
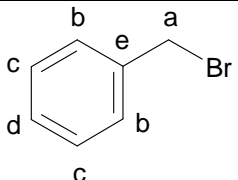


NMR SPECTROMETRY

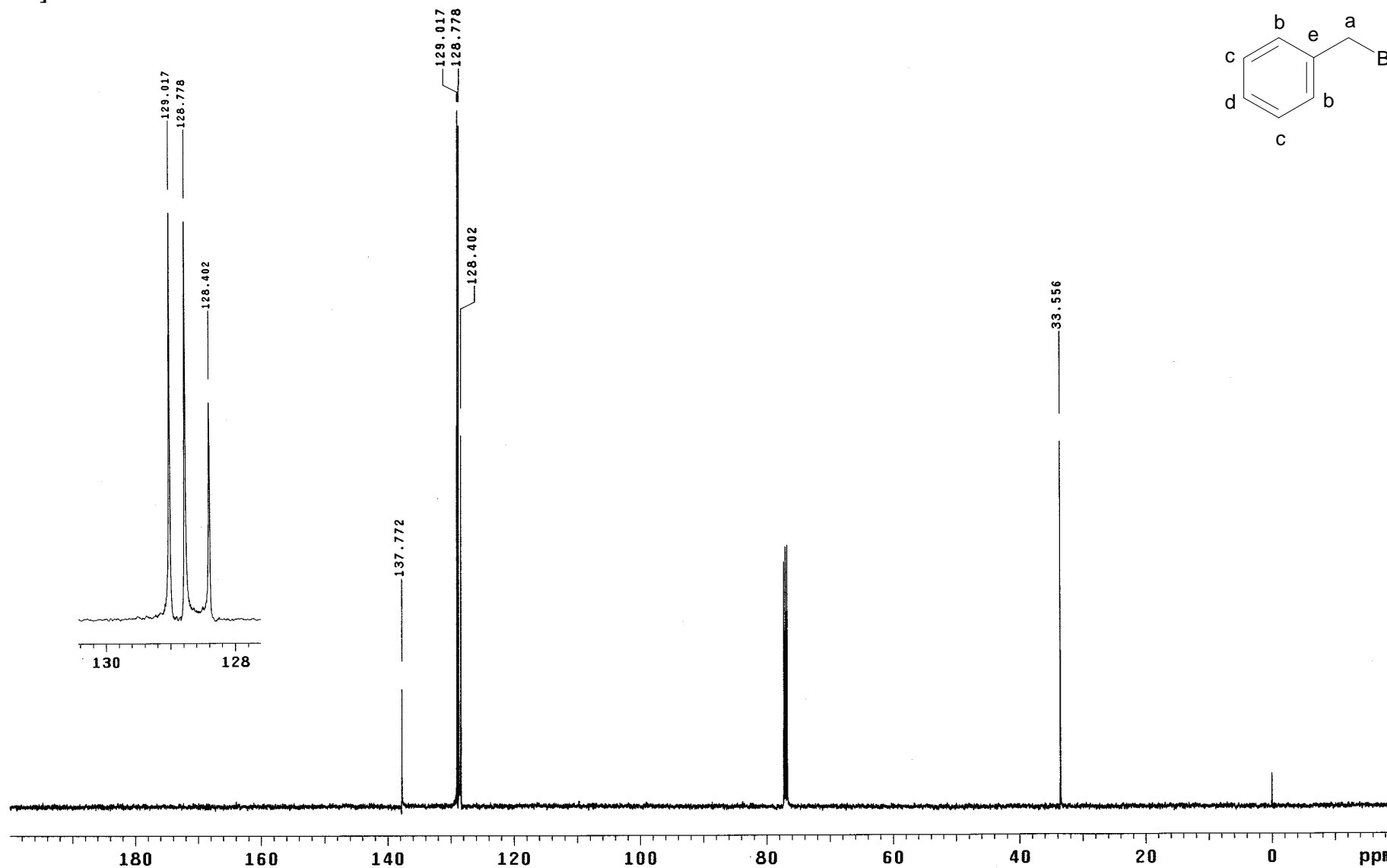
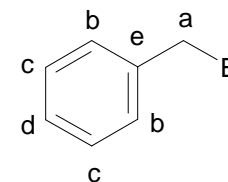
Contributor's name and address:		Verification Laboratory
Secretariat identification code	25-3-0014r (p1/3)	DSO National Laboratories
Signature		11 Stockport Road Singapore 117605
Chemical information:		
Chemical name	Benzyl bromide	
Schedule number		
CAS registry number	100-39-0	
Chemical structure with numbering of atoms		
Molecular formula	C ₇ H ₇ Br	
Sample information:		
Sample purity	>98 %	
Sample concentration	50 mg/mL	
Solvent	CDCl ₃	
pH	-	
Source	Fluka	
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)	35133.9	
Data points in Fourier transformed spectrum	65536	
Repetition time	2.5 s	
Pulse angle (μs and degrees)	6.463 μs, 45°	
Date of experiment	1 Jun 2005	
Data points in FID	35062	
Number of scans	720	
Baseline correction	Yes	
Spectral information:		
Chemical shifts (ppm) assigned except for acidic protons	Ca = 33.56, Cb = 129.02, Cc = 128.78, Cd = 128.40, Ce = 137.77	
Coupling constants (Hz)	-	

25-3-0014r (p2/3)

Benzyl bromide (C₇H₇Br)

[100-39-0]

¹³C{¹H} NMR



Res.Freq: 125.653 MHz
Solvent: CDCl₃
Temperature: 25°C
Concentration: 50 mg/mL
Reference: TMS (internal)

Spectral Width: 35133.9 Hz
Data points [FID]: 35062
Data points [Spectrum]: 65536
Pulse width: 4.463 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]	Nuc δ[ppm]
a: 33.56	d: 128.40
b: 129.02	e: 137.77
c: 128.78	

Benzyl bromide (C₇H₇Br)

[100-39-0]

