Electronic Supplementary Material (ESI) for ChemComm.

Unorthodox crystalline drug salts via the reaction amine-containing drugs with CO_2

Mohammad Soltani,[a] Brandon L. Mash,[b] Julian Henseler,[c] Sharhzad Badri,[a] Matthias Zeller,[b] E. Alan Salter,[a] Andrzej Wierzbicki,[a] Alexandra C. Stenson,[a] and James H. Davis, Jr.[a*]

Departments of Chemistry, (a) University of South Alabama, (b) Purdue University, and (c) Hochschule Aalen

SUPPORTING INFORMATION

Contents

Single Crystal X-ray Structure Determinations

Single crystals of the investigated compounds were coated with a trace of Fomblin oil and were transferred to either a Bruker Quest diffractometer with a fixed chi angle, a Mo Kα wavelength (λ = 0.71073 Å) sealed tube fine focus X-ray tube, single crystal curved graphite incident beam monochromator, and a Photon100 CMOS area detector, or onto a Bruker Quest diffractometer with kappa geometry, a Cu Kα wavelength (λ = 1.54178 Å) I-μ-S microsource X-ray tube, laterally graded multilayer (Goebel) mirror single crystal for monochromatization, and a Photon2 CMOS area detector. Both instruments were equipped with an Oxford Cryosystems low temperature devices and examination and data collection were performed at 150 K. Data were collected, reflections were indexed and processed, and the files scaled and corrected for absorption using APEX3, SAINT [1] and SADABS [2]. The space groups were assigned and the structures were solved by direct methods using XPREP within the SHELXTL suite of programs [3] and refined by full matrix least squares against F^2 with all reflections using Shelxl2018 [4] using the graphical interface Shelxle [5]. If not specified otherwise H atoms attached to carbon and nitrogen atoms as well as hydroxyl hydrogens were positioned geometrically and constrained to ride on their parent atoms. C-H bond distances were constrained to 0.95 Å for aromatic and alkene C-H moieties, and to 1.00, 0.99 and 0.98 Å for aliphatic C-H, CH_2 and CH_3 moieties, respectively. N-H bond distances were constrained to 0.91 Å for pyramidal (sp^3 hybridized) ammonium NH_2^+ and NH_3^+ groups. For "Despiramine-CO_2" the positions of ammonium NH_2^+ H atoms were refined and N-H distances were restrained to identical values. O-H distances of alcohols were constrained to 0.84 Å. Methyl CH_3, ammonium NH_3^+ and hydroxyl H atoms were allowed to rotate but not to tip to best fit the experimental electron density. In "Maproptilene-CO_2" a water molecule is disordered over two mutually exclusive positions related by an inversion center and was refined as half occupied. Water H atom positions were refined and O-H distances were restrained to 0.84(2) Å. U_{iso}(H) values were set to a multiple of U_{eq}(C) with 1.5 for CH_3, NH_3^+ and OH, and 1.2 for C-H, CH_2, and NH_2 units, respectively.

Additional data collection and refinement details are given in the table below. Complete crystallographic data, in CIF format, have been deposited with the Cambridge Crystallographic Data Centre. CCDC 1947399-1947402 contains the supplementary crystallographic data for this paper. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif.

[1] Bruker (2018). Apex3, Saint, Bruker AXS Inc.: Madison (WI), USA.

[2] Krause, L., Herbst-Irmer, R., Sheldrick G.M. & Stalke D. (2015). *J. Appl. Cryst.* **48**, 3-10.

[3] a) SHELXTL suite of programs, Version 6.14, 2000-2003, Bruker Advanced X-ray Solutions, Bruker AXS Inc., Madison, Wisconsin: USA b) Sheldrick GM. A short history of SHELX. *Acta Crystallogr A.* **2008**, *64(1)*, 112–122.

[4] a) Sheldrick GM. University of Göttingen, Germany, **2018**. b) Sheldrick GM. Crystal structure refinement with SHELXL. *Acta Crystallogr Sect C Struct Chem.* **2015**, *71(1)*, 3–8.

[5] Hübschle CB, Sheldrick GM, Dittrich B. ShelXle: a Qt graphical user interface for SHELXL. *J. Appl. Crystallogr.* **2011**, *44(6)*, 1281–1284.

Table 1. Experimental details

	Despiraminnium despiramine carbamate	Maproptilennium maproptilene carbamate hemihydrate	Nortryptilennium nortryptilene carbamate	Betahistidine carbamic acid
Crystal data				
Chemical formula	$C_{19}H_{21}N_2O_2 \cdot C_{18}H_{23}N_2$	$2(C_{21}H_{22}NO_2) \cdot 2(C_{20}H_{24}N) \cdot H_2O$	$C_{20}H_{20}NO_2 \cdot C_{19}H_{22}N$	$C_9H_{12}N_2O_2$
M_r	576.76	1215.61	570.74	180.21
Crystal system, space group	Monoclinic, $P2_1/n$	Triclinic, $P\bar{1}$	Monoclinic, $P2_1/n$	Triclinic, $P\bar{1}$
Temperature (K)	150	150	150	150
a, b, c (Å)	8.9559(3), 33.9149(10), 20.7715(6)	8.9101(4), 11.0141(5), 17.3483(8)	10.8194(6), 27.0609(15), 11.5232(6)	11.1385(7), 11.1376(6), 14.7537(9)
α, β, γ (°)	90, 97.3341(10), 90	84.2353(14), 78.5292(13), 85.5819(13)	90, 111.9021(18), 90	90.660(2), 90.947(2), 90.281(2)
V (Å^3)	6257.5 (3)	1657.22 (13)	3130.3 (3)	1829.89 (19)
Z	8	1	4	8
F(000)	2480	654	1224	768
D_x (Mg m^{-3})	1.224	1.218	1.211	1.308
Radiation type	Cu $K\alpha$	Cu $K\alpha$	Mo $K\alpha$	Mo $K\alpha$
No. of reflections for cell measurement	9806	9970	9244	9135

θ range (°) for cell measurement	4.5–72.1	2.6–80.2	2.4–28.8	2.3–33.2
μ (mm^{-1})	0.60	0.58	0.07	0.09
Crystal shape	Fragment	Block	Plate	Block
Colour	Colourless	Colourless	Colourless	Colourless
Crystal size (mm)	0.21 × 0.18 × 0.15	0.22 × 0.19 × 0.14	0.50 × 0.37 × 0.15	0.53 × 0.48 × 0.37
Data collection				
Diffractometer	Bruker AXS D8 Quest CMOS diffractometer with PhotonII charge-integrating pixel array detector (CPAD)		Bruker AXS D8 Quest CMOS diffractometer with Photon100 charge-integrating pixel array detector (CPAD)	
Radiation source	I-mu-S microsource X-ray tube		fine focus sealed tube X-ray source	
Monochromator	Laterally graded multilayer (Goebel) mirror		Triumph curved graphite crystal	
Detector resolution (pixels mm^{-1})	7.4074		10.4167	
Scan method	ω and phi scans			
Absorption correction	Multi-scan, *SADABS* 2016/2			
T_{min}, T_{max}	0.658, 0.754	0.658, 0.754	0.617, 0.746	0.683, 0.747
No. of measd, indep. and obsd. [$I > 2\sigma(I)$] reflections	35000, 11830, 10748	22153, 6778, 6205	89404, 8095, 7038	37070, 13618, 10357
R_{int}	0.029	0.034	0.042	0.033
θ values (°)	θ_{max} = 72.2, θ_{min} = 2.5	θ_{max} = 80.6, θ_{min} = 2.6	θ_{max} = 28.8, θ_{min} = 2.5	θ_{max} = 33.2, θ_{min} = 2.3
$(\sin\theta/\lambda)_{max}$ ($Å^{-1}$)	0.617	0.640	0.677	0.771
Range of *h*, *k*, *l*	*h* = -10→8, *k* = -39→32, *l* = -25→25	*h* = -11→9, *k* = -14→13, *l* = -21→20	*h* = -14→12, *k* = -36→36, *l* = -15→15	*h* = -17→17, *k* = -14→17, *l* = -22→22
Refinement				
Refinement on	F^2	F^2	F^2	F^2
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, *S*	0.040, 0.109, 1.05	0.042, 0.114, 1.10	0.053, 0.132, 1.09	0.049, 0.137, 1.04
No. of reflections	11830	6778	8095	13618
No. of parameters	791	424	391	477
No. of restraints	6	2	0	0
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement		H-atom parameters constrained	
Weighting scheme	$w = 1/[\sigma^2(F_o^2) + (0.0447P)^2 + 2.030P]$ where $P = (F_o^2 + 2F_c^2)/3$			
$(\Delta/\sigma)_{max}$	0.001	< 0.001	< 0.001	0.001
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e $Å^{-3}$)	0.20, -0.16	0.27, -0.19	0.34, -0.22	0.39, -0.27
Extinction method	None	*SHELXL2018*/3 (Sheldrick 2018),		None

		$Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$		
Extinction coefficient	n/a	0.0054 (7)	0.0070 (7)	n/a

Computer programs: Apex3 v2017.3-0, Apex3 v2018.7-2, Apex3 v2018.1-0 (Bruker, 2018), *SADABS* 2016/2 (Krause et al., 2015). *SAINT* V8.38A (Bruker, 2016), *SHELXS97* (Sheldrick, 2008), *SHELXL2018*/3 (Sheldrick, 2015, 2018), SHELXLE Rev946 (Hübschle *et al.*, 2011).

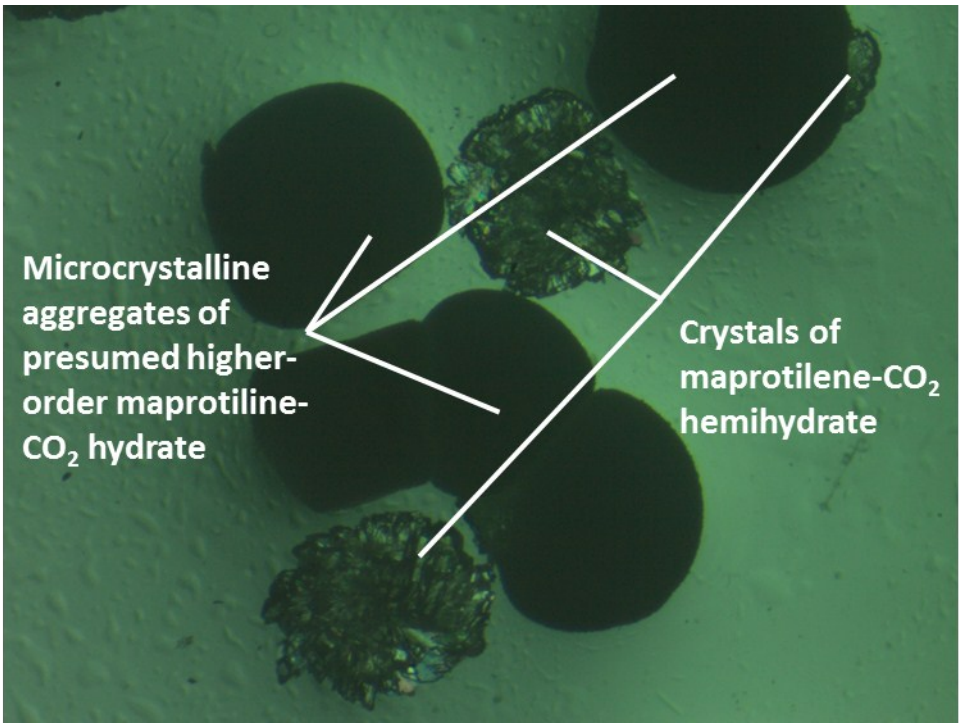
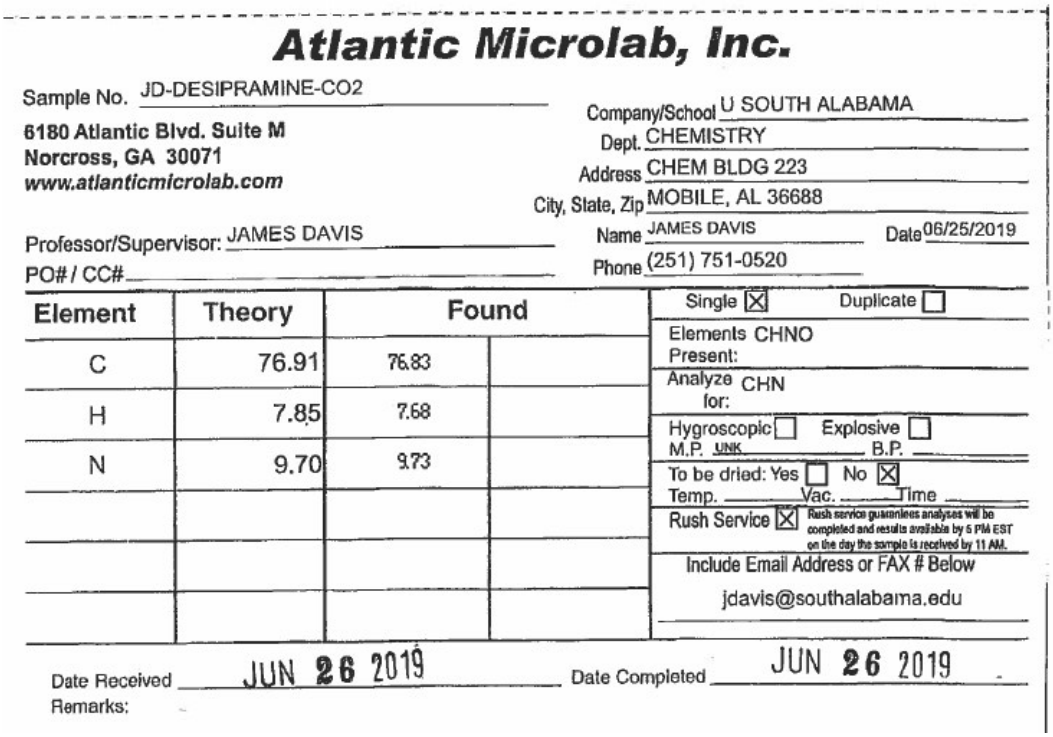


Figure S1. The two different crystal growth forms of the maprotilene-CO_2 product.



Atlantic Microlab, Inc.

Sample No. JD-DESIPRAMINE-CO2

6180 Atlantic Blvd. Suite M
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Professor/Supervisor: JAMES DAVIS
PO# / CC#

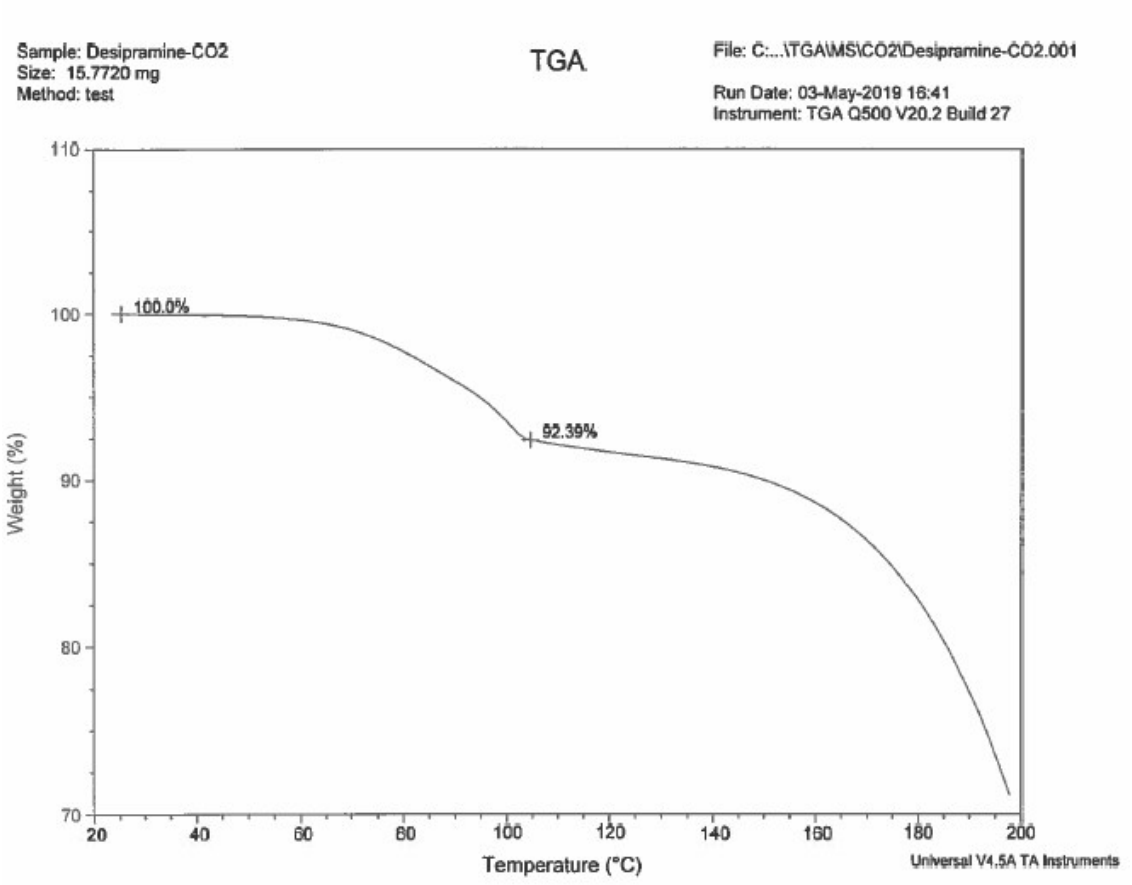
Company/School U SOUTH ALABAMA
Dept. CHEMISTRY
Address CHEM BLDG 223
City, State, Zip MOBILE, AL 36688
Name JAMES DAVIS Date 06/25/2019
Phone (251) 751-0520

Element	Theory	Found	
C	76.91	76.83	
H	7.85	7.68	
N	9.70	9.73	

Single ☒ Duplicate ☐
Elements Present: CHNO
Analyze for: CHN
Hygroscopic ☐ Explosive ☐
M.P. UNK B.P.
To be dried: Yes ☐ No ☒
Temp. Vac. Time
Rush Service ☒ Rush service guarantees analyses will be completed and results available by 5 PM EST on the day the sample is received by 11 AM.
Include Email Address or FAX # Below
jdavis@southalabama.edu

Date Received JUN 26 2019 Date Completed JUN 26 2019
Remarks:

Desipramine-CO_2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Size: 15.7720 mg
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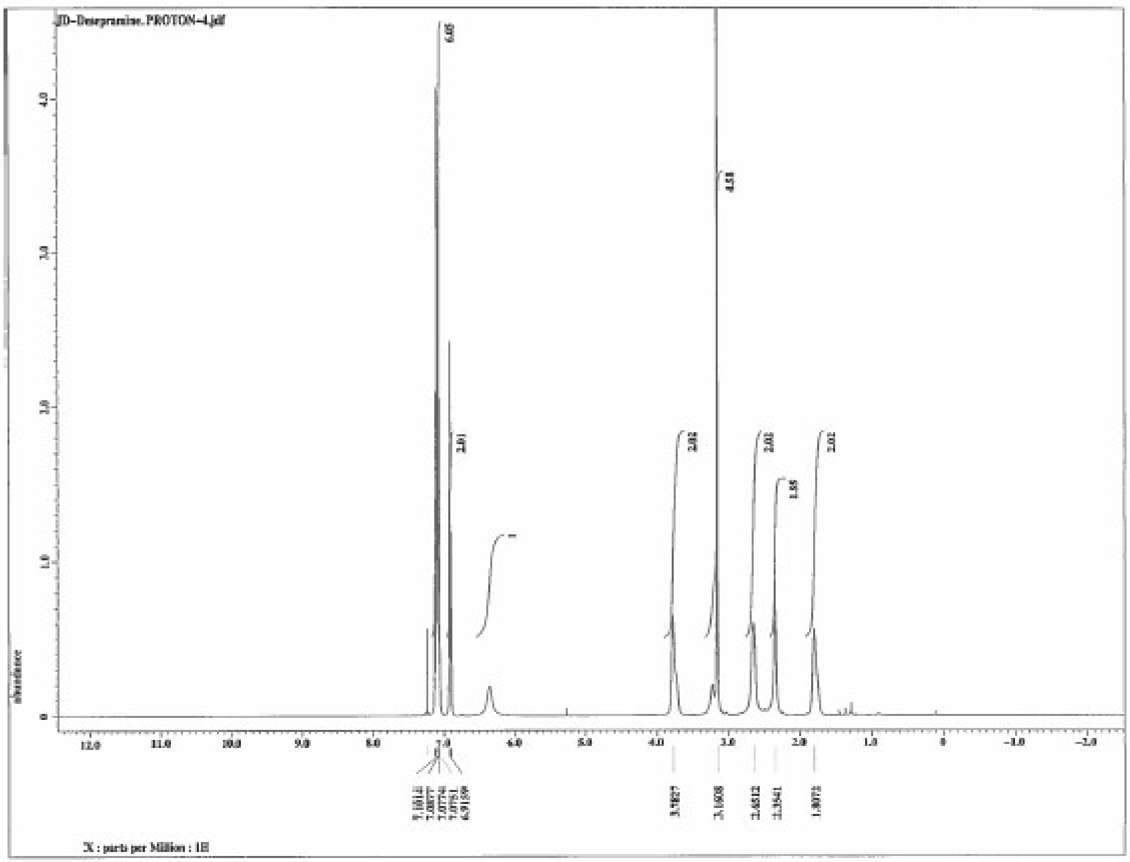
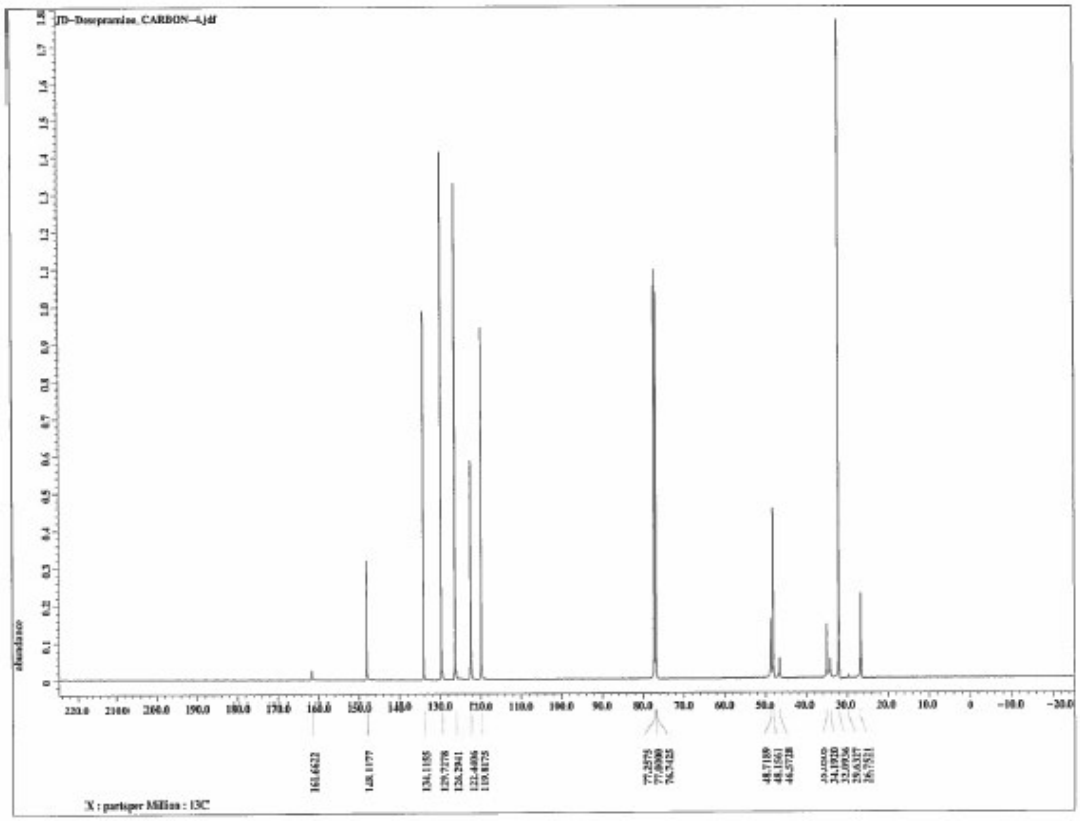
Universal V4.5A TA Instruments

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X : parts per Million : 13C

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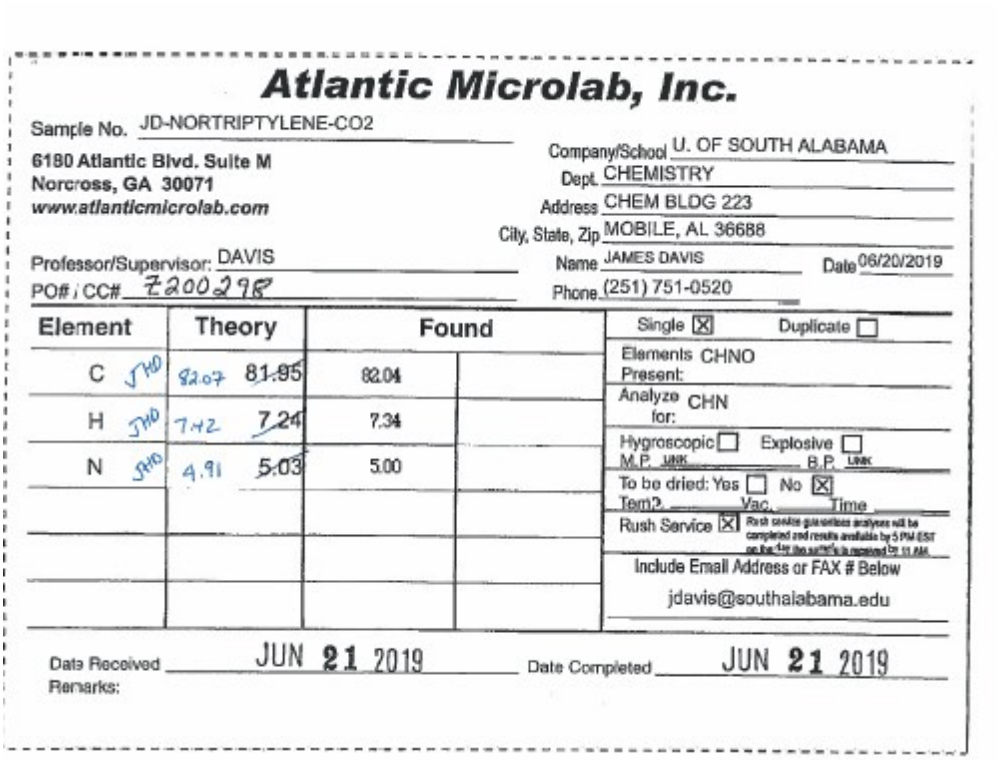

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Sample No. JD-NORTRIPTYLENE-CO2

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City, State, Zip MOBILE, AL 36688
Name JAMES DAVIS Date 06/20/2019
Phone (251) 751-0520

Professor/Supervisor: DAVIS
PO# / CC# Z200298

Element	Theory		Found	
C JHD	82.07	81.95	82.04	
H JHD	7.42	7.24	7.34	
N JHD	4.91	5.03	5.00	

Single ☒ Duplicate ☐

Elements Present: CHNO

Analyze for: CHN

Hygroscopic ☐ Explosive ☐
M.P. UNK B.P. UNK

To be dried: Yes ☐ No ☒
Temp. Vac. Time

Rush Service ☒ Rush service guarantees analyses will be completed and results available by 5 PM EST on the 1st day the sample is received by 11 AM.

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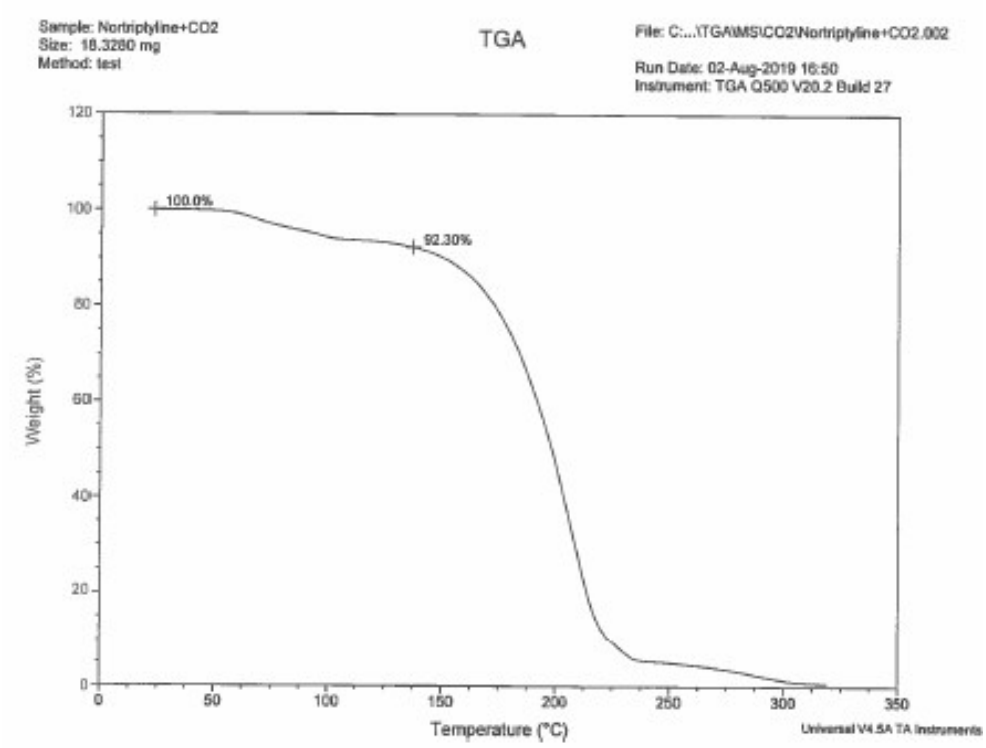
Date Received JUN 21 2019 Date Completed JUN 21 2019

Remarks: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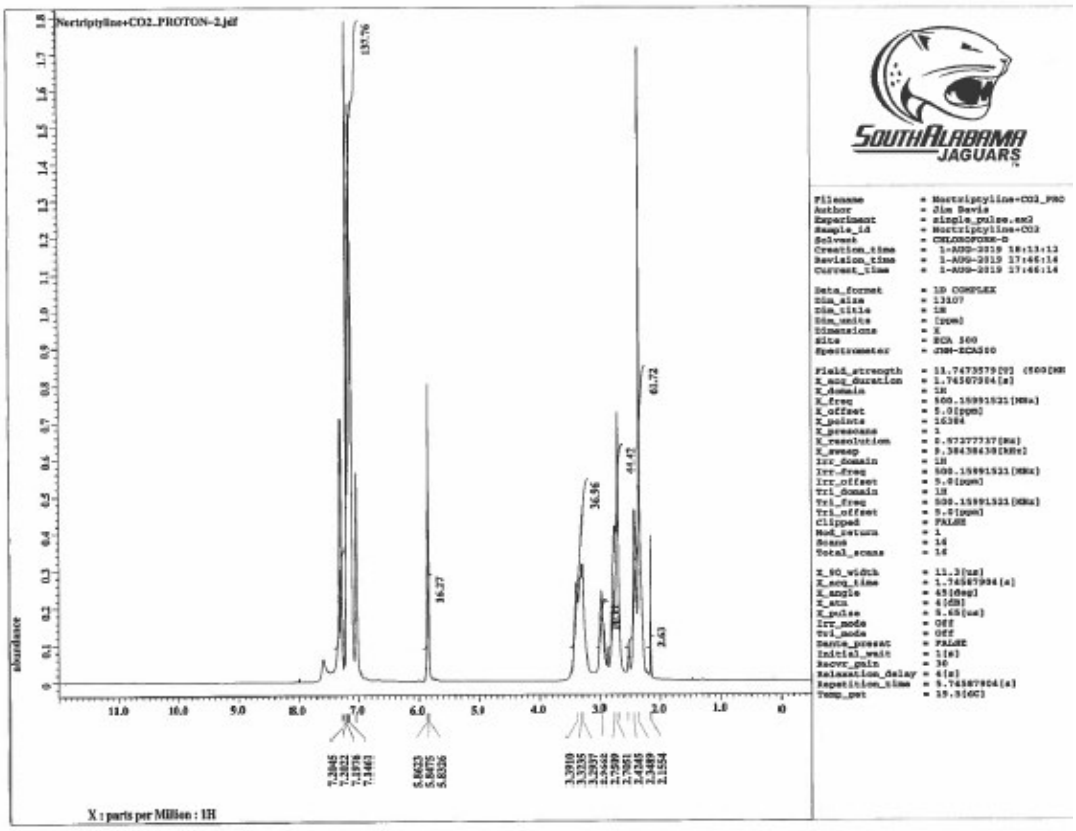
Weight (%)
Temperature (°C)
Universal V4.5A TA Instruments



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Spectrometer = JNM-ECA500

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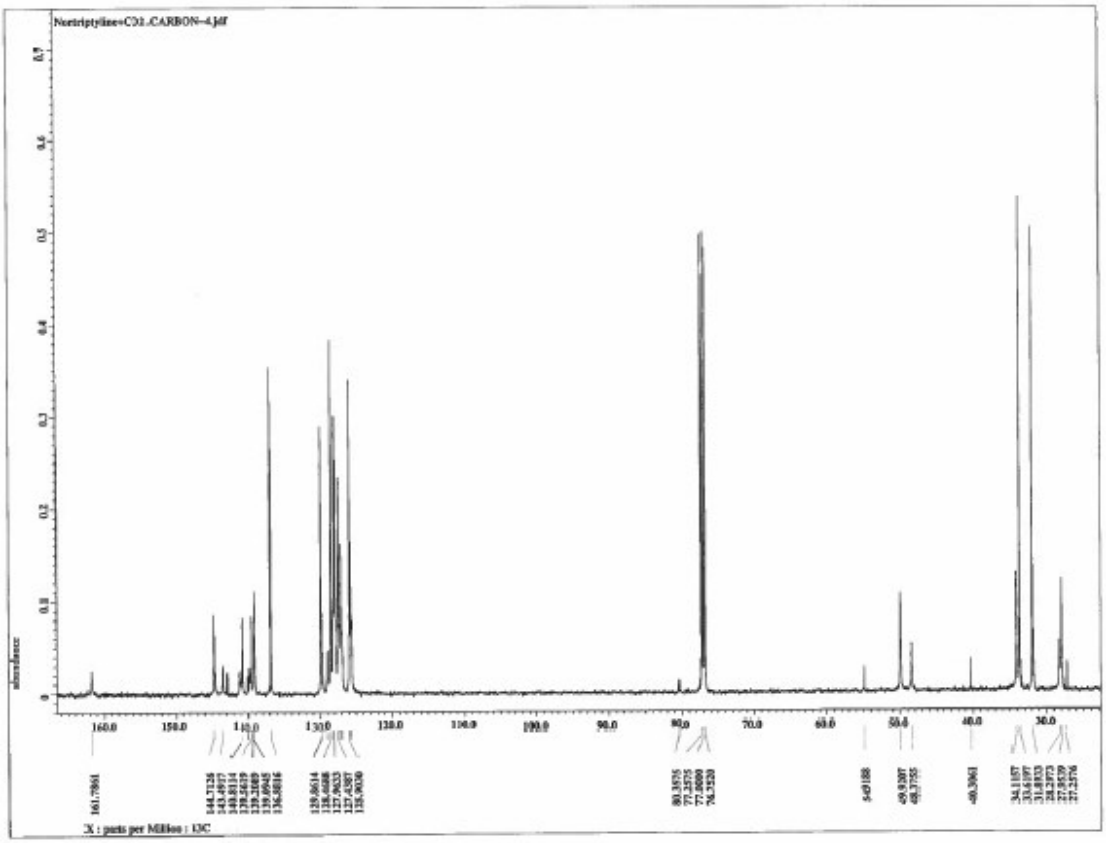

Maprotiline-CO_2

Atlantic Microlab, Inc.

Sample No. JD-MAPROPTILENE-CO2

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Professor/Supervisor: JAMES DAVIS
PO# / CC#

Name JIM DAVIS
Date 07/15/2019
Phone (251) 751-0520

Element	Theory	Found	
C	82.24	78.68	78.56
H	7.74	7.35	7.45
N	4.68	4.50	4.44
		NO CHARGE FOR DUPLICATES	

Single ☒ Duplicate ☐

Elements Present: CHNO

Analyze for: CHN

Hygroscopic ☒ Explosive ☐
M.P. UNK B.P. UNK

To be dried: Yes ☐ No ☒
Temp. ____ Vac. ____ Time ____

Rush Service ☒ Rush service guarantees analyses will be completed and results available by 5 PM EST on the day the sample is received by 11 AM.

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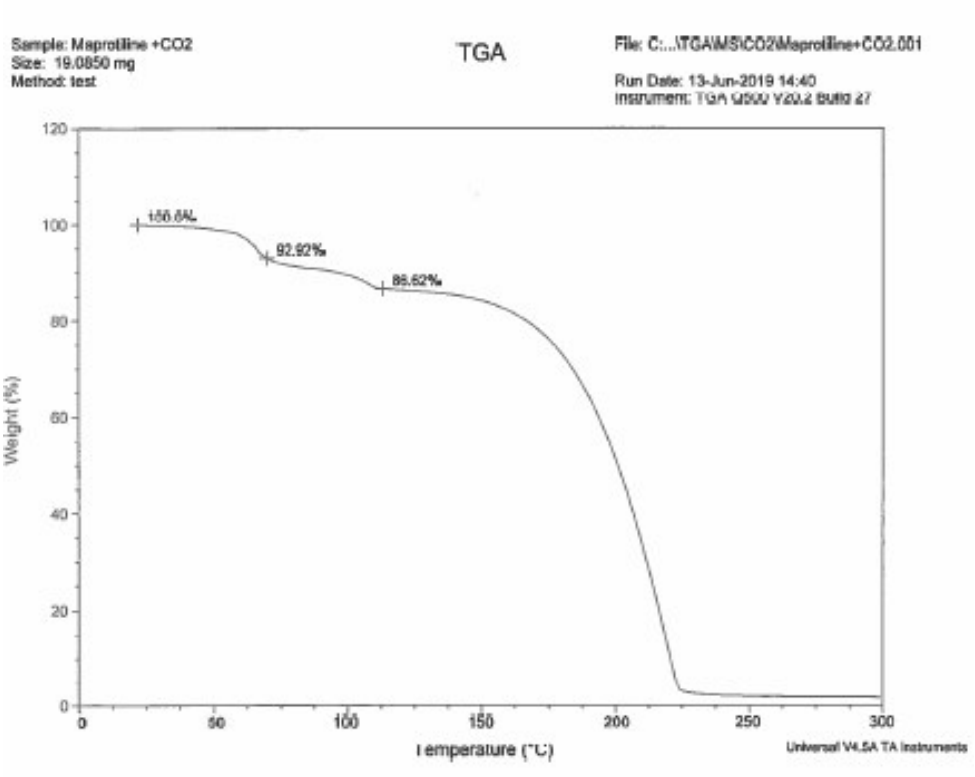
Date Received JUL 17 2019 Date Completed JUL 17 2019

Remarks:

checks ok for 1.5 hydrate: C = 78.36 H = 7.59, N = 4.69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Method: test
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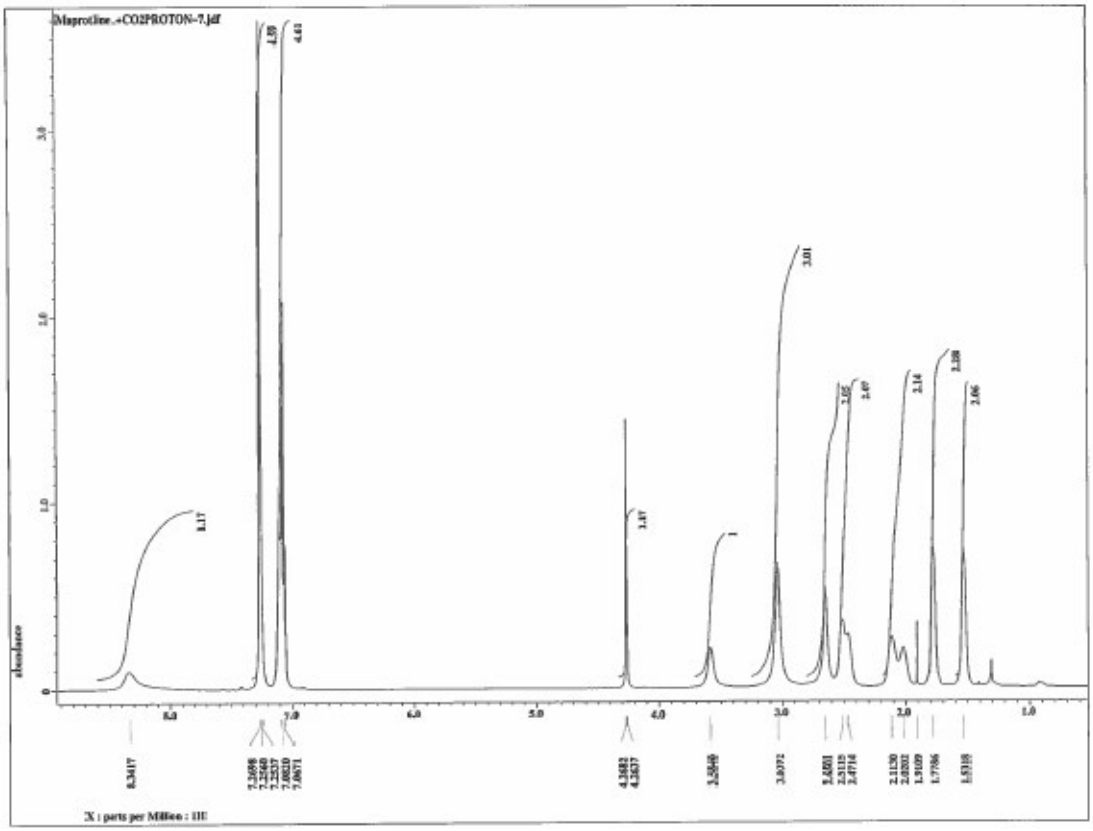
Weight (%)
Temperature (°C)
Universal V4.5A TA Instruments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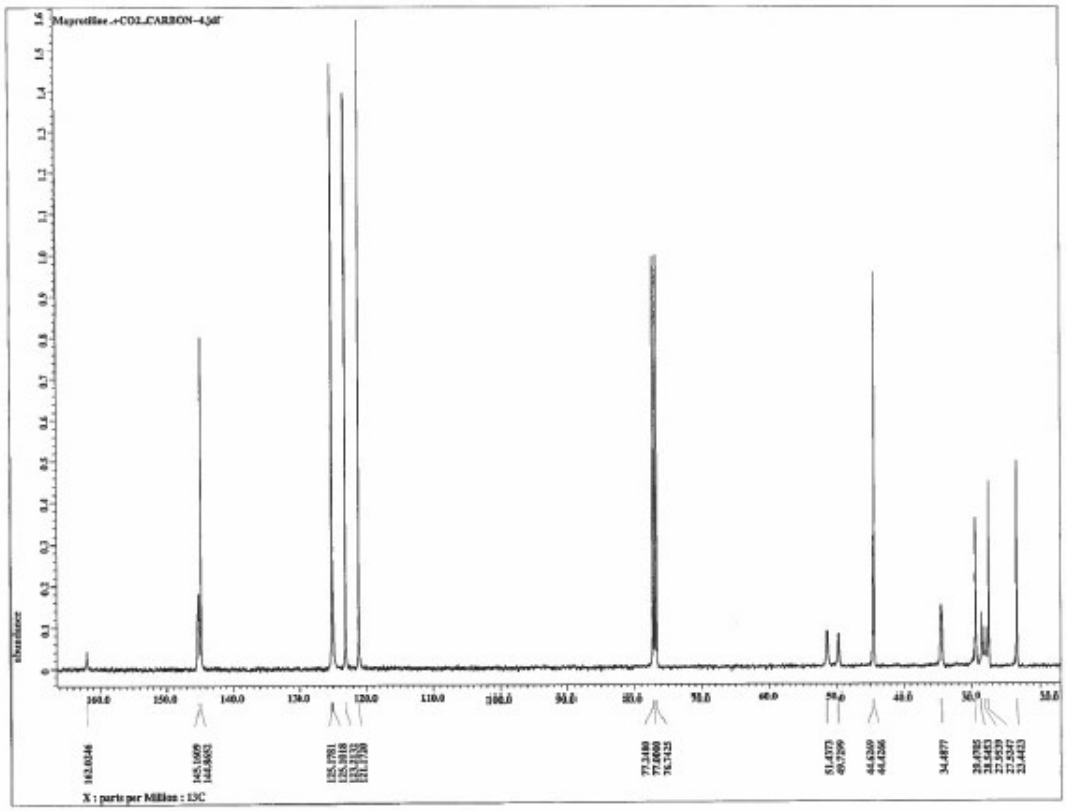
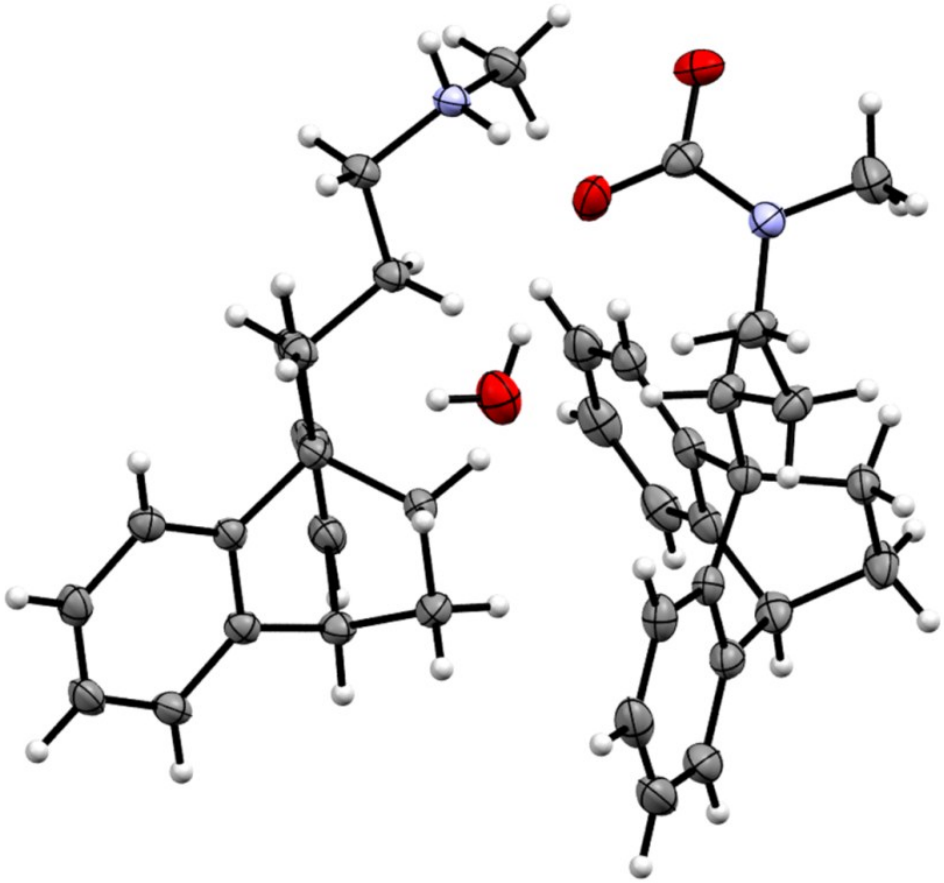
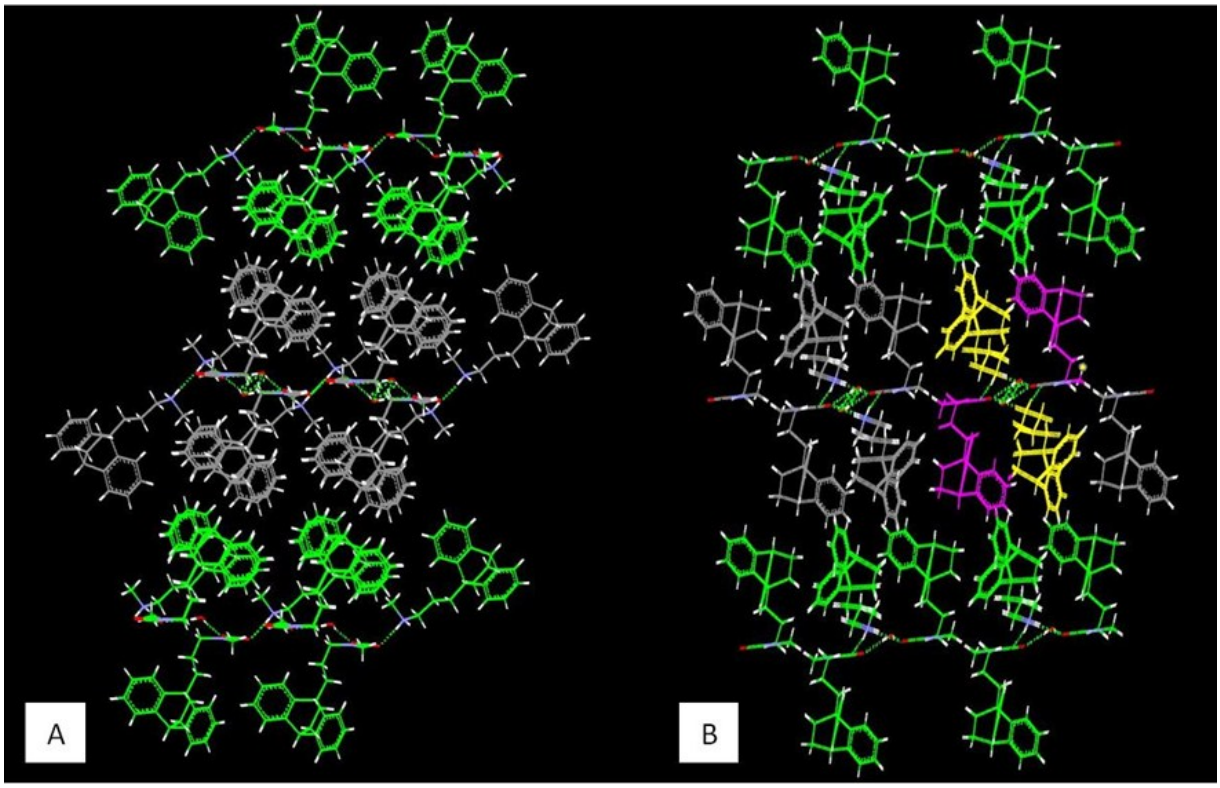
X : parts per Million : 1H



Maprotiline ORTEP and Crystal Packing





Maproptilene-CO_2: r(N-C) = 1.372 Å; a(O-C-O)= 124.2°. ORTEP drawing: The water position is 50% occupied. The crystal is made of ~16 Å-deep corrugated layers that slightly intermesh (Fig. A; three layers shown: middle layer (gray), upper and lower layers (green)). The layer surfaces are nonpolar, populated by nearly perpendicular phenyl groups that fit into the grooves of the next layer above/below; the layers are made of distinct upper and lower sublayers. Within a layer, all ionic groups and waters are found within a central ~5 Å region where the two sublayers meet and H-bonding (green dashes) occurs. The layers divide into subunits; each subunit consists of a stack of four parallel columns of ions that H-bond exclusively with one another. Fig. B is a 90° rotated view of Fig. A, looking down the columns of ions; one such subunit indicated: two columns of the protonated amine-species (yellow) and two columns of carbamate species (magenta). The columns are laced together by H-bonding along the central axis where the carbamates and amines of the four columns make contact.

Within the amine columns, there are H-pi interactions, where H belongs to the terminal methyl group of one ion and the pi system belongs to the next [r(H to phenyl's centroid) = 2.616 Å]. In addition, between adjacent amine and carbamate species (of the same sublayer), there are H-pi interactions between hydrogens of the former's aliphatic bridge moiety and the latter's phenyl group [r(H to phenyl's centroid) = 3.141, 3.143 Å].

Betahistine (Versec)-CO_2

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Sample No. JD-VERSEC-CO2

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Professor/Supervisor: JAMES DAVIS
PO# / CC# #201652

Name JAMES DAVIS
Phone (251) 751-0520
Date 08/05/2019

Element	Theory	Found	
C	59.99	59.36	59.23
H	6.71	6.52	6.64
N	15.55	15.75	15.74
		NO CHARGE FOR DUPLICATES	

Single ☒ Duplicate ☐

Elements Present: CHNO

Analyze for: CHN

Hygroscopic ☒ Explosive ☐
M.P. _____ B.P. _____

To be dried: Yes ☐ No ☒
Temp. _____ Vac. _____ Time _____

Rush Service ☒ Rush service guarantees analyses will be completed and results available by 5 PM EST on the day the sample is received by 11 AM.

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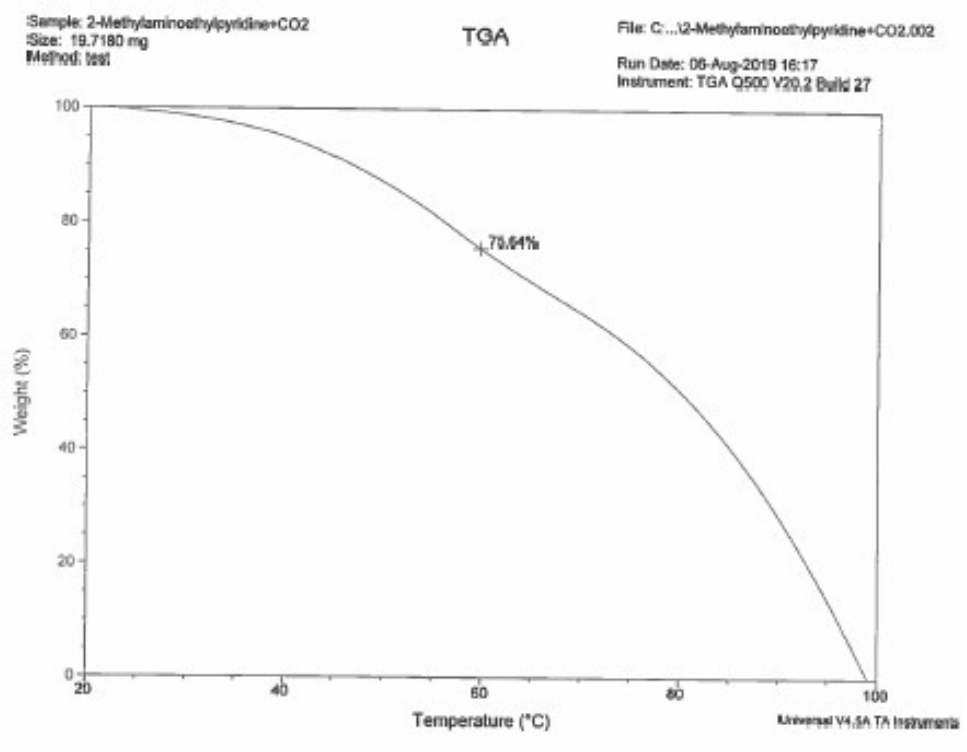
jdavis@southalabama.edu

Date Received AUG 06 2019

Date Completed AUG 06 2019

Remarks: slightly low on C, good X-Ray, NMR, TGA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Size: 19.7180 mg
Method: test
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File: C:...\2-Methylaminoethylpyridine+CO2.002
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Instrument: TGA Q500 V20.2 Build 27
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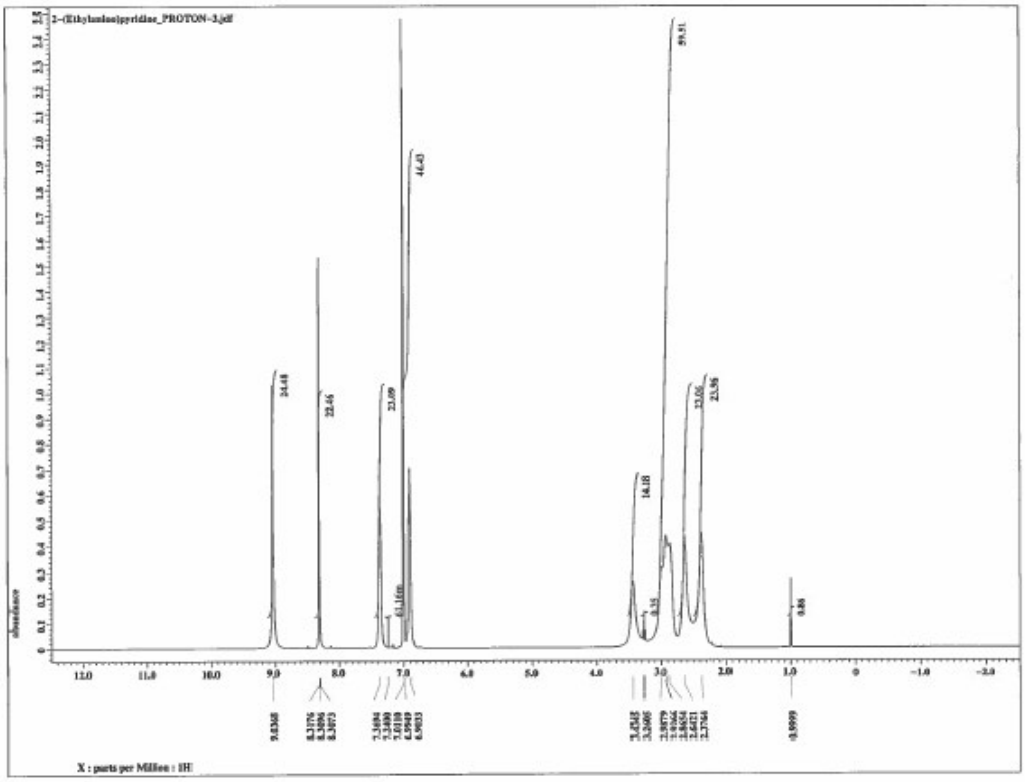
Weight (%)
Temperature (°C)
Universal V4.5A TA Instruments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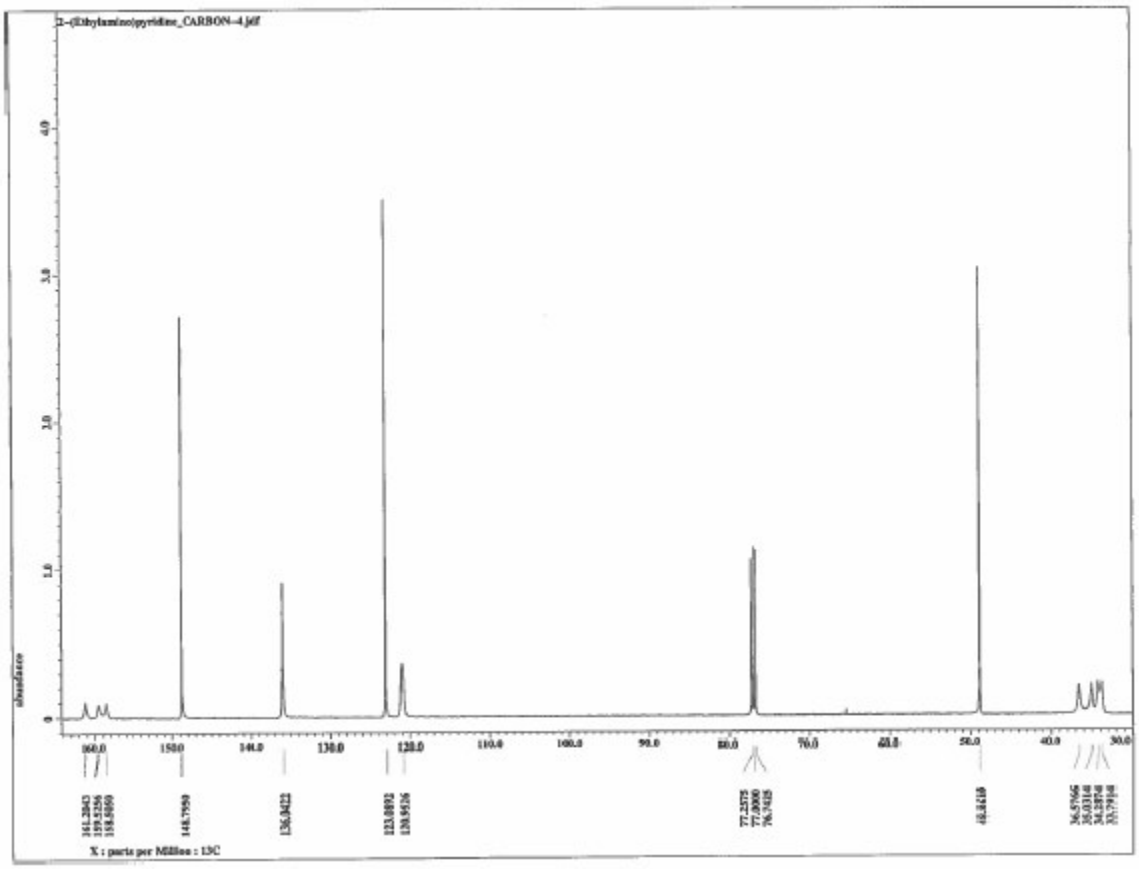
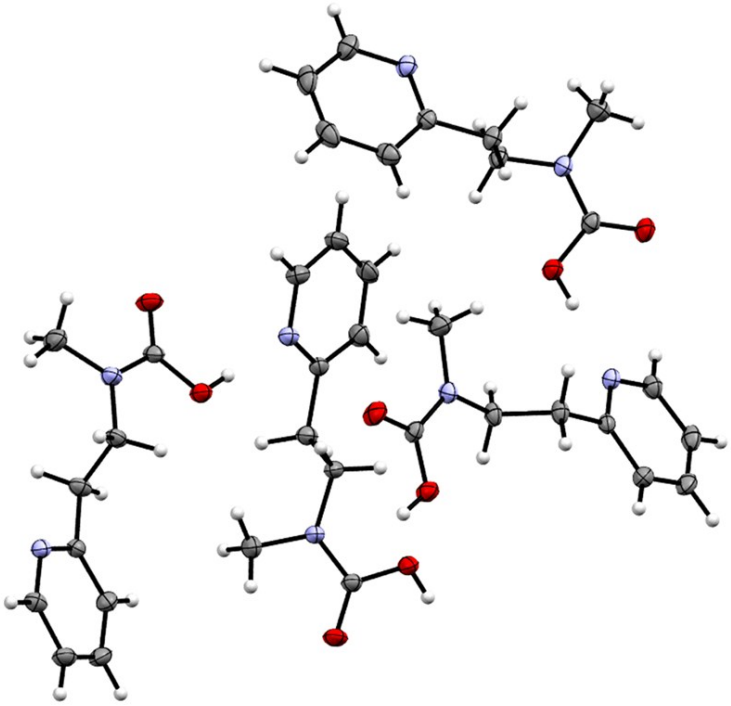
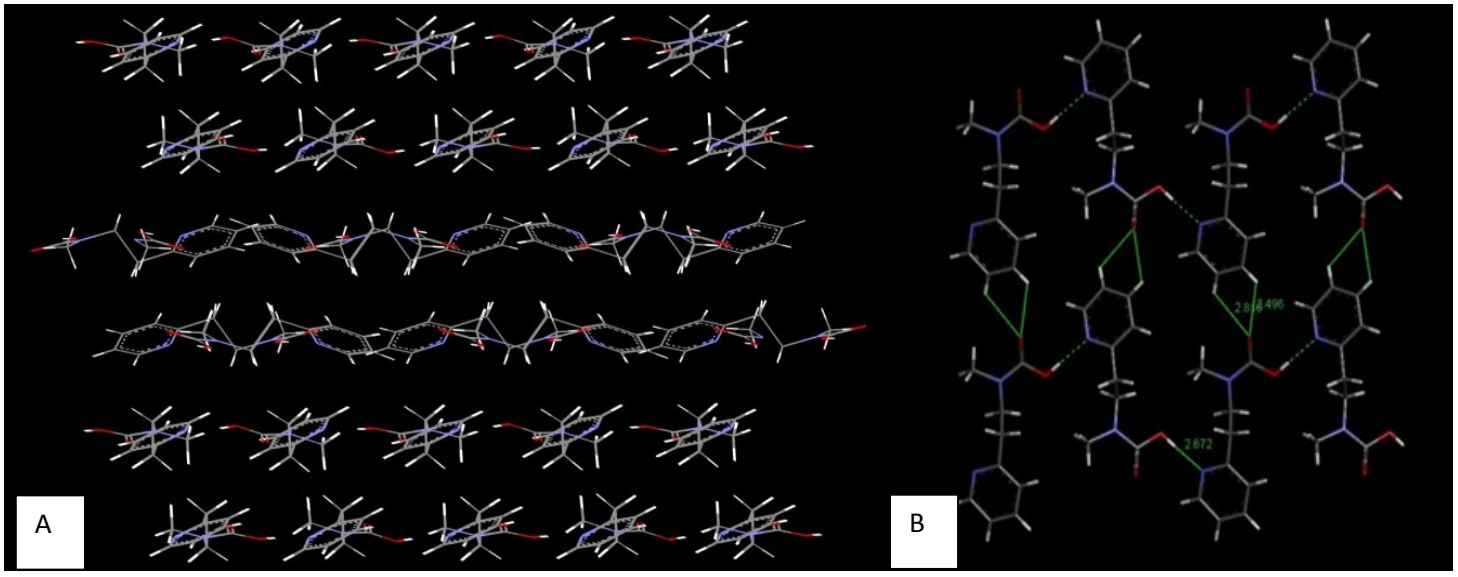
abundance
X : parts per Million : 1H


2-(Diethylamino)pyridine_CARBON-4.fid
abundance
X : parts per Million : 13C

Betahistine ORTEP and Packing



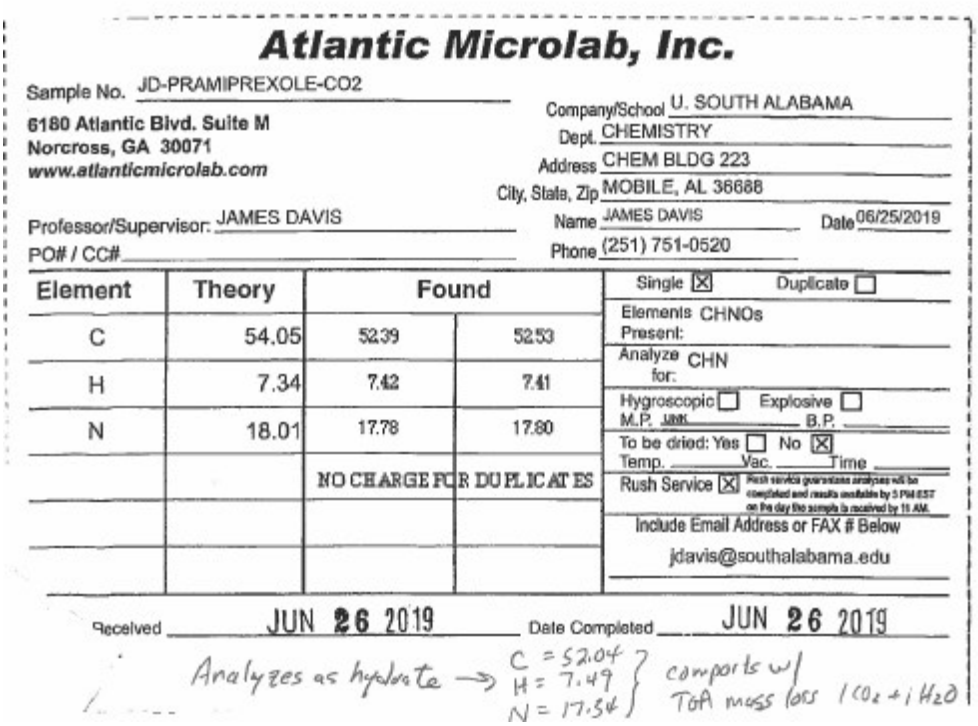


Betahistine-CO_2: r(N-C) = 1.353 Å; a(O-C-O)= 123.3°. The crystal is made of single-molecule layers (~ 3.4 Å) that repeat in pattern of four (Fig. A; six layers shown). Note that the acidic proton of the carbamic acid functional group is oriented to the right in the bottom layer, then left, then forward, then back, then to the right again in the rising succession of layers. Fig. B shows a plan view of the representative bottom layer of Fig. A. The carbamic acid moiety of each molecule is H-bonded to N(pyridine) of the

molecule to its right (green dashed lines) to form H-bonding chains running from left to right. The other carbonyl oxygen of each molecule interacts favorably the electron-poor aryl hydrogens of the neighbor molecule above/below (solid green lines) to cross link the H-bonded chains in the surface.

Most interlayer interactions involving the pyridine pi systems are H to pi, where H belongs to any of the three sets of H atoms present (H(aryl), H(methylamine), H(methylene)); however, between layers 2 and 3 (also, 4 and 5), there are N(carbamic acid) to pi interactions [r(N to pyridine's centroid) = 3.600 Å].

Pramipexole-CO_2



Atlantic Microlab, Inc.

Sample No. JD-PRAMIPREXOLE-CO2

6180 Atlantic Blvd. Suite M
Norcross, GA 30071
www.atlanticmicrolab.com

Company/School U. SOUTH ALABAMA
Dept. CHEMISTRY
Address CHEM BLDG 223
City, State, Zip MOBILE, AL 36688
Name JAMES DAVIS Date 06/25/2019
Phone (251) 751-0520

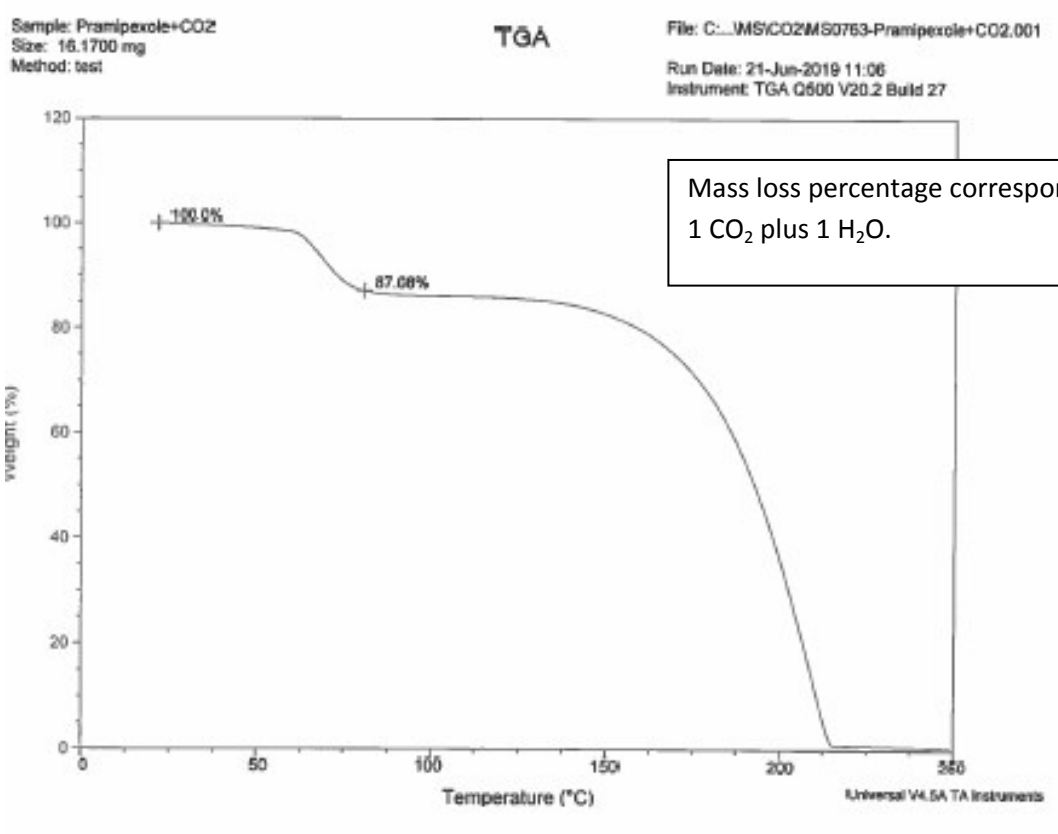
Professor/Supervisor: JAMES DAVIS
PO# / CC#

Element	Theory	Found	
C	54.05	52.39	52.53
H	7.34	7.42	7.41
N	18.01	17.78	17.80
		NO CHARGE FOR DUPLICATES	

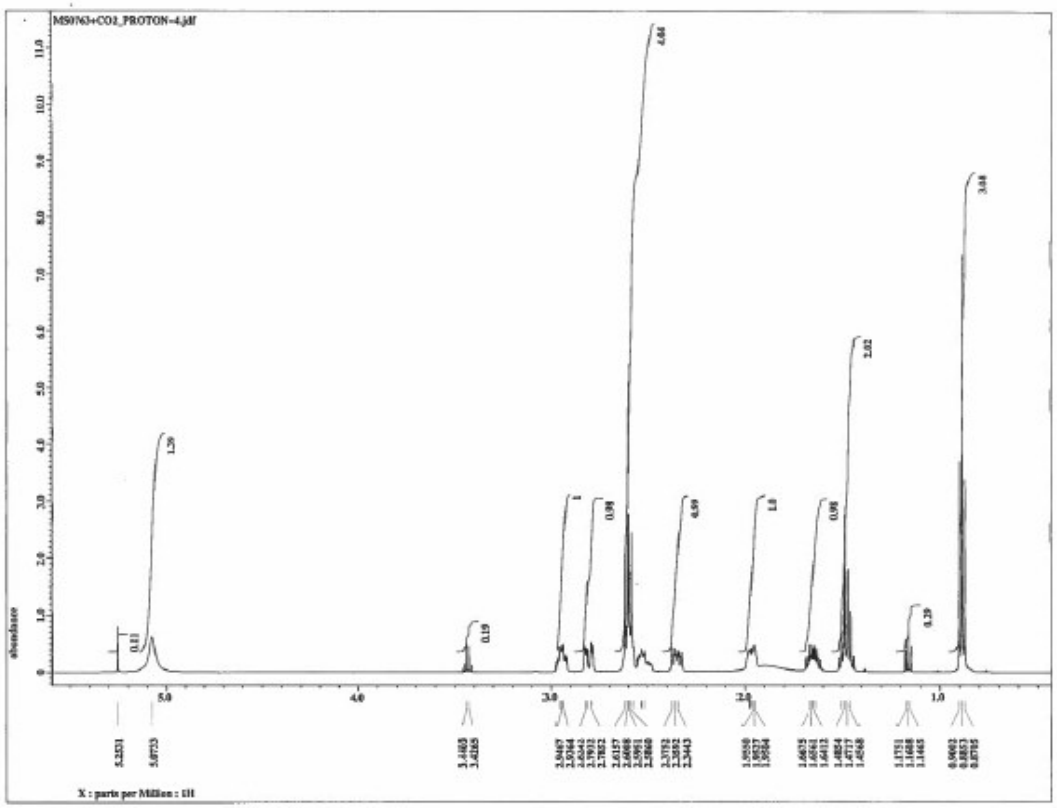
Single ☒ Duplicate ☐
Elements Present: CHNOs
Analyze for: CHN
Hygroscopic ☐ Explosive ☐
M.P. unk B.P.
To be dried: Yes ☐ No ☒
Temp. Vac. Time
Rush Service ☒ Rush service guarantees analyses will be completed and results available by 5 PM EST on the day the sample is received by 11 AM.
Include Email Address or FAX # Below
jdavis@southalabama.edu

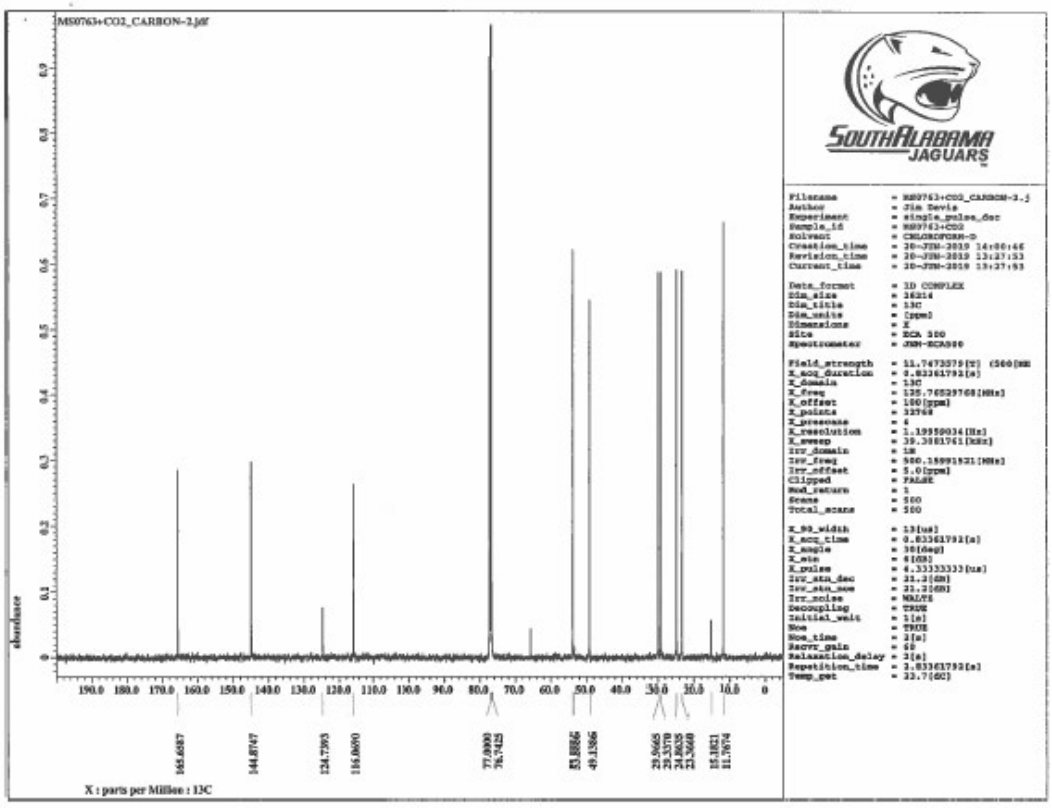
Received JUN 26 2019 Date Completed JUN 26 2019

Analyzes as hydrate → C = 52.04, H = 7.49, N = 17.54 } comports w/ TGA mass loss ($1 CO_2 + 1 H_2O$)



Mass loss percentage corresponds to 1 CO_2 plus 1 H_2O.


MS0763+CO2_PROTON-4.jdf
4.44
3.44
2.02
1.29
1
0.99
0.99
0.59
1.0
0.29
0.19
0.11
X : parts per Million : 1H



Ephedrine-CO_2

Atlantic Microlab, Inc.

Sample No. JD-EPHEDRINE-II-CO2

6180 Atlantic Blvd. Suite M
Norcross, GA 30071
www.atlanticmicrolab.com

Company/School U. SOUTH ALABAMA
Dept. CHEMISTRY
Address CHEM BLDG 223
City, State, Zip MOBILE, AL 36688
Name JAMES DAVIS Date 06/25/2019
Phone (251) 751-0520

Professor/Supervisor: JAMES DAVIS
PO# / CC#

Element	Theory	Found	
C	67.36	67.18	
H	80.09	8.10	
N	7.49	7.54	

Single ☒ Duplicate ☐

Elements Present: CHNO

Analyze for: CHN

Hygroscopic ☐ Explosive ☐
M.P. unk B.P.

To be dried: Yes ☐ No ☒
Temp. Vac. Time

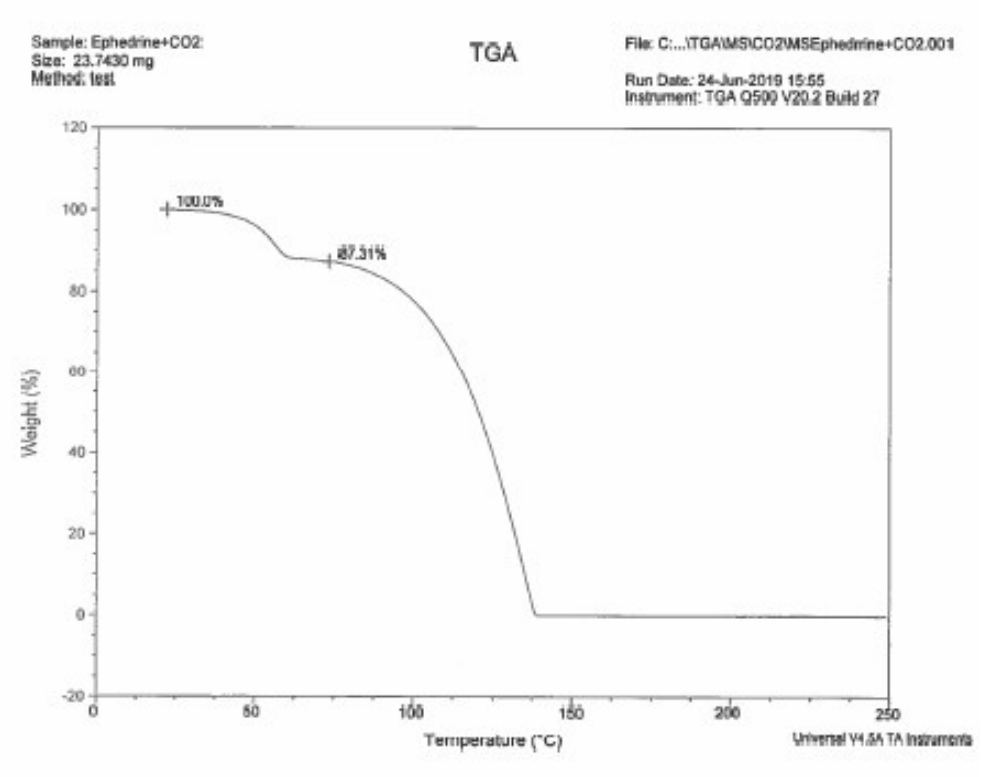
Rush Service ☒ Rush service guarantees analysis will be completed and results available by 5 PM EST on the day the sample is received by 11 AM.

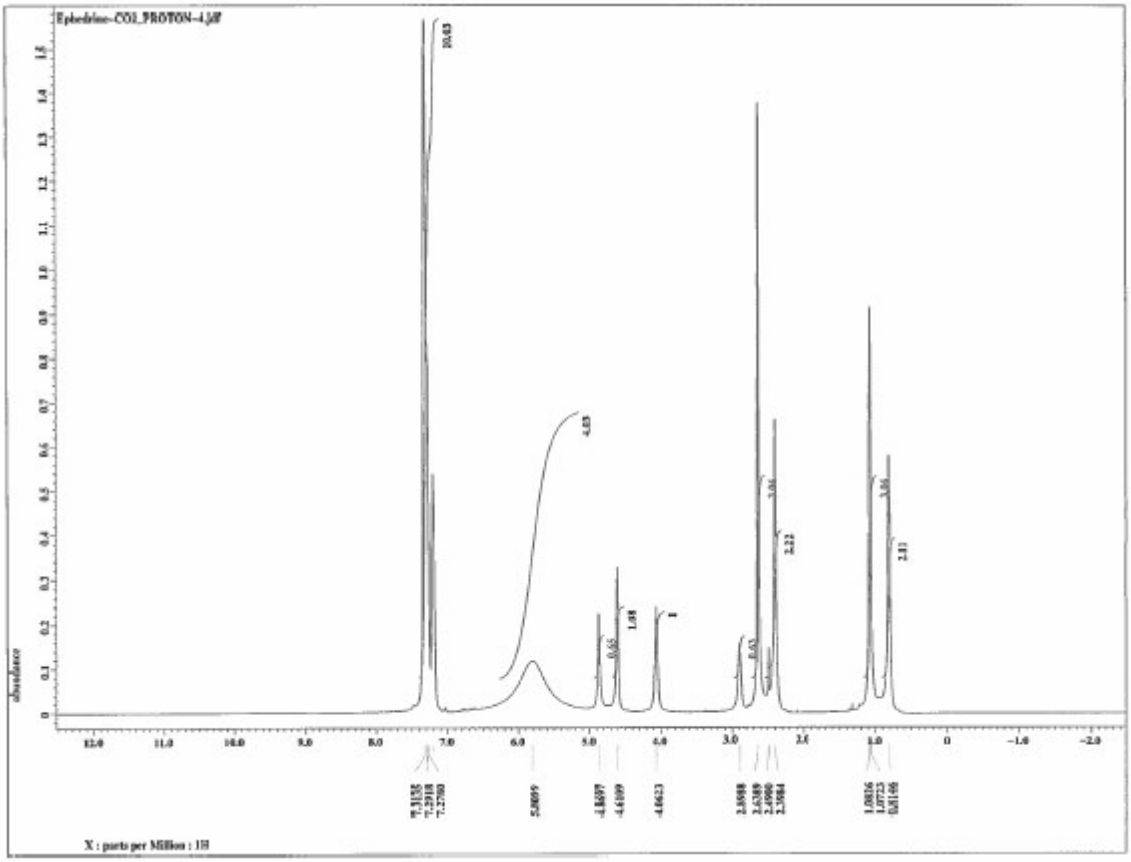
Include Email Address or FAX # Below

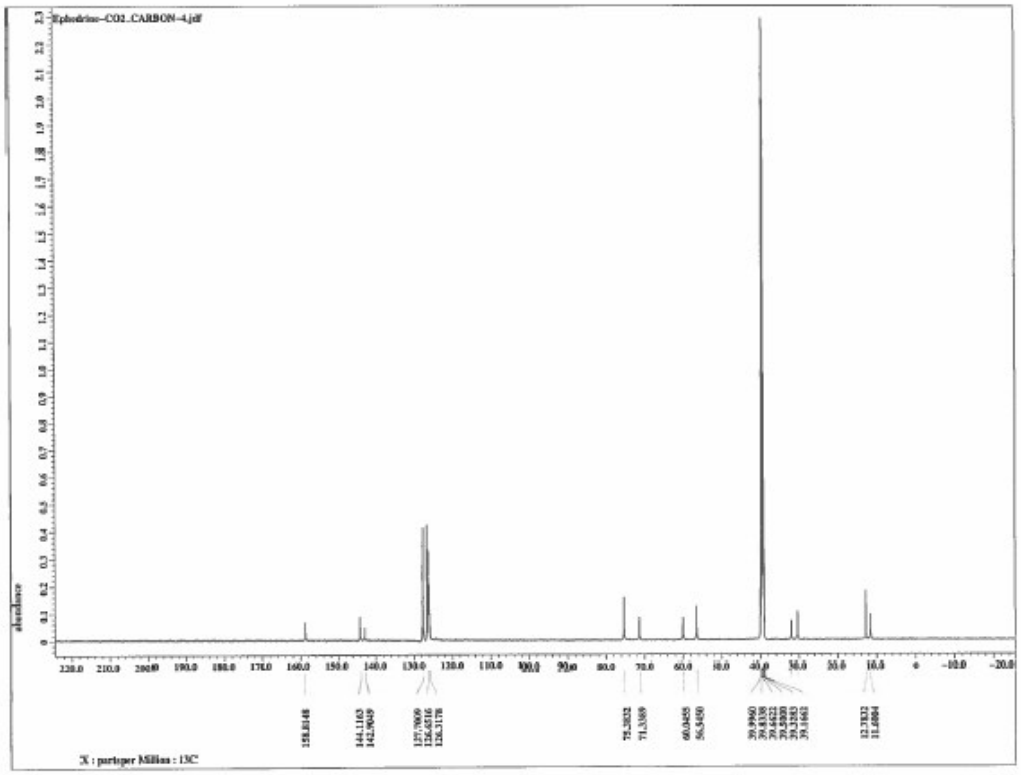
jdavis@southalabama.edu

Date Received JUN 26 2019 Date Completed JUN 26 2019

Remarks:


Sample: Ephedrine+CO2
Size: 23.7430 mg
Method: test
TGA
File: C:...\TGA\MS\CO2\MSEphedrine+CO2.001
Run Date: 24-Jun-2019 15:55
Instrument: TGA Q500 V20.2 Build 27
100.0%
87.31%
Weight (%)
Temperature (°C)
Universal V4.5A TA Instruments


Ephedrine-CO2_PROTON-4.10
absolute
X : parts per Million : 1H



Tranylcypromine-CO_2

Atlantic Microlab, Inc.

Sample No. JD-TRANYLCYPRO-CO2

6180 Atlantic Blvd. Suite M
Norcross, GA 30071
www.atlanticmicrolab.com

Company/School U SOUTH ALABAMA
Dept. CHEMISTRY
Address 223 CHEM BLDG
City, State, Zip MOBILE AL 36688
Name JAMES DAVIS Date 07/22/2019
Phone (251) 751-0520

Professor/Supervisor: DAVIS
PO# / CC# Z-220335

Element	Theory	Found	
C	73.52	73.29	
H	7.14	7.12	
N	9.03	8.99	

Single ☒ Duplicate ☐

Elements Present: CHNO

Analyze for: CHN

Hygroscopic ☐ Explosive ☐
M.P. _____ B.P. _____

To be dried: Yes ☐ No ☒
Temp. _____ Vac. _____ Time _____

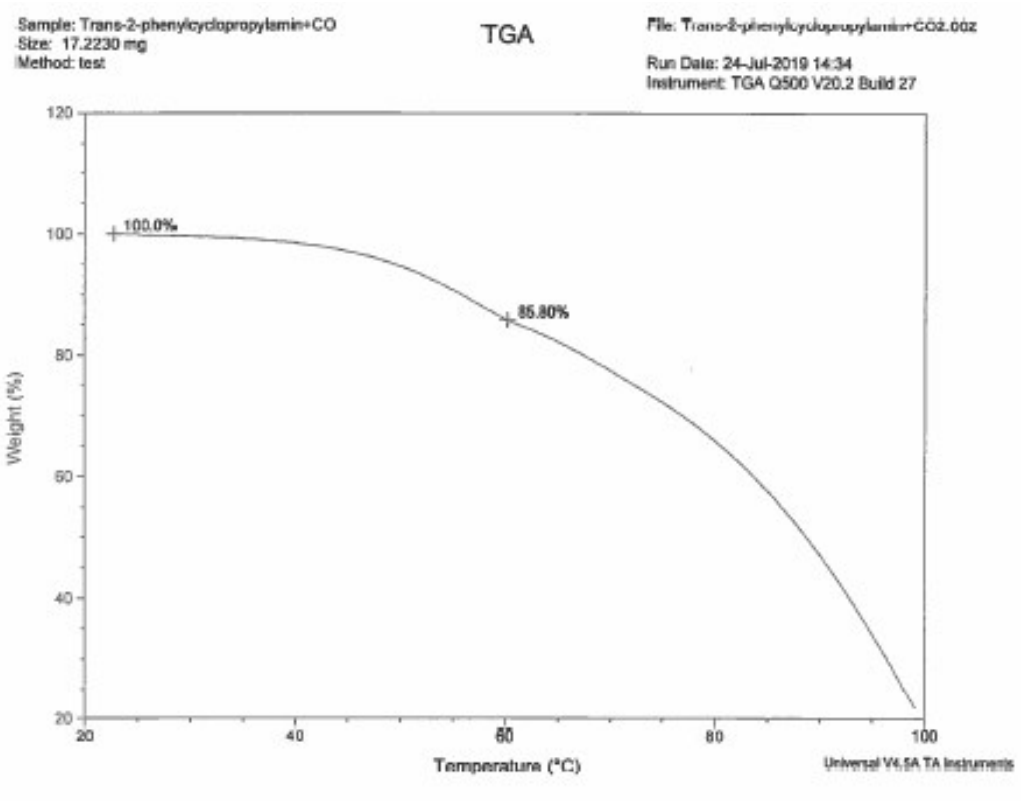
Rush Service ☒ Rush service guarantees analyses will be completed and results available by 5 PM EST on the day the sample is received by 11 AM.

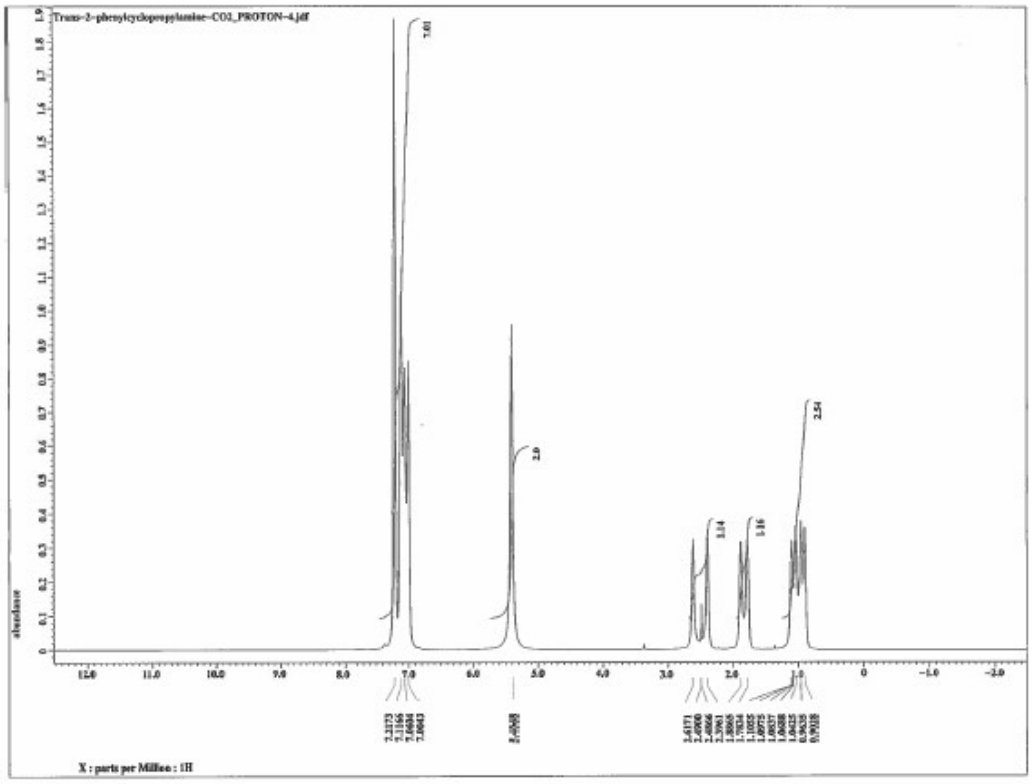
Include Email Address or FAX # Below

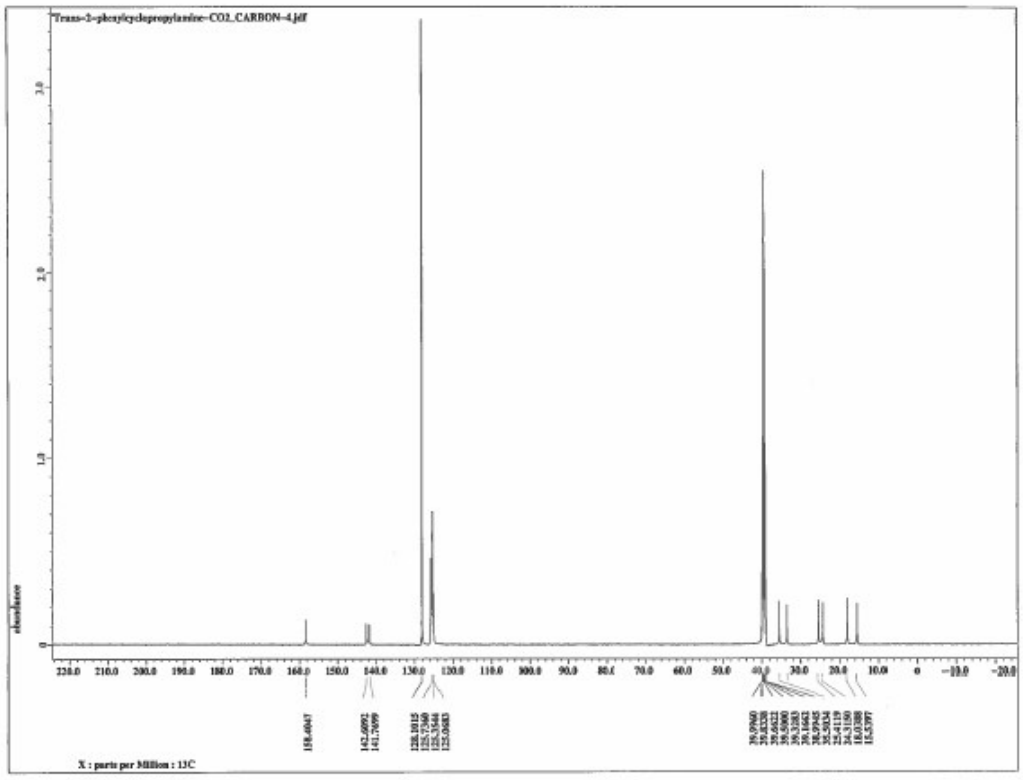
jdavis@southalabama.edu

Date Received JUL 24 2019 Date Completed JUL 24 2019

Remarks:


Sample: Trans-2-phenylcyclopropylamin+CO
Size: 17.2230 mg
Method: test
TGA
File: Trans-2-phenylcyclopropylamin+CO2.00z
Run Data: 24-Jul-2019 14:34
Instrument: TGA Q500 V20.2 Build 27
100.0%
85.80%
Weight (%)
Temperature (°C)
Universal V4.5A TA Instruments


Trans-2-phenylcyclopropylamine-CO2_PROTON-4.jdf
7.01
2.0
1.14
1.16
2.54
X : parts per Million : 1H


Trans-1-phenylcyclopropylamine-CO2_CARBON-4.jdf
X : parts per Million : 13C