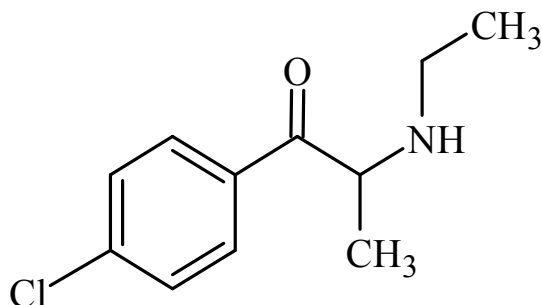




4-Chloroethcathinone

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-chlorophenyl)-2-(ethylamino)propan-1-one

CAS#: NA

Synonyms: 4-CEC, 4-chloro-N-ethylcathinone

Source: DEA Reference Material Collection

Appearance: White powder (HCl)

UV_{max}(nm): NA

2. CHEMICAL AND PHYSICAL DATA

2.1 CHEMICAL DATA

Form	Chemical Formula	Molecular Weight	Melting Point (°C)
Base	C ₁₁ H ₁₄ ClNO	211	NA
HCl	C ₁₁ H ₁₄ ClNO · HCl	248	253.4



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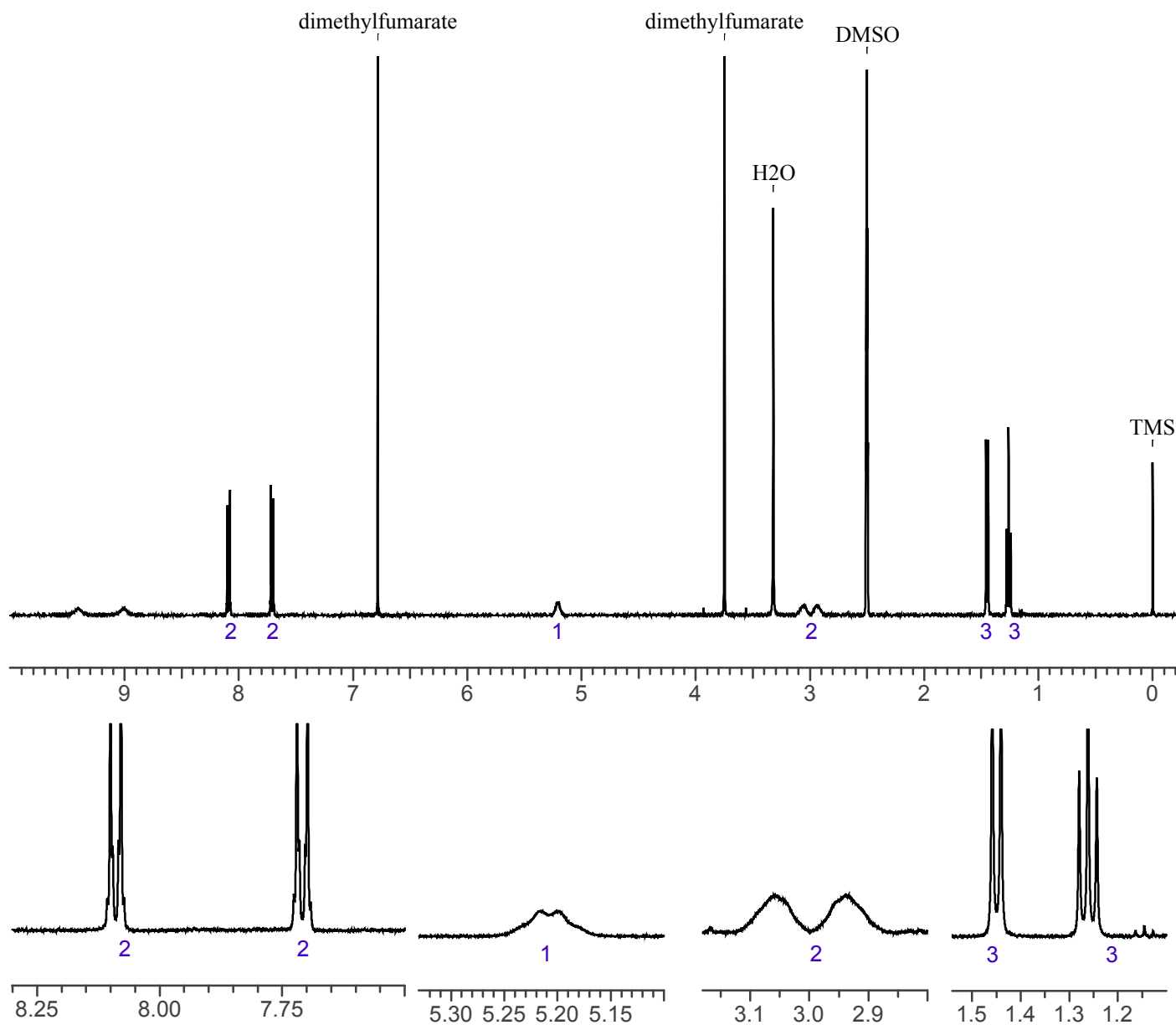
3. QUALITATIVE DATA

3.1 NUCLEAR MAGNETIC RESONANCE

Sample Preparation: Dilute analyte to ~5mg/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

¹H NMR: 4-Chloroethcathinone HCl Lot# 0478461-14; DMSO; 400MHz





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3.2 GAS CHROMATOGRAPHY/MASS SPECTROMETRY

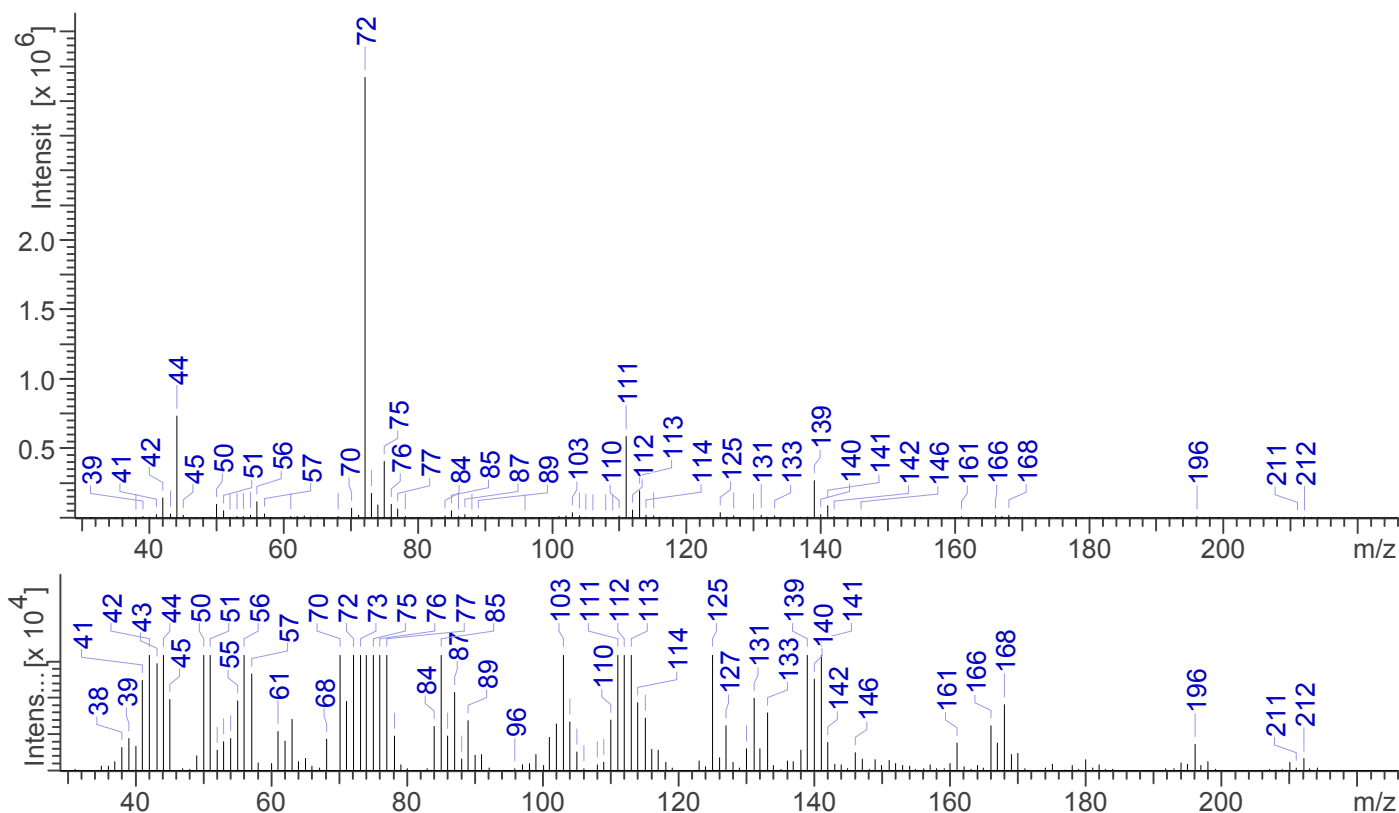
Sample Preparation: Dilute analyte ~4 mg/mL BE into chloroform.

Instrument: Agilent gas chromatograph operated in split mode with MS detector
Column: HP-5 (or equivalent); 30m x 0.25 mm x 0.25 μ m
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 280°C at 12 °C/min
3) Hold final temperature for 9.0 min

Injection Parameters: Split Ratio = 25:1, 1 μ L injected
MS Parameters: Mass scan range: 30-550amu
Threshold: 100
Tune file: stune.u
Acquisition mode: scan

Retention Time: 7.740min

EI Mass Spectrum: 4-Chloroethcathinone HCl Lot# 0478461-14





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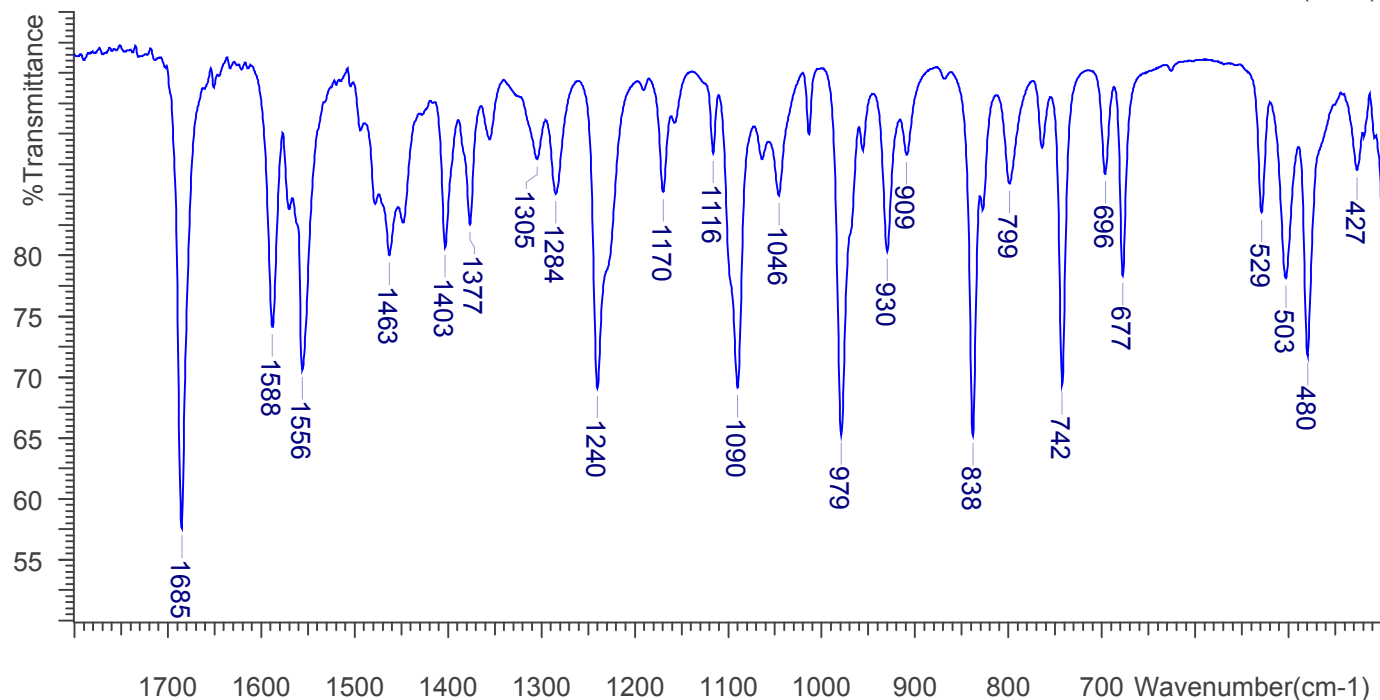
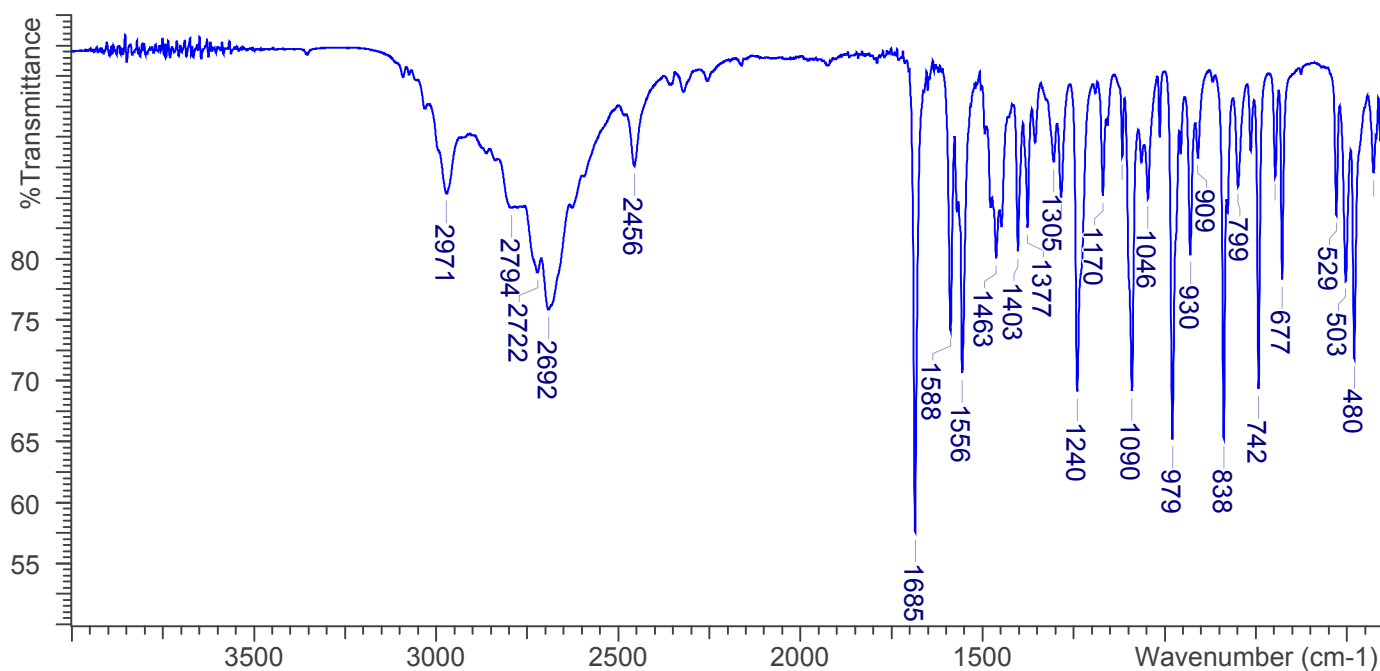


3.3 INFRARED SPECTROSCOPY (FTIR)

Instrument: FTIR with diamond ATR attachment (3 bounce)

Scan Parameters:
Number of scans: 32
Number of background scans: 32
Resolution: 4 cm⁻¹
Sample gain: 1
Aperture: 150

FTIR ATR (Diamond, 3 Bounce): 4-Chloroethcathinone HCl Lot# 0478461-14





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4. ADDITIONAL RESOURCES

No additional resources as of 10/13/16