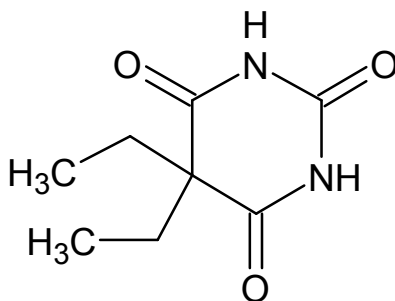




Barbital

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



1. GENERAL INFORMATION

IUPAC Name: 5,5-diethylpyrimidine-2,4,6(1H,3H,5H)-trione

CAS#: 57-44-3

Synonyms: Barbitone, Barb

Source: DEA Reference Material Collection

Appearance: White powder

UV_{max}(nm): Not Determined

2. CHEMICAL AND PHYSICAL DATA

2.1 CHEMICAL DATA

Form	Chemical Formula	Molecular Weight	Melting Point (°C)
Base	C ₈ H ₁₂ N ₂ O ₃	184.2	189.2
Sodium	C ₈ H ₁₂ N ₂ O ₃ Na	206.17	Not Determined



Barbital

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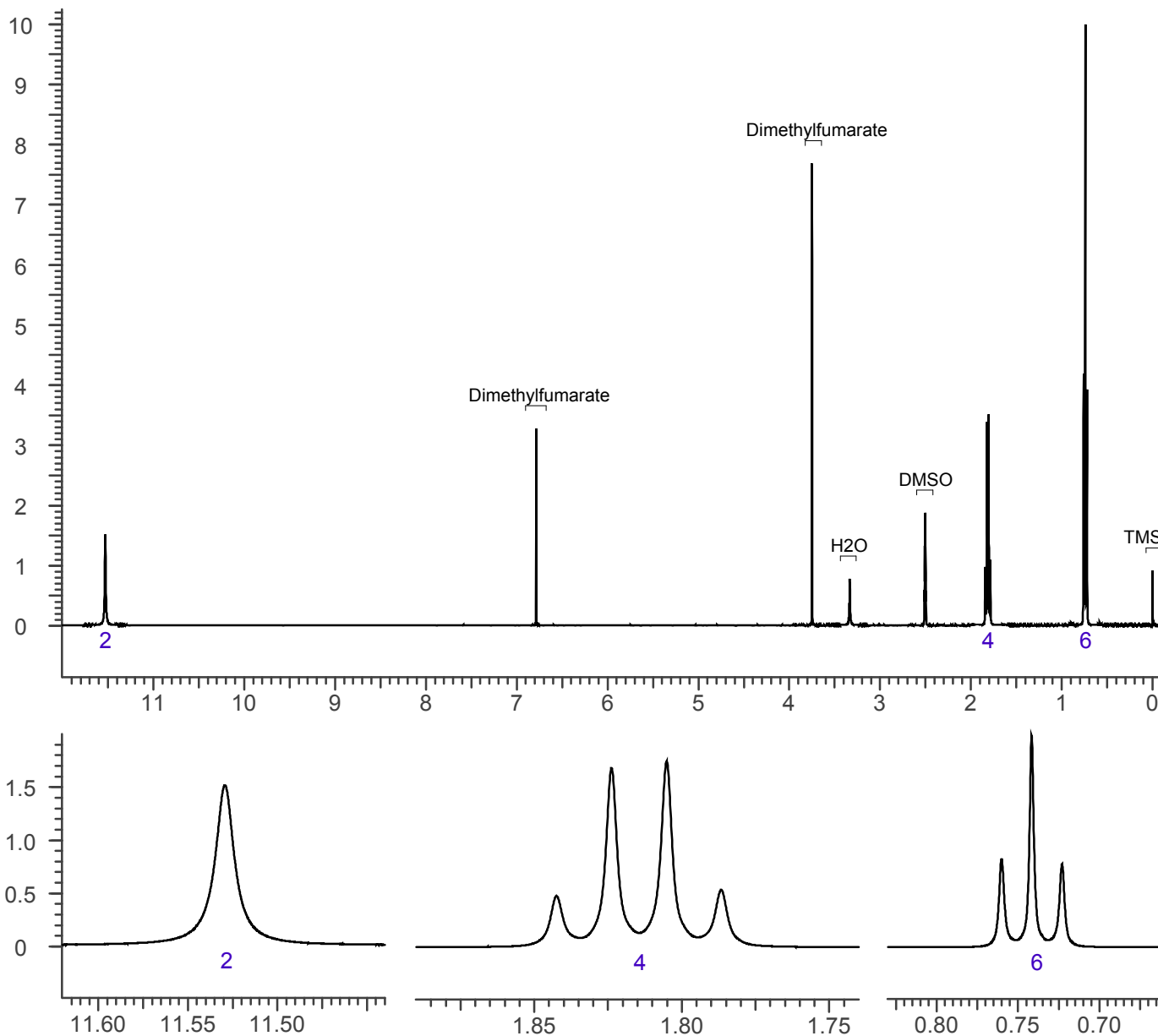
3. QUALITATIVE DATA

3.1 NUCLEAR MAGNETIC RESONANCE

Sample Preparation: Dilute analyte to ~12 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

¹HNMR: Barbital; Lot# 429050; DMSO; 400MHz





Barbital

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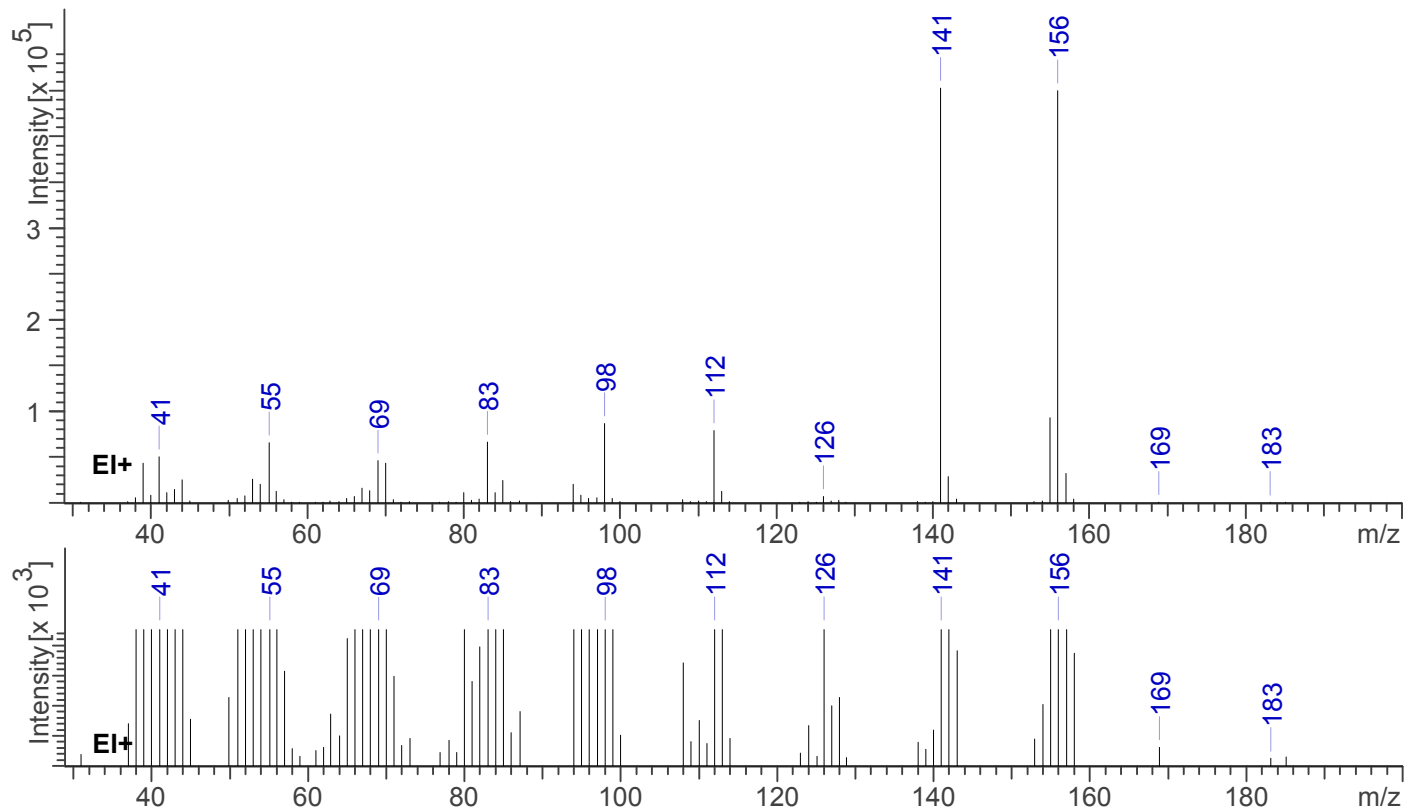
3.2 GAS CHROMATOGRAPHY/MASS SPECTROMETRY

Sample Preparation: Dilute analyte ~2 mg/mL in CHCl₃.

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

Retention Time: 7.141 min
EI Mass Spectrum: Barbital; Lot# 429050





Barbital

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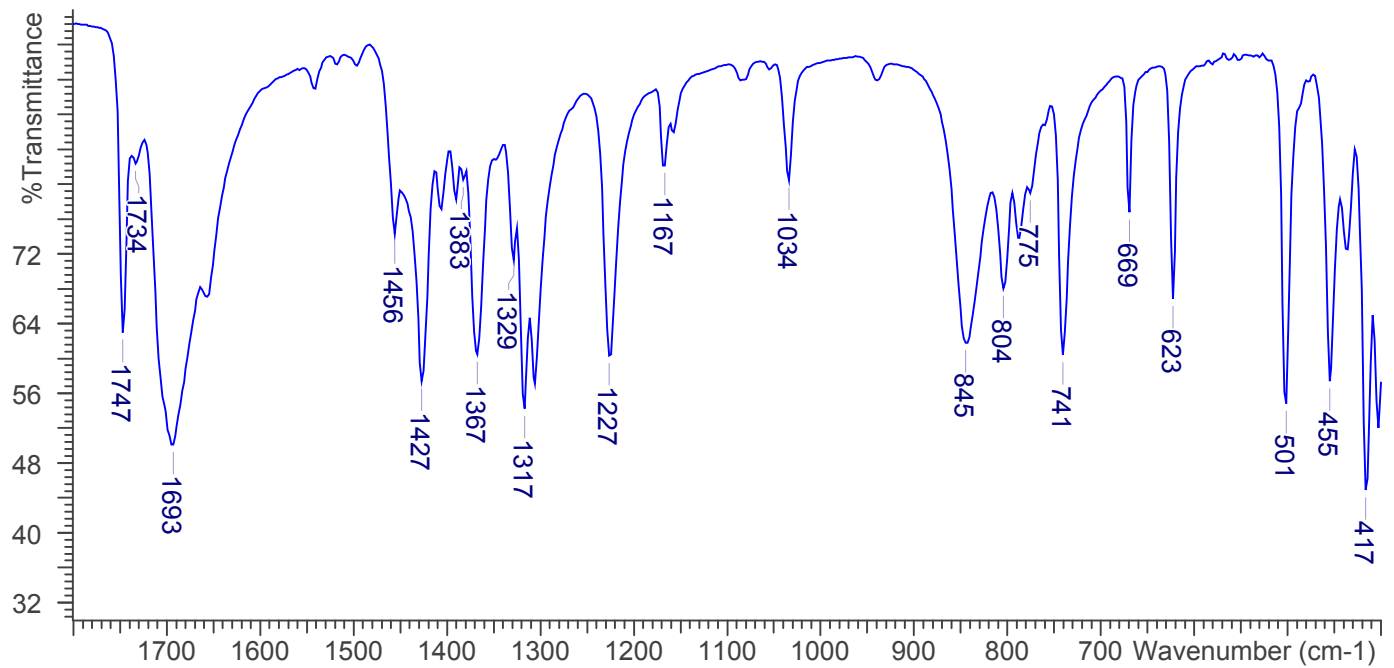
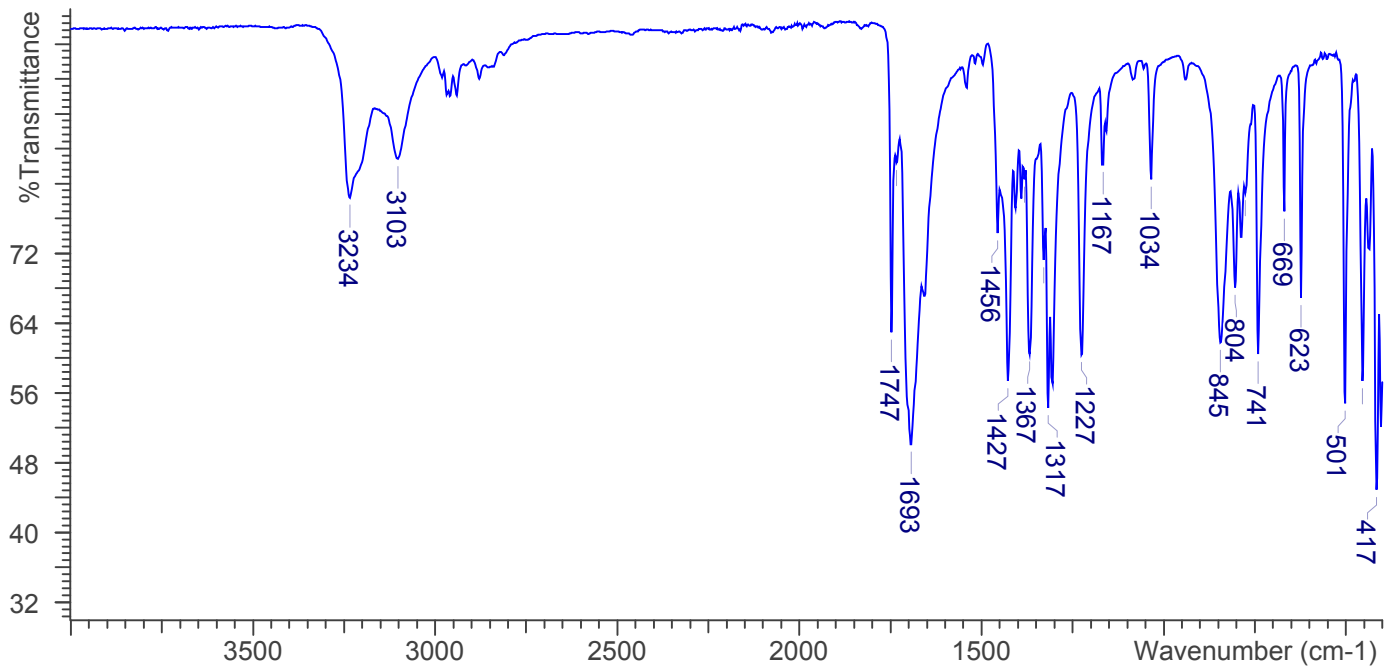


3.3 INFRARED SPECTROSCOPY (FTIR)

Instrument: FTIR with diamond ATR attachment (1 bounce)

Scan Parameters:
Number of scans: 32
Number of background scans: 32
Resolution: 4 cm⁻¹
Sample gain: 8
Aperture: 150

FTIR ATR (Diamond 1 Bounce): Barbital; Lot# 429050





Barbital

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4. ADDITIONAL RESOURCES

[*Forendex*](#)

[*Wikipedia*](#)