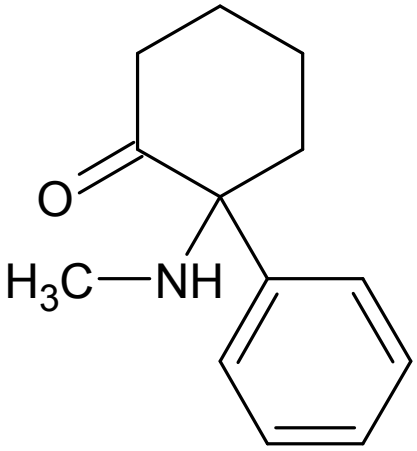
# Deschloroketamine

*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)-2-phenylcyclohexan-1-one

***CAS#:*** 4631-27-0

***Synonyms:*** 2'-oxo-PCM

***Source:*** DEA Reference Material Collection

***Appearance:*** White powder (HCl)

***$UV_{max}$(nm):*** Not Determined

## *2. CHEMICAL AND PHYSICAL DATA*

### 2.1 CHEMICAL DATA

| Form | Chemical Formula | Molecular Weight | Melting Point ($^{o}$C) |
|---|---|---|---|
| Base | $C_{13}H_{17}NO$ | 203 | Not Determined |
| HCl | $C_{13}H_{17}NO \cdot HCl$ | 240 | Not Determined |

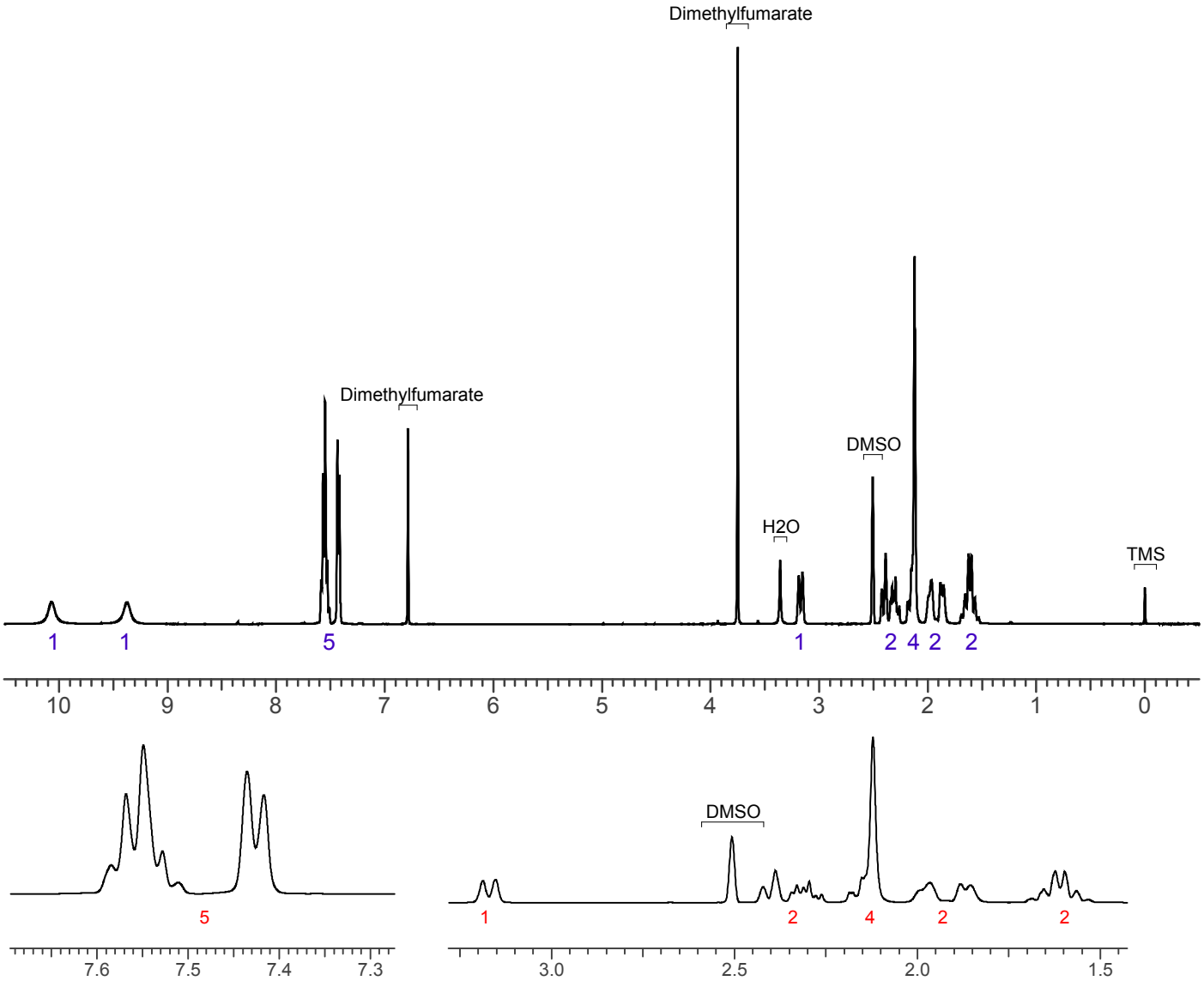
## *3. QUALITATIVE DATA*

### 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

$^{1}$H NMR: Deschloroketamine HCl Lot RM-151202-01; DMSO; 400 MHz

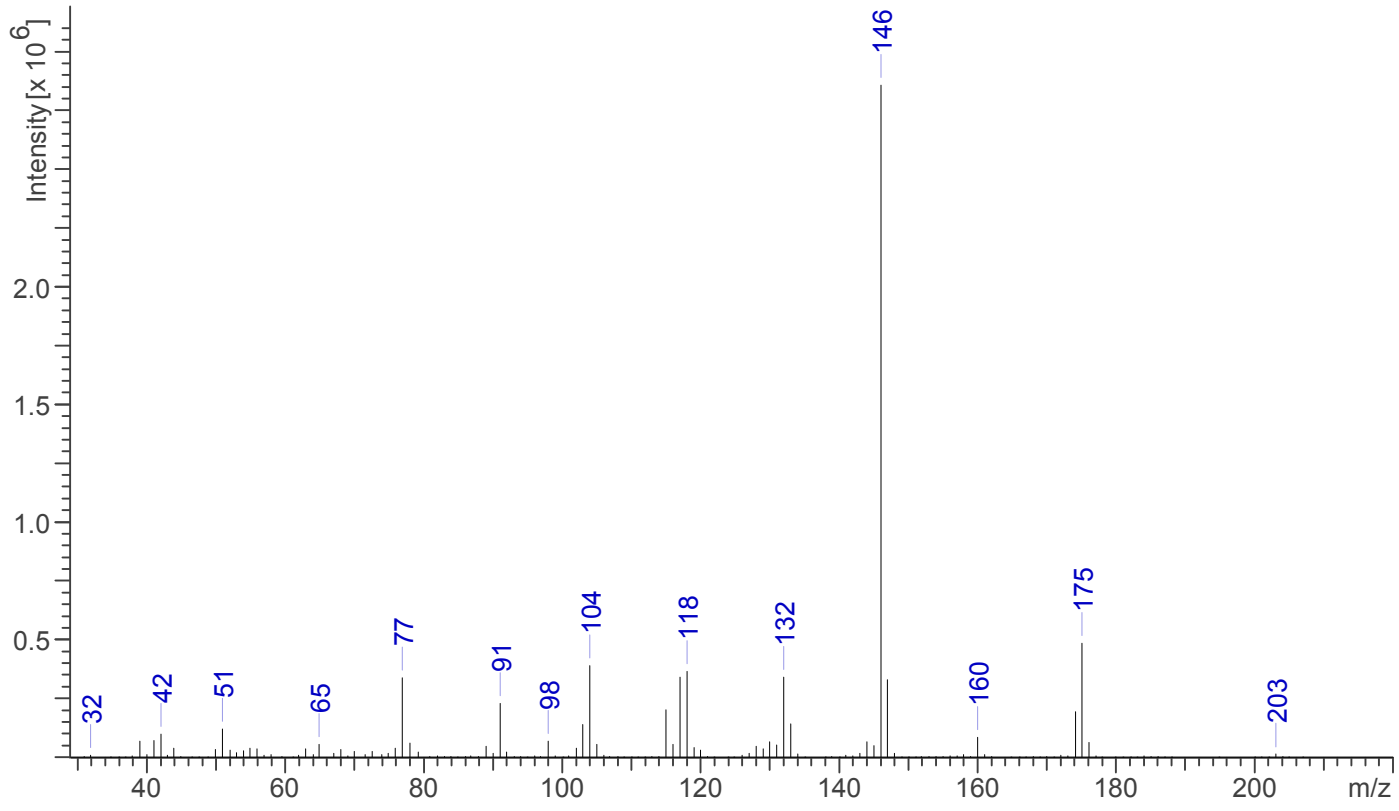


## 3.2 GAS CHROMATOGRAPHY/MASS SPECTROMETRY

*Sample Preparation:* Dilute analyte ~1 mg/mL in 1:1 CHCl3: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

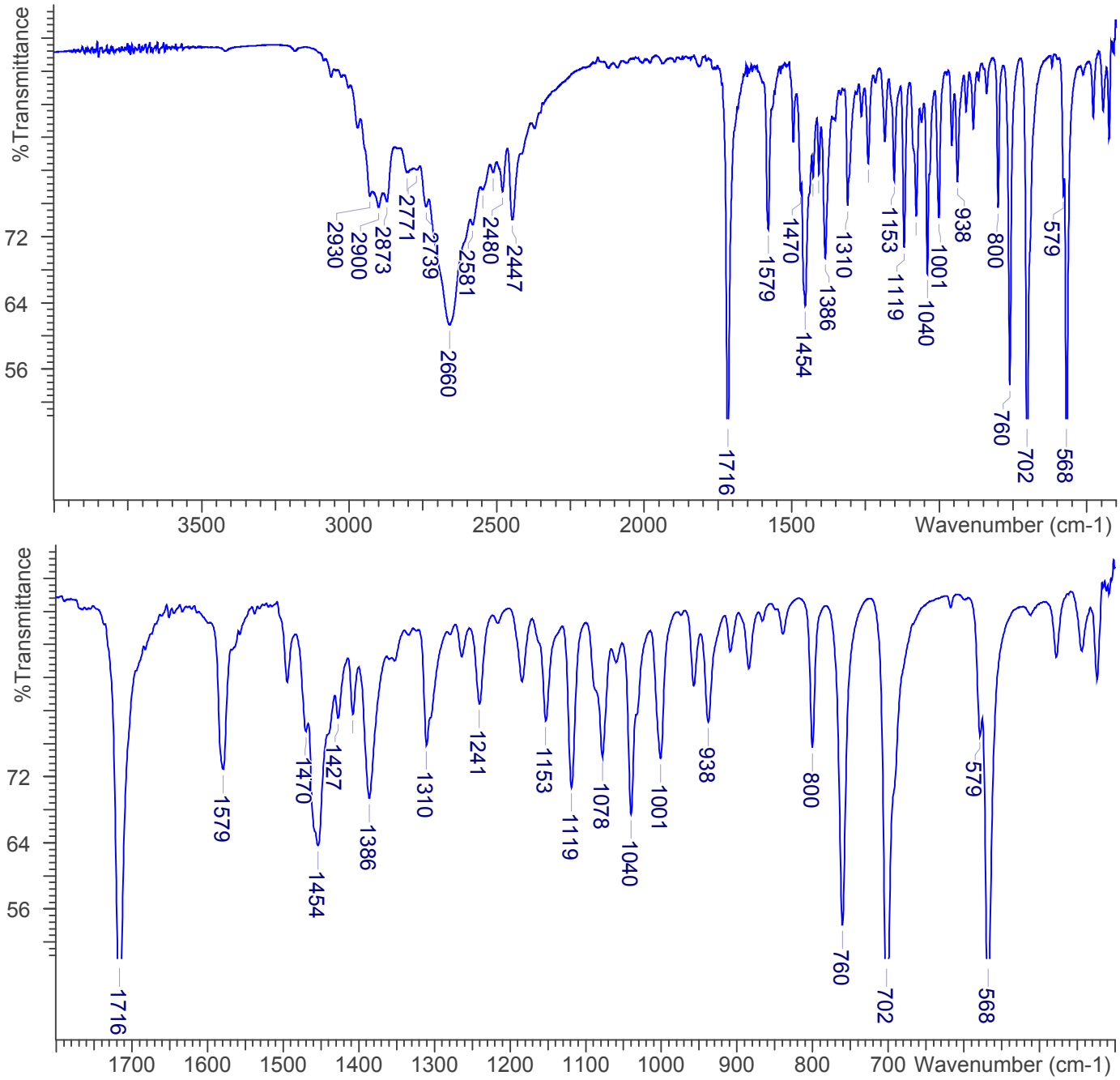


### 3.3 INFRARED SPECTROSCOPY (FTIR)

**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: 1
Aperture: 150

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



## *4. ADDITIONAL RESOURCES*

***Wikipedia***