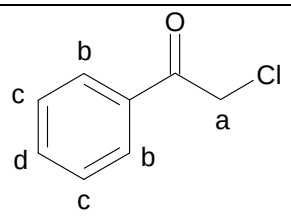
NMR SPECTROMETRY

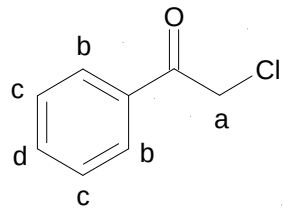
Contributor's name and address:	Verification Laboratory DSO National Laboratories 11 Stockport Road Singapore 117605
Secretariat identification code	25-3-0021r (p1/2)
Signature	
Chemical information:	
Chemical name	2-Chloroacetophenone
Schedule number	
CAS registry number	532-27-4
Chemical structure with numbering of atoms	
Molecular formula	C_8H_7ClO
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	^1H
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)	3.462 μs, 45°
Date of experiment	3 Jun 2005
Data points in FID	31480
Number of scans	16
Baseline correction	Yes
Spectral information:	
Chemical shifts (ppm) assigned except for acidic protons	Ha = 4.72, Hb = 7.96, Hc = 7.50, Hd = 7.62
Coupling constants (Hz)	$^3J_{\text{aromatic H}}$ = 8.0

25-3-0021r (p2/2)

2-Chloroacetophenone (C_8H_7ClO)

[532-27-4]

^{1}H NMR



Res.Freq: 499.662 MHz
Solvent: $CDCl_3$
Temperature: 25°C
Concentration: 49 mg/mL
Reference: TMS (internal)

Spectral Width: 5252.1 Hz
Data points [FID]: 31480
Data points [Spectrum]: 32768
Pulse width: 3.462 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:	4.72	
b:	7.96	^{3}Jaromatic H = 8.0
c:	7.50	
d:	7.62	