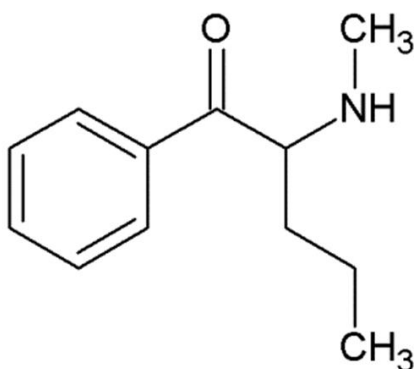




Pentedrone



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



1. GENERAL INFORMATION

IUPAC Name: 2-(methylamino)-1-phenylpentan-1-one

CAS #: 879669-95-1 (HCl)

Synonyms: α -methylaminovalerophenone

Source: DEA Reference Material Collection

Appearance: White powder (HCl)

UV_{max}: Not Determined

2. CHEMICAL AND PHYSICAL DATA

2.1 CHEMICAL DATA

Form	Chemical Formula	Molecular Weight	Melting Point (°C)
Base	C ₁₂ H ₁₇ NO	191	Not Determined
HCl	C ₁₂ H ₁₇ NO · HCl	227	176.8



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3. QUALITATIVE DATA

3.1 NUCLEAR MAGNETIC RESONANCE

Method NMR D₂O

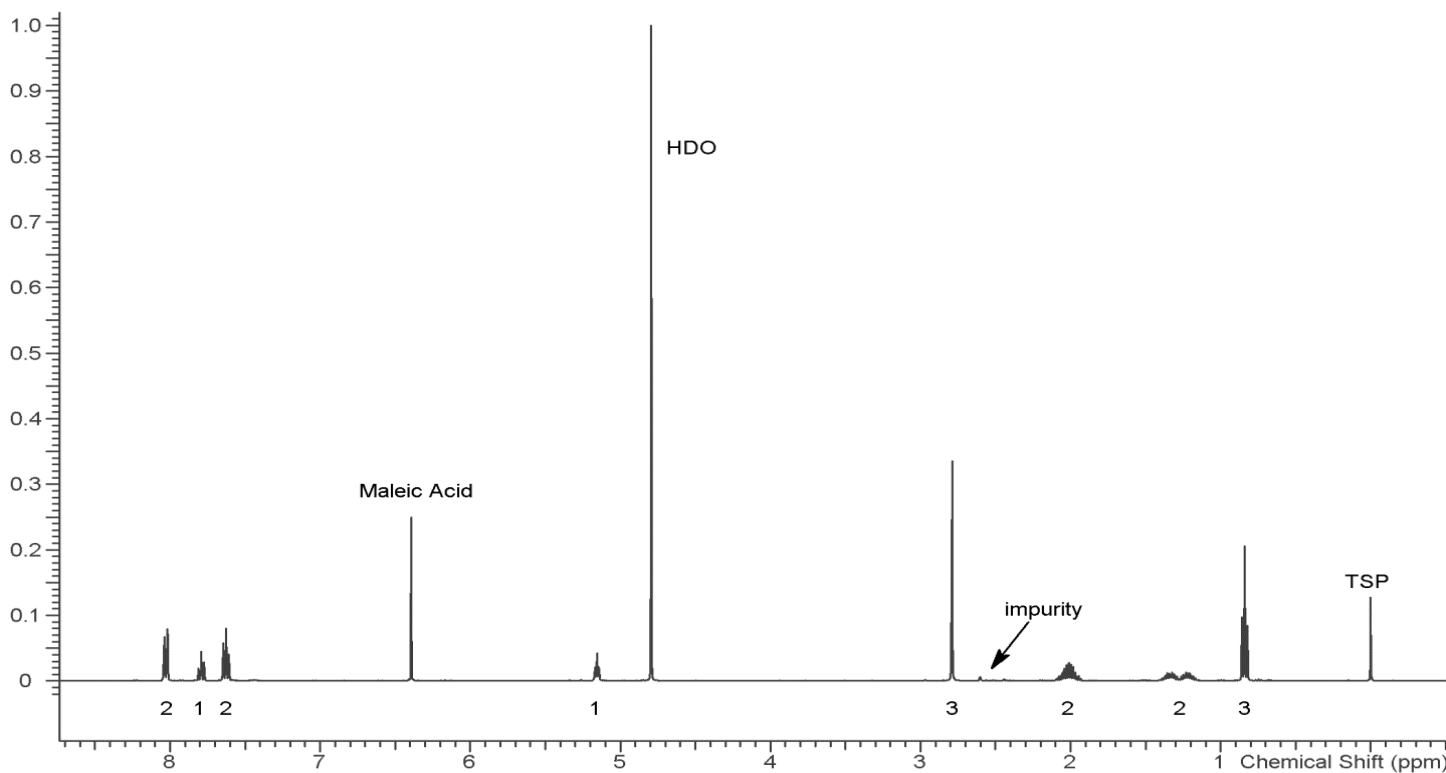
Sample Preparation: Dilute analyte to ~10 mg/mL in D₂O containing TSP for 0 ppm reference and maleic acid as quantitative internal standard.

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: Pentedrone HCl Lot # ALB225-6, D₂O, 400MHz



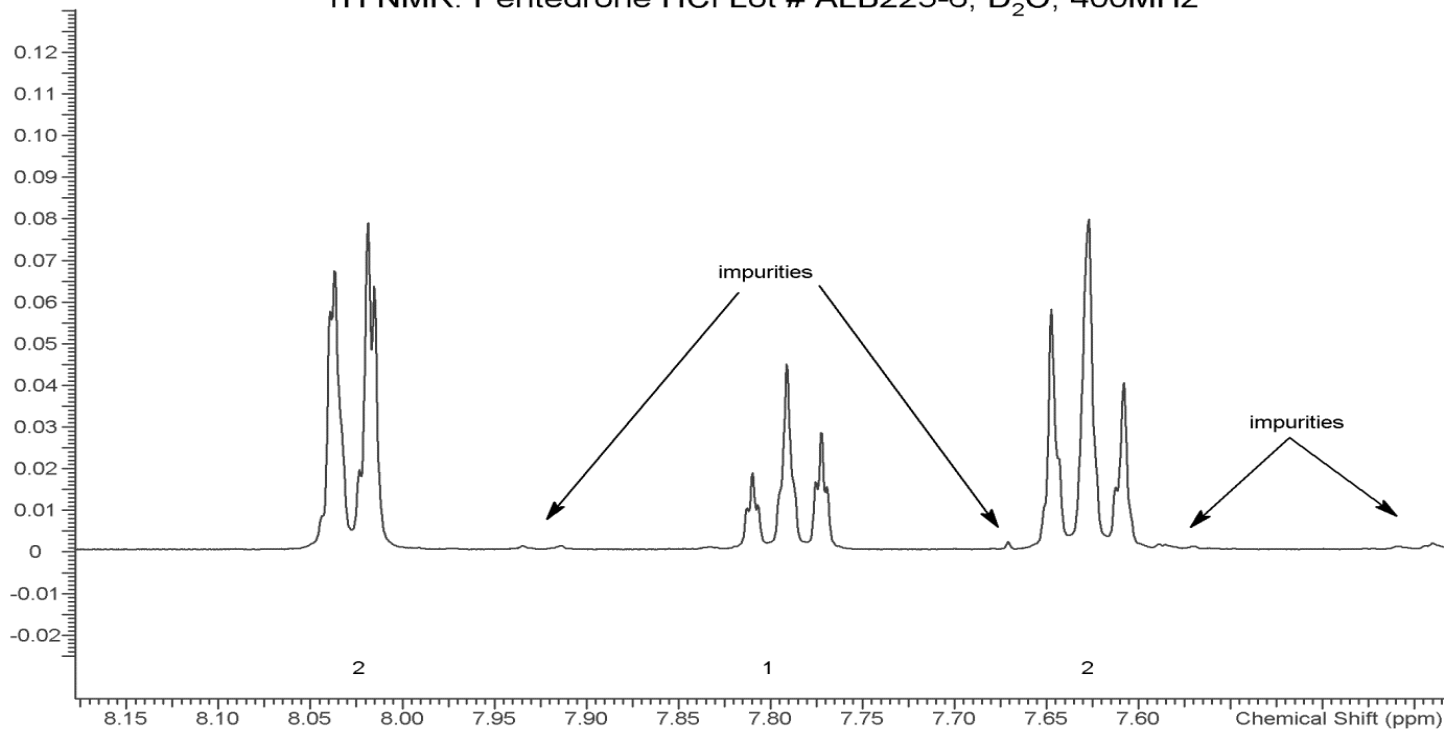


Pentedrone

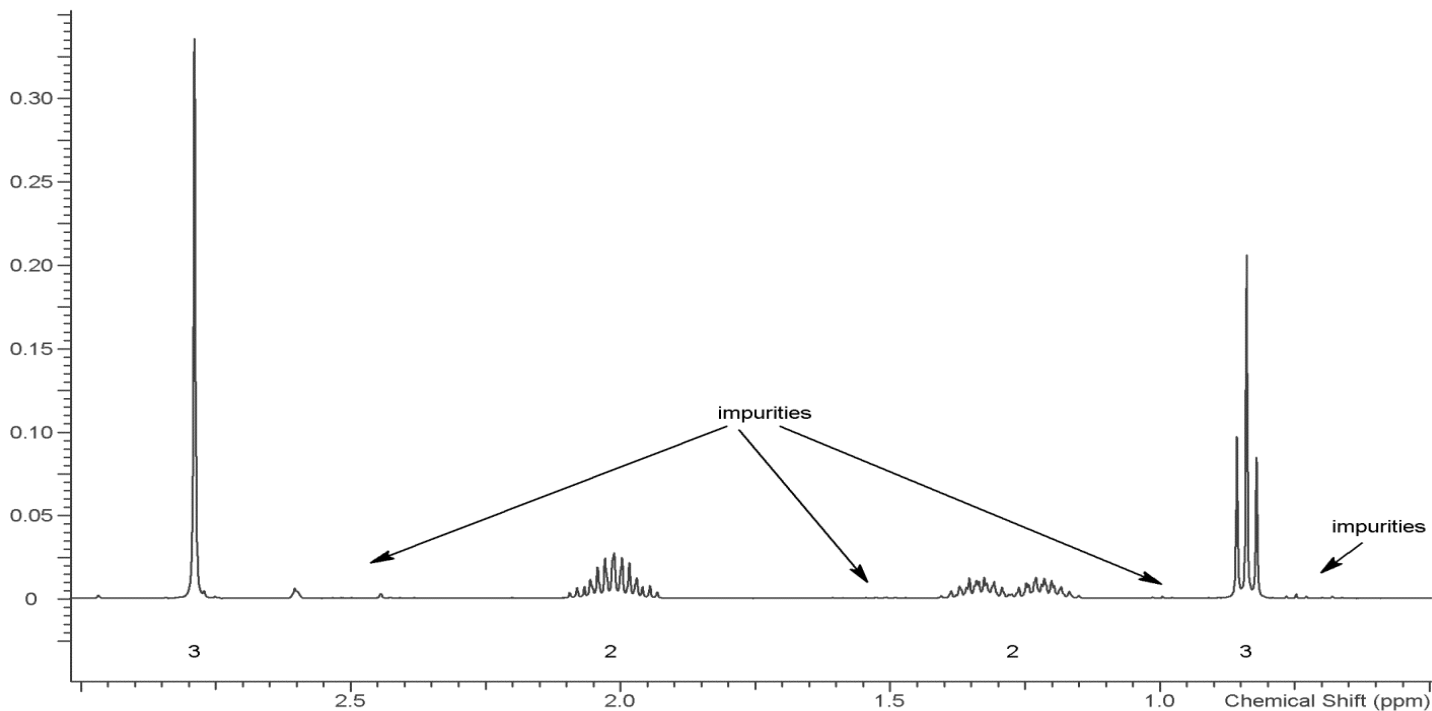


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¹H NMR: Pentedrone HCl Lot # ALB225-6, D₂O, 400MHz



¹H NMR: Pentedrone HCl Lot # ALB225-6, D₂O, 400MHz





Pentedrone

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3.2 GAS CHROMATOGRAPHY/MASS SPECTROMETRY

Sample Preparation: Dilute analyte to ~1 mg/mL base extracted in CHCl₃.

Instrument: Gas chromatograph operated in split mode with MS detector

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

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:

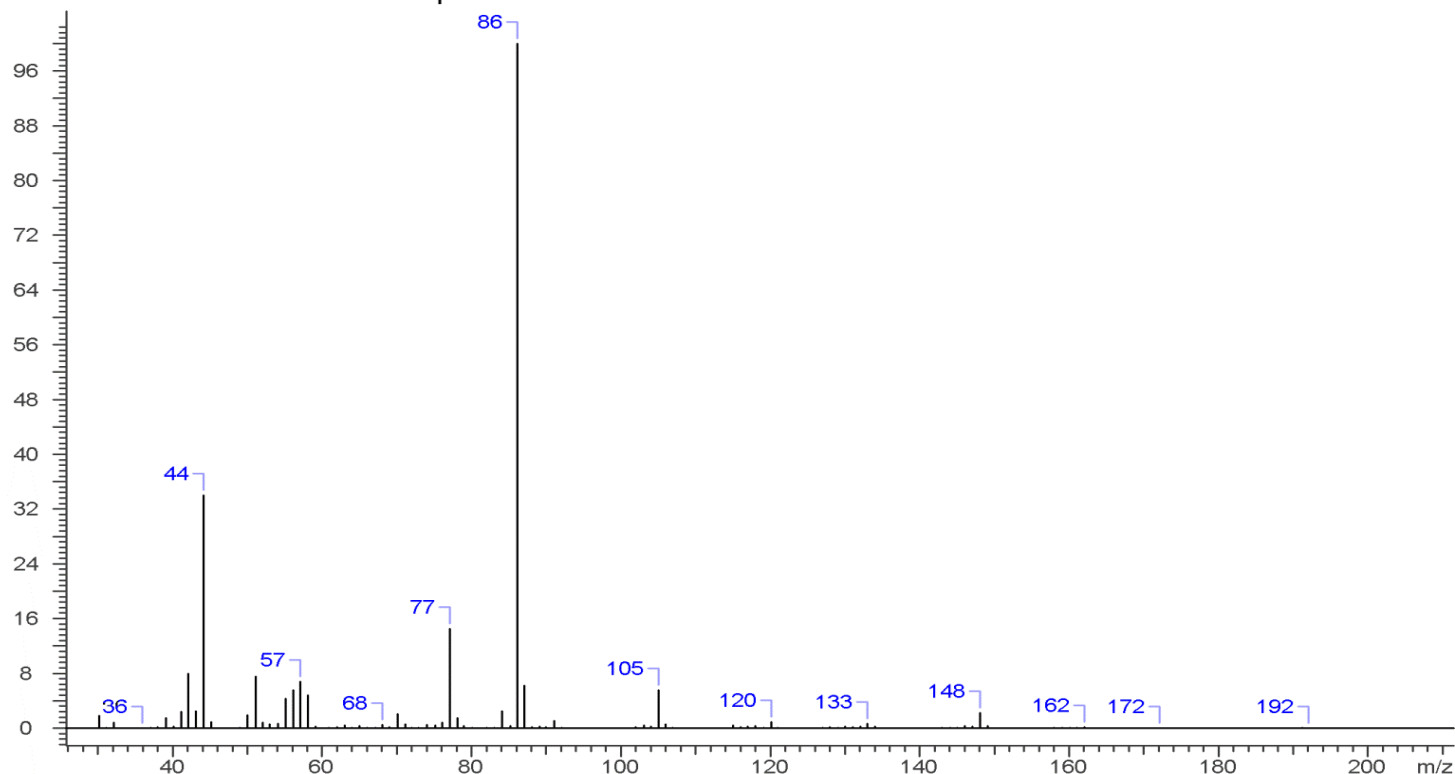
- 1) 100°C initial temperature for 1.0 min
- 2) Ramp to 300°C at 12°C/min
- 3) Hold final temperature for 9.0 min

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: 7.531 minutes

EI Mass Spectrum: Pentedrone HCl Lot # ALB225-6





Pentdrone

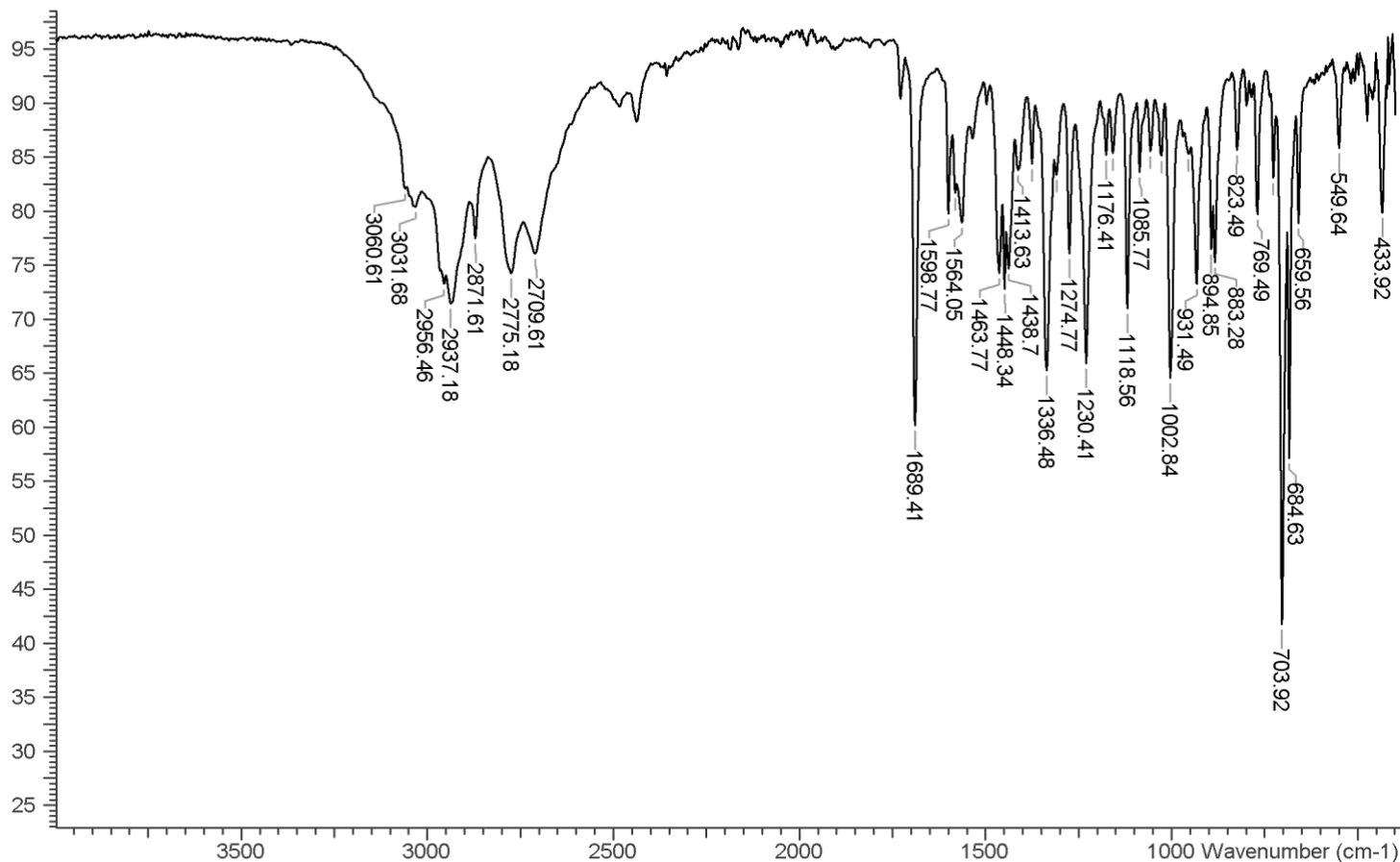
The Drug Enforcement Administration's Special Testing and Research Laboratory generated this monograph using structurally confirmed reference material.



3.3 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): Pentdrone HCl Lot #N1-P45EMG



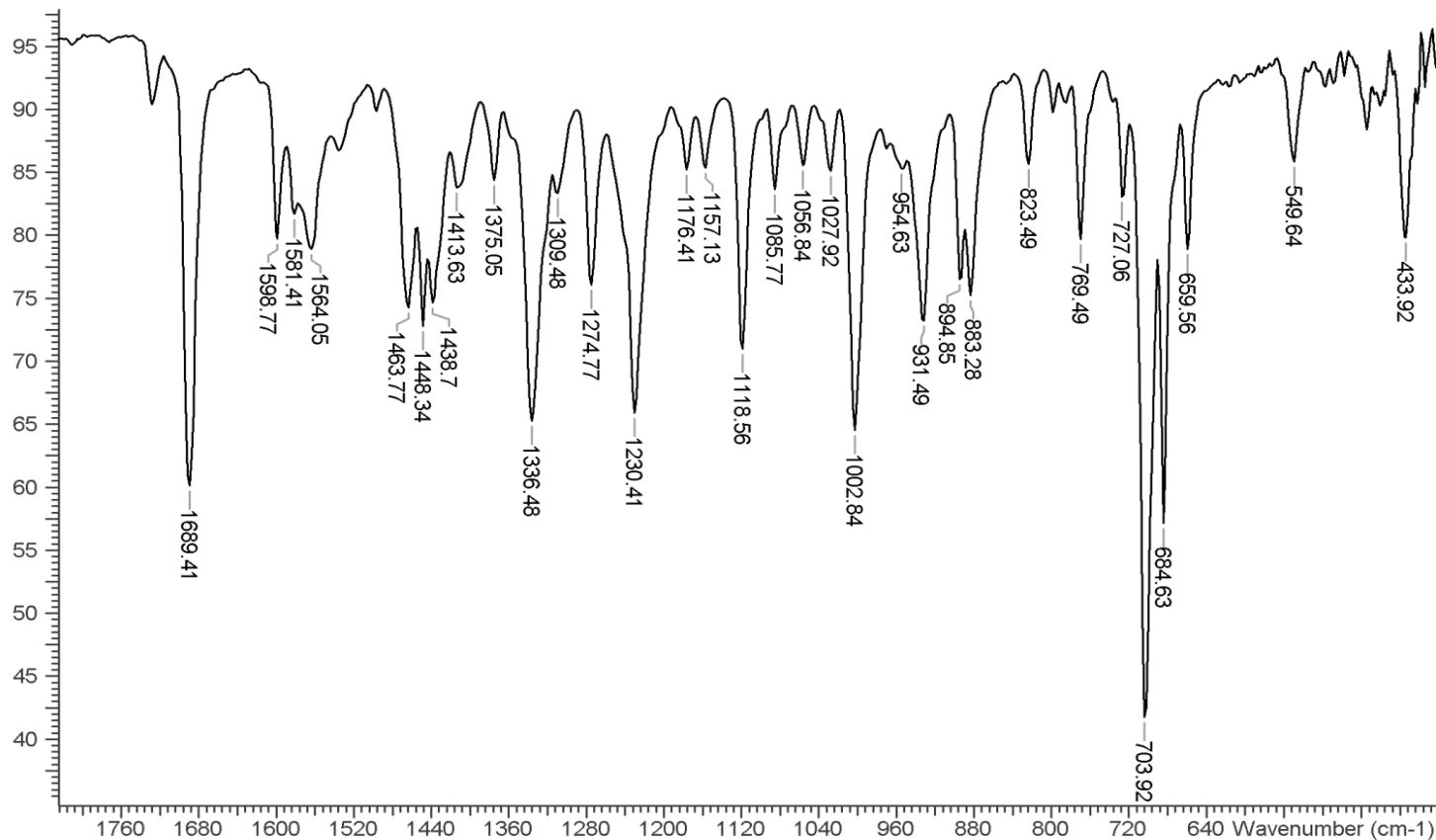


Pentadrone



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

FTIR ATR (Diamond, 3 Bounce): Pentadrone HCl Lot #N1-P45EMG



4. ADDITIONAL RESOURCES

[Forendex](#)

[Wikipedia](#)