
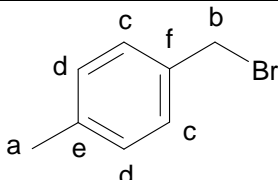


NMR SPECTROMETRY

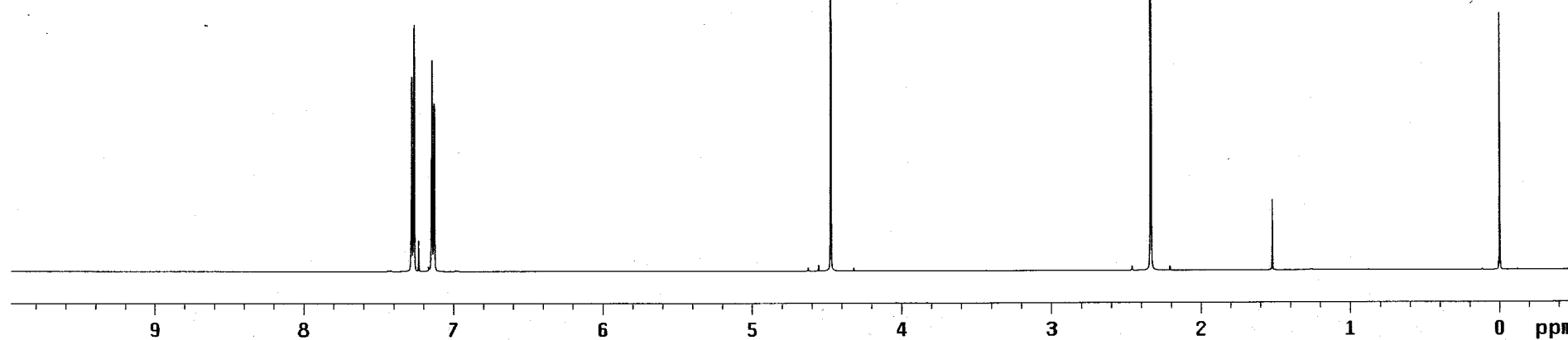
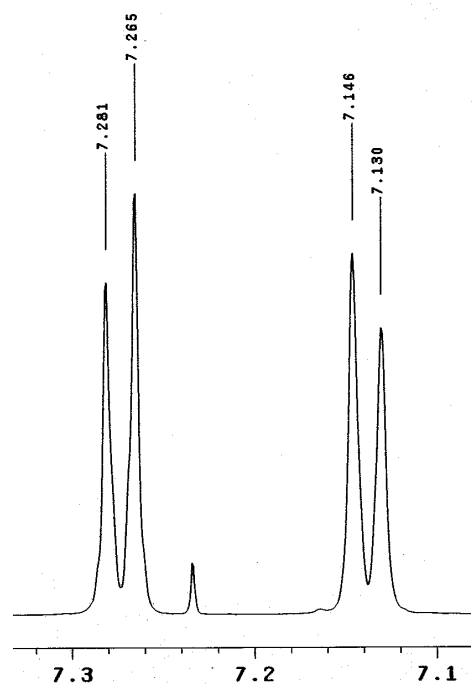
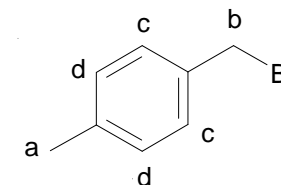
Contributor's name and address:		Verification Laboratory
Secretariat identification code	25-3-0019r (p1/2)	DSO National Laboratories
Signature		11 Stockport Road Singapore 117605
Chemical information:		
Chemical name	4-Methylbenzyl bromide	
Schedule number		
CAS registry number	104-81-4	
Chemical structure 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	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)	4.125 μs, 45°	
Date of experiment	18 Apr 2005	
Data points in FID	35062	
Number of scans	720	
Baseline correction	Yes	
Spectral information:		
Chemical shifts (ppm) assigned except for acidic protons	Ca = 21.22, Cb = 33.74, Cc = 128.96, Cd = 129.49, Ce = 138.37, Cf = 134.85	
Coupling constants (Hz)	-	

25-3-0019r (p2/2)

4-Methyl benzyl bromide (C₈H₉Br)

[104-81-4]

¹H NMR



Res.Freq: 499.662 MHz
Solvent: CDCl₃
Temperature: 25°C
Concentration: 50 mg/mL
Reference: TMS (internal)

Spectral Width: 5252.1 Hz
Data points [FID]: 31480
Data points [Spectrum]: 32768
Pulse width: 4.463 μs, 45°
Number of Scans: 16

Line broadening: no
Rep. time: 12 s
Resolution: 0.3 Hz (TMS)
Baseline correction: Yes
Instrument: Varian INOVA 500

Nuc	δ[ppm]	J[Hz]
a:	2.34	
b:	4.48	
c:	7.27	³ Jaromatic H = 7.9
d:	7.14	