
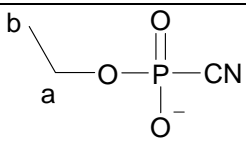


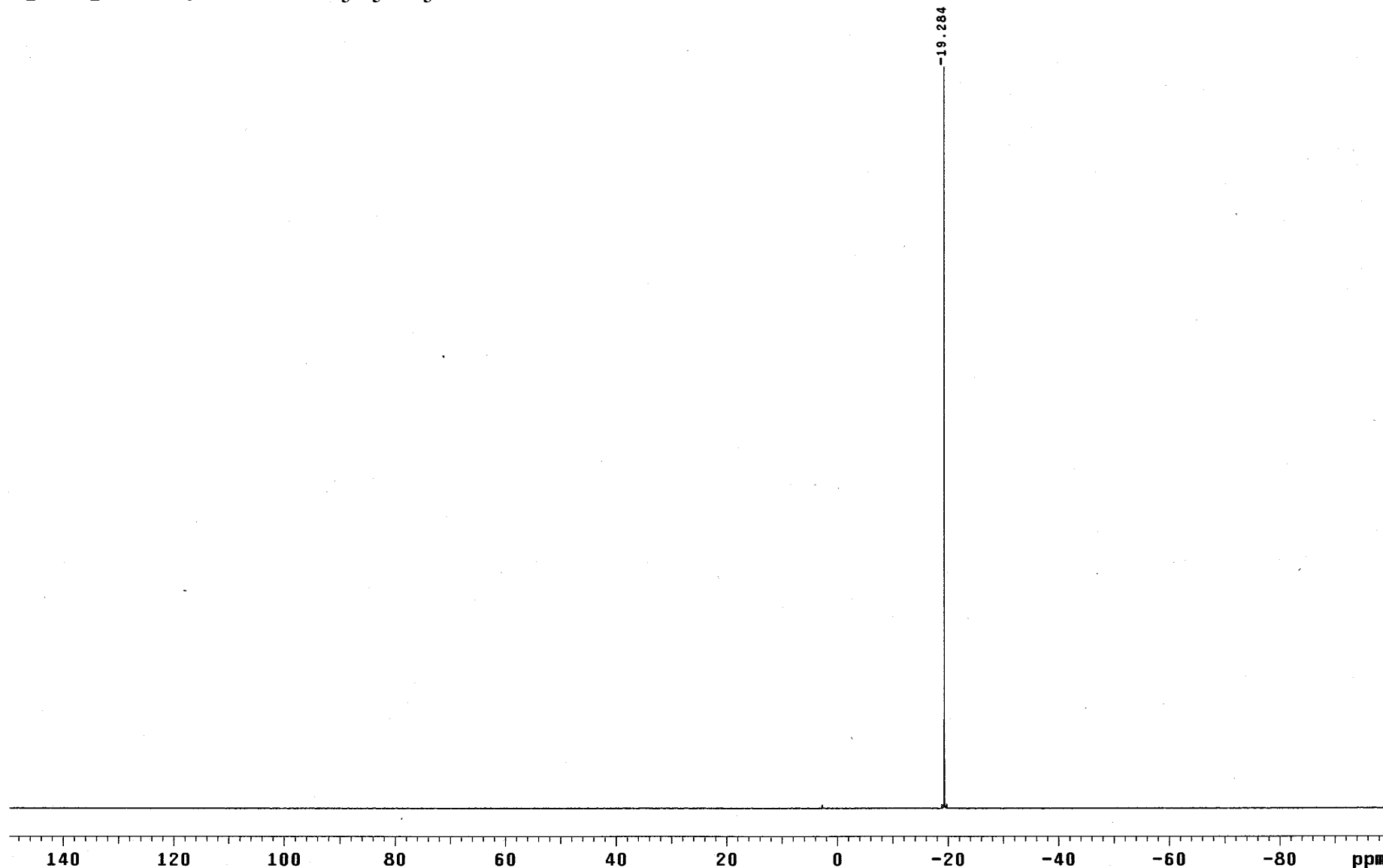
NMR SPECTROMETRY

Contributor's name and address:		Verification Laboratory
Secretariat identification code	25-3-0011r (p1/2)	DSO National Laboratories
Signature		11 Stockport Road Singapore 117605
Chemical information:		
Chemical name	Ethyl phosphorocyanidate	
Schedule number		
CAS registry number		
Chemical structure with numbering of atoms		
Molecular formula	C ₃ H ₅ NO ₃ P	
Sample information:		
Sample purity	96 %	
Sample concentration	30 mg/mL	
Solvent	D ₂ O	
pH	8.32	
Source	In-house synthesis YL30772	
Reference chemical shift (external)	H ₃ PO ₄ , 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	³¹ P{ ¹ H}	
Sample temperature	25 °C	
Spectral width (Hz)	50568.9	
Data points in Fourier transformed spectrum	131072	
Repetition time	14 s	
Pulse angle (μs and degrees)	8.875 μs, 45°	
Date of experiment	25 Jun 2005	
Data points in FID	101276	
Number of scans	64	
Baseline correction	Yes	
Spectral information:		
Chemical shifts (ppm) assigned except for acidic protons	P = -19.28	
Coupling constants (Hz)	-	

25-3-0011r (p2/2)

Ethyl phosphorocyanidate ($C_3H_5NO_3P$)

$^{31}P\{^1H\}$ NMR



Res.Freq: 202.271 MHz

Solvent: D2O

Temperature: 25°C

Concentration: 30 mg/mL

pH: 8.32

Reference: H_3PO_4 (external), 0ppm

Spectral Width: 50568.9 Hz

Data points [FID]: 101276

Data points [Spectrum]: 131072

Pulse width: 8.875 μs , 45°

Number of Scans: 64

Line broadening: 2

Rep. time: 14 s

Resolution: 0.77 Hz

Baseline correction: Yes

Instrument: Varian INOVA 500

Nuc δ [ppm]

P: -19.28

