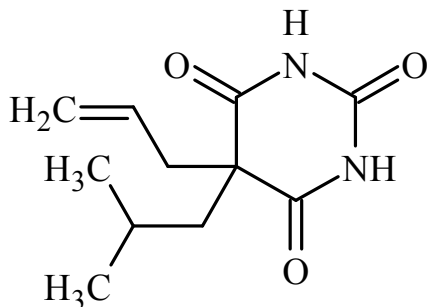




## Butalbital

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>	5-(2-methylpropyl)-5-(prop-2-en-1-yl)pyrimidine-2,4,6(1H,3H,5H)-trione
<b>CAS#:</b>	77-26-9
<b>Synonyms:</b>	Allylbarbital, 5-allyl-5-isobutylbarbituric acid, Itobarbital, Allylbarbituric Acid
<b>Source:</b>	DEA Reference Material Collection
<b>Appearance:</b>	White powder
<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>11</sub> H <sub>16</sub> N <sub>2</sub> O <sub>3</sub>	224	138.6



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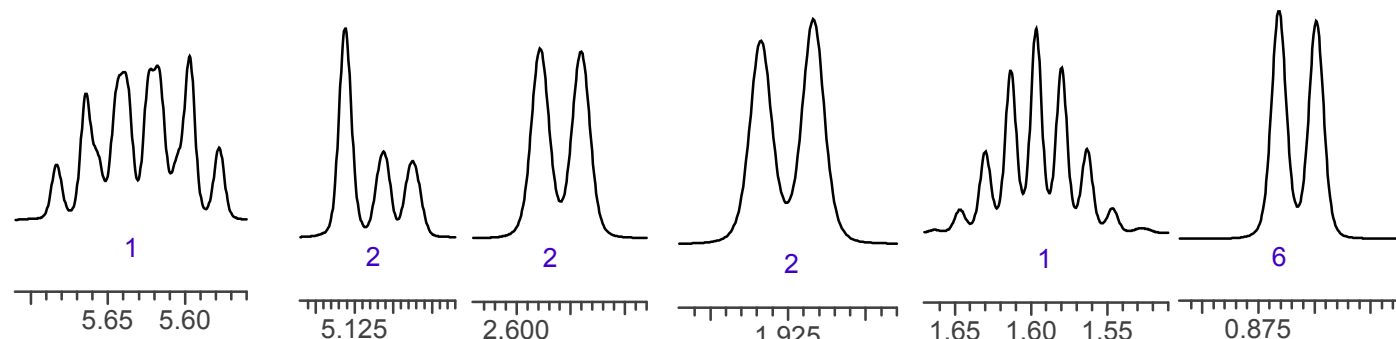
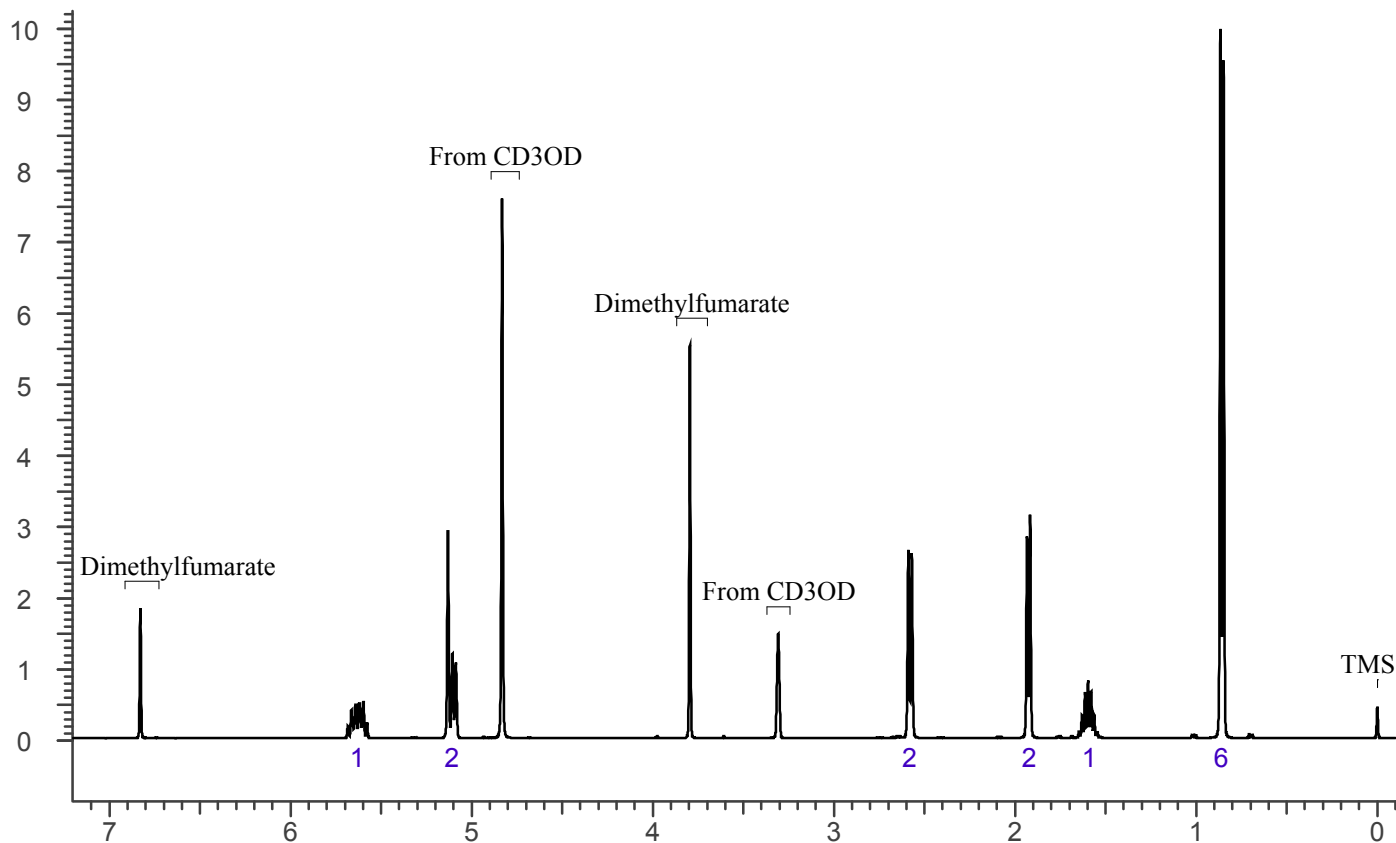
## 3. QUALITATIVE DATA

### 3.1 NUCLEAR MAGNETIC RESONANCE

**Sample Preparation:** Dilute analyte to ~25 mg/mL in CD<sub>3</sub>OD 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: Butalbital Lot A6A, CD<sub>3</sub>OD, 400MHz





## Butalbital

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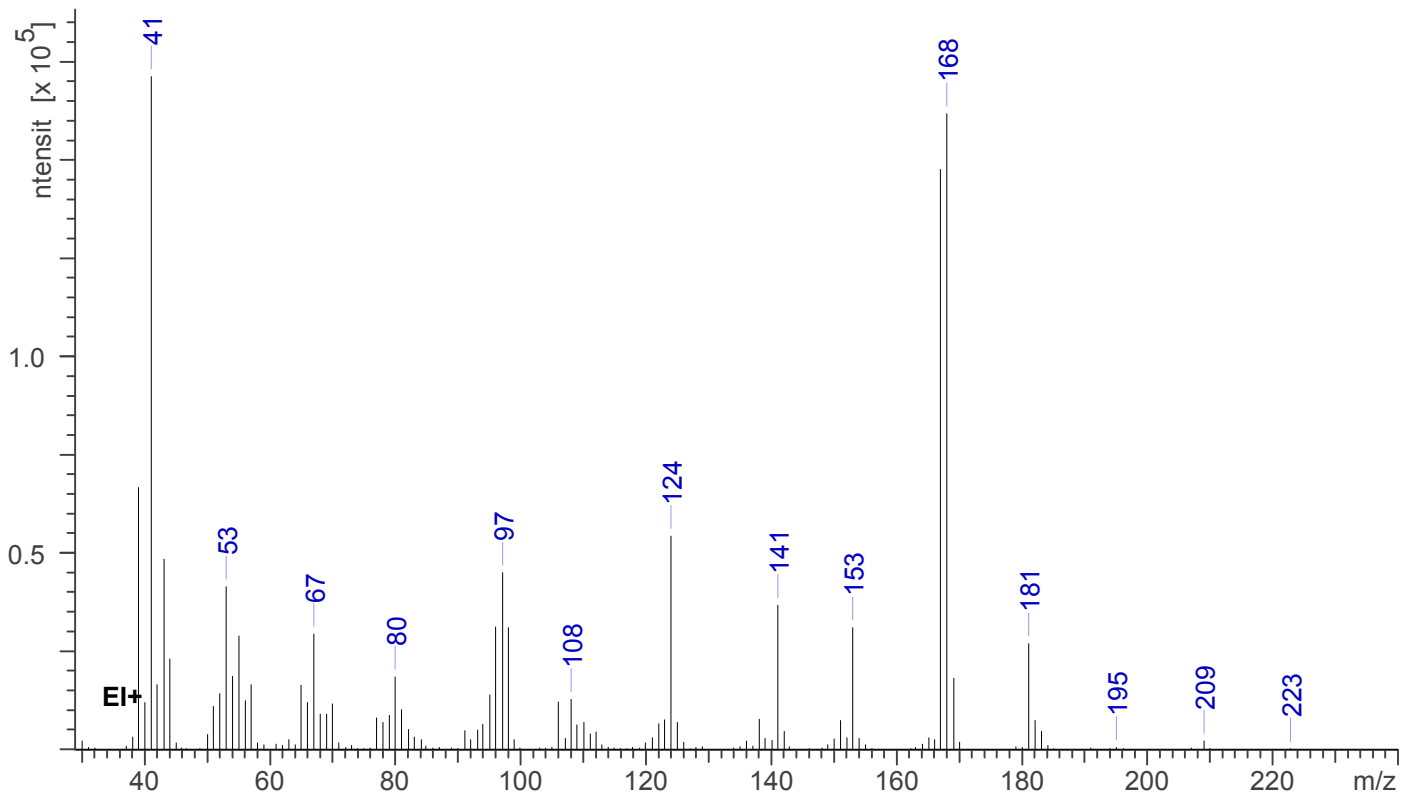
### 3.2 GAS CHROMATOGRAPHY/MASS SPECTROMETRY

*Sample Preparation:* Dilute analyte ~4 mg/mL in methanol.

**Instrument:** Agilent gas chromatograph operated in split mode with MS detector  
**Column:** DB-1 MS (or equivalent); 30m x 0.25 mm x 25  $\mu$ 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 300°C at 12 °C/min  
3) Hold final temperature for 9.0 min

**Injection Parameters:** Split Ratio = 20:1, 1  $\mu$ L injected  
**MS Parameters:** Mass scan range: 30-550 amu  
Threshold: 100  
Tune file: stune.u  
Acquisition mode: scan  
**Retention Time:** 8.328 min

EI Mass Spectrum Butalbital Lot A6A





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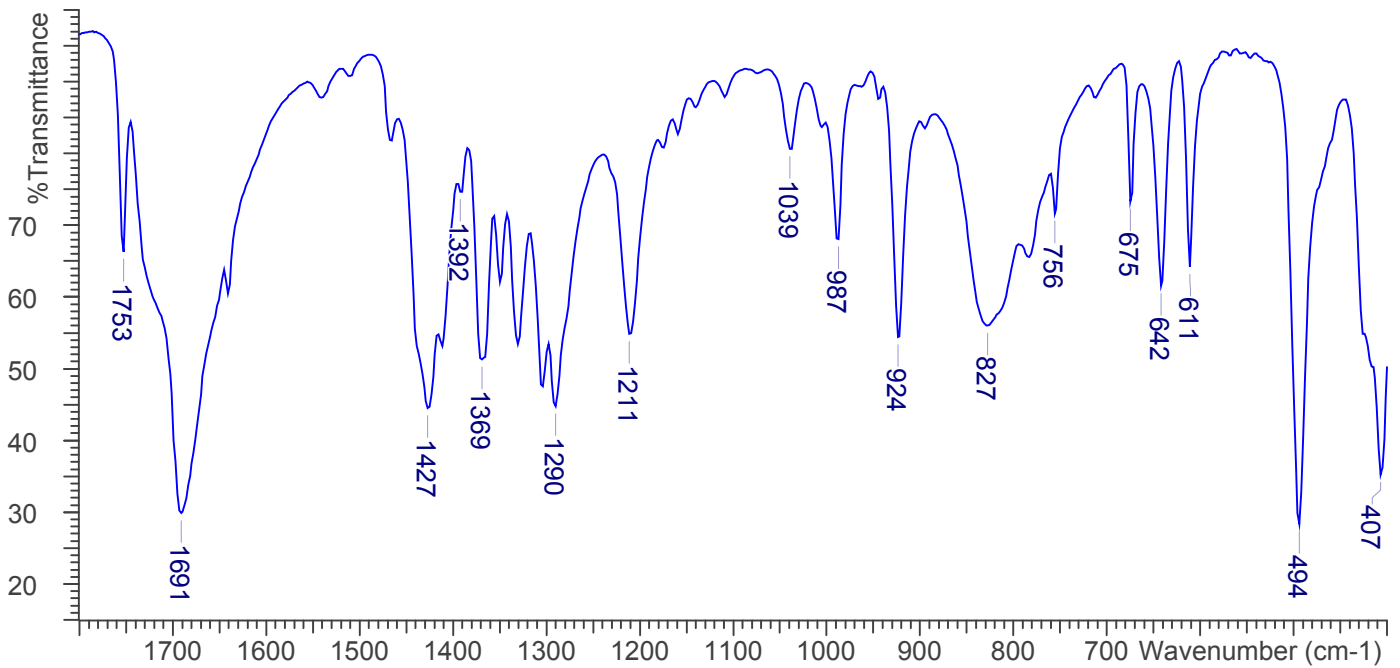
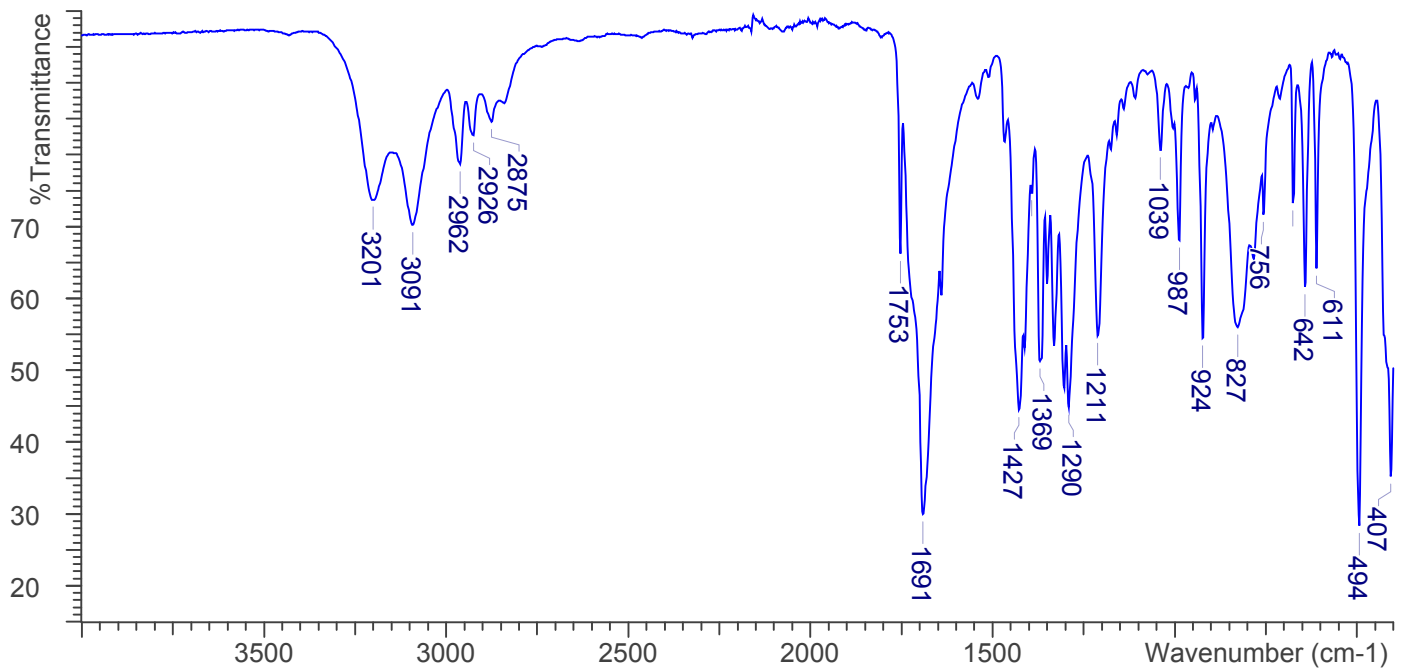


## 3.3 INFRARED SPECTROSCOPY (FTIR)

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

**Scan Parameters:**  
Number of scans: 32  
Number of background scans: 32  
Resolution: 4 cm<sup>-1</sup>  
Sample gain: 8  
Aperture: 150

FTIR ATR (Diamond, 1 Bounce) Butalbital Lot A6A





## **Butalbital**

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### **4. ADDITIONAL RESOURCES**

[\*Wikipedia\*](#)