

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



1. GENERAL INFORMATION

IUPAC Name: 1-(4-ethyl-2,5-dimethoxyphenyl)propan-2-amine

CAS#: 22004-32-6 (base)

Synonyms: DOET, DOE, Hecate

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	$C_{13}H_{21}NO_2$	223	Not Determined
HC1	C ₁₃ H ₂₁ NO ₂ · HCl	259	194

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3. QUALITATIVE DATA

3.1 NUCLEAR MAGNETIC RESONANCE

Sample Preparation: Dilute analyte to \sim 25 mg/mL in D₂O containing TSP for 0 ppm reference and maleic acid as quantitative internal standard.

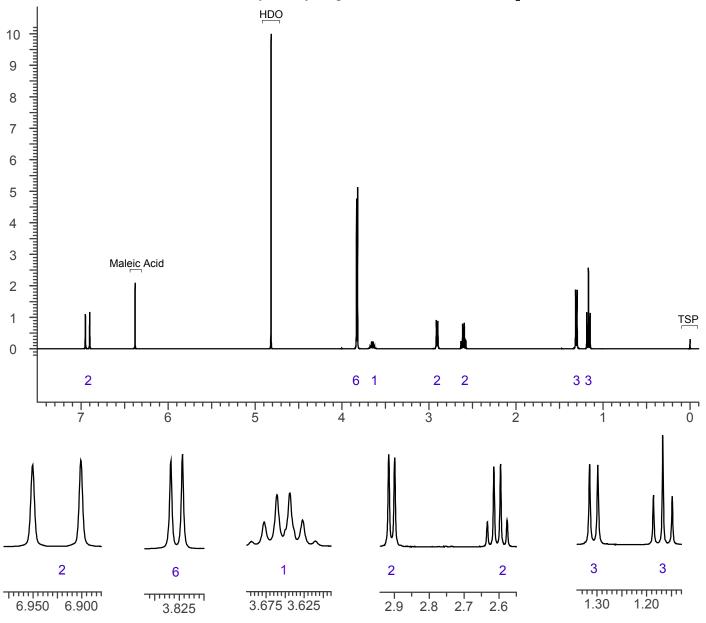
Instrument: 400 MHz NMR spectrometer

Parameters: Spectral width: at least containing -3 ppm through 13 ppm

Pulse angle: 90°

Delay between pulses: 45 seconds

¹H NMR: 2,5-dimethoxy-4-ethylamphetamine HCl Lot # J-1; D₂O; 400MHz



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3.2 GAS CHROMATOGRAPHY/MASS SPECTROMETRY

Sample Preparation: Dilute analyte ~4 mg/mL base extracted into chloroform.

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

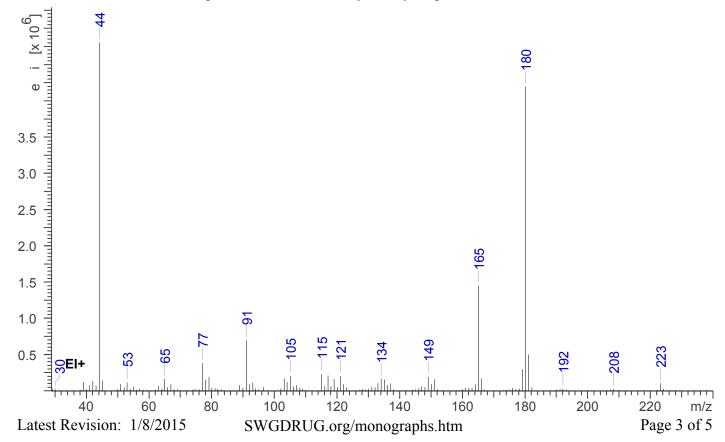
3) Hold final temperature for 9.0 min

Injection Parameters: Split Ratio = 20:1, 1 µL injected MS Parameters: Mass scan range: 30-550 amu

Threshold: 100
Tune file: stune.u
Acquisition mode: scan

Retention Time: 9.883 min

EI Mass Spectrum: 2,5-dimethoxy-4-ethylamphetamine HCl Lot # J-1





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3.3 INFRARED SPECTROSCOPY (FTIR)

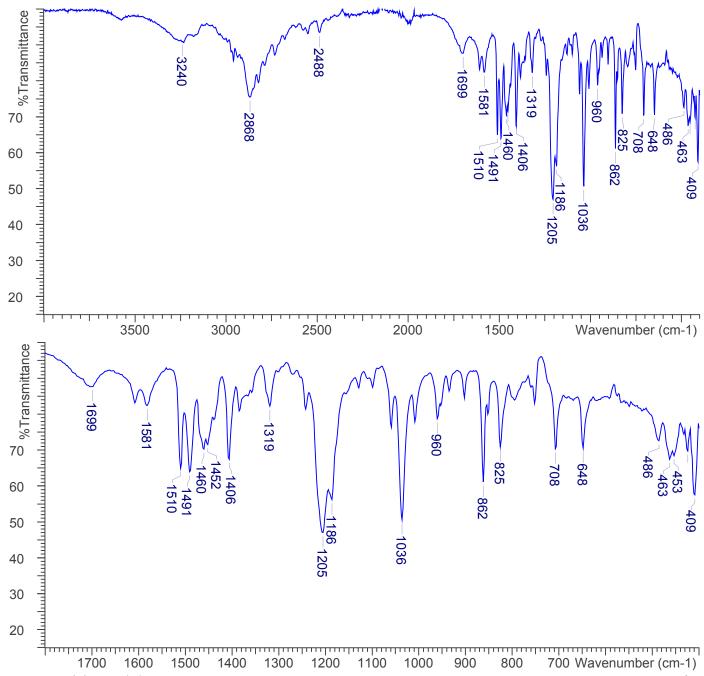
Insrument: FTIR with diamond ATR attachment (1 bounce)

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): 2,5-dimethoxy-4-ethylamphetamine HCl Lot # J-1



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4. ADDITIONAL RESOURCES

Forendex

Wikipedia