

Supporting information

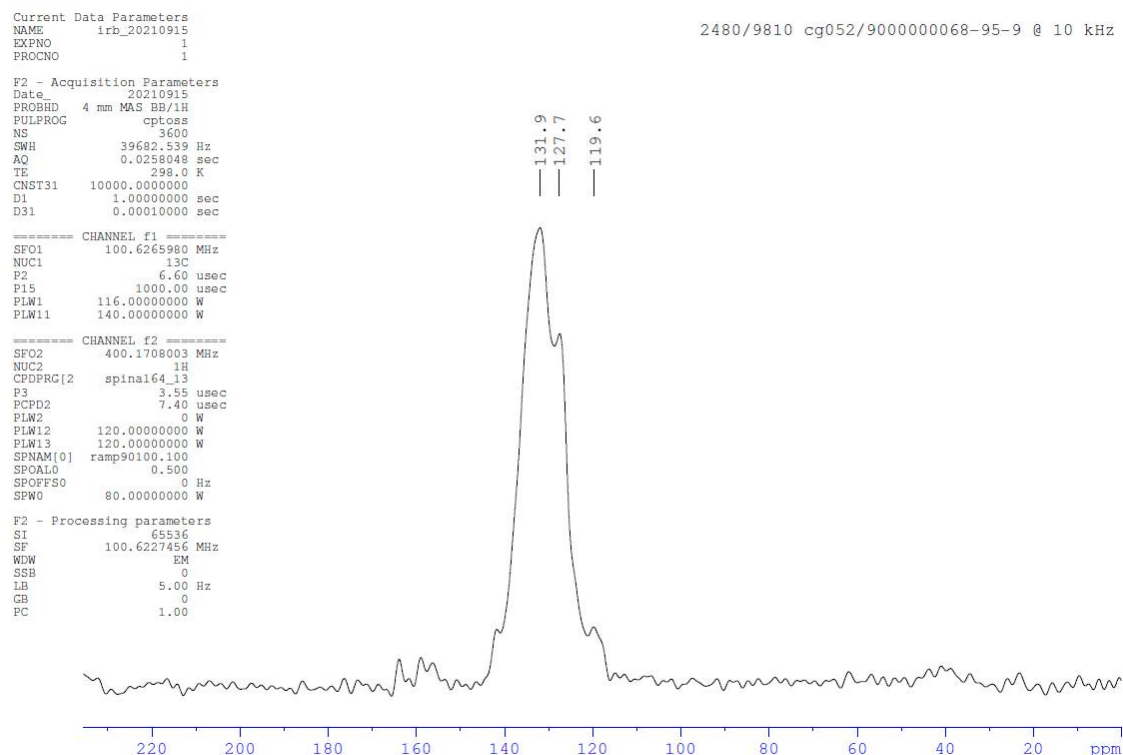
6-Chloro-3*H*-benzo[*d*][1,2,3]dithiazol-2-ium Chloride

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All data was recorded using a Bruker Avance III HD spectrometer operating at 400.1, 100.6 MHz for ¹H and ¹³C, respectively. Carbon-13 magic-angle spinning measurements were carried out at 100.6 MHz using a Bruker Avance III HD spectrometer and 4 mm (rotor o.d.) probe. Spectra were acquired at a spin rate of 10 kHz. Cross-polarisation (CP) spectra were recorded with TOSS spinning sideband suppression, 1 ms contact time and with a recycle delay of either 1 s. The recycle delay and contact time were optimised for each sample. Carbon spectral referencing is relative to neat tetramethylsilane, carried out by setting the high-frequency signal from an external sample of adamantane to 38.5 ppm. In addition to the CPTOSS spectrum, for cg052/9000000068-95-9 a phase inverted (cpqi_toss) experiment was performed to obtain negative CH₂, null CH, and positive C and CH₃. The difference between this and the original spectra is also provided.



Current Data Parameters
NAME irb_20210915
EXPNO 2
PROCNO 1

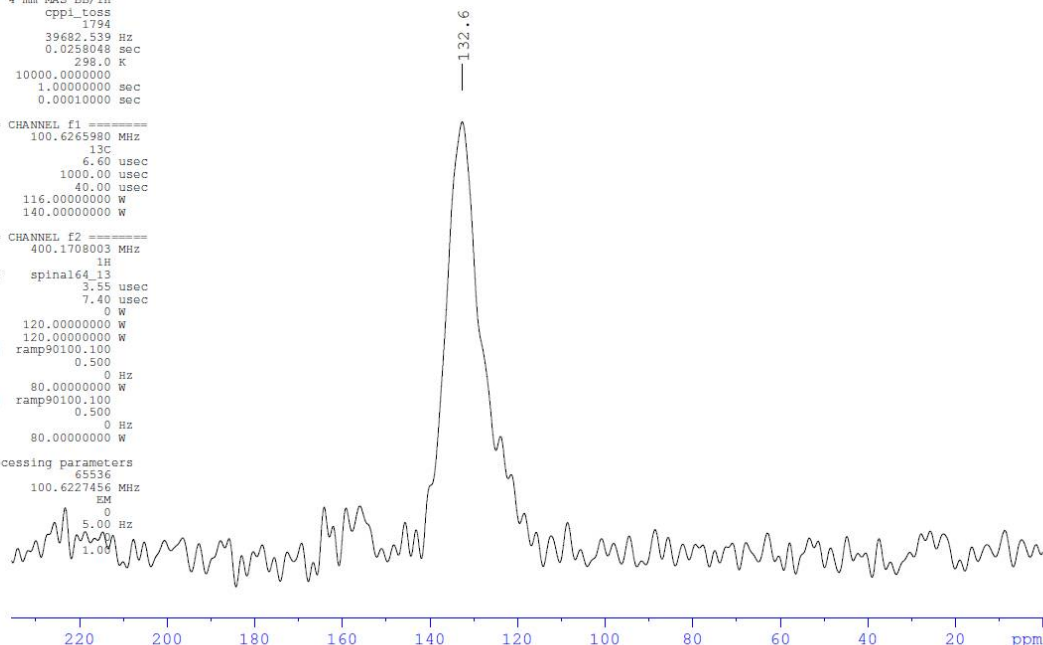
2480/9810 cg052/9000000068-95-9 @ 10 kHz

F2 - Acquisition Parameters
Date 20210915
PROBHD 4 mm MAS BB/1H
PULPROG cppl_toss
NS 1794
SWH 39682.539 Hz
AQ 0.0258048 sec
TE 298.0 K
CNST31 10000.000000 sec
D1 1.00000000 sec
D31 0.00010000 sec

===== CHANNEL f1 =====
SFO1 100.6265980 MHz
NUC1 13C
P2 6.60 usec
P15 1000.00 usec
P16 40.00 usec
PLW1 116.00000000 W
PLW11 140.00000000 W

===== CHANNEL f2 =====
SFO2 400.1708003 MHz
NUC2 1H
CPDPRG[2] spinal64_13
P3 3.55 usec
PCPD2 7.40 usec
PLW2 0 W
PLW12 120.00000000 W
PLW13 120.00000000 W
SPNAM[0] ramp90100.100
SPOAL0 0.500
SPOFFS0 0 Hz
SPW0 80.00000000 W
SPNAM[1] ramp90100.100
SPOAL1 0.500
SPOFFS1 0 Hz
SPW1 80.00000000 W

F2 - Processing parameters
SI 65536
SF 100.6227456 MHz
WDW EM
SSB 0
LB 5.00 Hz
GB 1.00
PC



Current Data Parameters
NAME irb_20210915
EXPNO 1001
PROCNO 1

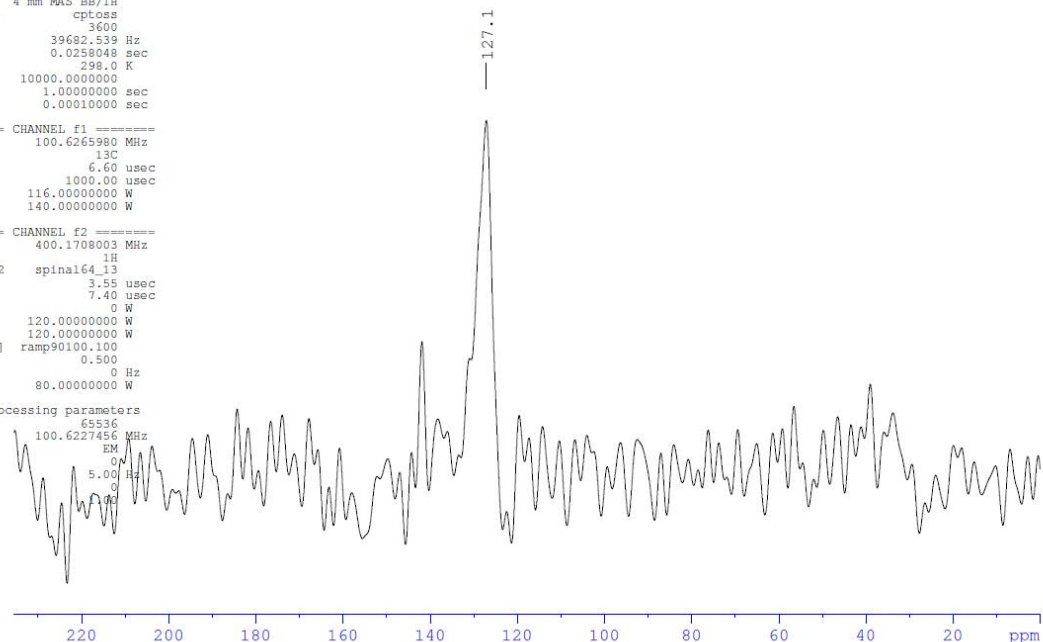
2480/9810 cg052/9000000068-95-9 @ 10 kHz
Difference

F2 - Acquisition Parameters
Date 20210915
PROBHD 4 mm MAS BB/1H
PULPROG cptoss
NS 3600
SWH 39682.539 Hz
AQ 0.0258048 sec
TE 298.0 K
CNST31 10000.000000 sec
D1 1.00000000 sec
D31 0.00010000 sec

===== CHANNEL f1 =====
SFO1 100.6265980 MHz
NUC1 13C
P2 6.60 usec
P15 1000.00 usec
PLW1 116.00000000 W
PLW11 140.00000000 W

===== CHANNEL f2 =====
SFO2 400.1708003 MHz
NUC2 1H
CPDPRG[2] spinal64_13
P3 3.55 usec
PCPD2 7.40 usec
PLW2 0 W
PLW12 120.00000000 W
PLW13 120.00000000 W
SPNAM[0] ramp90100.100
SPOAL0 0.500
SPOFFS0 0 Hz
SPW0 80.00000000 W

F2 - Processing parameters
SI 65536
SF 100.6227456 MHz
WDW EM
SSB 0
LB 5.00 Hz
GB 1.00
PC



Current Data Parameters
NAME irb_20210915
EXPNO 3
PROCNO 1

2480/9811 cg052/9000000069-20-3 @ 10 kHz

F2 - Acquisition Parameters
Date 20210915
PROBHD 4 mm MAS BB/1H
PULPROG cptoss
NS 762
SWH 39682.539 Hz
AQ 0.0258048 sec
TE 298.0 K
CNST31 10000.0000000
D1 1.00000000 sec
D31 0.00010000 sec

===== CHANNEL f1 =====
SFO1 100.6265980 MHz
NUC1 13C
P2 6.60 usec
P15 1000.00 usec
PLW1 116.00000000 W
PLW11 140.00000000 W

===== CHANNEL f2 =====
SFO2 400.1708003 MHz
NUC2 1H
CPDPRG[2] spinal64_13
P3 3.55 usec
PCPD2 7.40 usec
PLW2 0 W
PLW12 120.00000000 W
PLW13 120.00000000 W
SPNAM[0] ramp90100.100
SFOAL0 0.500
SPOFFS0 0 Hz
SPW0 80.00000000 W

F2 - Processing parameters
SI 65536
SF 100.6227456 MHz
WDW EM
SSB 0
LB 5.00 Hz
GB 0
PC 1.00

