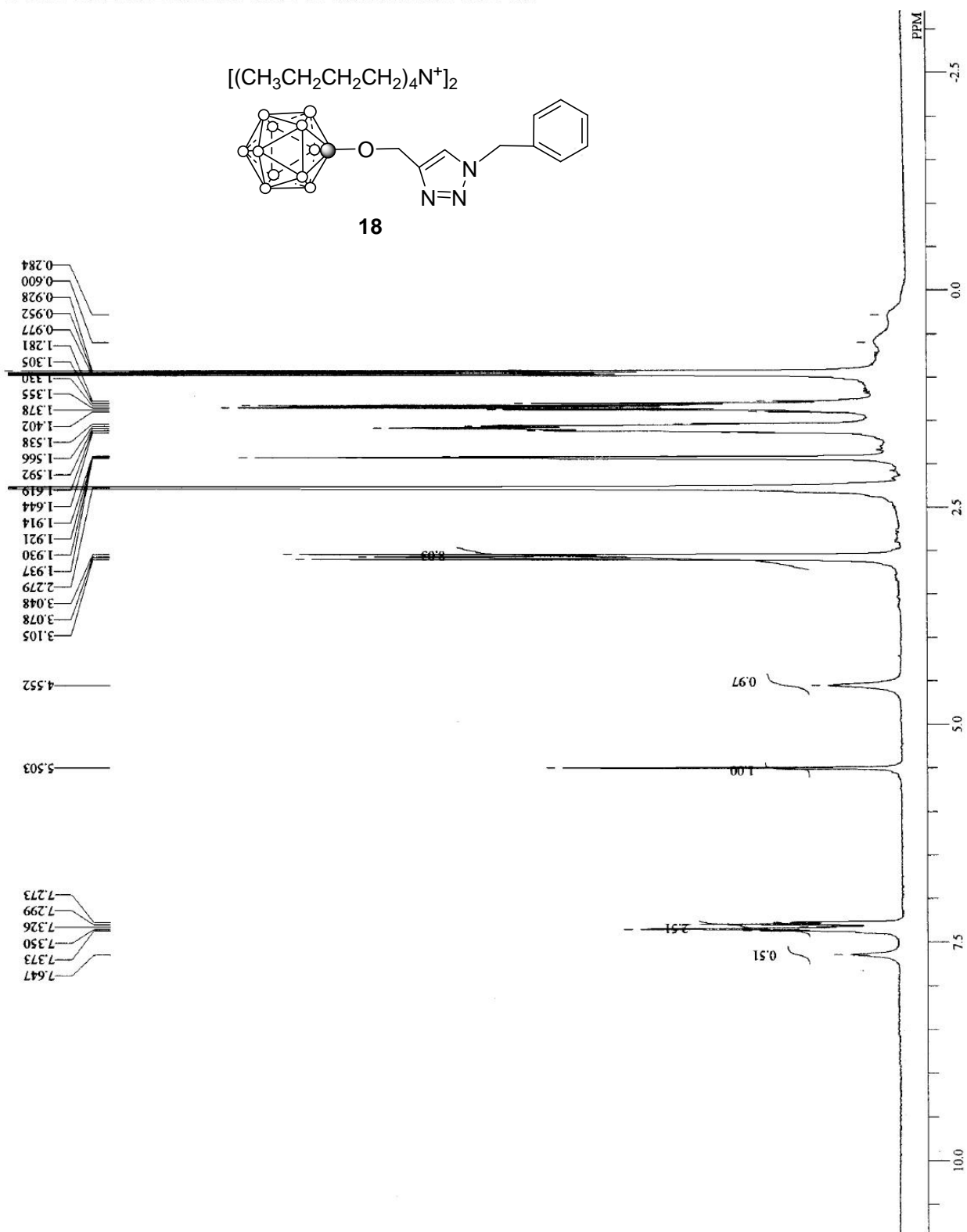
*O*-[1-benzyl-(1,2,3-triazol-4-yl)methyl]hydroxoundecahydro-*closo*-dodecaborate

(2-)

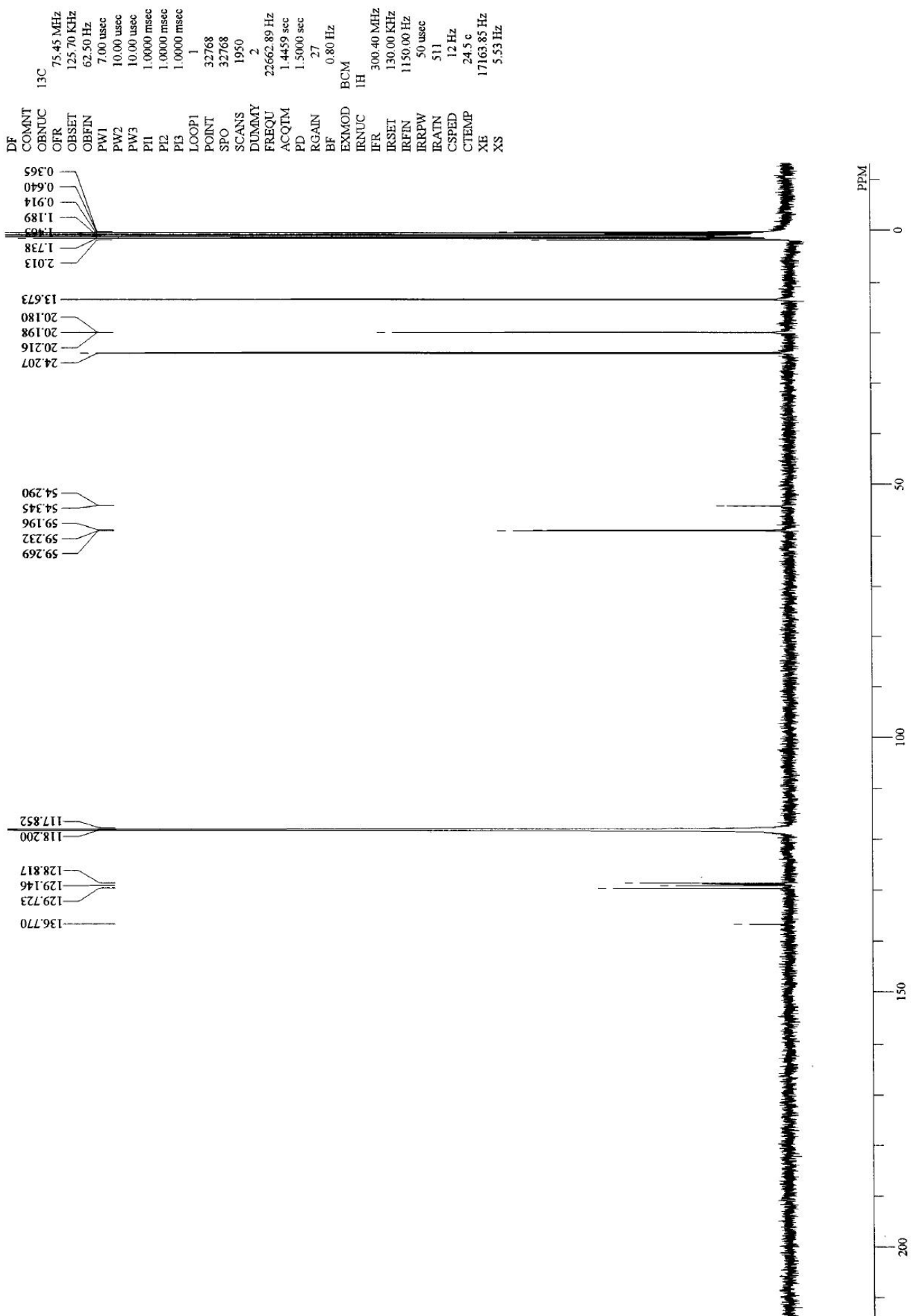
Ditetrabutylammonium Salt (**18**)

<sup>1</sup>H NMR (300 MHz, CD<sub>3</sub>CN)

DF COMNT 300.40 MHz  
 OBNUC 130.00 KHz  
 OFR 1150.00 Hz  
 OBSET 5.40 usec  
 OBFTN 10.00 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  
 SPO 32768  
 SCANS 8  
 DUMMY 1  
 FREQU 6015.04 Hz  
 ACQTM 5.4477 sec  
 PD 1.5510 sec  
 RGAIN 13  
 BF 0.80 Hz  
 EXMOD NON  
 EXNUC 1H  
 IFR 300.40 MHz  
 IRSET 130.00 KHz  
 IRFIN 1150.00 Hz  
 IRRPW 50 usec  
 IRAIN 511  
 CSPEP 14 Hz  
 CTEMP 23.6 c  
 XE 4229.51 Hz  
 XS 343.63 Hz



<sup>13</sup>C NMR (75 MHz, CD<sub>3</sub>CN)

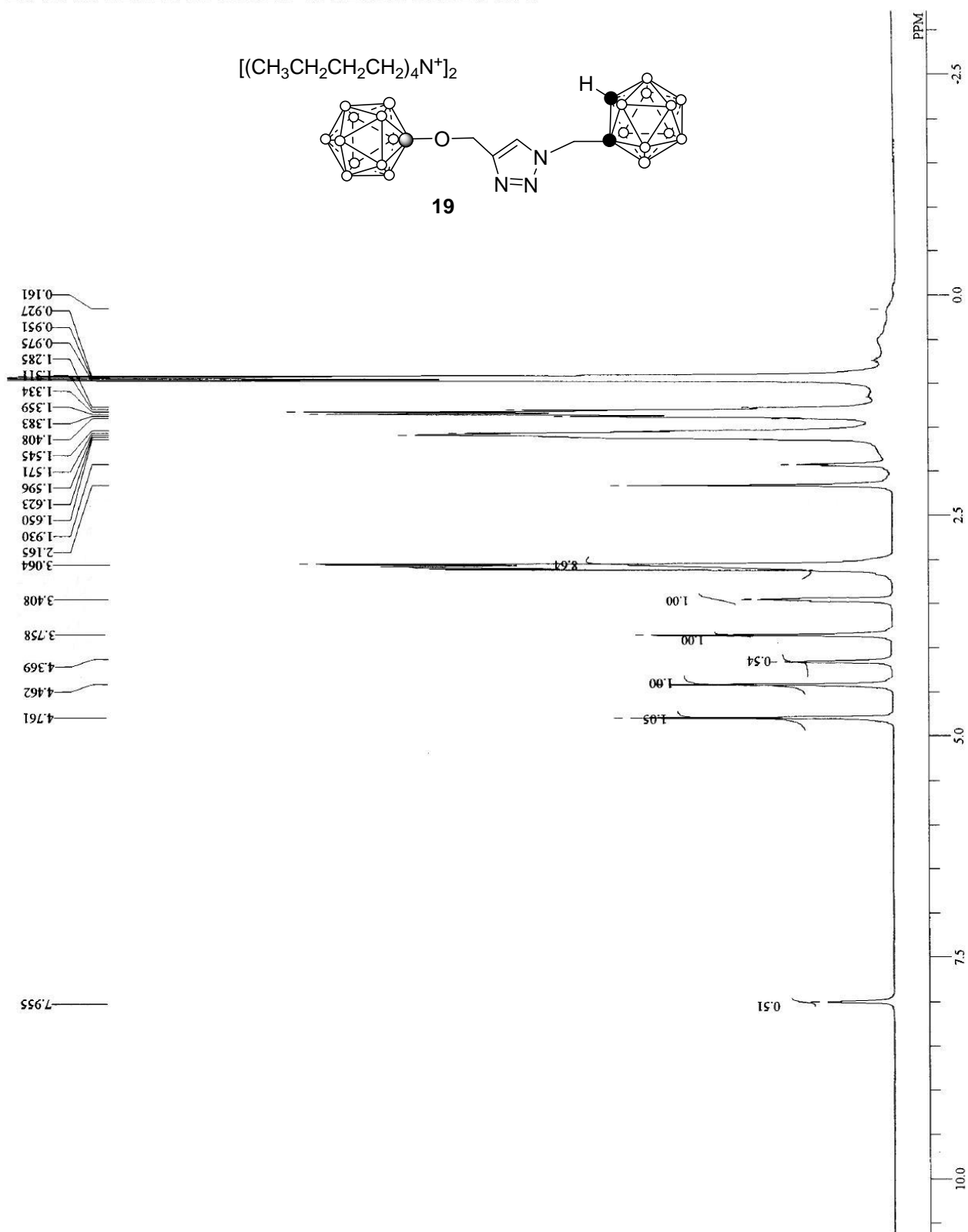


*O*-[1-(3-*o*-carboranylpropyl)-(1,2,3-triazol-4-yl)methyl]hydroxoundecahydro-*closo*-dodecaborate  
 Ditetabutylammonium Salt (**19**)

(2-)

<sup>1</sup>H NMR (300 MHz, CD<sub>3</sub>CN)

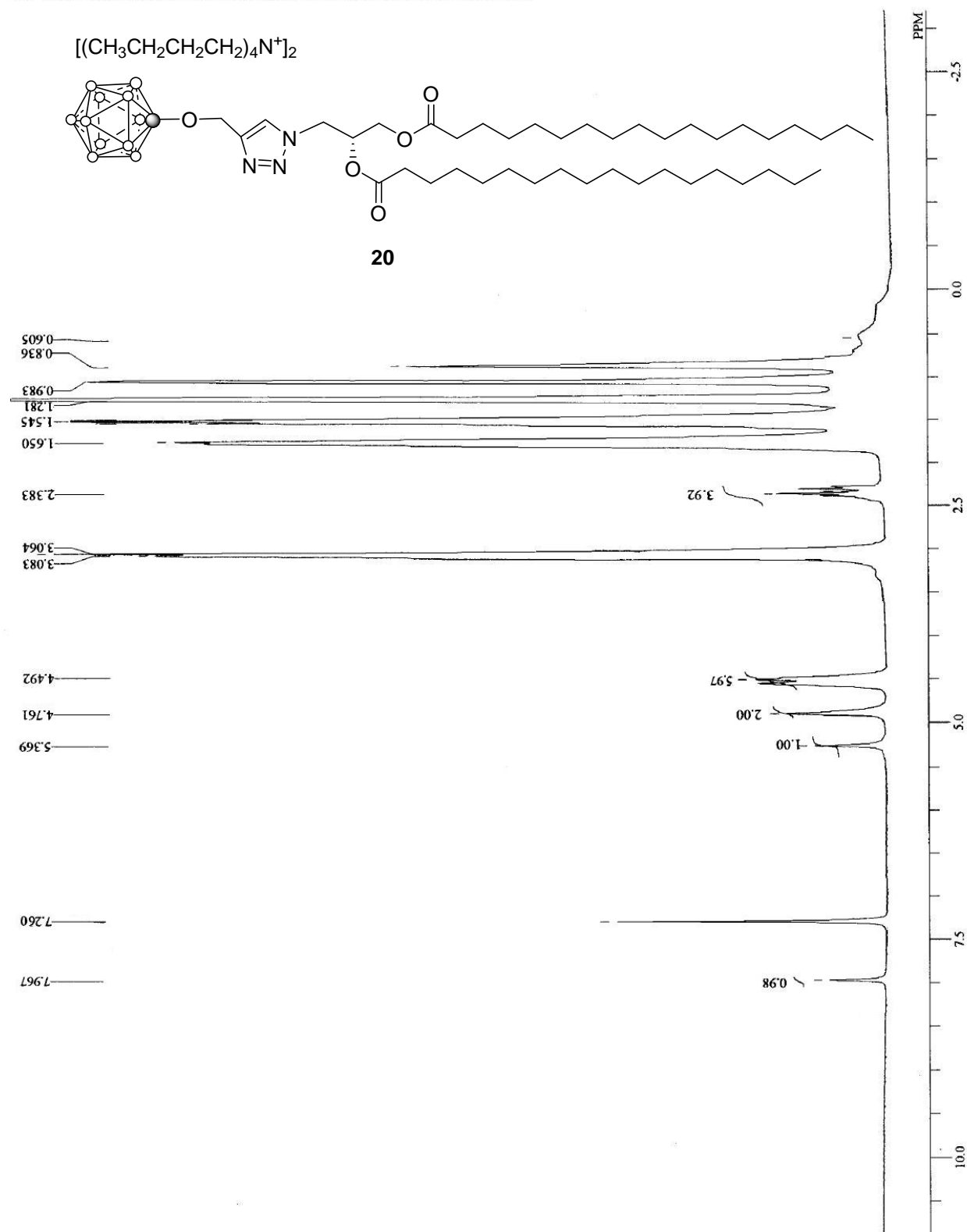
DF 300.40 MHz  
 COMNT 130.00 KHz  
 OBNLC 1150.00 Hz  
 OFR 5.40 usec  
 OBSET 10.00 usec  
 OBFIN 10.00 usec  
 PW1 1.0000 msec  
 PW2 1.0000 msec  
 PW3 1.0000 msec  
 P11 1.0000 msec  
 P12 1.0000 msec  
 P13 1.0000 msec  
 LOOP1 1  
 POINT 32768  
 SPO 32768  
 SCANS 8  
 DUMMY 1  
 FREQU 6015.04 Hz  
 ACQTM 5.4477 sec  
 PD 1.5510 sec  
 RGAIN 9  
 BF 0.80 Hz  
 NON  
 EXMOD  
 IRNUC 1H  
 IFR 300.40 MHz  
 IRSET 130.00 KHz  
 IRFIN 1150.00 Hz  
 IRRPW 50 usec  
 IRATN 511  
 CSPED 11 Hz  
 CTEMP 24.1 c  
 XE 4167.83 Hz  
 XS 374.47 Hz



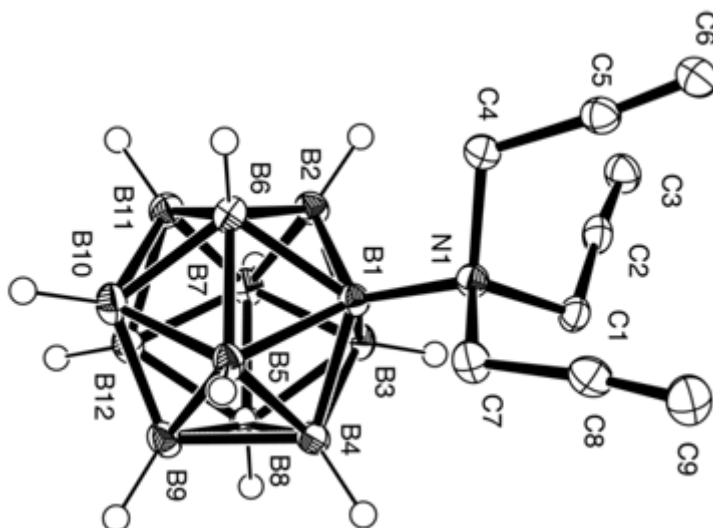
*O*-[1-(1,2-*O*-distearoyl-*sn*-3-glycerol)-(1',2',3'-triazol-4-yl)methyl]hydroxo-undecahydro-*closo*-dodecaborate  
 (2-) Ditetrabutylammonium Salt (**20**)

<sup>1</sup>H NMR (300 MHz, CD<sub>3</sub>CN)

DF COMNT 300.40 MHz  
 OBNUC 130.00 KHz  
 OFR 1150.00 Hz  
 OBSET 5.40 usec  
 OBFTN 10.00 usec  
 PW1 10.00 usec  
 PW2 10.00 usec  
 PW3 1.0000 msec  
 PFI 1.0000 msec  
 PL2 1.0000 msec  
 PE 1.0000 msec  
 LOOP1 1  
 POINT 32768  
 SPO 32768  
 SCANS 8  
 DUMMY 1  
 FREQU 6015.04 Hz  
 ACQTM 5.477 sec  
 PD 1.5510 sec  
 RGAIN 12  
 BF 0.80 Hz  
 EXMOD NON  
 IRNUC 300.40 MHz  
 IFR 130.00 KHz  
 IRSET 1150.00 Hz  
 IRRPW 50 usec  
 IRAIN 511  
 CSPED 13 Hz  
 CTEMP 25.0 c  
 XE 4241.25 Hz  
 XS 337.76 Hz

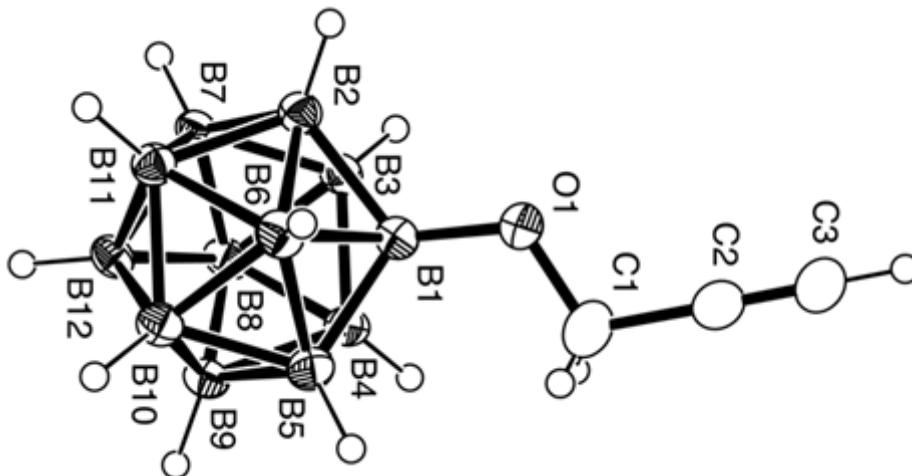


X-ray crystallographic structure and data of compound **2** (shelxl compound 2.cif)



ORTEP representation of anion **2**, showing 50% probability thermal ellipsoids (hydrogen atoms of the propyne groups are omitted for clarity).

X-ray crystallographic for the structure determination of compound **6** (shelxl compound 6.cif)



ORTEP representation of anion **6**, showing 50% probability thermal ellipsoids.