## CHE 344L Spectroscopic Analysis of an Unknown Spring 2014

Sect	ion L1—Dr. Fisher 9 students
1	Benzaldehyde
2	2-Propanol
3	Methyl ethyl ketone (2-butanone)
4	1-Hexene
5	1-Propanol
6	Methylbenzylamine
7	Ethyl acetate
8	Propanoic acid
9	tert-Butanol
Secti	on L2—Dr. Fisher 10 students
10	Propanoic acid
11	tert-Butanol
12	Benzaldehyde
13	1-Hexene
. 14	1-Propanol
15	Ethyl acetate
16	2-Propanol
17	Methylbenzylamine
18	Benzoic acid
19	Methyl ethyl ketone

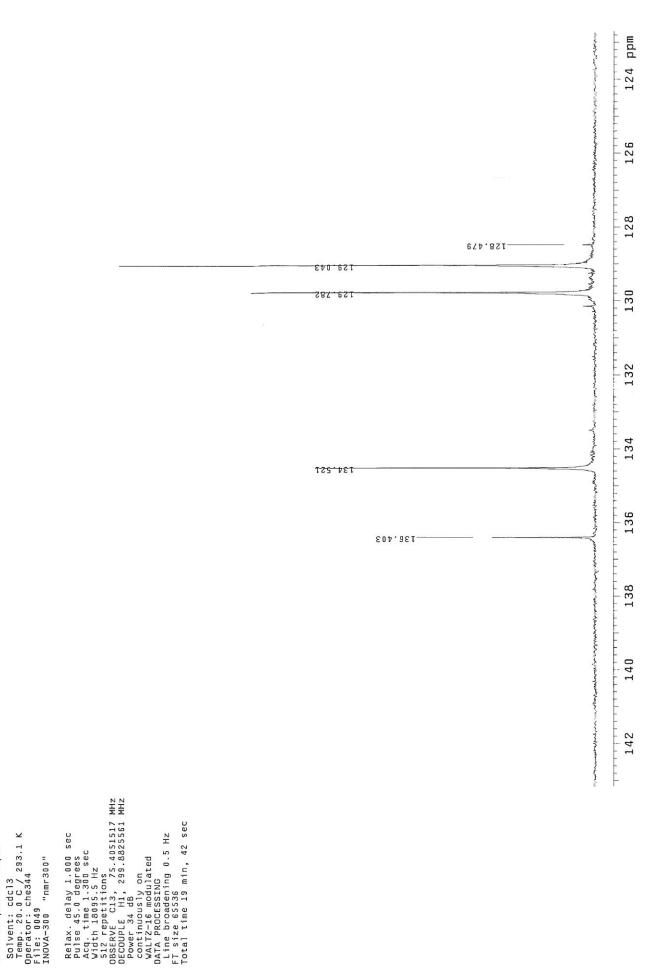
## Section L3—Dr. Fisher 10 students Propanoic acid 20 2-Propanol 21 Benzaldehyde 22 1-Propanol 23 Methylbenzylamine 24 25 1-Hexene 26 Ethyl acetate Benzoic acid 27 tert-Butanol 28 Methylbenzylamine 29

## Section L4—Ms Tsesarskaia 13 students

30	Benzoic acid
31	Benzaldehyde
32	Methylbenzylamine
33	1-Propanol
34	Methyl ethyl ketone (2-butanone)
35	1-Hexene
36	Ethyl acetate
37	Propanoic acid
38	Methyl ethyl ketone

- 39 2-Propanol
- 40 Methylbenzylamine
- 41 tert-Butanol
- **42** 1-Hexene

unk 1 spring 2014
Sample: unk 1 spring 2014
Sample ID: s\_20140404\_05
File: 0049.fid
Pulse Sequence: s2pul
Solvent: cdc13
Temp. 20.0 C / 293.1 K
Operator: che344
File: 0049 "nmr300"
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Vidth 18095.5 Hz
S12 repetitions
OBSERVE C13, 75.4051517 MHz
DECOUPLE H1, 299.8825561 MHZ
DATA FROCESSING
Line Decodening 0.5 Hz
FI size 65536



Sample: unk 1 spring 2014 Sample ID: s\_20140404\_05 File: 0049.fid

unk 1 spring 2014

Pulse Sequence: s2pul

unk 🕹 spring 2014

Sample: unk **Z** spring 2014 Sample ID: s\_20140404\_07 File: /home/che344/vnmrsys/data/che344spring2014/unk2c13-256scans.fid

Pulse Sequence: s2pul Solvent: cdcl3 Temp. 20.0 C / 293.1 K Operator: che34 File: unk2c13-256sans INOVA-300 "nmr300" Relax. delay 1.000 sec Pulse 45.0 degrees Acq. time 1.300 sec Width 18095.5 Hz 256 repetitions OBSERVE C13, 75.4051517 MHz DECOUPLE H1, 299.8825561 MHz Power 34 dB continuously on WALTZ-16 modulated DATA PROCESSING Line broadening 0.5 Hz FT size 65536 Total time 9 min, 51 sec

		,

Sample: unk **J.** spring 2014 Sample ID: s\_20140404\_07 File: /home/che344/vnmrsys/data/che344spring2014/unk2c13-256scans.fid

Solvent: cdcl3 Temp. 20 0 C / 293.1 K Operator: che34 File: unk2c13-256sans INOVA-300 "nmr300"

Pulse Sequence: s2pul

unk **2** spring 2014

*		

Sample: unk \$\ \pi\rightarrow \pi\ri

Solvent: cdc13 Temp. 20.0 C / 293.1 K Operator: che344 File: unk3013-5kscans INOVA-300 "nmr300"

Pulse Sequence: s2pul

unk **3** spring 2014

		,

шdd 323. T 10 20 29.216 792.62 29.304 30 28.85 888.83 36.642 40 50 09 7 0 058.77 703.77 287.87 80 Relax. delay 1.000 sec Acq. time 1.300 sec Acq. time 1.300 sec Width 18095.5 Hz 5000 repetitions OBSERVE CI3, 75.4051517 MHz DECOUDLE H1, 299.8825561 MHz POWER 34 dB CONTINUOUSLY ON WALTZ-16 modulated DATA PROCESSING Line broadening 0.5 Hz FT size 65536 Total time 3 hr, 12 min, 27 sec

Sample: unk **3** spring 2014 Sample ID: s\_20140404\_08 File: /home/che344/vnmrsys/data/che344spring2014/unk3c13—5kscans.fid

Solvent: cdc13
Temp. 20.0 C / 293.1 K
Operator: che34
File: unks:13-5kscans
INOVA-300 "nmr300"

Pulse Sequence: s2pul

unk 3 spring 2014

		<b>s</b> *
		ž.

шdd 0 13.954 22.22 671.18 33,552 40 09 880.77 880.77 80 100 011-011 120 140 139.230 160 180 200 220 MHZ

unk 4spring 2014

Sample: unk 4 spring 2014 Sample ID: s\_20140406\_01 File: /home/Che344/vnmrsys/data/che344spring2014/unk4c13-256scans.fid

Pulse Sequence: s2pul
Solvent: cdc13
Temp. 20.0 C / 293.1 K
Operator: che344
File: unk4c13-256scans
INOVA-300 "nmr300"

Relax. delay 1.000 sec Acq time 1.300 sec Acq time 1.300 sec Vidth 18095.5 Hz 256 repetitions 0BSERVE C13, 75.4051517 MH DECOUPLE H1, 299.8825561 MH Power 34 dB continuously on WALTZ-16 modulated DATA PROEESSING Line broadening 0.5 Hz FT size 65536 Total time 9 min, 51 sec

Sample: unk 4 spring 2014 Sample ID: s\_20140406\_01 File: /home/che344/vnmrsys/data/che344spring2014/unk4c13-256scans.fid

Solvent: cdcl3 Temp. 20.0 C / 293.1 K Operator: che344 File: unk4.13-256scans INOVA-300 "nmr300"

Pulse Sequence: s2pul

unk 4spring 2014

шdd 13.954 20 22,229 30 31.149 33-552 40 50 09 \$50.77 \$50.77 LINE STATE OF THE PARTY OF THE 80 MHZ

unk 4spring 2014

Sample: unk 4 spring 2014 Sample ID: s\_20140406\_01 File: /home/che344/vnmrsys/data/che344spring2014/unk4c13-256scans.fid Pulse Sequence: s2pul

Solvent: cdcl3
Temp. 20.0 C / 293.1 K
Operator: che34
File: unk4cl3-256scans
INOVA-300 "nmr300"

Relax. delay 1.000 sec Pulse 45.0 degrees Acq. time 1.300 sec Width 18095.5 Hz 256 repetifions 0858VE C13, 75.4051517 MH DECOUDLE H1, 299.8825561 MH Power 34 dB continuously on WALTZ-16 modulated DATA PROCESSING Line broadening 0.5 Hz FT size 65536 Total time 9 min, 51 sec

unk 5spring 2014

Sample: unk 5 spring 2014 Sample ID: s\_20140406\_02 File: /home/che344/vnmrsys/data/che344spring2014/unk5c13-256scans.fid

Solvent: cdcl3 Temp. 20 0 C / 293.1 K Operator: che34 File: unkSc13-256scans INDVA-300 "nmr300"

Pulse Sequence: s2pul

unk 5spring 2014

Sample: unk 5 spring 2014 Sample ID: s\_20140406\_02 File: /home/che344/vnmrsys/data/che344spring2014/unk5c13-256scans.fid

Pulse Sequence: s2pul Solvent: cdcl3 Temp. 20.0 C / 293.1 K Operator: che34 File: unkSc13-256sans INOVA-300 "nmr300"

шdd 20 25.803 40 778.18 09 TT8.87-808. 80 487.77-100 120 128.530 125.530 140 T06'27T-160 180 200 220 Relax. delay 1.000 sec Pulse 45.0 degrees Acq. time 1.300 sec Width 18095.5 Hz 256 repetitions OBSERVE C13, 75.4051517 MHz DECOUPLE H1, 299.8825561 MHz Power 34 dB Continuously on WALT2-16 modulated DATA PROCESSING Line broadening 0.5 Hz FT size 55536 Total time 9 min, 51 sec

Sample: unk 6 spring 2014 Sample ID: s\_20140406\_03 File: /home/che344/vnmrsys/data/che344spring2014/unk6c13-256scans.fid

Solvent: cdcl3
Temp 20.0 C / 293.1 K
Operator: che344
File: unksc13-256scans
INOVA-300 "nmr300"

Pulse Sequence: s2pul

unk 6spring 2014

шdd 25.803 30 40 50 178.12-09 7.0 778.97-808.44 **Δε**Γ. ΓΓ-80 90 100 110 120 126.838 125.747 128,530 130 Relax. delay 1.000 sec Pulse 45.0 degrees Acq. time 1.300 sec Width 18095.5 Hz 256 repetitions OBSERVE C13, 29.8825561 MHz DECOUPLE H1, 299.8825561 MHz Power 34 dB Continuously on WALTZ-16 modulated DATA PROCESSING Line broadening 0.5 Hz FT size 65536 Total time 9 min, 51 sec

Sample: unk 6 spring 2014 Sample ID: s\_20140406\_03 File: /home/che344/vnmrsys/data/che344spring2014/unk6c13-256scans.fid

Solvent: cdc13
Temp. 20 0 C / 293.1 K
Operator: che344
File: unk6c13-255scans
INOVA-300 "nmr300"

Pulse Sequence: s2pul

unk Sspring 2014

unk 7spring 2014

Sample: unk 7 spring 2014 Sample ID: s\_20140406\_04 File: /home/che344/vnmrsys/data/che344spring2014/unk7c13-256scans.fid

Pulse Sequence: s2pul Solvent: cdc13 Temp. 20.0 C / 293.1 K Operator: che344 File: unk7c13-256scans INOVA-300 "nmr300" Relax. delay 1.000 sec Pulse 45.0 degrees Acq. time 1.300 sec Width 18095.5 256 repetitions OBSERVE C13, 75.4051517 MHz DECOUPLE H 1. 299.8825561 MHz Power 34 dB, continuously on WALTZ-16 modulated DATA PROCESSING Line broadening 0.5 Hz FT size 65536 Total time 9 min, 51 sec

N.		

шdd 14.034 A SECTION OF THE PROPERTY AND ADDRESS OF THE PROPERTY AND 20 20-816 30 40 50 09 502.09 والمنافرة والمراج والمرافرة والمنافرة والمراج والمعارض والمراجعة والمرافرة والمواجعة والمرافزة والمراجعة والمداور 7.0 619.17 917.97 202.77 MHZ MHZ Relax. delay 1.000 sec Acq. time 1.300 sec Acd. 18095.5 Hz 256 repetitions OBSERVE C13, 75.4051517 MH DECOUPLE H1, 299.8825561 MH Power 34 db continuously on WALTZ-16 modulated DATA PROCESSING Line Broadening 0.5 Hz FT size 65536 Total time 9 min, 51 sec

Sample: unk 7 spring 2014 Sample ID: s\_20140406\_04 File: /home/che344/vnmrsys/data/che344spring2014/unk7c13-256scans.fid

Solvent: cdc13
Temp. 20.0 C / 293.1 K
Operator: che344
File: unK7c13-256scans
INOVA-300 "nmr300"

Pulse Sequence: s2pul

unk 7spring 2014

0 127.8 20 121.151 40 9 £49.87-890.55 80 100 120 140 160 180 748.181-200 220 Relax. delay 1.000 sec Pulse 45.0 degrees Acq. time 1.300 sec Width 18095.5 Hz 5000 repetitions OBSERVE C13, 75.4051517 MHz DECOUPLE H1, 299.8825561 MHz Power 34 db continuously on WALTZ-16 modulated DATA PROCESSING Line broadening 0.5 Hz FT size 65536 Total time 3 hr, 12 min, 27 sec

шdd

unk 8spring 2014

Sample: unk 8 spring 2014 Sample ID: s\_20140406\_05 File: /home/che344/vnmrsys/data/che344spring2014/unk8c13-5kscans.fid

Solvent: cdc13
Temp. 20.0 C / 293.1 K
Operator: che344
File: unk843-5kscans
INOVA-300 "nmr300" Pulse Sequence: s2pul

unk 8spring 2014

Sample: unk 8 spring 2014 Sample ID: s\_20140406\_05 File: /home/che344/vnmrsys/data/che344spring2014/unk8c13-5kscans.fid

Solvent: cdcl3 Temp. 20.0 C / 293.1 K Operator: che34L File: unk8013-5kscans INOVA-300 "nmr300" Pulse Sequence: s2pul

Relax. delay 1.000 sec Aq. time 1.300 sec Aq. time 1.300 sec Width 18095.5 Hz 5000 repetitions 5000 repetitions DECOUPLE H1, 299.8825561 MHz Dower 34 db continuously on WALTZ-16 modulated DATA PROCESSING Line broadening 0.5 Hz FT size 85536 Total time 3 hr, 12 min, 27 sec

unk 9spring 2014

Sample: unk 9 spring 2014 Sample ID: s\_20140407\_01 File: /home/che344/vnmrsys/data/che344spring2014/unk9c13-256scans.fid

Pulse Sequence: s2pul Solvent: cdcl3 Temp. 20.0 C / 293.1 K Operator: che34 File: unk9c13-256scans INOVA-300 "nmr300" Relax. delay 1.000 sec Pulse 45.0 degrees Acq. time 1.300 sec Width 18095.5 Hz 256 repetitions OBSERVE C13, 75.4051517 MHz DECOUPLE H1, 299.8825561 MHz Power 34 dB continuously on WALTZ-16 modulated DATA PROCESSING Line broadening 0.5 Hz FT size 65536 Total time 9 min, 51 sec

unk 9spring 2014

Sample: unk 9 spring 2014 Sample ID: s\_20140407\_01 File: /home/che344/vnmrsys/data/che344spring2014/unk9c13—256scans.fid

Pulse Sequence: s2pul Solvent: cdcl3 Temp. 20 0 C / 293.1 K Operator: che344 File: unk9c13-255scans INOVA-300 "nmr300" Relax. delay 1.000 sec Pulse 45.0 degrees Acq. time 1.300 sec Vidth 18095.5 Hz 256 repetitions OBSERVE C13, 75.4051517 MHz DECOUPLE H1, 299.8825561 MHz Power 34 db continuously on WALTZ-16 modulated DATA PROCESSING Line broadening 0.5 Hz FT size 65536 Total time 9 min, 51 sec

unk 18 spring 2014
Sample: unk 18 spring 2014
Sample: unk 18 spring 2014
File: /home/Che344/vnmrsys/data/che344spring2014/unk18c13-256scans.fid
Pulse Sequence: s2pul
Solvent: cdc13
Temp. 20.0 C / 293.1 K
Operator: che344
File: unk18c13-256scans
INOVA-300 "nmr300"
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 18095.5 Hz
256 repetitions
OBSERVE C13, 75.4051517 MHz
DECOUPLE H1, 299.8825561 MHz
DECOUPLE H1, 299.8825561 MHz
Continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 65536

Sample: unk 18 spring 2014 Sample ID: s\_20140407\_02 File: /home/che344/vnmrsys/data/che344spring2014/unk18c13-256scans.fid

unk 18 spring 2014

Pulse Sequence: s2pul Solvent: cdcl3 Temp. 20.0 C / 293.1 K Operator: che344 File: unk: 18613-255scans INOVA-300 "nmr300" Relax. delay 1.000 sec Pulse 45.0 degrees Acq. time 1.300 sec Width 18095.5 Hz 2.56 repetitions OBSERVE C13, 75.4051517 MHz DECOUPLE H1, 299.8825561 MHz Power 34 db Continuously on WALTZ-L6 modulated DATA PROCESSING Line broadening 0.5 Hz FT size 65536 Total time 9 min, 51 sec

	₹	