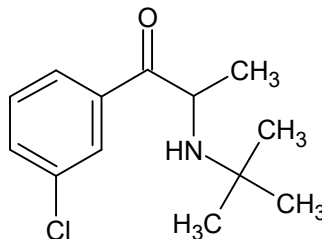




Bupropion

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



1. GENERAL INFORMATION

IUPAC Name: 2-(*tert*-butylamino)-1-(3-chlorophenyl)propan-1-one

CAS#: 34911-55-2 (base), 31677-93-7 (HCl)

Synonyms: 3-chloro-N-*tert*-butyl- β -ketoamphetamine, Amfebutamone, Voxra, Zyban

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 ₁₃ H ₁₈ ClNO	239.74	Not Determined
HCl	C ₁₃ H ₁₈ ClNO HCl	276.20	229-234 (Charred)



Bupropion

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



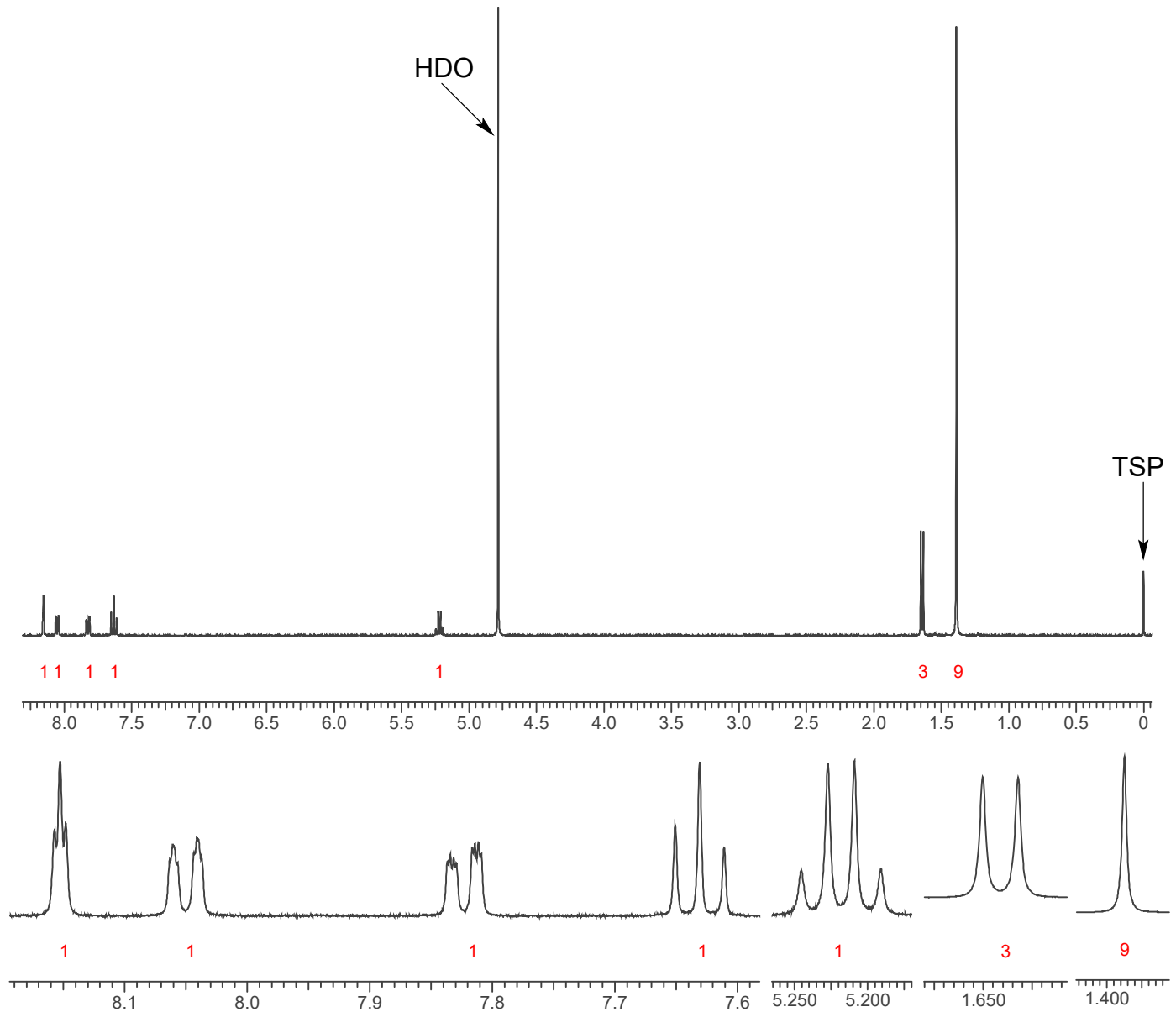
3. QUALITATIVE DATA

3.1 NUCLEAR MAGNETIC RESONANCE

Sample Preparation: Dilute analyte to ~7 mg/mL in D₂O containing TSP for 0 ppm reference.

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: Bupropion HCl; Lot# 0421509-4; D₂O; 400MHz





Bupropion

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



3.2 GAS CHROMATOGRAPHY/MASS SPECTROMETRY

Sample Preparation: Dilute analyte ~4 mg/mL in MeOH

Instrument: Agilent gas chromatograph operated in split mode with MS detector

Column: DB-1 MS (or equivalent); 30m x 0.25 mm x 0.25 μ m

Carrier Gas: Helium at 1.5 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

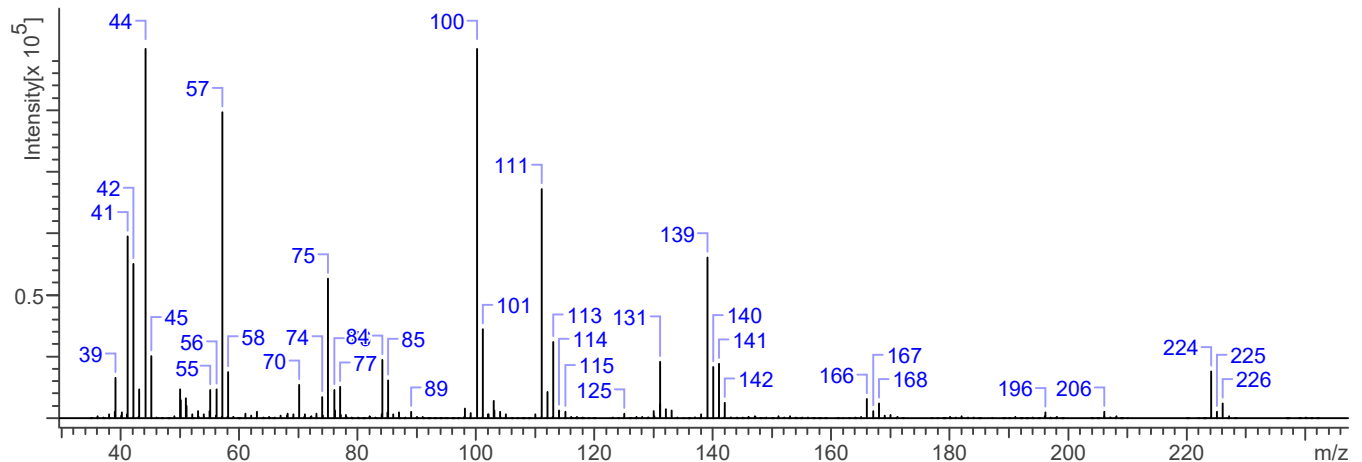
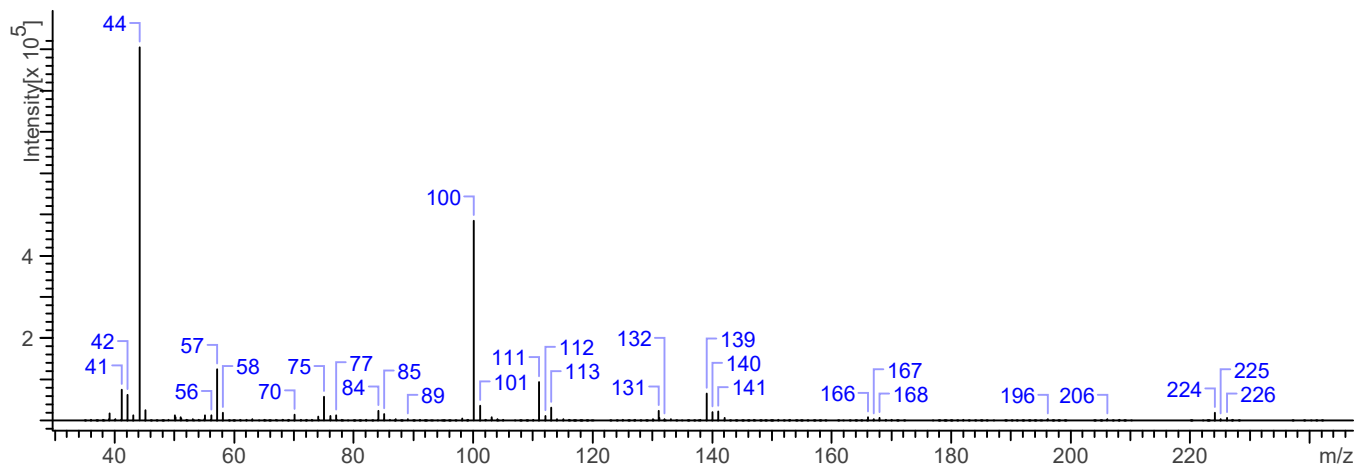
Injection Parameters: Split Ratio = 25:1, 1 μ L injected

MS Parameters: Mass scan range: 30-550 amu Threshold: 100

Tune file: stune.u Acquisition mode: scan

Retention Time: 8.748 min

EI Mass Spectrum: Bupropion HCl; Lot# 0421509-4





Bupropion

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

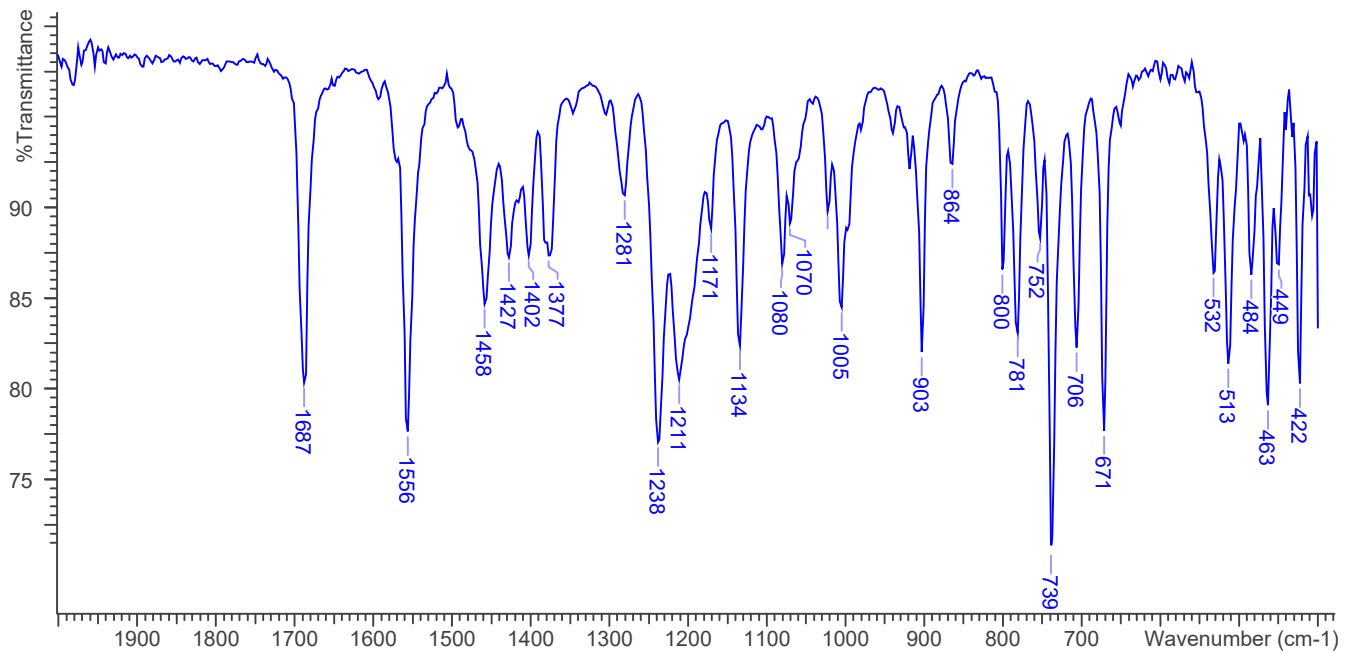
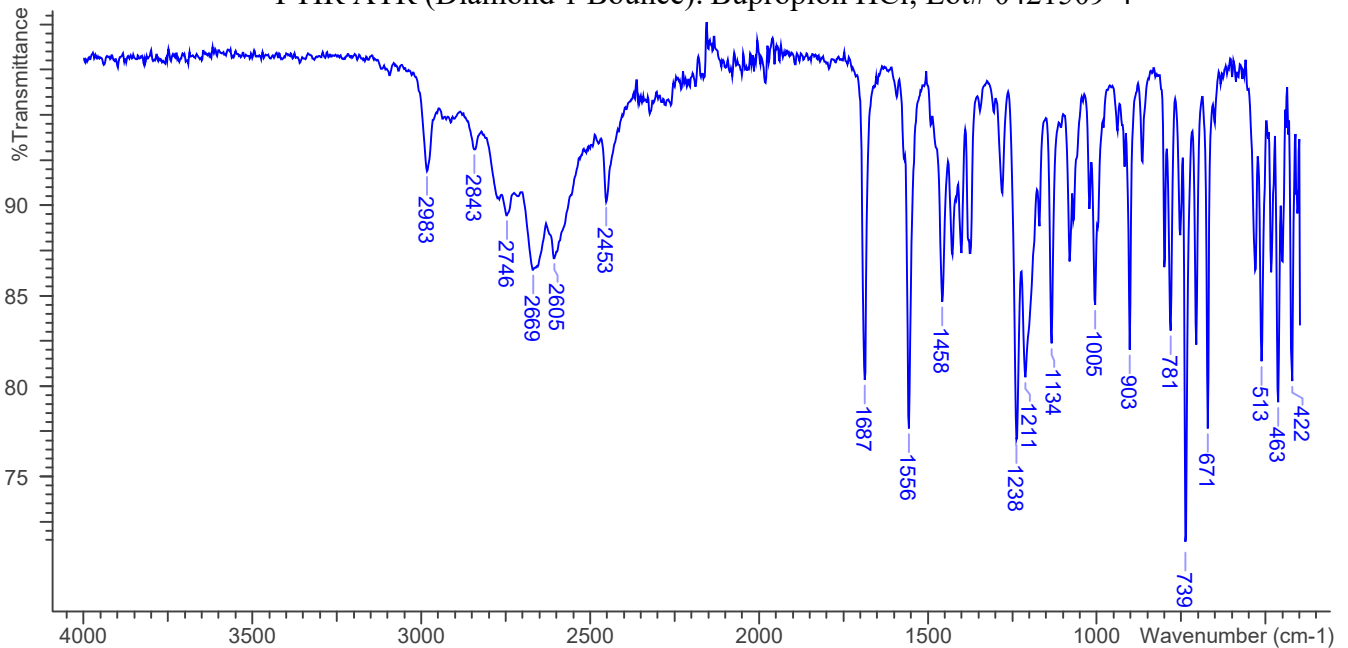


3.3 INFRARED SPECTROSCOPY (FTIR)

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): Bupropion HCl; Lot# 0421509-4





Bupropion

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



4. ADDITIONAL RESOURCES

[*Wikipedia*](#)