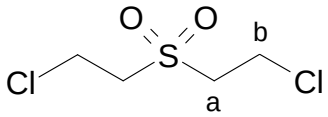
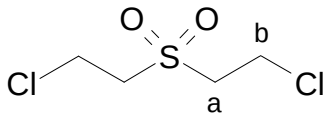
NMR SPECTROMETRY

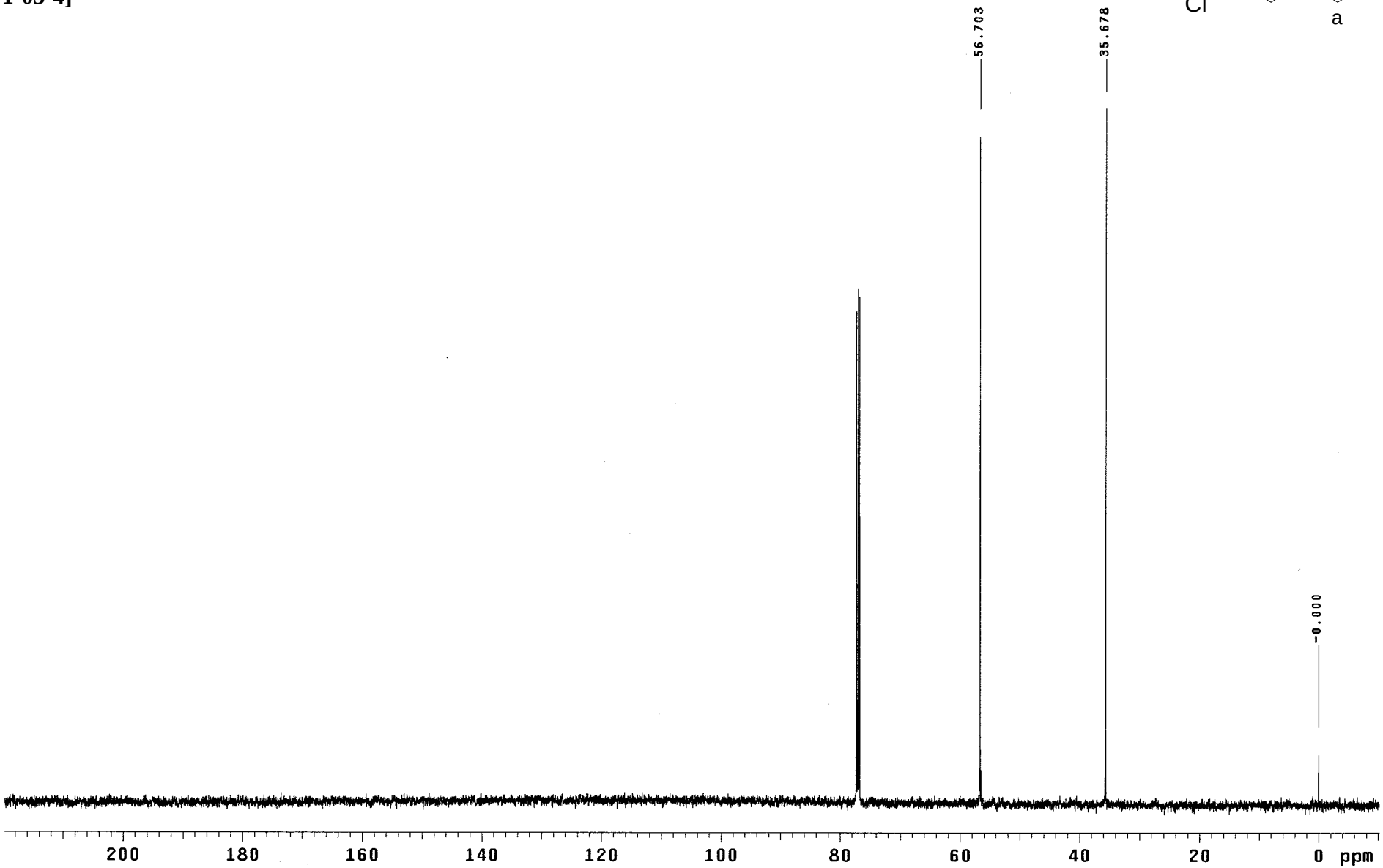
Contributor's name and address:	Verification Laboratory DSO National Laboratories 11 Stockport Road Singapore 117605
Secretariat identification code	25-3-0034r (p1/2)
Signature	
Chemical information:	
Chemical name	Bis(2-chloroethyl)sulfone
Schedule number	
CAS registry number	471-03-4
Chemical structure with numbering of atoms	
Molecular formula	$C_4H_8Cl_2O_2S$
Sample information:	
Sample purity	95 %
Sample concentration	35 mg/mL
Solvent	$CDCl_3$
pH	-
Source	In-house synthesis YL21791
Reference chemical shift (internal)	TMS, 0 ppm
Instrument information:	
Manufacturer	Varian, Inc.
Model	Inova 500 MHz
Spectrometer frequency	500 MHz
Software version	VNMR version 6.1C
Experimental information:	
Nucleus measured	$^{13}C\{^{1}H\}$
Sample temperature	25 °C
Spectral width (Hz)	28891.3
Data points in Fourier transformed spectrum	32768
Repetition time	2.5 s
Pulse angle (μs and degrees)	6.463 μs, 45°
Date of experiment	2 Jun 2005
Data points in FID	28832
Number of scans	720
Baseline correction	Yes
Spectral information:	
Chemical shifts (ppm) assigned except for acidic protons	Ca = 56.70, Cb = 35.68
Coupling constants (Hz)	-
Impurities marked with asterisks	

Bis(2-chloroethyl)sulfone ($C_4H_8Cl_2O_2S$)

[471-03-4]

$^{13}C\{^1H\}$ NMR





Res.Freq: 125.653 MHz
Solvent: $CDCl_3$
Temperature: 25°C
Concentration: 35 mg/mL

Reference: TMS (internal)
Spectral Width: 35133.9 Hz
Data points [FID]: 28832
Data points [Spectrum]: 32768

Pulse width: 6.463 µs, 45°
Number of Scans: 720
Line broadening: 2
Rep. time: 2.5 s

Resolution: 1.07 Hz (TMS)
Baseline correction: Yes
Instrument: Varian INOVA 500

Nuc δ[ppm]
a: 56.70
b: 35.68