
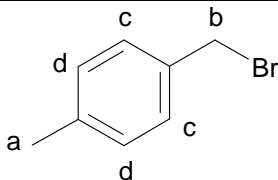


NMR SPECTROMETRY

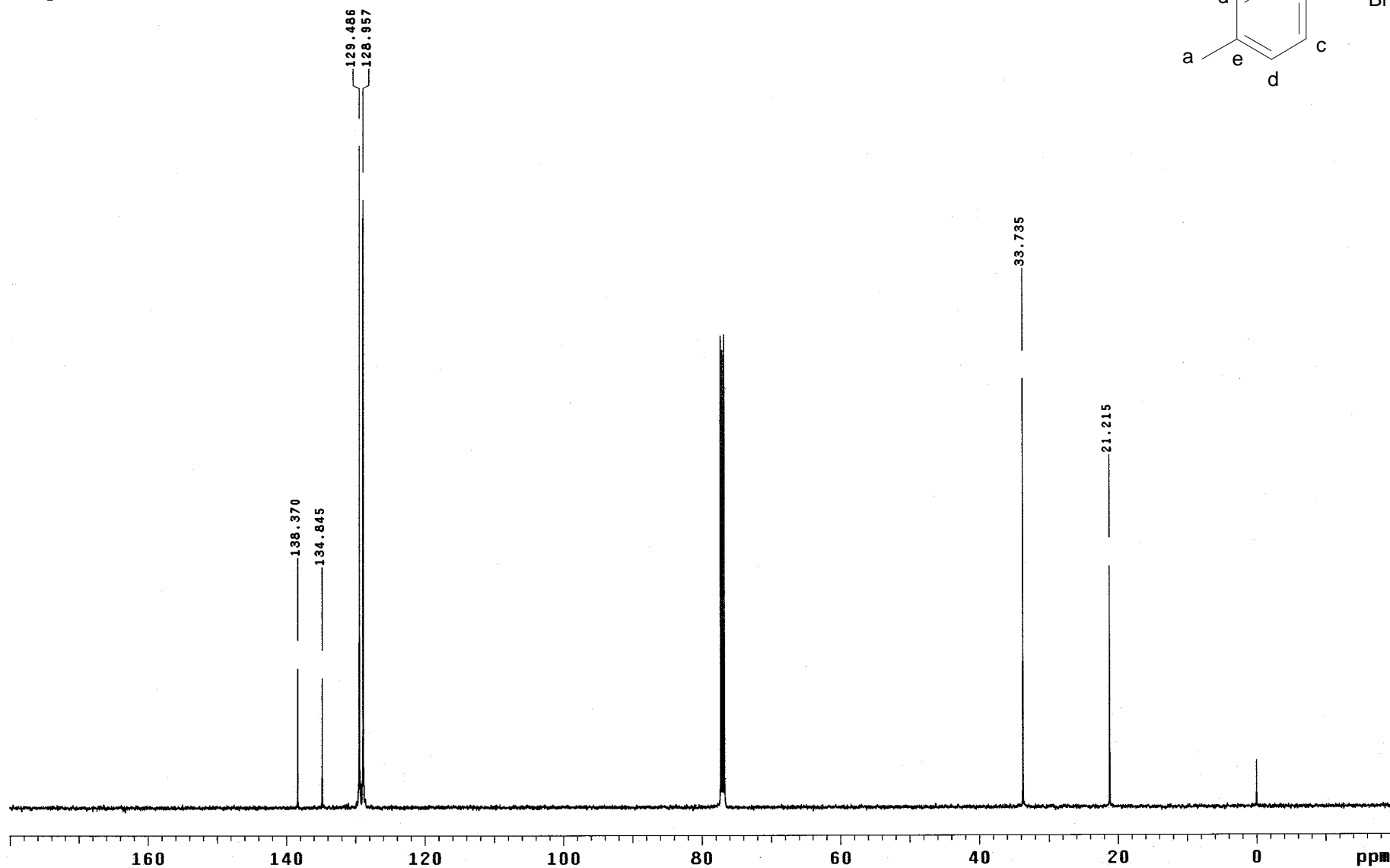
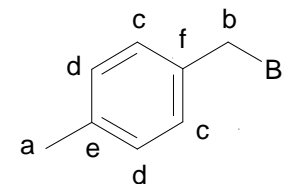
Contributor's name and address:		Verification Laboratory
Secretariat identification code	25-3-0020r (p1/3)	DSO National Laboratories
Signature		11 Stockport Road Singapore 117605
Chemical information:		
Chemical name	4-Methylbenzyl bromide	
Schedule number		
CAS registry number	104-81-4	
Chemical structure with numbering of atoms		
Molecular formula	C ₈ H ₉ Br	
Sample information:		
Sample purity	98%	
Sample concentration	50 mg/mL	
Solvent	CDCl ₃	
pH	-	
Source	Alfa Aesar	
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	¹ H	
Sample temperature	25 °C	
Spectral width (Hz)	5252.1	
Data points in Fourier transformed spectrum	32768	
Repetition time	12 s	
Pulse angle (μs and degrees)	4.463 μs, 45°	
Date of experiment	18 Apr 2005	
Data points in FID	31480	
Number of scans	16	
Baseline correction	Yes	
Spectral information:		
Chemical shifts (ppm) assigned except for acidic protons	Ha = 2.34, Hb = 4.48, Hc = 7.27, Hd = 7.14	
Coupling constants (Hz)	³ J _{aromatic H} = 7.9	

25-3-0020r (p2/3)

4-Methyl benzyl bromide (C₈H₉Br)

[104-81-4]

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: 4.125 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: 21.22
b: 33.74
c: 128.96
d: 129.49

Nuc δ[ppm]
e: 138.37
f: 134.85

4-Methyl benzyl bromide (C_8H_9Br)

[104-81-4]

