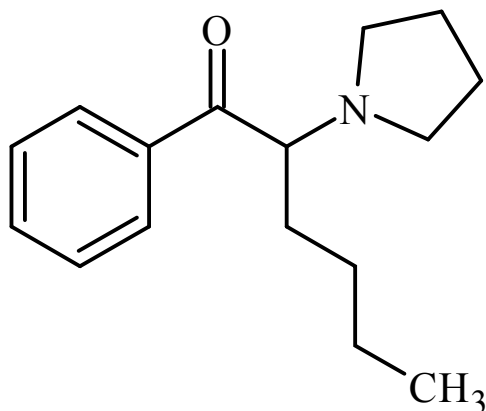




## a-PHP

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



### 1. GENERAL INFORMATION

<b>IUPAC Name:</b>	1-phenyl-2-(pyrrolidin-1-yl)hexan-1-one
<b>CAS#:</b>	13415-59-3 (HCl)
<b>Synonyms:</b>	$\alpha$ -pyrrolidinohexanophenone, $\alpha$ -pyrrolidinohexiophenone, 2-(1-pyrrolidinyl)hexanophenone, PV-7
<b>Source:</b>	DEA Reference Material Collection
<b>Appearance:</b>	Tan powder
<b>UV<sub>max</sub>(nm):</b>	Not Determined

### 2. CHEMICAL AND PHYSICAL DATA

#### 2.1 CHEMICAL DATA

Form	Chemical Formula	Molecular Weight	Melting Point (°C)
Base	C <sub>16</sub> H <sub>23</sub> NO	245	Not Determined
HCl	C <sub>16</sub> H <sub>23</sub> NO HCl	281	Not Determined



## a-PHP

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### 3. QUALITATIVE DATA

#### 3.1 NUCLEAR MAGNETIC RESONANCE

**Sample Preparation:** Dilute analyte to ~20 mg/mL in D<sub>2</sub>O containing TSP for 0 ppm reference and maleic acid as quantitative internal standard.

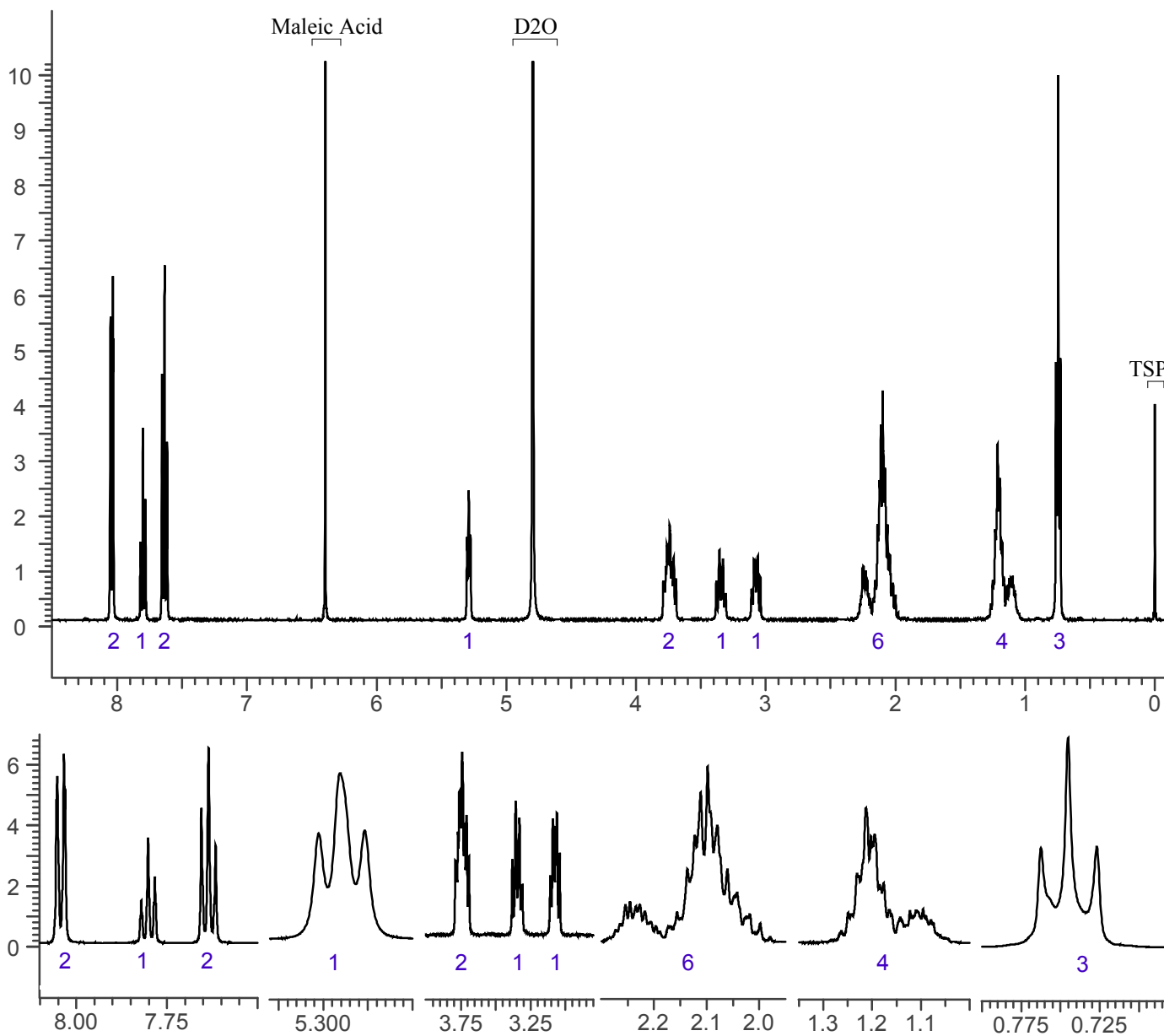
**Instrument:** 400 MHz NMR spectrometer

**Parameters:** Spectral width: at least containing -2.9 ppm through 13.2 ppm

Pulse angle: 90°

Delay between pulses: 45 seconds

<sup>1</sup>H NMR: α-PHP HCl Lot#RM-150116-01





## a-PHP

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### 3.2 GAS CHROMATOGRAPHY/MASS SPECTROMETRY

*Sample Preparation:* Dilute analyte ~5 mg/mL in CHCl<sub>3</sub> base extracted with 1N Sodium Hydroxide

**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 = 20:1, 1 μL injected

**MS Parameters:** Mass scan range: 30-550 amu

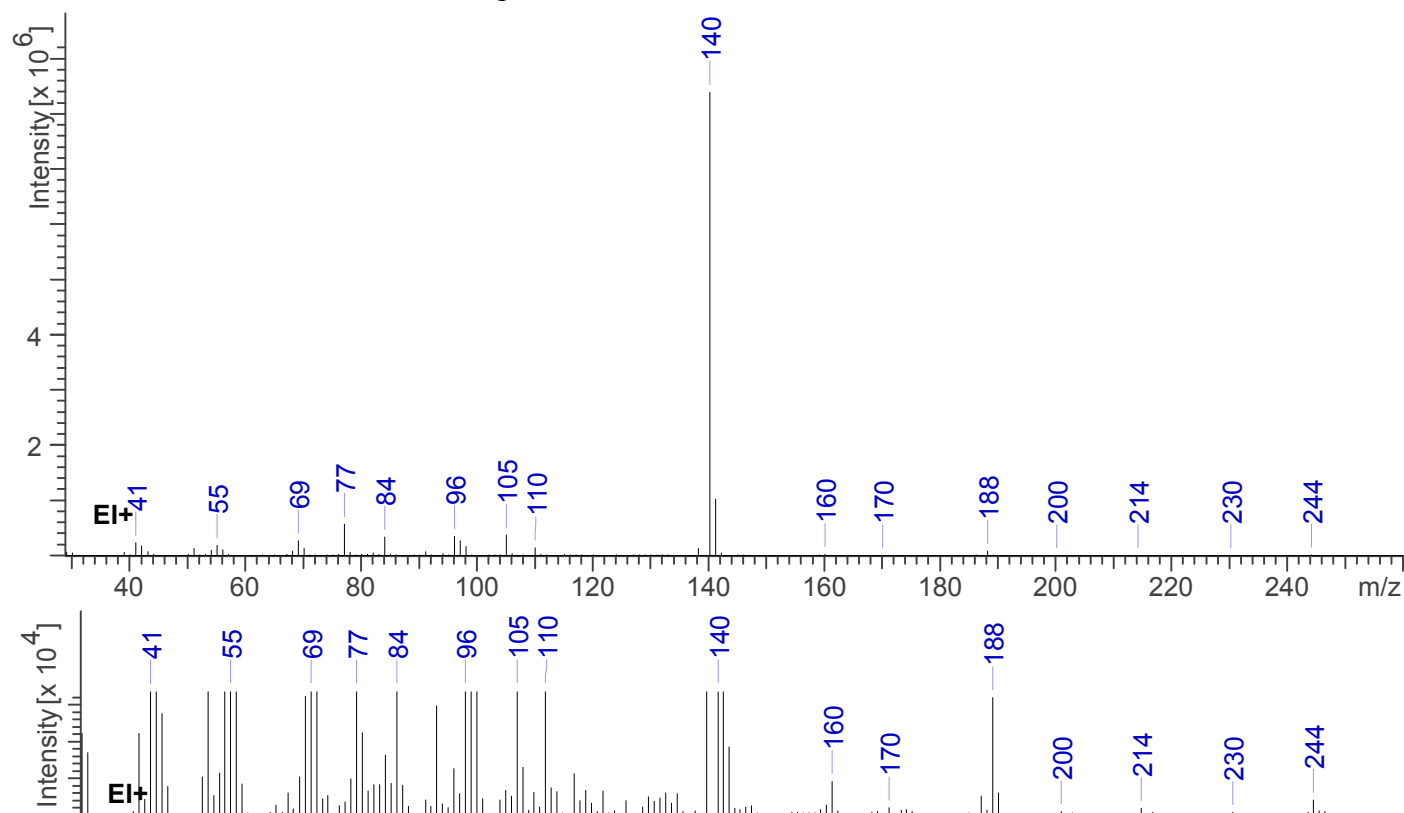
Threshold: 100

Tune file: stune.u

Acquisition mode: scan

**Retention Time:** 11.401 min

EI Mass Spectrum: α-PHP HCl Lot# RM-150116-01





## a-PHP

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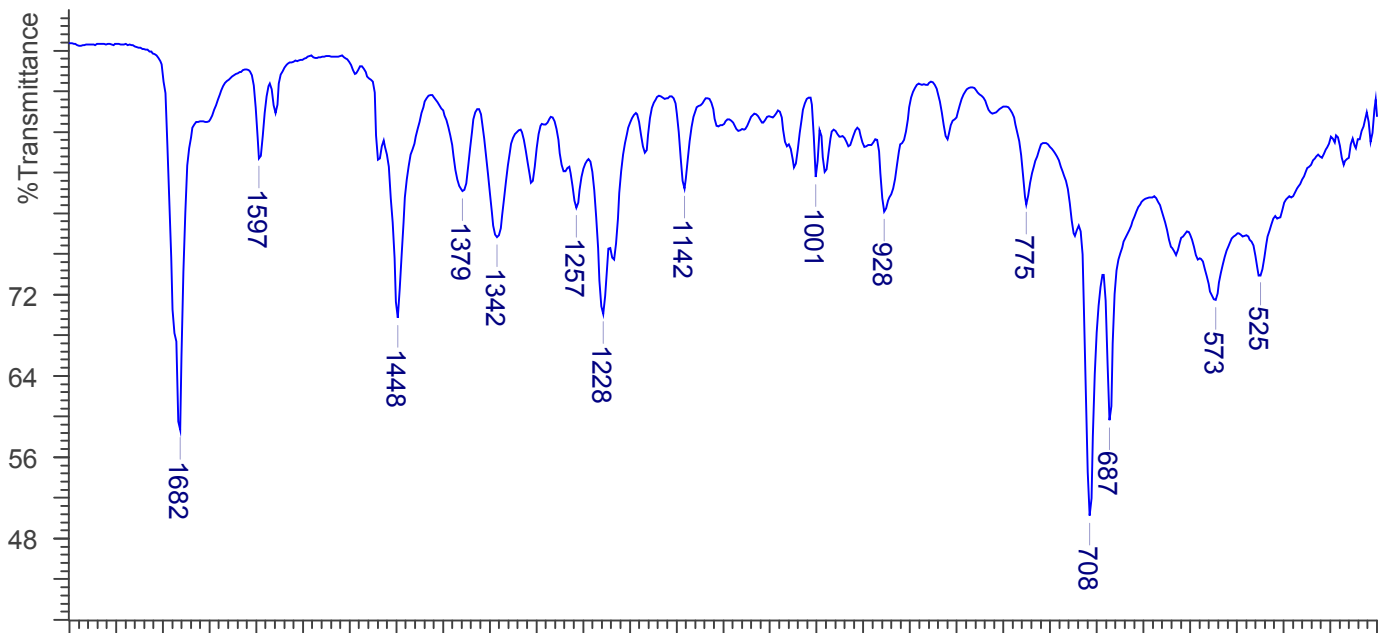
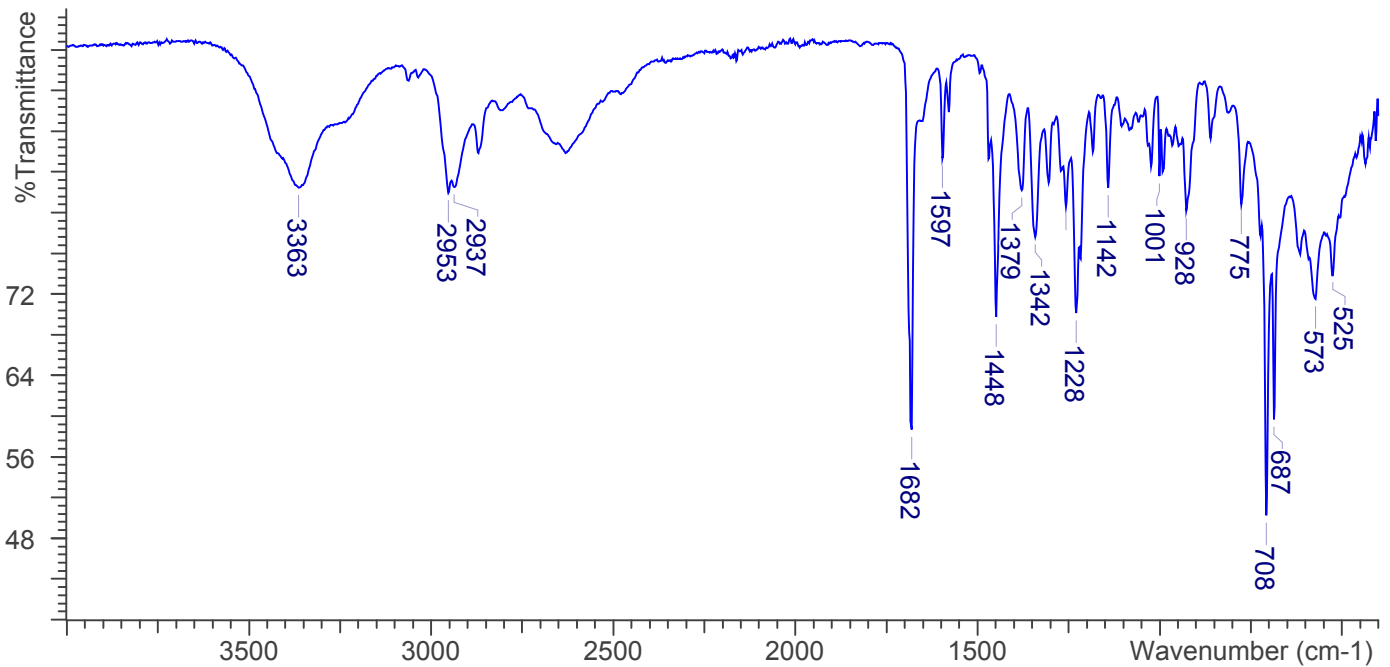


### 3.3 INFRARED SPECTROSCOPY (FTIR)

**Instrument:** FTIR with diamond ATR attachment (1 bounce)

**Scan Parameters:**  
Number of scans: 16  
Number of background scans: 16  
Resolution: 4 cm<sup>-1</sup>  
Sample gain: 8  
Aperture: 150

FTIR ATR (Diamond, 1 Bounce): α-PHP HCl Lot# RM-150116-01





## **a-PHP**

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



### **4. ADDITIONAL RESOURCES**

[\*Wikipedia\*](#)