
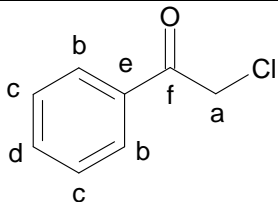


NMR SPECTROMETRY

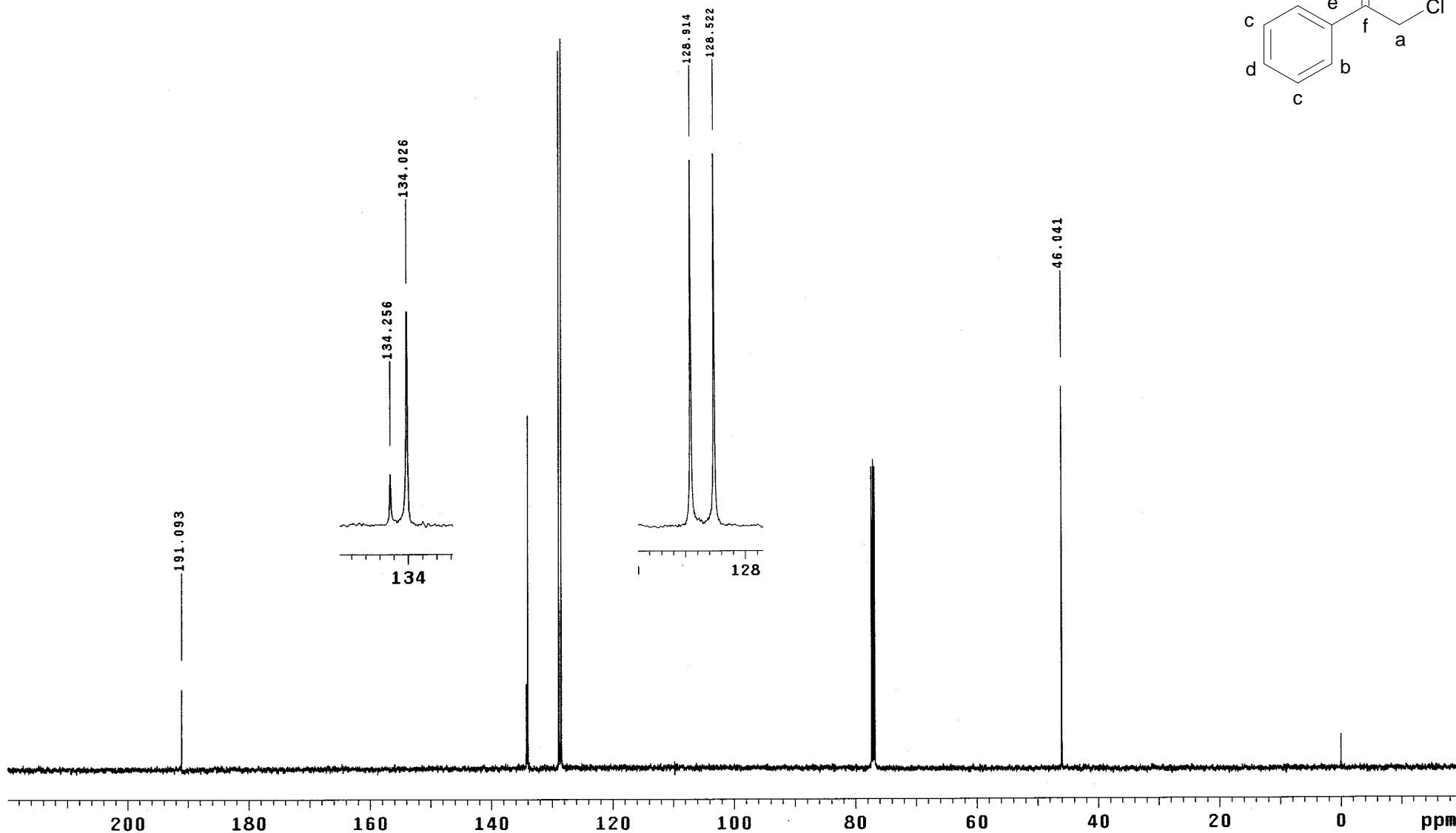
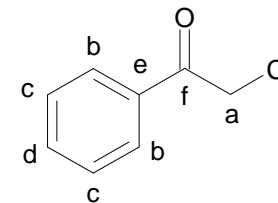
Contributor's name and address:		Verification Laboratory
Secretariat identification code	25-3-0022r (p1/3)	DSO National Laboratories
Signature		11 Stockport Road
		Singapore 117605
Chemical information:		
Chemical name	2-Chloroacetophenone	
Schedule number		
CAS registry number	532-27-4	
Chemical structure with numbering of atoms		
Molecular formula	C ₈ H ₇ ClO	
Sample information:		
Sample purity	98 %	
Sample concentration	49 mg/mL	
Solvent	CDCl ₃	
pH	-	
Source	Merck	
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	3 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 = 46.04, Cb = 128.52, Cc = 128.91, Cd = 134.03, Ce = 134.26, Cf = 191.09	
Coupling constants (Hz)	-	

25-3-0022r (p2/3)

2-Chloroacetophenone (C₈H₇ClO)

[532-27-4]

¹³C{¹H} NMR



Res.Freq: 125.653 MHz
Solvent: CDCl₃
Temperature: 25°C
Concentration: 49 mg/mL
Reference: TMS (internal)

Spectral Width: 35133.9 Hz
Data points [FID]: 35062
Data points [Spectrum]: 65536
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]
a: 46.04
b: 128.52
c: 128.91
d: 134.03

Nuc δ[ppm]
e: 134.26
f: 191.09

25-3-0022r (p3/3)

2-Chloroacetophenone (C₈H₇ClO)

[532-27-4]

