
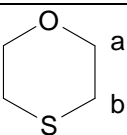


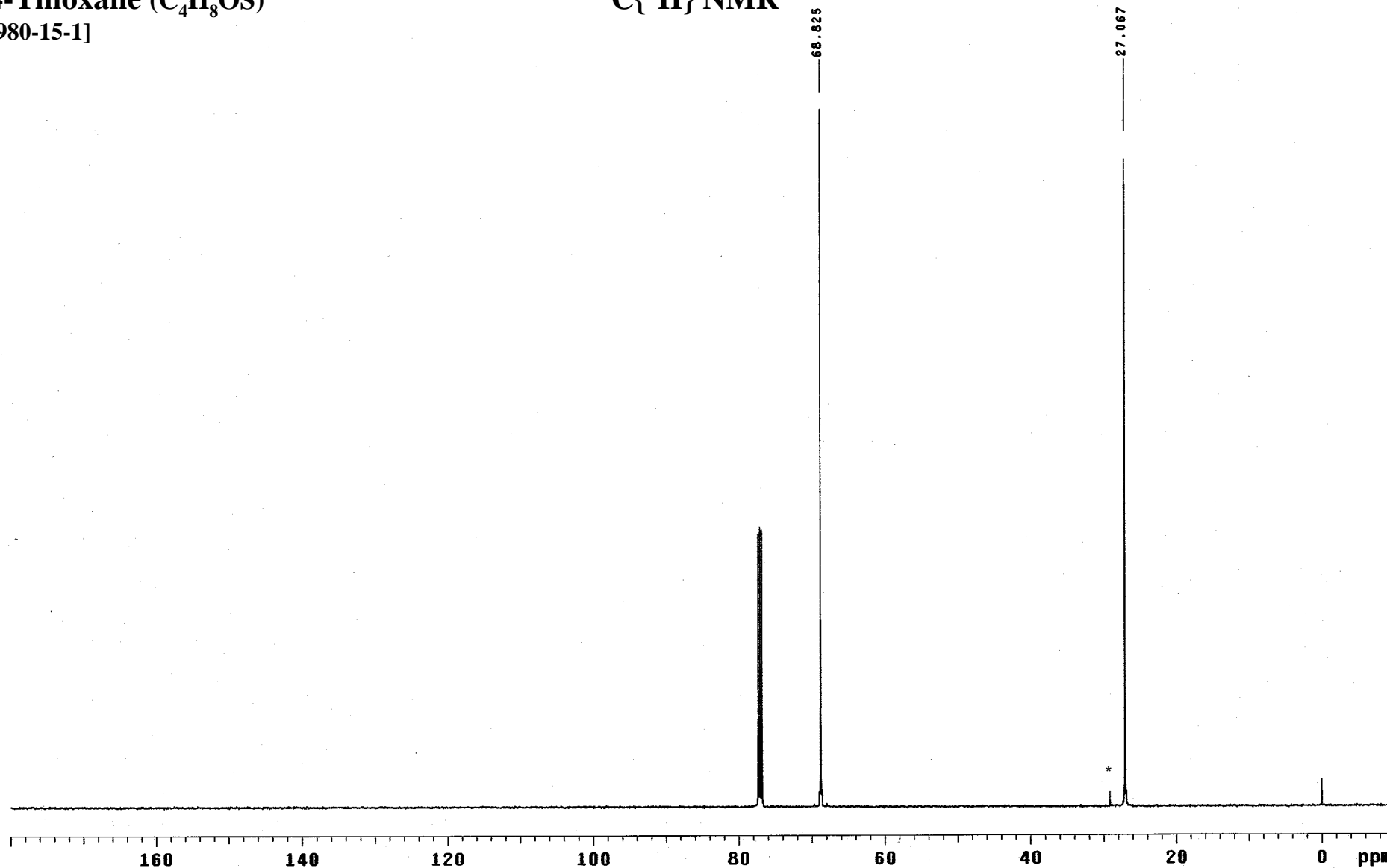
## NMR SPECTROMETRY

<b>Contributor's name and address:</b>		Verification Laboratory
Secretariat identification code	25-3-0008r (p1/2)	DSO National Laboratories
Signature		11 Stockport Road Singapore 117605
<b>Chemical information:</b>		
Chemical name	1,4-Thioxane	
Schedule number		
CAS registry number	15980-15-1	
Chemical structure with numbering of atoms		
Molecular formula	C <sub>4</sub> H <sub>8</sub> OS	
<b>Sample information:</b>		
Sample purity	98 %	
Sample concentration	56 mg/mL	
Solvent	CDCl <sub>3</sub>	
pH	-	
Source	Aldrich	
Reference chemical shift (internal)	TMS, 0 ppm	
<b>Instrument information:</b>		
Manufacturer	Varian, Inc.	
Model	Inova 500 MHz	
Spectrometer frequency	500 MHz	
Software version	VNMR version 6.1C	
<b>Experimental information:</b>		
Nucleus measured	<sup>13</sup> C{ <sup>1</sup> 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)	4.125 μs, 45°	
Date of experiment	12 Apr 2005	
Data points in FID	23874	
Number of scans	720	
Baseline correction	Yes	
<b>Spectral information:</b>		
Chemical shifts (ppm) assigned except for acidic protons	Ca = 68.83, Cb = 27.07	
Coupling constants (Hz)	-	

25-3-0008r (p2/2)

**1,4-Thioxane (C<sub>4</sub>H<sub>8</sub>OS)**  
[15980-15-1]

**<sup>13</sup>C{<sup>1</sup>H} NMR**



Res.Freq: 125.653 MHz  
Solvent: CDCl<sub>3</sub>  
Temperature: 25°C  
Concentration: 56 mg/mL  
Reference: TMS (internal)

Spectral Width: 23923.4 Hz  
Data points [FID]: 23874  
Data points [Spectrum]: 32768  
Pulse width: 4.125 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: 68.83  
b: 27.07

