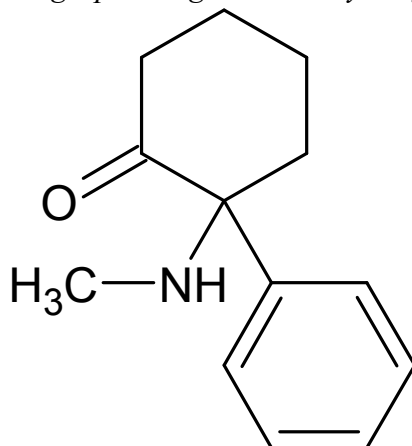




## Deschloroketamine

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>	2-(methylamino)-2-phenylcyclohexan-1-one
<b>CAS#:</b>	4631-27-0
<b>Synonyms:</b>	2'-oxo-PCM
<b>Source:</b>	DEA Reference Material Collection
<b>Appearance:</b>	White powder (HCl)
<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>13</sub> H <sub>17</sub> NO	203	Not Determined
HCl	C <sub>13</sub> H <sub>17</sub> NO · HCl	240	Not Determined



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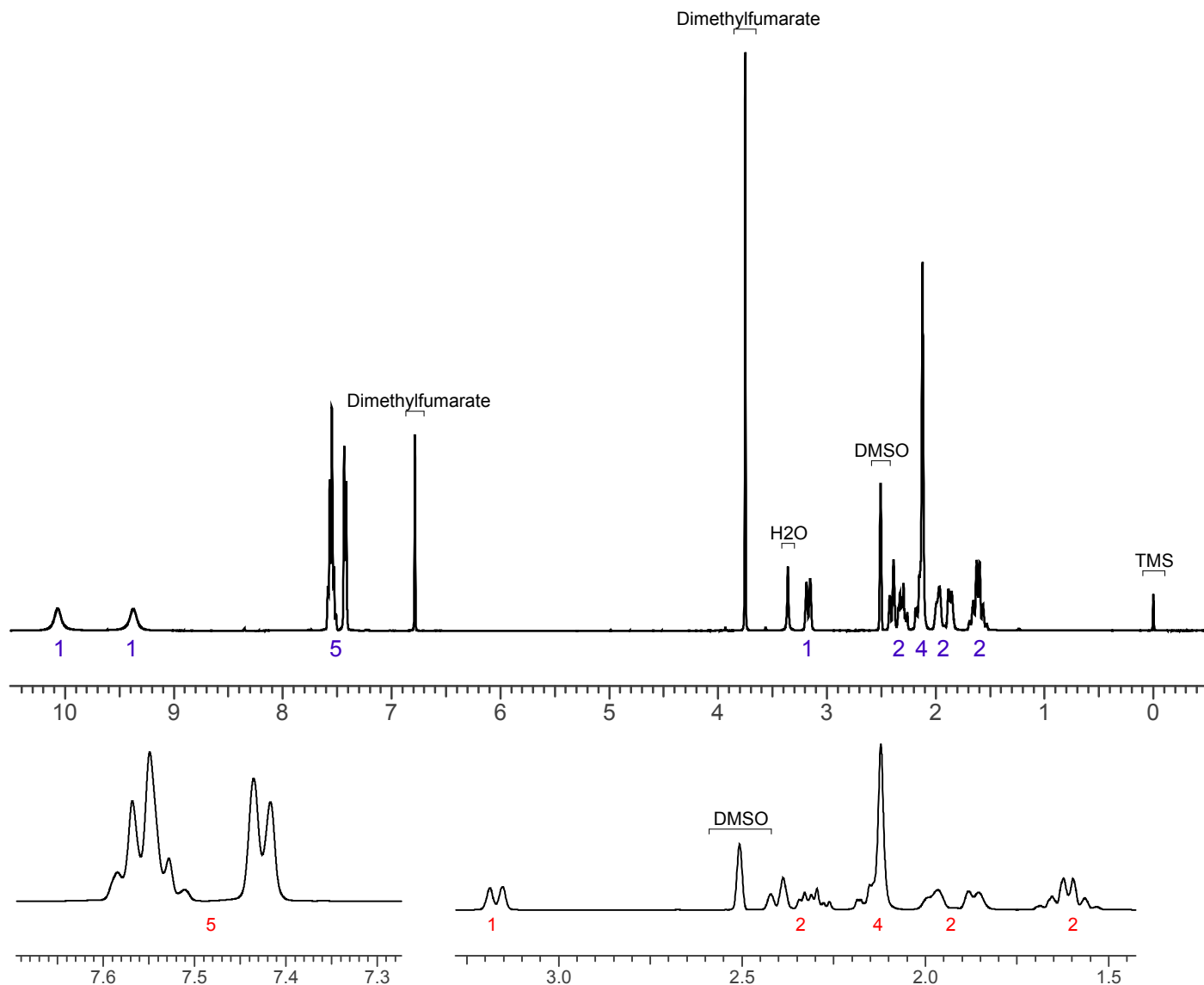
## 3. QUALITATIVE DATA

### 3.1 NUCLEAR MAGNETIC RESONANCE

**Sample Preparation:** Dilute analyte to ~20 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

<sup>1</sup>H NMR: Deschloroketamine HCl Lot RM-151202-01; DMSO; 400 MHz





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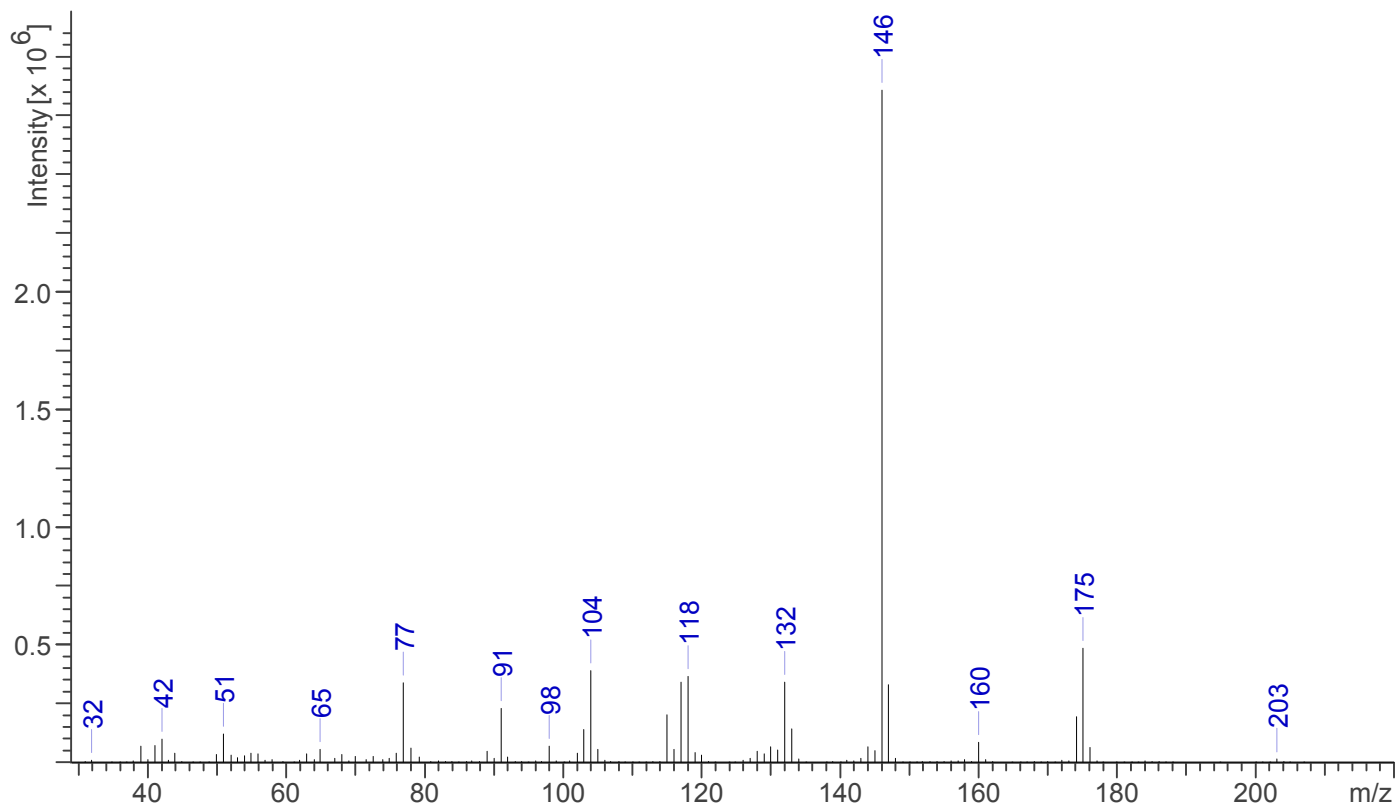


### 3.2 GAS CHROMATOGRAPHY/MASS SPECTROMETRY

*Sample Preparation:* Dilute analyte ~1 mg/mL in 1:1 CHCl<sub>3</sub>:MeOH.

**Instrument:** Agilent gas chromatograph operated in split mode with MS detector  
**Column:** DB-5 MS (or equivalent); 15m 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: 250°C  
MS Quad: 150°C  
Oven program:  
1) 100°C initial temperature for 1.0 min  
2) Ramp to 280°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: 150  
Tune file: stune.u  
Acquisition mode: scan  
**Retention Time:** 6.462 min

EI Mass Spectrum: Deschloroketamine HCl Lot RM-151202-01





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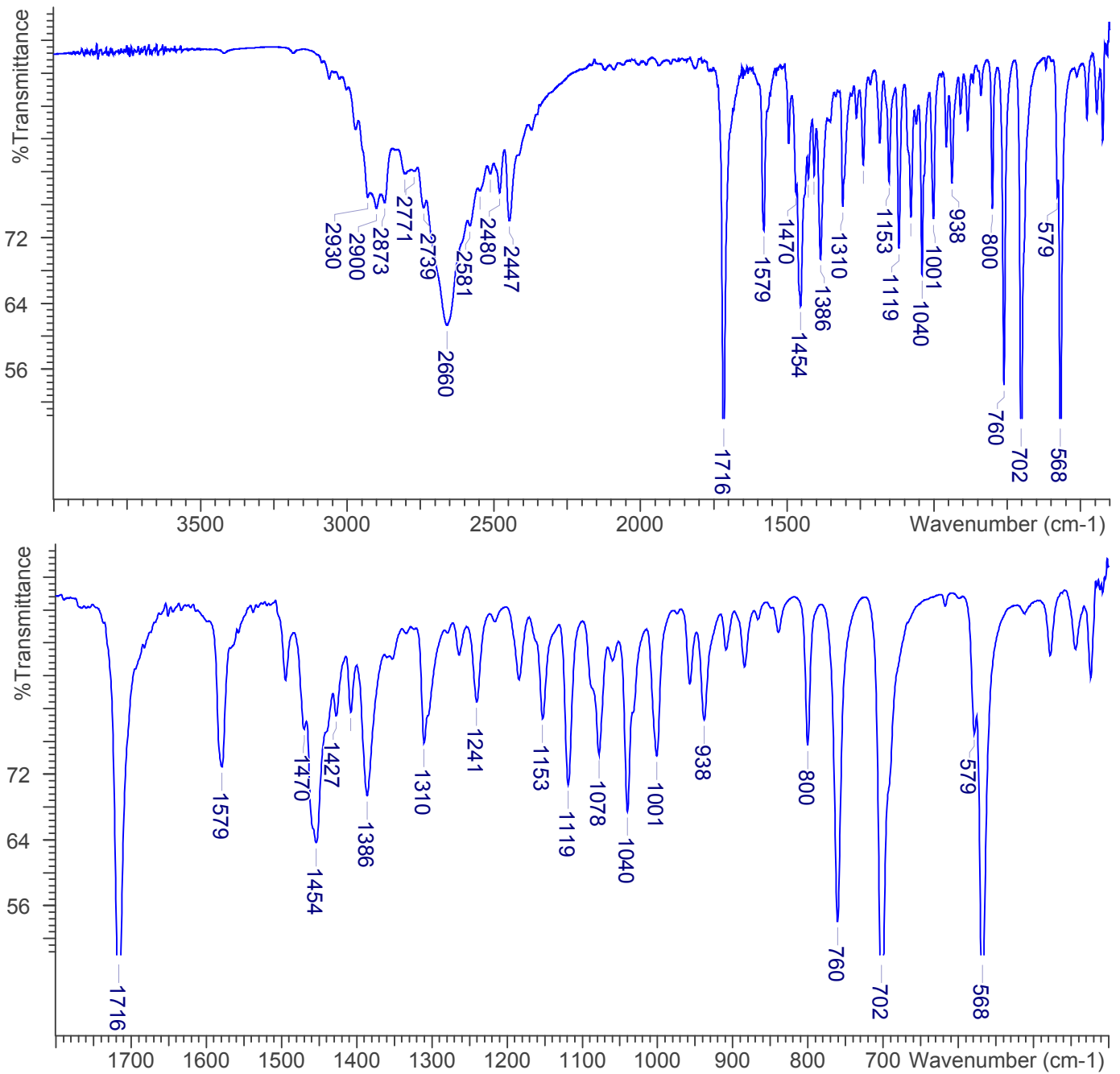


## 3.3 INFRARED SPECTROSCOPY (FTIR)

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

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

FTIR ATR (Diamond, 1 Bounce): Deschloroketamine HCl Lot RM-151202-01





## Deschloroketamine

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### 4. ADDITIONAL RESOURCES

[Wikipedia](#)