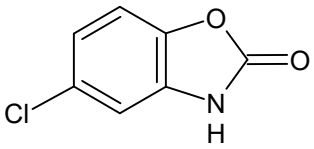
Chlorzoxazone

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



1. GENERAL INFORMATION

IUPAC Name: 5-chlorobenzo[d]oxazol-2(3*H*)-one

CAS#: 95-25-0

Synonyms: 5-chloro-2-benzoxazolone, 5-chloro-2-benzoxazolol, 5-chloro-2(3*H*)-benzoxazolone, 5-chloro-1,3-benzoxazol-2(3*H*)-one

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 (^{o}C)
Base	$C_7H_4ClNO_2$	169.56	190.97

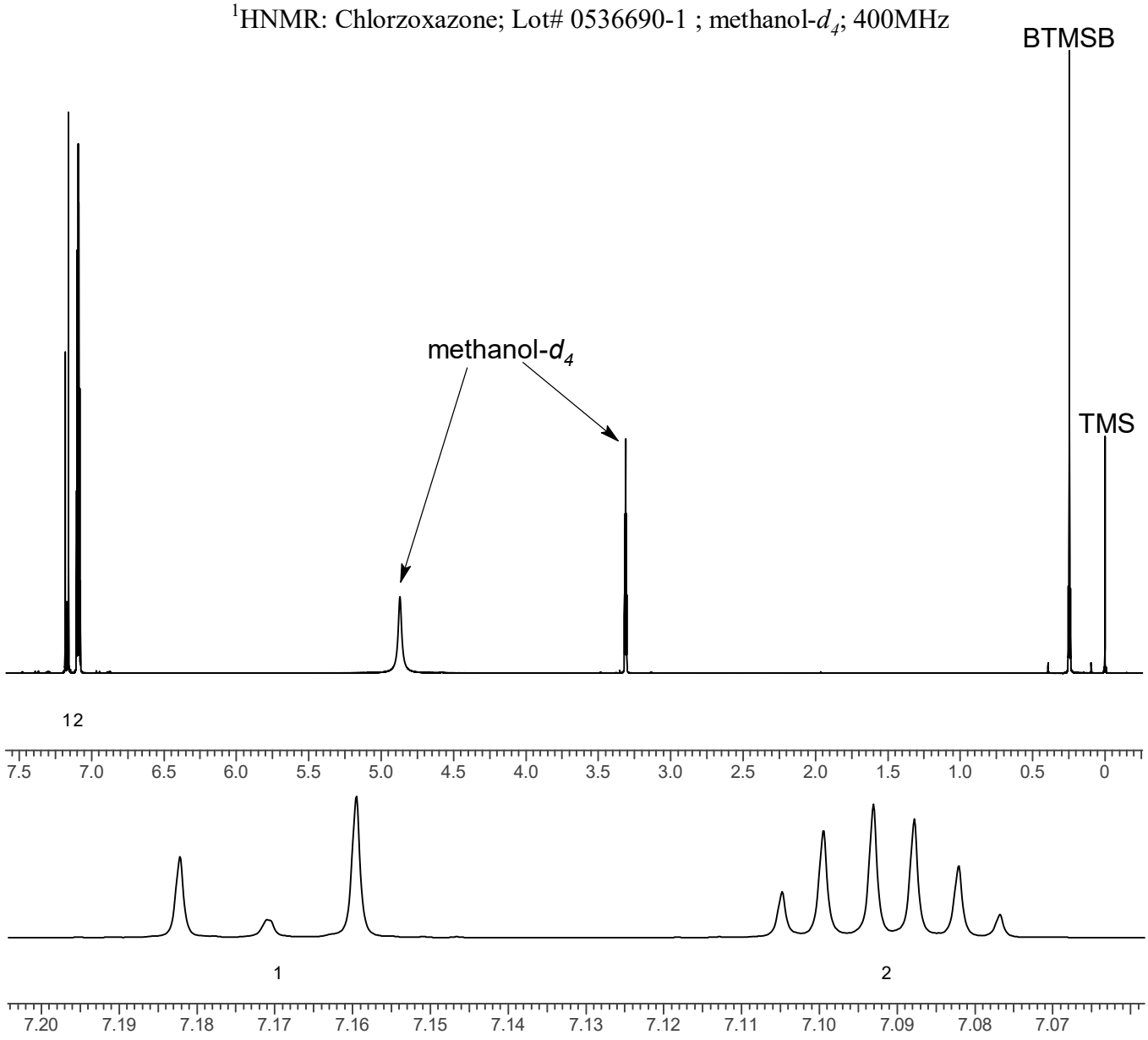
3. QUALITATIVE DATA

3.1 NUCLEAR MAGNETIC RESONANCE

Sample Preparation: Dilute analyte to ~12 mg/mL in methanol-d_4 containing TMS for 0 ppm reference and 1,4-BTMSB-d_4 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

^{1}HNMR: Chlorzoxazone; Lot# 0536690-1 ; methanol-d_4; 400MHz

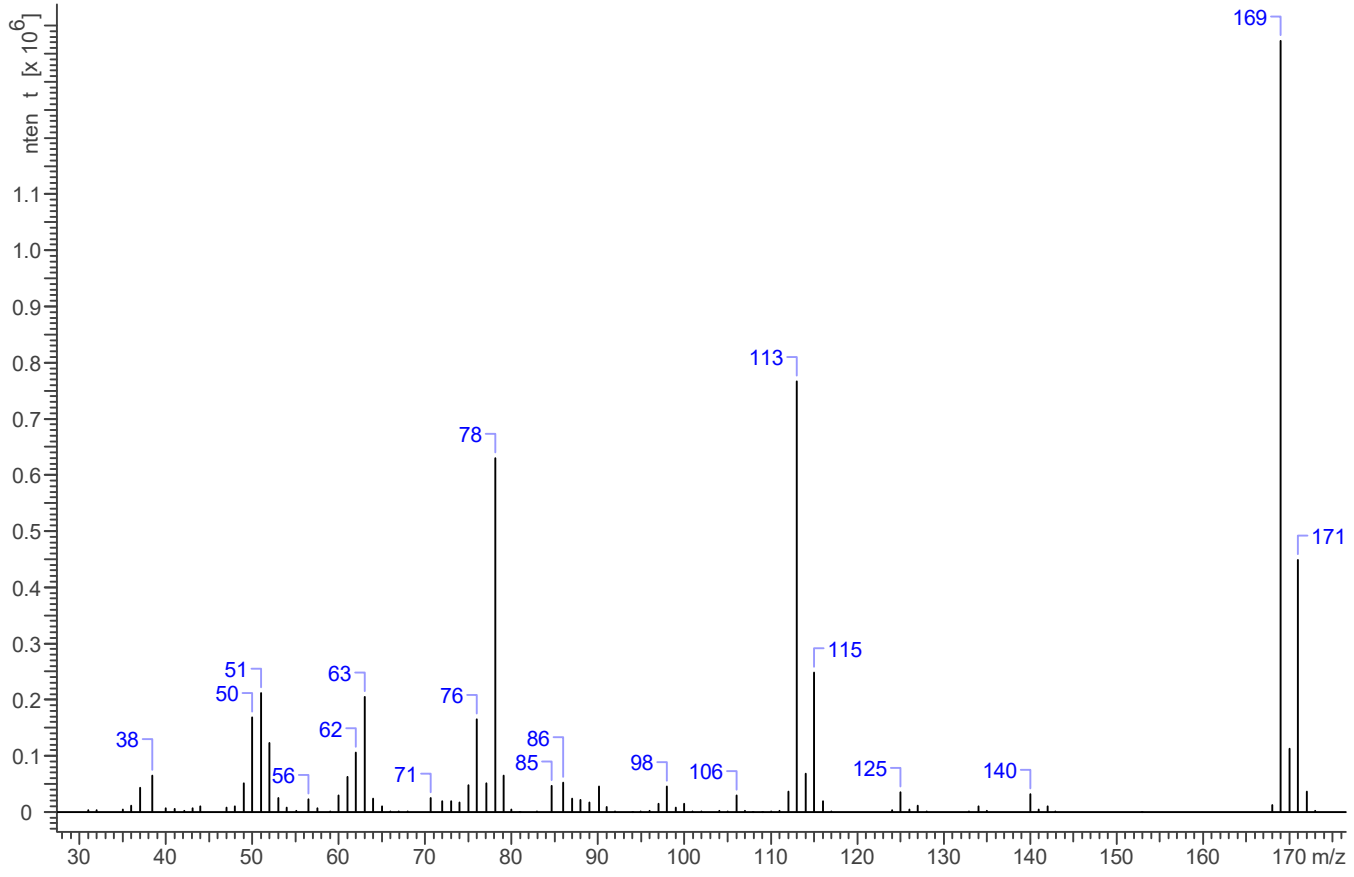


3.2 GAS CHROMATOGRAPHY/MASS SPECTROMETRY

Sample Preparation: Dilute analyte ~3 mg/mL in MeOH

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 1.5 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 µL injected	
MS Parameters:	Mass scan range: 30-550 amu	Threshold: 150
	Tune file: stune.u	Acquisition mode: scan
Retention Time:	9.16 min	

EI Mass Spectrum: Chlorzoxazone; Lot# 0536690-1



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): Chlorzoxazone; Lot# 0536690-1