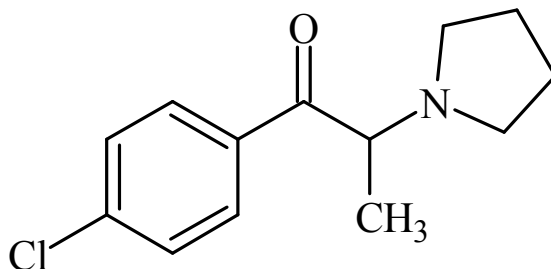




4'-Chloro- α -pyrrolidinopropiophenone

The Drug Enforcement Administration's Special Testing and Research Laboratory generated this monograph using structurally confirmed reference material.



1. GENERAL INFORMATION

IUPAC Name: 1-(4-chlorophenyl)-2-(pyrrolidin-1-yl)propan-1-one

CAS#: Not Available

Synonyms: 4'-Chloro- α -PPP, 4'-Chloro-PPP

Source: DEA Reference Material Collection

Appearance: Light brown powder

UV_{max}(nm): Not Determined

2. CHEMICAL AND PHYSICAL DATA

2.1 CHEMICAL DATA

Form	Chemical Formula	Molecular Weight	Melting Point (°C)
Base	C ₁₃ H ₁₆ ClNO	237.725	Not Determined
HCl	C ₁₃ H ₁₆ ClNO HCl	274.186	Not Determined



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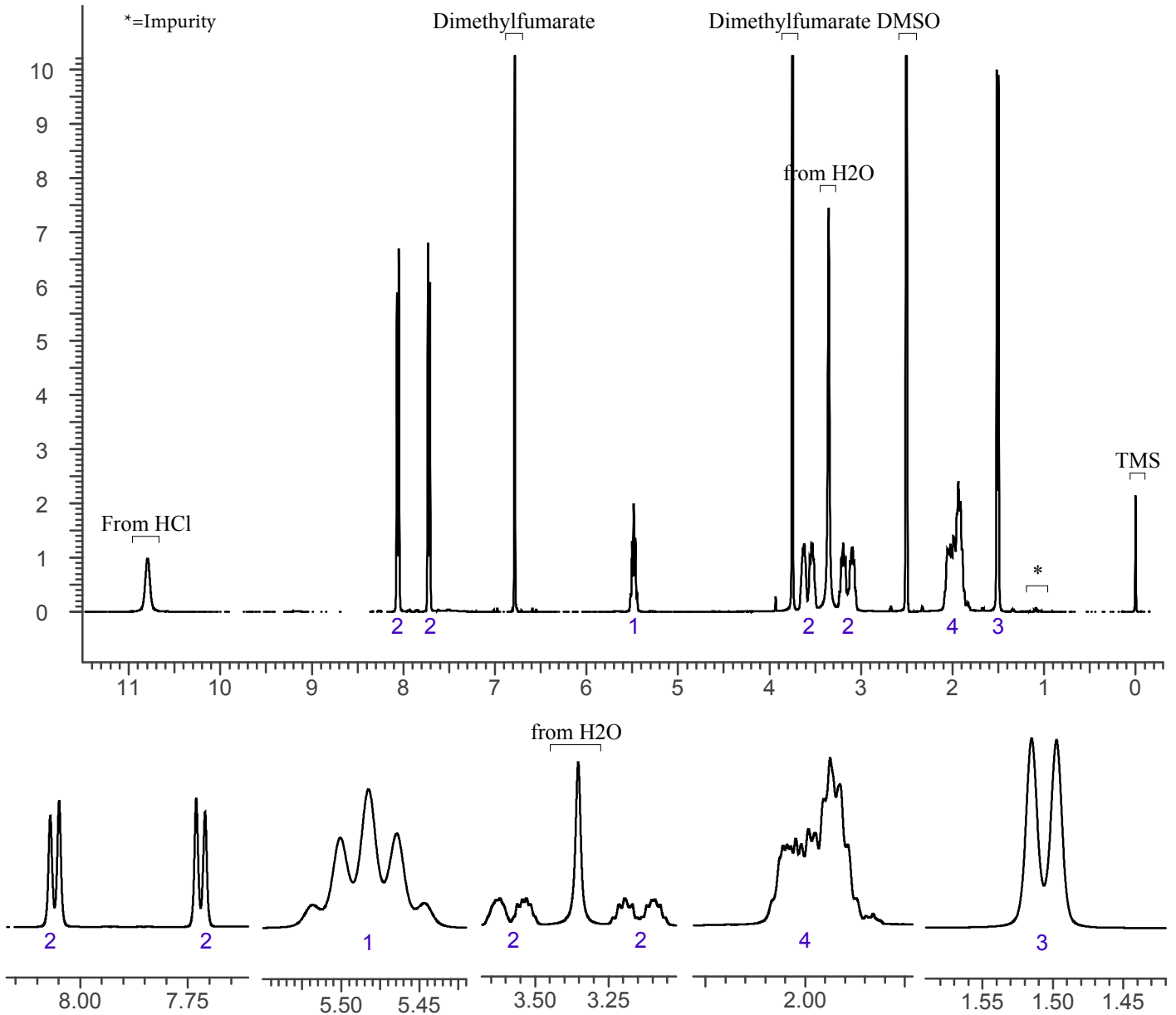
3. QUALITATIVE DATA

3.1 NUCLEAR MAGNETIC RESONANCE

Sample Preparation: Dilute analyte to ~5 mg/mL in DMSO containing TMS for 0 ppm reference and dimethylfumarate as quantitative internal standard.

Instrument: 400 MHz NMR spectrometer
Parameters: Spectral width: at least containing 3 ppm through 13 ppm
Pulse angle: 90°
Delay between pulses: 45 seconds

¹HNMR: 4 Chloro- α -Pyrrolidinopentiophenone HCl Lot 0464674-27, 400MHz





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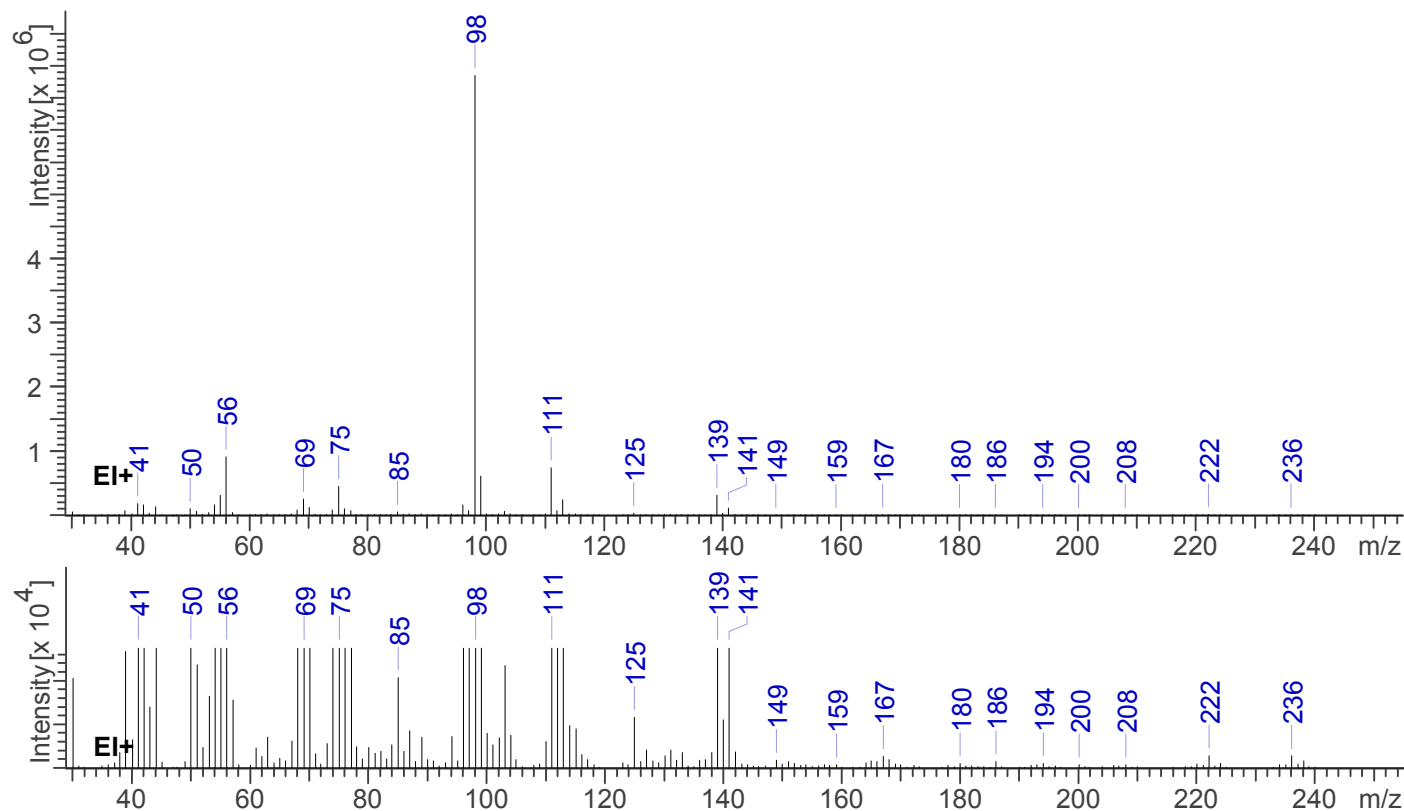
3.2 GAS CHROMATOGRAPHY/MASS SPECTROMETRY

Sample Preparation: Dilute analyte ~4 mg/mL in base extracted CHCl_3 .

Instrument: Agilent gas chromatograph operated in split mode with MS detector
Column: HP-5 MS (or equivalent); 30m x 0.25 mm x 0.25 μm
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 = 25:1, 1 μL injected
MS Parameters: Mass scan range: 30-550 amu
Threshold: 100
Tune file: stune.u
Acquisition mode: scan
Retention Time: 9.914 min

EI Mass Spectrum: 4'-Chloro- α -pyrrolidinopropiophenone HCl, Lot 0464674-27





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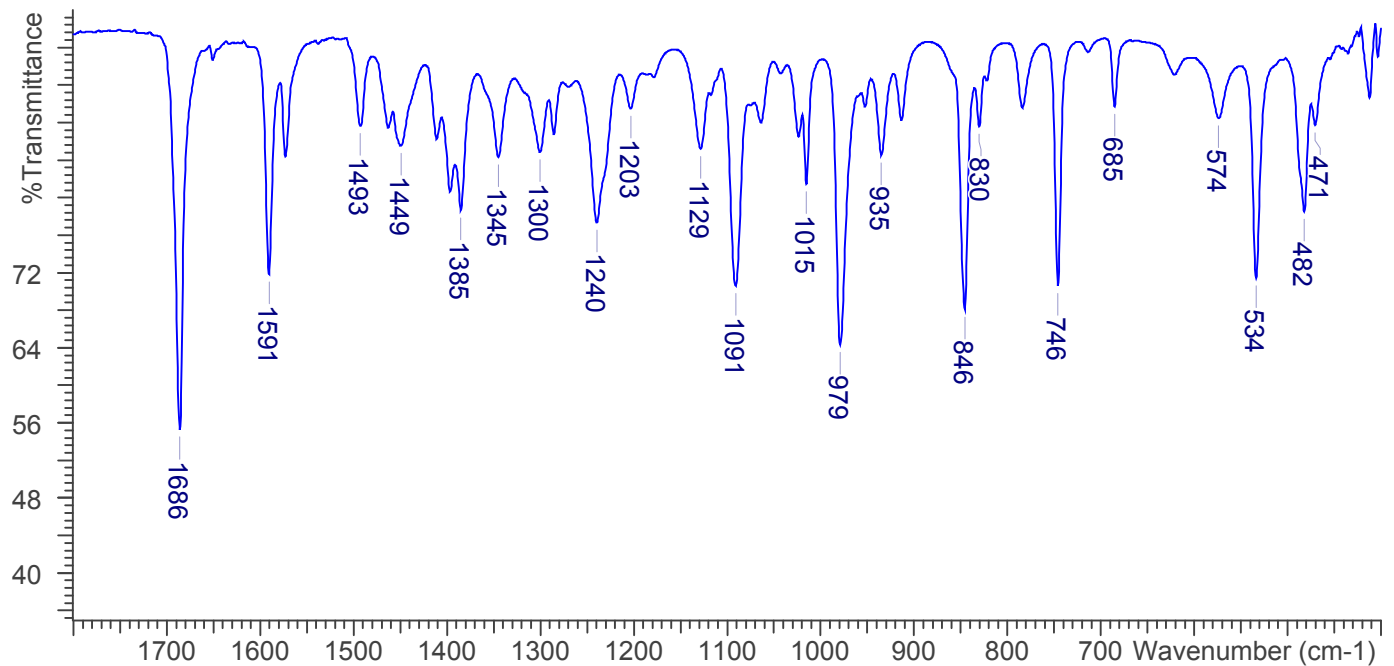
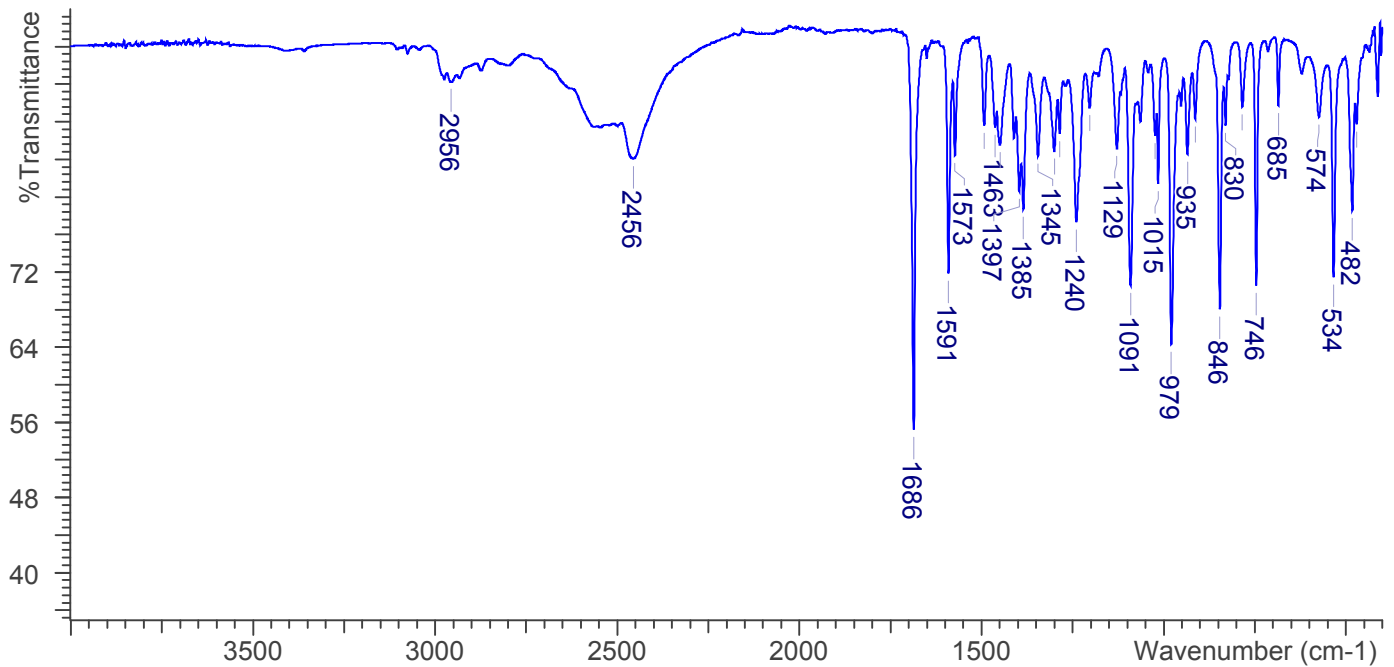


3.3 INFRARED SPECTROSCOPY (FTIR)

Instrument: FTIR with diamond ATR attachment (1 bounce)

Scan Parameters:
Number of scans: 32
Number of background scans: 32
Resolution: 4 cm^{-1}
Sample gain: 8
Aperture: 150

FTIR ATR (Diamond, 1 Bounce): 4-Chloro- α -Pyrrolidinopentiophenone HCl, Lot 0464674-27





4'-Chloro- α -pyrrolidinopropiophenone

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4. ADDITIONAL RESOURCES

No Literature as of 06/2016