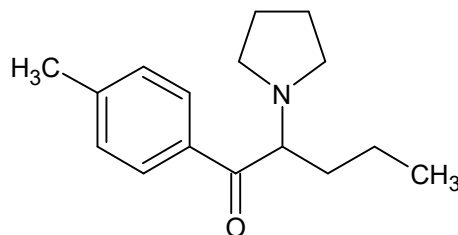




Pyrovalerone

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-methylphenyl)-2-(pyrrolidin-1-yl)pentan-1-one

CAS#: 3563-49-3

Synonyms: Centroton, 4-Methyl-B-detone-prolintane, Thymergix, O-2371, Valerophenone

Source: DEA Reference Material Collection

Appearance: NA (sample in solution)

$UV_{max}(nm)$: Not determined

2. CHEMICAL AND PHYSICAL DATA

2.1 CHEMICAL DATA

Form	Chemical Formula	Molecular Weight	Melting Point (°C)
Base	$C_{16}H_{23}NO$	245	Not Determined
HCl	$C_{16}H_{23}NO \text{ HCl}$	281	Not Determined



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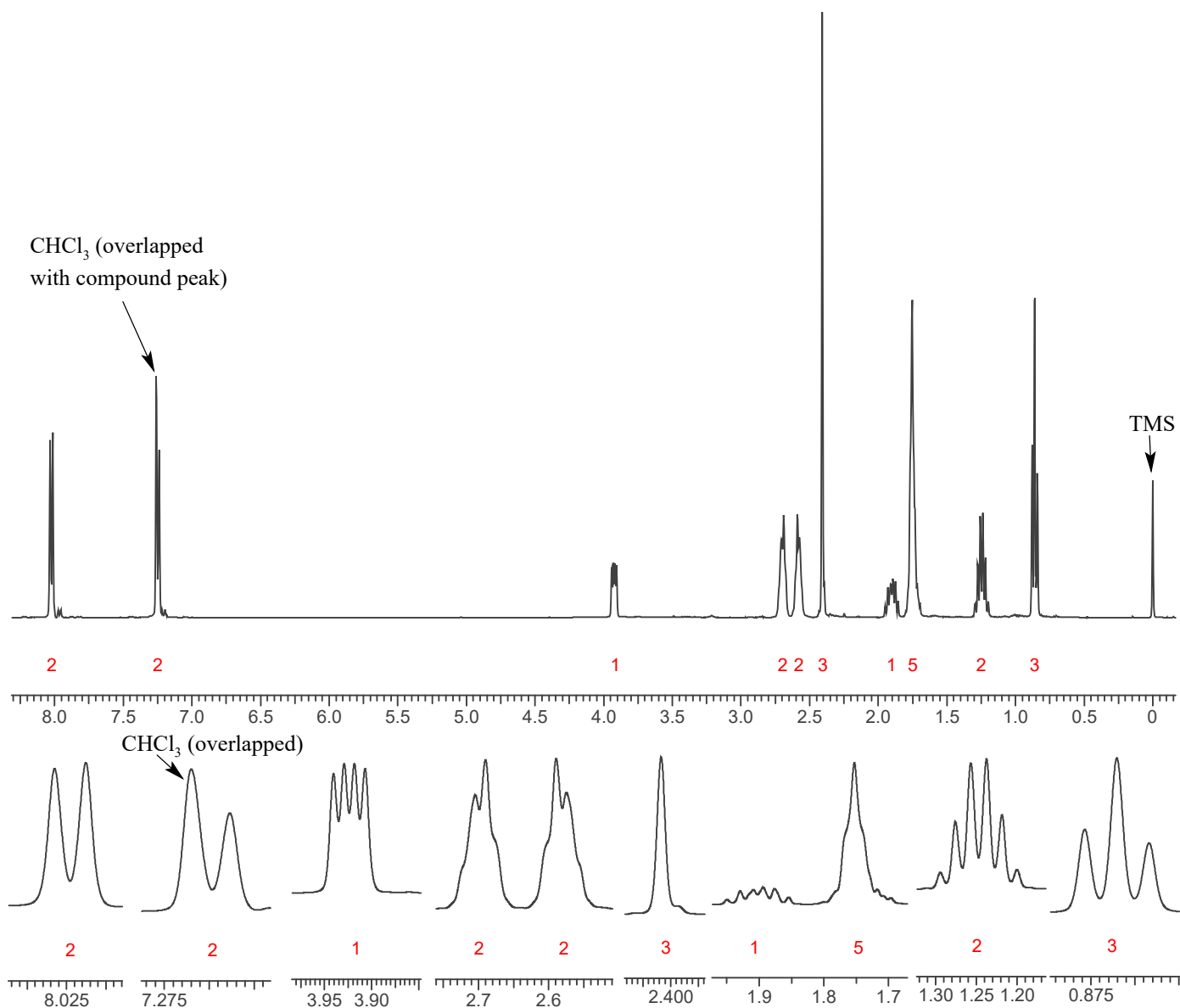
3. QUALITATIVE DATA

3.1 NUCLEAR MAGNETIC RESONANCE

Sample Preparation: Dilute analyte to ~9 mg/mL in CDCl_3 containing TMS for 0 ppm reference.

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

^1H NMR: Pyrovalerone; Lot# 0427898-21; CDCl_3 ; 400MHz





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3.2 GAS CHROMATOGRAPHY/MASS SPECTROMETRY

Sample Preparation: Dilute analyte ~ 2 drops in 1 mL CHCl₃

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

Column: DB-1 MS (or equivalent); 30m x 0.25 mm x 0.25 μm

Carrier Gas: Helium at 1.0 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

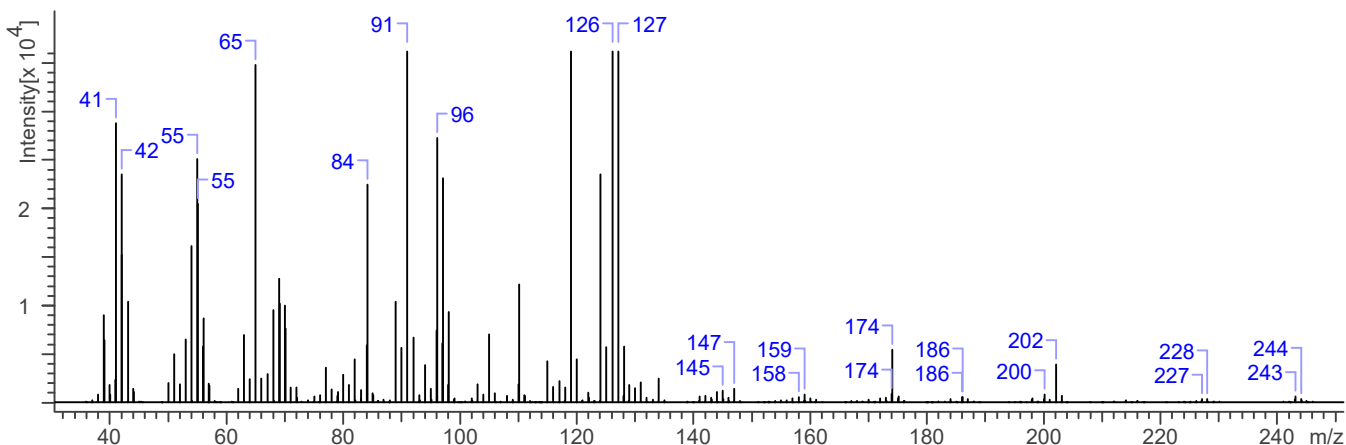
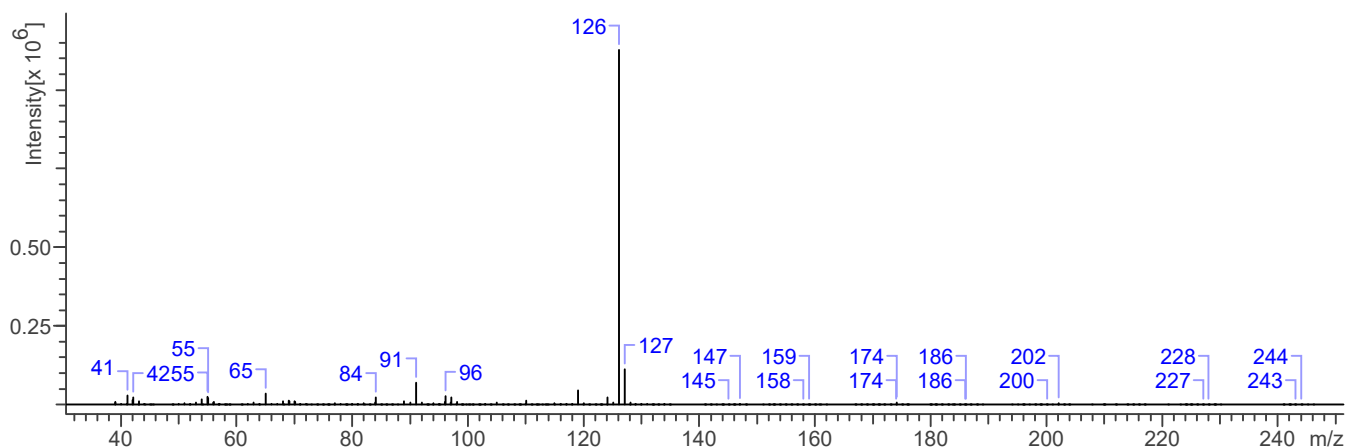
3) Hold final temperature for 30.0 min

Injection Parameters: Split Ratio = 25:1, 1 μL injected

MS Parameters: Mass scan range: 30-550 amu Threshold: 150
Tune file: stune.u Acquisition mode: scan

Retention Time: 11.332 min

EI Mass Spectrum: Pyrovalerone; Lot# 0427898-21





Pyrovalerone



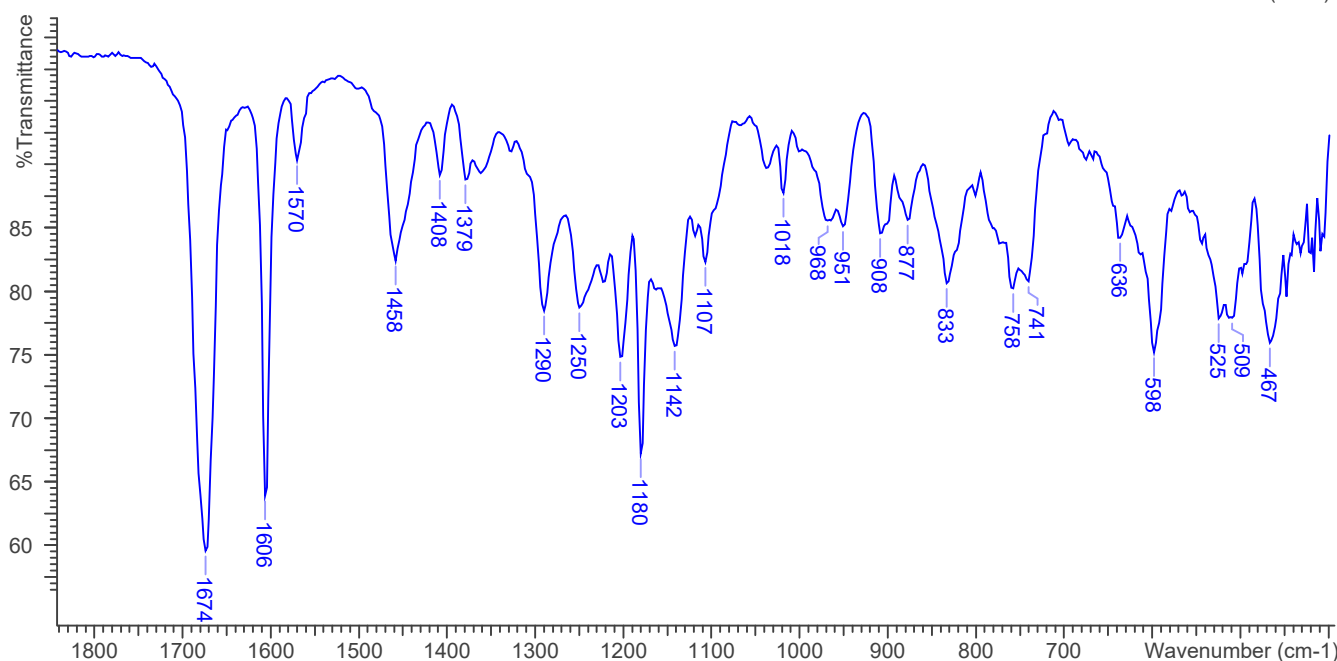
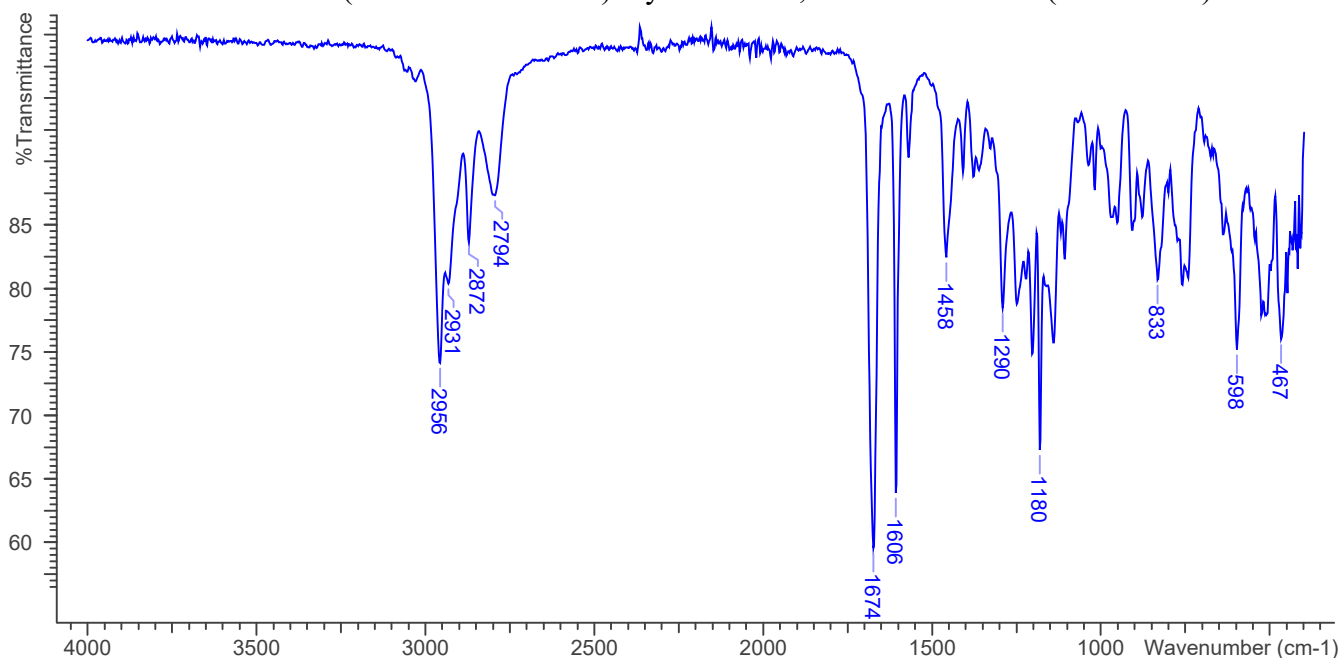
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3.3 INFRARED SPECTROSCOPY (FTIR)

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): Pyrovalerone; Lot# 0427898-21 (dried down)





Pyrovalerone

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4. ADDITIONAL RESOURCES

[*Wikipedia*](#)

[*Forendex*](#)