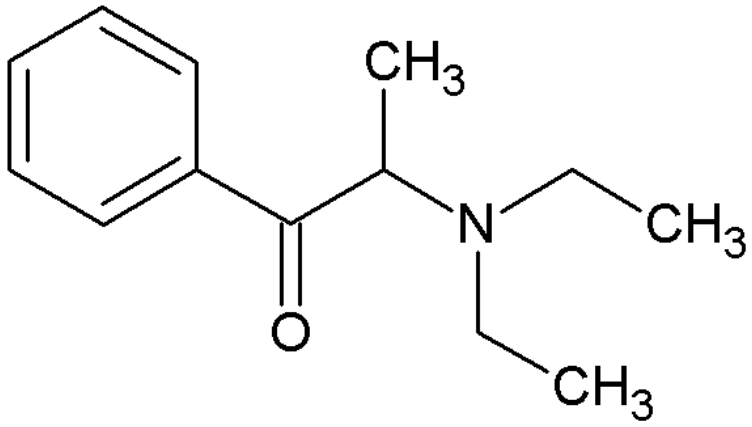
Diethylcathinone

Latest Revision: March 18, 2013



1. GENERAL INFORMATION

IUPAC Name: 2-(Diethylamino)-1-phenylpropan-1-one

CFR: Schedule IV

CAS #: Base: 90-84-6; HCl: 134-80-5

Synonyms: Diethylpropion; Amfepramone

Source: DEA Reference Material Collection

Appearance: Off-white powder (HCl)

Kovat's Index: Pending

UV_{max}: 253.2 nm

2. CHEMICAL AND PHYSICAL DATA

2.1 CHEMICAL DATA

Form	Chemical Formula	Molecular Weight	Melting Point (°C)
Base	$C_{13}H_{19}NO$	205	Not Determined
HCl	$C_{13}H_{19}NO.HCl$	242	172.0

3. ADDITIONAL RESOURCES

Forendex

Wikipedia

4. QUALITATIVE DATA

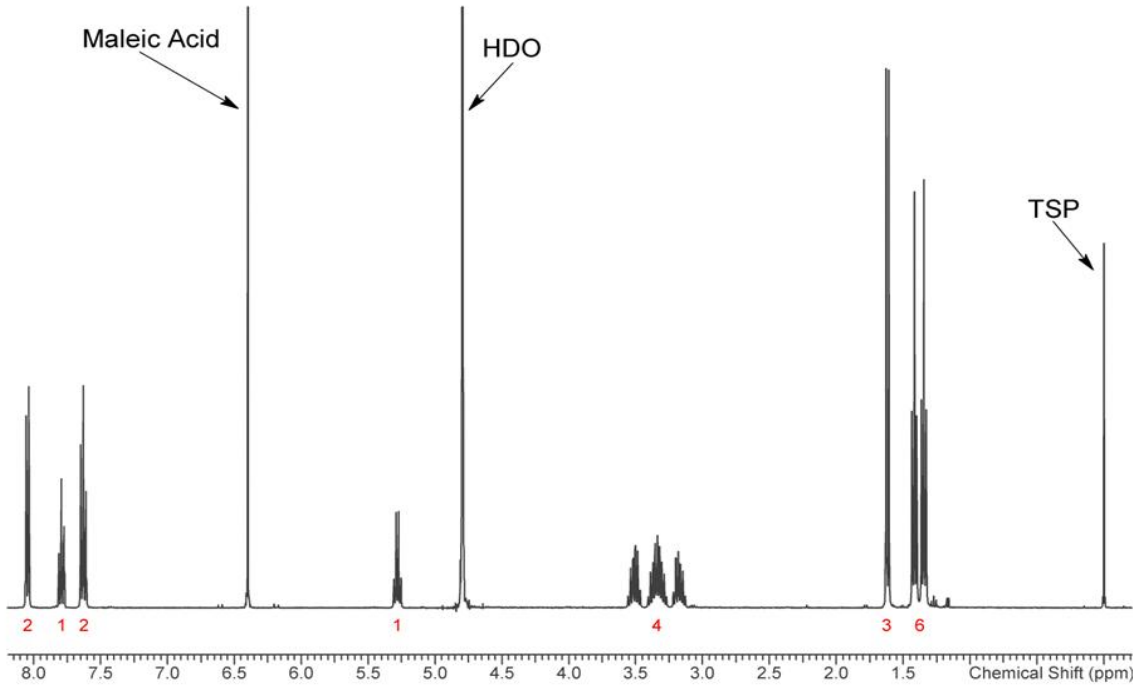
4.1 NUCLEAR MAGNETIC RESONANCE

Method NMR D_2O

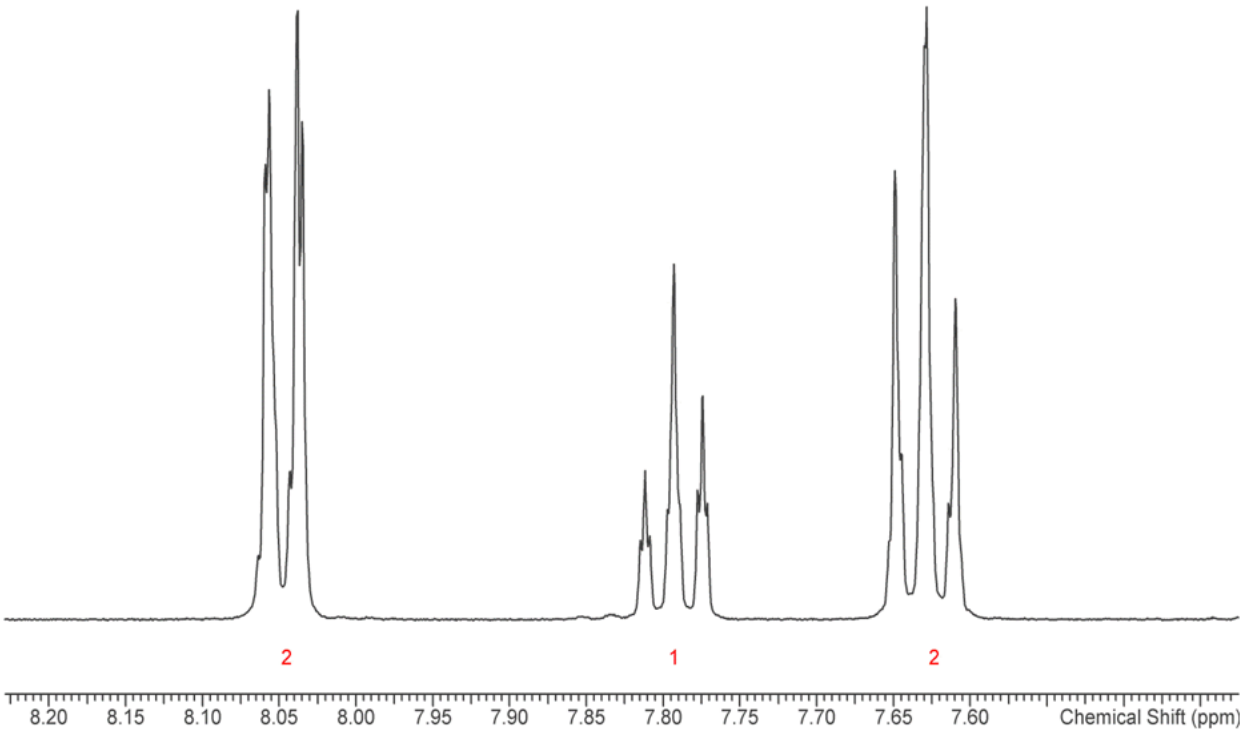
Sample Preparation: Dilute analyte to ~10 mg/mL in D_2O containing TSP for 0 ppm reference and maleic acid as quantitative ISTD.

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: Diethylcathinone HCl Lot # TADMAR94 D_2O, 400MHz



1H NMR: Diethylcathinone HCl Lot # TADMAR94; D_2O; 400 MHz



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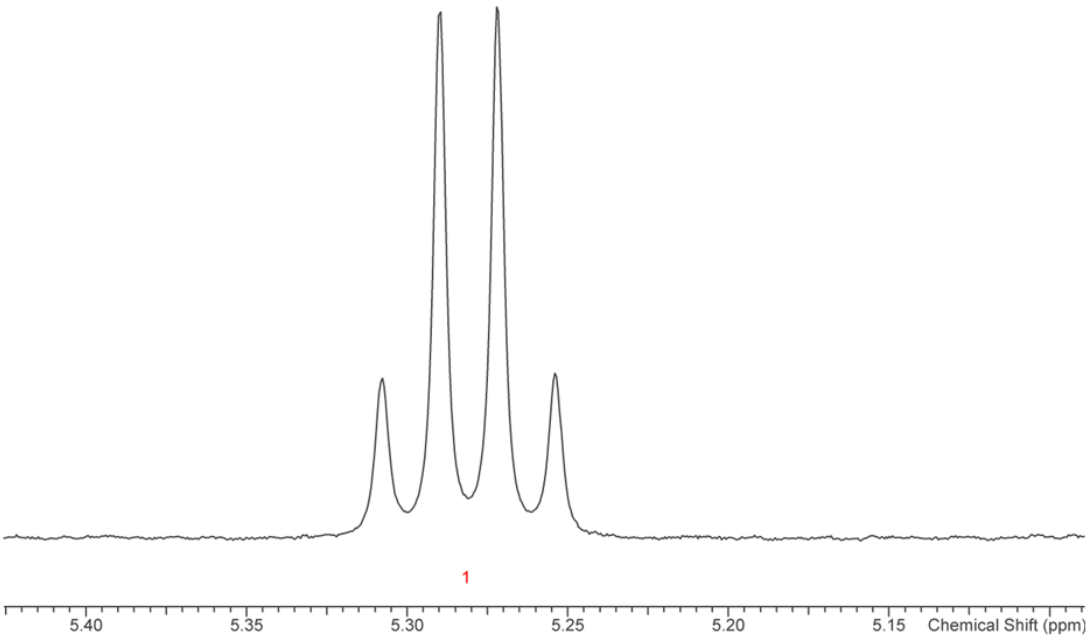

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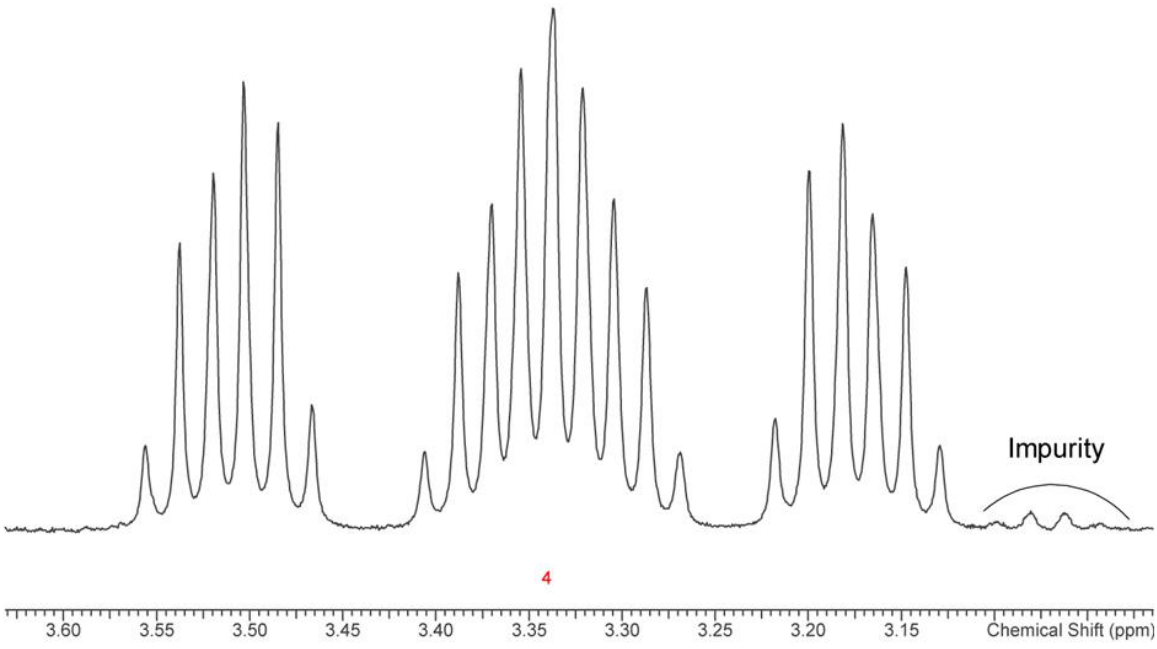
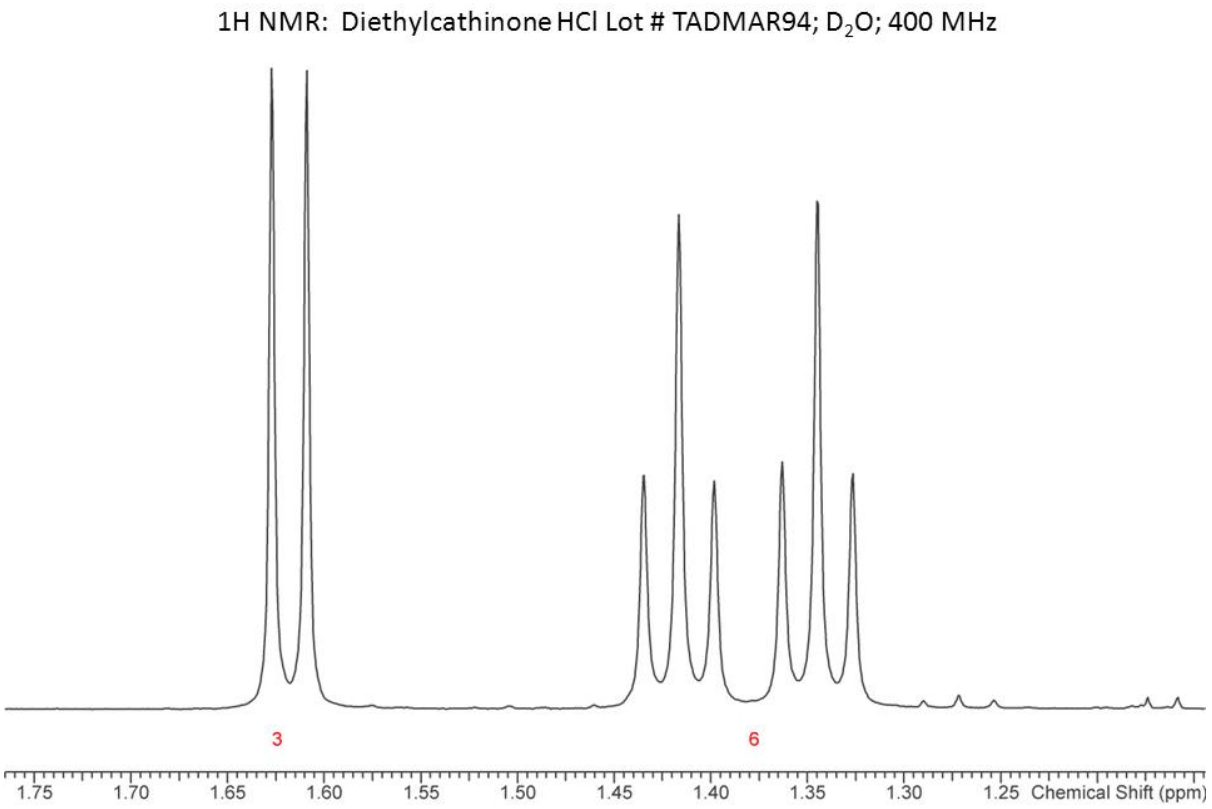
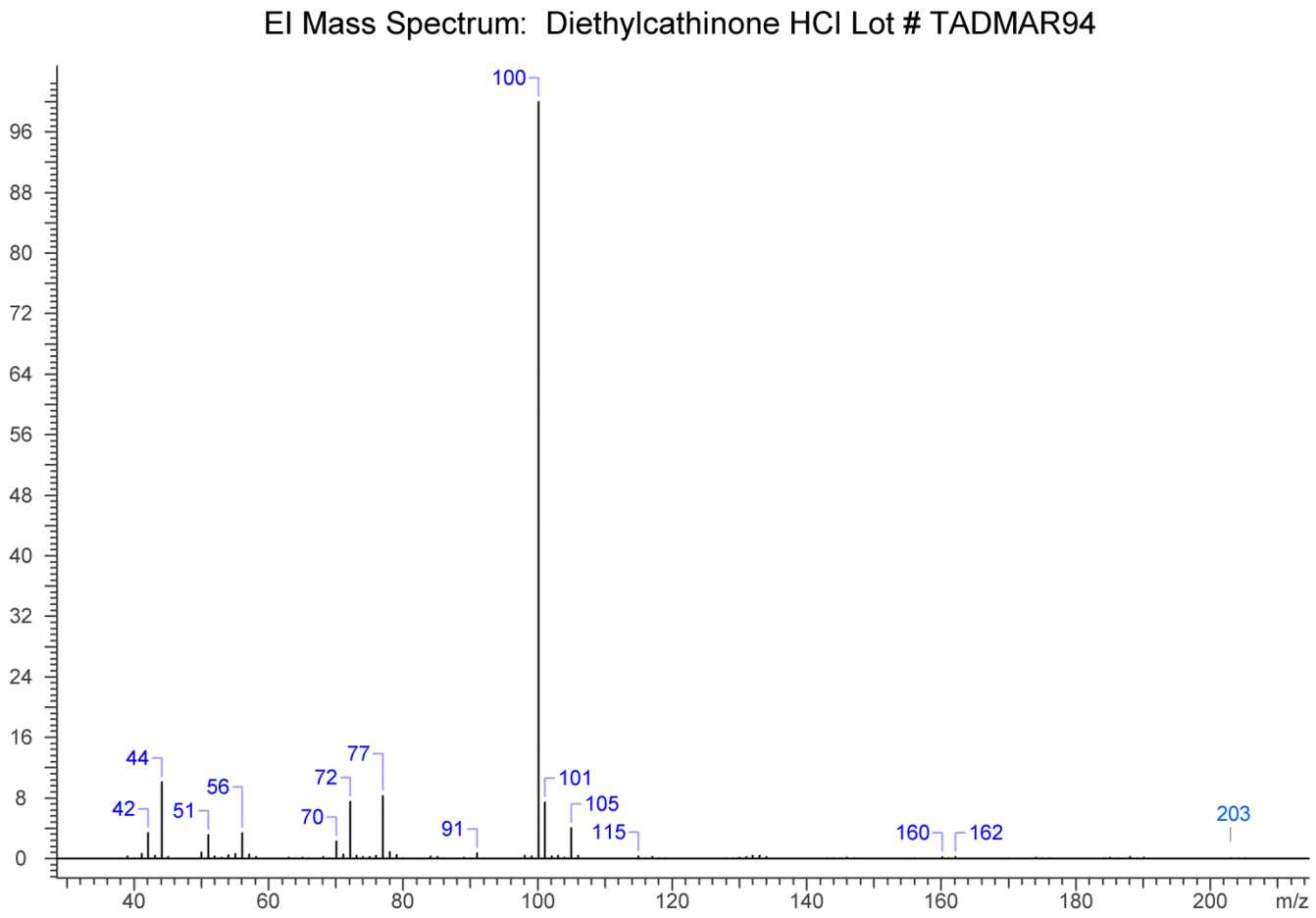




4.2 GAS CHROMATOGRAPHY/MASS SPECTROMETRY

Sample Preparation: Dilute analyte to ~1 mg/mL in $CHCl_3$.

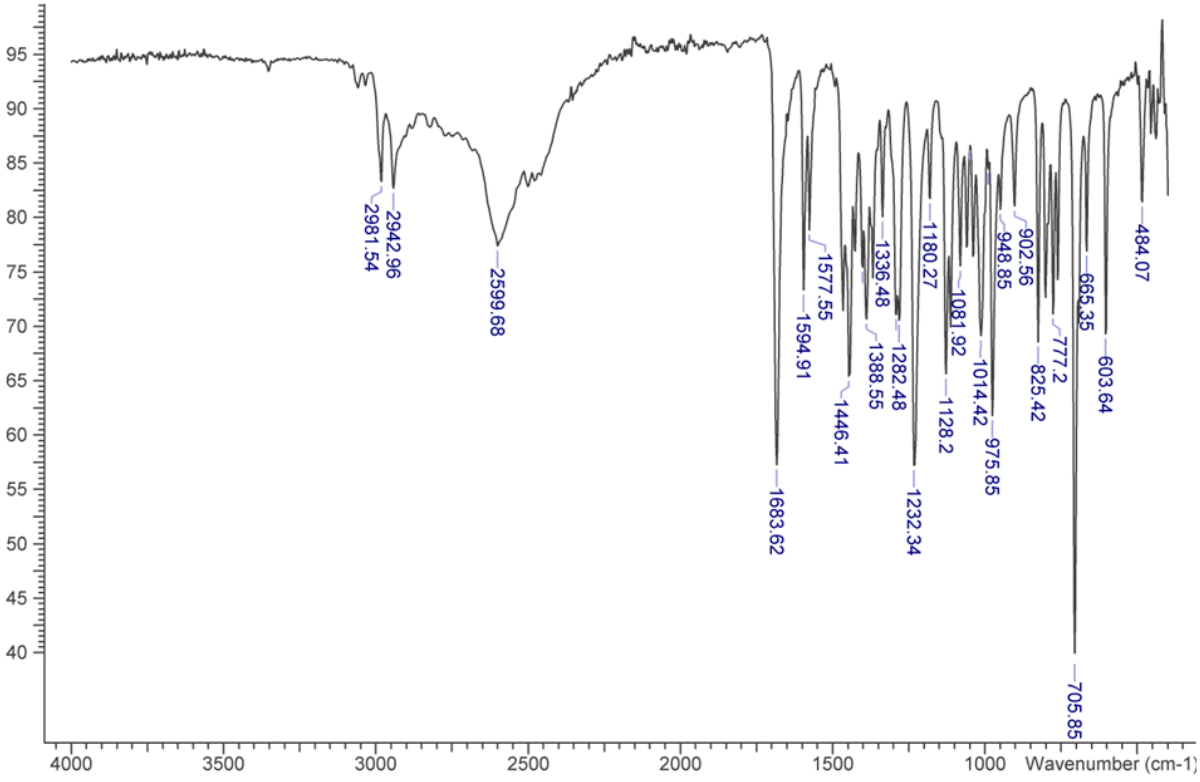
Instrument:	Gas chromatograph operated in split mode with MS detector
Column:	DB-1 MS 30m x .25mm x .25µm
Carrier gas:	Helium at 1 mL/min
Temperatures:	Injector: 280°C MSD transfer line: 280°C MS Source: 230°C MS Quad: 150°C Oven program: 1) 100°C initial temperature for 1.0 min 2) Ramp to 300°C at 12°C/min 3) Hold final temperature for 9.0 min
Injection Parameters:	Split Ratio = 20:1, 1 µL injected
MS Parameters:	Mass scan range: 34-550 amu Threshold: 100 Tune file: stune.u Acquisition mode: scan
Retention Time:	7.802 min



4.3 INFRARED SPECTROSCOPY (FTIR)

Instrument:	FTIR with ATR attachment
Scan Parameters:	Number of scans: 32 Number of background scans: 32 Resolution 4 cm^{-1} Sample gain: 8 Aperture: 150

FTIR (Diamond ATR, 3 Bounce): Diethylcathinone HCl Lot # TADMAR94



FTIR (Diamond, 3 Bounce): Diethylcathinone HCl Lot # TADMAR94