

1. GENERAL INFORMATION

IUPAC Name:	1-phenyl-2-(1-pyrrolidinyl)-1-pentanone
CFR:	Not Scheduled (01/2013)
CAS #:	14530-33-7 (base); 5485-65-4 (HCl)
Synonyms:	α-pyrrolidinopentiophenone, α-pyrrolidinovalerophenone , O-2387
Source:	DEA Reference Material Collection
Appearance:	White powder (HCl)
Kovat's Index:	Pending
UV_{max} (nm):	253.0

2. CHEMICAL AND PHYSICAL DATA

2.1 CHEMICAL DATA

Form	Chemical Formula	Molecular Weight	Melting Point (°C)
Base	C ₁₅ H ₂₁ NO	231	Not Determined
HCl	C ₁₅ H ₂₁ NO · HCl	267	161.3

3. *ADDITIONAL RESOURCES*

[Forendex](#)

[Wikipedia](#)

4. *QUALITATIVE DATA*

4.1 NUCLEAR MAGNETIC RESONANCE

Method NMR D₂O

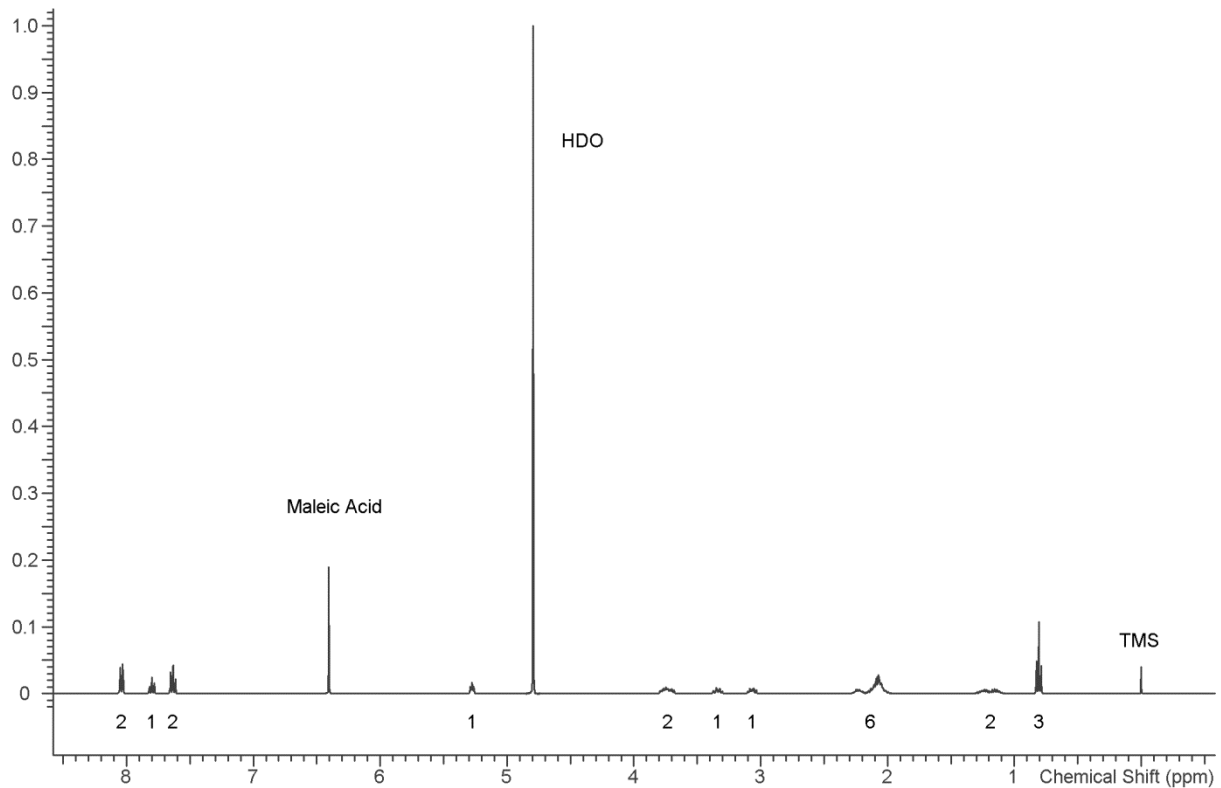
Sample Preparation: Dilute analyte to ~10 mg/mL in D₂O containing TSP for 0 ppm reference and maleic acid as quantitative internal standard.

Instrument: Varian Mercury 400 MHz NMR spectrometer with proton detection probe

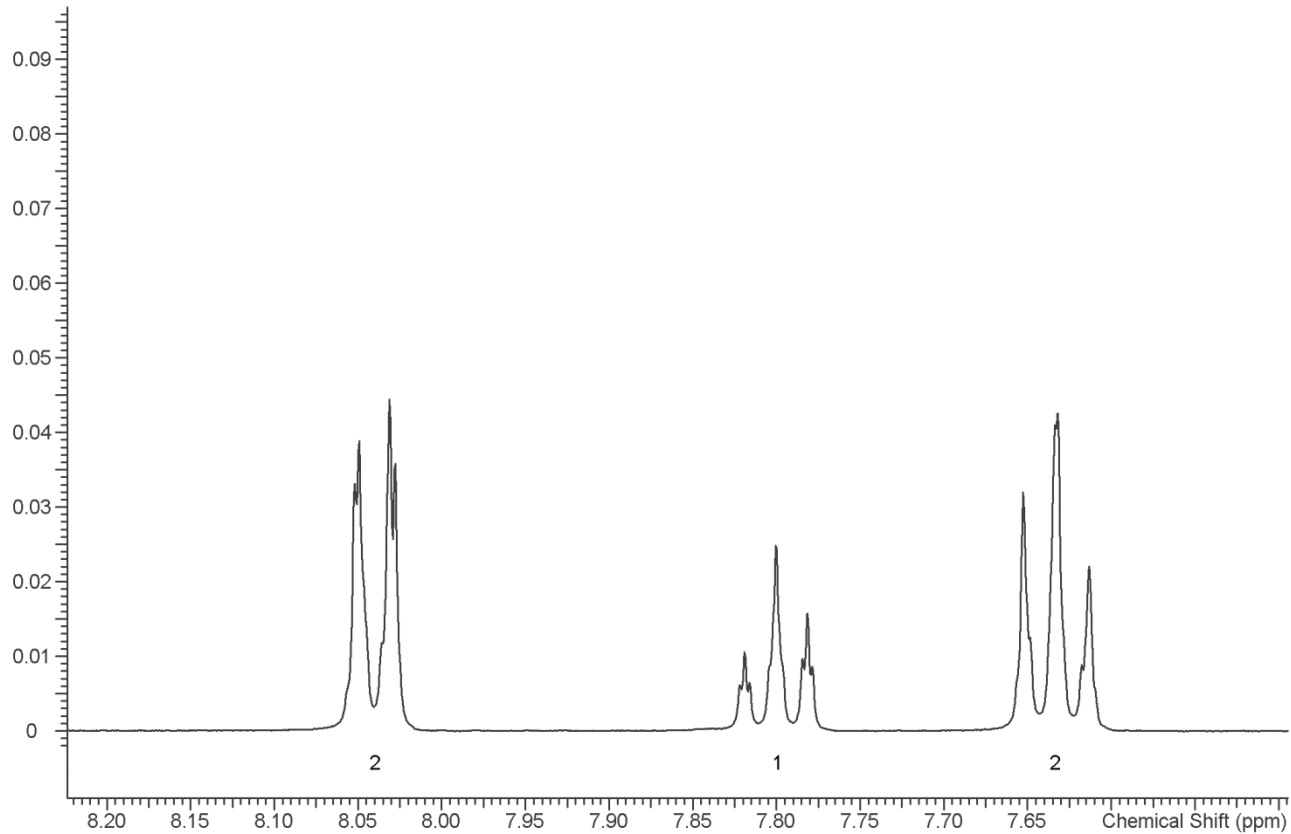
Parameters:

- Spectral width: at least containing -3 ppm through 13 ppm
- Pulse angle: 90°
- Delay between pulses: 45 seconds
- Number of scans (NT): 8
- Number of steady state scans: 0
- Oversampling: 4 or more
- Shimming: automatic gradient shimming of Z1-4 shims
- Phasing, Drift Correction: automatic or manual

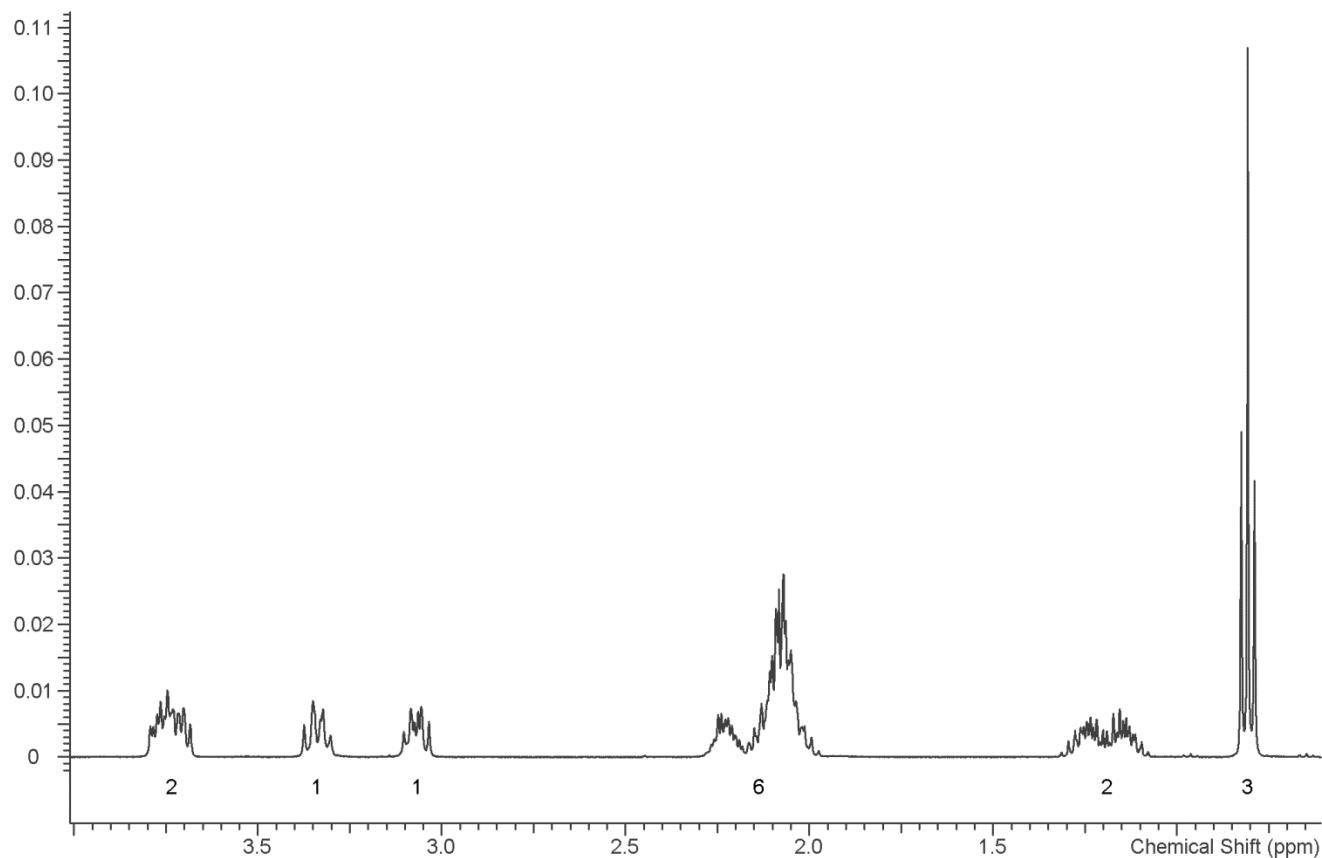
1H NMR: alpha-PVP HCl Lot # N17-P29H, D₂O, 400MHz



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4.2 GAS CHROMATOGRAPHY/MASS SPECTROMETRY

Sample Preparation: Dilute analyte to ~1 mg/mL in MeOH.

Instrument: Agilent gas chromatograph operated in split mode with MS detector

Column: DB-1 MS; 30m x .25mm x .25 μ m

Carrier Gas: Helium at 1 mL/min

Temperatures:
Injector: 280°C
MSD transfer line: 280°C
MS Source: 230°C
MS Quad: 150°C

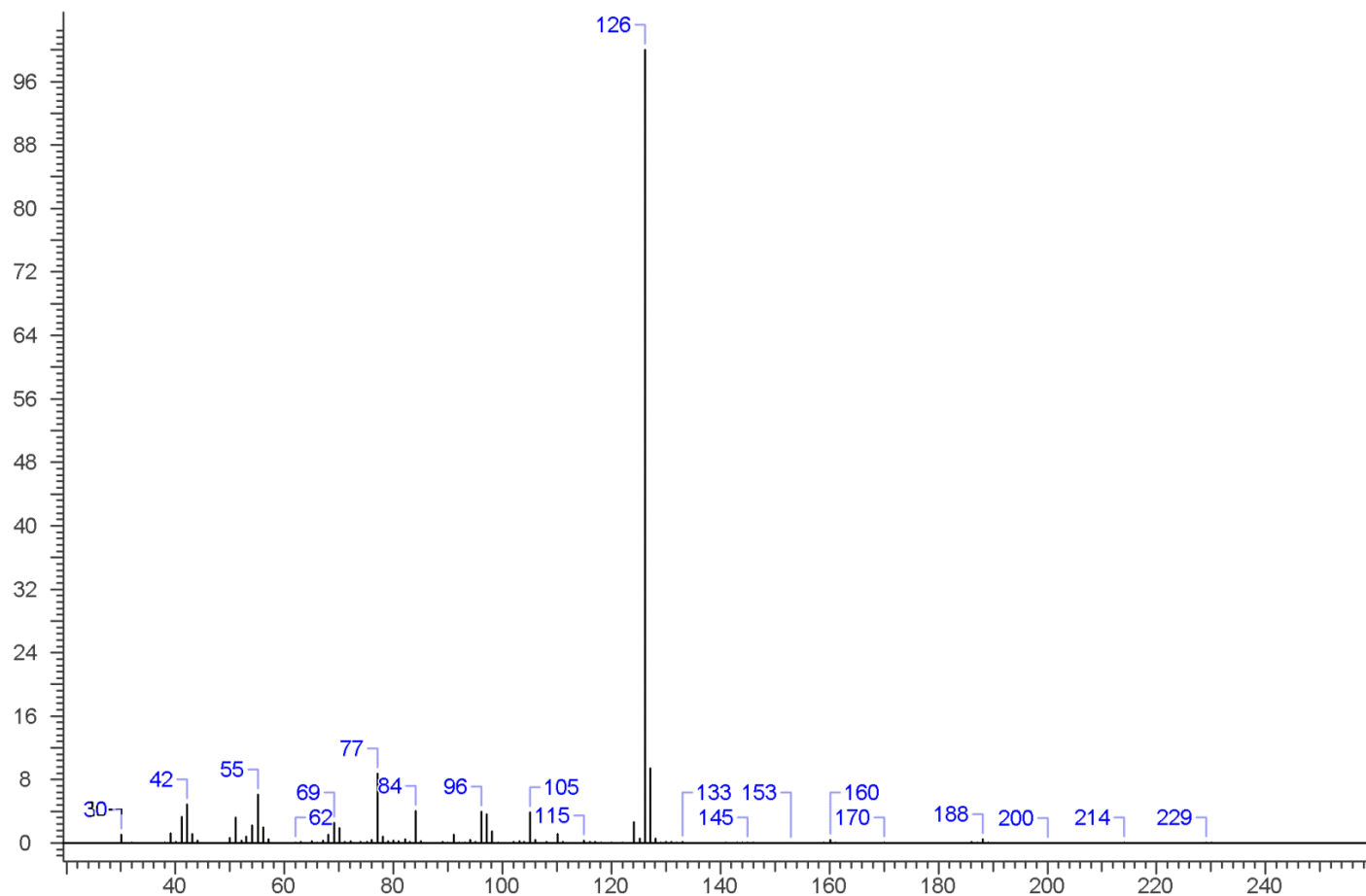
Oven program:
1) 100°C initial temperature for 1.0 min
2) Ramp to 300°C at 12°C/min
3) Hold final temperature for 9.0 min

Injection Parameters: Split Ratio = 20:1, 1 μ L injected

MS Parameters:
Mass scan range: 30-550 amu
Threshold: 100
Tune file: stune.u
Acquisition mode: scan

Retention Time: 10.208 minutes

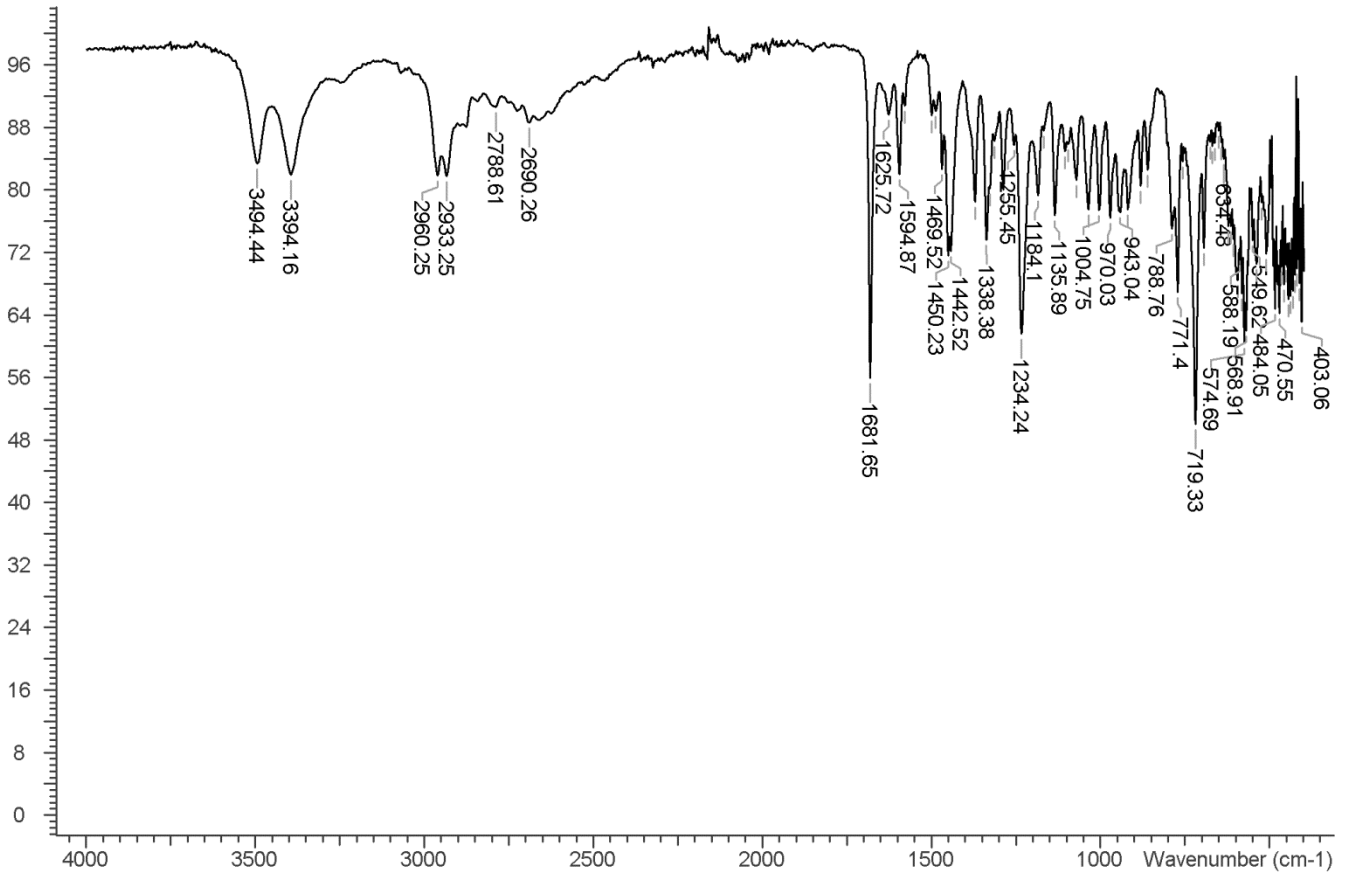
EI Mass Spectrum: alpha-PVP HCl Lot # N17-P29H



4.3 INFRARED SPECTROSCOPY (FTIR)

Instrument: FTIR with diamond ATR attachment (3 bounce)
Scan Parameters: Number of scans: 32
Number of background scans: 32
Resolution: 4cm^{-1}
Sample gain: 8
Aperture: 150

FTIR ATR (Diamond, 3 Bounce): alpha-PVP HCl Lot # N17-P29H



FTIR ATR (Diamond, 3 Bounce): alpha-PVP HCl Lot # N17-P29H

