
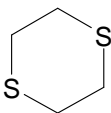


NMR SPECTROMETRY

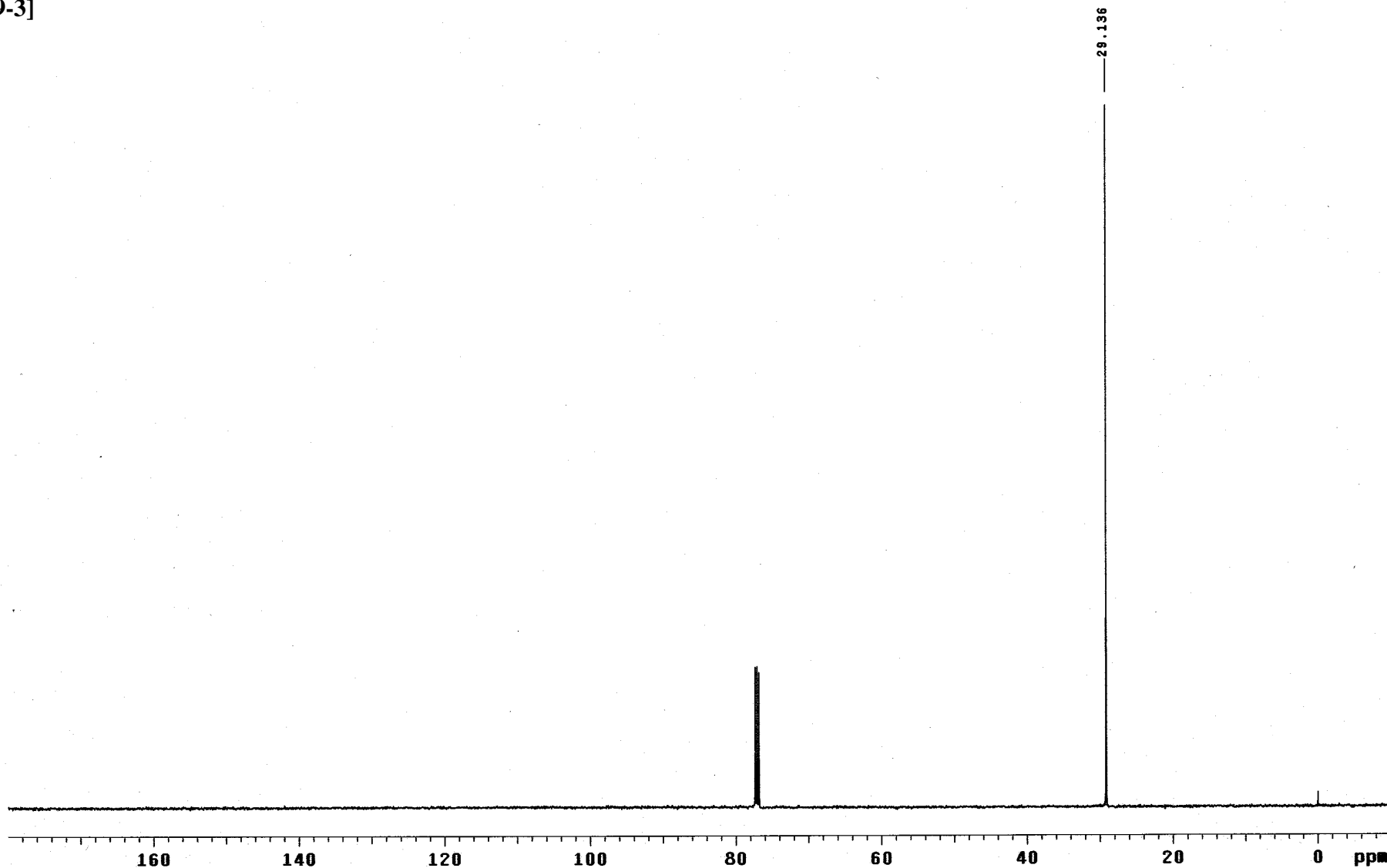
Contributor's name and address:		Verification Laboratory
Secretariat identification code	25-3-0006r (p1/2)	DSO National Laboratories
Signature		11 Stockport Road Singapore 117605
Chemical information:		
Chemical name	1,4-Dithiane	
Schedule number		
CAS registry number	505-29-3	
Chemical structure with numbering of atoms		
Molecular formula	C ₄ H ₈ S ₂	
Sample information:		
Sample purity	97 %	
Sample concentration	48 mg/mL	
Solvent	CDCl ₃	
pH	-	
Source	Aldrich	
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)	23923.4	
Data points in Fourier transformed spectrum	32768	
Repetition time	2.5 s	
Pulse angle (μs and degrees)	6.463 μs, 45°	
Date of experiment	24 Jun 2005	
Data points in FID	23874	
Number of scans	720	
Baseline correction	Yes	
Spectral information:		
Chemical shifts (ppm) assigned except for acidic protons	C = 29.14	
Coupling constants (Hz)	-	

25-3-0006r (p2/2)

1,4-Dithiane (C₄H₈S₂)

[505-29-3]

¹³C{¹H} NMR



Res.Freq: 125.653 MHz
Solvent: CDCl₃
Temperature: 25°C
Concentration: 48 mg/mL
Reference: TMS (internal)

Spectral Width: 23923.4 Hz
Data points [FID]: 23874
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]
C: 29.14

