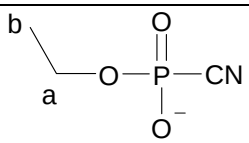
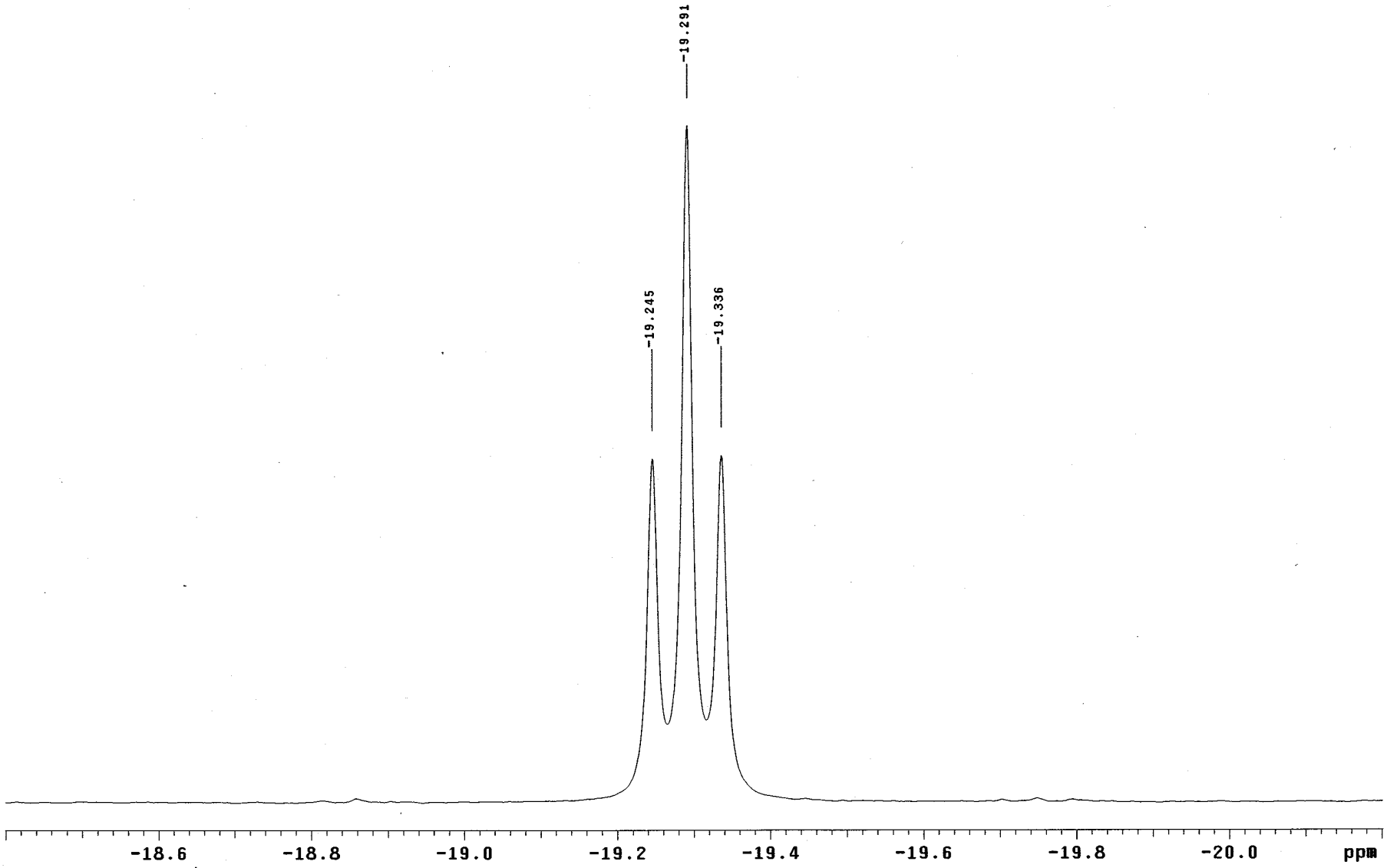
NMR SPECTROMETRY

Contributor's name and address:	Verification Laboratory DSO National Laboratories 11 Stockport Road Singapore 117605
Secretariat identification code	25-3-0012r (p1/2)
Signature	
Chemical information:	
Chemical name	Ethyl phosphorocyanidate
Schedule number	
CAS registry number	
Chemical structure with numbering of atoms	
Molecular formula	$C_3H_5NO_3P$
Sample information:	
Sample purity	96 %
Sample concentration	30 mg/mL
Solvent	D_2O
pH	8.32
Source	In-house synthesis YL30772
Reference chemical shift (external)	H_3PO_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
Sample temperature	25 °C
Spectral width (Hz)	50568.9
Data points in Fourier transformed spectrum	524288
Repetition time	16 s
Pulse angle (μs and degrees)	8.875 μs, 45°
Date of experiment	25 Jun 2005
Data points in FID	303414
Number of scans	64
Baseline correction	Yes
Spectral information:	
Chemical shifts (ppm) assigned except for acidic protons	P = -19.29
Coupling constants (Hz)	J(Ha,P) = 9.16

Ethyl phosphorocyanidate ($C_3H_5NO_3P$) ^{31}P 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]: 303414
Data points [Spectrum]: 524288
Pulse width: 8.875 μs, 45°
Number of Scans: 64

Line broadening: 2
Rep. time: 16 s
Resolution: 0.19 Hz
Baseline correction: Yes
Instrument: Varian INOVA 500

Nuc δ[ppm]
P: –19.29
J(Ha,P) = 9.16 Hz